A SYSTEMATIC APPROACH TO THE DESIGN OF PLANT-WIDE CONTROL STRATEGIES FOR CHEMICAL PROCESSES

by

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ABSTRACT

Synthesis of plant-wide control structures entails identification of control objectives that are consistent with the overall production goals and formulation of control strategies in a multivariate environment. Formal techniques have been developed which address issues such as: the progressive generation of relevant process control tasks and control objectives, verification of the feasibility of control structures, decision making in a multi-objective setting, formulation of control schemes to address a range of process phenomena over time-scales of various lengths and generation of control strategies in multivariable processes. These techniques have been integrated to derive a systematic approach to the synthesis of plant-wide control structures for chemical process plants.

A conceptual hierarchical framework is proposed for the analysis of process operations and synthesis of plant-wide control structures. It is recommended that the plant be vertically decomposed into a set of process representations of varying degree of abstraction of the detailed process. Starting from the coarsest viewpoint such as the input-output representation, a control structure which addresses issues associated with the overall production plan can be developed. Then, moving down onto the next level, the process viewpoint, the control objectives and the control strategies are being systematically refined. This procedure is repeated until all details in the plant are revealed in the most detailed viewpoint. In this way, a hierarchy of control strategies which account for both the long-range operational requirements and short-range dynamic control specifications can be developed. The synthesis of control strategies at each level of the hierarchy respects the multivariate nature of the plant system. Using a goal-oriented approach, engineering preferences and design trade-offs are formally accounted for in a multi-objective manner. The control objectives are distinctively associated with manipulated variables and so the control structure is relatively transparent and easily comphrensible. The hierarchy of control structures are then integrated to form a multi-horizon control system where the control strategies which account for long term material and energy balances in the plant are implemented independently from those which are associated with the process dynamic transient regulation.

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The most incomprehensible thing about the world is that it is comprehensible. — Albert Einstein

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Christine Ng
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Table of Contents

List of Figures

List of Tables

Chapter 1
Introduction

1.1 Introduction to Plant Control

The importance of a reliable control system for the safe, smooth and economical operation of a chemical process cannot be overstated. In today's chemical plants, the function of a control system goes far beyond basic process monitoring and regulation of the plant at steady state, in the presence of continuous process disturbances. The control system is now seen by the industry as a device to drive the process to its limit of highest quality of production using the exiting process equipment, while simultaneously safeguarding the process operation from unsafe terrain and disallowed emissions to the environment. It has long been recognized that a carefully designed process control system can bring out the best performance in a plant. In today's competitive markets, with the increasing trend of process units integration, the control system plays a crucial role in plant operation and hence the design of such system must be carried out carefully.

The design of process control system consists of two aspects. The first aspect is related to *control system formulation* and the second aspect deals with *control system implementation*. Control system formulation refers to the process by which the set of strategies that are needed to accomplish all the operational requirements are generated. At this stage of the design, the associations between manipulated variables and control objectives are synthesized. The set of associations form the control strategies and these strategies together define a process control structure. Once the control strategies are developed, they must be implemented by means of some kind of control algorithms and this is performed in the second stage of the design. This second stage of control system synthesis deals with the interconnection structure between measured and manipulated variables and this task has received a tremendous amount of attention from academia and industry. With the level of advancement in this particular direction, at present, there is a variety of algorithms available to the designer. Depending on the skill of the designer, the tightness of the required process operational specifications and the amount of time the designer would like to invest in the controller design phase, he or she can choose from a simple proportional-integral-derivative control to the more sophisticated optimal control algorithms like a variant of the model-based predictive control. The point is that, at present, there exists a great deal of theoretical knowledge on how to design control algorithms that are "robust", "resilient" and "adaptive", given a set of manipulated and controlled variables. However, the question of how to define a set of suitable control strategies for a given plant, which is related to the first stage of the control system design, has not been addressed satisfactorily. Ironically, this is the question that is most frequently faced by a chemical engineer.

1.2 Past Methods of Control Systems Design and Research Motivation

The existence of the gap between the advancement of process control methodologies in academia and the actual requirement for control system design in process industry has been pointed out in several classic papers on the critique of chemical process control theory some twenty years ago (Foss, 1973; Lee and Weekman, 1976; Kestenbaum et al. 1976). These papers have in fact initiated interests in academia to study the problem of control structure synthesis for chemical plants and a number of approaches have emerged. Over the years, methodologies of varying degree of "complexity" have been put forward and they have ranged from the unit-operation based methods favored in the 70's to the more globally oriented, structural-based typed of approaches developed in the past decade (Morari, 1980a, 1980b, 1980c; Johnston, R.D., 1985a, 1885b; Calandrains, 1988, Georgiou, 1989; Johnston, J.E., 1991) and the plant-wide based tiered framework in recent years (Price and Georgakis, 1993; Poton and Liang, 1993)

Although many of the existing methodologies have contributed significant insight to the problem of control structure synthesis and have led to deeper understanding of issues in structural controllability for chemical plants, interaction among variables and the problem of selection of controlled and manipulated variables, their impact on the chemical process operations has been minimal. The use of local, unit-operation based approaches is still favored in industry. It is believed that the failure of the past work to address goals directly related to production requirements in a clear and precise manner and the lack of a mechanism to reduce the complexity of the plant-wide control problem to a manageable size have contributed to such consequence. Furthermore, the perceived or real need for modeling an entire plant has created an apprehension on the part of the control system designer in undertaking more global approaches.

1.3 Research Objectives

In view of the above, the goal of this research is to formalize a framework in which issues related to plant-wide process control can be suitably addressed and to develop a systematic approach to the synthesis of plant-wide control structures and control strategies for chemical processes. The methodology should be *useful* in that it is supported by unambiguous analytical aids that guide the designer from the selection of controlled and manipulated variables to the formulation of specific control structures in a systematic manner. Furthermore, the methodology should also be *implementable*. A mechanism must exist to fight the complexity of the plant-wide design problem. Specifically, the objectives of the research are:

1. To identify the fundamental issues associated with the design of plant-wide control systems and strategies for chemical processes.
2. To develop a suitable framework for the *analysis* of the control system design problem and for the *synthesis* of plant-wide control structures and control strategies.
3. To develop formal techniques which are needed to address issues at various stages of control system design.
4. To assemble a systematic methodology for the synthesis of plant-wide control structures and control strategies.

1.4 Contributions of the Present Work

In this research, the key issues associated with the synthesis of plant-wide control strategies have been identified. A hierarchical framework is proposed for the study of plant operation. Within this hierarchical approach, a systematic methodology for the design of plant-wide control structures have been formulated. Plant control strategies are systematically synthesized in an evolutionary manner. Techniques which address issues such as:

- identification of specific control tasks and control objectives which are consistent with the overall production plan
- verification of the feasibility of control strategies
- decision making in a multi-objective setting
- formulation of control schemes to meet long-range operational requirements and short-range dynamic control specifications
- generation of control strategies in a multivariate environment

have been formalized. These techniques form the basis of a generic framework for the design of plant-wide control strategies.

1.5 Thesis Organization

This thesis is organized has follows. Chapter 2 gives an overview of the issues which are important in plant operation and plant-wide control system design. A detailed review of the past work on the development of methodologies for control system design is given, as well as a summary of the shortcomings and weaknesses in the existing methods. Chapter 3 presents an overview of the generic framework for the design of plant-wide control strategies. Chapters 4 through 6 discuss the specific techniques which can be used to address different issues at various stages of the design problem. Applications of the techniques introduced in Chapters 4 through 6 to address fundamental plant-wide control issues will be presented in Chapter 7. Chapter 8 presents the complete methodology for the synthesis of plant-wide control strategies for chemical plants. Chapters 9, 10 and 11 demonstrate the application of the proposed methodology to develop control structures for several industrial processes. Chapter 12 highlights the relationship between plant design and control performance, and suggests a formalism to determine process modifications that could improve control performance. Chapter 13 summarizes the contribution of this research and addresses future research opportunities.

Chapter 2
Issues In Plant-wide Control Systems Design

2.1 A Typical Plant-wide Control Problem

Control structure synthesis is that step of engineering work during control system design where the associations among controlled variables and manipulated variables in the plant are generated. This set of associations together form a control structure whose function is to guarantee stable plant operation and ensure production related goals are delivered. One begins the synthesis process wiih an imprecisely stated problem definition of production requirements as illustrated in Figure 2-1. The process control engineer is generally given a process flowsheet that shows the interconnections among the different unit operations in the plant. The job of the control engineer is to decide how to accomplish the production goals given the inputs to the process and satisfy the plant operational constraints in the presence of various types of process disturbances. Generally, production goals at this stage of the design can only be expressed informally (e.g. minimum cost, maximum plant throughput or high quality products), and these goals could have no direct relation to any one particular process variable.

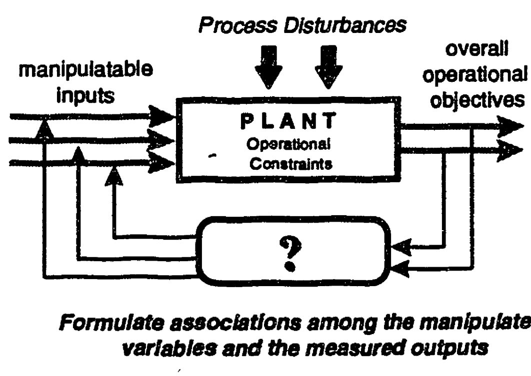


Figure 2 - 1: The Plant-wide Control Problem

The design of a control system for a process plant can often be an overwhelming task. Modern plants are usually designed with economic objectives in mind. Frequently, economic incentives force efficient use of resources and so the cost-optimal plant configuration is usually composed of individual unit-operations linked together not only along the forward path, but also in the feedback direction via the use of material recycle streams. Application of a certain degree of integration of heat sources and heat sinks is also quite common. The size of the plant, the inter-coupling of unit-operations, and the variety of plant control objectives all contribute to the complexity of the control design problem.

The issues which are important in the design of a control systems for the complete plant can be best described by studying a typical problem that is presented to a designer. Figure 2-2 shows the flowsheet of the hydrodealkylation of toluene (HDA) process studied by Douglas (1988). The HDA process represents a fairly typical chemical plant: conversion of raw materials in the reactor is incomplete, unreacted raw materials are recycled and there exists some extent of heat integration. In this plant, pure toluene feed, make-up hydrogen (95% pure) are mixed and combined with recycled toluene and recycled gas streams. The combined stream is pre-heated and is fed to a plug-flow reactor where the materials react according to the following exothermic reactions:

$$\text{Toluene} + \text{Hydrogen} \rightarrow \text{Benzene} + \text{Methane}$$
$$2\ \text{Benzene} \rightarrow \text{Diphenyl} + \text{Hydrogen}$$

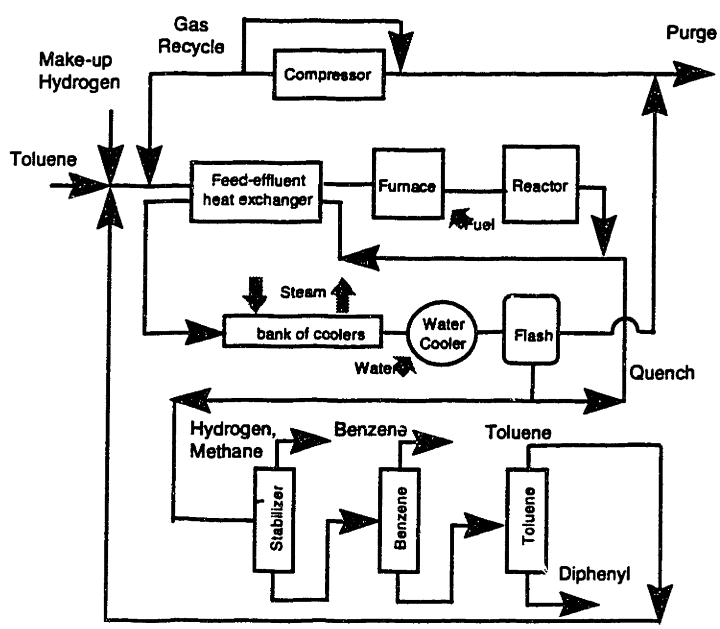


Figure 2 - 2: Process Flowsheet of the Hydrodealkylation of Toluene Process

The reactor effluent is immediately quenched and is followed by a vapor-liquid phase equilibrium separation. The vapor coming off from the separator is hydrogen-rich. A large portion of this stream is recycled back to the reactor area and the rest of the stream is purged. Some of the liquid from the separator is used to quench the reactor effluent while the rest is being sent to the downstream separation train where benzene is recovered. Unreacted toluene is removed and is recycled as well. It is the goal of the operation to:

- maintain plant materials and energy balances
- produce benzene at the desired production rate
- produce benzene at the desired purity
- minimize process variations
- avoid violation of equipment constraints
- meet process constraints
- minimize production cost

Note that it may not always be possible to meet all production objectives and a critical component in the task of control structure synthesis is the evaluation of design trade-offs. In order to develop a control system for the HDA plant which can best meet the production objectives listed above, several key issues must be addressed by the designer. These issues are discussed in the next few sections.

Identification of Specific Process Controlled Variables

Generally, production objectives at the initial stage of the design can only be expressed informally. It is very common to find that the initial production objectives of the plant are defined in terms of the overall production objectives/goals of the plant rather than a set of process variables that are to be regulated. Notice that the production objectives for the HDA example can be generalized into two classes:

1. *Explicit Objectives*: An explicit objective can be directly expressed in terms of a specific process variable or can be easily defined in mathematical terms. Examples are: flow rates, component compositions, stream or vessel temperatures, vessel pressures, ratios of feeds or products. These objectives can be used directly as controlled variables in the control system. Implicit objectives are *lumped* objectives.
2. *Implicit Objectives*: An implicit objective is defined by a set of process variables and it is related to the overall behavior of the process. Common examples are: maintenance of materials and energy balances, optimization or economic objectives. The attainment of an implicit objective requires coordination of a large number of process variables in the plant in a consistent manner.

Figure 2-3 depicts the scopes of the two classes of objectives. The extent of an explicit objective (such as OBJ-1_{Explicit} or OBJ-2_{Explicit}) is localized to a specific process stream or unit while the scope of an implicit objective (such as $\text{OBJ}_{\text{Implicit}}$) could extend to the entire plant and hence it is a global objective. The specific process variables that are related to each of the implicit objectives are often not obvious. A crucial part of the synthesis task is to identify the specific process variables that are to be regulated in order to achieve the overall design objectives.

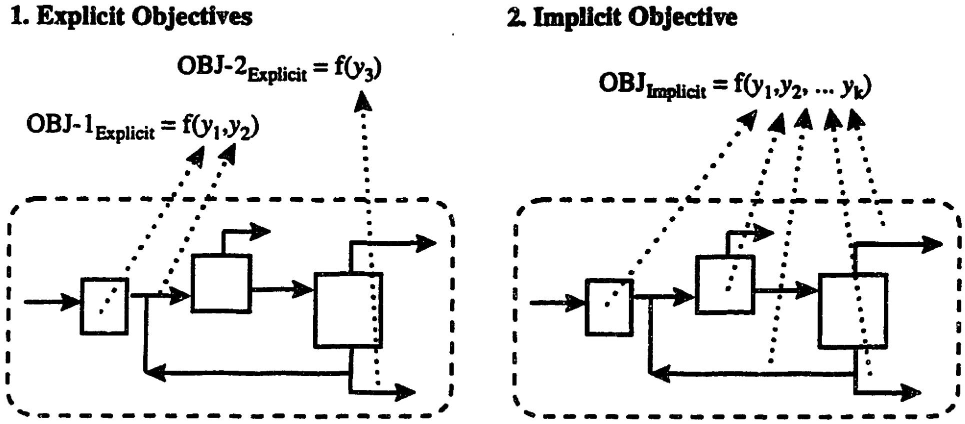


Figure 2 - 3: Explicit versus Implicit Objectives

Maintain internal consistency in the overall design

The importance of having internal consistency between the overall plant control structure and the overall production objectives has often been neglected. The design of a plant-wide control structure is not just an exercise to determine what inputs should be used to regulate what outputs in order to keep the plant under control. A plant-wide control structure is a device to assists the plant personnel to deliver their production objectives. Thus, the set of control strategies formulated should have direct relation to each of the goals of the plant operation.

Treatment of the Multivariable and Multi-objective Design Problem

In the operation of a chemical plant, such as the HDA process, there are invariably multiple goals that one would like to simultaneously accomplish. It should be clear that these goals are not of equal importance. It is of top priority to ensure that the plant is operating within its safe-operating limits. Goals which are related to product specifications should precede those which are related to the optimization of the plant. In a multivariable setting, these goals are likely to be inter-related and some of them may even be conflicting with some other objectives. The designer must then systematically resolve this issue during the synthesis.

Diversion of Process Disturbances from Plant Objectives

Chemical processes are typically bombarded by various disturbances from the environment even during a normal day of operation. Disturbances arise from the variations of feed purity, feed flow rates that cannot be controlled, daily variations of temperatures at the plant site, variations in the temperatures of the coolant or steam being used, etc. None of these are within the range of control of the engineer. Once the disturbances have entered the process, they cannot be eliminated. The only effective way to deal with the effects of the disturbance is by carefully diverting the disturbances to the less critical locations of the plant until they leave the process. The presence of a control system in the plant in fact offers another source of disturbances. By virtue of its role in process regulation, the control system transforms the variation of the process from the regulated variables to a different part of the plant, depending on its choice of manipulated variables (Moore, 1991). This idea is pictorially shown in Figure 2-4 (example originated from Downs, 1993b). The feed to the reactor is to be pre-heated by a heat-exchanger to a certain temperature. The temperature control loop attempts to maintain the outlet temperature at the required setpoint under possible variation of the upstream temperature. The result of the presence of this control loop is that the original effect of the disturbance is being diverted from the outlet temperature of the reactor feed to the variation of the flow rate of the hot process stream. Thus, it is important to keep in mind that the diversion of disturbance propagation in the plant is the heart of the control strategy design (Moore, 1991) and a good control strategy should exploit its ability to transform the process in order to "push" the undesirable effects to the less critical part of the plant.

It is important to clarify that the issue of how effective the control system is on the execution of production specification changes is a command-following question and it is as important as the problem of process regulation. In fact, the effects of the disturbances and the command signals on the control output are exactly identical. Variations that are otherwise propagated to the process outputs are being diverted to the actuators of the controllers. Thus, it is important to keep in mind that part of the function the control structure is to modify the topography of the disturbance rejection pathways in the plant so that they propagate in a desirable manner.

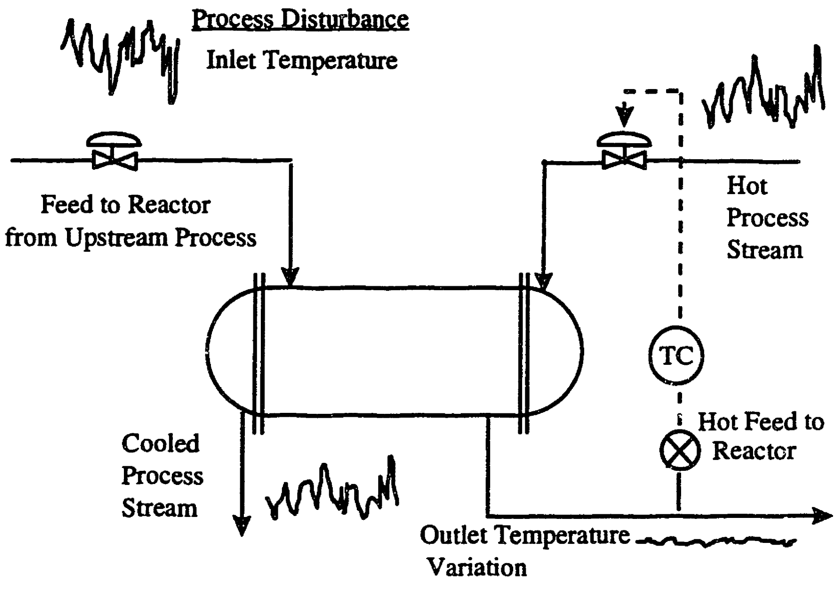


Figure 2 - 4: Propagation of Disturbances in a Heat-exchanger System (from Downs, 1993b)

Complexity of the Plant-wide Control Structure

Plant operators form an integral part of the operation of a chemical process. Any successful design methodology must be developed with the notion that operators are the ultimate users of the final product. Thus, the control system, when implemented, must have an identifiable structure which works with a mechanism that is relatively transparent.

Only such types of structures will prospectively become an aid to the operators and help to facilitate the delivery of production goals. Switching control from automatic to manual mode is a very frequent response to an esoteric and implicit control system.

2.2 A Methodology for the Synthesis of Plant-wide Control Systems

Chemical plants being built today are becoming more and more complex. With increased competitions in the market, there is great incentive to minimize both the operating cost. Thus, increasingly, more and more plants are built with some extent of material integration and heat integration with tight process operating constraints and multiple plant objectives. Not only do such forces make identification of suitable control strategies difficult, they also have the tendencies to drive the process to its operable limits, making it hard to maintain the stability of the plant during large upsets (Arkun, 1980; Narraway, 1993). Thus, a systematic method is needed to help the designer to address the issues of plant-wide control highlighted above. Specifically, a methodology for the synthesis of plant-wide control structures should :

- use a globally oriented approach which allows the designer to make evaluation on the plant as a whole at every step of the design;
- provide a mechanism by which specific process controlled variables that are consistent with the overall plant production goals be derived from production goals that are only vaguely defined;
- address the propagation of disturbances in plant-wide control;
- have a feature that allows the designer to incorporate the multiple plant objectives into the design in their order of importance;
- account for the fact that a chemical plant is a truly multivariable system;
- provide unambiguous rules to assist the designer in the synthesis process;
- and, generate a set of control strategies which together form an identifiable and relatively transparent control structure that can be easily understood by plant operators.

In the aerospace industry, a sophisticated control system designed specifically for a particular aircraft can be directly applied to any aircraft of the same type. However, the same is not true in the process industry. Generally, each chemical process plant has been designed for the particular environment in which it operates. A control structure which works well for a particular plant may not work in a different plant even if both plants produce the same product. Thus, a useful methodology should be one that is flexible enough that allows the designer to handle a wide variety of processes by allowing he or she to address the particularity of each control problem.

2.3 Review of Past Work

Since Foss (1973), Lee and Weekman (1976) and others pointed out the underdevelopment of control principles which guide the synthesis of control structures for chemical plants, a number of attempts have been made by researchers to address the plant-wide control design problem. Proposed methodologies have ranged from simple, unstructured set of heuristics which serve as guiding principles to the more systematic structured approaches. The various proposed design methods can be loosely classified according to the design viewpoint being employed and the type of approach being used in the development of design criteria.

2.3.1 Design Viewpoints

Design methodologies can be classified according to the position from which unit-operations are being viewed and according to the group of unit-operations which are being compared and judged. Unit-based focus and plant-wide focus have been the two most popular design viewpoints.

Unit-based focus

The development of design methodologies using the unit-based viewpoint come naturally from the experience that engineers have acquired on the control of unit operations. As a testimony to the widely available methodologies for the control of units like distillation columns, Umeda (1978) and Niida (1986) first formalized methodologies using the unit-based design viewpoint. Their basic idea was to decompose the plant horizontally into individual unit of operation (Figure 2-5 (a)); generate the best control structure for each unit (Figure 2-5 (b)); at the end, combine all these structures to form a complete one for the entire plant (Figure 2-5 (c)). Thus, unit-based control structure synthesis is essentially a *bottom-up* approach.

Although the unit-based focus directly utilizes our experience of the control of individual unit-operations, the major drawback with approaches which employ this viewpoint is that control structures of different parts of the plant that have been synthesized separately may not be compatible with one another. Thus, to maintain global consistency of the resulting structure of control loops, the designer has to identify and resolve conflicts such as those arising when a stream was selected for both control and manipulation by two different loops or the same output is being controlled by the two different controllers (see Figure 2-5 (c)). Since well-defined and sound rules are not available, the critical job still relies on the individual's experience. Secondly, there is no mechanism in this approach to ensure that the final control configuration is actually consistent with the overall plant-wide production objectives. Although Niida (1986) has provided rules to help designers to identify control loops in different unit-operations that will help to ensure overall objectives are being met and to avoid conflicts, it is still unclear how one can accomplish production goals and ensure that overall control system is feasible. The need for resolving conflicts is the major weakness in methodologies based on unit-based focus. The question of how one can remove conflicts while maintaining control requirements is still unanswered. With increasing application of material and heat integration in the plant and the use of multiple recycle streams together with complex heat-exchanger networks, chemical plants are becoming more and more complex. One can no longer isolate the effects of control to within the unit itself. Unit-based synthesis methods have become impractical for modern times so focus of research in the past decade has been shifted to plant-wide methods.

Figure 2-5 (a)

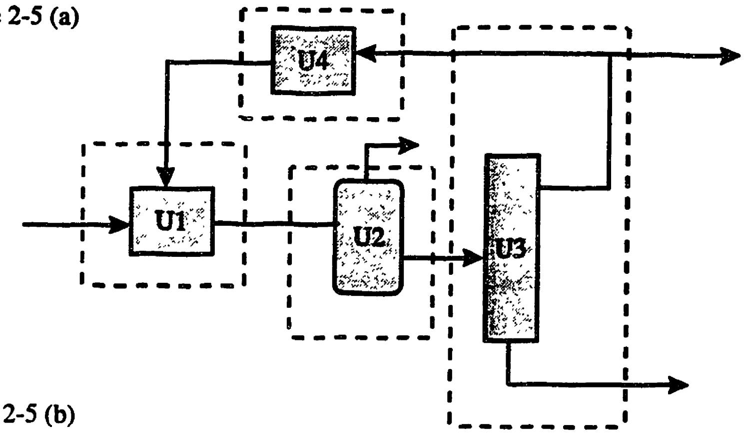


Figure 2-5 (b)

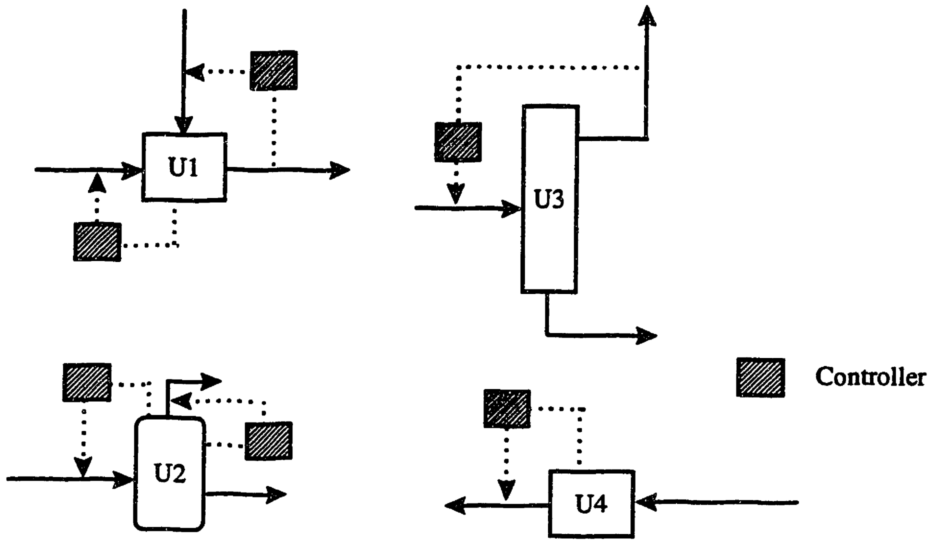


Figure 2-5 (c)

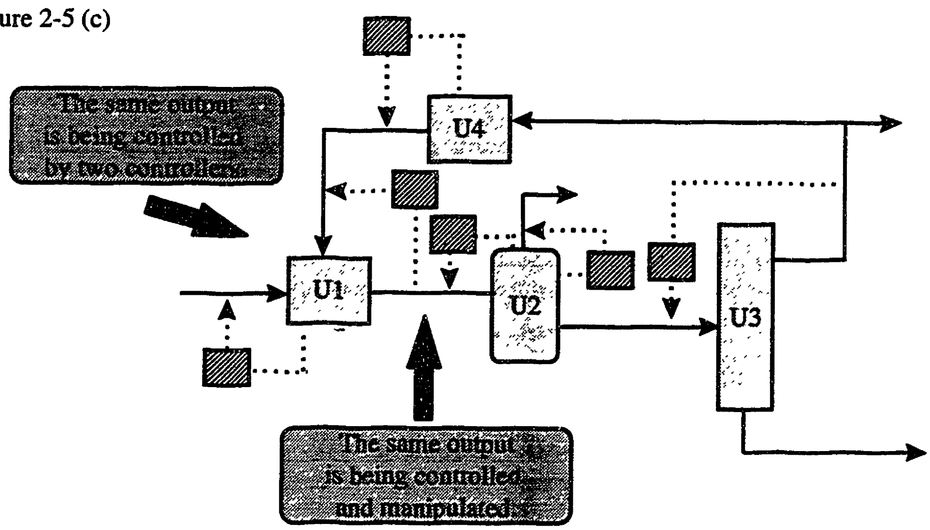


Figure 2 - 5: Unit-based Design Viewpoint

Plant-wide Focus

In the unit-based design methodologies, the complexity of the plant-wide control design problem is reduced by decomposing the plant by unit-operations. In the plant-wide based design methodologies, the entire plant is the object of study at every step of the synthesis procedure. The complexity of the design problem is reduced by decomposing the control structure either by functions of the loops in the control system or by the speed of the control loops.

The very first of this approach can be dated back to Buckley's division of the control structure synthesis problem into (1) material balance control system for the entire plant and (2) product quality control system for the entire plant (Buckley, 1964). The control of material inventories (handled by the first system) takes precedence and is considered to be important to prevent accumulation or depletion of materials in holding tanks. The second system is aimed at controlling the thermodynamic states to ensure the regulation of product quality. The rationale behind the decomposition is based on the fact that the material balance control system is called on to compensate for very low frequency disturbances (e.g. changes in production rates once every few days) while the product quality control system is called on to ensure the operation of the plant against higher-frequency disturbances (such as variation in temperature or pressure once every few minutes, or even seconds). Since the two systems address the rejection of disturbances that are widely different in ranges of frequencies (typically, an order of magnitude apart or more), there is generally minimal interaction between the material balance and product quality controls. Figure 2-6 shows the amplitude ratio versus frequency for the material balance and product quality control systems of a typical process plant. Although the approach to the decomposition of control task is useful, Buckley (1964) has offered little guidance on how the actual control loops (mainly single-input, single-output type) should be structured. Much of the synthesis work was still left to the designer's experience and skills.

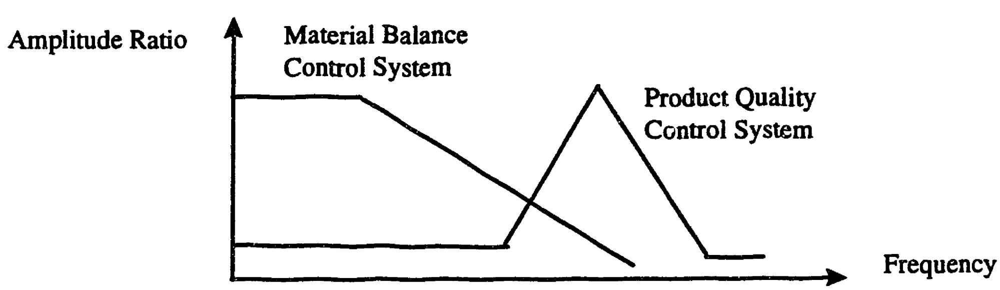


Figure 2 - 6: Sketch of Amplitude Ratio versus Frequency of Material Balance Control System and Production Quality Control System in Typical Process Plants

Shunta (1981) published the control design methodology practiced in DuPont and it can be regarded as an extension of Buckley's methodology. The list of control tasks were expanded to include the following:

1. Identification of special features in the plant.

2. Development the overall material balance control scheme.
3. Development the controls for secondary flows and temperatures.
4. Development the overall product quality control scheme.
5. Development constraint controls for equipment.
6. Development controls for startup.
7. Development process modeling and carrying out dynamic studies.

Again, there is no formal guidance on how each task should be carried out. Nevertheless, Shunta's work reflects the diversity of control objectives that are faced by the control system designer.

Recently, several groups of researchers have attempted to formalize methodologies using the plant-wide based focus in a *tiered framework*. In the tiered framework, complexity of the design is reduced through *decomposition of control structure by functions* or *decomposition by the speed of the control loop*. As a direct descendant of Buckley's (1964) method, Price and Georgakis (1993) and Layman and Georgakis (1995) address the control problem in stages corresponding to the goals and tasks of the control system. Each goal defines a subset of control loops and these control subsets are designed one at a time. A set of typical tiers useful for chemical process plants are:

1. Inventory control / production rate control. (lowest tier)
2. Product specification control.
3. Equipment and operating constraints.
4. Economic performance enhancement.

Their tiers correspond to a certain economic orders of magnitude within a plant. Control failure of a lower tiers would incur greater cost penalties than a similar failure at a higher layer. In their methodology, they propose that one should first develop the inventory control structure. For each inventory control structure, the additional controls which must be implemented to manipulate product quality are examined.

McAvoy and Ye (1994), have decomposed the control tasked according to the speed of the decentralized single-input, single-output (SISO) control loops. Their tiered framework consists of:

1. Level control loops.
2. Temperature, pressure control loops (non-composition, not related to production rate).
3. Composition control, production rate control.

Their methodology recommends the designer to first identify level control loops and other temperature, pressure control loops base on good understanding of the process. Then, the control loops for composition control and production rate control are selected based on a disturbance impact analysis. A tiered framework had been used by Banerjee and Arkun (1995).

In principle, a *decomposition-by-functions* approach should allow one to design control structures that are consistent with the overall production objectives. However, the guidelines that have been developed are based primarily on good understanding of the process. When the plants get larger and larger, like those that are common in the petro-chemical industry, one tends to lose his or her perspective of the function of each manipulation in the plant and the task of synthesis becomes difficult.

Hierarchical Focus

The hierarchical framework extends the plant-wide methods into multiple viewpoints. Rather than viewing the design issue as just one flat representation in the traditional plant-wide methods, this approach motivates the designer to decompose the plant into a set of representations. Invariably, all hierarchical approaches exploits the fact that each process representation capture a certain aspect of the plant operation. Thus, the complexity of the design is reduced as the designer is able to focus on one aspect of plant operation in each process viewpoint. The hierarchical framework is being commonly employed in many disciplines to solve very large scale problems.

Morari et al. (1980a, 1980b, 1980c) were the first to introduce the use of hierarchical decomposition for large-scale systems to deal with the complexity of the design of control structures for chemical plants. Their method has been based on the multilayer-multiechelon optimization theory developed by Mesarovic(1970) and Fiedeisen (1979). Morari et al. (1980a, 1980b, 1980c) recognize that different disturbances affect the plant at different frequencies as shown in Figure 2-7. Using a set of comprehensive mathematical rules to classify controlled variables into ones which are related to plant optimization (such as those affected by d_1 in Figure 2-7) and ones which are related to plant regulation (such as those affected by d_2 in Figure 2-7), the effects of the *slowly-varying* disturbances which have a relatively large economic impact on the system and the *fast-varying* disturbances with low economic impact can be separately identified. In this way, control objectives which must be controlled to reject various types of disturbances are categorized in a multilayer fashion to form a multi-scale hierarchy such as the one shown in Figure 2-7. However, in his methodology, regulatory control structures are synthesized by generating control structures to some horizontally divided sub-problems of the plant via structural arguments (see Section 2.3.2) alone.

Although Morari recognizes the fact that some control objectives are more important than others, the classification is mainly based on their economic impact on the plant. Johnston (1991) proposed a methodology that gives explicit treatment of the multiobjective nature of production. His approach uses a *top-down* hierarchy that is similar to the one that has been introduced by Douglas (1995) for process design. The plant is progressively modeled by: (a) an overall input-output system, (b) a recycled structure with generalized reaction and separation systems, (c) a detailed flowsheet with all unit operations. A set of logically sound guidelines has been provided to aid the design from the identification of initial production objectives to the selection of a feasible set of manipulated variables in a systematic manner.

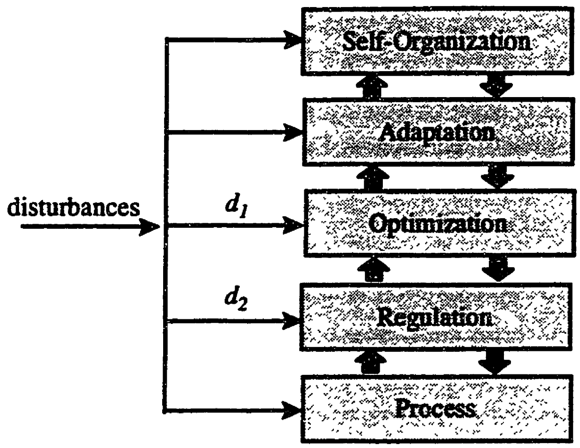


Figure 2 - 7: Morari et al's (1980a; 1980b; 1980c) Multilayer Decomposition of the Control Tasks

The main driving force in the mechanism of Johnston's methodology is diversion of disturbances to less critical locations of the plant. Thus the control strategies are synthesized on the basis of the effects of the structure on the topography of the disturbances propagation in the plant. The plant-wide nature of the design problem is retained by formulating specific procedures that translate initial objectives and refine control decisions from the top layer down the hierarchy. In this manner, the global objectives are ultimately being transformed into more specific control objectives at a, possibly, local level, which can be handled by a controller via a set of manipulated variables. The multiobjective nature of the problem is handled by always treating the objectives of higher priority first. Regulation of control objectives is handled by choosing manipulated variables that will divert disturbances from the more important variables to the less critical ones. Structural controllability analysis (see Section 2.3.2) is performed to ensure that the final control configuration is feasible. By following the hierarchical decomposition, only control structure alternatives that are consistent with the overall production goals will be retained for final screening. Thus, the set of alternatives is largely reduced.

Ponton and Laing (1993) have recently proposed the use of a hierarchical approach to the design of plant-wide control structures. Their methodology involves the integration of a control system design hierarchy with the process synthesis hierarchy that has been advocated by Douglas (1985). The methodology proposed by Douglas (1985) for the synthesis of process flowsheet requires a sequential elaboration of the plant from a single block with only feed and product streams to a full process flowsheet. In brief, the process design hierarchy can be divided into the following stages :

- Design of the input-output structure
- Design of the recycle structure
- Design of the separation sequencing
- Design of the energy integration

The corresponding control system design hierarchy proposed by Ponton et al. (1993) is:

- Feed and product rate control
- Recycle rates and composition control

- Product and intermediate stream composition control
- Temperature and energy balance control
- Inventory regulation

Analysis at the first two levels of the hierarchy establishes the basic control structure that forms the basis of the computer control system. The details of the control system can be filled in when one proceeds to the more elaborate levels of the process design hierarchy (e.g. the stages that are involved with the sequencing of the separation units and the integration of energy). The selection of control alternatives from the available choices is based on heuristics and qualitative understanding of the process. Much of the synthesis work has to be relied on the designer's own experience of the process itself. Decisions are being made in a fairly non-systematic, *ad hoc* fashion.

It should be noted that in Ponton's (1993) work, the regulation of inventory is being regarded to be the least important type of control and it is to be examined after all "strategic" control systems have been specified. This approach is contrary to what Buckley (1964), Shunta (1981) and Price and Georgakis (1993) have proposed. In the works by these earlier researchers, they have considered the synthesis of the part of the control structure to handle inventory control to be more critical to the success of the operation than the part of the control structure for the control of product quality.

2.3.2 Design Approaches

Once a design framework has been chosen, criteria must be developed to enable the selection and allocation of manipulated variables to control objectives, i.e. the synthesis of a control structure. The next few sections will summarize the various approaches that have been used by researchers.

Heuristically Based Approaches

Most design methodologies developed before 1980s have been based heavily on design heuristics, such as those methods developed by Buckley (1964), Shunta (1981), Umeda (1978) and Niida (1986). Allocation of manipulated variables to control objectives are based primarily on factors such as the size of the process gain; the size of the process time constants and the size of the deadtime. Little regard is given to the multivariable nature of the process plant as well as the impact of these decision to the performance of the close-loop control structure.

Recently, Price and Georgakis (1993) have developed design rules which considers the interactive nature of process variables in the plant. Some of their rules include:

- Inventory control structure should be *self-consistent* and directed along the primary process path where a structure is said to be self-consistent if it is able to propagate a production rate change throughout the process (see Figure 2-8).
- Use process internal flows as throughput manipulators.
- Composition manipulators should be closed to the controlled variable.

Luyben and co-workers (Luyben, 1993a; 1993b; 1993c; 1994; Luyben and Luyben, 1996; Tyreus and Luyben, 1993) have also investigated the effect of recycles and fresh feeds in process plants and they proposed that:

- One flowrate somewhere in the recycle loop should be flow controlled to prevent the buildup of material in the recycle stream.
- Fresh feed make-up of any component cannot be fixed unless the component undergoes complete single-pass conversion.
- Reactor composition control is required. Use fresh components to hold the reactor level or to maintain composition.

All these rules allow the generation of design alternatives which are potentially promising but further evaluation through dynamic simulations is required to determine the best candidate control structure(s).

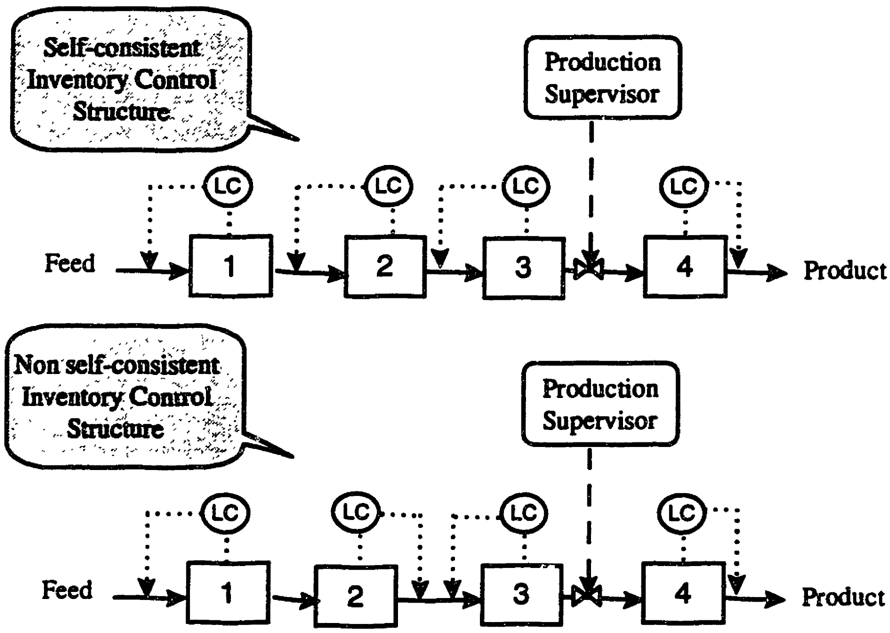


Figure 2 - 8: Self-consistent and Non self-consistent Inventory Control Structure

Structural Approaches

Structural arguments have been used extensively for the synthesis of feasible plant-wide control structures in both the unit-based or plant-wide design framework. The work by Govind and Powers (1976, 1977, 1978, 1982) marked the beginning of a much more systematic structural approach to the formalization of plant-wide control. They proposed the use of cause-and-effect digraphs based on the incidence matrix[1] of the steady-state material and energy balances for a given processing scheme. The digraph represents the interaction among the different process variables and information flow is presented through a network of nodes and edges. Nodes are the process variables and the edges represent directional causality[2]. These graphs contain information of the steady-state gains, dominant time constants and deadtimes. Synthesis of control structure begins with a

[1] Incidence matrix is essentially a structural array which shows the dependence of each output on various inputs. More details about incidence matrix will be given in Chapter 4.

[2] The notion of causality is intended as the property that the present value of the output (effect) of a physical system is not affected by future values of the input (cause).

statement of process objectives from the designer. If they are properly stated, they can be translated into the process variables that might be controlled. The method uses the cause-and-effect graph to systematically derive alternative sets of measured objectives either in the downstream or upstream direction. The control requirements are propagated forward or backward via *Boolean* type of arguments in order to identify logical linkages between controlled objectives - measured variables and manipulated variables. Screening of the final set of alternative structures relies on practical heuristics and simple dynamic considerations.

The structural approach has many attractive features, since it has an intuitive inferencing set of procedures and the synthesis process can be carried out systematically. However, the major weakness is that it lacks a mechanism which will ensure that (1) the final control structure will satisfy controllability requirements and that (2) there is no overspecification of control objectives. At times, infeasible control structure can be generated (Morari and Stephanopoulos, 1980b; Johnston, R.D. and Barton, 1985a).

Johnston, R.D. and Barton (1985a, 1985b) proposed an alternate algorithm that is also based on structural argument but included a procedure to ensure that the degrees of freedom are met and that the final control structure is feasible.

The notion of structural controllability was first introduced by Lin (1976) who made use of structural matrices (equivalent to incidence matrices). The adaptation of this idea for control structural synthesis was first proposed by Morari and Stephanopoulos (1980b). Johnston, R.D. and Barton (1985a, 1985b) adopted the structural controllability arguments in Morari's (1980b) work for the selection of sets of manipulated variables for the various control objectives. The difference between the two methods lies in the way that consistent sets of manipulated variables are being selected. Morari creates manipulation sets for the units sequentially, resolving conflicts as they arise. Johnston, R.D. et al. expanded Morari's idea by the explicit use of a coordinator matrix which acts as a high level decision maker to help eliminate the generation of conflicts and infeasible structures early in the design by monitoring the assignment process. One big advantage of the presence of the coordinator is that the assignment process becomes non-iterative.

Both of the above approaches have set the stage of structural analysis of plant-wide control methods for the more recent developments in this area. Georgiou and Floudas (1989) and Türkay, et al. (1993) have formulated the control synthesis problem as a mixed-integer linear programming problem for the global plant. Their methods make use of the structural controllability (Morari et al., 1980b; Johnston, R.D., 1985a) and functional controllability (Russell and Perkins, 1987) as explicit constraints for the optimization problem.

In these structurally based design methodologies, after the set of feasible control structures have been generated, they have to be further analyzed using additional output performance related criteria to determine which of these is the best control structure for the plant. Thus, this type of methodologies has several shortcomings. First, the task of generating the complete set of feasible control structures could be enormous for large complex plants. Second, the number of feasible control structures for the plant could be large and a good structure can only be identified through further systematic screenings. Hence, much of the effort that has been invested into generating the complete set of feasible control structures does not amount to much efficiency in the synthesis of the best control structure for the plant.

The synthesis of control configurations based on the analysis of the *disturbance load paths* of the process has been used by Calandranis and Stephanopoulos (1988). Although their methodology has been developed primarily for the design of control systems in heat exchanger networks (HEN), the fundamental concept behind their approach is quite applicable to other types of system as well.

The design process is divided into two stages. The first stage deals with the design of the configuration of control loops in a network of heat-exchangers (the DESIGN problem). The second stage deals with the sequencing of the control action of the loops to accommodate set-point changes and to reject load disturbances (the OPERATIONAL problem).

In their work, they have exploited, in an explicit manner, the rich analytical knowledge derived from the structure of a HEN and its operability characteristics in order to identify routes through the HEN structure that can allocate *loads* (disturbances, or set-point changes) to *available sinks* (external coolers or heaters). These routes are the disturbance load paths.

Through a series of illustrative examples, they have demonstrated that a disturbance load path that is suitable for "nominal" operating conditions may not be operable when the magnitude of the anticipated disturbance becomes significant. Furthermore, a disturbance load path may be *nonconvex* so that is usable at end parametric conditions but not operative for a range of intermediate values of the varying parameter. Also, the occurrence of a pinch temperature "jump" during the transition of the process from one state to another may make the originally selected disturbance load path unsuitable if minimum utility consumption is to be achieved. Thus, in their work, they have emphasized the need of a supervisory system that continually updates its information about the operation of the network and evaluates better structural alternatives using suitable *control logic*. Their methodology goes beyond the selection of the necessary control elements (measurements and manipulations) from within the HEN. Their methodology also provides guidelines for the determination of the structure of a set of SISO loops which are capable of transferring the network from one steady state to another in some "optimal" manner. The control structure is an inherently variable one, where the active configuration connecting the controlled variables and the manipulations depend upon the specific control task. The result is that the set of SISO loops emulates multivariable control through a logical sequence of control actions but the control structure at large and the operation of each control loop are quite transparent to the human operator.

The selection of the manipulated variables is based on simple heuristic arguments using parameters like the open-loop static gains, delays and time constants. Guidelines are available to assist the design of steady-state control structures and the implementational strategies. However, whenever conflicts arise, *ad hoc* judgemental knowledge from the designer is required. Nevertheless, their work has demonstrated the power of structural analysis and the superiority of a variable control configuration over a fixed control structure.

The use of disturbance load paths for the synthesis of plant-wide control structure has been further developed by Johnson, J.E. (1991) within the structural framework. His methodology allows the designer to select potential manipulated variables that can be used for the maintenance of various control objectives by tracing the topography of the propagation of process disturbance in terms of the plant's causal pathway (structural) network.

Multivariable Design Approaches

With the exception of the work by Johnston, J.E. (1991), the control structure synthesis methods described previously are designed primarily to generate control configurations suitable for single-input, single-output control loops. None of the above approaches paid any attention to issues related with the dynamic interactions among the control loops, either. Another avenue that has been taken by several researchers is that the plant-wide control system synthesis problem should be viewed as a large-scale, multivariable control problem. Multi-input, multi-output controllers (MIMO) of various degrees of decentralization have been proposed. The review of the predominant methodologies given below of such an approach is by no means complete, since all these methodologies are variants of the same theme, i.e. design of MIMO controllers, for which an enormous amount of research work has been carried out over the last 30 to 40 years. In the subsequent paragraphs, only those approaches which have explicitly stated that they were intended for the design of very large-scale MIMO systems, such as a complete chemical plant will be discussed.

Centralized Multivariable Control

Lau, et al. (1985) proposed the use of singular value decomposition (SVD) technique as a tool to tackle the problem of loop selection for the synthesis of control structures in a systematic and rigorous manner. Control structures are synthesized using the *condition number* (which is the ratio of the maximum singular value to the minimum singular value) and the *total interaction measure*. Ideally, the selected structure of control loops should correspond to a system with a small condition number and a small amount of interaction. Processes with nearly triangular (lower, or upper) input-output models, exhibit little or no interaction and allow the formulation of a natural structure of non-interacting loops. When the system does not have a natural structure, structural compensators can be designed to exploit system interaction. Thus, Lau (1985) provides prescription for the design of control structures from pairing of sets of controlled variables with sets of manipulated variables to the actual control laws that will be used.

Decentralized Multivariable Control

Daoutidis and Kravaris (1992) suggested the use of *relative orders* of input-output pairs of a multivariable nonlinear system as a measure of sluggishness. A multi-loop structure can then be formed by arranging input-output pairings in such a way that the pair itself forms a relative order that is lower than the relative orders between the input and the other system outputs.

Banerjee and Arkun (1995) have developed a systematic way to determine the input-output pairings based on the amount of cross-feed performance degradation resulted from not using a full scale multivariable design. In the first step, a subset of measurements and manipulations are selected based on a necessary condition for robust stability. Then, all possible pairings for the subset of control variables that made it past the first step are tested for nominal stability and small cross feed performance degradation. The key design criterion is that the candidate configurations should not suffer much performance degradation as a result of decentralization.

Block Decentralized Approach

Centralized MIMO control has the potential of achieving global optimality as there is an absence of segregation in the original problem. Decentralized approaches, on the other hand, reduce the complexity of the problem by allowing the sub-problems to be handled individually. To take advantage of the relative strengths of both approaches, Manousiouthakis, et al. (1986) put forward a *block decentralization* strategy for control structure synthesis. The original system is to be partitioned into blocks of aggregates of control loops of various dimensions that have no interactions among themselves. This idea is in fact very similar to Morari's method (Morari, 1980a) of decomposition of a plant into subgroups of same functionality with minimal interactions (and therefore minimal coordination effort).

In the approach by Manousiouthakis (1986), the best case would be a completely decentralized plant with SISO loops and the worst case would be a fully centralized one. In the algorithm, *block relative gain* (BRG) is used as a means to measure the amount of interaction among the various possible blocks.

2.4 Strengths and Weaknesses in Past Work

In the previous section, the pros and cons of the various types of methodologies have been pointed out. In this section, the strengths and weaknesses in the work developed in the past are further summarized. The usefulness of the methodologies have been evaluated based how well do they address some of the issues discussed in Sections 2.1 and 2.2 as well as the degree of formalization accomplished.

Identification of Specific Process Controlled Variables and Maintaining internal consistency in the overall design

The most critical assumption that has been made by many past researchers is that the designer has a good idea of the process variables to be regulated in each unit-operation. This is in fact rarely the case. As demonstrated earlier in Section 2.1, the designer is often only given the overall production goals, which may or may not be related directly to a set of specific output variables. The issue of the identification of controlled variables is extremely important for very large plants that are common in petro-chemical industries. It is not always obvious what variables have direct contribution to high product purity and maximum product throughput. However, even if the designer can identify the possible set of variables that must be maintained at desired values for stable operation, the choice of a set of variables that it is consistent with the initial production objectives is very often non-trivial. Thus, to ensure that the final control structure of the plant is consistent with the overall production objectives, it is of the utmost importance that a methodology can begin from production goals that are only vaguely defined and be able to refine the initial objectives systematically into specific sets of variables to be regulated. Furthermore, the methodology should maintain a plant-wide viewpoint so as to ensure that the final control structure is feasible, conflict-free and related to the overall production objectives. Through such an approach, plant-wide requirements are being retained during the synthesis process. The works by Morari et al. (1980a) and Johnston, J.E. (1991), Price and Georgakis (1993), Lyman and Georgakis (1995), McAvoy and Ye (1994) have demonstrated the benefit of a plant-wide framework. Marari et al. (1980a) and Johnston, J.E. (1991) have shown how process controlled variables which are associated with the production objectives can be systematically identified.

Treatment of the Multi-objective Design Problem

Real life decision making for a large-scale problem is often an extremely complex process. There are usually several objectives that one would like to accomplish during the operation of chemical plants and some of them may even have to be optimized. There are also some other issues that are crucial to the success of the operation but need not be optimized and are only required to be brought to a satisfactory region. Not only do these multiple objectives facing the engineer may not have direct correspondence to each other, they may even be in conflict with each other and each may dictate different treatment by the control system. The control of a chemical plant is in fact one such type of a problem and any useful methodology must have a feature that allows the designer to incorporate the multiple objectives into the control system design. The main focus of the research in this area has been the formulation of control structures using fully decentralized SISO control structures. The use of multivariable control in a plant has not been fully explored. With the exception of the work done by Morari, et al. (1980a) , Johnston, J.E. (1991), Lau, et al. (1985) and the recent work by Price and Georgakis (1993), none of the past work explicitly recognize that not all of the plant's objectives are of equal importance.

Complexity of the Plant-wide Control Structure

To reduce the complexity of the plant-wide control structure, past researchers have limited themselves to the employment of the SISO loops. As described in the previous section, the use of MIMO structures for process controlled should be explored. The control structure should be one which adequately accounts for process interaction but at the same time retains a recognizable and relatively transparent structure so that its function can be easily understood by plant operators.

Systematic nature of the methodology

With the exception of the methodologies which treat the plant-wide control problem as a monolithic multivariable design problem, most methods that have been recently developed relies quite heavily on design heuristics and generic rules to synthesize potential plant-wide control structures. Examples of these works include Price and Geogakis (1993), Lyman and Geogakis (1995), Luyen and co-workers (Luyben, 1993a; 1993b; 1993c; 1994; Luyben and Luyben, 1996; Tyreus and Luyben, 1993). These workers have relied on dynamic simulations to help them to determine the best control structure from the set of alternatives. Furthermore, it is doubtful that heuristically based methods can be conveniently applied to large scale systems.

Structurally based methodologies such as those by Johnston, R.D. (1984) and Georgiou and Floudas (1989) are very systematic. However, work which have been developed to date only allows the synthesis of a set of feasible control structures for the plant. The issue of how to identify the best control structure from the set of potential ones have not been satisfactorily addressed.

Among all the methods described in the previous section, only Johnston's method (Johnston, 1991) provides a systematic means for the identification of control objectives that are conflict-free and are consistent with the full set of overall plant production goals. The use of a hierarchical framework helps to retain the overall plant-characteristics at every stage of the synthesis process. Again, the weakness in Johnston's work (Johnston, 1991) is that only the structural aspect of the design problem has been explored. Structural representation of the process only shows the relations among variables. When there are multiple alternatives for the control of certain objective, Johnston has only provided qualitative arguments for the selection of suitable manipulated variable for control. Furthermore, there is little consideration of process dynamics. Interaction of control actions in a multivariable system is again addressed in a qualitative manner.

2.5 Approach in this work

At this point, it should be clear that control structure synthesis is not merely a process of obtaining optimal pairing between inputs and outputs of the plant. It is, in fact, a creative process by which a set of control strategies which creates desirable pathways for the propagation of disturbances and ensures a conflict-free delivery of overall production objectives is determined. It is the objectives of this research to develop a methodology which addresses the above fundamental issues.

In this research, a systematic methodology for the synthesis of plant-wide control structures which uses Johnston's ideas (Johnston, 1991) as the basis has been developed. The hierarchical framework is a suitable one for solving large-scale problems. It will be shown, in the next few chapters how a comprehensive method can be developed by incorporating specific quantitative rules that are suitable for a multiobjective, multivariable setting. It will also be shown how control strategies that are suitable for both long-range and short-range regulation of the plant be developed in the hierarchical framework and how the use of such multiple control schemes can benefit plant operation. It will be demonstrated later that the proposed methodology allows the designer to generate a set of control strategies that are consistent with the overall plant wide control objectives and that these strategies together, work with a mechanism that is relatively transparent which can be understood by plant operators and addresses the operational needs of today's chemical process plants.

Chapter 3
A Generic Framework for the Design of Plant-wide Control Structures

3.1 Introduction

The task of control structures synthesis can be described as follows. Given a fixed flowsheet, a vector of process disturbances $\boldsymbol{d} \in \mathbf{D}$ that are expected for the plant, a vector of measured process outputs $\boldsymbol{y} \in \mathbf{Y}$ and a vector of manipulated inputs $\boldsymbol{u} \in \mathbf{U}$, a control structure for the plant is to be derived so that the plant production objectives are met in the most desirable manner. It has been pointed out in Chapter 2 that there are two main types of plant objectives:

1. Type I : Explicit production objectives - $\beta \in \mathbf{I} \subseteq \mathbf{Y}$

   An explicit objective is a local objective which can be directly related to a measurable variable.
2. Type II : Implicit production objectives - $\kappa \in \mathbf{II}$

   An implicit objective is a global objective which represents the overall behavior of the process. The state of the implicit objective can be related to a number of measurable outputs $y_i \in \mathbf{Y}$ in various locations of the plant, i.e.:

$$\kappa_j = f_j(y_i)\,, \quad \kappa_j \in \mathbf{II}, y_i \in \mathbf{Y} \qquad [3\text{-}1]$$

   where $f_j(\cdot)$ is some function.

Hence, the goal of the *overall control system* of the plant is to minimize the following vector of objectives:

P1: $\Phi = \min_{u} F = [F_k] \quad \forall k \in F_k \equiv F_I \cup F_{II}$

subject to:

plant dynamics
process constraints
process disturbances

where :

$$F_{I,i} \in F_I \quad \forall i \in \mathrm{I}, \quad F_{I,i} = \left\| \beta_{i,sp} - \beta_i \right\| \qquad [3\text{-}2]$$

$$F_{II,j} \in F_{II} \quad \forall j \in \mathrm{II}, \quad F_{II,j} = \left\| \kappa_{i,sp} - \kappa_i \right\| \qquad [3\text{-}3]$$

The design of a control structure that will optimally solve the problem P1 on-line for continuous changes in the vector of disturbances $\boldsymbol{d}$ and vectors of desired objectives $\boldsymbol{\beta}$ and κ is non-trivial. In this chapter, a generic framework which allows designer to systematically identify a control structure to tackle the P1 will be described.

In Section 2.1, typical plant-wide design problem was presented using the Hydrodealkylation (HDA) plant. The HDA example shows that the task of designing plant-wide control strategies poses several challenges to the control engineer. These include:

1. *Not all the specific process control objectives are known.* Implicit objectives (e.g. minimize production rate, minimize process variations) create obstacles in the design. Without knowing the set of process variables which define the global behavior represented by an implicit objective, we cannot easily incorporate a control mechanism that will maintain the objective at its desired state. Thus, part of the task of the designer is to identify the set of specific process variables which must be coordinated to achieve the global objective, κ_j in Equation [3-1].
2. *It is a multi-input multi-output (MIMO) design problem.* Changing one manipulated variable may have effects in a number of areas in the plant. It is not obvious which ones of these designs would help us to best accomplish the general production objectives that we have listed.
3. *It is a large scale design problem.* Changes in a manipulated variable produce both local and global effects in the plant. The recycle streams in the process modify the dynamics of the global system and introduce slow process dynamics within the plant, causing the ultimate effects of some process changes to be only observable in the long time-horizon. By taking a global viewpoint of the plant, we are able to account for both the local and global characteristics of the process. However, this viewpoint contains a lot of detailed information that is required to be processed, increasing the complexity of the synthesis. On the other hand, if we focus our design on the individual unit-operations, we may lose our perspective of the plant as a whole and fail to account for objectives which are global in nature.

It has been found by many researchers (Simon, 1969; Mesarovic et al., 1970; Fideisen et al.,1979; Lasdon, 1964; Haimes, 1973; 1975; Sage, 1977; Maximov and Meystel, 1992;

Douglas, 1985; Morari et al., 1980a; Johnston, J.E., 1991; Ponton et al., 1993 and others) that the complexity of the design problem can be reduced by posing the design issues in a hierarchical framework. In the next section, an overview of the hierarchical analysis is presented, which will be followed by specific description of how each of the issues mentioned above can be addressed within the hierarchical framework.

3.2 Overview of Hierarchical Analysis

Figure 3-1 gives an overview of the organization of a hierarchical analysis applied to the synthesis of plant-wide control structures. A control structure is derived from a *hierarchy of stratification* of the overall system which consists of a set of process representations that range from coarse process abstraction to detailed plant descriptions. The higher strata correspond to a longer time horizon of the process operation while the lower strata correspond to a shorter time horizon of the operation. At each stratum, there is a set of production goals which are derived from the overall production objectives. This set of goals form a hierarchy and a control structure which address these goals is to be synthesized. The control of each goal in the hierarchy functions like a decision-making unit which must be coordinated among other decision-making units (control of other goals). As each stratum corresponds to a distinct time-scale of the problem, the control structure synthesized at each stratum corresponds to a different layer of the overall control system. The focus of this work is on the control tasks immediately related to process regulation.

The proposed framework uses a "total system viewpoint" in the design. A stratified model of the entire system is derived on one hand, while the overall control system is decomposed into layers (long-horizon and short-horizon) on the other hand. The tasks of the units comprising the *multiechelon system* (goals) are then defined with reference to the representation and the decision problem at each stratum (Mesarovic et al., 1970). The organization approach displayed in Figure 3-1 uses several notions of levels that has been introduced by Mesarovic et al. (1970) to describe hierarchical systems. In general :

1. The concept of strata is introduced for the modeling purpose.
2. The concept of layers is introduced in reference to the vertical decomposition of a decision problem into sub-problems. Layers are essentially levels of decision making complexity (Haimes et al., 1990).
3. The concept of echelons refers to the mutual relationship between decision-units comprising a system.

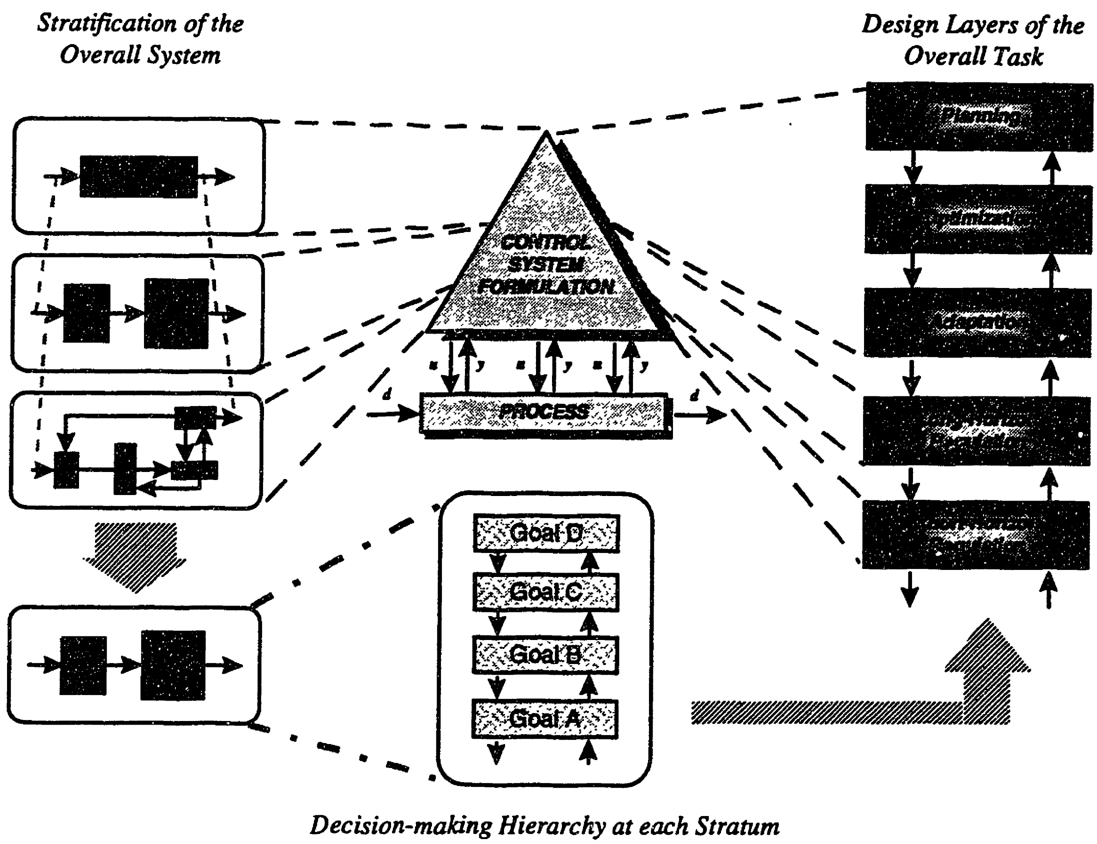


Figure 3 - 1: The Organization of a Hierarchical Analysis applied to the Synthesis of Plant-wide Control Structures

3.3 Modeling Complex Chemical Plants by Hierarchical Stratification

Hierarchical stratification is used to resolve dilemma in describing a large complex system. The dilemma is between simplicity in modeling (and consequently in the solution strategy applied) and competence in accounting for the large complex system's numerous behavioral aspects (Haimes et al., 1990). Using a multistrata framework, a process plant can be described by a family of representations, each representation is concerned with the behavior of the system as viewed from a different level of abstraction. Each stratum has its own set of relevant variables and is governed by its own concepts and principles. A subsystem on a given stratum is a system on the stratum below (Figure 3-2). Stratification allows one to study the internal operation of the plant at the level of detail represented by the stratum, relatively independent of other strata. As we move down the hierarchy, we obtain a more detailed explanation of the process, while in moving up the hierarchy, we obtain a deeper understanding of the significance of various parts of the plant (Mesarovic et al., 1970).

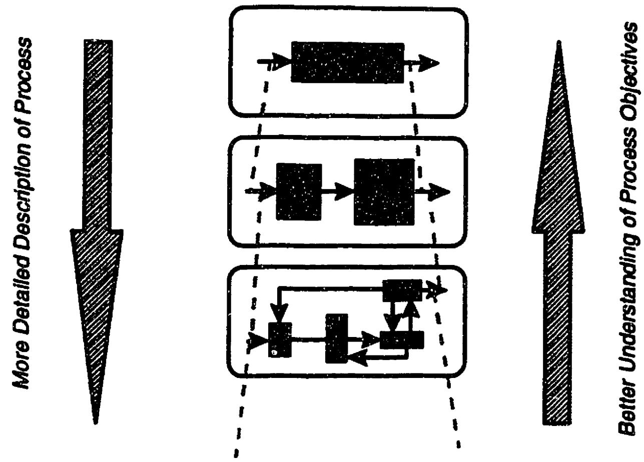


Figure 3 - 2: Hierarchical Stratification

The HDA plant presented in Section 2.1 can be decomposed into a hierarchy of plant representations, similar to those used in conceptual design of chemical plants (Douglas, 1988) as shown in Figure 3-3. By examining only the information that can be derived from a particular representation, the focus of the plant control design is being shifted to that particular range of characteristics. This series of process representations of the HDA plant provides a spectrum of *visual resolution* which can suitably address both the local explicit objectives (Type I: β) and the global implicit objectives (Type II: κ). Level and stratum will be used interchangeably throughout the discussion.

1. *Level 1: Input-Output Representation of the Plant*

   The *input-output* representation is the most abstract viewpoint of the plant (Figure 3-3 (a)). It gives a unique perspective of the overall purpose of the production plan, that is, to transform the feed streams into the desired product(s) using the available resources of utilities. This particular representation allows the designer to focus on the overall process objectives and corporate management decisions that affect interactions between the environment and the plant as a whole. Issues and objectives that are important at this level of representation include the overall materials and energy balances of the process, production rate and the steady-state product quality control.

2. *Level 2: Recycle Structure of the Plant*

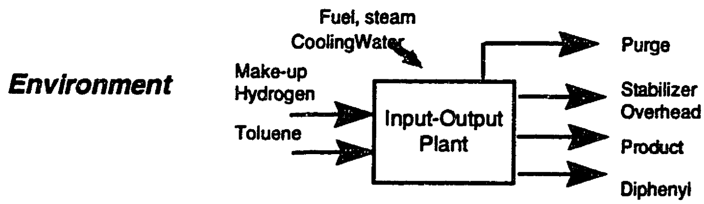
   At the next level, the main block, input-output plant, is decomposed into two sub-blocks by grouping the activities which are dynamically similar into two areas. One block represents the generalized reaction unit and the other the generalized separation system (see Figure 3-3 (b)). With this decomposition, the recycle structure of the plant is exposed. In this viewpoint, the effects of variations in the recycle flows on the overall system can be studied.

3. *Level 3: Refined Representations of the Plant*

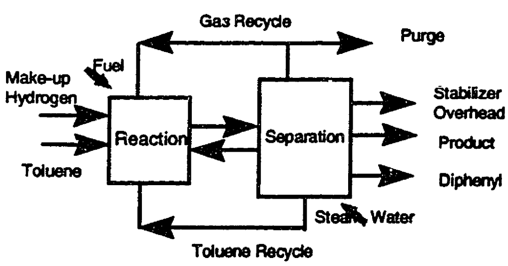
   At Level 3, the sub-blocks of the reaction and separation systems are expanded in stages through a series of refined representations of the plant. The role of the process units in the plant are being systematically evaluated in these viewpoints. For example, at Level 3a (Figure 3-3 (c)), we can examine how the division of materials in the generalized phase-separation unit plays a role in the process; at Level 3b (Figure 3-3 (d)), we take a closer look at the reaction section; at Level 3c (Figure 3-3 (e)), the interaction between the separation system and the rest of the plant is being emphasized. As the these representations become more refined, more and more of the details in the plant are being exposed. Objectives and constraints which are localized to individual unit-operations become issues in the design.

4. *Level 4: Detailed Representation of the Plant*

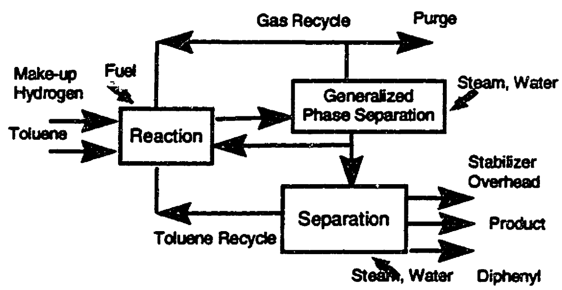
   At the detailed level (Figure 3-3 (f)), individual unit-operations are the basic blocks in the representation. The analysis focuses on the immediate changes in the different operating-units. Process behaviors that are localized to the unit-operations predominate in this representation. The dynamics of product recovery in the separation system can also be studied.



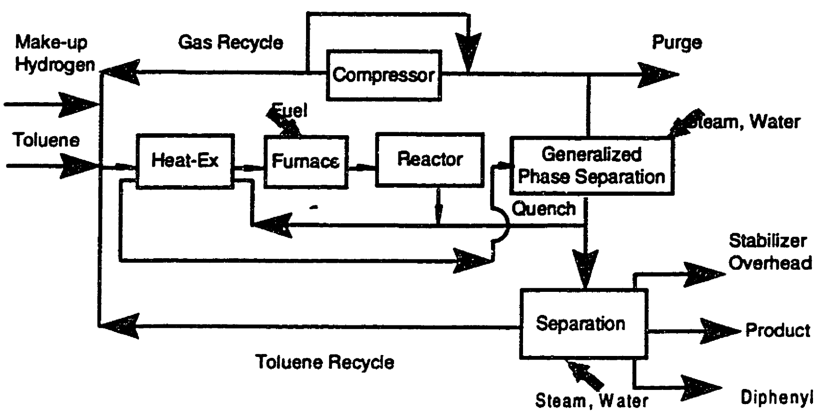
(a) Level 1: Input-Output Plant



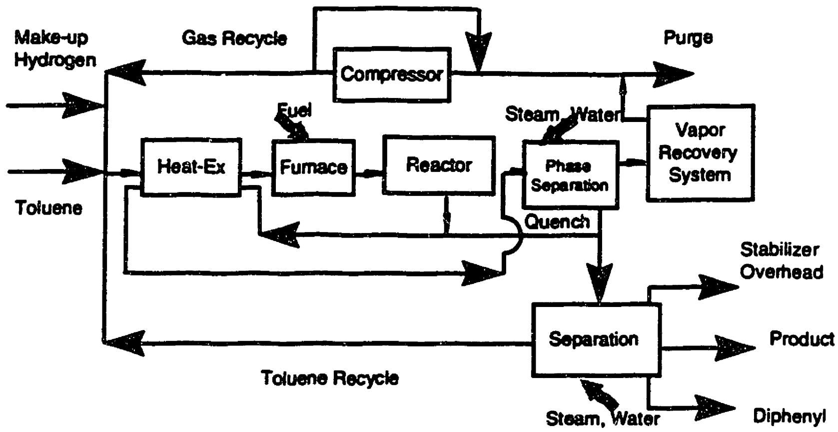
(b) Level 2: Recycle Structure



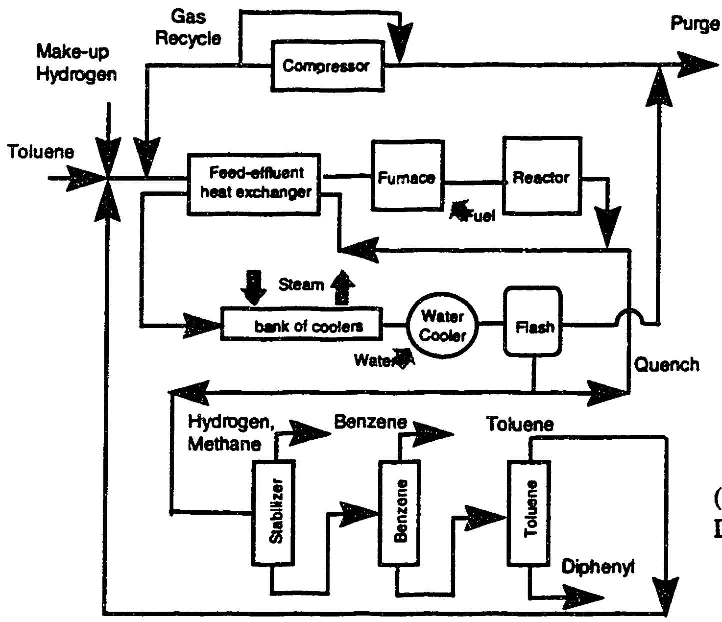
(c) Level 3a: Generalized Reaction - Expanded Separation



(d) Level 3b: Detailed Reaction - Generalized Separation System



(e) Level 3c: Detailed Reaction - Expanded Separation



(f) Level 4: Detailed Reaction - Detailed Separation

Figure 3 - 3: Process Representation of the HDA Process

3.3.1 Formalization of the Concept of Strata

The description on multistrata system has been quite conceptual so far. The core ideas can be been formulated mathematically. Given a plant: **P**: **U** × **D** → **Y**, the set **U** (manipulated variables), **D** (external disturbances) and **Y** (measured outputs) can be decomposed into families of sets :

$$\begin{aligned} &\mathbf{U}_i,\ 1 \le i \le n \\ &\mathbf{D}_i,\ 1 \le i \le n \\ &\mathbf{Y}_i,\ 1 \le i \le n \end{aligned} \qquad [3\text{-}4]$$

such that :

$$\begin{aligned} \mathbf{U} &= \mathbf{U}_1 \times \mathbf{U}_2 \cdots \times \mathbf{U}_n \\ \mathbf{D} &= \mathbf{D}_1 \times \mathbf{D}_2 \cdots \times \mathbf{D}_n \\ \mathbf{Y} &= \mathbf{Y}_1 \times \mathbf{Y}_2 \cdots \times \mathbf{Y}_n \end{aligned} \quad [3\text{-}5]$$

where each set $\{\mathbf{U}_i, \mathbf{Y}_i\}$ represents manipulated variables and measured outputs that are observable from the i^{th} stratum and below only and $\mathbf{D}_i$ represents external disturbances that are significant to the i^{th} stratum. The highest level is represented by $i = 1$, the lowest level is represented by $i = n$. Then, the behavior of the i^{th} stratum can be described by $\mathbf{U}_1$, $\mathbf{U}_2$ … $\mathbf{U}_i$, $\mathbf{Y}_1$, $\mathbf{Y}_2$ … $\mathbf{Y}_i$ and $\mathbf{D}_i$. The i^{th} stratum is a system represented as mapping $\mathbf{P}_i$:

$$\begin{aligned} &\mathbf{P}_1 : \mathbf{U}_1 \times \mathbf{D}_1 \times \omega_1 \rightarrow \mathbf{Y}_1 \\ &\mathbf{P}_i : \mathbf{U}_1 \times \ldots \mathbf{U}_i \times \mathbf{D}_i \times \omega_i \rightarrow \mathbf{Y}_1 \times \ldots \mathbf{Y}_i ,\ 1 < i < n \\ &\mathbf{P}_n : \mathbf{U}_1 \times \ldots \mathbf{U}_n \times \mathbf{D}_n \rightarrow \mathbf{Y}_1 \times \ldots \mathbf{Y}_n \end{aligned} \quad [3\text{-}6]$$

The set ω_i represents the set of inter-level stimuli from the strata immediately below the i^{th} stratum. Thus, there exists a mapping $h_i : \mathrm{Y}_{i+1} \times \omega_{i+1} \rightarrow \omega_i$, $1 < i < n$ such that responses from the stratum below is passed to the level above.

A complete decoupling can rarely be fully justified in practical application and a complete understanding of the system behavior as a whole usually requires the study of the cross-strata interdependence as well. In the modeling of chemical plants, ω_i represents the set of measured outputs that must be passed from stratum i+1 to stratum i in order to fully represent the behavior of the system at a higher degree of abstraction. It will be shown later that these variables are generally related to the unstable and integrating dynamics of the plant which cannot be abstracted into a model which represents a long time horizon of the process. Let the set of such variables be $\mathbf{Y}^*$, then:

$$\begin{aligned} \mathbf{Y}^* &= h_{n-1}\,(\mathbf{Y}_1 \ldots \mathbf{Y}_n) \\ \mathbf{Y}^* &= h_i\,(\mathbf{Y}_1 \ldots \mathbf{Y}_{i+1}, \mathbf{Y}^*) \\ \mathbf{Y}^* &= h_1\,(\mathbf{Y}_1 , \mathbf{Y}_2, \mathbf{Y}^*) \end{aligned} \quad [3\text{-}7]$$

and the relevant output responses at each stratum are given by :

$$\begin{aligned} &[\mathbf{Y}_1 , \mathbf{Y}^*] = \mathrm{S}_1\,(\mathbf{U}_1, \mathbf{D}_1) \\ &[\mathbf{Y}_1 \ldots \mathbf{Y}_i , \mathbf{Y}^*] = \mathrm{S}_i\,(\mathbf{U}_1 \ldots \mathbf{U}_i , \mathbf{D}_i) \\ &[\mathbf{Y}_1 \ldots \mathbf{Y}_n] = \mathrm{S}_n\,(\mathbf{U}_1 \ldots \mathbf{U}_n , \mathbf{D}_n) \end{aligned} \quad [3\text{-}8]$$

By definition, $\mathbf{Y}^*$ must be observable at the n^{th} stratum.

Description of Process at Each Stratum

The detailed dynamics of the overall process can be described by the following generic set of differential and algebraic equations (DAEs) :

$$\dot{x} = f(x,u,d) \quad [3\text{-}9]$$

$$y = g\,(x, u, d) \quad [3\text{-}10]$$

where :

x = vector state variables of the process
y = vector of measurable outputs of the process, $y \in Y$
d = vector of process disturbances , $d \in D$
u = vector of manipulatable inputs, $u \in u$

As we remove the details of the process and from abstract description of the plant, some of the inputs and outputs of the process become unobservable. At the i^{th} stratum, the observable inputs and outputs of the system are confined to the following sets :

$$\begin{aligned} u^i &\in \mathrm{U}^i = \mathrm{U}_1 \times \mathrm{U}_2 \ldots \times \mathrm{U}_i \\ y^i &\in \mathrm{Y}^i = \mathrm{Y}_1 \times \mathrm{Y}_2 \ldots \times \mathrm{Y}_i \times \mathrm{Y}^* \\ d^i &\in \mathrm{D}^i = \mathrm{D}_i \end{aligned} \quad [3\text{-}11]$$

Recall that set Y^* corresponds to the set of measurable outputs which must be made observable at all levels of abstraction to ensure proper description of the overall behavior of the system. These variables have strong associations with the unstable and integrating modes of the system. The determination of such set of variables and the reasons why these variables must be passed to higher levels will be explained later. Then, following the description in the previous section, at an abstract level, the process is described by :

$$\dot{x}^i = f(x^i,u^i,d^i) \quad [3\text{-}12]$$

$$y^i = g\,(x^i, u^i, d^i) \quad [3\text{-}13]$$

where :

x^i = vector of aggregate state variables at the i^{th} stratum
y^i = vector of measurable outputs observable at the i^{th} stratum
d^i = vector of disturbances relevant at the i^{th} stratum
u^i = vector of manipulated inputs available at the i^{th} stratum

Strata with high degree of abstraction are concerned with broader aspects of the overall systems behavior, thus, these are also concerned with the slower aspects of the overall systems. The higher levels cannot respond to variations in either the environment or the process itself, which are faster than the variations of concern to the lower levels, since the latter are reacting faster and are concerned with more particular, or local, changes (Mesarovic et al., 1970). Assuming external disturbances are being described in terms of frequency spectra of their time variations, vector $\boldsymbol{d}^i$ at the i^{th} stratum corresponds to the set of external disturbances with time variations that are comparable to the time horizon represented by the i^{th} stratum.

Description of the Process at Abstract Levels

At the abstract process representation, we capture the behavior of the process over a long-horizon. Thus, the process is essentially at its steady-state. When a process is at steady-state, nothing is being accumulated. Thus, equations [3-12] and [3-13] can be reduced to:

$$\mathbf{0} = \boldsymbol{f}^i\,(\boldsymbol{x}^i_{ss}, \boldsymbol{u}^i, \boldsymbol{d}^i) \qquad [3\text{-}14]$$

$$\boldsymbol{y}^i = \boldsymbol{g}^i\,(\boldsymbol{x}^i_{ss}, \boldsymbol{u}^i, \boldsymbol{d}^i) \qquad [3\text{-}15]$$

where $\boldsymbol{x}^i_{ss}$ is a vector of steady-state values of the aggregate state variables corresponding to the representation at the i^{th} stratum.

For strictly stable systems, given initial values of the states and any finite changes of $\boldsymbol{u}^i$ and $\boldsymbol{d}^i$, finite $\boldsymbol{x}^i_{ss}$ values can be obtained from equation [3-14]. For systems with unstable modes and for systems with integrating modes, $\boldsymbol{x}^i_{ss}$ values may not be finite for some changes of $\boldsymbol{u}^i$ and $\boldsymbol{d}^i$ and we must introduce control actions to stabilize the system and to contain the integrating modes at all strata:

$$\begin{aligned} \boldsymbol{u}_u(t) &= \boldsymbol{c}_u\,(\boldsymbol{y}_u^*),\ \boldsymbol{u}_u \in \mathbf{U}^i \\ \boldsymbol{u}_o(t) &= \boldsymbol{c}_o\,(\boldsymbol{y}_o^*),\ \boldsymbol{u}_o \in \mathbf{U}^i \end{aligned} \qquad [3\text{-}16]$$

where $\boldsymbol{y}_u^*$ is associated with the unstable modes and $\boldsymbol{y}_o^*$ is associated with the integrating modes in the process. With the implementation of the stabilizing control law (Equation 3-16]):

$$\begin{aligned} &\left(\frac{y_u^{\bullet}}{u_j}\right)_{\substack{t\to\infty \\ u_u(t)=c_u(y_u),\,u\neq j}} \rightarrow \text{finite},\ \ \forall u_j \in \mathbf{U}^i \\ &\left(\frac{y_o^{\bullet}}{u_j}\right)_{\substack{t\to\infty \\ u_o(t)=c_o(y_o),\,o\neq j}} \rightarrow \text{finite},\ \ \forall u_j \in \mathbf{U}^i \end{aligned} \qquad [3\text{-}17]$$

Substituting equations [3-16] into [3-15], we obtain :

$$\boldsymbol{y}^{\mathrm{i}} = \boldsymbol{g}^{\mathrm{i}}\,[\,\boldsymbol{x}_{\mathrm{ss}}\,,\, \boldsymbol{c}_{\mathrm{u}}(\boldsymbol{y}_{\mathrm{u}}^*),\, \boldsymbol{c}_{\mathrm{o}}(\boldsymbol{y}_{\mathrm{o}}^*),\, \boldsymbol{u}^{\mathrm{i}},\, \boldsymbol{d}^{\mathrm{i}}] \qquad [3\text{-}18]$$

With equations [3-16] defined, equation [3-18] can be used to study the behavior of the system at the i^{th} stratum.

Determination of Y^*

Consider the following linear dynamic system described by the following set of differential and algebraic equations :

$$\begin{aligned} \dot{x} &= Ax + Bu + Ed \\ y &= Cx + Du + Fd \end{aligned} \qquad [3\text{-}19]$$

Without loss of generalization, assume $d = 0$ in the rest of our discussion. Then, let :

$$x(0) = \xi \neq 0 \qquad [3\text{-}20]$$

$$Av_i = \lambda_i v_i \qquad [3\text{-}21]$$

$$w_i^T A = \lambda_i w_i \qquad [3\text{-}22]$$

where v_i and w_i are the right and left eigenvectors corresponding to eigenvalue λ_i of the system. $x(t)$ is given by :

$$x(t) = \sum_{i=1}^{n} e^{\lambda_i t} v_i w_i^T \xi + \sum_{i=1}^{n} \sum_{k=1}^{m} w_i^T b_k v_i \int_0^{\tau} e^{\lambda_i (t-\tau)} u_k(\tau) d\tau \qquad [3\text{-}23]$$

which can be further partitioned into :

$$\begin{aligned} x(t) = &\sum_{i=1}^{n_s} e^{\lambda_{s_i} t} v_i w_i^T \xi + \sum_{i=1}^{n_s} \sum_{k=1}^{m} w_i^T b_k v_i \int_0^{\tau} e^{\lambda_{s_i} (t-\tau)} u_k(\tau) d\tau \\ &+ \sum_{i=1}^{n_u} e^{\lambda_{u_i} t} v_i w_i^T \xi + \sum_{i=1}^{n_u} \sum_{k=1}^{m} w_i^T b_k v_i \int_0^{\tau} e^{\lambda_{u_i} (t-\tau)} u_k(\tau) d\tau \\ &+ \sum_{i=1}^{n_o} e^{\lambda_{o_i} t} v_i w_i^T \xi + \sum_{i=1}^{n_o} \sum_{k=1}^{m} w_i^T b_k v_i \int_0^{\tau} e^{\lambda_{o_i} (t-\tau)} u_k(\tau) d\tau \end{aligned} \qquad [3\text{-}24]$$

where : $\quad \lambda_{s_i} < 0 \,;\; \lambda_{u_i} > 0 \,;\; \lambda_{o_i} = 0$

There are n_s stable eigenvectors, n_u unstable eigenvalues and n_o eigenvalues at zero. Then, as $t \to \infty$,

$$
\begin{aligned}
e^{\lambda_{s_i} t} &\rightarrow 0 \\
e^{\lambda_{u_i} t} &\rightarrow \infty \\
e^{\lambda_{o_i} t} \rightarrow 1 &\Rightarrow \int_0^{\infty} e^{\lambda_{o_i}(t-\tau)} u_k(\tau) d\tau \rightarrow \infty
\end{aligned}
\qquad [3\text{-}25]
$$

Since y is related to the states by equations [3-19], the states and measurable outputs that have strong associations with the non-negative eigenvalues of the system no not reach finite steady-state values at long-horizon. Since,

$$
\begin{aligned}
y_j(t) = &\sum_{i=1}^{n_s} e^{\lambda_{s_i} t} (c_j^T v_i) w_i^T \xi + \sum_{i=1}^{n_s} \sum_{k=1}^{m} w_i^T b_k (c_j^T v_i) \int_0^{\tau} e^{\lambda_{s_i}(t-\tau)} u_k(\tau) d\tau \\
&+ \sum_{i=1}^{n_u} e^{\lambda_{u_i} t} (c_j^T v_i) w_i^T \xi + \sum_{i=1}^{n_u} \sum_{k=1}^{m} w_i^T b_k (c_j^T v_i) \int_0^{\tau} e^{\lambda_{u_i}(t-\tau)} u_k(\tau) d\tau \\
&+ \sum_{i=1}^{n_o} e^{\lambda_{o_i} t} (c_j^T v_i) w_i^T \xi + \sum_{i=1}^{n_o} \sum_{k=1}^{m} w_i^T b_k (c_j^T v_i) \int_0^{\tau} e^{\lambda_{o_i}(t-\tau)} u_k(\tau) d\tau
\end{aligned}
\qquad [3\text{-}26]
$$

$(c_j^T v_i)$ dictates how much the i^{th} mode shows up is observed in the j^{th} output of the system. Thus, for each unstable mode i (i = 1, .. , n_u and unstable modes are those modes whose eigenvectors correspond to λ_{u_i}), determine the outputs y_j whose corresponding $(c_j^T v_i)$ are relatively large. Then these outputs form vector y_u^*. Similarly, for each integrating mode, i (i = 1, .. , n_o and integrating modes are those modes whose eigenvectors correspond to λ_{o_i}), determine the outputs y_j whose corresponding $(c_j^T v_i)$ are relatively large. Then these outputs form vector y_o^*.

$$
\mathbf{Y}^* \equiv y_u^* \cup y_o^* \qquad [3\text{-}27]
$$

$\mathbf{Y}^*$ is the set of measurable outputs which do not have finite steady-state gains for changes in manipulated variables u :

$$
\begin{aligned}
\left(\frac{y_u^*}{u_j}\right)_{t\rightarrow\infty} &\rightarrow \infty, \ u_j \in \mathbf{U} \\
\left(\frac{y_o^*}{u_j}\right)_{t\rightarrow\infty} &\rightarrow \infty, \ u_j \in \mathbf{U}
\end{aligned}
\qquad [3\text{-}28]
$$

Then, at high level of abstraction where the set $y_i \in \mathbf{Y}^*$ is not directly observable, we must explicitly introduce control actions at all strata:

$$\boldsymbol{u}_{\mathrm{u}}(t) = \boldsymbol{c}_{\mathrm{u}}(\boldsymbol{y}_{\mathrm{u}}^{*}) \qquad [3\text{-}29a]$$
$$\boldsymbol{u}_{\mathrm{o}}(t) = \boldsymbol{c}_{\mathrm{o}}(\boldsymbol{y}_{\mathrm{o}}^{*}) \qquad [3\text{-}29b]$$

so that:

$$\begin{aligned} \left(\frac{y_u^{*}}{u_j}\right)_{\substack{t \to \infty \\ u_u(t)=c_u(y_u),u \neq j}} &\to \text{finite}, \ \boldsymbol{u}_j \in \mathbf{U} \\ \left(\frac{y_o^{*}}{u_j}\right)_{\substack{t \to \infty \\ u_o(t)=c_o(y_o),o \neq j}} &\to \text{finite}, \ \boldsymbol{u}_j \in \mathbf{U} \end{aligned} \qquad [3\text{-}30]$$

3.3.2 Control Tasks in the Multistrata system

The set of process representations provide a proper framework in which specific process control tasks can be generated. At the Level 1, the focus of the design is on objectives which specify the overall process behavior and those which deal with the interactions of the plant with the external environment. As we move down the hierarchy to the next level, it is of paramount importance that objectives at the lower levels are consistent with the overall production plan. Control objectives at Level 1 must be *translated* to the new level. Thus, the objectives at a high level constrain the behavior at a lower level, ensuring that the consistency among the hierarchy of viewpoints is maintained. New objectives may also become observable at the new viewpoint as more details of the plant are being exposed. Objectives translated from Level 1 may be *refined* or *spawned* to reflect the added details in the new viewpoint. Such procedures are repeated at the next level and the level below the next, etc. Through this process, we systematically shift the focus of the design from a global viewpoint to a more local one. This enables us to reduce the complexity of the design problem and to generate a plant control system which accounts for both the peculiarity of the unit-operations and the desired global behavior.

Thus, based on the overall production plant, we can generate control objectives which are relevant to the particular representation being dealt with. The set of control objectives in turn define the *tasks* of the control structure at that level of representation. The set of control objectives of the production is the dual of the control tasks of the control system. Control objectives and control tasks will be used interchangeably in our discussion. The relationship between production plan and control objectives; the relationship between control objectives and control tasks, as well as the process by which control tasks at each representation are generated are illustrated in Figure 3-4.

3.3.3 Progressive Generation and Modification of Plant Control Objectives

In this section, the procedure through which plant control objectives at each stratum (or level) of process representation are generated will be outlined. The specific mechanisms (developed by Johnston, J.E., 1991) used for the translation, refinement and spawning of objectives will be presented.

The overall control system has been defined in Problem P1 and the overall production goals have been defined in equations [3-2] and [3-3]. At the first stratum, our model represents the input-output structure of the overall plant, thus, the goals that are relevant at level one are :

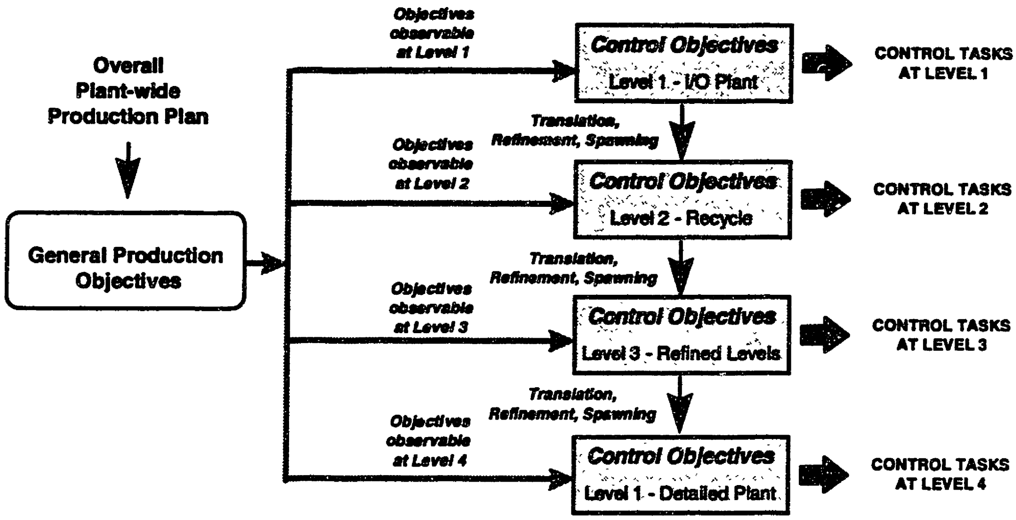


Figure 3 - 4: Generation of Control Tasks

$$F^1_{I,k} = \left\| \beta_{k,sp} - \beta_k \right\|, \ \forall \beta_k \in Y^1 \qquad [3\text{-}31]$$

$$F^1_{II,j} = \left\| \kappa_{j,sp} - \kappa_j \right\|, \ \forall \kappa_j \in \Pi \qquad [3\text{-}32]$$

$\mathbf{Y}^1$ represents the set of measured output that are observable at Level 1. Relevant explicit objectives are those that are observable at the first stratum and those that must be controlled to maintain the stability and contain the integrating modes in the plant, i.e., $\beta_k \in \mathbf{Y}^1$. All implicitly objectives in set Π are relevant at all strata since they represent the overall behavior of the plant.

Beyond the first stratum, control objectives are defined by progressively modifying the control objectives defined at the earlier levels.

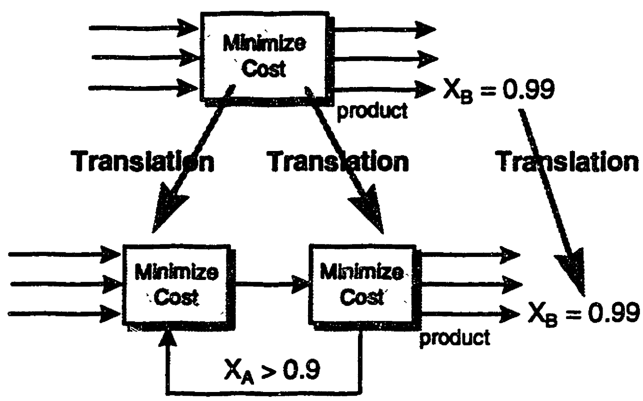
Translation

Control objectives are updated by direct translation. Since explicit objectives are "local" objectives and are attributes of process units or streams, they are translated (or allocated) only to the sub-blocks containing the associated process variables. Implicit objectives are translated (or allocated) to all sub-blocks for which the objectives apply. With the revelation of some of the internal structure of the plant, new objectives become observable and the are included in the list of control objectives at the new level as well. Figure 3-5 gives several examples of objectives created for direct translation.

Once objectives have been translated to the new viewpoint, they are checked to see if they can be further modified. Objectives can be progressively modified by either *refinement* or *spawning*.

Refinement

An implicitly defined objective is refined to one or several more specific process objective(s) when we can associate specific variable(s) within the sub-block to the lumped objective. For example, in Figure 3-6, sensitivity analysis may show that in order to minimize the operating cost, we should minimize the loss of products and raw materials from the process. These new objectives are finer description of the cost objectives. Even though their descriptions are still "fuzzy", they reflect the added details at the recycle structure viewpoint.



New Objective observable at refined level

Figure 3 - 5: Translation of Control Objectives

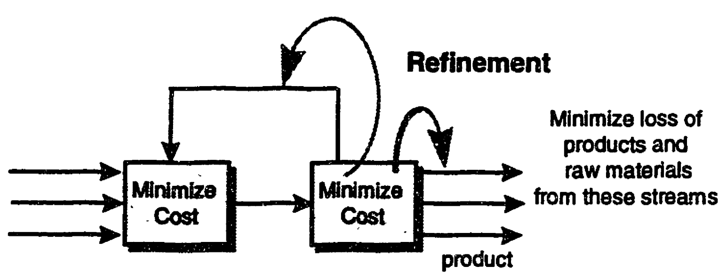


Figure 3 - 6: Refinement of Control Objectives

Spawning

When the achievement of a process objective requires a constraint on the input system of a unit, spawning occurs. New objective(s) are generated onto other sub-block(s) to *replace* the original objective when it cannot be met in that sub-block. New objective(s) are also generated onto other sub-block(s) to *supplement* the original objective. Such situations are identifiable when one examines the pathways of disturbances propagation in the plant (see Chapter 4, 5 and 7 for more details on this). The idea of spawning is illustrated in Figure 3-7. In the top schematic, the original objective lies in Unit C where the outlet temperature of the stream is to be controlled. Unit C is an isothermal process and there is no manipulation available in the vicinity of Unit C for that purpose. If the control of the inlet temperature can be accomplished in Unit A, a new objective can be spawned to replace the original objective which cannot be met in Unit C. In the bottom schematic, a new objective is spawned because the disturbance propagation pathway indicates that a disturbance affecting Unit A has a direct influence on Unit B. Hence, introducing a control objective in Unit A will ensure earlier diversion of the disturbance away from the original objective.

Thus, objectives associated with representations at the lower level of the hierarchy are either newly observable objectives or are objectives which have been generated via one or more of the mechanisms described above. Thus, by construction, our objectives are always consistent with those at the higher levels and the internal consistency among the sets of control tasks in the control system is being maintained.

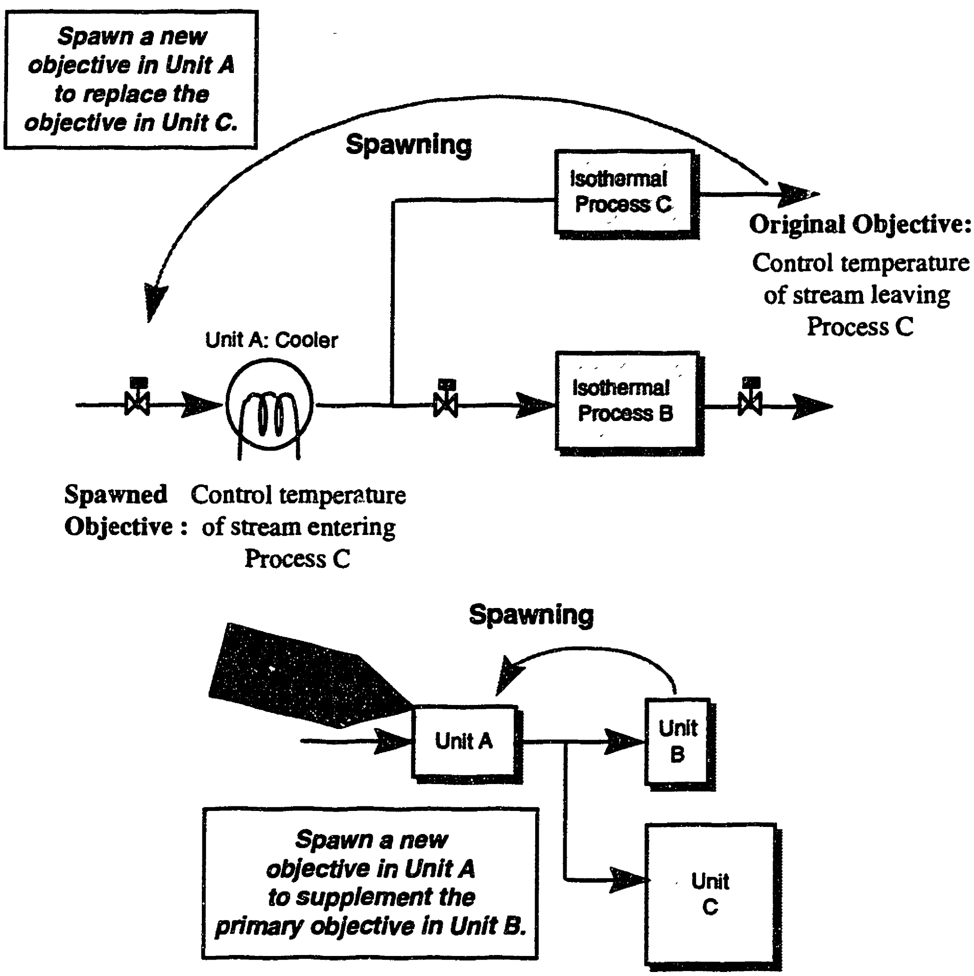


Figure 3 - 7: Spawning of Control Objectives

3.4 The Multilayer Hierarchy: Time Horizons of Control Tasks

A typical functional hierarchy for decision making and control is made up of the following layers:

1. Planning
2. Optimization
3. Learning and Adaptation
4. Direct Regulation — control tasks associated with various process characteristics significant at various time-horizons

Each stratum corresponds to a distinct time scale of the plant operation, the control structure synthesized at each stratum addresses issues important to a different layer of the overall control task. The focus of this research is on the control tasks immediately related to process regulation, which is the layer that has direct interaction with the process.

As pointed out by Simon (1969), the benefit of constructing the hierarchy of viewpoints is that we have separated the higher-frequency dynamics (or those effects which are important in the short time-horizon) involving internal structure of the components, from the lower-frequency dynamics (or those effects which are only important in the long time-horizon) involving interactions among component at the more abstract levels. Thus, the range of process phenomena with which the designer is concerned have been divided according to their associated time-horizons, each of which is characterized by one of the representations in our hierarchy of plant stratification. The hierarchy of process representations in the multistrata system provides a framework in which sets of consistent control tasks are displayed in viewpoints which match their relevant *time-scales*. The relevant time-horizons characterized by each viewpoint in the hierarchy are shown in Figure 3-8. Within this *time resolution*, we have partitioned the disturbances which impact the system according to their frequencies of variations. Below is a summary of the different issues that are of relevance at the various process representations.

1. *Level 1: input-output level*

   The input-output model represents the longest time-scale of operation which allows the designer to focus on the slowest dynamics in the plant. Disturbances (and exogenous inputs) that vary at low frequencies (e.g. changes in operating point, persistent process disturbance) are important here. This is the viewpoint in which we evaluate the long-term *static feasibility* of the process. The control tasks that address the process steady-state behavior can be developed using the input-output plant.

2. *Level 2: The recycle structure*

   At this level, the characteristic time-scales of operation of the individual blocks are smaller than that of the overall process. The difference in time-scales between the Level 1 and Level 2 representations could be of an order of magnitude Luyben (1993a).

3. *More refined process representations*

   As we move down the hierarchy, the viewpoints become more refined and each individual block represents yet shorter time-scales of operation. The planning horizon associated with each level at a lower level decreases in time and space. The interaction among the different process blocks that are needed to bring about changes in the overall process can be studied within these refined representations.

4. *The most detailed representation*

   The detailed level reveals the higher order dynamics of the plant (such as inverse responses, capacitors in series). In addition, this viewpoint also exposes the high-frequency disturbances affecting local process variables like flow rates, compositions, temperatures, pressures or tank levels. This is the level at which the *dynamic operability* of both the overall process and the individual operating-units can be studied.

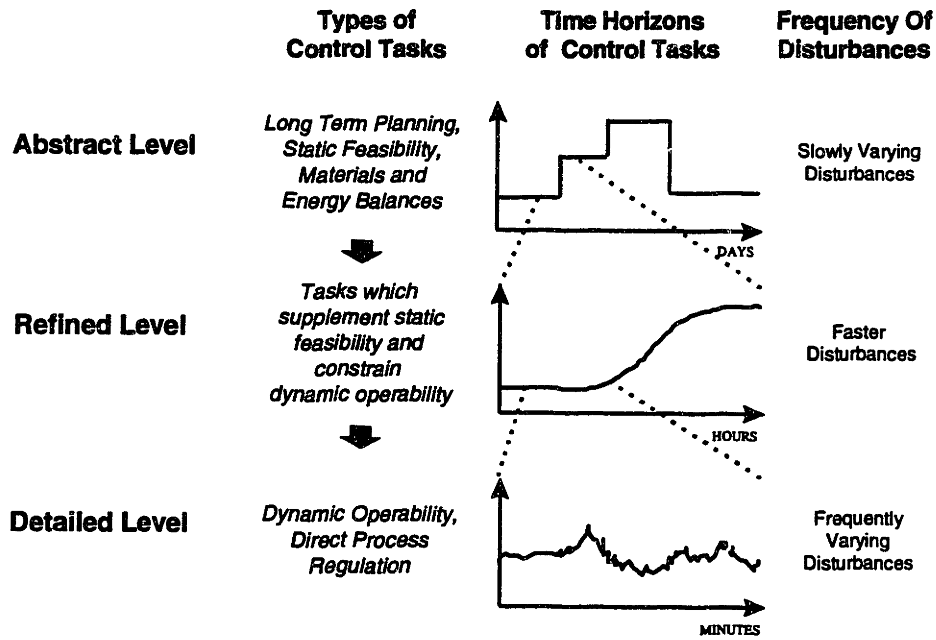


Figure 3 - 8: Time-horizons and Hierarchical View of Control Tasks

3.4.1 The Hierarchical Cascade Control System

The control objectives at each level define the set of *control tasks* which are to be attained using some kind of *control strategies.* By control strategies, we refer to the "plan" or "method" through which the control tasks would be accomplished. *In general,* this "plan" may consist of a set of decentralized single-input, single-output (SISO) loops, or a fully multivariable controller, or some combination of the two. The set of control strategies, together, specifies the *control structure* (or control configuration) for that level of representation. The set of control structures can be integrated to form the plant *control system.* The control structures at different levels are inter-related:

- *The control structure at a lower level assists the control structures at the higher levels.* Each level of representation accentuates disturbances that fall into a particular range of frequencies, the corresponding control structure is therefore suited for eliminating disturbances in that particular range. Faster disturbances are being eliminated by control structures at the lower levels. The control structures at the higher level only has to reject the more slowly varying disturbances. Controlling the refined objectives at a lower level therefore assists the control of the a overall objectives observable at the higher levels.

- *Control objectives at a lower level are related to the control objectives at the higher levels.* Control Objectives at a higher level dictates control objectives at the lower levels. As control objectives at a refined level are generated as described in Section 3.3, the control structure that we form at a refined level try to accomplish the same objectives as those at a higher level, but with a set of more refined control strategies.

A *hierarchy cascade control system* consists of a set of control structures, arranged in a graded series shown in Figure 3-9.

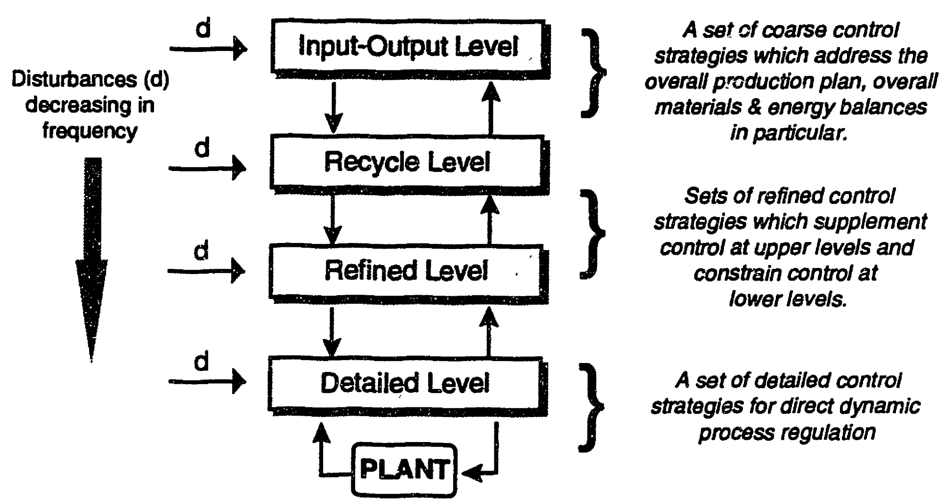


Figure 3 - 9: Hierarchical Cascade Control System

3.5 A Decision-Making Multiechelon Hierarchy for Plant Control Objectives

As noted earlier in Section 2.1, in the operation of a chemical plant, there are invariably multiple number of production objectives that one would like to simultaneously covered. Generally, plant control objectives can be grouped into categories according to their functions, such as:

- regulation of materials and energy balances
- plant production and product quality
- process operation and equipment constraints
- process safety constraints
- environmental regulations
- economic goals

Obviously, the various categories of plant objectives are not of equal importance. For example, the maintenance of materials and energy balances in the plant are always of the highest priorities. One must ensure there is a balance between the inflows and outflows of materials and energy streams or materials will start accumulating or depleting in the process. Severe accumulation can cause fluids to overflow in tanks, pressures to build up in vessels and inerts to accumulate in the process. Of the next level of importance are those objectives which are to guard against violation of process operation, equipments, environmental and safety constraints. Objectives that are related to product specifications (like production rate and product quality) are of higher priorities than the economic objectives. A plant may not be able to sell the off-spec products to their contracted customers, or that further processing would be needed to achieve the required specifications. If this production unit is part of a multi-plant, manufacturing of off-spec products may have a long-range effects on other downstream processes.

3.5.1 The Notion of a Multiechelon Hierarchy

The set of plant control objectives form a multiecheloon hierarchy. At the i^{th} stratum of plant representation, there is a set of goals which are to be accomplished via some manipulations of the process inputs:

$$
\begin{aligned}
F^{i}_{\mathrm{I},k} &= \left\|\beta_{k,sp} - \beta_k\right\| \quad \forall \beta_k \in \mathrm{I}^{i} \\
F_{\mathrm{II},j} &= \left\|\kappa_{j,sp} - \kappa_j\right\| \quad \forall \kappa_j \in \mathrm{II} \\
F^{*}_{\mathrm{I},p} &= \left\|y^{*}_{p,sp} - y^{*}_{p}\right\| \quad \forall y^{*}_{p} \in \mathbf{Y}^{*}
\end{aligned}
\qquad [3\text{-}33]
$$

where I^i is the set of explicit objectives relevant at the i^{th} stratum. $\mathbf{Y}^*$ is the set of process variables that are not observable from the i^{th} stratum but must be made observable at the i^{th} stratum in order to properly describe the process behavior (see Section 3.3.1 for details). These set of goals, when arranged in their order of importance, form a decision-making hierarchy:

$$
\mathbf{L}^{i}\!: \{\, \mathrm{L}_1^{\,i} > \mathrm{L}_2^{\,i} > \ldots > \mathrm{L}_w^{\,i} \,\},\ \mathbf{W}^{i} \equiv \mathbf{Y}^{*} \cup \mathrm{I}^{i} \cup \mathrm{II} \qquad [3\text{-}34]
$$

where $\mathbf{L}^i$ is a finite hierarchical family of goals for the i^{th} stratum in the set $\mathbf{W}^i$. Set $\mathbf{W}^i$ is a finite index set and " >" is a strict partial ordering of $\mathbf{L}^i$. The ordering ">" is such that $\mathrm{L}_k^{\,i} > \mathrm{L}_j^{\,i}$ if and only if $\mathrm{L}_k^{\,i}$ has priority of action over $\mathrm{L}_j^{\,i}$. Note that each decision making unit has primary interest only in some aspect of the process. However, due to the multivariate nature, the end result of its action depends on the entire process (Mesarovic et al., 1970).

Thus, in a multiechelon hierarchy, there is a family of interacting subsystems (in this case, the plant control objectives) which are recognized explicitly. Furthermore, the subsystems can be defined to be decision making units (such as control strategies used to accomplish the objectives). Finally, the decision units can be arranged hierarchically, in the sense that some of them are influenced or controlled by others (due to the multivariable nature of plant operation).

In plant-wide control system design, the hierarchy of objectives define the list of practical operational requirements that are to be met through the use of a control system. There are three main aspects that this control system design must address:

1. *The interaction of variables in a multi-input, multi-output (MIMO) system.*

   Appreciation of the interaction phenomenon in a multivariable or MIMO system is important. Undesirable effects may result if interaction is not accounted for during a MIMO control system design. In the mild cases, interactions may degrade the expected performance of the control system; under the worst circumstances, interaction my generate hidden feedback effects in the plant and destabilizes the process.

2. *The multiobjective character of the design problem.*

   To properly address the hierarchy of plant control objectives, the control system should be developed in such a way that the engineering preferences and trade-offs are being accounted for.

3. *Ease of maintenance of the control system.*

   The individuality of each control objective should be preserved as much as possible for easy maintenance.

Multiobjective design problems can be solved with flexibility in the *modular multivariable design framework* (Meadowcroft et al., 1992). A detailed description of this framework is given in Chapter 6. A brief introduction of the essential ideas of this approach is followed.

3.5.2 The Modular Multivariable Design Framework

The Modular Multivariable Controller (MMC) design methodology (Meadowcroft et al., 1992) uses a priority-driven design approach and is based on the solution of multiobjective optimization problems using the strategy of *lexicographic goal programming* (Ijiri, 1965; Jääskelainen, 1972, Ignizio, 1976, 1982). Suppose a simple MIMO process has four measured outputs (y_1, y_2, y_3 and y_4) and five inputs (m_1, m_2, m_3, m_4 and m_5). Using the MMC design methodology, a MIMO control system can be developed as follows:

Step 1: Define Control Goals

Suppose our control tasks involves maintaining all four outputs at their respective set-points ($\beta_{i,sp}$, i = 1, 2, 3, 4) and $\beta_i = y_i$. Then, it is our goals (L_i, i = 1, 2, 3, 4) to achieve the following:

$$L_1:\ a_1 = \min |\beta_1 - \beta_{1,sp}|$$
$$L_2:\ a_2 = \min |\beta_2 - \beta_{2,sp}|$$
$$L_3:\ a_3 = \min |\beta_3 - \beta_{3,sp}|$$
$$L_4:\ a_4 = \min |\beta_4 - \beta_{4,sp}|$$

The values of a_i (i = 1, 2, 3, 4) are measures of the *levels of achievement* of our goals.

Step 2: Prioritize Control Goals

Goals are arranged according to their order of importance by injecting our engineering preferences and trade-offs into the design. In our illustration, suppose:

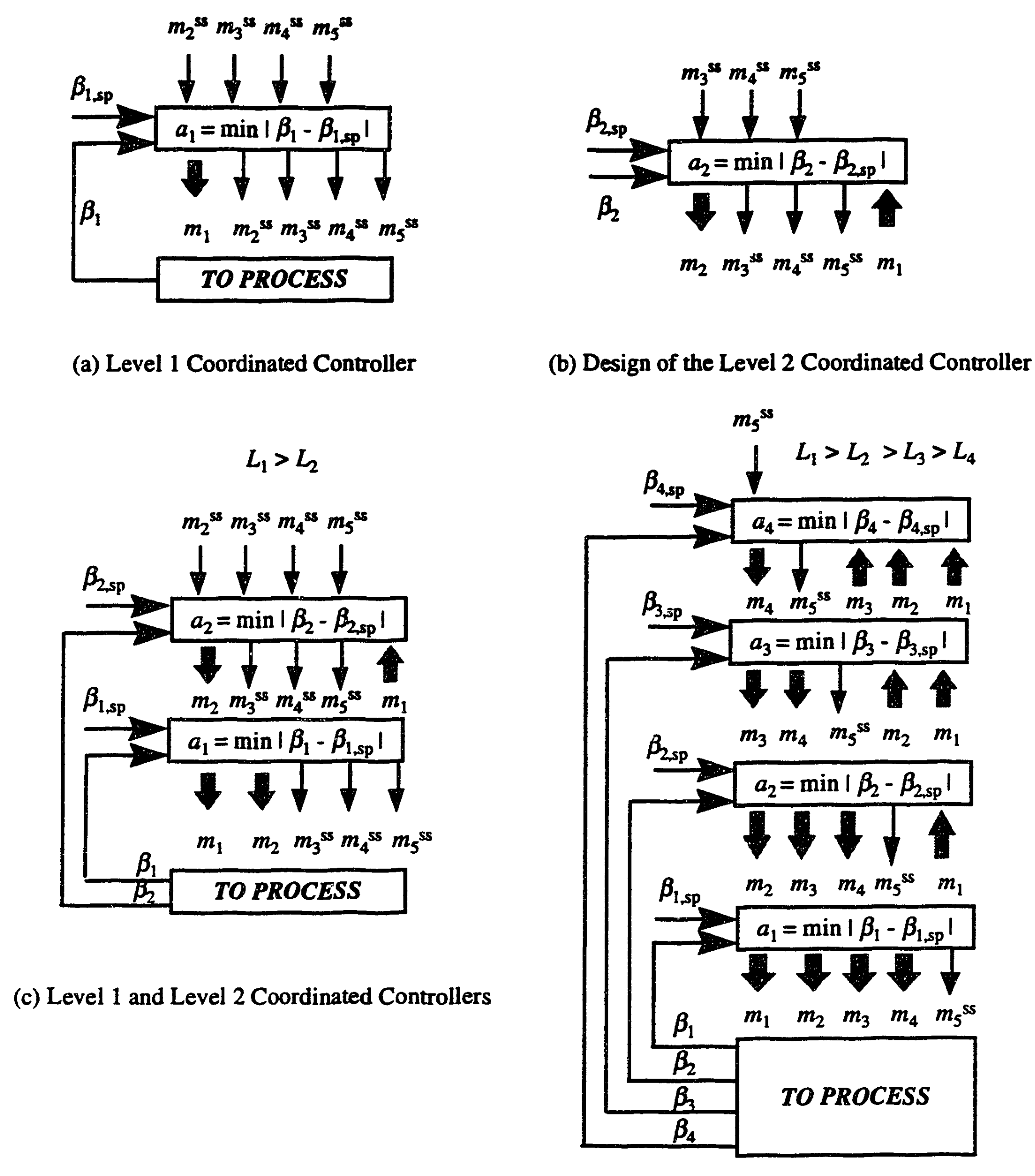
$$L_1 > L_2 > L_3 > L_4$$

where "A > B" indicate that A is more important than B. $L_1, \ldots, L_4$ form a multiechelon hierarchy.

Step 3: Synthesize Control System

A control configuration for the MIMO system is then developed using a priority-driven approach by means of sequential satisfaction of goals. The overall MMC configuration is composed of a series of what they called, *coordinated controllers* (Popiel et al., 1986; Meadowcroft et al., 1992).

Synthesis begins from the most important objective, i.e. L_1 in this case. In a multivariable system, one or more inputs in the system may have some effects on the output y_1 and therefore can potentially have some influence on a_1, the level of achievement of L_1. In the MMC design, only one degree of freedom in the process is assigned to each goal and that degree of freedom becomes the *primary manipulated variable* for that goal (in Chapter 6, the advantages of this approach will be further explained). Suppose m_1 is the *best* manipulated variable for controlling L_1. Then, m_1 is the primary manipulated variable for L_1 and a *coordinated controller* can be formed by associating m_1 to y_1. The Level 1 coordinated controller (CC-1) is shown in Figure 3-10 (a). In the figure, m_2^{ss}, m_3^{ss}, m_4^{ss} and m_5^{ss} represent steady-state values of the rest of the manipulated variables which are not yet involved in the design.



(a) Level 1 Coordinated Controller

(b) Design of the Level 2 Coordinated Controller

(c) Level 1 and Level 2 Coordinated Controllers

(d) The Overall MMC Design

Figure 3 - 10: Evolution of the MMC Design

With that set up, we move on to the next most important goal, which is L_2 in this case. The coordinated controller for L_2 is designed by choosing the best manipulated variable to control y_2 *while* y_1 *is under perfect control by* m_1. In this way, the interaction between m_1 and y_2 is explicitly being accounted for in the design. Suppose m_2 is the best input for this purpose, it then becomes the primary manipulated variable for y_2. The Level 2 coordinated controller (CC-2) is depicted in Figure 3-10 (b). This controller, is then coupled with CC-1 as shown in Figure 3-10 (c) for simultaneous control of both y_1 and y_2. Notice the interaction between m_2 and y_1 is now being taken into account by CC-1.

Similarly, this structure can be easily expanded to incorporate the control of Goals 3 and 4. The overall MMC control configuration for our simple MIMO process is shown in Figure 3-10 (d). We have assumed m_3 and m_4 to be the primaries for L_3 and L_4 respectively. Only four manipulated variables are being used in the design, m_5 remains to be a degree of freedom.

Hence, in the proposed work, a control strategy is referred to the method or plan by which a control task is being accomplished through a coordinated controller using the assigned primary manipulated variable. Coupled coordinated controllers form a multivariable control system.

Selection of Primary Manipulated variables

The selection of primary manipulated variables plays a pivotal role in the MMC design. It is through these selections that we define the performance of the closed-loop system. We choose the primary for the most important objective from the largest set of possible manipulated variables and the primary is the "best" manipulation for control purposes among all possible choices. By reserving this "best" manipulated variable for the most important objective, we have used our resources to ensure that the control system would best meet our goal of the highest priority. Similarly, the primaries for the other plant control objectives are selected sequentially, *in the order of importance*. Thus, through the MMC design, very explicitly, the "good" properties of control have been associated with the more important objectives.

The structure and functionality of the modular multivariable design methodology will be detailed in Chapter 6. The background, the control theory upon which the development had been based and the methods to be used for the selection of primary manipulated variables will also be provided.

3.6 The Hierarchy of Modeling Needs

Models which define the *fundamental interconnections* or/and *cause-and-effect relationships* among process variables (inputs and outputs) in the system are useful for *analysis* of the process and *synthesis* of control strategies for the plant. As such, the models to be used at each level of plant representation should be consistent with the level of detail observable from the viewpoint; the relevant time-horizon specific to this level in the hierarchy and the goal of the analysis or synthesis.

It has been pointed out that the amount of information which is contained in a problem formulation is one of the most critical factors in acquiring a problem solution (Greenfield and Ward, 1967). At different stages of the design, we are required to identify the process trends, determine the feasibility of a proposal, evaluate the suitability of the design, screen alternatives, construct the basic control structure, synthesize detail control laws or implement the control structure. Different models would be needed to address different needs. Models of a number of different types would be needed at different stages of the design. Simple, logical models are useful for characterizing the general behavior of the system while more complex, analytical models describe the plant in more quantitative terms.

3.6.1 Logical Models

Logical models are used to model qualitative system behavior. They capture the "connectivity" relationships among variables, the "signs", the "directions" and the "propagation pathways" of process effects created by changing various variables in the plant. These models are structurally based graphs and Boolean representation of the system. They are useful when it is needed to perform qualitative analysis on the process. Qualitative analysis is performed to improve our understanding of the plant and to identify the major process trends. It is also used throughout the design to screen alternatives, whenever necessary. In Chapter 4, the construction of various graphs and Boolean models for qualitative analysis of the physical system will be elaborated.

3.6.2 Analytical Models

Analytical models are essentially quantitative models which describe the amounts and magnitudes of the information flow and the quality of the transmissions. They can be articulated in terms of mathematical relations between process inputs and outputs and they are *input-output* representations which relate process inputs (like manipulated variables or any measurable disturbances or exogenous inputs) with process outputs (measurable and unmeasurable process variables).

A range of quantitative information can be included in any one model. Simpler models characterize the steady-state behavior of the process are suitable for capturing the long-horizon characteristics of plant behavior or the behavior that is excited by inputs of very low frequencies. More detailed models emphasize the phenomena observed at the detailed process representation, such as the transient behavior of the plant. In Chapter 5, the various types of analytical models that are useful for control structure synthesis will be described.

3.7 Integrating the Hierarchies: A Generic Framework for Control System Design

In the previous sections, a various number of hierarchies have been presented. Each hierarchy serve to capture one aspect of the plant-wide control design problem. The hierarchy of strata defines a *visual resolution* of the chemical plant in terms of a series of plant representations. The multilayer hierarchy defines a *temporal resolution* in terms of planning horizons. The two hierarchies of resolutions are integrated to define the generic framework the synthesis of plant-wide control strategies as depicted in Figure 3-11.

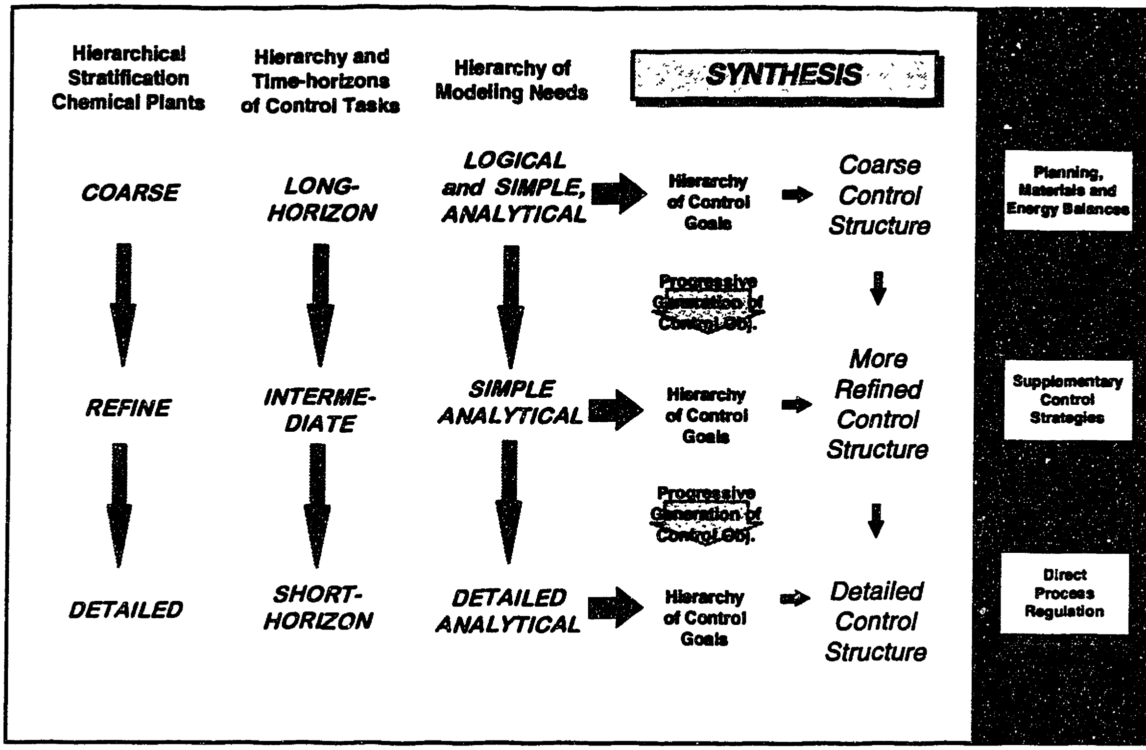


Figure 3 - 11: The Generic Framework for the Design of Plant-wide Control Structures

3.7.1 Methodology Overview

The design of plant control strategies is made more manageable by vertically decomposing the plant into a hierarchy of representations, from coarse to detailed. This hierarchy defines the visual resolution. Each of these representations corresponds to a specific temporal span. Coarser representations characterize long-horizon behavior of the process, more detailed viewpoint expose the faster dynamics in the plant. Hence, the models which are needed for the analysis and synthesis of control strategies should vary according to the visual span and time span of the viewpoint. Logical models are used to detect the general process trends and feasibility of alternatives, simple models are used to quantify the information flow while more detailed analytic models describe the quality of the process response during transient.

At each level of the hierarchy, we are only concerned with objectives which are observable from the corresponding representation. These objectives define the tasks of the control system. Some of these tasks are more important than others. The maintenance of some process constraints could also be crucial to the plant. We express our engineering preferences and trade-offs by explicitly prioritizing our goals in their order of importance.

Once control goals at each level have been identified and prioritized, a set of control strategies can be synthesized using the modular multivariable design framework. The resulting set of control strategies defines a control structure that is suitable for attaining the control tasks corresponding to that particular process viewpoint. As in all variants of hierarchical cascade control systems, the control structure that we develop at the top is imprecise, at the intermediate levels, the control structures are more refined but they still do not contain all the necessary details. At the bottom, the control structure has the required precision for process regulation (Maximov and Meystel, 1992).

At the top of the hierarchy where we visualize the input-output representation of the process, we have the best understanding of the overall "production plan" and are most able to define a set of relevant control objectives that are consistent with this production plan. When we move to the next level of representation, such as the recycle structure, the control objectives should be updated to reflect the added details in the model. Objectives are translated, refined or spawned to the new level.

The different control structures that we have synthesized for each of the process representations are inter-related by virtual of the consistent definition of plant viewpoints, process models and control tasks associated with the representations. Thus, they can be cascaded to form a hierarchical control system. Each control structure is associated with a certain time-scale of operation, so it is a *multi-horizon control system*. At the top of the hierarchy, the focus of the control structure is the long-term planning, material and energy balance control of the plant. At the intermediate levels, the control structures define supplementary control tasks which assist the accomplishment of control tasks at the higher levels and help to define the control tasks for the lower levels. At the detailed level, the control structure is concerned with direct regulation of the process. As we move down the hierarchy, the frequencies of control actions increase in anticipation of the more frequent changes of process disturbances and exogenous inputs. The details of the construction of the multi-horizon control system will be discussed in Chapter 8.

3.7.2 Assumptions used in the Proposed Methodology

It has been implicitly assumed in the methodology that the following basic information is either available to the designer or can be developed based upon his/her understanding of the process:

1. Logical models such as structural representations of the plant and causal models are available or can be easily developed. These models are useful for the identification of the global process trends, for the determination of the stability of the open-loop process, for studying the feasibility of alternatives designs and for visualizing the topography of the propagation of disturbances in the plant.
2. Static models which capture the long-horizon characteristics of the process can be obtained. These are useful for analysis at the abstract levels of the plant.
3. Other dynamic characteristics about the plant which characterize the transient behavior can be developed.
4. Modeling uncertainty is known. It will be shown in Chapter 6 that accounting for model uncertainty introduces robustness in the design.
5. External process disturbances and expected exogenous inputs are known. Knowledge of the pattern of process disturbances and exogenous inputs expected for the plant allows the design of a control system that minimizes their effects on the production objectives.

The utilization of these items will be explained in the Chapters 4 through 8.

Chapter 4
Structural Aspects of Control Systems Analysis

4.1 The Use of Structural Analysis in Process Systems Engineering

Structural analysis is commonly employed in process systems engineering as a design aid and as an alternative route to rigorous numerical analysis of the system under investigation. A typical plant is described by hundreds of differential and algebraic equations, both linear and non-linear. When the number of equations and variables involved are large, it is advantageous to begin the analysis based on the invariant structural properties of the system as there are relatively easy ways to identify infeasible design configurations based on structural models.

A structural model of a plant is composed of components and interconnections and it is a *graph-theoretic* based representation of the system. A process maybe defined by the following equations :

$$
\begin{aligned}
y_1 &= f(a,b,c) = 4a + \exp(b - c/a) + 475 \\
y_2 &= f(a,d,g) = ag - 439/d
\end{aligned}
\qquad [4\text{-}1]
$$

The set of equations in [4-1] can be compactly represented in a structural matrix which consists of elements of fixed zeros or independent free parameters "×" as shown in Table 4-1:

Table 4 - 1: A Typical Structural Matrix

	y_1	y_2	a	b	c	d	g
Equation 1	×		×	×	×		
Equation 2		×	×			×	×

The matrix in Table 4-1 is also known as the *incidence matrix*. Each row in the matrix represents an equation while each column represents a variable. The presence of a "x" in an entry signifies that the variable represented by that column is related to the other variables in that row which also have "x"s in their respective columns. A "null" entry signifies no such relationship exists. In this representation, the dependence of the numerical values of the system parameters and the functional forms of the equations have been abstracted out. The remaining is a compact representation of the interdependence of variables involved in the process. Analysis based on such a representation has the following advantages :

1. Results of structural analysis is not dependent on the actual values of many of the plant parameters. Error in the estimation of plant parameters will not lead to incorrect conclusion.
2. The exact functional form of the relationships among variables do not play any part in the structural analysis. Thus, incorrect conclusion due to mis-representation of the physical system is avoided.
3. This representation is suitable for both linear and non-linear systems of equations.
4. Modeling large systems in structural form is much easier and it allows the designer to focus on the components and interconnections of the system rather than the exact numerical values in the equations.
5. There are efficient algorithms available for analyzing structural matrices whereas numerical rank determination is a non-trivial problem.

Structural analysis allows one to identify infeasible designs that are due to the inherent structure of the physical system, regardless of the numerical values of the plant parameters or the operating conditions of the plant. These infeasibilities remain no matter how the plant is being operated. Thus, control structures that do not pass the structural test of a particular criterion can be eliminated for further consideration.

Structural state controllability has been a popular "first screening test" for feasibility of control structures. This was first derived by Lin (1976) and has been used by Morari and Stephanopoulos (1980b), Johnston and Barton (1985) and Georgiou and Floudas (1989) as a criterion for synthesis of plant-wide control structures. As noted in Chapter 2, these methodologies allow the determination of a set of feasible control structures for a process plant. These set of control structures must be evaluated to determine which one of them can best meet the control objectives of the production unit.

In the proposed work, the generation of the entire feasible control structures is avoided by employing quantitative and numerical information about the process during control structure synthesis (see Chapter 5). Structural analysis is mainly used to assist the consistent generation of control objectives (recall Section 3.3.2) and the formulation of causal process models for acquiring an understanding of important process trends and for the selection of controlled and manipulated variables. In section 4.1.1, the fundamentals of structural representations of processes will be presented. Then, the structural aspects that are useful for control systems design in the proposed methodology will be discussed in the sections to follow. The focus of this chapter is on the presentation of the techniques. Direct application to control structure synthesis we be discussed in Chapters 7 and 8.

4.1.1 Structural Representations: Boolean Incidence Matrix

A typical plant is described by hundreds of differential and algebraic equations of the following type :

$$\begin{aligned}
\dot{x}_1 &= f_1(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d}) \\
\dot{x}_2 &= f_2(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d}) \\
&\vdots \\
\dot{x}_k &= f_k(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d}) \\
y_1 &= h_1(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d}) \\
y_2 &= h_2(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d}) \\
&\vdots \\
y_n &= h_n(\boldsymbol{x},\boldsymbol{u},\boldsymbol{d})
\end{aligned} \qquad [4\text{-}2]$$

where :

$$\begin{aligned}
\boldsymbol{x} &= [x_1 \quad x_2 \quad \cdots \quad x_k]^{\mathrm{T}} = \text{states of the system} \\
\boldsymbol{y} &= [y_1 \quad y_2 \quad \cdots \quad y_n]^{\mathrm{T}} = \text{outputs of the system} \\
\boldsymbol{u} &= [u_1 \quad u_2 \quad \cdots \quad u_m]^{\mathrm{T}} = \text{inputs of the system}
\end{aligned}$$

To correctly represent a dynamic system in structural terms, the state derivatives must be related to the states of the system by additional relationships :

$$x_i = \left\{ \int_0^{\tau} \dot{x}_i(t)d\tau; x_i(t=0) = x_{i,o} \right\} = f(\dot{x}_i) \;\; \forall i = 1,\cdots,n \qquad [4\text{-}3]$$

Equation sets [4-2] and [4-3] can be combined and transformed to a structural matrix representation in which each row corresponds to an equation, each column represents a variable in the system. For each equation, we place an "X" in all those columns where the corresponding variables are involved in the equation. The following examples illustrates how this can be done.

EXAMPLE 4-1

Given the following system of equations:

$$\begin{aligned}
\dot{x}_1 &= f_1(F_1,T_1,x_1) \\
\dot{x}_2 &= f_2(F_2,T_2,x_2) \\
k &= f_3(x_1,x_2)
\end{aligned} \qquad [4\text{-}4]$$

In order to represent the dynamical system correctly, the following additional equations must be defined to relate the states x_1 and x_2 to their derivatives through:

$$x_i = f(\dot{x}_i) \;\; \forall i = 1,2 \qquad [4\text{-}5]$$

Then, we can represent the above dynamic system by the following structural matrix shown in Table 4-2:

Table 4 - 2: Example 1 - Structural Matrix of a system of Dynamic Equations

	$\dot{x}_1$	$\dot{x}_2$	x_1	x_2	k	F_1	F_2	T_1	T_2
(1)	×		×			×		×	
(2)		×		×			×		×
(3)			×	×	×				
(4)	×		×						
(5)		×		×					

This matrix can be easily transformed to represent a system at steady state by simply deleting the columns corresponding to the derivatives of the state and the rows which relate the states to their derivatives. Note that the matrix consists of four distinct parts. The first part consists of the state derivatives. The second part is made up of the state variables and the outputs or any intermediate variables of the system. The third part contains the manipulated variables of the system and the fourth part consists of the disturbances and variables of the plant that are externally specified.

4.2 From Boolean to Directed Graphs: Defining Physical Causality

There is a direct correspondence between system representations in terms of Boolean matrices (matrix representations) and networks of nodes and edges (pictorial representations). Both of these representations are instantiation of the *graph-theoretic* concepts. A *graph* is a mathematical abstraction of structural relationship between discrete objects and it is represented by a collection of *nodes*. Existence of a relationship between two nodes is represented by an *edge*. Discrete nodes and the relationships between them can represent something physical, such as units and streams in a process, or they may be something more abstract such as chemical intermediates and their precedence relationship (Mah, 1990). Associated with each pictorial graph is a *Boolean matrix*, ***R***, with the rows representing the nodes and the columns representing the edges in the graph. The element $r_{ij} = 1$ (or "×") if there is an edge between vertices *i* and *j*, otherwise it is zero (or blank).

A typical graph is depicted in Figure 4-1(a). Depending on the application, it may be useful to include additional attributes associated with the edges and vertices. A common attribute is the direction of information flow associated with the edges. Graphs with edges which have directions are *digraphs*, or *directed graphs*. Figure 4-1(b) is an example of a digraph. Undirected graphs are useful for representing symmetric relationships among the vertices, but in may applications, the relationships between discrete objects are asymmetrical (such as the direction of material flow in a process) so digraphs capture this feature in the problem formulation.

Graph-theoretic concepts are very useful in process system analysis. Pictorial representations offer an additional advantage over matrix representations since they provide better visualization of the process, making it easier to assimilate information. However, as the pictorial representations get large, they lose their intuitive appeal. In that case, Boolean matrix representations offer a computational advantage as computer-aided algorithms based on these matrices can be developed to assist system analysis.

In the next sub-sections, the use of graph-theoretic representations of system to aid development of plant control strategies will be described.

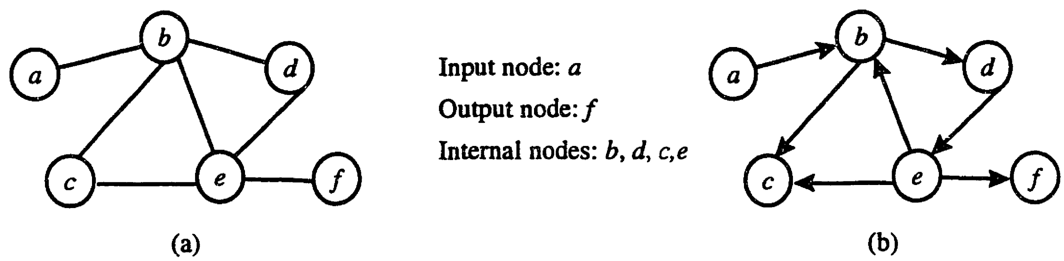


Figure 4 - 1: A Typical graph (a) Un-directed graph; (b) Directed graph

4.2.1 Representing Process Behavior using Causal Pathway Networks

Behavioral description of a process is based on input-output models of the process. Thus, the internal workings of an object are not important as long as one can describe fully the input-output behavior of the discrete objects (Johnston, 1991). The ultimate goal of any plant control system is to modify the process behavior in such a way that the controlled objectives are always being maintained at their desired state, in the presence of external process disturbances. Thus, an important part of the development of process control strategies requires analyzing the process behavior and studying how the behavior can be modified. Johnston, J.E. (1991) has developed a formal representation in which process behavior can be reasoned.

A unit *causal pathway network* (CPN) is network representation for process behavior. Nodes of the network are variables associated with the input and output attributes of a process unit, and a directed edge between two nodes exists if a change in the input node induces a change in the output node. Figure 4-3 gives the CPN developed by Johnston (1991) for a simple heat-exchanger shown in Figure 4-2. The unit consists of input ports and output ports where input streams (cold-feed and hot-feed) and output streams (cold-effluent and hot-effluent) enter and leave the unit, respectively. The input-output behavior represents the *static* description of how input disturbances (manipulatable or un-manipulatable) propagate through the unit from input stream attributes to output stream attributes, in the same sense as what a quantitative equation-based model would describe. In the network representation, there are edges linking hot-feed-temperature to cold-effluent-temperature and hot-effluent-temperature. Thus, changes in the temperature of the hot-feed stream cause changes in the temperatures of the cold and hot-effluent streams. The causal relationships in the network can be identified through: (i) input-output plant data; (ii) physical reasoning or (iii) a system of modeling equation describing the relationships among the process variables.

Individual unit networks in a plant can be constructed in a similar manner. These networks, when combined, form the *plant* CPN for process behavior. When combining the networks, nodes associated with an output port of a unit are linked to an input port of another unit if there exists a stream between these two units in the process flowsheet. An example which illustrates such connectivity given by Johnston (1991) has been reproduced in Figure 4-4.

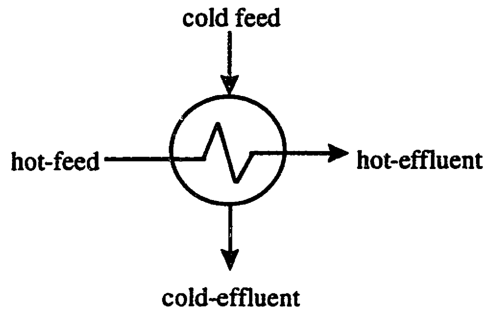


Figure 4 - 2: A Simple Heat-exchanger

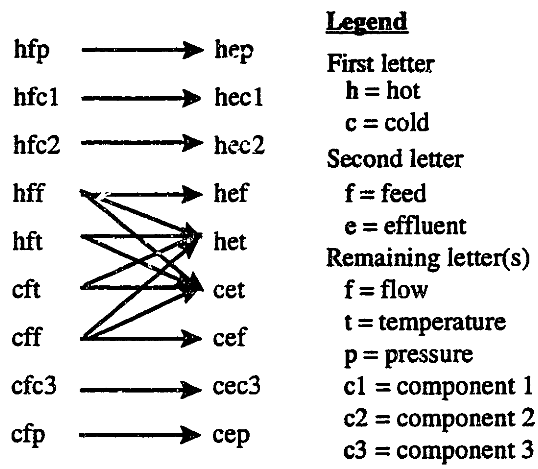


Figure 4 - 3: Network Representation for a Heat-exchanger

The CPN can be used to trace out the pathways of causal relationships through the plant and define the process behavior. *Process behavior* refers to the state of a process which can be defined in terms of what variables are disturbed (or affected) when a set of input effects enters the process. Using the CPN for the heat-exchanger and flash process shown in Figure 4-4, we can deduce that a change in hot-feed-flow affects hot-effluent-flow, hot-effluent-temperature and cold-effluent-temperature. Hot-effluent-flow then in turns affects flash-feed-flow which has an effect on flash-vapor-flow and flash-liquid-flow. Hot-effluent-temperature also has an influence on flash-feed-temperature which then affects flash-vapor-flow, flash-vapor-component1, flash-vapor-component2, flash-vapor-temperature, flash-liquid-flow, flash-liquid-component1, flash-liquid-component2 and flash-liquid-temperature. We can further deduce from this CPN that flash-vapor-pressure can only be affected by a change in hot-feed-pressure.

The role that CPNs play in the synthesis of plant control strategies can be summarized as follows:

1. *Identify the set of manipulated variables which influence a process variable.* While it is relatively easy to name the potential manipulated variables which are located close to a particular control objective of interest, it becomes hard to recognize manipulated variables which influence the control objective through some long-range effects in the plant. The identification task is made more manageable when we formally depict the causal-relationships in the plant in terms of a network.
2. *Study the disturbance load paths in the system.* Disturbance load paths refer to the routes through which process variations propagate in the system. It is a consistent, uniformed way of representing any parameter deviations (temperatures and/or flowrates) from their nominal values (Calandranis and Stephanopoulos, 1988). CPN is a tool (although not the only kind) for tracing such pathways. More about disturbance load paths will be discussed in Section 4.2.2.

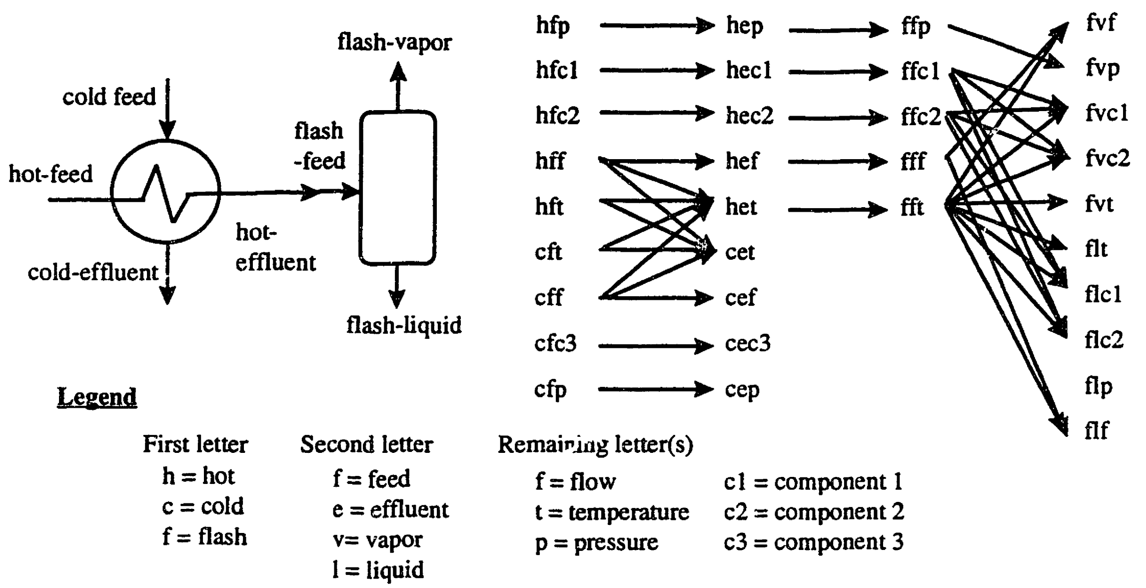


Figure 4 - 4: Expanded Network Representation for a Plant Section (from Johnston, 1991)

4.2.2 Using Disturbance Load Paths to guide the selection of controlled and manipulated variables

A causal pathway network (CPN) is a tool that can be used to trace out the process variations and study how the variations can be modified. The importance of managing process variations in a chemical plant has been discussed in Section 2.1, where we pointed out that an important plant control objective is to divert process variations caused by external disturbances in such a way that the variations in product and quality are minimized. A CPN depicts the *topography* and the *directionality* of the system. In the context of a chemical plant, topography refers to the structural relationships among process variables in the plant; directionality refers to the course on which process variations in the system travels.

Disturbance Load Paths of Open and Closed-loop Systems

Suppose there is a disturbance which causes variation in the temperature of the cold water feed of the simple heat-exchanger in Figure 4-2. Based on the corresponding CPN (Figure 4-3), we can deduce that variation in cold-feed-temperature produces variations in cold-effluent-temperature and hot-effluent temperature. Figure 4-5 depicts the direction of flow of these temperature variations. The route along which temperature variation travels is called the *disturbance load path*. What we see in Figure 4-5 is the effect of the disturbance on the uncontrolled system. Thus, it represents the *open-loop effect*.

A control loop such as the one shown in Figure 4-6 can be placed in the system to minimize the variation of temperature in cold-effluent. As a result of the implementation of the control loop, temperature variation in the cold feed that would have otherwise passed on to the temperature of the cold effluent is now being diverted to the flow of the hot feed and hence the temperature and flow of the hot-effluent. Furthermore, the control loop also diverts variations in cold-feed-flow and hot-feed-temperature away from the hot effluent. Thus, the control loop has transformed the process behavior by modifying the topography of the disturbance load path. The direction of flow of temperature variation of the modified process can be found in Figure 4-7. The pathways represent the directionality of the *closed-loop system*. By virtue of the control-loop, we have additionally transformed some of the temperature variation into flow variations in hot-feed and hot-effluent.

The transformation of the system directionality by the control structure is depicted in the CPN of the heat-exchanger (Figures 4-8 (a) and (b)). The broken lines in Figure 4-8 (a) represent the original directions that had been affected by the control loop. The gray thick lines in Figure 4-8 (b) are the new directions in the modified system. Nodes [*hff*], [*hft*], [*cft*] and [*cff*] are the *disturbance sources* of variation in node [*cet*]. The control system has *deactivated* the paths which go from the disturbance sources to [*cet*] (i.e. the broken lines in Figure 4-8 (a)) and has placed them with new paths which bring the variation from the disturbance sources to [*hef*] and [*het*], the *disturbance sinks*.

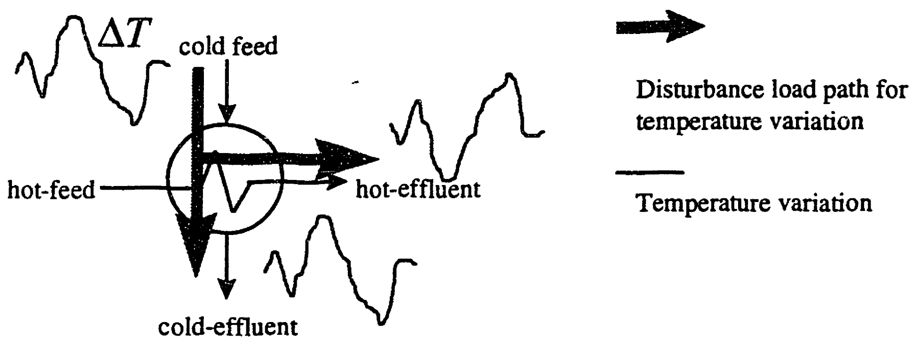


Figure 4 - 5: Directionality of the Simple Heat-exchanger

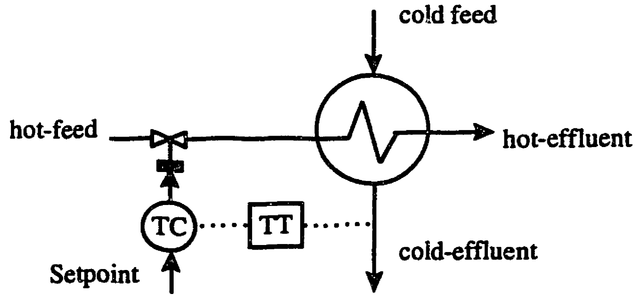


Figure 4 - 6: Feedback control loop for the Heat-exchanger

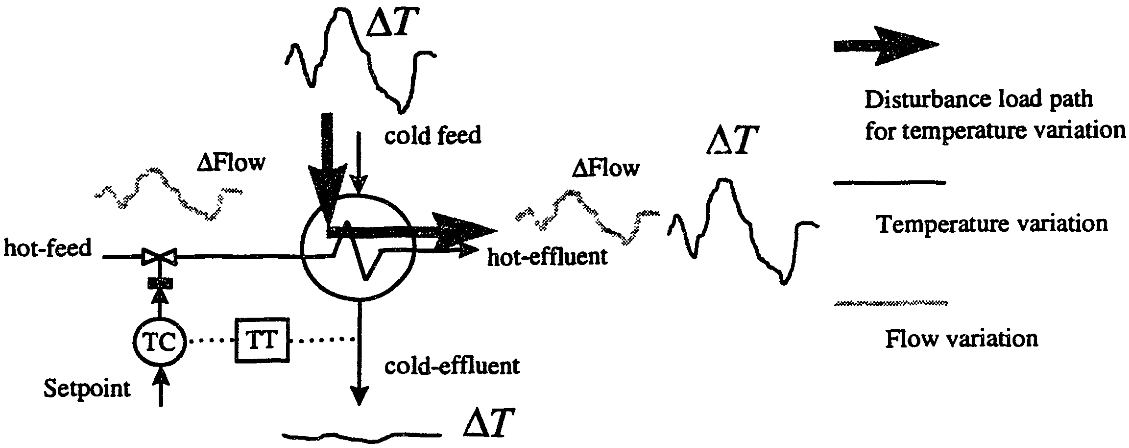


Figure 4 - 7: Directionality of the Closed-loop System

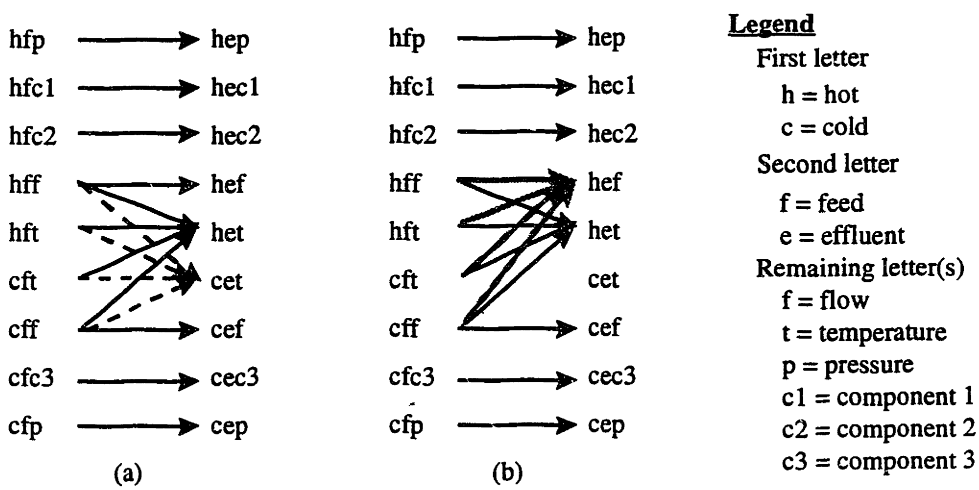


Figure 4 - 8: Transformation of Process CPN (a) CPN of the open-loop system; (b) Modified CPN of the closed-loop system (adapted from Johnston, 1991)

Boolean Representation of Disturbance Load Paths

The disturbance load path can also be depicted in a Boolean representation of the system. The following set of steady-state equations models the physical behavior of the heat-exchanger shown previously in Figure 4-2:

$$(het - hft)\, hff * \alpha_1 = Q \qquad [4\text{-}6]$$

$$(cet - cft)\, cff * \alpha_2 = Q \qquad [4\text{-}7]$$

$$Q = UA\, \Delta T \qquad [4\text{-}8]$$

$$\Delta T = \frac{(hft - cft) - (het - cet)}{\ln\left\{\dfrac{(hft - cft)}{(het - cet)}\right\}} \qquad [4\text{-}9]$$

where:

α_i = constants

ΔT = approach temperature

U = heat transfer coefficient of the heat-exchanger

A = heat transfer area

Boolean representation corresponding to Equations [4-6] to [4-9] is shown in Figure 4-9 (a). Variables on the right side of the table are process inputs and those on the left side are process outputs. The symbol "⊗" indicates an output assignment. In general an *output assignment* is the output variable of a particular equation. Thus, we can view that the variable corresponding to the column of that output assignment is to be computed from the equation that is represented by that row in the matrix. The set of "⊗" is called the *output set assignment*. Each equation should have exactly one output variable and each variable on the left side of the matrix should appear as the output variable of exactly one equation. It is not always possible to solve the set of equations sequentially by computing one output after another. In practice, the equations often have to be solved simultaneously, but by selecting an output set, we have imposed a directionality to the system of equations, very similar to the direction in a CPN. Output assignment algorithms can be found in Mah (1990).

In Figure 4-9 (b), we have traced out the disturbance load path through which [*cft*] affects [*cet*]. After implementing a control loop, this path is disabled (see Figure 4-9 (c)). Instead, the variation travels from [*cet*] (where the setpoint of the outlet temperature is defined) to the flow of the hot stream [*hff*]. The flow of the hot stream is now an "output" of the controller.

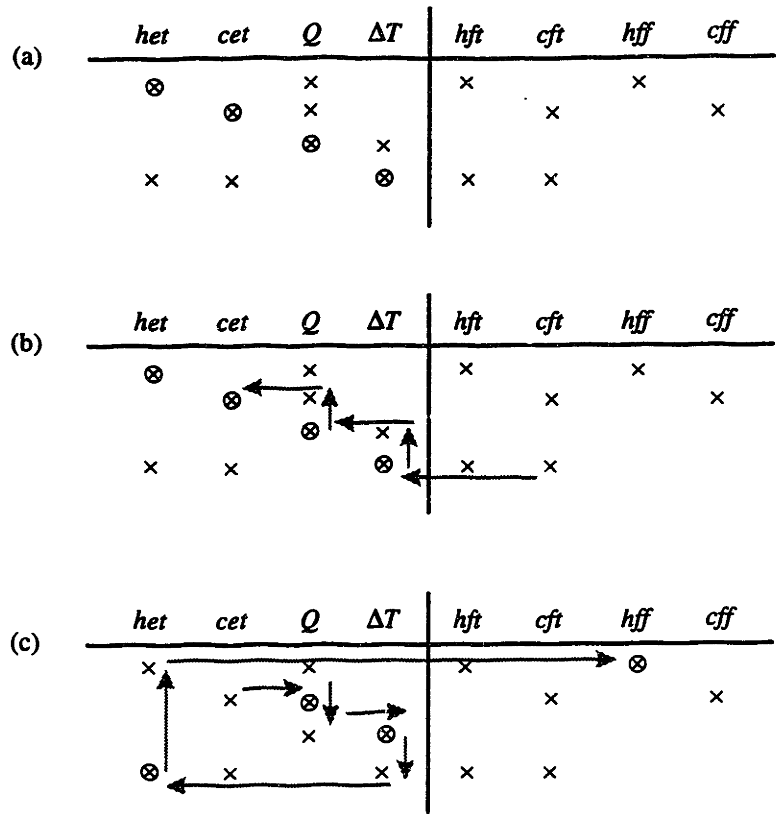


Figure 4 - 9: Boolean representation of the CPN (a) Boolean representation of the open-loop system; (b) Disturbance load path in the open-loop system; (c) Disturbance load path in the closed-loop system

Application of the Concept of Disturbance Load Paths to Control Systems Design

In this section, practical applications of the concept of disturbance load paths for the synthesis of plant-wide control structures are described.

1. *Identify ways to transform process variation*
   When modifying process variation, the goal is to divert variation toward "non-critical" process variables. By studying the disturbance load paths in the closed-loop system formed by each of the potential manipulated variables, the manipulated variable that can best minimize variations in the critical process variables can be identified.
2. *Identify supplementary controlled variables which help to minimize process variation*
   Disturbance load paths are useful for deriving special control strategies to minimize process variation at a specific location. Figure 4-10 shows a portion of a plant which consists of a flash, a reactor and a multicomponent distillation column. The following reactions happen in the reactor:

$$C_1 + C_2 \rightarrow C_4$$
$$C_1 + C_4 \rightarrow C_5$$
$$C_3 \rightarrow C_6$$

The reactor is being maintained at isothermal condition. C_1, C_2, C_3 and C_6 go preferentially to the distillate, with C_3 and C_6 being the lightest materials. Feed to the reactor comes from the liquid product of an upstream unit (a flash unit). The corresponding CPN of this section of the process is shown in Figure 4-11. We can judge from the CPN that in order to minimize variation in DV6, variations in RE6 and RF3 must also be minimized. Since there is no manipulated variable which would affect RE6 in the vicinity of the unit, we must spawn a new control objective to maintain RE3 at some fixed value using manipulated variables available from the upstream unit. This activity is an example of the concept of spawning that was introduced in Section 3.3.2. The purpose of this spawning is to generate a new objective to help minimizing variation in DV6.

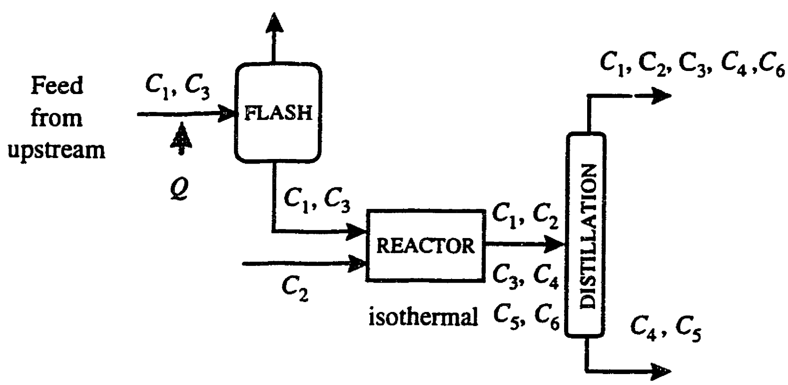


Figure 4 - 10: Flash, reactor and distillation process

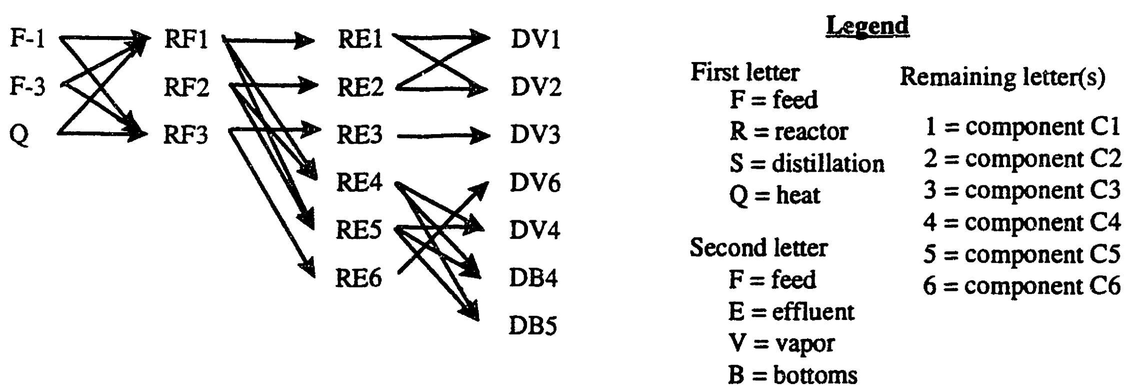


Figure 4 - 11: CPN of the flash, reactor and distillation process

The examples and illustrations in this section have the following implications :

1. Uncontrollable disturbances entering the plant can only leave the process through the streams that link the process to the environment.

2. The pathways through which the disturbances travel are being modified by the plant control structure. Thus, the control strategies of the system transform the topography of the propagation of the disturbances in the system.
3. Structural matrices offer a medium in which the alteration of the diversion of disturbances in the plant can be studied.

An ideal plant control structure should divert the undesirable effects of process disturbances to the less critical locations in the plant. As illustrated in the heat-exchanger example, under closed-loop control, the effects of process disturbances are being propagated to the chosen manipulated variables for process control. In a square system (i.e. a plant such that the number of inputs equals the number of outputs), all manipulated variables are being used for process control and all inputs will be affected. Thus, diversion of disturbances can only be discussed with respect to complete sets of manipulated variables being selected for control. Obviously, there will only be a finite number of these sets in non-square systems such that the number of inputs exceeds the number of outputs. The inputs which are being used for process control in a non-square system are being affected by the process disturbances.

4.2.3 Performing Qualitative Simulation using Signed Causal Models

A common approach to process simulation is by performing numerical computation on a set of equations describing the physical system. However, characterization of the physical system and solving of a set of non-linear equations numerically are expensive tasks that can only be justified if precise process behavior is crucial for the engineering tasks. In many domains, qualitative reasoning is superior to formulating and solving a system of quantitative equations because reasoning based on qualitative models and data is sufficient for performing the desired task and requires less computation (Palowitch, 1987).

Qualitative Reasoning of Process Behavior

Qualitative reasoning of process behavior can be done based on a signed causal model of the process. A *signed causal model* is pictorial graph of the process form by nodes and arcs, but with a *sign attribute* associated with the arcs. Graphs of various form can be developed for a process. The CPN that we discussed in previous section is one form of graph which captures only the input-output behavior of the process with the internal variables of the process ignored. To be useful for qualitative process simulation, internal variables are important. The reason for this will be obvious in the later discussion.

A signed causal model is constructed base on the set of mathematical modeling equations describing the process. Process variables form nodes; related nodes are linked by arcs. A directed arc represents how a change in the initial node is propagated to the terminal node. Sign attribute is added to the arcs to characterize the direction of deviation of the process variables at the arc's initial and terminal nodes. A "+" sign indicates that the terminal node deviates in the same direction as the initial node. A "-" sign indicates that the terminal node varies in a direction that is opposite from that of the initial node. Palowicth (1987) has called such a causal model a *single-staged directed graph* (SDG).

In general, mathematical equations specify equality relationships but contain no information on how changes in an individual process variable or parameter directly affects other system variables. Thus, knowledge of the physical principles and mechanisms behind each equation is necessary to specify causality (Palowitch, 1987). The next example will demonstrate the basic idea behind a SDG. For more details on the construction of SDGs, refer to Palowitch (1987).

EXAMPLE 4-2

The heat flux in a conductor can be described by the following driving force equation:

$$T_1 - T_2 = q/k \qquad [4\text{-}10]$$

where T_1 and T_2 are the temperatures on two sides of the conductor, q is the heat flux in the conductor and k is the heat conductivity of the material. Causal influences can be specified from the understanding of the fundamental physical principles governing the equation. Heat flux results from a difference in the temperatures on both sides of the conductor, which is the driving force of the flow of heat. 1/k is a measure of the resistively. It is a physical characteristic of the conductor so it is independent on q and ΔT. Based on this physical understanding, we can develop the following causal relationships:

$$q = f(-\ 1/k)$$
$$q = f(+\ T_1)$$
$$q = f(-\ T_2)$$
$$T_1 = f(-\ q)$$
$$T_2 = f(+\ q)$$

such that $A = f(-B)$ means that increasing B decreases A. The above causal relationships can be used to construct the signed causal digraph shown in Figure 4-12. This example shows that the causal relationships can only be developed witn an understanding of the physical system.

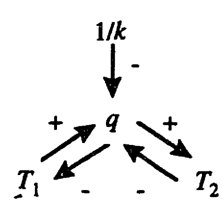


Figure 4 - 12: Signed Causal Digraph (SDG) of Heat Flow through a Conductor

Performing Qualitative Process Simulations

The single-staged directed graph (SDG) shows the physical relationships among process variables and the nature of process variation occurring in the process. Using this graph, important qualitative process trends in the plant can be uncovered by simulating the effects caused by changes in specific variables in the plant.

While constructing the SDG for qualitative simulation, care should be taken when deciding which nodes to include and which nodes to exclude from the model. Adding digraph nodes will give greater knowledge about a physical system and reduce the number of spurious interpretations. However, an increased level of detail may eliminate information that constrains qualitative parameter states and adds spurious interpretations to the network (Palowitch, 1987). Thus, it is important to select an appropriate model which captures the characteristics to be analyzed in the process.

Palowitch (1987) has pointed out that the causal digraph is not unique. Depending on the chosen modeling parameters, one may come up with a different causal representation of the process. Also, ambiguities may arise in the causal digraphs. When multiple paths with opposite net signs influence a particular node, one cannot determine from the causal digraph with certainty the absolute behavior of that node. The next two examples illustrate the explanatory power of SDGs.

EXAMPLE 4-3

Figure 4-13 shows a cooler and the corresponding SDG of this process. Fluid of concentration C_A leaves the tank by overflow. From this simple SDG, we can deduce the following:

1. An increase in the inlet flow (F_1, +) decreases the outlet temperature (T,-).
2. An increase in the flow of the cooling water (F_{cw}, +) decreases the outlet temperature (T,-).
3. Increasing the inlet flow (F_1, +) increases the outlet flow (F_1, +).
4. Material A in F_1 travels with the bulk flow so an increase in the concentration of A in the inlet stream (C_{A1}, +) increases the concentration of A in the outlet stream (C_{A2}, +).

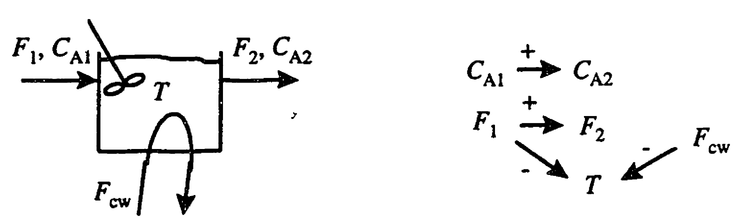


Figure 4 - 13: SDG of a Cooler

EXAMPLE 4-4 (from Oyeleye, 1990)

Figure 4-14 shows a causal model which represents an exothermic first order irreversible ($A \rightarrow B$) reaction that takes place in a continuous stirred tank reactor (CSTR) equipped with a cooling jacket. Reactor level and coolant temperate are assumed to be constant. Then, the following can be deduced from the digraph. (The process variable and its qualitative deviation are enclosed in parentheses):

1. An increase in the concentration of A of the inlet stream (C_{A0}, +) raises the concentration of A in the CSTR (C_A, +).
2. Increasing the concentration of A in the CSTR (C_A,+) increases the rate of reaction which increases the temperature of the materials (T, +) in the CSTR.

3. An increase in temperature (T, +) increases the reaction further and causes the concentration of A in the CSTR to decrease (C_A, -).

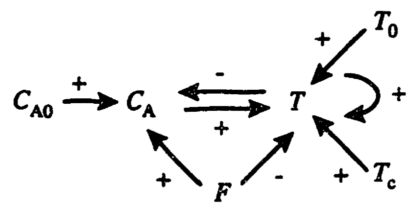


Figure 4 - 14: SDG of CSTR (from Oyeleye, 1990)

Examples 4-3 and 4-4 have illustrated how SDGs provide a medium in which qualitative process trends in the plant can be systematically studied. Its application in a plant-wide setting will be demonstrated in Chapter 7.

4.3 Structural issues in the Hierarchical Propagation of Control Objectives

In Section 3.3.2, we described several mechanisms which allows control objectives identified at one level of process representation to be systematically updated and modified at the next level of the hierarchy. These mechanisms maintain consistency in the specification of control objectives for the plant. In this section, we introduce the structural counterparts to these mechanisms.

4.3.1 Structural Interpretation of Translation of Control Objectives

Control objectives defined at an abstract level are being translated or allocated to some sub-blocks in a more detailed representation. Earlier, we developed the following rules for translation: (i) an explicitly defined objective at one level is translated only to the sub-block associated with that process variable; (ii) an implicit objective is global in nature so it is translated to all the sub-blocks for which the objective applied. The structural equivalence of these two statements can be illustrated in the next two examples.

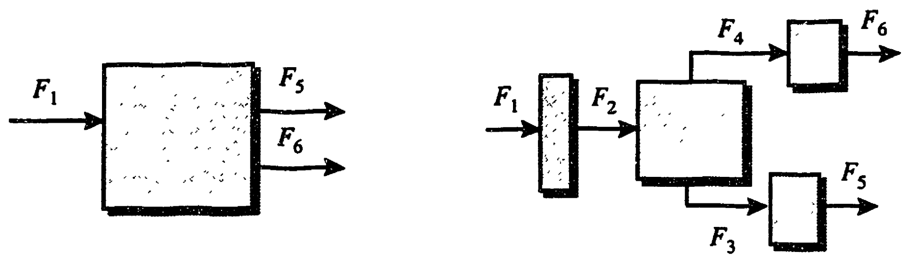
EXAMPLE 4-5

In an abstract view of a simple flow system (Figure 4-15 (a)), it is required to maintain the production rate, P, at some pre-specified value. P is directly related to F_5. This simple system can be transformed into the following structural representation:

$$\begin{array}{c} \begin{array}{cccc} F_1 & F_5 & F_6 & P \end{array} \\ \begin{pmatrix} \times & \times & \times & \\ & \times & & \otimes \end{pmatrix} \end{array}$$

where $\otimes$ represents the control objective of the system. By selecting P to be the control objective, we have taken away one degree of freedom in the process. The abstract view of the process can be expanded to incorporate more details of the plant at a lower level of representation, such as the one shown in Figure 4-15 (b). An explicit objective is one that is directly related to a measurable variable in the plant, if it is observable at one level, it must necessarily be observable at all other lower levels in the hierarchy. Based on this fact, and based on our rule for translation of explicit objectives, we can say that the column corresponding to P in the structural matrix representing the detailed level must also be a control objective:

$$
\begin{array}{ccccccc}
F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & P
\end{array}
$$
$$
\begin{pmatrix}
\times & \times & & & & & \\
 & \times & \times & \times & & & \\
 & & \times & & \times & & \\
 & & & \times & & \times & \\
 & & & & \times & & \otimes
\end{pmatrix}
$$



(a) (b)

Figure 4 - 15: A simple flow system (a) Abstract view; (b) Detailed view

EXAMPLE 4-6

Suppose it is also desired to maintain the overall material balance in the process shown in Figure 4-15 (a). Material balance (M) is a global, implicit objective as it represents the overall behavior of the process and that the determination of the material balance involves a large number of process variables in the system. Structurally, its relation to the process at the abstract level is described by:

$$
\begin{array}{ccccc}
M & F_1 & F_5 & F_6 & P
\end{array}
$$
$$
\begin{pmatrix}
\otimes & \times & \times & \times & \\
 & & \times & & \otimes
\end{pmatrix}
$$

such that both M and P (P is a requirement specified in Example 4-5) are control objectives. As we move down to the more detailed level (Figure 4-15 (b)) , M, the implicit objective is translated to all sub-blocks for which the objective applies. This means, for each sub-block i where a material balance equation can be written, we create a corresponding subgoal M_i. Thus, we develop the following structural matrix for the detailed level:

$$
\begin{array}{c}
\begin{array}{ccccccccccc} M_1 & M_2 & M_3 & M_4 & F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & P \end{array} \\
\begin{pmatrix}
\otimes & & & & \times & \times & & & & & \\
& \otimes & & & & \times & \times & \times & & & \\
& & \otimes & & & & \times & & \times & & \\
& & & \otimes & & & & \times & & \times & \\
& & & & & & & & \times & & \otimes
\end{pmatrix}
\end{array}
$$

4.3.2 Structural Interpretation of Generation of new Control Objectives

As mentioned in Section 3.3.2, new control objectives can be generated via either refinement or spawning of implicit objectives. Refinement of an implicit objective occurs when specific variables within a sub-block can be associated to the original objective. For example, a cost optimization objective for the abstract unit may be refined into one which requires minimization of loss of raw materials in the product stream at a detailed level. Such refinement requires sensitivity analysis of the different variables related to the cost function which does not have a structural counterpart. Spawning is another mechanism in which new objectives can be generated. As spawning only occurs when there is a fundamental relationship between the original objective and the potential new variables, it can be explained in structural terms. In fact, it has already been demonstrated in Section 4.2.2 how new control objective which can be spawned to help to minimize process variation of an important process goal can be identified by studying the disturbance load paths in the plant. The next two examples further illustrate the concept of spawning.

EXAMPLE 4-7

It has been illustrated in Chapter 3 how spawning can take place to *replace* an original objective with a new one. A process and its corresponding CPN is shown in Figure 4-16. T_{in} represents the temperature of the stream entering the cooler, T_A is the temperature of the stream leaving the cooler, T_B and T_C represent the temperatures of the streams leaving the isothermal processes B and C. It is desired to maintain T_C at some fixed value. As shown in the CPN, there is not a manipulated variable in the vicinity of Process C. Also, T_C is directly influenced by T_A which can be directly controlled by the heat flux to the cooler. Hence, we can spawn a new objective to control the temperature of the stream leaving Unit A. As T_C is not influenced by any other process variables, this new objective will replace the original objective.

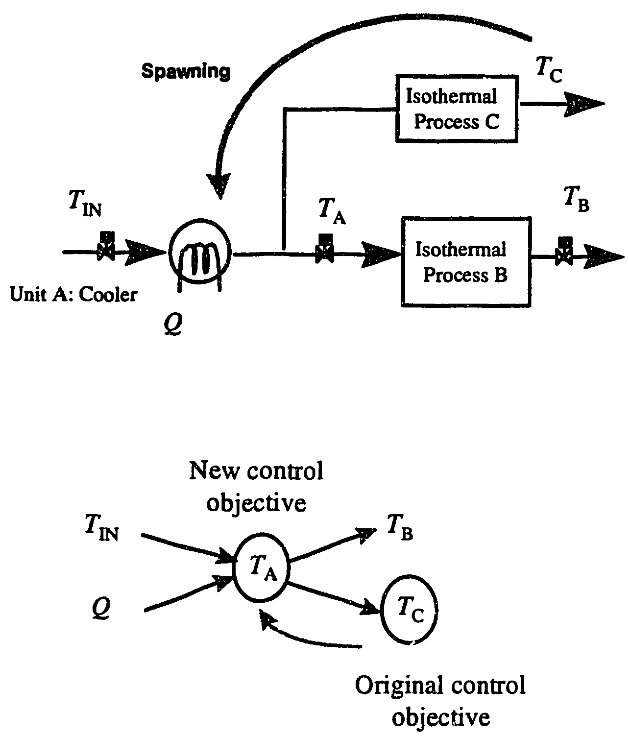


Figure 4 - 16: Structural interpretation of spawning (to replace a control objective)

EXAMPLE 4-8

In Figure 4-17, we show a process that consists of three reactors. F_0 and $F_0{}^*$ enter unit A where the materials react to produce product A. Product A undergoes isomerization in unit B to form product B. Product A is also mixed with D in unit C to form product C. The goal is to maintain the F_B at fixed value. From the CPN, we see that F_B is influenced by both F_A and T_A. F_0 and Q are the only manipulated variables in the process. Notice that T_A is influenced by a disturbance T_0. Variation in T_A propagates to F_B and T_B. Thus, to minimize variation in F_B, we should try to minimize variations in both F_A and T_A. Variation in T_A caused by T_0 could be easily diverted away from F_B though the use of Q. Hence, we spawn a new objective, T_A (which could be controlled by Q) to supplement the control of F_B.

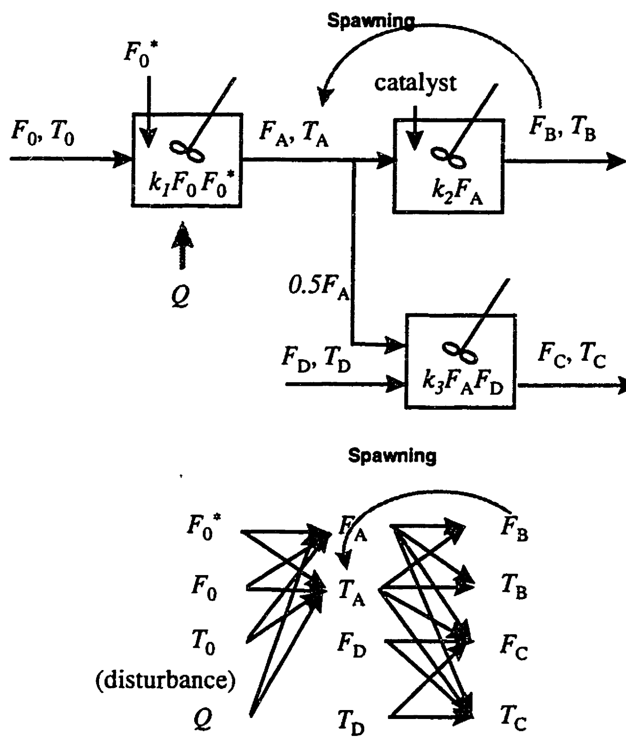


Figure 4 - 17: Structural interpretation of spawning (to supplement a control objective)

Examples 4-7 and 4-8 have shown how structural analysis can aid the generation of control objectives through spawning.

EXAMPLE 4-7

It has been illustrated in Chapter 3 how spawning can take place to *replace* an original objective with a new one. A process and its corresponding CPN is shown in Figure 4-16. T_{in} represents the temperature of the stream entering the cooler, T_A is the temperature of the stream leaving the cooler, T_B and T_C represent the temperatures of the streams leaving the isothermal processes B and C. It is desired to maintain T_C at some fixed value. As shown in the CPN, there is not a manipulated variable in the vicinity of Process C. Also, T_C is directly influenced by T_A which can be directly controlled by the heat flux to the cooler. Hence, we can spawn a new objective to control the temperature of the stream leaving Unit A. As T_C is not influenced by any other process variables, this new objective will replace the original objective.

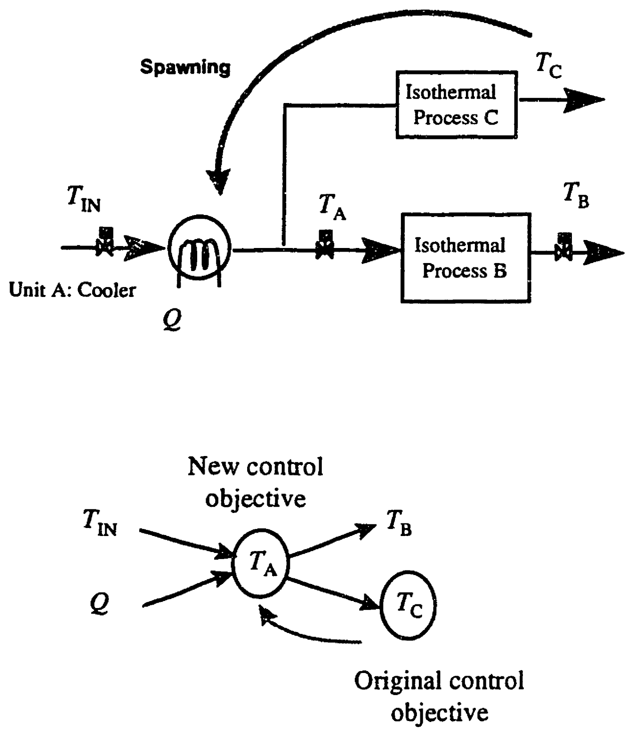


Figure 4 - 16: Structural interpretation of spawning (to replace a control objective)

Chapter 5
Quantitative Aspects of Control Systems Analysis

5.1 Quantitative Analysis of Plant Behavior

A hierarchical framework for the design and synthesis of plant-wide control structures was presented in Chapter 3. In this framework, the chemical plant is studied through a hierarchical stratification which consists of a series of process representations. Analysis and synthesis of plant-wide control structures begins from coarse process representations. In an evolutionary manner, details of the process are gradually incorporated to the process viewpoint, enabling control structures of finer details to be synthesized. As noted earlier, the coarser viewpoints capture the longer time-horizon characteristics about the plant behavior while those viewpoints with more details capture the dynamic behavior of the process. Thus, tools which allows the evaluation of process behavior in various time-horizons are required. This is the subject of this chapter.

In Chapter 4, structural techniques have been introduce for studying process trends, identifying disturbance load paths and for systematically identifying relevant control objectives as well as potential manipulated variables in the process. However, performing structural analysis on the plant *alone* is not sufficient as such methods fail to discriminate effective designs from the merely probable ones. In this chapter, the modeling requirements for formal quantitative analysis of plant behavior at various time-scale will be introduced.

5.2 Modeling the Process for Long-Horizon Analysis

At the top of the hierarchy, the process plant is being represented by coarse viewpoints. Figures 5-1 (a) and (b) give examples of two coarse viewpoints of a process which produces acetic anhydride. According to the formalism for the multistrata system described in Chapter 3, the only process variables which are significant to a particular viewpoint are those variables that are associated with the inlet and outlet process streams, i.e. the observable process variables. Thus, the essential characteristics of the coarse viewpoints can be captured by the corresponding material and energy balances of the systems. These balance equations are useful for studying the long-horizon characteristics of the plant.

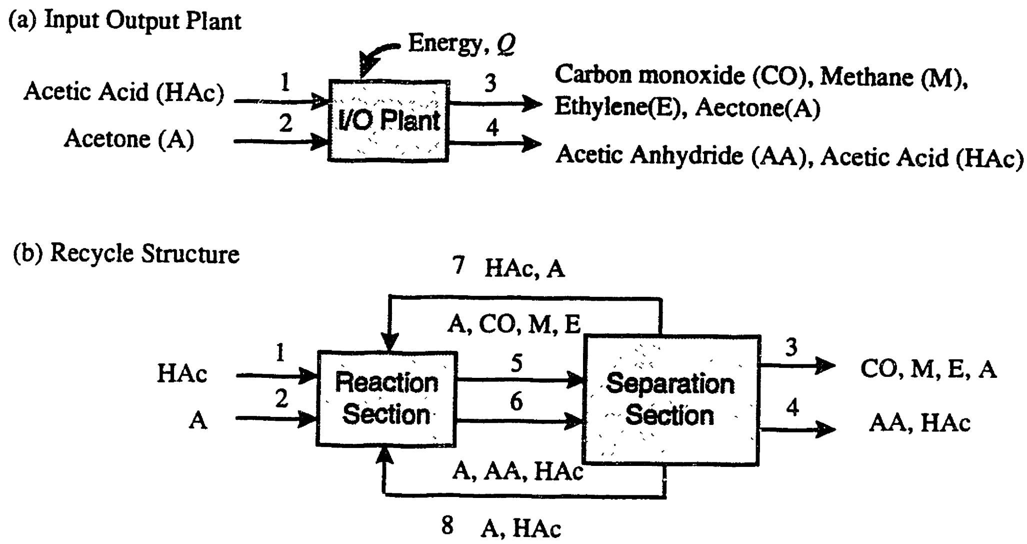


Figure 5 - 1: Representations of a process which produces Acetic Anhydride (a) Level 1: Input-Output Plant; (b) Level 2: Recycle Structure

5.2.1 Describing the Long-horizon Characteristics by Material and Energy Balances

Each block in a particular viewpoint can be described by one energy balance and a set of independent material balances. The number of material balances that is required to fully describe the system is given by:

$$N_{MB} = N_C - N_R + N_I \qquad [5\text{-}1]$$

where:

N_{MB} = number of independent material balances
N_C = number of reactive components in the system
N_R = number of independent reactions
N_I = number of inert components in the system

The next example demonstrates how material and energy balances are developed for the coarse process viewpoints using only variables observable from the viewpoint.

EXAMPLE 5-1

Recall that the following reactions take place in the HDA process shown previously in Figure 2-2:

R1: Toluene (T) + Hydrogen (H) $\rightarrow$ Benzene (B) + Methane (M)
R2: 2 Benzene (2B) $\rightarrow$ Diphenyl (D) + Hydrogen (H)

There is no inert in the process. The letter(s) in parenthesis are the symbols for the corresponding materials.

Since there are 5 reactive components and 2 reactions, we can write 3 independent material balances for each block in any viewpoint (from equation 5-1). Writing material balances for components T, H and M and the overall energy balance will completely describe each block in the viewpoint.

Level 1: Input-Output Level (Figure 5-2 (a))

The following is a generalized material balance:

$$A_{in} + A_{genearted} = A_{reacted} + A_{unreacted} \quad [5\text{-}2]$$

where A is the molar flow of a material and the subscripts refer to the types of flows. Then, for Level 1, we can write the following balances:

Material balance of toluene (T):

$$F_2\, x_{2,T} = F_5\, x_{5,B} + F_3\, x_{3,B} + F_4\, x_{4,B} + 2\, F_6\, x_{6,D} + F_3\, x_{3,T} + F_5\, x_{5,T} + F_6\, x_{6,T} \quad [5\text{-}3]$$

where F_i is the molar flow of stream i and $x_{i,j}$ is the molar composition of material j in stream i. ($F_5\, x_{5,B} + F_3\, x_{3,B} + F_4\, x_{4,B}$) is the amount of benzene produced in R1 that is not converted to diphenyl in R2. For every mole of diphenyl produced, 2 moles of benzene are required, which require 2 moles of toluene (i.e. 2 $F_6\, x_{6,D}$).

Material balance of hydrogen (H) :

$$F_1 x_{1,H} + F_6 x_{6,H} = F_4\, x_{4,B} + F_5\, x_{5,B} + F_3\, x_{3,B} + 2F_6\, x_{6,D} + F_3\, x_{3,H} + F_4\, x_{4,H} \quad [5\text{-}4]$$

Material balance of methane (M):

$$F_1\, x_{1,M} + F_4\, x_{4,B} + F_3\, x_{3,B} + 2F_6\, x_{6,D} = F_3\, x_{3,M} + F_4\, x_{4,M} + F_5\, x_{5,M} \quad [5\text{-}5]$$

The energy balance of the input-output viewpoint can be written as follows:

$$H_1 + H_2 + Q_{fuel} + Q_{steam} + Q_{cw} = H_4 + H_5 + H_6 \quad [5\text{-}6]$$

where H_i is the molar enthalpy of stream i.

Equations [5-3] through [5-7] together describe the process at the input output level.

Level 2: Recycle Structure (Figure 5-2 (b))

In a similar manner, material and energy balances for the recycle level can be developed. The material balances for toluene are:

Reaction Section:

$$F_{2,T} + 2F_{7,D} + F_{7,T} + F_{7,B} + 2F_{9,D} + F_{9,T} + F_{9,B} + 2F_{11,D} + F_{11,T} + F_{11,B}$$
$$= F_{10,B} + 2F_{10,D} + F_{10,T} \qquad [5\text{-}7]$$

Separation Section:

$$F_{10,T} + F_{10,B} + 2F_{10,D} = F_{8,T} + F_{8,B} + 2F_{8,D} + F_{5,T} + F_{5,B}$$
$$+ 2F_{5,D} + F_{6,T} + F_{6,B} + 2F_{6,D} + F_{9,T} + F_{9,B} + 2F_{9,D}$$
$$+ F_{11,T} + F_{11,B} + 2F_{11,D} + F_{4,T} + F_{4,B} + 2F_{4,D} \qquad [5\text{-}8]$$

T-junction:

$$F_{8,T} + F_{8,B} + 2F_{8,D} = F_{7,T} + F_{7,B} + 2F_{7,D} + F_{3,T} + F_{3,B} + 2F_{3,D} \qquad [5\text{-}9]$$

For simplicity, $F_{i,j}$ is used to describe the molar flow rate of component j in F_i, i.e. $F_i\, x_{i,j}$. Notice that adding equations [5-7] through [5-9] gives equation [5-3], as expected. Material balances for other components can be written in a similar manner.

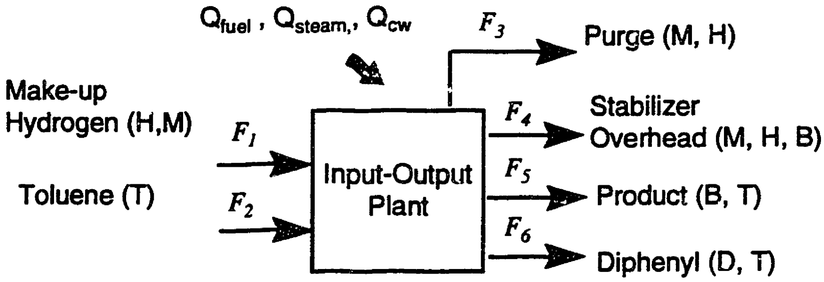
The energy balances are simply:

Reaction: $H_1 + H_2 + H_7 + H_{11} + H_9 + Q_{Fuel} = H_{10}$ [5-10]

Separation: $H_{10} + Q_{Steam\text{-}(b)} + Q_{cw\text{-}(b)} = H_4 + H_5 + H_6 + H_8 + H_{11} + H_9$ [5-11]

T-Junction: $H_8 = H_3 + H_7$ [5-12]

(a) Level 1: Input-Output Plant



(b) Level 2: Recycle Structure

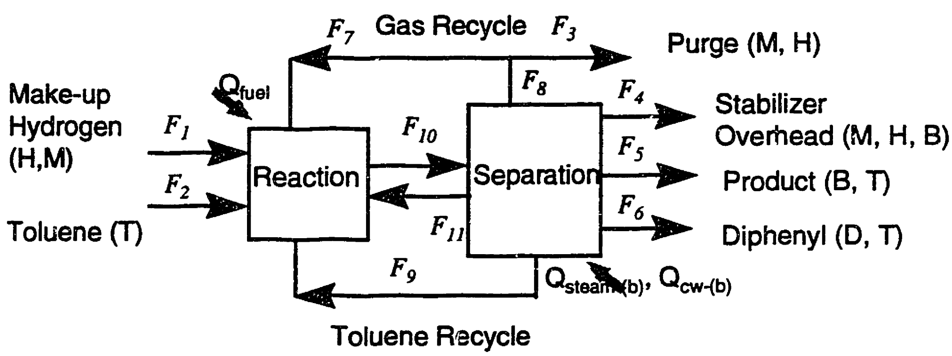


Figure 5 - 2: Coarse Viewpoints of the HDA plant

5.2.2 Quantifying Long-horizon Process Characteristics

When the chemical plant is described by a coarse viewpoint, the primary focus of the control system design is on the maintenance of the energy and material balances. Thus, we are interested in modeling how the accumulations of materials are affected by changes in the process variables. Component flows are the key variables in the material balances. A component flow can be varied by adjusting either the total flowrate of the stream or the composition of that component in the stream. The *steady-state gains* of the residuals of the balance equations are computed based on the procedure described below.

Computing the open-loop gain of the residual of a balance equation

Suppose a process block consists of a feed stream F_1 and two outlet streams F_2 and F_3. Additionally, a chemical reaction takes place such that:

$$i \rightarrow j \qquad [5\text{-}13]$$

Suppose perfect separation between i and j is achievable. Then, the following material balance can be written:

$$F_1 x_{1,i} = F_2 x_{2,i} + F_3 x_{3,j} \qquad [5\text{-}14]$$

where $x_{h,g}$ is again the composition of g in stream h. The residual of material i, r_i, in the process is simply given by:

$$r_i = F_1x_{1,i} - F_2x_{2,i} - F_3x_{3,j} \qquad [5\text{-}15]$$

At nominal steady-state, r_i should be zero. When the system is perturbed slightly by a small change in, say $\delta x_{2,i}$, with all other variables remain constant, the rate of change of the residual is simply:

$$\delta r_{i,x_{2,i}} = -F_2\delta x_{2,i} \qquad [5\text{-}16]$$

where the second subscript of δr signifies the type of perturbation made. Similarly, the rate of change of the residual for a change in the flow, say F_3 would be:

$$\delta r_{i,F_3} = -x_{3,i}\delta F_3 \qquad [5\text{-}17]$$

The rate of change, $\delta r_{i,k}$, can be regarded as the *open-loop integrating gain* of the residual of the balance equation for material i for a perturbation in k . The use of this terminology is further explained in Section 5.3.1 and is based on the work by Arkun et al. (1990).

Scaling Process Gains

From the discussion above, it is easy to see that the size of $\delta r_{i,k}$ is a function of the size of the perturbation δk. Hence, perturbation gains are scale dependent. To ensure a fair comparison can be made, the perturbation gains must be properly scaled. The scaling guidelines are as follows:

1. For a flowrate manipulation (such as perturbing F_3), if the size of the valve of that stream is known, we compute $\delta r_{i,F_3}$ for a 1% change in valve position, otherwise, we take a 1% change of the flow from its nominal value.
2. For a composition manipulation, such as a change in $x_{2,i}$, we compute $\delta r_{i,x_{2,i}}$ for a 1% change in the original value of the composition.

The important thing is to ensure that $\delta u/u$ stays constant for any u, where u is a potential manipulated variable in the system.

Note that if the stream valves of a process have not been installed, when scaling has been properly done, $\delta r_{i,x_{j,i}}$ equals $\delta r_{i,F_j}$ and both values measure the impact of the variation of the flow of component i in stream j on the residual of the balance equation for i. If the stream valves of the process have not been installed, flow changes are the only direct manipulations. Note that if the compositions of a stream are externally defined (such as a feed stream), stream compositions are not process manipulated variables so $\delta r_{i,x_{j,i}}$ of the components do not exist. One must compute $\delta r_{i,F_j}$ to estimate the effect of varying individual component flows on the system.

5.2.3 Uncertainty in Models for Long-horizon Analysis

The analytical forms of the material and energy balances describing the coarse process viewpoints can be fully determined. However, uncertainty in the open-loop process gains can arise from the variations of the compositions of materials in the process streams. For example, $x_{1,i}$ in equation [5-14] could be the composition of material i of the feed stream. This composition may vary according to the upstream condition. Then, the open-loop gain of the residual of i in the real system, i.e. $\delta r_{i,F_1}$ would vary as well and there is modeling uncertainty associated with the gain computed from the nominal material balance. When the steady-state operating point changes, both the flows and compositions of many streams in the process will change as well, introducing another source of model uncertainty. Furthermore, static gains are not constants for processes which are not time-invariant. The magnitudes of the gains may change as a result of process change. If the process is non-linear, the magnitudes of the static gains may only be valid in the vicinity of the region in which the model had been obtained, even though the process could be time-invariant. As the quality of the control system design is strongly dependent on the reliability of the models which we use to describe the process behavior, knowledge of the expected variations in the gains would allow the quantification of the amount of uncertainty associated with the models and hence the introduction of robustness in the design. In Chapter 6, the utilization of model uncertainty for the synthesis of process control structures will be discussed.

5.3 Modeling the Process for Short-Horizon Analysis

At the hierarchical strata which are represented by more elaborated process description, the dynamics in the plant become observable and must be incorporated into the process models used in control structure synthesis.

The complex dynamics of most chemical processes is a result of the combined effects of various dynamic and steady-state elements in the plant. Detailed dynamic modeling of a plant based on a set of differential and algebraic equations describing the physico-chemical behavior is an extremely intensive engineering task. Often, the engineer has to deal with an incomplete set of modeling parameters. The resulting input-output model may also not necessarily be suitable for making a number of decisions related to the design issues of plant control structures. It is recommended in this research that an evolutionary approach be used for the modeling of process dynamics. By modeling the different aspects of process dynamics separately, decisions that are associated with different aspects of process dynamics can be made explicitly at different design stages. Such a gradual introduction of dynamic aspects into the modeling of a plant represents an approach that is feasible and guided and relevance-oriented.

In the next few sections, the various dynamic aspects in the plant that are of relevance to control structure synthesis will be discussed.

5.3.1 Process Integrating Elements

If a plant consists of one or more integrating elements, some outputs will exhibit integrating behavior to perturbation of some process inputs. An integrating process is one which cannot balance itself and has no natural equilibrium or steady-state. If the inflow of mass or energy deviates from the outflow even by a very small amount, some of the outputs will grow linearly with time in an unbounded fashion. Thus, an integrating process is *non-self-regulating*. The usual steady-state gains for these process are therefore undefined. In linear system theory, a process which contains integrator(s) has one or more poles in the origin.

Integrators are very common in chemical processes. These elements are typically associated with storage tanks whose outflows are not dependent on the amount of the materials in the tanks, examples include: continuous stirred-tank reactors, flash drums, bottoms of separation columns, condensers of distillation columns, etc. Since flow measurements and flow actuators in field are never perfect. The inflows and outflows of an integrating process can never be set manually to be at the same value so an integrating process cannot be left unattended and a feedback control scheme must be utilized to maintain the inventory of mass or energy to be within some desired bounds at all times. For this reason, the control of the integrators in the plant are one of the highest priorities in the hierarchy of process objectives under dynamic consideration.

In general, a *pure* integrating process can be described by:

$$g(s) = \frac{g_i}{s} \qquad [5\text{-}18]$$

The output increases in a ramp with a slope of g_i (in the output-time plot) for a step change in the input. Arkun and Downs (1990) called g_i the *integrator gain*. Next are several formal statements concerning integrating systems, based on some definitions given in Arkun and Downs (1990).

Definition 5-1 (from Morari and Zafiriou, 1989)

Let $g(s)$ be the open-loop scalar transfer function and let m be the largest integer for which:

$$\lim_{s \to 0} s^m g(s) \neq 0 \qquad [5\text{-}19]$$

Then, the system $g(s)$ is said to be type m. A type m system has m poles at the origin.

Definition 5-2 (from Arkun and Downs, 1990)

A type m system can be expanded into the following form:

$$g(s) = \sum_{i=1}^{m} \frac{g_i}{s^i} + \tilde{g}(s) \qquad [5\text{-}20]$$

where the constant g_i is called the i^{th} *order integrator gain* of $g_i(s)$ and $\tilde{g}(s)$ is called the *non-integrating gain* of $g(s)$.

Definition 5-3 (from Arkun and Downs, 1990)

Let $G(s)$ be an $n \times n$ transfer matrix with m poles at the origin. Then:

$$G(s) = \sum_{i=1}^{m} \frac{G_i}{s^i} + \tilde{G}(s) \qquad [5\text{-}21]$$

where the constant matrix G_i is called the i^{th} *order integrator gain matrix* of $G(s)$ and $G(0)$ is called the *non-integrating gain matrix* of $G(s)$.

According to Definition 5-3, for a MIMO system with $m = 1$, the transfer function matrix $G(s)$ has the following general form:

$$G(i,j)(s) = \frac{G_1(i,j)}{s} + \tilde{G}(i,j)(s) \qquad [5\text{-}22]$$

$\tilde{G}(i,j)$ is stable if the system is stable except for the non-self-regulating integrators (Arkun and Downs, 1990). Hence, for a unit step change in the j^{th} input, after a sufficiently long time, the i^{th} output will asymptotically follow a ramp with slope equal to the integrator gain $G_1(i,j)$. The time response of several process outputs can be found in Figure 5-3. Line (a) represents a pure integrator such that $\tilde{G}(0) = 0$; curve (b) is another integrating process but $\tilde{G}(0) \neq 0$; curve (c) is a self-regulating output and $G_1 = 0$. Hence, if an output is affected by integrator(s), after some period of time, the time-response of that output is solely determined by the magnitude of the integrator gain. Thus, the sensitivity of an integrating outputs to different inputs for "large time" can be determined in much the same way they were determined for self-regulating processes at steady-state (Arkun and Downs, 1990). The size of the integrator gain is equivalent to the slope of the output-time response curve and can be easily measured from a plot of the time response, generated by conducting a simulation experiment on the plant and perturb the process inputs. A large integrator gain means that a small change in the input has a strong effect on the output. So integrator gains can be interpreted similarly as steady-state gains.

A procedure developed by Arkun and Downs (1990) for the analytical computation of integrator gains based on state-space models is given below.

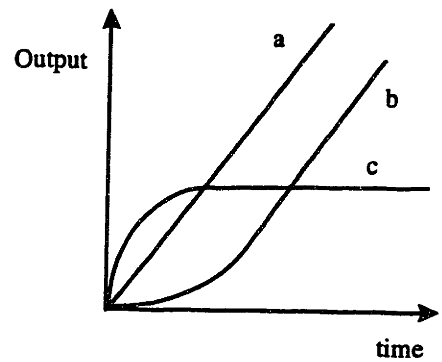


Figure 5 - 3: Step responses of several outputs (a) pure-integrator; (b) integrating; (c) self-regulating (from Arkun and Downs, 1990)

Computing Integrator gains based on state-space process description

For a system with the following state-space description and transfer function matrix:

$$\dot{x} = Ax + Bu \qquad [5\text{-}23]$$

$$y = Cx + Du \qquad [5\text{-}24]$$

and

$$G(s) = C(sI - A)^{-1}B + D \qquad [5\text{-}25]$$

Arkun and Downs (1990) have shown that the first order integrator gain matrix of $G(s)$ can be computed from:

$$G_1 = C\left[I - U\begin{pmatrix} I \\ 0 \end{pmatrix}\left[V^T U\right]_r^{-1}\begin{pmatrix} I & 0 \end{pmatrix}V^T\right]B \qquad [5\text{-}26]$$

and U and V are obtained from single value decomposition of A such that:

$$A = U\Sigma V^T \qquad [5\text{-}27]$$

where U is an $n \times n$ orthogonal matrix of the eigenvectors of AA^T , V is an $n \times n$ orthogonal matrix of the eigenvectors of A^TA, and Σ is an $n \times n$ diagonal matrix:

$$\Sigma = \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} \qquad [5\text{-}28]$$

where Σ_r is an $r \times r$ diagonal matrix whose elements are the non-zero singular values of A. Then, $[V^TU]_r$ in equation [5-26] is the first $r \times r$ block of the $n \times n$ matrix V^TU.

For prove of this and the computation of higher-order integrator gains from state-space models, refer to Arkun and Downs (1990).

5.3.2 Process Deadtime

In chemical processes, deadtime commonly occur as a result of the transportation of mass and energy along the pipelength, producing *transportation lag* or *pure delay*. Deadtime can also result from lag caused by delay in output measurement. In a multicapacitor process that is composed of a large number of capacitors in series, the process output may also appear to lag the input, giving an *apparent deadtime* in the process. Even there is no explicit delay in the multicapacitor process, the initial response is often approximated by a pure deadtime.

Figure 5-4 gives the generic internal control structure such that $G(s)$ is the transfer function representation of the plant, $\tilde{G}(s)$ is the plant model and $G_c(s)$ is the internal model controller. Based on internal model control theory for linear systems, perfect control depends on the invertibility of the process (Morari and Zafiriou, 1989). Under perfecting modeling assumption, $\tilde{G}(s) = G(s)$. The closed-loop response of the output is given by:

$$y = GG_c(y_{sp} - d) + d \qquad [5\text{-}29]$$

where y and y_{sp} respectively represent the vectors of outputs and setpoints, d is the vector of process disturbances. The dependence on frequency have been omitted in the presentation for brevity. It has been shown (Morari and Zafiriou, 1989) that perfect control can be achieved if the controller is set to be the inverse of the process, i.e.

$$G_c = G^{-1} \qquad [5\text{-}30]$$

Many processes may contain elements which are noninvertible, making Equation [5-30] a non-achievable stipulation. By factoring the process into an invertible part G_- and a noninvertible (i.e. non-causal) part G_+, i.e.:

$$G = G_+ G_- \qquad [5\text{-}31]$$

such that G_-^{-1} is stable, causal and invertible, and by setting:

$$G_c = G_-^{-1} \qquad [5\text{-}32]$$

the closed-loop transfer function is simply:

$$y = G_+(y_{sp} - d) + d \qquad [5\text{-}33]$$

This expression clearly indicates that the non-invertible part of the process determines the closed-loop performance of the control system.

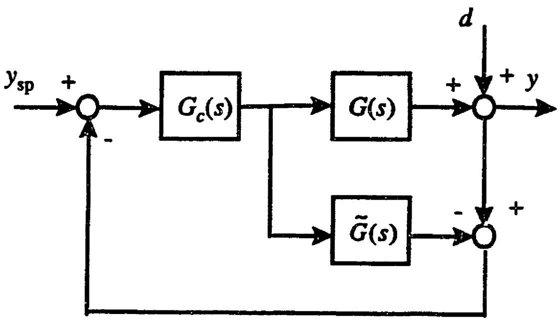


Figure 5 - 4: The Internal Model Control Structure

The inversion of deadtime makes the system non-causal, and therefore unstable; a process with deadtime is non-invertible. For single-input, single-output systems, the detrimental effect of deadtime has been found to increase monotonically with its magnitude. For multi-input, multi-output systems, not only are the magnitudes of the deadtimes important, but also their distribution within the transfer function matrix (Holt and Morari, 1985). Thus, processes with large deadtimes create problems in control. Hence, deadtime can serve as a rough indicator of the achievable quality of control. When delays of isolated process outputs are significant, it suggests the possibility of decomposition between connected parts of a process for decoupled control considerations.

Knowledge of the size of the process deadtime helps the designer to determine if the design of control strategies for certain section of the plant can be isolated from the rest of the plant due to the presence of a large deadtime. Furthermore, based upon the size of the deadtime, the designer can identify those inputs that are more suitable to be used as manipulated variables.

It is relatively straight forward to measure the deadtime in the process as it is simply the time it takes for the output to first respond to changes in the input. Deadtime can be easily taken from a plot of input and output versus time such as the one shown in Figure 5-5. Such a plot can be generated from either a dynamic simulation of the process or based on historical plant data, if available. Very often, the magnitude of the deadtime in the process can be estimated from our understanding of the physical process. Transportation lag can be estimated if the average flow rate, the lengths of the pipes through which the material travels and the residence times of the materials in the process units through which it passes are known. Delays caused by lags in measurements are usually known exactly. Apparent deadtimes caused by multiple capacitors in series have to be determined experimentally (through computer simulation or based on input-output plant experiments).

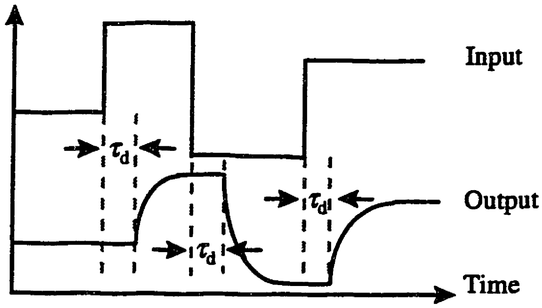


Figure 5 - 5: Measuring Process Deadtime

5.3.3 Dominant Time Constants

The speed at which inventory of mass, energy or inertia can change is indicated by the capacity of the process. Generally, chemical processes are composed of more than one process capacitors, usually arranged in series or in parallel. The overall response corresponds to the compounded dynamics between the manipulated variable and controlled variable. The dominant time constant can be thought of as the time constant of the slowest sub-process in the system. Being the slowest sub-process, it has the largest time constant so it roughly characterizes the time it takes for the effects caused by the manipulated variable to complete. In fact, the experience from the process industry is that most processes can be modeled with reasonable faithfulness by a combination of deadtime and capacitor (Shinskey, 1988):

$$y(s)=\frac{\hat{K}e^{-\hat{\theta}s}}{(s+\hat{a})}u(s) \qquad [5\text{-}34]$$

The deadtime element captures the combined effects of pure delay and apparent delays produced by capacitors in series. The capacitor of the model defines a characteristic time constant which define the shape of the output response in a crude manner. The resulting model serves as a good indicator of the general process trend.

Controlling the process with a slow input would require moving the input quickly and with bigger action. With the incorporation of time constant in the model, a finer scale is given to the designer to model to discriminate inputs which change the process slowly from those which change the process quickly.

5.3.4 Inverse Response

Inverse response, often known as *non-minimum phase* behavior, is associated with the inherent characteristic of the plant. Due to the presence of two opposing forces running in parallel that response at different speeds, in opposite directions and produce different gains on the output, the output of the process will initially move in a direction opposite to where it eventually ends up, for step changes in the input. The ultimate response of the output is determined by the sub-process which produces a higher gain on the output but the initial speed and direction are induced by the faster sub-process.

For SISO systems, in terms of terminology for linear systems, inverse response indicates the presence of an odd number of right-half plane (RHP) zeroes in the process (see Figure 5-6). Since inversion of a SISO system with RHP zeroes generates RHP poles, RHP zeroes are non-invertible elements. Hence, RHP zeroes also limit the closed-loop performance of the system. Zeroes are invariant under state and output feedback, they must simply be tolerated (Kwakernaak and Sivan, 1972). Perfect feedback control is unrealizable for systems with RHP zeroes. The output must deviate from its setpoint for a certain period of time. Under the assumption of no modeling error, Frank (1974) found that the integrated squared error of the output response under optimal control to be a function of the RHP zeroes:

$$\mathrm{ISE} = \sum_{i=1}^{m} \frac{2}{z_i} \qquad [5\text{-}35]$$

where z_i is the RHP zero. Thus, zeroes which are close to the origin lead to greater loss than those far away. Systems with zeroes at the origin are structurally uncontrollable (Holt and Morari, 1985).

The existence of RHP zeroes and the number of RHP zeroes that are present in the SISO system can be easily determined based on the shape of the output response (recall Figure 5-6). Using input-output data obtained from the open-loop step tests (either from plant experiment or computer simulations), the location of the RHP zeroes can be determined by fitting the data set to a model of the following form:

$$y(s) = \frac{\hat{K}(-s+\hat{z})e^{-\hat{\theta}s}}{(s+\hat{a})(s+\hat{b})}u(s) \qquad [5\text{-}36]$$

where $\hat{K}$, $\hat{\theta}$, $\hat{a}$, $\hat{b}$ and $\hat{z}$ are model parameters. The model described by equation [5-36] is suitable for describing a process with one RHP zero. For processes with more than one RHP zeroes, the number of lead-lag elements in the model must be increased appropriately.

By incorporating RHP zeroes in the model, we have increased the precision of the modeling. The process response is being described by a model with higher level of details. The RHP zeroes, together with the deadtime, define all the non-invertible elements in the plant and they allow the identification of manipulated variables which the best achievable closed-loop performance.

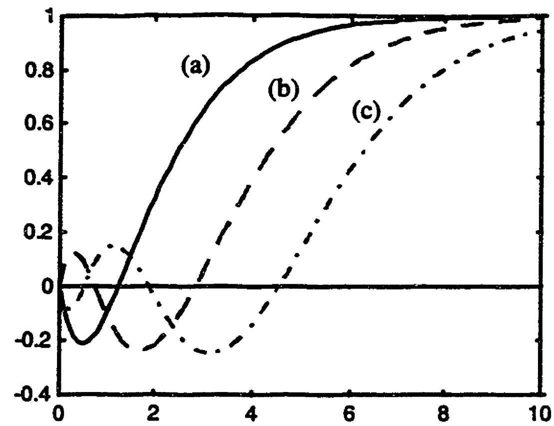


Figure 5 - 6: Response of $\frac{1}{(s+1)}\left(\frac{-s+1}{s+1}\right)^i$ (a) $i = 1$; (b) $i = 2$; (c) $i = 3$ (from Holt and Morari, 1985)

Multivariable zeros are located at frequencies such that the overall multivariable system exhibits characteristics similar to those we have described for the SISO system. These are called right-half plane transmission (RHPT) zeroes. MacFarlane and Karcanias (1976) defined transmission zeroes to be those values of s for which the rank of $G(s)$ drops below its nominal rank. Numerical software packages such as MATALB™ will also compute the RHPT zeroes given $G(s)$. A procedure for the computation of RHPT zeroes of a transfer function matrix $G(s)$ is given in Maciejowski (1989).

5.3.5 Higher-order Dynamics

At the detailed level of process representation, higher-order dynamics that are neglected in a simple first-order plus dead-time model or in a simple inverse response process model should be included. Higher order-dynamics can be captured by increasing the order of the model until the required precision of the output response is established. Using plant input-output data, the additional parameters in a model which includes higher order dynamics can be estimated.

5.3.6 Uncertainty in Models for Short-horizon Analysis

Dynamic models developed based on a nominal operating point are prone to error primarily because a number of dynamic aspects in the model are functions of the flow rate of the material. Examples of dynamic elements which are dependent on process flow rate include:

- deadtime caused by transportation lag
- time constants which measure the size of the capacitors

Furthermore, in a reaction medium, the time constant is influenced by the rate of reaction. In an energy transfer medium, the time constant is influenced by the rate of heat transfer which could be function of fouling and other physical state of the system. Similar sources also cause variation in the model parameters of an inverse response process as inverse response is simply a result of sub-processes running in parallel. Similarly, parameters which define the higher-order dynamics in the process could contain error for similar reasons as well. Thus, the time constant, gain and deadtime of the individual sub-process may change as a result of changes in the process conditions which affect the parameters that define an inverse response.

The amount of uncertainty associated with the model parameters should be quantified whenever it is possible to do so. The utilization of such information for control system design will be discussed in Chapter 6.

5.4 A Consistent Modeling of Process Behavior

Figure 5-7 summarizes a hierarchy of analytical models which are representations of the process in the *time-domain*. These models are useful at various stages of control structure synthesis. For non-integrating processes, the most primitive information about the process is its static gain. Next, the quality of the transmission of information can be roughly captured by the dominant time constant of the process. Additional details are revealed with the knowledge of the sub-processes which produce inverse response. Finally, the higher order dynamics are included in the model to improve the accuracy of the process description. Notice that simpler models capture characteristics of a larger space and time and are more suitable for performing analysis on the abstract views of the plant. More complex models describe process details of a finer time-span, so they are more suitable for addressing the control tasks at the detailed plant representations. This hierarchy of models matches with the hierarchies of process representations and time-scales introduced in Chapter 3.

While developing distinct process models for different resolutions to capture various aspects of process behavior, care must be taken so that the models are consistent with each other. Thus, it is important to provide consistent descriptions of process trends at various levels, e.g. from long-horizon description to short-horizon characterization. A dynamic model may describe the process behavior during transient. This dynamic model should agree with the corresponding long-horizon static description at time equals infinity.

The concept of multi-scale consistent modeling can be applied to ensure consistency in process modeling. In the next section, basic concept of multi-scale systems theory for process modeling will be discussed. This will be followed by a discussion of how multi-scale systems theory can be utilized to construct process models which are consistent at various time-horizons.

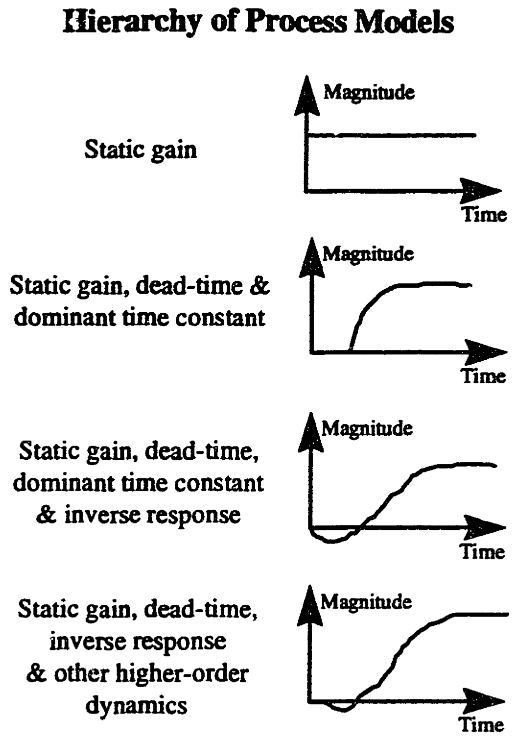


Figure 5 - 7: The Hierarchy of Process Modeling Needs for Control Structure Synthesis

5.5 Multi-scale Systems Theory

Research has shown that multi-scale models of processing systems offer an attractive alternative to the conventional models in the time or frequency domain for process simulation, estimation and control. The basic principles of multi-scale systems theory discussed in this section is based on research by Stephanopoulos (1996). In general, multi-scale systems theory provides a set of principles for describing a system at different time resolutions by enabling the construction of a set of consistent models to describe the process at a different resolution, a means to relate models and states at different time-resolutions, and consistent definitions regarding the notions of transfer functions, stability, controllability and observabilty in dynamic systems. Furthermore, Stephanopoulos (1996; 1997) have found that application of multi-scale systems theory reduces exaggeration of model uncertainty when projecting long-horizon process behavior using a model developed at very fine time-scale and prevents aliasing effect in models developed based on data collected over a large sampling interval.

5.5.1 Defining a Process on a Binary Tree

Figure 5-8 shows how a binary tree is utilized to represent the values of the states of a system at different model scales. At the zeroth level, the states of the process are sampled at an interval of T, the smallest possible sampling period. The vector of n states $[x_0\ x_1\ x_2\ \ldots\ x_{k-3}\ \ x_{k-2}\ x_{k-1}\ x_k\ x_{k+1}\ x_{k+3}\ \ldots\ x_{n-1}]$ at the zeroth level over a period of time $(n-1)T$ represents the progression of the process in time. At a more regressed model scale, such as Level -1, the process is described by a vector of $n/2$ states, each node represents the *state* of the process over a time period of $2T$. At each reduction of model scale, the resolution of the model reduces by one half. The existence of formal relationships among states of models at different scales allows the representation of the set of scaled model on a binary tree. Defined on trees, multi-scale models capture the essential features of the systems' dynamic behavior, localized in time and scale.

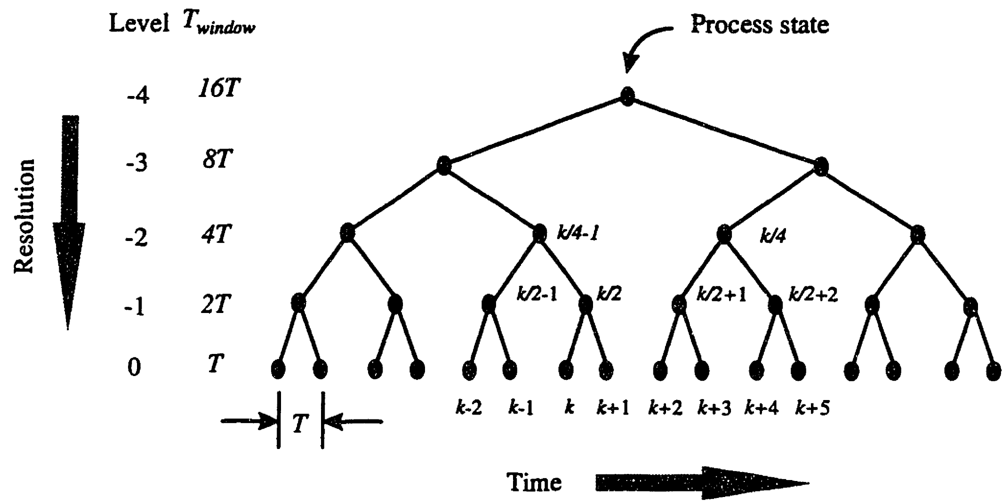


Figure 5 - 8: Process States represented on a Binary Tree

For a first order homogeneous system sampled at an interval of T (Level 0) and described by:

$$x_{k+1} = Ax_k \quad [5\text{-}37]$$

where A is some state transition matrix. Stephanopoulos (1996) has shown that the following relationships are true:

$$x_{k+1} = A(Ax_{k-1}) = A^2 x_{k-1} \quad [5\text{-}38]$$

$$x_k = A(Ax_{k-2}) = A^2 x_{k-2} \quad [5\text{-}39]$$

Adding [5-38] and [5-39] gives:

$$x_{k/2} = A^2 x_{k/2-1} \quad [5\text{-}40]$$

where:

$$x_{k/2} = \tfrac{1}{2}(x_k + x_{k+1}) \quad [5\text{-}41]$$

$$x_{k/2-1} = \tfrac{1}{2}(x_{k-1} + x_{k-2}) \quad [5\text{-}42]$$

Equation [5-40] is a model of the system at Level -1. It describes the original process at Level 0 with a lower scale (lower resolution). Each state vector of the model in [5-40] captures the average behavior of the process over an interval of $2T$. Equations [5-41] and [5-42] denote the Haar-averaged state of the system over the expanded discretization interval (Stephanopoulos, 1996). States $x_{k/2}$ and $x_{k/2-1}$ are two consecutive samples at Level -1. Models at even lower resolution can be developed based on Equation [5-40], in terms of a state representation over an interval that is some multiple of T, specifically 2^nT, where n corresponds to the level of resolution.

The relationships among the states at various time and at various model scale have been indicated on the binary tree in Figure 5-8. The index $k/2$ represents states which correspond to a process description whose resolution is half of the highest resolution. The notation $x^{(-m)}_{\frac{k}{2^m}-i}$ can be used to describe the i^{th} sample of a model at the $-m^{th}$ scale. Alternatively, we can let x_k^{-n} to represent any arbitrary state vector k at Level $-n$. The scaled model at Level $-n$ of a 1st order homogeneous system is simply:

$$\text{Level } -n \quad x^{(-n)}_{k+1} = A^{2^n} x_k \qquad [5\text{-}43]$$

Relationships which describe the models in time at different scales for higher order systems can be developed. For example, the set of relationships between model at Level 0 and model at Level -1 for the 2nd and 3rd order systems are simply:

$$\begin{aligned} &\text{Level } 0 \quad x^{(0)}_{k+1} = Ax_k + Bx_{k-1} \\ &\text{Level } -1 \quad x^{(-n)}_{k+1} = (A^2 + 2B)x_k + (-B^2)x_{k-1} \end{aligned} \qquad [5\text{-}44]$$

and

$$\begin{aligned} &\text{Level } 0 \quad x^{(0)}_{k+1} = Ax_k + Bx_{k-1} + Cx_{k-2} \\ &\text{Level } -1 \quad x^{(-n)}_{k+1} = (A^2 + 2B)x_k + (2AC - B^2)x_{k-1} + C^2 x_{k-2} \end{aligned} \qquad [5\text{-}45]$$

respectively. In all cases, multi-scale theory preserves the order of the system during scale reduction.

Figure 5-9 shows the response of the scalar process: $x_{k+1} = 0.4x_k$; $x_0 = 5$ computed using models of different scales. Model predictions based on models of higher scale follow closely the trajectory of the states at the finest model scale.

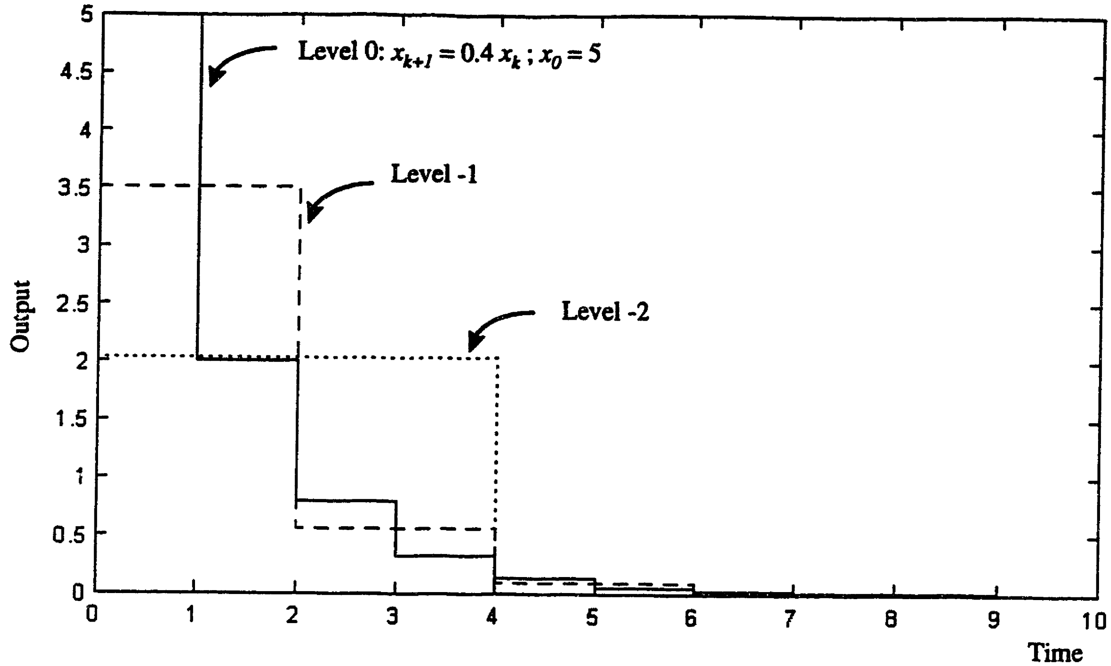


Figure 5 - 9: Representation of a 1st homogeneous system at different model scale

5.5.2 Relationships Between States on a Binary Tree

An important component of the formalism for multi-scale modeling is the relationship which exists among states at different scales on the binary tree. Stephanopoulos (1996) have shown using Equation [5-37] through [5-43] that states for a 1st order homogeneous system at Level -1 are related to those at Level 0 by (refer to Figure 5-8):

$$\begin{aligned} x_{k+1} &= 2(I + A)^{-1} A x_{k/2} \quad \text{right node} \\ x_k &= 2(I + A)^{-1} x_{k/2} \quad \text{left node} \end{aligned} \qquad [5\text{-}46]$$

Equations in [5-46] indicate that we can define the evolution of the state of a system on a binary tree, each node of which captures the value of the state at a give time-interval and a given time-scale.

Figure 5-10 to defines the convention used to describe the directional shift from a state at a lower level to a higher level. For a general tree node ρ, the following relationships are true:

$$\begin{aligned} x_\rho &= A_\alpha \bar{\alpha} x_\rho + A_\beta \bar{\beta} x_\rho \\ x_\rho &= A_\alpha x_{\rho\bar{\alpha}} + A_\beta x_{\rho\bar{\beta}} \end{aligned} \qquad [5\text{-}47]$$

where $\bar{\alpha}$ and $\bar{\beta}$ are shift operators which define upward or downward movement in the tree, A_α and A_β are coefficients which are functions of the model parameters describing the model at the level corresponding to the tree node ρ. A_α is simply $2(I+A)^{-1}$ for a 1st order homogeneous system. For any given ρ, only one of the $\rho\bar{\alpha}$ and $\rho\bar{\beta}$ exists. Therefore, in [5-47], only one of the terms on the right-hand side is non-zero. Generalizing [5-47] to a n^{th} order system, the tree node ρ is simply given by:

$$x_\rho = A_1 x_{\rho\bar{\gamma}} + A_1 x_{\rho\bar{\gamma}^2} + \cdots + A_n x_{\rho\bar{\gamma}^n} \qquad [5\text{-}48]$$

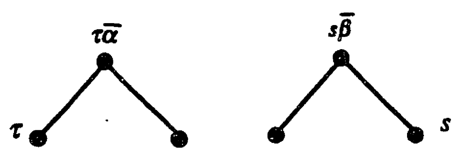


Figure 5 - 10: Directional Shift from a State at a Lower level to a Higher level

5.5.3 Scaling Forced Dynamical Systems

The formalism presented above can be extended to forced dynamical systems. For a 1st order forced system sampled at an interval of T:

$$x_k = Ax_{k-1} + Bu_{k-1} \qquad [5\text{-}49]$$

The model at the next lower scale where each state represents the process over an interval (T_{window}) of $2T$ has been found to be described by:

$$x_{k/2} = A^2 x_{k/2-1} + (I + A)Bu_{k/2-1} \qquad [5\text{-}50]$$

where $u_{k/2-1}$ is the averaged value of the input, given by the following averaging scheme:

$$u_{k/2-1} = 1/2(I + A)^{-1}\{Au_{k-2} + (I + A)u_{k-1} + Iu_k\} \qquad [5\text{-}51]$$

The averaging scheme in [5-51] is model-dependent (see the presence of A).

In general, at Level $-n$:

$$x_{k+1}^{-n} = A^{2^n} x_k + (I + A)(I + A^2)\cdots(I + A^{2^{n-1}})Bu_k \qquad [5\text{-}52]$$

Thus, the dynamics of a linear forced system can be described by any scale through a linear system. Note that for the system described by [5-52], if all eigenvalues of A is less than unity, then at some n, $|A^{2^n}| \to 0$. It has been shown by Stephanopoulos et al. (1996) that:

$$x_{ss} = (I - A)^{-1}Bu_{ss} = Ku_{ss} \qquad [5\text{-}53]$$

where x_{ss} is the value of the state at steady-state, u_{ss} is the input at steady-state and K is simply the process gain of x for a step change in u. Thus, as the scale incrases, the value of the state given by [5-52] approaches the steady-state value.

Stephanopoulos (1996) has shown that the following multi-scale models can be generated from the discrete time model of Equation [5-49]:

$$\begin{aligned} x_{k+1} &= 2(I+A)^{-1}Ax_{k/2} + (1+A)^{-1}Bu_k \\ x_k &= 2(I+A)^{-1}x_{k/2} - (1+A)^{-1}Bu_k \end{aligned} \qquad [5\text{-}54]$$

In general, for a 1st order process with delay that is described by:

$$x_{k+1} = Ax_k + Bu_{k-p}\ ; \quad p \geq 0 \qquad [5\text{-}55]$$

for a time scale of T. The model at time scale $2T$ is:

$$\begin{aligned} x_{k/2} &= A^2 x_{\frac{k}{2}-1} + (I+A)Bu^R_{\frac{k}{2}-1-\frac{p}{2}} \quad \text{for } p = 0, \text{even} \\ x_{k/2} &= A^2 x_{\frac{k}{2}-1} + (I+A)Bu^L_{\frac{k}{2}-1-\frac{p-1}{2}} \quad \text{for } p = \text{Odd} \end{aligned} \qquad [5\text{-}56]$$

where the superscripts R and L denote two scaling processes (see Stephanopoulos, 1996 for details).

5.5.4 Properties of Multi-scale Systems

In the pervious section, the dynamic relationship among the states at different scales has been demonstrated (Equations [5-48] and [5-54]). These relationships imply a binary tree, which can be seen as the domain for the definition of process dynamics. Any dynamic system defined in a set of time points can be transformed into a dynamic system defined on the nodes of a binary tree. Benveniste et al. (1990) have shown that this tree is a homogeneous tree and possesses certain interesting isometries which allow the rigorous definition of a distance between two nodes, which is essential in the definition of shift operators on the tree (such as $\overline{\alpha}$ and $\overline{\beta}$ in Equation [5-47]). Using these shift operators, Stephanopoulos (1996) has shown the following properties for the multi-scale system of Equation [5-52]:

1. Steady-state

   As the scale increases, the value of the state given by [5-52] approaches the steady-sate value of $(I-A)^{-1}B$.

2. Stability

   If the dynamic system (Equation [5-49]) is stable (strictly stable), so is the multi-scale system of [5-52], and vice versa. Therefore, the value of the state at any node of the binary tree is bounded or/and approaches a steady state as it moves upward on the tree.

3. Controllability

If the system [5-49] is controllable, so is the multi-scale system [5-52] independently of whether the final state is at a higher scale (upward controllability) or a lower scale (downward controllability) with respect to the initial state.

4. Observability

If the system [5-49] is observable with the output equation $y_k = Cx_k$, so is the multi-scale system [5-52]. However, the measurement structure for a multi-scale system may involve measurements at different sampling intervals. In such cases, the output equation can be written as $y(t) = C^* x(\tau)$ where C^* defines the measurement structure at the scale of the node, τ. Observabilty is guaranteed at each level if and only if the corresponding observability gramian is invertible. Thus, there is a significance difference in the ability to observe a system's dynamics as we move upwards or downwards on the tree, i.e. observability of a coarser state is always guaranteed by the available measurements at the finest scale under consideration, while the observabilty of the finer states from data at larger scales requires specific measurement structures, expressed by C^*.

5.6 From Steady-State Description to Dynamic Characterization

In the hierarchical framework, process behavior is being analyzed through a series of process viewpoints, from coarse process representation to detailed process description. Earlier in Section 5.2, long-horizon process characteristics are essentially represented by static process models. Supposed an output y, representing the state of the process, is related to a manipulated variable u at steady-state through the following relationship:

$$y = Ku \qquad [5\text{-}57]$$

and for a unit change in u, y is at $y_{ss} = K$. K is simply the process gain.

Based on the multi-scale systems theory and Equation [5-57], K is the average value of the output to a unit step change in u, $\bar{y}$, over a very long period of time, say T^* as illustrated in Figure 5-11. On the binary tree, the average output value over the infinite horizon represents the top of the tree at Level $-\infty$ as shown in Figure 5-12. At each step of increment of model resolution, the process response represented is obtained by computing average output values over a time horizon that is half of the time horizon used at the previous level. When the window over which each data is being averaged, i.e. T_{window}, is still relatively large, all data are very close to the steady-state value and there is no advantage in incorporating dynamic characteristics in the process trend. Expansion of the binary tree is only carried out along the left node. At some level of model scale (such as Level $-m$-1), where the first data represents the average value of the output over a time period of $t_{dynamic}$, the deviation of the first data (which represents the average value of the output from $t = 0$ to $t_{dynamic}$) from the steady-state value becomes significant. Further increase in model resolution must incorporate the effect of the process dynamics. From this point onward, the binary tree expands from both the left node and right node.

In the sections that follow, a guideline which help to determine when the effects of process dynamics should be incorporated into the process description will be presented.

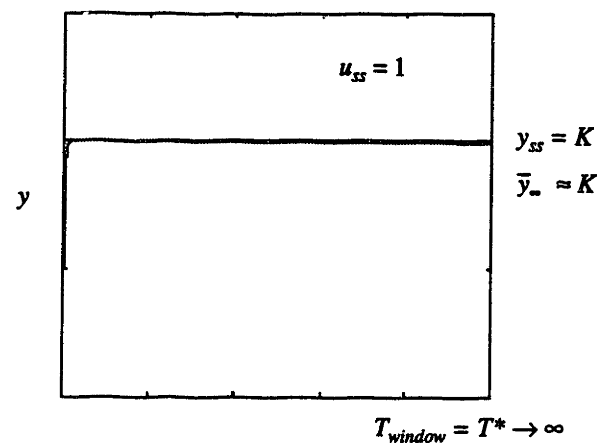


Figure 5 - 11: Process Response Curve over an Infinite Time Horizon

5.6.1 First Approximation of Process Dynamics

Given a real process described by:

$$y(s) = \frac{1}{10s+1} u(s) \qquad [5\text{-}58]$$

Assuming that the static gain has been accurately determined to be 1 unit at Level $-\infty$ such that the process is being modeled by:

$$y_k^{-\infty} = u_{k-1}^{-\infty} \qquad [5\text{-}59]$$

At some model scale level, the dynamic of the step response becomes significant and the model structure in [5-59] needs to be modified to incorporate the process dynamic characteristics. The time horizon over which we begin incorporation of model dynamics is $t_{dynamic}$.

It has been found that varying $t_{dynamic}$ may affect the quality of the dynamic model. Table 5-1 shows the 1[st] order approximations of the process in Equation [5-58] based step response data for different $t_{dynamic}$. A first order representation of the process is simply:

$$y_{k+1}^{-m} = \hat{a}^{-m} y_k^{-m} + \hat{b}^{-m} u_k^{-m} \qquad [5\text{-}60]$$

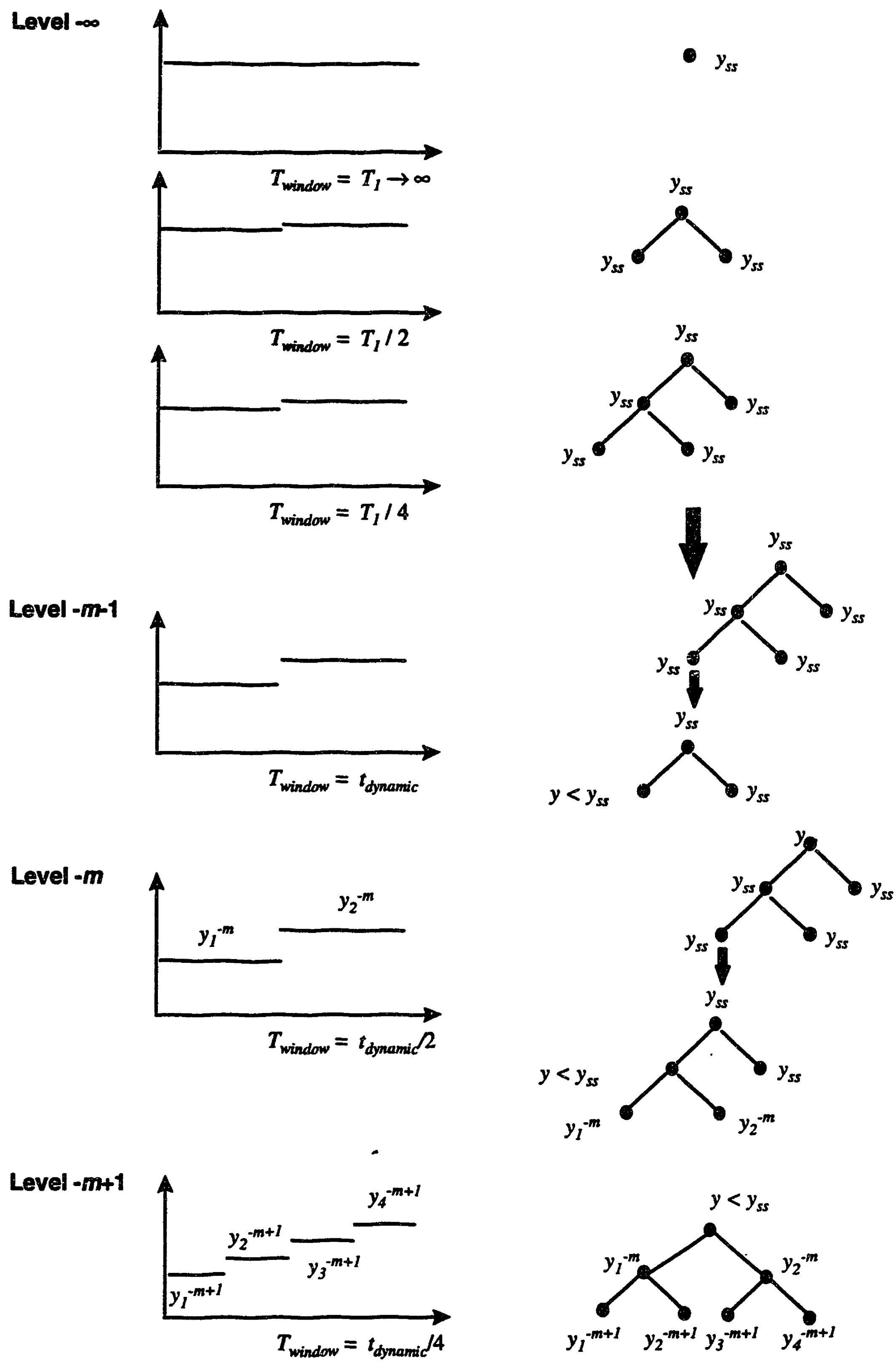


Figure 5 - 12: Expansion of Binary Trees at Different Model Scale

Table 5 - 1: First order approximation of Process in Equation [5-58] using various $t_{dynamic}$

$t_{dynamic}$	$\bar{y}_1^{-m}$	$\bar{y}_2^{-m}$	y_1^{-m-1}	$\hat{a}^{-m}$	$\hat{b}^{-m}$	Equivalent τ	%error	a^{-m}	b^{-m}
				(estimates)				(true values)	
150	0.8733	0.9999	0.9366	0.0008	0.9992	10.4977	4.98	0.0006	0.9994
140	0.8643	0.9999	0.9321	0.0007	0.9993	9.7047	-2.95	0.0009	0.9991
130	0.8539	0.9998	0.9269	0.0014	0.9986	9.8579	-1.42	0.0015	0.9985
120	0.8419	0.9996	0.9208	0.0025	0.9975	10.0343	0.34	0.0025	0.9975
110	0.8278	0.9993	0.9136	0.0041	0.9959	9.9903	-0.10	0.0041	0.9959
100	0.8111	0.9987	0.9049	0.0069	0.9931	10.0425	0.42	0.0067	0.9933
90	0.7911	0.9977	0.8944	0.0110	0.9890	9.9802	-0.20	0.0111	0.9889
80	0.7666	0.9957	0.8812	0.0184	0.9816	10.0147	0.15	0.0183	0.9817
70	0.7365	0.9920	0.8643	0.0304	0.9696	10.0154	0.15	0.0302	0.9698
60	0.6988	0.9850	0.8419	0.0498	0.9502	10.0009	0.01	0.0498	0.9502
50	0.6509	0.9713	0.8111	0.0822	0.9178	10.0062	0.06	0.0821	0.9179
40	0.5889	0.9444	0.7667	0.1352	0.8648	9.9967	-0.03	0.1353	0.8647
30	0.5076	0.8901	0.6989	0.2232	0.7768	10.0019	0.02	0.2231	0.7769
20	0.3990	0.7789	0.5890	0.3679	0.6321	10.0002	0.00	0.3679	0.6321

Each process model in Table 5-1 predicts the response of a process whose average output value is $\bar{y}_1^{-m}$ from time $t = 0$ to $t_{dynamic}/2$ and $\bar{y}_2^{-m}$ from $t = t_{dynamic}/2$ to $t_{dynamic}$. The rest of our discussion will employ terminology defined in Figure 5-12. Using Equation [5-49], [5-50] and [5-53], it can be shown that:

$$\hat{a}^{-m} = \frac{K - \bar{y}_2^{-m}}{K - \bar{y}_1^{-m}} \; ; \quad \hat{b}^{-m} = K(1 - \hat{a}^{-m}) \qquad [5\text{-}61]$$

To maintain *consistency* between the process static model and dynamic model, a constraint has been placed on the dynamic model such that the *process gain based on the dynamic model is equivalent to the process gain observed over the infinite horizon.* At $t = \infty$, the gain of the model in Equation [5-60] is the same as the process gain K. Note that uncertainty in the process gain would translate to the dynamic model as well. If the error bounds of the process gain are known, the limit of model uncertainty of the time constant for the first order approximation can also be computed. For example, in the process examined in Table 5-1 the process gain over the infinite horizon may only be known with an uncertainty of $\pm$ 0.005 unit. Then, using $t_{dynamic}$ = 60 time unit as the window over which we estimate the process dynamics, the estimated process time constant could vary from 8.5358 to 11.1869 time unit.

It can be seen from Table 5-1 that the error in the estimate of the τ of this first order system is large when $t_{dynamic}$ is large. The true process dynamics cannot be observed from y_1^{-m} and y_2^{-m} as their average value, y_1^{-m-1}, is relatively close to the steady-state value of the step change. Reasonable approximation can be obtained for cases whose $t_{dynamic}$ is between 6τ to 2τ. Although the illustration here is based on a true 1st order system that is free of uncertainty in data, similar exercises have shown that when y_1^{-m-1}, the average value of the output from $t = 0$ to $t_{dynamic}$, is about 85% of the value of the output at steady-state, a good first order approximation of the process can be obtained for other types of system by introducing process dynamic at Level *-m* (see the case studies in Section 5.7).

5.7 Evolutionary Modeling of Process Dynamics

Once we have reached the level at which the process dynamics is observable and significant, a dynamic model is required to describe the process trend. As one increases the level of the model resolution (i.e. lower the scale of the model), faster process dynamics will be exposed and the 1st order process approximation that we developed at Level *-m* may need to be updated. Incorporation of additional process dynamics will be done at a gradual manner so that we can separate dynamics that are relevant at different time scales. The creation of models at different scales which can sufficiently capture various process dynamics while maintaining consistency among models will be illustrated below.

5.7.1 Developing Dynamic Models in the Multi-scale Framework

In the multi-scale framework, due to the structure of the binary tree, model resolution increases by a factor of 2 as we move down one level of model scale. At Level *-n*, T_{window}^{-n}, the width of the window over which each data point represents, is 2^n times the length of the smallest sampling period. Then, for a process which can be sampled at a rate of 1 time unit, T_{window}^{-n}, the width of the window at Level *-n*, is simply $2^n \times 1$ time unit. Thus, the first step in developing a first order approximation of the dynamic process is to find Level *-m*-1 such that the first data for a representation of the step response, i.e. y_1^{-m-1} is approximately 0.85 of the steady-state value of the step change. Then, T_{window}^{-m-1}, i.e. 2^{m+1} (sampling period), is $t_{dynamic}$. At Level *-m*, we develop a first order dynamic approximation of the process response curve using data which covers the range from $t = 0$ to $t_{dynamic}$. The time span is the time span over which development of all dynamic models at all levels of details will be based upon.

Case 1: True Process is First Order

The order and structure of the process models developed according to the multi-scale systems theory are preserved. Thus, if the true process is first order, the process at any resolution can be derived based on the 1st order approximation obtained at Level *-m*-1 together with the relationship in Equation [5-60].

Let us study a process which is truly first order and has a time constant of 10 minute with a gain of 1. It will be assumed that the size of the process gain is known with certainty. Extension to process approximation with error in the process gain is straight forward. The process can be sampled at a rate of no faster than 1 minute. The dynamic model will be developed based on the process response curve to a step change of the input.

The first step in process modeling is to choose a time span $t_{dynamic}$. When modeling processes using the multi-scale systems theory, $t_{dynamic}$ must be a multiple of 2^n times the sampling period. Based on data in Table 5-1, $t_{dynamic}$ can be set to 64 min for the purpose of our analysis and this is Level -*m*-1. At Level -*m*, T^{-m}_{window} is 32 min. The resolution of the process response over $t_{dynamic}$ is described by two states: y_1^{-m} (0.7150) and y_2^{-m} (0.9884). The best first order approximation is given by (the symbol ^ indicating an estimate of a model parameter will be omitted in the rest of the presentation):

$$\hat{y}_k^{-m} = Ay_{k-1}^{-m} + Bu_{k-1}^{-m};\quad T^{-m}_{window} = 32\,\text{min};\ A = 0.0407;\ B = 0.9593 \qquad [5\text{-}62]$$

which has the following equivalent continuos model:

$$\hat{y}(s) = \frac{1}{9.9954s+1}u(s)\ (\text{gain} = 1) \qquad [5\text{-}63]$$

At Level -*m*+1, the model of the next higher resolution has the structure:

$$\hat{y}_k^{-m+1} = ay_{k-1}^{-m+1} + bu_{k-1}^{-m+1};\quad T^{-m}_{window} = 16\,\text{min} \qquad [5\text{-}64]$$

Based on Equations [5-49] and [5-50], the coefficients in [5-62] and [5-64] are related by:

$$A = a^2;\ B = b(1+a) \qquad [5\text{-}65]$$

If the model at Level -*m* accurately describes the process dynamics at Level -*m*+1, the coefficients in [5-64] are simply:

$$a = 0.2017;\ b = 0.7983 \qquad [5\text{-}66]$$

States at Level -*m* (i.e. y_1^{-m}, y_2^{-m}) are also related to states at Level -*m*+1 (i.e. y_1^{-m+1}, y_2^{-m+1}, y_3^{-m+1}, y_4^{-m+1}) through the relationships in [5-54]:

$$y_k = \frac{2}{1+a}y_{k/2} - \frac{b}{1+a}u_k;\ y_{k+1} = \frac{2a}{1+a}y_{k/2} + \frac{b}{1+a}u_k \qquad [5\text{-}67]$$

where y_k are states at Level -*m*+1 and $y_{k/2}$ are states at Level -*m*. With *a* and *b* determined, equation [5-67] can be used to compute the values of y_i^{-m+1} based on y_1^{-m}, y_2^{-m}. The validity of this multi-model structure at Level -*m*+1 is verified by comparing y_i^{-m+1}, the true sampled values, with those predicted based on Equations [5-67]. This comparison can be found in Table 5-2. As shown, the error in the states at Level -*m*+1 computed based on Equation [5-67] is within the limit of numerical error in statistical approximation. One can therefore conclude that a first-order response model is an appropriate structure to describe the model response at Level -m+1. It can be easily verified that similar transformations based on equation [5-65] gives good approximation of process state at Level -m+2, Level -m+3 ... Level 0. Based on such results, one can conclude that the true process is 1st order.

Table 5 - 2: True state values versus model predictions using [5-67]

Interval (min)	States	Output based on sampled value	Output computed from coefficients in [5-67]
0 to 16	y_1^{-m+1}	0.5257	0.5257
17 to 32	y_2^{-m+1}	0.9042	0.9043
33 to 48	y_3^{-m+1}	0.9807	0.9807
49 to 64	y_4^{-m+1}	0.9961	0.9961

Case 2: True process is 1st order plus deadtime

If the true process is not 1st order, the 1st order approximation that we develop at Level -m+1 where $T_{window}^{-m} = t_{dynamic}/2$ will not be able to give good prediction of process trend at a higher resolution as other process dynamics are revealed at a lower level.

Suppose the true process is a 1st order process with a time constant of 10 min and a deadtime of 8 min. At Level -m, T_{window} = 32 min, the following first order approximation is obtained:

$$y_{k+1}^{-m} = 0.0498 y_k^{-m} + 0.9502 u_k^{-m} \quad (\tau = 10.66 \text{ min}) \qquad [5\text{-}68]$$

which gives a good prediction of the process trend at Level -m. Similar models at other levels can be generated using Equation [6-65]. As in Case 1, using Equation [5-67], the values of the states at other scales can also be computed based on the model at Level -m. The prediction of the process trends at Level -m+1 and at Level -m+2 are compared with the true process trend in Table 5-3. The first order approximation developed at Level -m gives reasonable prediction at Level -m+1 but the error in the prediction for the earlier part of the process response trend becomes unacceptably large at Level -m+2. We can conclude that the 1st order approximation is *insufficient* to describe the process trend at Level -m+2. The structure of the process model must be modified if it is desired to capture other process dynamics in the model.

Since y_1^{-m+2} is zero, the effect of deadtime in the process becomes *visible* at Level -m+2. We can develop another process model using a 1st order plus deadtime structure (Equation [5-55]):

$$y_{k+1}^{-m+2} = 0.4493 y_k^{-m+2} + 0.5507 u_{k-1}^{-m+2} \quad [5\text{-}69]$$

This model allows good prediction of process trends at Level -*m*+2 as well as at other lower levels.

Table 5 - 3: True state values versus model predictions of a 1st order plus deadtime process

Level -*m*+1				Level -*m*+2			
$y_{k+1}^{-m+1} = 0.2231 y_k^{-m+1} + 0.7769 u_k^{-m+1}$				$y_{k+1}^{-m+2} = 0.4724 y_k^{-m+2} + 0.5276 u_k^{-m+2}$			
Interval (min)	States	True State Values	Predicted Values	Interval (min)	States	True State Values	Predicted Values
0 to 16	y_1^{-m+1}	0.1728	0.1494	0 to 8	y_1^{-m+2}	0	-0.1554
17 to 32	y_2^{-m+1}	0.7869	0.8102	9 to 16	y_2^{-m+2}	0.3455	0.4542
33 to 48	y_3^{-m+1}	0.9570	0.9576	17 to 24	y_3^{-m+2}	0.7059	0.7422
49 to 64	y_4^{-m+1}	0.9913	0.9906	25 to 32	y_4^{-m+2}	0.8697	0.8782
				33 to 40	y_5^{-m+2}	0.9406	0.9425
				41 to 48	y_6^{-m+2}	0.9733	0.9728
				49 to 56	y_7^{-m+2}	0.9880	0.9872
				57 to 64	y_8^{-m+2}	0.9946	0.9939

Case 3: True process is 2nd order

Suppose the true process is 2nd order and it can be accurately described by the following model in the frequency domain:

$$y(s) = \frac{1}{(80s+1)(5s+1)} u(s) \quad [5\text{-}70]$$

At Level -*m*, T_{window}^{-m} = 256 min; the process trend can be represented by the following 1st order approximation:

$$y_{k+1}^{-m} = 0.0411 y_k^{-m} + 0.9589 u_k^{-m} \quad [5\text{-}71]$$

which is equivalent to a process governed by a time constant of 80.1832 min. Table 5-4 compares the predictions of the process step response curve at various resolutions using the 1st order approximation developed at Level -*m* and utilizing the relationships between states at different scales. As shown in Table 5-4, our 1st order model gives good prediction of process trend at low resolution. As the resolution increases, model estimates begin to deviate from the true state values. Through a series of transformation using Equation [5-65], the model at Level -*m*+4 is given by:

$$y_{k+1}^{-m+4} = 0.8191 y_k^{-m+4} + 0.1809 u_k^{-m+4} \quad [5\text{-}72]$$

At this level, the initial state values of the step response become noticeably different from the corresponding true state values. This suggests that a 1st order approximation is inadequate to describe the process trend at higher resolution. A change in model structure is therefore necessary to model process response.

Using a 2nd order model which requires two past states and two past inputs to describe the process response, we obtain the following more refined description of the process:

$$y_{k+1}^{-m+4} = 0.8618\,y_k^{-m+4} - 0.0350\,y_{k-1}^{-m+4} + 0.1284\,u_k^{-m+4} + 0.0447\,u_{k-1}^{-m+4} \quad [5\text{-}73]$$

which is equivalent to a process that is controlled by time constants of 80.1832 min and 5.0748 min. At a lower scale where T_{window} is shorter, the dynamics of faster time constants becomes significant. The model in [5-72] derived based on the model developed at Level -*m* only captures the dynamic of the slower time constant. In fact, the coefficients for the past states in the second order model is related to the coefficient of the past state in the first order model. Suppose the 1st order approximation developed at Level -*m* is translated to Level -*h* ($h < m$) as:

$$y_{k+1}^{-h} = a^{-h} y_k^{-h} + b^{-h} u_k^{-h} \quad [5\text{-}74]$$

and the 2nd order process description is given by:

$$y_{k+1}^{-h} = c^{-h} y_k^{-h} + d^{-h} y_{k-1}^{-h} + e^{-h} u_k^{-h} + f^{-h} u_{k-1}^{-h} \quad [5\text{-}75]$$

It can be shown using *z*-transform that the model in [5-74] is related to the 2nd order process model in [5-75] by the following relations:

$$c^{-h} = a^{-h} + R^{-h}; \quad d^{-h} = -a^{-h} * R^{-h} \quad [5\text{-}76]$$

where R^{-h} is solely a function of the faster process time constant. At a higher level, such as Level -*m*, the effect of the faster dynamics (R^{-m}) is insignificant and R^{-m} approaches zero, allowing the dynamics to be described by one past state y_k. A consistent augmentation of the first order dynamic model at Level -*h* derived from the model developed at higher level would require the following to hold:

$$c^{-h} - a^{-h} \approx \frac{-d^{-h}}{a^{-h}} \quad [5\text{-}77]$$

It can be easily verified that the models described in [5-72] and [5-73] satisfy the consistency rule in [5-77].

Table 5 - 4: Prediction of Process State value using a 1st order approximation at various resolutions

Level -*m*+1; T_{window} =128 min

$y_{k+1}^{-m+1} = 0.2026 y_k^{-m+1} + 0.7974 u_k^{-m+1}$

Time (min)	True State Value	Estimated State Value
y_1	0.4736	0.4735
y_2	0.8932	0.8933
y_3	0.9784	0.9784
y_4	0.9956	0.9956

Level -*m*+2; T_{window} = 64 min

$y_{k+1}^{-m+4} = 0.4502 y_k^{-m+4} + 0.5498 u_k^{-m+4}$

Time (min)	True State Value	Estimated State Value
y_1	0.2751	0.2739
y_2	0.6721	0.6731
y_3	0.8527	0.8529
y_4	0.9338	0.9338
y_5	0.9703	0.9702
y_6	0.9866	0.9866
y_7	0.994	0.9940
y_8	0.9973	0.9973

Level -*m*+3; T_{window} = 32 min

$y_{k+1}^{-m+4} = 0.6709 y_k^{-m+4} + 0.3291 u_k^{-m+4}$

Time (min)	True State Value	Estimated State Value
y_1	0.1357	0.1309
y_2	0.4144	0.4169
y_3	0.6074	0.6088
y_4	0.7369	0.7375
y_5	0.8236	0.8239
y_6	0.8818	0.8818
y_7	0.9207	0.9207
y_8	0.9469	0.9468
y_9	0.9644	0.9643
y_{10}	0.9761	0.9761
y_{11}	0.984	0.9839
y_{12}	0.9893	0.9892
y_{13}	0.9928	0.9928
y_{14}	0.9952	0.9951
y_{15}	0.9968	0.9928
y_{16}	0.9978	0.9951

Level -*m*+4; T_{window} = 16 min

$y_{k+1}^{-m+4} = 0.8191 y_k^{-m+4} + 0.1809 u_k^{-m+4}$

Time (min)	True State Value	Estimated State Value
y_1	0.0573	0.0444
y_2	0.2141	0.2173
y_3	0.356	0.3589
y_4	0.4727	0.4748
y_5	0.5683	0.5698
y_6	0.6466	0.6477
y_7	0.7106	0.7114
y_8	0.7631	0.7636
y_9	0.806	0.8064
y_{10}	0.8412	0.8414
y_{11}	0.87	0.8701
y_{12}	0.8935	0.8936
y_{13}	0.9128	0.9128
y_{14}	0.9286	0.9286
y_{15}	0.9416	0.9415
y_{16}	0.9522	0.9521
y_{17}	0.9608	0.9608
y_{18}	0.9679	0.9679
y_{19}	0.9737	0.9737
y_{20}	0.9785	0.9784
y_{21}	0.9824	0.9823
y_{22}	0.9856	0.9855
y_{23}	0.9882	0.9881
y_{24}	0.9903	0.9903
y_{25}	0.9921	0.9920
y_{26}	0.9935	0.9935
y_{27}	0.9947	0.9947
y_{28}	0.9957	0.9956
y_{29}	0.9964	0.9920
y_{30}	0.9971	0.9935
y_{31}	0.9976	0.9947
y_{32}	0.9981	0.9956

Case 4: Process has other higher order dynamics

Suppose the true process is 2^{nd} order with a positive zero at 0.01428 and it is described by the following model in the frequency domain:

$$y(s) = \frac{-70s+1}{(80s+1)(5s+1)} u(s) \qquad [5\text{-}78]$$

At Level $-m$, $T_{window}^{-m} = 256$ min. The process trend can be represented by the following 1st order approximation:

$$y_{k+1}^{-m} = 0.0420 y_k^{-m} + 0.9580 u_k^{-m} \qquad [5\text{-}79]$$

which is equivalent to a 1st order process with a time constant of 80.7757 min. Based on the relationships between states at different scales, we can make predictions of process trends at various resolutions based on model in Equation [5-79]. Table 5-5 compares the true state values with the predictions of the process step response curve at various resolutions using the 1st order approximation developed at Level $-m$. Again, our 1st order model gives good prediction of process trend at low resolution. As the resolution increases, model estimation begin to deviate from the true state value. Through a series of transformations similar to the one shown in Equation [5-65], the model at Level $-m+3$ is given by:

$$y_{k+1}^{-m+3} = 0.6729 y_k^{-m+3} + 0.3271 u_k^{-m+3} \qquad [5\text{-}80]$$

At this level, the initial state values of the step response become noticeably different from the true state value. This suggests that a 1st order approximation is inadequate to describe the process trend at higher resolution. A change in model structure is therefore necessary to model process response.

Using a 2nd order model which requires two past states and two past inputs to describe the process response, the following more refined description of the process is obtained:

$$y_{k+1}^{-m+3} = 0.6745 y_k^{-m+3} - 0.0011 y_{k-1}^{-m+3} - 0.3075 u_k^{-m+3} + 0.6341 u_{k-1}^{-m+3} \qquad [5\text{-}81]$$

which corresponds to a 2nd order process governed by two time constants (80.7757 min and 4.9609 min) and a zero at 0.015. The 2nd order process model is consistent with the 1st order approximation in that Equation [5-77] holds:

$$c^{-h} - a^{-h} \approx \frac{-d^{-h}}{a^{-h}} \approx 0.0016 \qquad [5\text{-}82]$$

Table 5 - 5: Prediction of Process State of an Inverse Response process using a 1st order approximation at various resolutions

Level $-m+1$; $T_{window} = 128$ min			Level $-m+3$; $T_{window} = 32$ min		
$y_{k+1}^{-m+1} = 0.2050 y_k^{-m+1} + 0.7950 u_k^{-m+1}$			$y_{k+1}^{-m+3} = 0.6729 y_k^{-m+3} + 0.3271 u_k^{-m+3}$		
Time (min)	True State Value	Estimated State Value	Time (min)	True State Value	Estimated State Value
y_1	0.0439	0.0405	y_1	-0.4972	-0.5792
y_2	0.7998	0.8033	y_2	-0.0978	-0.0626
y_3	0.9596	0.9597	y_3	0.2639	0.2850
y_4	0.9918	0.9917	y_4	0.5066	0.5189
			y_5	0.6693	0.6762
Level $-m+2$; $T_{window} = 64$ min			y_6	0.7783	0.7821
$y_{k+1}^{-m+2} = 0.4528 y_k^{-m+2} + 05472 u_k^{-m+2}$			y_7	0.8514	0.8534
y_1	-0.2975	-0.3209	y_8	0.9004	0.9014
y_2	0.3853	0.4019	y_9	0.9332	0.9336
y_3	0.7238	0.7292	y_{10}	0.9552	0.9553
y_4	0.8759	0.8774	y_{11}	0.97	0.9699
y_5	0.9442	0.9445	y_{12}	0.9799	0.9798
y_6	0.9749	0.9749	y_{13}	0.9865	0.9864
y_7	0.9887	0.9886	y_{14}	0.991	0.9908
y_8	0.9949	0.9948	y_{15}	0.9939	0.9938
			y_{16}	0.9959	0.9959

5.7.2 Summary

There are many approaches available for process modeling. For process systems analysis in the hierarchical framework, regardless of the modeling approach employed, one must ensure that models describing the same process at various levels are consistent. The previous section has demonstrated how one can utilize the multi-scale systems theory to identify when the dynamics in a process becomes significant and warrants the use of dynamic models to describe the process behavior. Furthermore, it has been shown that at low resolution, the step response of a process can be described by a 1st order approximation. If the true process is not 1st order, the 1st order model structure must be updated to incorporate more details process dynamics into the model in order to describe the process at a higher resolution. As demonstrated in the case studies, using the relationships between process states of scaled models of various resolutions on the binary tree, we can determine when a model structure becomes inadequate to capture process dynamics which are significant over a shorter time horizon. When the assumed model form cannot capture observable process dynamics, the only way to incorporate these dynamics into the process model is to change the model structure. The availability of a set of consistent models which conform to the multi-scale systems properties allows the synthesis of consistent process control strategies at various time-scale resolution. Implementation of control strategies at various time-horizons can also be carried out by utilizing the set of consistent models (Stephanopoulos, 1997).

Chapter 6
Multi-objective Control System Design

6.1 The Plant-wide Control Structure Design Problem

A typical chemical plant is quite large, consists of a large number of process variables and many manipulated variables. For plant-wide control, the designer essentially has to synthesize a set of control strategies for a large multi-input, multi-output (MIMO) process. In Chapter 2, we have identified the following aspects that are important in the design of a control system for a complete chemical plant:

1. The multivariate nature of the design problem.

   The multivariate nature of the design problem makes the task of control structure synthesis a difficult and non-trivial one. Faced with possibly a numerous number of feasible control configurations, the designer must derive a scheme to discriminate the best control structure(s) from the set of a feasible ones. The inter-coupling nature of the unit-operations further complicates the problem. The quality of control of one output can be affected by the control of one or more outputs in other locations of the plant by virtue of process interactions. It is not obvious how manipulated variables should be associated with process outputs in order to generate a control structure that can best address the production objectives. The control structure synthesis method should account for this multivariable interaction.

2. Multiobjective character of the control structure synthesis problem.

   The main function of the control system is to compute control actions that are required to ensure that the production objectives are met, through the manipulation of some process variables. A suitable control system would be one which associates the manipulated variables with the process outputs in such a way that the plant production objectives can be optimally achieved in the presence of external influences. Typically, in a process plant, there are a multiple number of plant productions objectives that we wish to attain. As pointed out in Chapter 2, some production objectives are related to product quality; some are related to plant operational limits; others are related to the overall behavior of the process and there are additional goals related to the satisfaction of government or environmental regulations. For each objective, there is a certain target value at which the plant must be maintain. As the various categories of plant objectives do not all have equal importance, the control system must be designed in such a way that our engineering preferences and trade-offs are being accounted for.

Formalization which addresses the aforementioned multivariable and multiobjective nature of the control design problem is needed. In this chapter, a goal oriented approach to multiobjective design issues will be described and a useful framework for the design of plant-wide control systems will be presented.

6.2 Multi-objective Analysis for the Multiechelon Hierarchy of Control Objectives

In general, the control actions which must be executed in order to attain all the production objectives can be computed by solving the optimization problem P1 presented in Section 3.1. P1 can be rewritten to include the specific variables for optimization as follows:

$$\text{P2:} \quad \min_{\Delta m_1, \Delta m_2, \cdots, \Delta m_m} \sum_{k=1}^{p} [F_1(k) \quad F_2(k) \quad \cdots \quad F_n(k)] \qquad [6\text{-}1]$$

s.t.

$$g(\Delta m_1, \Delta m_2 \ldots, \Delta m_m) \le 0$$
$$h(\Delta m_1, \Delta m_2 \ldots, \Delta m_m) = 0$$
$$m_{\text{lower}} \le m_i \le m_{\text{upper}} \quad \text{for } i = 1 \text{ to } m$$

where F_k again represents a control objective (k = 1 to n with n being the total number of objectives); p is the control horizon; Δm_1 to Δm_m are vectors of incremental control actions over the period of control horizon; g and h represent the physical constraints which define the model of the process. The control actions of the manipulated variables must also be confined to be within their permissible bounds. In addition to classifying control objectives into explicit and implicit types (refer to Section 3.1), objectives can also be divided into the following classes:

1. Class I: Outputs to be maintained at their setpoints

   Objectives which are accomplished by regulating specific outputs at their desired setpoints, such as maintaining $y_i(k)$ at $y_{i,sp}(k)$, where k is the value of the output at the k^{th} sample. These objectives can be easily translated into deviation variables $F_i(k)$:

$$F_i(k) = \left\| y_i(k) - y_{i,sp}(k) \right\| \quad i \in \text{I} \qquad [6\text{-}2]$$

2. Class II: Outputs to be maintained within a bounded region

   Objectives which are concerned with the maintenance of outputs to be within some bounded limits, i.e.:

$$y_{j,lo} \le y_j(k) \le y_{j,up} \quad j \in \text{II} \qquad [6\text{-}3]$$

The definition of objectives in Class II given by equation [6-3] treats the outputs as *hard* constraints where no excursion outside the feasible region is allowed. Alternatively, a *soft* representation like the one below can be used:

$$F_j(k) = \text{neg}(y_j(k) - y_{j,lo}) + \text{pos}(y_j(k) - y_{j,up}) \quad j \in \text{II} \qquad [6\text{-}4]$$

where

$$\text{pos}(x) \equiv \begin{Bmatrix} x; x > 0 \\ 0, x \le 0 \end{Bmatrix}; \quad \text{neg}(x) \equiv \begin{Bmatrix} 0, x \ge 0 \\ x, x < 0 \end{Bmatrix} \qquad [6\text{-}5]$$

If $F_j(k)$ is forced to be zero, no excursion is allowed and equation [6-4] is equivalent to equation [6-3]. For objectives which are bounded from above only, the use of $\text{pos}(\cdot)$ alone is sufficient to define the soft representation. Similarly, for objectives which are bounded from below only, the use of $\text{neg}(\cdot)$ is sufficient.

3. Class III: Optimization Objectives

   All optimization objectives can be written in the following form:

$$Q_h = \min F_h(\cdot) \quad h \in \text{III} \qquad [6\text{-}6]$$

where $F_h(\cdot)$ is some objective function defined in terms of the process variables.

Obviously, some of the objectives are more important than the others and attempting to treat all objectives undiscriminatively may lead to designs that are either over-conservative or non-practical in essence. The set of control objectives $\{F_k\}$ can be cast into a multiechelon hierarchy. The notion of a multiechelon hierarchy for control objectives has been discuss in Section 3.5.1. A multiobjective design approach useful for control structure synthesis will be described next.

6.2.1 A Goal-Oriented Multiobjective Design Approach

In a multiobjective optimization, it is required to locate the solution within the feasible region such that the set of objectives can be satisfied in the most optimal manner. Figure 6-1 depicts the solution space of a similar multiple optimization for two objectives $F_1(z)$ and $G_2(z)$ with respect to z. The shaded region represents the set of all the feasible solutions, $\Re$. Point S_1 is a feasible solution and point S_2 is an infeasible solution. An optimal solution of the problem must fall onto the line from A to B. Any solution on this line is a *noninferior* solution because no improvement of any one objective can be made without simultaneously degrading the value of another. This region is called the *pareto optimal subspace*, $\Re^P$. As any point in the pareto optimal subspace represent an equally optimal solution (in the pareto optimal sense), the most desirable solution is the one based upon our subjective judgment of the relative importance of the minimization of $F_1(z)$ and $F_2(z)$. Thus, a supply of the preferences of the designer is essential in any multiple objective decision analysis.

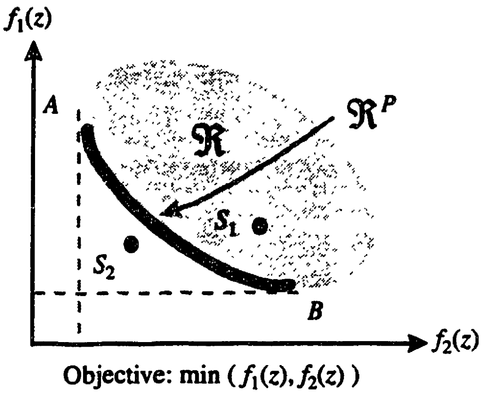


Figure 6 - 1: Pareto Optimal Surface of a Two Dimensional Problem

Approaches which require *a priori* supply of preference information have been found to be useful for control system design (Meadowcroft, 1992). A common approach to *a priori* multiple objective design is to transform the vector of objectives in [6-1] into a scalar utility function defined in terms of some weights:

$$\text{P3:} \quad \min_{\Delta m_1, \Delta m_2, \cdots, \Delta m_j} \sum_{k=1}^{p} w_1 F_1(k) + w_2 F_2(k) + \cdots + w_n F_n(k) \qquad [6\text{-}7]$$

s.t.

$g(\Delta m_1, \Delta m_2 \ldots, \Delta m_m) \leq 0$

$h(\Delta m_1, \Delta m_2 \ldots, \Delta m_m) = 0$

$m_{lower} \leq m_q \leq m_{upper}$ for $q = 1$ to m

The relative magnitudes of the weights, w_i, for the objectives reflect their relative importance in the design. Although this method is computationally attractive, the numerical value of each of the weights only reflects the designer's subjective judgment of the *level* of importance of each objective versus the rest.

An alternative way of defining preferences *a priori* is by mimicking the inherently goal-oriented nature of decision making by simply asking the objectives be ranked according to their perceived importance (Ignizio, 1982). This ranking establishes a multiechelon hierarchy of control objectives in the design. The Modular Multivariable Controller (MMC) Design Framework (Meadowcroft, 1992) introduced in Section 3.5.2 uses the *lexicographic goal programming* (introduced by Ignizio, 1976) to handle multivariable control problems. The key steps in the MMC design framework can be summarized as follows:

1. Define control goals.

   Our control goals are to minimize the deviation variables such as F_i as defined in [6-2], F_j as defined in [6-4] and our optimization objectives such as F_h as defined in [6-6]. The values of the deviation variables and F_h measure the levels of achievements with respect to the corresponding objectives that they represent. Control goals are a_k, where $a_k \equiv F_p$ and $k = 1, \ldots n$; $p = 1, \ldots, n$ (n being the total number of constraints that belong in classes I, II and III).

2. Prioritize control goals.

   The level of achievement, i.e. min (a_k), of each control objective is viewed as a goal in the design. According to our engineering preferences and perceived design trade-offs, goals are arranged according to their order of importance so that a_1 is of higher priority than a_2, a_2 is of higher priority than a_3, etc. This preference order forms a hierarchy of goals (or equivalently objectives).

3. Satisfy the multiechelon hierarchy of control goals sequentially.

   The design approach is priority-driven. Starting from the most important goal, a manipulated variable which has the best potential to maintain the level of achievement of the goal at its highest level is selected to be the *primary manipulated variable*. This primary will be responsible for the attainment of the first control objective. Then, the design proceeds to the second most important goal. From the remaining set of manipulated variable, the one that can best maintain the second goal at its highest level of achievement *without* degrading that of the more important goal (i.e. the first goal in this case) is the primary for the second goal. Assignment of primaries to other goals are made in a similar manner.

Mathematically, the goal-oriented optimization is a lexicographic minimization and can be stated as:

$$\text{P4:} \quad \underset{\Delta m_1, \Delta m_2, \cdots, \Delta m_m}{\text{lexico min}} \sum_{k=1}^{p} \boldsymbol{a}(k) = [a_1(k) \quad a_2(k) \quad \cdots \quad a_n(k)] \qquad [6\text{-}8]$$

$$\text{s.t.}$$
$$\boldsymbol{g}(\Delta \boldsymbol{m}_1, \Delta \boldsymbol{m}_2 \ldots, \Delta \boldsymbol{m}_m) \le 0$$
$$\boldsymbol{h}(\Delta \boldsymbol{m}_1, \Delta \boldsymbol{m}_2 \ldots, \Delta \boldsymbol{m}_m) = 0$$
$$\boldsymbol{m}_{\text{lower}} \le \boldsymbol{m}_q \le \boldsymbol{m}_{\text{upper}} \quad \text{for } q = 1 \text{ to } m$$

Here, $\boldsymbol{a}(k)$ is an ordered achievement vector at the k^{th} sample and a_1 is assumed to be preferred over a_2 which is preferred over a_3, etc. The solution to P4 is simply the lexicographic minimum $\boldsymbol{a}^*$.

Definition 6-1: Lexicographic Minimum (Meadowcroft et al., 1992)

Given an ordered array of $\boldsymbol{a}$, the solution $\boldsymbol{a}^{(1)}$ is preferred to the solution $\boldsymbol{a}^{(2)}$ if for the goal F_k at any priority level k (k= 1, ... , n) the following is true:

$$\boldsymbol{a}_k^{(1)} \text{ is preferred to } \boldsymbol{a}_k^{(2)}$$

while for all goals of priority higher than k,

$$\boldsymbol{a}_j^{(1)} \text{ as desirable as } \boldsymbol{a}_j^{(2)}, j < k \quad \text{(higher priority)}$$

The lexicographic minimum, $\boldsymbol{a}^*$, is the solution which is preferred over any other.

In a sequential fashion, manipulated variables are assigned to the hierarchy of production objectives, in the order of their importance. Thus, very explicitly, this methods allows the reservation of the "better" manipulated variables for the achievement of the more important plant control goals, shifting the emphasis of the design to the more important objectives. This sequential objective-satisfaction approach offers an attractive framework for solving control design problems for the following reasons:

1. The control structure synthesis problem involves the satisfaction of a distinct number of control objectives which are noncommensurable.
2. In most real problems, the task of deciding which control objective is more important should not be difficult. On the other hand, it would be more challenging for one to arrive at a set of weights for each of the objectives that accurately reflect the preference of the designer. In the case where not all objectives can be attained, rather than sacrificing one or more objectives to accomplish all desirable outcomes in an average sense, only the most important ones will be considered in the design.
3. The sequential objective-satisfaction approach offers an attractive framework for solving control design problems. Instead of generating a multivariable controller design which may not result in an identifiable structure, the prioritizing methods, when judiciously employed, allows the synthesis of a set of control strategies that forms a plant control structure that is relatively transparent.

Note that by sequentially assigning one manipulated variable to one production goal, the set of control strategies synthesized at the end in fact has an identifiable structure. Each control objective has been assigned to a primary manipulated variable whose variation has the most contribution to the control of that objective. The issues that may make the proposed approach for the synthesis of plant-wide control strategy not a viable one have been addressed by Meadowcroft et al. (1992):

1. The difficulty in priority assignment.

   The premise of the propose framework is the existence of a hierarchy of production goals of various levels of priorities. Thus, one may argue that the proposed framework would fail if such a hierarchy of goals does not exist, or, if the designer is not able to distinguish the different levels of importance among the goals. In practice, however, it is believed that the operation of chemical plant generally involves several basic operational objectives whose levels of importance should be unambiguous. Objectives that are related to the safety of the plant are undeniably the most important ones. Goals related to product specifications should receive more attention than those that are related to plant optimization. With a good understanding of the operational objectives in the plant, prioritization of goals should be straight forward.

2. Ability to evaluate the design trade-offs.

   By strict interpretation of the proposed method, assignment of primary manipulated variables to important goals are made early in the design. Thus, one would not in fact compare complete design alternatives and evaluate the trade-offs for each of the goal in terms of compete designs. It can be argued that the proposed approach does not limit comparison of design trade-offs. First of all, in a multiobjective framework, there would be little justification for equal emphasis on *all* of the objectives. Thus, designs that allow better control ability of more important objectives are preferred. Under the present proposal, the trade-offs will be biased toward the more important objectives. If, at any priority level, one determines that there are several equally attractive design alternatives, one can generate decision trees and retain all the alternatives until it becomes obvious at a lower priority which particular branch leads to a superior outcome.

6.2.2 Objective Ranking of Plant Control Objectives

As noted in Section 3.5, for chemical plant operations, objectives which are associated with the regulation of materials and energy inventories in the plant should be of the highest priorities. Objectives related to the prevention of the violation of equipment constraints, environmental regulations and other process safety constraints should precede those which are related to production and product quality. Optimization objectives should only be investigated after all other objectives have been met. Further division of each category of objectives into goals of finer priority level would require understanding of the context of the operation. For instance, in a given context of operation which involves large production changes, objective A may be more important than objective B. In another context where changes in the distribution of produced products are critical, objective B may be more important. Often, the inability to decide the relative importance of process goals is primarily due to lack of understanding of the plant operation (Meadowcroft et al., 1992).

The ranking of objectives in the above discussion had been based on experience and insight of operation of chemical processes. Although there are no precise rules which guide the assignment of objectives to their proper priority levels according to their preference of importance, the *paired comparison method* (Morris, 1964; Ignizio, 1976) provides a framework for an "objective" means of ranking. In essence, objectives are compared, two at a time. Each time, we ask the question, *"which objective would we rather sacrifice if there were only one degree of freedom available for satisfaction of one objective?"*. The objective which we would rather sacrifice is given a lower priority. In this way, a *hierarchy of plant control objectives* can be established. If more than one decision maker is involved, more sophisticated objectives ranking procedures may be employed (Satty et al., 1985).

6.2.3 Preemptive Priorities

The assumption that has been used so far in the discussion is that each control objective will be assigned a distinct level of priority. It was noted by Ignizio (1976) that such a treatment might be unrealistic since: (1) it is rare for a well constructed real life problem to have more than even five priority levels; (2) it would be rare indeed to be able to satisfy any objectives assigned such a low level of priority as, say P_{10} without degrading the achievements of the more important objectives. A problem which involves a large number of different objectives can be better represented by reducing the number of priority levels to a minimum that is consistent with the true characteristics of the actual problem under consideration. This can be achieved by arranging objectives according to ordered sets that can be assigned to preemptive priorities such that $P_k >> P_{k+1}$. The achievement of the set of objectives at any one preemptive priority is *immeasurably* preferred to the achievement of the objectives set at any lower preemptive priority (Ignizio, 1976). Objectives which belong in the same priority levels may be combined into a scalar utility function via the use of weights.

6.3 Quantitative Analysis: Assignment of Primary Manipulated Variables to Control Objectives

Within the modular multivariable controller design framework, plant-wide control design alternatives which address the multiple objectives in the production can be systematically generated. The selection of primaries for each of the objectives plays a pivotal role in the synthesis process. By identifying sets of potential primary manipulated variables for the individual control objectives, sequentially starting from the most important ones, control design alternatives which place heavier emphasis on the more important plant production goals can be generated. In general, a preferred primary should possess some of the favorable attributes, such as the ability to reject deviations within its range of operations, the quality of the expected output response, etc. Through these selections, we define the potential closed-loop performance of the entire system.

As a complex process plant is being analyzed in the hierarchical framework through a hierarchy of process representations, Different sets of design criteria is therefore needed to address the different observable characteristics at different levels of the design hierarchy. The methodology that one could employ for the selection of primary manipulated variables will be discussed next.

6.3.1 Generating Control Structures for Long-horizon Control

Coarse process viewpoints in the multistrata hierarchy capture the characteristics of the plant which are observable at a long time-horizon. In the previous chapter, it was pointed out that long-horizon process behavior can be captured by means of static models of the plant, i.e. steady-state gains. The potential achievement level of each of the control objectives by any of the available manipulated variables can be evaluated using steady-state gains and a model of the process. The essential properties of manipulated variables for the maintenance of control objectives in the long-horizon are described below.

Range of Operation of the Manipulated Variables

Most of our control objectives involves minimizing the deviation variables defined in Class I (Equation [6-2]) and Class II (Equation [6-4]). Such objectives can be translated goals which require the maintenance of the process outputs as closed to the targets as possible. In the long-horizon of the production plan, it is important that the process can be maintained at the set of desired setpoints and that the control structure is able to move the plant to a new steady-state, i.e. a new set of setpoints. Thus, for long-horizon control of the plant, the control structure should be able to maintain the plant outputs at their targets over a broad operation range without saturating the manipulated variable. When a manipulated variable is at its operational limit, one degree of freedom is lost in the design. Hence, it is preferred that manipulated variables which have relatively wide ranges of operation be used as primaries. A manipulated variable would be easily saturated if (1) its nominal operation point is close to the limit of its operation (i.e. its saturation limits), or (2) it produces a small gain on the output that is associated with the objective under consideration. Obviously, if an output is controlled by an input that gives a large gain and has a wide range of manipulation, there is a better potential for us being able to carry out large changes in the output that may be required during process operation.

The "steady-state gains" which are used to describe our process through a static input-output models are really open-loop gains, i.e. they represent the gains of the outputs when a manipulated variable is changed in the process by one unit (k_{ij}, gain of output i for a unit change in input j). However, the "gains" that are used for analysis should be consistent with the lexicographic goal programming framework. That means, measures which describe how each manipulated variable affect the concerned output when outputs that should be of higher priorities are being controlled by their respective primaries should be used. Closed-loop gains describe exactly this effect on the system. By computing the effect of each of the manipulated variable on the concerned output when all the more important outputs are under perfect control by their corresponding primary manipulated variables, the interaction effect in the multivariate environment is being accounted for.

Impact of Model Uncertainty on Robustness of Control System Design

The quality of the selection of primary manipulated variable is a function of how good the static models are. The actual values of the static closed-loop gains may deviate from the nominal ones if: (1) we have error in our models, or (2) the plant under investigation is very non-linear so a small deviation from the nominal operating point may result in considerable amount of changes in the values of the gains, or (3) presence of input disturbances to the plant changes the gains. Thus, instead of selecting primary manipulated variables based on the nominal static closed-loop gains alone, the expected ranges of variation of the gains should be included in the analysis.

The amount of uncertainty in the model (and hence the confidence level in our selection based on the size of the static gain) can be captured by a *robustness measure* (Meadowcroft, 1992) which is defined to be:

$$C_g = \frac{|G_{max}|}{|G_{min}|} \qquad [6\text{-}9]$$

where:

C_g = condition number for static robustness measure

G_{max} = the maximum magnitude that the closed-loop gain can take on

G_{min} = the minimum magnitude that the closed-loop gain can take on

The computation of G_{max} and G_{min} will be discussed later in this section. C_g is an explicit measure of the robustness between the given input and output and its value can vary from 1 to ∞. When C_g has a value of unity, it indicates that that the possible uncertainty in the open-loop model (i.e. error in k_{ij}), if any, has no effect on the closed-loop gain. At the other extreme, when $C_g = \infty$, it indicates that the true value for the gain may be of a different sign to the modeled (nominal) value, a situation of minimum robustness.

Computing Closed-loop gains and Robustness measures

The use of "closed-loop" gains in the analysis is consistent with the multiobjective lexicographic goal optimization framework being employed. Assignment of primary manipulated variables to an output that is of a lower priority is made by assuming all objectives of higher priorities are being maintained at their best achievement levels, i.e. zero static deviation. In other words, the achievement levels of the more important objectives are not compromised as a result of interaction.

Consider a plant of n control objectives, all of which are concerned with the minimization of the vector of outputs from their setpoints. Let this vector of outputs be $\boldsymbol{y}$ = [y_1, y_2 , …, y_n] , arranged in the order of importance. Assuming that there are p manipulated variables $\boldsymbol{m}$ = [m_1, m_2, … , m_n] , where $n \le p$. Let $\boldsymbol{K}$ be the matrix of open-loop gains of the plant, i.e. :

$$\boldsymbol{K} = [k_{ij}] = \left(\frac{\partial y_i}{\partial m_j}\right)_{m_q \; q=1,\cdots,p,\, q\neq j} \qquad [6\text{-}10]$$

Designate the columns of $\boldsymbol{K}$ by $\boldsymbol{k}_i$ (i=$1,2,...p$), and define $K^i_{p_1 p_2 \cdots p_i}$ to be the $i \times i$ matrix made up to the first i rows of the matrix:

$$\begin{bmatrix} \boldsymbol{k}_{p_1} & \boldsymbol{k}_{p_2} & \cdots & \boldsymbol{k}_{p_p} \end{bmatrix}_{nxi} \qquad [6\text{-}11]$$

where the subscript p_m denotes the primary manipulated variable for the m^{th} controlled variable. Define the "closed-loop" gain, G_i between a controlled output y_i and its primary manipulated variable m_{p_i}, by :

$$G_i = \left[\frac{\partial y_i}{\partial m_i}\right] \quad [6\text{-}12]$$

Assuming that all the more important outputs, that is y_k for $k=1,2,\ldots,i-1$, are under perfect control by the previously designated primary manipulated variables and all manipulated variables that are not already designated as primaries are held constant, that is, m_h = constant, $h = p_1, p_2, \ldots, p_{i-1}$. Then, Meadowcroft et al. (1992) have shown that :

$$G_i = \left[\frac{\det(A)}{\det(A')}\right] \quad [6\text{-}13]$$

where $A = K^{i}_{p_1 p_2 \cdots p_i}$ and $A' = K^{i-1}_{p_1 p_2 \cdots p_{i-1}}$. A' is the largest principal minor of A.

Introduction of model uncertainty and model variation into the above description would mean that the open-loop gains k_{ij} can vary (either in a correlated or an uncorrelated fashion) between some upper and a lower bounds. A range of values of G_i , det(A) and det(A') will be possible. The robustness measure, C_g, is defined by the limits of this range. Under variations of the open-loop gains, if det(A) changes sign, then $|G_{min}| = 0$ and $C_g(G_i)$ = ∞. If det(A') changes sign under gain variations, $|G_{max}| = \infty$ and $C_g(G_i)$ = ∞ as well. There are several ways in which gains in the open-loop gain matrix, $\boldsymbol{K}$, can vary. They are :

Case I. Uncorrelated Perturbations of Gains (Unstructured Uncertainty)

Each k_{ij} is assumed to vary independently within a range of values. This is the most conservative assumption

Case II. Unidimensional Correlation of Gain Perturbations (Structured Uncertainty)

The perturbation of a static gain is assumed to be correlated with those of other gains along the same row or column. One situation would be the effect of one manipulated input vary in a correlated manner is the entire column in matrix $\boldsymbol{K}$.

Case III. Multi-Dimensional Correlation of Gain Perturbations.

In some cases, the perturbations of a static gain can be correlated with those of other gains distributed over several rows and columns.

Meadowcroft et al. (1992) have developed methods in which the robustness measure for each of the cases listed above can be estimated.

In summary, for each control goal, the potential primary manipulated variables should have the following characteristics:

- have high expected performance by being an input that is far away from its saturation limits and has a large gain on goal i when all goals from 1 to (i-1) are under perfect control by the previously assigned primary manipulated variables.
- have minimal effects of model uncertainty with a robustness measures, C_g, that is close to unity.

When identifying potential primary manipulated variables, the two criteria above may give conflicting recommendations that a decision of which variable to select may not be obvious. By generating decision trees, we maintain all equally attractive alternatives and carry out all the options to the selection of the next set of primaries until it becomes obvious which alternatives will lead to a better overall outcome in the end.

6.3.2 Generating Control Structures for Short-horizon Control

Following the hierarchical multilayer approach, control strategies and control structure for the plant are being continuously refined to complement the time scales of operation defined by the abstract models in the hierarchy. In the later stages of the design, the dynamics of the plant becomes relevant in the process representations and short-horizon analysis is employed in the synthesis of control structures. Detailed dynamic models that bring out the transient behavior of the process will be required in this phase of analysis. Furthermore, in the short-horizon timespan, the primary interest is to minimize process deviations as fast as possible and in a smooth manner. Consequently, primary manipulated variables must be selected based on the quality of transient response that they produce on the outputs. The attributes to be considered will be described in the next few sections.

Attributes in Primary Manipulated Variables for Short-horizon Control

To evaluate potential manipulated variables quantitatively, in a systematic manner, measurements which allow the designers to evaluate the merit of the use of each of the available inputs have been developed and these are presented below.

Integrator Gain

As shown in Section 5.3.1, process integrator can be modeled by the rate of change of the corresponding output, known as the integrator gain. Thus, the larger the integrator gain, the faster the response of the output for changes in the input. For integrating outputs, it is preferred that inputs which produce large integrator gains be used as primary manipulated variables, i.e. which have small $V_{integrator}$:

$$V_{ingegrator} = 1/\text{ (integrator gain)} \qquad [6\text{-}14]$$

Process Deadtime

As noted earlier in Section 5.3.2, process deadtime is a non-invertible element so it is desirable to minimize the deadtime in the closed-loop response by judicious choice of primary manipulated variable. The presence of am exceedingly large deadtime between the process input and output automatically implies that the input is an unsuitable choice for feedback dynamic control purposes. Thus, one should choose inputs whose effects on the output are characterized by small deadtimes:

$$V_{\text{deadtime}} = T_i \quad [6\text{-}15]$$

where T_i is the deadtime.

Time Constant

The dominant time constant gives a rough measure of the time it takes for the completion of the changes in the output in an open-loop manner. Although the size of the dominant time constant does not affect the quality of the closed-loop output response, it determines the transient of the control action. In the internal model control framework, the transient control action is given by (Morari and Zafiriou, 1989):

$$m(s) = G_-^{-1}(s)F(s)y_{sp}(s) \quad [6\text{-}16]$$

where $m(s)$ is the process input, $F(s)$ is a filter and $G_-(s)$ is the invertible part of the process model. Time constant is an invertible element so it is part of $G_-(s)$ and would appear as a negative zero in $G_-^{-1}(s)$. This means, to obtain the same quality of output response, an input which causes the output to move slowly would need to change quickly and use a large control action. Thus, it is always preferred to choose inputs whose effects on the output are characterized by small dominant time constants τ:

$$V_{\text{dominant}} = \tau \quad [6\text{-}17]$$

Right-half Plane (RHP) Zeroes

The presence of RHP zeroes (or RHP transmission zeroes for MIMO systems) in the system cause performance degradation and limits the performance of the closed-loop system as they are non-invertible elements. It had been explained in Section 5.3.4 that under the assumption of optimal control, the integrated squared error of the output response under optimal control is a function of the RHP zeroes (Frank, 1974):

$$\text{ISE} = \sum_{i=1}^{k} \frac{2}{z_i} = V_{RHP} \quad [6\text{-}18]$$

Hence, it is preferred to chose inputs in such a way that the overall system contains the least offending RHP (transmission) zeroes, i.e. a small V_{RHP}.

Range of Operation of the Manipulated Variables

It is desirable to use a manipulated variables which has a large range of operation with nominal steady-state value that is far away from their saturation limits. During dynamic control of the process, the manipulated variables may have to produce large deviations from their original steady-state values in order to force the system to eliminate deviations as fast as possible (this is particularly true for slow processes). The input should be far away from the saturation limits of the variable. In long-horizon analysis, the magnitudes of the static gains are used to measure the likelihood of the input hitting the saturation limits for large changes in the setpoint. The size of the static gain, however, is not indicative of the likelihood of input saturation during transient control. For short-horizon analysis, a more direct measure is used. If the nominal value of the manipulated variable is X_0 and that it must be confined in the range from X_{lower} to X_{upper}. Then,

$$V_{range} = [\ \min \{ (X_{upper} - X_0),\ (X_0 - X_{lower}) \}\ ]^{-1} \qquad [6\text{-}19]$$

represents the inverse of the minimum range of operation that this manipulated variable can provide. Thus, $V_{range} = \infty$ for any input that has its nominal value at saturation.

Model Uncertainty

To be consistent with the lexicographic goal programming approach, the selection of primary manipulated variable for each objective is based on a system which has all of the objectives that are of higher priorities under perfect control. This means, similar to the long-horizon analysis, the selection should be made based on a model of the "closed-loop" system as well. The impact of model uncertainty on the performance of the closed-loop system is shown below.

Consider the k^{th} step in the sequential design procedure on the following general plant (tilda omitted from now on for brevity):

$$\begin{bmatrix} \boldsymbol{y} \\ y_k \end{bmatrix} = \boldsymbol{G} \begin{bmatrix} \boldsymbol{m} \\ m_k \end{bmatrix} + \begin{bmatrix} \boldsymbol{h} \\ h_k \end{bmatrix} \qquad [6\text{-}20]$$

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{b} \\ \boldsymbol{c} & d \end{bmatrix} \qquad [6\text{-}21]$$

where :

$\boldsymbol{y}$ = the vector of goals 1 to (k-1), arranged in order of importance

$\boldsymbol{m}$ = the vector of primary manipulated variables that have previously been assigned to the vector of output $\boldsymbol{y}$ and m_i is the primary for y_i, $i = 1.....(k\text{-}1)$

y_k = the output to which a primary manipulated variable is to be assigned

m_k = a candidate manipulated variable for assignment.

$\boldsymbol{h}$ = a vector of disturbances influencing outputs $\boldsymbol{y}$

h_k = a disturbance influencing output y_k

$\boldsymbol{G}$ = the transfer function matrix describing $[\boldsymbol{y} \quad y_k]^T$ by $[\boldsymbol{m} \quad m_k]^T$

$\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c}, d$ = subsets of $\boldsymbol{G}$ of appropriate dimensions

Submatrix A of the matrix G is the closed-loop description of the plant for the 1 to $(k$-1) goals. It can be assumed to have the following pre-defined factorization:

$$A = A_- A_+ \qquad [6\text{-}22]$$

where A_+ is a previously defined non-invertible matrix for the transfer function matrix for goals 1 to $(k$-1). Let ,

$$Q = F_{k-1}[A_-]^{-1} \qquad [6\text{-}23]$$

be the controller for goals 1 to $(k$-1) such that

$$m = Qy_{sp} \qquad [6\text{-}24]$$

where y_{sp} is a vector of setpoint for the outputs defined in vector y.

The MMC design methodology leads to the following closed-loop description of the plant:

$$\begin{bmatrix} y \\ y_k \end{bmatrix} = G_+ F \begin{bmatrix} y_{sp} - h \\ y_k - h_k \end{bmatrix} \qquad [6\text{-}25]$$

$$G_+ = \begin{bmatrix} A_+ & 0 \\ c(A_-)^{-1}(1 - G_{k+} f_k) & G_{k+} \end{bmatrix} \qquad [6\text{-}26]$$

such that :

$$G_k = (d - cA^{-1}b) = (d - cA^{-1}b)_-(d - cA^{-1}b)_+ = G_{k-}G_{k+} \qquad [6\text{-}27]$$

G_k is a 1 × 1 transfer function of y_k by m_k and the factorization of $G_k = G_{k-}G_{k+}$ is unique. G_+ is the non-invertible part of matrix G. The characteristics of $[y \quad y_k]^T$ is determined by this matrix. Since m_1 to m_{k-1} have been previously determined in a similar fashion, y_k is only a function of G_{k+} and f_k. Thus, the response of y_k can be optimized by choosing an m_k from the remaining set of free manipulated variables such that G_+ possesses certain desirable characteristics.

Under the assumption of perfect modeling, the system described by equation [6-21] is uni-directionally decoupled. Changes in the set-points (or disturbances affecting the outputs) of the less important objectives do not affect the behavior of the more important objectives. However, due to imperfect modeling, such decoupling will not be perfect. The true description may look something like the following:

$$G_{+} = \begin{bmatrix} A_{+} & S \\ c(A_{-})^{-1}(1-G_{k+}f_k) & G_{k+} \end{bmatrix} \qquad [6\text{-}28]$$

where $S \neq 0$.

One can view S as a disturbance acting on output vector $\boldsymbol{y}$. S can be quantified by the *decoupling sensitivity* of output k to changes in the setpoint of output j (all other setpoints being constant):

$$S_{k,j}(z) = \frac{y_k(z)}{(y_{j,sp}(z) - h_j(z))} \qquad [6\text{-}29]$$

such that k is of higher priority than j. If one assumes additive errors for A and b in [5-16], i.e.:

$$A = \tilde{A} + \Delta A \; ; \; b = \tilde{b} + \Delta b \qquad [6\text{-}30]$$

It has be shown by Meadowcroft et al. (1992) that the decoupling sensitivity to be described by the following equation:

$$S_{k,j} = \frac{1 - f_k \tilde{G}_{k+}}{1 + (G_k - \tilde{G}_{k+})c_k} [\Delta b - \Delta A \tilde{A}^{-1} \tilde{b}]_{kth\ row} \frac{f_j}{\tilde{G}_{j-}} \qquad [6\text{-}31]$$

Then, S_{kj} is small if the vector $[\Delta b - \Delta A \tilde{A}^{-1} \tilde{b}]_{kth\ row}$ is small (which only occurs in rare cases when effects of errors in model cancel out each other), or both Δb and ΔA tend to zero (which requires a small amount of uncertainty in A and a small amount of uncertainty in b) or the value of $f_k \tilde{G}_{k+}$ is close to unity. The last condition requires G_k to be completely invertible with very little uncertainty. Hence, in order to ensure a small decoupling sensitivity, we must choose $m_k = m^*$ such that ΔA is small and choose $m_j = m^{**}$ such that both Δd and Δb are small. For a system of n outputs, the manipulated variables should be selected in such a way that there is a least amount of uncertainty in the models between the selected input and all the outputs that are of more importance in order to ensure small decoupling sensitivity and preserve as much unidirectional decoupling as possible in our design framework.

The uncertainty in the models between the selected input and all the outputs that are more important should be small. Let Δ_i (i = 1 to 3) be the norm of the amount of uncertainty in A, b and d in the matrix G (equation [6-21]). Then,

$$V_{uncertainty} = \Sigma\, \Delta_i \qquad [6\text{-}32]$$

Selecting Primary Manipulated Variables for Short-horizon Control

In the previous section, a number of attributes which contribute to the performance of the closed-loop system have been introduced and ways to quantify the various effects on control performance have been in Equations [6-14], [6-15], [6-17], [6-18], [6-19] and [6-32]. Some of these measurements defined may provide indication that certain inputs are unsuitable. For examples, inputs which have exceedingly large $V_{deadtime}$, large V_{range} or large V_{RHP} suggest that they are poor candidates for dynamic transient control. For the rest of the inputs, a quantitative evaluation procedure can be applied. One practical approach would be to use a heuristic rule like the one below:

$$V = \sum_i w_i \left| \frac{Vi}{N_i} \right| \qquad [6\text{-}33]$$

where i = integrator, deadtime, dominant, RHP, range or uncertainty (any attributes that apply in the case under consideration)

w_i = a value that represents the relative importance of each of the attribute for the plant under consideration

N_i = a normalization factor since V_i is scale dependent.

The normalization factor N_i should be chosen to make all V_i/N_i to be of roughly the same order of magnitudes. Depending on what attribute is viewed as more important in the particular application, w_i can be adjusted accordingly to reflect that preference. The next example illustrates the use of these measurements.

EXAMPLE 6-1

Suppose it is desired to choose a set of potential manipulated variables to control a particular output from a set of four. The following information about the effect of each of the inputs on the output of interest are given:

Input	A	B	C	D
nominal position (0-100)	72	54	8	28
deadtime	10	5	5	1
dominant time constant	110	28	32	60

V_i have been computed as follows:

Input	A	B	C	D	$\overline{V_i}$ average
V_{range}	0.0139	0.0185	0.125	0.0357	0.04828
$V_{deadtime}$	10	5	5	1	5.25
$V_{dominant}$	110	28	32	60	57.5

V_{range} and $V_{dominant}$ can be normalized to values which are comparable to $V_{deadtime}$ by dividing their values by N_{range} and $N_{dominant}$ respectively, where:

$$N_i = \overline{V_i} \;/\; V_{deadtime} \text{ for } i = \text{range and dominant}$$

Using $N_{range} = 0.009196$; $N_{deadtime} = 1$ and $N_{dominant} = 10.95$, the following V_i/N_i for each of the inputs have been obtained:

Input	A	B	C	D
V_{range} / N_{range}	2.27	3.79	11.37	4.55
$V_{deadtime} / N_{deadtime}$	10	5	5	1
$V_{dominant} / N_{dominant}$	10.043	2.5565	2.9217	5.4783

Notice that all values have been normalized to roughly the same order of magnitude so that a legitimate comparison can be made. For dynamic control, it is more important that we minimize the deadtime between the input and output. Also, the range of manipulation that can be made by the individual input is also important as we would like to be able to handle large movements that may be required during transient control. Using $w_{deadtime} = 5$; $w_{dominant} = 1$ and $w_{range} = 3$, the following V values for the inputs have been obtained:

Input	A	B	C	D
$V = \Sigma\, w_i\, \lvert V_i / N_i \rvert$	64.57	33.60	68.70	22.13

Based on our preferences, inputs B and D are two promising candidates. Note that although the effect of inputs B and C on the output are essentially the same, the fact that input C has a much smaller range of operation makes B a more desirable choice.

6.4 Synthesizing Plant-wide Control Structures

6.4.1. The Control Input Assignment Process

The design criteria which capture the attributes that characterize the quality of closed-loop control have been developed based upon fundamental control theory, combined with practical considerations. Within the goal-oriented design framework, in a sequential manner, inputs that are good candidates for control of each of the production objectives can be identified. Thus, a plant-wide control structure can generated based on the results obtained from the long-horizon or short-horizon analysis. The type of analysis employed will depend of the level on details in the hierarchy of process representation.

Figure 6-2 is a visualization of the control input assignment process. At each level of process representation, beginning from the most important objective (i.e. Goal 1 in the figure), we access all the available input against the design criteria. The best input is assigned to this goal. Then, the next important goal is being considered. Since input 1 has been selected to be the primary for Goal 1, we no longer need to include this manipulation in the picture. The remaining inputs are compared against the design criteria. The properties that we use for comparison should account for the fact that Goal 1 is under perfect control by input 1, in other words, closed-loop properties should be used. The best manipulation (such as input 2 in this illustration) is assigned to be the primary manipulated variable for the second most important objective. This process is repeated until no more degrees of freedom are available. If there are excess degrees of freedom, they can be used to achieve the optimization objectives.

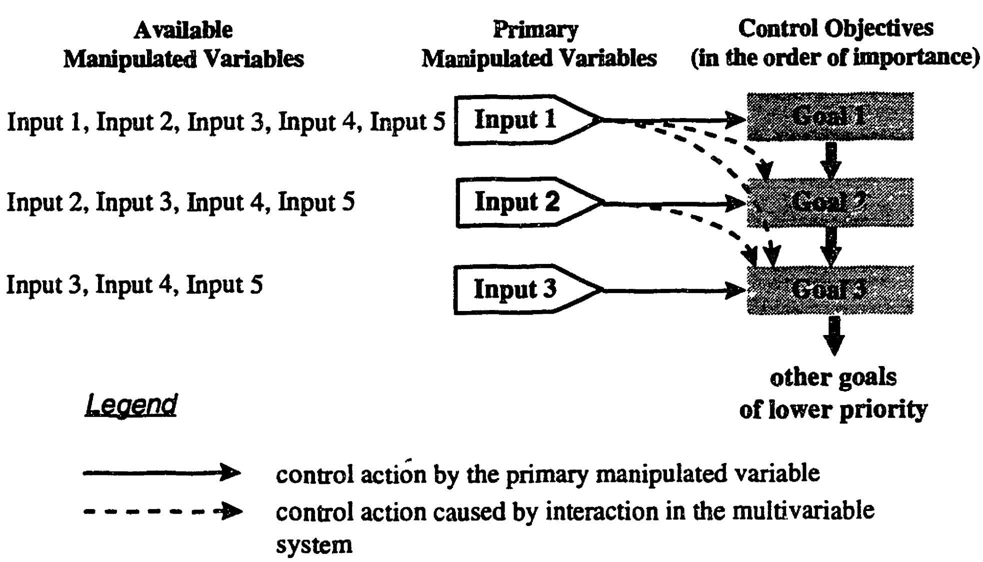


Figure 6 - 2: Visualization of the Control Input Assignment Process

Whenever multiple design alternatives are encountered, all alternatives will be maintained by initiating branching and generate a decision tree. Branching is stopped whenever it becomes obvious a certain decision path (a decision path is one which identifies a set a control input assignments to a set of prioritized control objectives) would lead to a better outcome at a later stage of the design (i.e. a control objective/goal being evaluated at a later stage). Branching is stopped at this point as a more desirable path from the set of alternatives has been identified. The next goal will only need to consider the extension of this desirable path.

6.4.2 Types of Plant-wide Control Structures

Modular Multivariable Control Structures

The design methodology proposed in this chapter consists of two main features: (1) manipulated variables are assigned sequentially to the control objectives in the order of their importance; (2) the interaction among process variables are being accounted for during the assignment. Thus, the control scheme derived can be directly implemented as a modular multivariable controller. As shown in Figure 6-3, the modular multivariable controller (MMC) is a truly MIMO design (see the expanded view shown on the right-hand side). The computation of control actions systematically shifting emphasis to the more important objectives, while taking into account the interaction among process variables. As a result of the sequential assignment of manipulated variables to each individual production objective, there are distinct associations between control objectives and manipulated variables. Unlike other multivariable controller, the MMC design maintains a fairly transparent and easily comprehensible control structure.

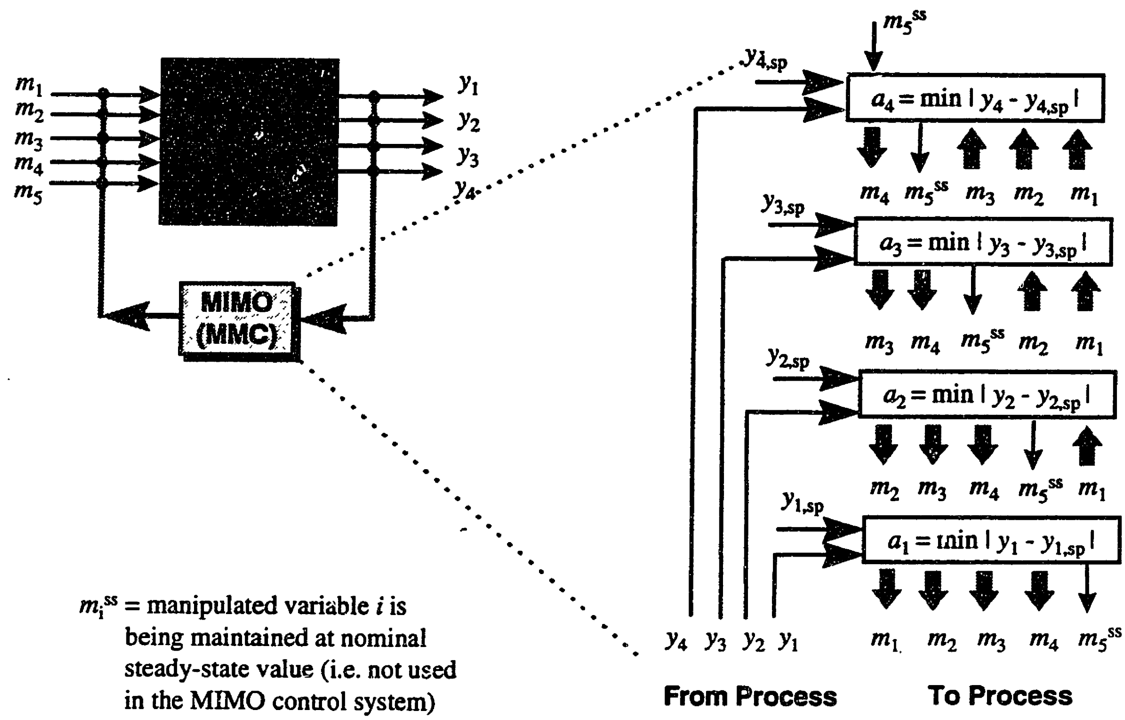


Figure 6 - 3: A MIMO control structure

Single-Input Single-Output Control Structures

Although the use of a fully multivariable controller in the plant is perhaps the most ideal implementation, such a strategy may not be suitable for certain applications. For example, systems which exhibit fast dynamic behavior require frequent update of control actions. If computational power that is required by the multivariable design is not available, a simpler control structures may be desirable. The assignments that we have made though the systematic selection method can be implemented as a set of SISO loops in the plant if the amount of interactions among the process variables is tolerable. Interactions measures such as the static and dynamic relative gain arrays can be used to analyze the suitability of a SISO implementation.

Mixed Control Structures

In most chemical processes, one could find a wide range of process dynamics. Some process variables will react very quickly to changes in process disturbances, others will react slowly. The effect of some process variations can be detected immediately, while other process variations will only be obvious after a long time span has passed. Thus, it is not uncommon that fast control actions are required for the control of process objectives which exhibit fast transient dynamics and slower control actions can be used for those objectives which vary slowly. In such cases, a mixed SISO-MIMO plant control structure such as the one shown in Figure 6-4 can be employed. Fast varying control objectives can be controlled by SISO loops if the amount of interaction among these process variables is tolerable. The slowly varying control objectives can be controlled by a MIMO control structure, such as a MMC.

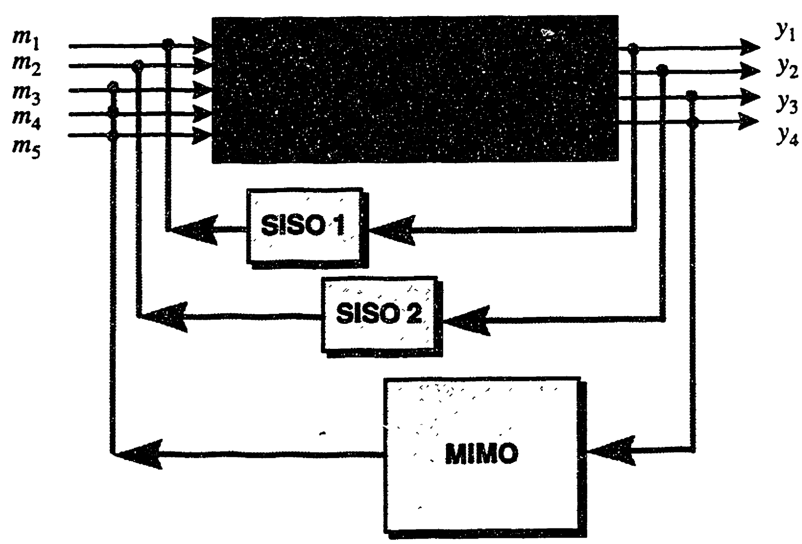


Figure 6 - 4: A mixed SISO-MIMO control structure

6.5 Implementing a Modular Multivariable Controller

The MIMO control of the controlled objectives can be accomplished by the Modular Multivariable Controller (MMC; Mdeadowcroft, 1992; 1997) so that the implementation conforms to the multiobjective approach. A MMC is essentially a model predictive controller (MPC) that is being designed in the goal programming framework. A brief description of the implementation of such controller is described in this section. More details of the implementation can be found in Meadowcroft et al. (1992, 1997).

Suppose a 2 × 2 system can be represented by the following linearized models of the plant of the following form:

$$\hat{y} = \boldsymbol{M}\,\boldsymbol{u} + \boldsymbol{L}\,\boldsymbol{u_o} \qquad [6\text{-}34]$$

where: $\hat{y}$ = vector of predicted outputs (controlled objectives)

$\boldsymbol{u}$ = vector of future control actions

$\boldsymbol{u_o}$ = vector of past control inputs

$\boldsymbol{M}$ = impulse response matrix of output y by the future control action

$\boldsymbol{L}$ = matrix which describes the effect of past control actions on the future outputs

Matrices $\boldsymbol{M}$ and $\boldsymbol{L}$ can be computed using standard techniques described in Prett and Garcia (1988).

The control actions for the two goals are computed through a series of linear programming (LP) optimizations. The objective functions are the 1-norm of the error of the predicted output from the setpoint $\boldsymbol{r_i}$ of goal $\boldsymbol{i}$ over some prediction horizon P, i.e. :

$$a_i = \left\| r_i - \hat{y}_i \right\|_1 \qquad [6\text{-}35]$$

where $\hat{y}_i(m)$ is the vector of predicted outputs over prediction horizon P. At time-step m ($m \leq P$), let $r_i(m) - y_i(m) = k_i^+(m) - k_i^-(m)$, where $k_i^+(m)$ and $k_i^-(m)$ are both greater than or equal to zero. Then, the objective function of goal i is simply:

$$a_i = \sum_{m=1}^{P} k_i^+(m) + k_i^-(m) \qquad [6\text{-}36]$$

The first optimization solves for the control actions for the first objective (one of the higher priority) as follows:

$$\text{P5:} \quad a_1^{(1)} = \min_{u_1, k_1^+, k_1^-} \sum_{m=1}^{P} k_1^+(m) + k_1^-(m) \qquad [6\text{-}37]$$

s.t.:

$$M_{11}u_1 + k_i^+ - k_i^- = r_1 - L_{11}u_{o,1} + e_1$$
$$u_1(1+C) = \ldots = u_1(P) = u_1(C)$$
$$k_i^+(m) \geq 0 \ \forall\, m = 1 \text{ to } P,\ i = 1$$
$$k_i^-(m) \geq 0 \ \forall\, m = 1 \text{ to } P,\ i = 1$$

where M_{11} is the impulse response matrix of y_1 by u_1, L_{11} is the matrix of past control action of $u_{o,1}$ on $\hat{y}_1$. Vector e_1 is the model error in a standard MPC algorithm, defined as the difference between the measured output and the predicted output. C is the control horizon and P is the prediction horizon such that $C \leq P$. Optimization P5 computes the optimal value of $u_1^{(1)}$ for the control of y_1 over the horizon P. The achievement level of the first objective is simply $a_1^* = a_1^{(1)}$.

Having obtained the achievement level of the first objective (regardless of the achievement level of the second objective), the control actions for both objectives 1 and 2 can be re-computed by imposing the requirement that the incorporation of control actions for the second objective will not degrade the performance of the first objective, which is of higher priority.

$$\text{P6:} \quad a_2^{(2)} = \min_{u_1, u_2, k_1^+, k_1^-, k_2^+, k_2^-} \sum_{m=1}^{P} k_2^+(m) + k_2^-(m) \qquad [6\text{-}38]$$

s.t.:

$$\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} k_1^+ \\ k_2^+ \end{bmatrix} - \begin{bmatrix} k_1^- \\ k_2^- \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} - \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} u_{o,1} \\ u_{o,2} \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}$$
$$\sum_{m=1}^{P} k_1^+(m) + k_1^-(m) \leq a_1^*$$
$$u_1(1+C) = \ldots = u_1(P) = u_1(C)$$
$$u_2(1+C) = \ldots = u_2(P) = u_2(C)$$
$$k_i^+(m) \geq 0 \ \forall\, m = 1 \text{ to } P$$
$$k_i^-(m) \geq 0 \ \forall\, m = 1 \text{ to } P$$

M_{ij} is the impulse response matrix of output i by u_j. L_{ij} is the matrix which describe the effect of u_{oj} on y_i. Vector e_2 is the model error in a standard MPC algorithm, defined as the difference between the measured output and the predicted output. P6 gives the control actions u_1^* and u_2^* which will minimize the error in the outputs and give preference to the more important objective. Extension to a $n \times n$ MMC design is straight forward.

Chapter 7
Application of Design Techniques to Plant-wide Control System Design

7.1 Introduction

In Chapters 4 through 6, a number of design techniques that are useful for the analysis and synthesis of plant-wide control problems have been presented. The application of these techniques to address various important aspects of the plant-wide control design problem will be demonstrated in this chapter.

7.2 Issues in Operational Stability of Process Plants

So far in the presentation, it has been assumed that the process plant under study is open-loop stable. However, this will not be true for all cases. Plants which contain unstable dynamics are generally harder to control. When a plant is open-loop unstable, it means that if the states are slightly away from their nominal values, the process would not attain a new steady-state by itself but would go exponentially away from the original operating point. Thus, it is important to determine the operational stability of the process plant under study priori to developing the plant-wide control structure for it (the reason for this will be explained in Chapter 8).

Instability in a chemical process plant is typically caused by either:

1. the presence of an inherently unstable unit-operation, like a continuous-stirred tank reactor being operated at an unstable operating point;
2. or the circumstantial interconnections of the plant through the material recycle loops or heat-integration which generate *positive feedback* in the system (Morud and Skogestad, 1994a, 1994b). Positive feedback has the tendency to move eigenvalues toward the right direction and make the response slower (if the eigenvalues stay in the left-half plane) or even unstable (if the eigenvalues cross the imaginary axis and enter the right-half plane).

The former cause generates local effects in the plant while the latter cause produces global phenomena in the process by virtue of the plant interconnections. It will be demonstrated in this section how one can determine if the interconnections of the plant generate unstable dynamics in the overall system without performing rigorous numerical analysis. Particularly, the application of simple structural techniques will be illustrated.

7.2.1 Modification of Process Dynamics by Material or Energy Recycles

Continuous chemical plants generally utilize material recycle streams and make use of some extent of heat-integration of energy sources and sinks. Material recycles are typically introduced to improve yield or conversion, to reuse solvent, intermediates or other liquid/vapor heat carriers, and for economic reasons (Tyreus, 1993a). Heat-integration is primarily done for energy conservation.

Material recycle streams and heat-integration networks give rise to complex interconnections in the plant. They are sources of feedback effects in the system and therefore they modify the dynamics of the individual unit-operations and possibly introduce complex dynamic behavior to the overall system. The next two sections demonstrates how process dynamics is being modified by the feedback mechanism caused by material recycle or heat-integration. Simple techniques can be used to examine the stability of the open-loop process.

7.2.2 Material Recycles and Positive Feedback

Consider a simple recycle system shown in Figure 7-1. Feed A combines with the recycle (assume pure A) is partly converted into B in the reactor. The reaction mixture is separated and a fraction of A is recycled back to the reactor. A simple local numerical simulation can illustrate how the material recycle creates positive feedback in the system in this idealized system. The values indicated in Figure 7-1 are the nominal flowrates of the various components in the system. Using the process specifications and relations summarized in Table 7-1, the transient of the various flows in the system to a step change in the molar flow of A into the reactor have been computed and summarized in Table 7-1. In the local numerical dynamic simulation, it has been assumed that the reactor is being kept at isothermal condition so that the pure material recycle effects can be demonstrated. Also, all units in the plant are open-loop stable so any positive effect is due to the interconnections in the plant. For simplicity, it is also assumed that a fixed fraction of A is being recycled back to the reactor (it can be easily shown that this assumption does not alter the results).

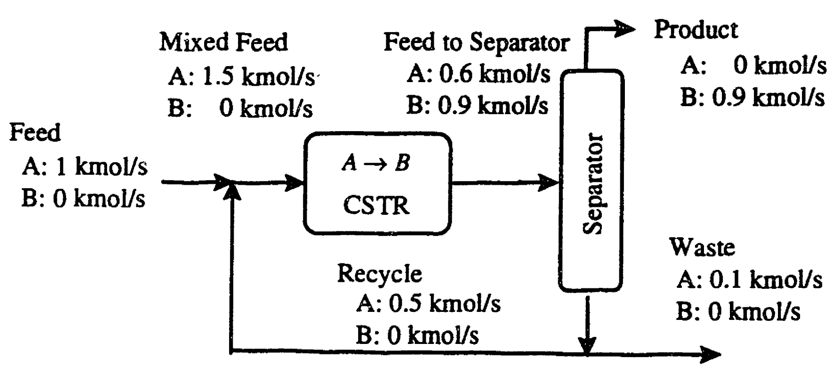


Figure 7 - 1: A simple recycle system

Table 7 - 1: Local Numerical Dynamic Simulation of the Material Recycle Loop

Stream	Feed	Mixed Feed	Feed to Separator	Product	Recycle	Waste
component (mol/s)	A	A	A	B	A	A
(nominal)	1	1.5	0.6	0.9	0.5	0.1
(step up)						
1st round	2	2.5	1	1.5	0.8	0.2
2nd round	2	2.8	1.12	1.68	0.896	0.224
3rd round	2	2.896	1.584	1.738	0.927	0.232
4th round	2	2.927	1.171	1.759	0.937	0.234
5th round	2	2.937	1.175	1.762	0.939	0.235
6th round	2	2.939	1.176	1.764	0.941	0.235
7th round	2	2.941	1.176	1.764	0.941	0.235

Reactor: CSTR
Reactor volume (V_R): 1.5 m^3
Volumetric flow of feed: 1 m^3/s
Initial concentration of A in feed: 1 mol/m^3
kinetic rate constant (k): 1 s^{-1}

Physical Relationships used:
A in Mixed Feed = A in Feed + A in Recycle
A in Feed to Separator = A in Mixed Feed / ($V_R k$+1)
B in Product = A in Mixed Feed - A in Feed to Separator
A in Recycle = (0.5/0.6) * A in Product
A in Waste = (0.1/0.6) * A in Product

See that increasing the concentration of A in the feed increases the molar flow of A in the recycle stream (when A in feed is increased to 2 kmol/s, the amount of A in the recycle increased to 0.8 kmol/s initially), which leads to an reinforcement of the original increase of A in the mixed feed which further increases the molar flow of A in the recycle. The material recycle generates a positive feedback effect. However, the amount of increases per cycle diminishes and so the overall system eventually stabilized to a new steady-state. This quick and simple local numerical analysis shows that this positive feedback does not destabilize the system. Alternatively, Morud and Skogestad (1994b) have shown that a system that consists of a first order reaction in x_i in an isothermal CSTR and a recycle can be described by the following generic equation:

$$\frac{dx}{dt}=\frac{1}{\tau_0}(z_i-(1-\alpha)x_i)-kx_i \qquad [7\text{-}1]$$

and

$$\lambda = -\frac{1}{\tau_0} - k + \frac{\alpha}{\tau_0} \qquad [7\text{-}2]$$

where: x_i = concentration of i in reactor

z_i = concentration of i at the inlet of reactor

k = reaction rate constant

τ_0 = residence time in the reactor (always > 0)

α = fraction of recycled materials ($0 \leq \alpha \leq 1$),

$\alpha = 1$ when all of i is recycled

λ = eigenvalue (root of the equation)

When there is no recycle, (i.e. $\alpha = 0$), $\lambda = -1/\tau_0 - k$ which is always less than zero. When all of i is recycled (i.e. $\alpha = 1$), $\lambda = -k$ and is also less than zero. Thus, this system is always stable. Positive feedback (α / τ_0) makes the response more sluggish by moving the eigenvalue towards the origin but does not destabilize the system.

Now, one of the assumptions is relaxed by allowing the temperature in the reactor to vary. Then, consider an increase in temperature of the feed to the process. An higher inlet temperature would result in a higher adiabatic rise from the exothermic reaction which leads to a higher outlet temperature. The recycle stream is therefore of a higher temperature. Mixing the recycle stream with the feed would reinforce the temperature increase and a positive feedback is again created. Whether this positive feedback would lead to instability in the overall system would depend on the amount of heat generated in the reaction. Morud and Skogestad (1994b) showed that an energy balance for an adiabatic CSTR with a 0^{th} order exothermic reaction, i.e. $r=k(T)$ (0^{th} order reaction was chosen to show the pure temperature effect) yield:

$$\frac{dT}{dt} = \frac{1}{\tau_0}(T_{in} - T) + f(T) \qquad [7\text{-}3]$$

$$f(T) = k(-H_{rxn}) / c_p = kT_{ad} \qquad [7\text{-}4]$$

where:

H_{rxn} = heat of reaction

T_{in} = feed temperature

T = reactor temperature

T_{ad} = adiabatic rise = ($-H_{rxn} / c_p$)

c_p = heat capacity

k = kinetic rate constant

τ_0 = residence time

The root of this equation has been found to be:

$$\lambda = -\frac{1}{\tau_0} + T_{ad} k'(T) \qquad [7\text{-}5]$$

where

$$k'(T) = \frac{dk(T)}{dT} = \frac{kE}{RT^2} \qquad [7\text{-}6]$$

and E (in J/kmol) is the activation energy. This model suggests that the temperature dependency of the reaction has introduced positive feedback and it has moved the eigenvalue to the right, making the response slower or even unstable if $T_{ad}\ k'(T) > 1/\tau_0$. The positive feedback from material recycle has been caused by heat effect so it is in fact a form of *energy recycle*. Effects of energy recycle and heat integration in a plant will be detailed next.

7.2.3 Positive Feedback from Energy Recycle and Heat integration

Energy recycle can occur within the material recycle system in the plant as demonstrated in the previous section, or it can arise as a result of an explicit transfer of energy from heat sources to heat sinks through a heat integration system in the plant. Energy recycle can produce complex behavior in the plant. A physical system studied by Tyreus (1993b) illustrates some phenomenon produced by heat-integration. Consider the reactor pre-heater system shown in Figure 7-2. This process consists of an adiabatic catalytic packed-bed tubular reactor where a *highly* exothermic reaction takes place. For economic reason, a pre-heater has been installed to make use of the heat generated from the reaction to preheat the feed. The stability of this system can be examined though a *qualitative simulation* based on the signed causal digraphs of the system.

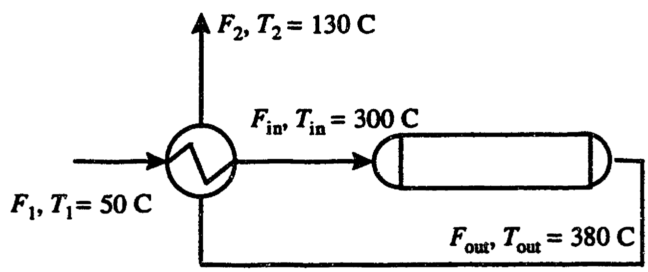


Figure 7 - 2: Reactor pre-heater system, Streams at Design Steady-state Temperatures (from Tyreus, 1993b)

Step 1: Choose the Level of Modeling Detail

The purpose of this qualitative simulation is to determine if heat accumulates in the integrated loop upon changes of the heat content of the inlet stream. Accumulation of heat in the system leads to process instability. Heat content of the feed stream is a function of both the flow rate and the temperature of the stream. To simplify the analysis and to avoid ambiguities, causal models will be developed assuming all flows are constant. If it is found that the system is stable with respect to changes in T_1, the models will be expanded to include the influence of flowrates on the system.

Step 2: Construct the Causal Models

A single staged directed graph (SDG) for the entire process can be constructed by combining the SDGs of individual units (refer to Section 4.2.3 for background about this modeling method).

Feed Pre-heater

The feed is pre-heated by transferring the energy from F_{out} to F_1 in a counter-flow heat exchanger. The flow relations describing the fundamental principles governing the unit are as follows:

$$H_1 + Q_{ex} = H_{in} \qquad [7\text{-}7]$$

$$H_{out} = H_2 + Q_{ex} \qquad [7\text{-}8]$$

$$Q_{ex} = UA\Delta T \qquad [7\text{-}9]$$

$$\Delta T = [\ (T_2 - T_1) - (T_{out} - T_{in})\ /\ [\ln\ (T_2 - T_1)\ /\ (T_{out} - T_{in})] \qquad [7\text{-}10]$$

where: ΔT = the approach temperature of the streams involved in the feed pre-heater

U = heat-transfer coefficient

A = heat-transfer area

$R_h = 1/UA$ = resistance

From our understanding of the physical systems we can develop the following causal interactions:

$$H_{in} = f(+H_1) \qquad [7\text{-}11]$$

$$H_2 = f(+H_{out}) \qquad [7\text{-}12]$$

$$\Delta T = f(-H_1) \qquad [7\text{-}13]$$

$$\Delta T = f(-H_{out}) \qquad [7\text{-}14]$$

$$Q_{ex} = f(+\Delta T) \qquad [7\text{-}15]$$

$$H_{in} = f(+Q_{ex}) \qquad [7\text{-}16]$$

$$H_2 = f(-Q_{ex}) \qquad [7\text{-}17]$$

$$Q_{ex} = f(-R_h) \qquad [7\text{-}18]$$

where $A = f(-B)$ means an decrease in B causes an increase in A. R_h is constant at constant flows, when fouling is ignored

Reactor

This is an adiabatic reactor so the energy balance is given by:

$$H_{in} + Q_{rxn} = H_{out} \qquad [7\text{-}19]$$

$$Q_{rxn} = f(T_{in}) \qquad [7\text{-}20]$$

which can be transformed into the following qualitative interactions:

$$H_{out} = f(+H_{in}) \quad [7\text{-}21]$$
$$Q_{rxn} = f(+H_{in}) \quad [7\text{-}22]$$
$$H_{out} = f(+Q_{rxn}) \quad [7\text{-}23]$$

The SDG for the entire plant is shown in Figure 7-3. It is formed by combining the qualitative interactions for both the pre-heater and the reactor.

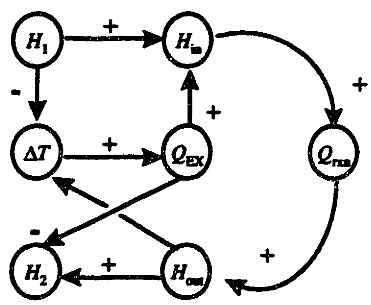


Figure 7 - 3: Single-staged Directed Graph for the Reactor Pre-heater System in Figure 7-2

Step 3: Perform Qualitative Simulation

At constant F_1, increasing T_1 increases H_1. As H_1 is increased, there is a path which directly increases H_{in} and another path which decreases ΔT and ultimately causes a decrease in H_{in}. Thus, the initial effect of a rise in H_1on H_{in} is ambiguous and a quantitative sensitivity analysis is required to determine if an increase in T_1 causes an increase in H_{in}. It is known that the reactor exhibits inverse response to step down in inlet temperature (Tyreus, 1993b). Thus, whether a rise in H_1 causes an increase or decrease in H_{in}, H_{out} increases initially, regardless. Thus, is can be assumed that an increase in T_1 results in a rise in H_{in}. As H_{in} increases, Q_{rxn} increases and therefore H_{out} is higher than before. This increases ΔT and therefore causes a rise in H_{in} again. Positive feedback has been created in the system and the increase of H_{in} caused by a rise in T_1 is being reinforced. Since the reaction is *highly* exothermic (Tyreus, 1993b), the increase in H_{in} caused by the increase in Q_{rxn} would be larger than the increase caused by the increase in T_1 (whose gain would be not exceed one unit). Thus, energy begins to accumulate in the system and the system is open-loop unstable.

The conclusion arise from the qualitative simulation agrees with the numerical stability analysis performed by Tyreus (1993b).

7.2.4 Qualitative Simulation versus Rigorous Numerical Analysis

With the availability of a dynamic model for the entire plant, one could easily test the stability of a system by rigorously determining the eigenvalues or the system or by direct numerical simulation. However, qualitative simulation using causal models offers an attractive alternative. Through systematic examination of the *direct cause* of the instability, feedback stabilizing control strategy can be easily identified. For example, in the tubular reactor-heat exchanger process studied in Section 7.2.3, the system is open-loop unstable. To prevent plant runaway, the heat content somewhere in the energy loop must be maintained at some fixed value. The ability to identify the direct cause of the instability is very important. When the process plant is large, there are many possible sources of process instability the plant may have multiple material and energy recycles, creating complex interconnections. Merely knowing the presence of positive eigenvalues will not assist the designer in correctly identifying where the instability originates.

7.3 Managing Material and Energy Flows in Process Plant

Many researchers and practitioners (Buckley, 1964; Shunta, 1981; Price and Georgakis, 1993; Layman and Georgakis, 1995, Downs, 1993a) have identified that the management of materials and energy in the plant to be the most fundamental process control issue. Buckley (1964) stated that the purpose of material balance control is to meet the specification on plant production level as well as to maintain a proper coordination of material flows in the process plant. Energy balance control, although less emphasized by past researchers, plays an equivalent role in the proper operation of the plant. Accumulation or depletion of energy in the system may lead to plant runaway. In the sections that follow, the peculiarity of plant materials and energy management will be illustrated.

7.3.1 Controlling Material Inventories

In a complex process plant that is composed of units interconnected by forward process streams and recycles, materials accumulate in many holding tanks. The overall material in the plant is distributed into multiple inventories. Each non self-regulating inventory is a process integrator. The flows in and out of each inventory must be balanced to prevent accumulation in that part of the plant. Hence, inventory control in a plant relies on proper coordination of the control of individual distributed inventories.

Downs (1993a) illustrated through a simple process with a recycle stream that improper coordination of unit inventory control strategies will create operational problems. Consider the process shown in Figure 7-4 (a). Suppose there is an increase in the flow of F_1 in the diagram. The control inventory control strategy for Unit A will react by increasing the flow of F_2. As the flow of F_2 increases, the inventory control strategy for Unit B will respond by increasing the flow of F_4. Any increase of F_4 will reinforce the original upset caused by an increase in F_1, creating a positive feedback in the plant that is not going to diminish. Although the inventories in the units are being maintained at fixed levels, materials in the plant accumulate in streams 2 and 4 and will eventually lead to problems in the operation. Even though the control of the individual distributed inventories in the plant are locally stable, globally the two control strategies are incompatible and generate destabilizing effect in the plant. Inconsistency exists in the inventory control structure for this process. A *globally integrative* system has been produced. Hence, it is important to maintain a global perspective and account for both long and short-range interactions during the design of control structures for large complex systems. Similar analysis on the control strategies used in Figure 7-4 (b) to (c) will show that they are both *globally stabilizing.*

The pitfall in the control design demonstrated in Figure 7-4 (a) could have been prevented if a systematic analysis had been performed on the system. The next two sub-sections will demonstrate the application of the structural and quantitative techniques introduced in Chapters 4, 5 and 6 to design *feasible* material inventory control system for this process plant.

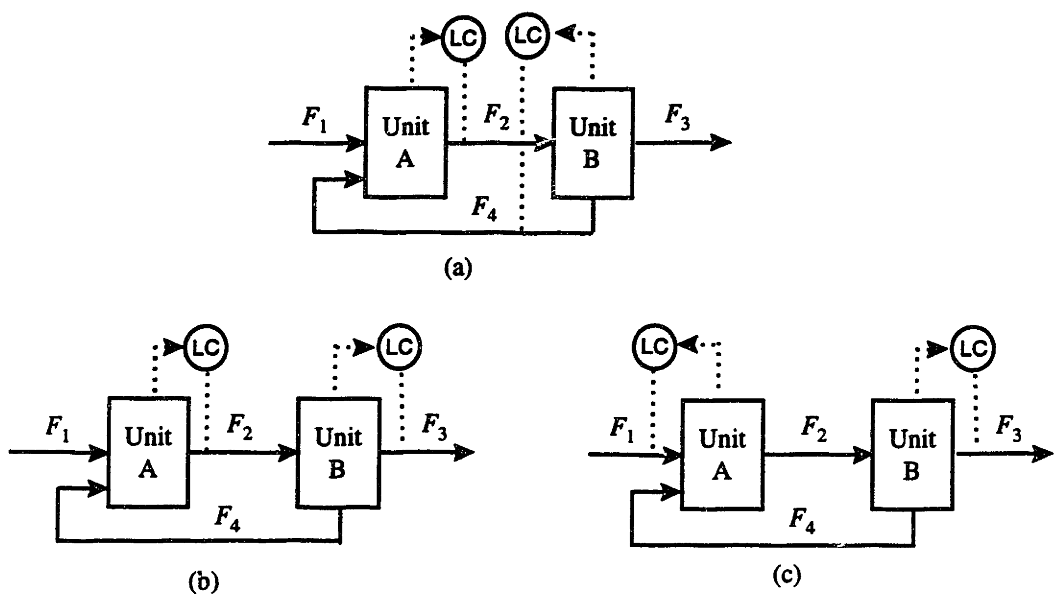


Figure 7 - 4: Inventory Control Strategies for a Process with Recycle (from Downs, 1993a)

Structural Representation of Material Flows in Process Plants

A Boolean (structural) representation of the plant can be constructed using "+1" to represent incoming arcs and "-1" to represent outgoing arcs as in Table 7-2.

Table 7 - 2: Structural matrix for the process in Figure 7-4 (Open-loop)

	F_1	F_2	F_3	F_4
Unit A	+1	-1		+1
Unit B		+1	-1	-1

The control structure in Figure 7-4 (a) has assigned F_2 to control the inventory in Unit A. In a multivariable system, selection of manipulated variables for the subsequent control objectives must account of the interaction effect from the known control assignments. The effect of the control of inventory in A using F_2 can be accounted for by substituting the influence of F_2 on A into the second row of the matrix. The updated matrix is found in Table 7-3. Table 7-3 reflects the fact F_2 has been selected as a manipulated variable in the control system and is no longer an available degree of freedom for the control of the inventory in B. Additionally, F_1 has been identified to be a manipulated variable as a result of the interaction in the closed-loop system. While we have gained a manipulation through interaction, we have also lost F_4 for the same reason. This matrix correctly indicates that only F_1 and F_3 are feasible choices. One can conclude that the control structure shown in Figure 7-4 (a) is clearly unacceptable. The control structure used in Figure 7-4 (b) would be a feasible one.

Table 7 - 3: Unit A controlled by F_2

	F_1	F_2	F_3	F_4
Unit A				
Unit B	+1	n/a	-1	

The structure shown in Figure 7-4 (c) uses F_1 to maintain the inventory in Unit A. Since F_1 has no direct influence on the inventory in Unit B (see Table 7-2), the structural representation for the inventory in Unit B does not have to be adjusted and it is simply identical to the original description as shown in Table 7-4. The matrix shows that either F_2, F_3 or F_4 are feasible choices. This confirms that structure used in Figure 7-4 (c) is a workable solutions.

Table 7 - 4: Unit A controlled by F_1

	F_1	F_2	F_3	F_4
Unit A				
Unit B	n/a	+1	-1	-1

Quantitative Analysis in the Modular Multivariable Design Framework

Structural analysis is helpful in identifying feasible control alternatives, but it does not offer us any additional insight as to how to evaluate our choices. The quantitative analysis presented in Chatper 5 can be combined with the modular multivariable control design framework introduced in Chapter 6 to resolve this issue.

The process shown in Figure 7-4 consists of only one component with the following nominal stream flow rates: F_1 = 22 mol/hr, F_2 = 30 mol/hr, F_3 = 22 mol/hr and F_4 = 8 mol/hr. In the long-horizon, it is desired to maintain the material inventory in the system at steady-state. The residuals (r_A and r_B) of the material balance equations can be written as follows:

Unit A: $r_A = F_1 + F_4 - F_2$ [7-24]

Unit B: $r_B = F_2 - F_4 - F_3$ [7-25]

The open-loop gain of r_A and r_B for a unit change (1% change) of each of the streams is simply given by:

$$\delta r_{k,F_i} = x\delta F_i \quad k = \text{A or B} \qquad [5\text{-}17]$$

where x is the composition of the material of interest. In this case, x is equal to 1 since we are dealing with a single-component process. The open-loop gains have been computed in Table 7-5.

Table 7 - 5: Open-loop Gains for the Process in Figure 7-4

F_i	F_1	F_2	F_3	F_4
r_{A,F_i}	0.22	-0.30	0	0.08
r_{B,F_i}	0	0.30	-0.22	-0.08

The design criteria for long-horizon control stated in Section 6.3.1 suggest that a control objective should be assigned to a manipulated variable which has a large gain and has the minimal effects of model uncertainty. Without loss of generalization, it will be assumed for the time being that the maintenance of the inventory in Unit A is more important. Also for simplicity, it will be assumed that there is no error in our models. Primary manipulated variables to each of the control objectives based solely on the size of the gain as a measure of the likelihood of the input reaching its saturation limits. Clearly, F_2 has the largest gain and is the best input for the maintenance of inventory in Unit A.

Having the primary for Unit A selected, the gains of the residual of the inventory balance in Unit B must be updated to reflect the closed-loop control of the inventory in Unit A by F_2. The closed-loop gain of the inventory of Unit B can be computed by:

$$G_i = \left[\frac{\det(A)}{\det(A')}\right] \qquad [7\text{-}26]$$

where $A = K^i_{p_1 p_2 \cdots p_i}$

$A' = K^{i-1}_{p_1 p_2 \cdots p_{i-1}}$

$K^i_{p_1 p_2 \cdots p_i}$ = $i \times i$ open-loop gain matrix of the first i^{th} objectives, with manipulated variables p_1 , p_2 … p_{i-1} selected as the primary manipulated variables for goal 1, 2,… (i-1)etc. p_i is the manipulated variable being considered as a candidate for goal i.

Using Equation [7-26], the closed-loop gain of the inventory in Unit B for a change in F_1 is computed as shown below:

$$A: \quad \begin{array}{c} \\ \delta r_A \\ \delta r_B \end{array} \begin{array}{c} \begin{array}{cc} F_2 & F_1 \end{array} \\ \begin{bmatrix} -0.30 & 0.22 \\ 0.30 & 0 \end{bmatrix} \end{array} \tag{7-27}$$

$$A': \quad \begin{array}{cc} & F_2 \\ \delta r_A & [-0.3] \end{array} \tag{7-28}$$

Then, det(A) = -(0.3)(0.22), det(A') = -0.3. The closed-loop gain of the inventory of A for a unit change of F_1 is therefore 0.22. The closed-loop gains by other inputs are given in Table 7-6.

Table 7 - 6: Closed-loop Gains (Unit A by F_2)

	F_1	F_2	F_3	F_4
Unit B	0.22	0	-0.22	0

By explicitly accounting for the interaction caused by the control of the inventory in Unit A by F_2, one can correctly identify that F_2 is no longer an available manipulated (since the size of the closed-loop gain is zero). Furthermore, Table 7-6 indicates that a manipulation F_1 is gained as a result of interaction and F_4 is an infeasible choice. Since the magnitudes of the closed-loop gains for F_1 and F_3 are the same, either F_1 or F_3 can be assigned to be the primary manipulated variable for Unit B. Hence, using the modular multivariable design framework with the given nominal flowrates, the following structures have been identified to be promising candidates for the system:

1. Structure 1:
   - Control inventory in Unit A by F_2
   - Control inventory in Unit B by F_1
2. Structure 2:
   - Control inventory in Unit A by F_2
   - Control inventory in Unit B by F_3

By designing control structures within the modular multivariable design framework, control alternatives that can best accomplish the control objective can be systematically identified. The selection of inconsistent control structures has also been prevented by explicitly accounting for the interaction produced by closed-loop control of plant objectives.

7.3.2 Controlling Throughput

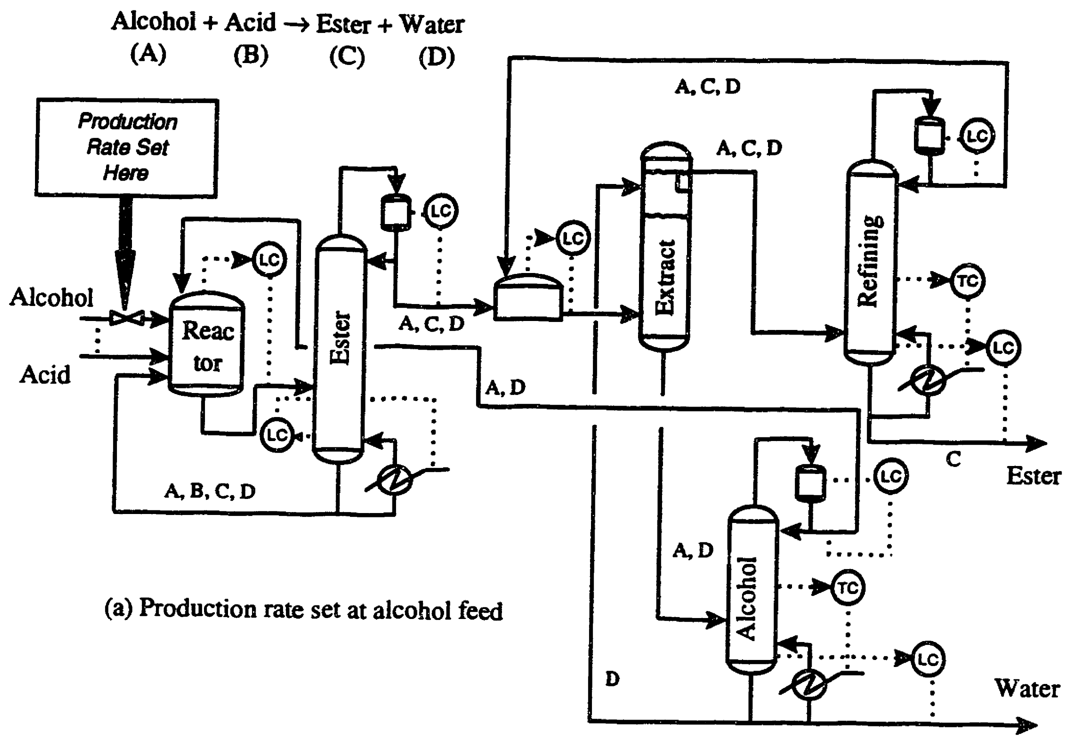
It has been suggested by Downs (1993c) that the location at which the production rate is set has a great influence on the operation of the inventory control system. Figure 7-5 shows two different overall inventory control schemes for the esterification process which Downs (1993c) has studied. The following reaction takes place in the reactor (the letters in parenthesis are symbols which will be used to refer to the various compounds the in the rest of the discussion in this section):

$$\text{Alcohol (A)} + \text{Acid (B)} \rightarrow \text{Ester (C)} + \text{Water (D)} \qquad [7\text{-}29]$$

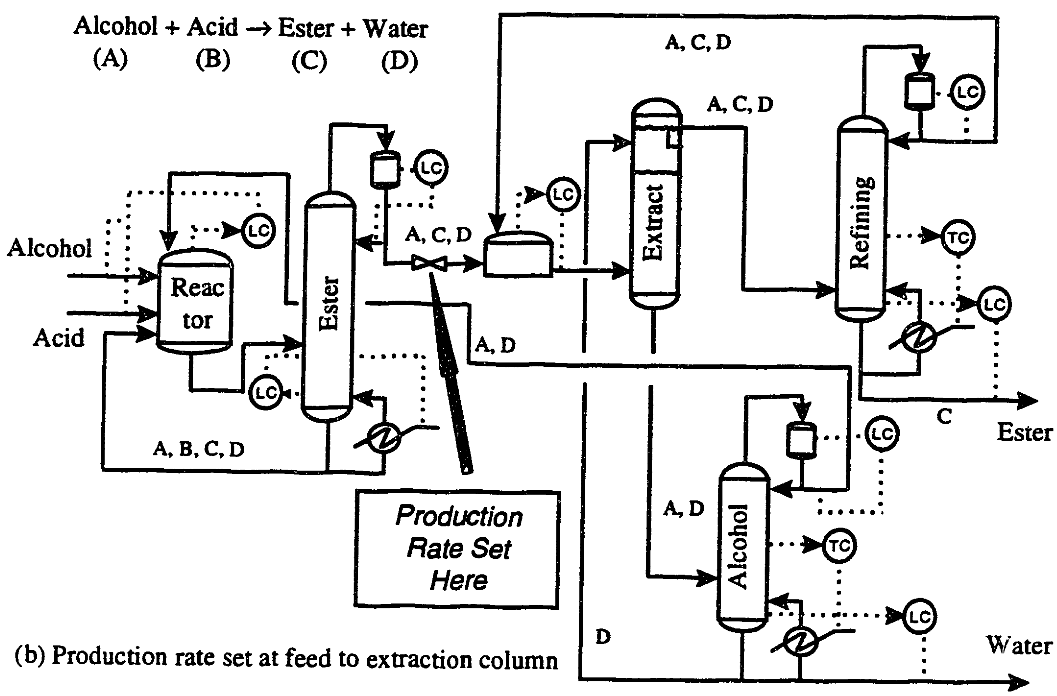
In the esterification process, acid reacts with alcohol in the reactor to produce ester and water. The reaction mixture is processed in the ester column where acid is separated. The distillate of the ester column contains the product, ester, as well as water and alcohol. Using water as the solvent in the extraction column, part of the alcohol is separated from the mixture. The top stream coming off from the extraction column has a higher concentration of ester but there is still a large amount of impurities. This stream is further refined in the refining column where ester is purified in the bottom. The distillate of this column contains mostly alcohol and water and a small amount of ester. This stream is recycled back to the extraction column for further ester recovery. The bottoms of the extraction column is a mixture of alcohol and water. Alcohol in this stream is being separated from the water in the alcohol column and is recycled back to the reactor.

In Figure 7-5 (a), the production rate of the process is set at the feed (alcohol). Except for the level of the esterification column which is controlled by the steam, all other distributive inventories are controlled by the outlet streams. In Figure 7-5 (b), the production rate is set at the feed to the extraction column. Then, the levels of the distributive inventories upstream of the location where production rate is set have to be controlled by manipulating the inlet streams.

It has been found by Downs (1993c) that the overall inventory control scheme in Figure 7-5 (a) to exhibit some undesirable phenomenon which centers in the recycle stream that sends the distillate of the refining column back to the intermediate storage tank for further ester purification.



(a) Production rate set at alcohol feed

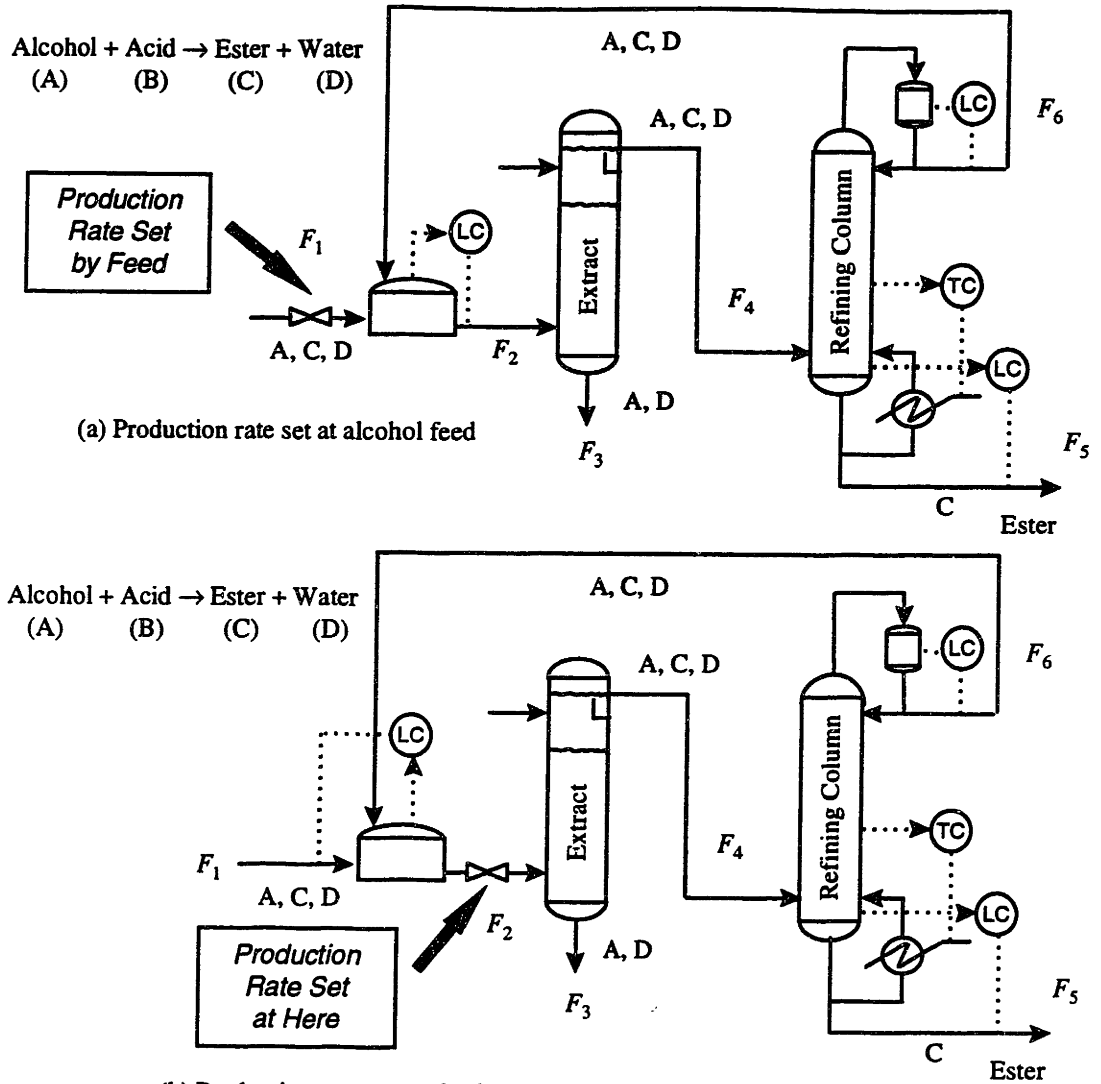


(b) Production rate set at feed to extraction column

Figure 7 - 5: Esterification Process (from Downs, 1993c)

Down (1993c) has offered an explanation of the root cause of the stability problem in the control structure in Figure 7-5 (a). Consider the problematic area isolated in Figure 7-6 (a). Since the control scheme sets the production rate at the feed, by virtue of the inventory controls at the reactor and the condenser of the esterification column, the feed to the intermediate storage tank is directly affected by the production rate, i.e. F_1. When the production rate is increased, F_1 will increase which causes the level of the intermediate storage tank to rise. The inventory control scheme will cause F_2 to go up as well. F_2 consists of a mixture of alcohol, water and ester. As shown in the diagram, ester (the product) will go preferentially to the top layer. The level of the top layer is controlled by a weir at the top of the vessel and the excess amount leaves the vessel by overflow. The top level is therefore self-regulating. As the rate of product increases, the rate of ester entering the extraction column increases as well and the flow of F_4 will rise as a result of an increased rate of ester entering the unit. F_4 contains ester as well as alcohol and water. Since the separation of ester from the mixture in the refining column is not perfect, there will be an increase of accumulation of material in the condenser of the refining column and the flow F_6 will rise as a result of that. Notice that F_6 is being recycled back to the intermediate storage tank, causing the level of inventory to increase further. A positive feedback loop has been created in the system. From Equation [7-2], for a non-reactive systems with the reaction constant equal (such as this portion of the esterification process), the amount of increase in the flow of F_6 should diminish in each cycle of the "loop" so the positive feedback will not generate instability in the system. However, positive feedback from the recycle loop does increase the sluggishness of the plant response. Furthermore, Downs (1993c) noted that during plant operation, an sudden increase in the production rate may cause flooding in the extraction column. Also, if the control valve on F_6 has not been sized to account for the potential increase in flow of F_6 as a result of production rate increase, F_6 may hit its saturation limit before the new steady-state is reached. When that happens, there is no feasible solution for the increase in production rate.

Alternatively, if the production rate is set at the feed to the extraction column (see Figure 7-6 (b)), an increase in production rate would only impact the process upstream. The extraction column and the recycle stream F_6 are not affected. This inventory control scheme does not generate positive feedback in the system.



(a) Production rate set at alcohol feed

(b) Production rate set at feed to extraction column

Figure 7 - 6: Esterification Process - Isolated Separation Section (from Downs, 1993c)

Systematic Study of Interaction Between Throughput Control and Material Inventory Control

Implicit in Downs' study of the esterification process (Downs, 1993c) is that the inventory control scheme is designed *independently* and *after* the location for production rate control has been selected. It will be shown in this section that by systematically accounting for the effect of the closed-loop inventory control in the system, one can arrive at a production rate control strategy that complements the inventory control strategy in the plant.

Consider the problematic area in the esterification process as shown in Figure 7-6 (a). Confining the analysis to the recycle loop, there are three distributed inventories: the material inventory in the intermediate storage tank (r_A); the material inventory in the ester-rich phase of the extraction column (r_B); and the material inventory in the condenser of the refining column (r_C). The material inventories in this portion of the esterification process can be represented by the Boolean (structural) matrix in Table 7-7. Again, a value of "+1" is used to represent streams entering the inventory, "-1" for streams leaving the inventory.

Table 7 - 7: Open-loop Structural Description of the Esterification Process

	F_1	F_2	F_3	F_4	F_5	F_6
r_A	+1	-1				+1
r_B		+1		-1		
r_C				+1		-1

In this illustration, the inventory control systems derived by Downs (1993c) in Figures 7-6 (a) and (b) will be reproduced. The most suitable locations to set the plant throughput for both cases will by systematically determined.

Case I: Control r_A by F_2

F_2 is assigned to be the primary manipulated variable for r_A to reproduce the control scheme shown in Figure 7-6 (a). The structural matrix in Table 7-8 represents the effect of the system when r_A is under closed-loop control by F_2. As result of the interaction, F_1 and F_6 have gained influence on the inventory in r_B.

Table 7 - 8: M_A controlled by F_2

	F_1	F_2	F_3	F_4	F_5	F_6
r_A						
r_B	+1	n/a		-1		+1
r_C		n/a		+1		-1

Notice that the inventory of r_B is in fact self-regulating. The level is being maintained at the desired height by a weir at the top of the tower. The flow of F_4 adjusts according to the rate at which the level is rising. In effect, it is like F_4 has been selected to the primary manipulated variable to control the inventory in r_B. Since F_2 has no direct influence on r_C, the row which corresponds to r_C in the matrix does not have to be updated. Having identified the self-regulating feature, the structural matrix which indicates the effect of the remaining manipulations on r_C when both r_A and r_B are under closed-loop control is shown in Table 7-9:

Table 7 - 9: r_A controlled by F_2; r_B controlled by F_4

	F_1	F_2	F_3	F_4	F_5	F_6
r_A						
r_B						
r_C	+1	n/a		n/a		

Downs's control structure (Downs, 1993c) assigned F_6 to maintain the inventory r_C. The structural matrix in Table 7-9 indicates that due to process interaction, F_6 is in fact not a feasible choice. The results is not surprising given the knowledge of Downs' study which was discussed earlier. F_1 is the only manipulated variable which can be used to maintain the inventory r_C without upsetting the plant. Thus, systematic analysis of the closed-loop effect of the control of the individual distributed inventories has prevented generation of a problematic control structure.

Note that in the portion of the system under investigation, there are 6 inputs and 3 material balance equations. F_1, F_2 and F_4 are involved in the material balance control scheme. The values of the other three streams must be defined for the system to be completely specified. The flows of F_3 and F_5 have been specified elsewhere in the plant, not shown in Figure 7-6 (a). Therefore, the remaining stream F_6 is the location at which the production rate of the process should be set.

Case II: Control r_A by F_1

To reproduce the inventory control scheme used in Figure 7-6 (b), F_1 is assigned to be the primary manipulated variable for the control of inventory in r_A. With this selected, the structural matrix in Table 7-7 should be adjusted to reflect the closed-loop control of this objective as shown in Table 7-10.

Table 7 - 10: Control r_A by F_1

	F_1	F_2	F_3	F_4	F_5	F_6
r_A						
r_B	n/a	-1		-1		
r_C	n/a			+1		-1

Since F_1 has no direct influence on r_B and r_C, the rows which concerns r_B and r_C in the updated matrix is identical to the ones for the open-loop process. Once again, the material inventory of r_B is self-regulating and F_4 is directly related to the rate of flow of the inlet stream. Given this, the structural matrix is further adjusted to reflect the maintenance of r_B by F_4:

Table 7 - 11: Control r_A by F_1; control r_B by F_4

	F_1	F_2	F_3	F_4	F_5	F_6
r_A						
r_B						
r_C	n/a	-1		n/a		-1

In this case, either F_2 or F_6 are feasible choices. Selecting F_6 to control the inventory in r_C would reproduce the control structure shown in Figure 6-7 (b) which had been found by Downs (1993a) to be a stabilizing control strategy. The flows of F_3 and F_5 are set externally. F_2 is the location at which the production rate should be set.

Conflict demonstrated in the control structure used in Figure 7-6 (a) is prevented by systematically accounting for the closed-loop effect produced by each element in the inventory control system. As shown in the case studies, the location where the throughput rate is set is intricately related to the plant's inventory control scheme. The production rate must be set by a stream whose value can be freely adjusted without generating any conflict with the inventory control system. The two case studies have shown that structural techniques can be used to identify these closed-loop influences. Naturally, a quantitative analysis of the system within the modular multivariable framework would explicitly account for these effects as well (recall example in Section 7.3.1). One must ensure the control strategies for throughput and inventory control are compatible with each other.

7.3.3 Controlling Inventories of Individual Components

Applications of design techniques presented in Chapters 4 through 6 to synthesize feasible overall material balance control schemes have been demonstrated in Sections 7.3.1 and 7.3.2. Overall material balance control is usually sufficient to prevent accumulations in individual unit-operations. For a process plant, Downs (1992) observed that material balance must be maintained not only from an overall viewpoint, but also for each component in the system. In general, the following relationship holds for each component in the system:

Accumulation = Input enters through system boundary
+ Generation within the system
- Output which leaves through the system boundary [7-30]
- Consumption within the system

The accumulation term in Equation [7-30] must be equal to zero for strictly stable steady-state operation. If the rate at which the component leaves the system is a function of the amount of the component present within the system, the component inventory is self-regulating, otherwise, it is integrating.

Trace components recycle to extinction. In some cases, the rate of accumulation or depletion of a component is so slow that the balance can be re-established by periodically replenishing any lost amount or discharge the excess batchwise. For components which present in the plant in significant quantities, the control strategy must take the component balance control into account. Downs (1992) has shown that the control strategies employed in the individual unit-operations are tied closely to the overall process control of component inventories. For example, a level control scheme for materials in a simple process vessel maintains an overall balance of materials in the tank. By virtue of this level controller, the individual component inventory in the tank are also being maintained at fixed values. Increase in the inflow of one component will be corrected by the level controller which will increase the outflow of the vessel, and thus the outflow of that component.

Improperly designed overall material inventory control scheme may not account for all component inventories in the plant. When the scope of process control is expanded to the entire plant, there will be more opportunities for individual components to accumulate or deplete in the system. Down (1992; 1993a) has shown how seemingly acceptable plant-wide control schemes may cause one or more components to accumulate in the process. Down's processes will be used in the next two case studies to show how one can systematically generate control configurations which are compatible with component balance control.

Case Study: Methanol Recovery Process

Figure 7-7 shows the plant-wide control structure for a methanol recovery process which Downs (1992; 1993a) has studied. In this process, stream 1 is a 10 mol/h water feed used to scrub a 100 mol/h nitrogen offgas stream; stream 2 contains 10 mol% methanol. The scrubbed nitrogen is vented and the water-methanol mixture is sent to a distillation column where methanol is concentrated in the distillate to 90 mol%. The water at the bottom of the distillation column is recycled back to the scrubber.

Downs (1992; 1993a) proposed a control system which maintains the levels at the base of the scrubber and distillation column by manipulating the bottoms flows. There is a composition control strategy at the top of the distillation column to ensure the product specification can be met. Feed flows are set at fixed values. The component inventory table corresponding to the closed-loop system is shown in Table 7-12 (Downs, 1993).

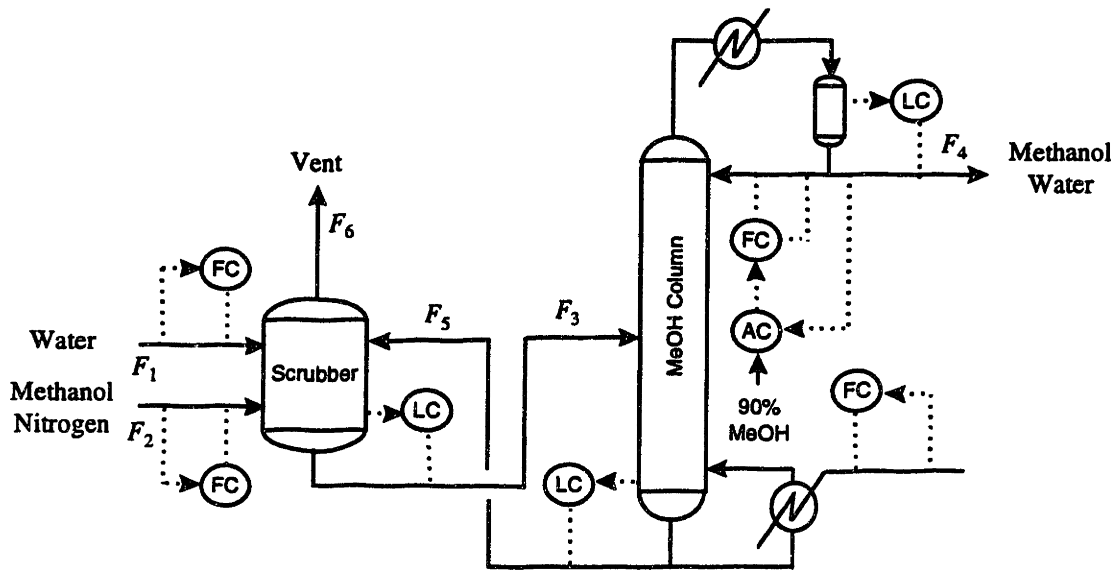


Figure 7 - 7: Plant-wide control Structure for a Methanol Recovery Process (from Downs, 1993a)

Table 7 - 12: Component Inventory table for the Controlled Methanol Recovery Process in Figure 7-7

	Input	+ Generation	- Output	- Consumption	=Accumulation
Component	Enters through system boundaries	Produced within the system	Leaves through system boundaries	Consumed within the system	Inventory controlled by?
Water	F_1	0	F_4 and small amount in F_6	0	Not self-regulating
Methanol	F_2	0	F_4	0	Self-regulating via the distillation comp. control
Nitrogen	F_2	0	F_6	0	Self-regulating via the vent to atmosphere

Under the proposed control scheme, the component inventory control of water is not self-regulating. The composition controller has set the rate of water and methanol leaving the process to be at 90/10. Thus, there will only be a balance of water in the system if the ratio of the rate of water to rate of methanol entering the scrubber is also at exactly 90/10. Since this is not the case, there is no mechanism in the plant which will account for the variation in the water to methanol feeds ratio. Consider the case where the ratio of the water feed to methanol is greater than 90/10. Since the composition of the column distillate is being maintained at 90% of methanol, any excess water must be passed to the bottoms, causing the level to rise. As the level goes up, the level controller at the bottom of the distillation column will force water to be recycled back to the scrubber. A positive feedback has been created. Water begins to accumulate in the recycle stream.

Downs (1993a) suggested that the water inventory control problem could be remedied by choosing water feed to control the level in the scrubber as shown in Figure 7-8. In the improved control structure, once water begins to accumulate in the scrubber, causing the level to rise, the rate of water entering the process will be reduced by the level controller, restoring the balance of the water inventory in the system.

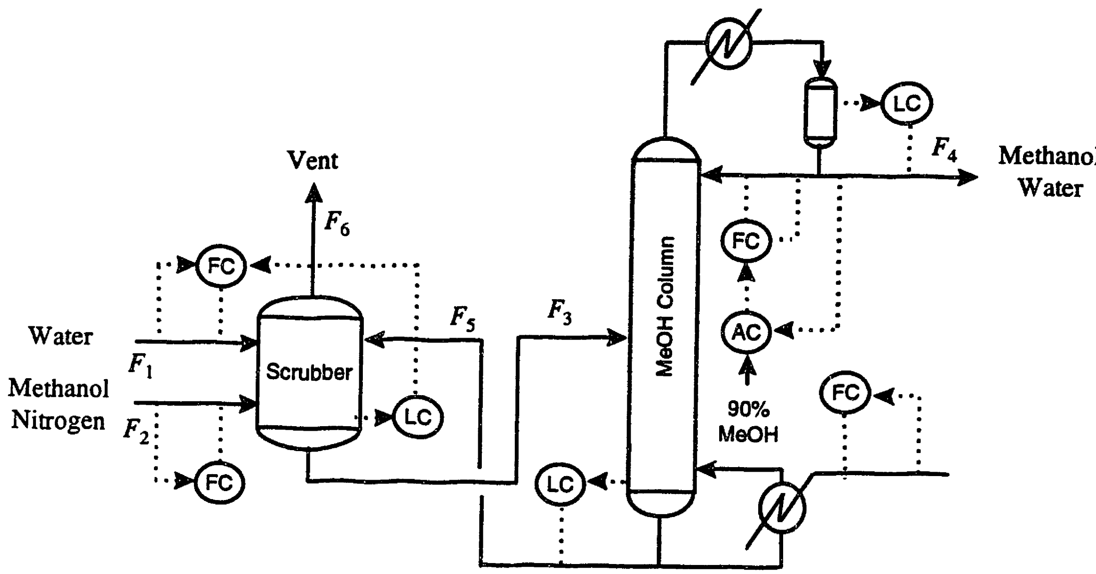


Figure 7 - 8: Improved plant-wide control structure for a methanol recovery process (from Downs, 1993a)

The methanol recovery process can be systematically analyzed using techniques introduced in Chapters 4 through 6. First, the complexity of the design problem can be reduced by studying the input-output representation of the process (Figure 7-9). At the input-output representation of the plant (Figure 7-9) only F_1, F_2 F_4 and F_6 are observable. There are 3 components in the process, none of them are reactive so according to equation [5-1], 3 individual material balances are required to completely defined the material balance at the input-output level. These material balances (MBs) are:

MB for H_2O: $r_{\text{overall, H2O}} = F_{1,\text{H20}} - F_{6,\text{H2O}} - F_{4,\text{H20}}$ [7-31]

MB for MeOH: $r_{\text{overall, MeOH}} = F_{2,\text{MeOH}} - F_{4,\text{MeOH}}$ [7-32]

MB for N_2: $r_{\text{overall, N2}} = F_{2,\text{N2}} - F_{6,\text{N2}}$ [7-33]

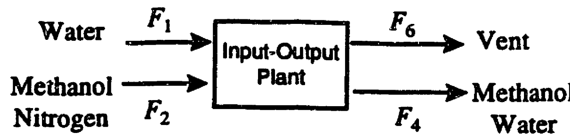


Figure 7 - 9: Input-Output Representation of the Methanol Recovery Process

Again, $F_{i,j}$ is the molar flow of component j in stream i. If F_1 and F_2 remain to be fixed (following Downs' (1992; 1993a) stipulations), only F_6 and F_4 are manipulatable inputs. Then, $F_{6,N2}$ must vary to maintain the $r_{overall,\ N2}$ to be at zero. Similarly, $F_{4,MeOH}$ must be manipulated in order to keep $r_{overall,\ MeOH}$ at zero for any variation in $F_{2,MeOH}$. For the material balance of water, either $F_{6,H2O}$ or $F_{4,H2O}$ can be use to maintain $r_{overall,\ H2O}$ at zero. However, we expect only a trace amount of water will leave the process via the vent (F_6) so $F_{4,H2O}$ is the preferred choice. Our analysis indicates that mechanisms must exist to separately adjust the flows of $F_{6,N2}$, $F_{4,MeOH}$ and $F_{4,H2O}$ in order to balance the residuals of the material balance equations. Other than the nitrogen balance, there is no internal mechanism that will adjust $F_{4,MeOH}$ and $F_{4,H2O}$ according to the level of accumulations of water and methanol. We must provide some feedback control schemes to accomplish these tasks. Thus, $F_{4,H2O}$ and $F_{4,MeOH}$ must vary independently. Hence, the control structure shown in Figure 7-7 which fixes the flows of both feed streams and set the composition of methanol in F_4 by a composition controller violates the material balance constraints. As the ratio of $F_{4,H2O}$ to $F_{4,MeOH}$ must be fixed at 10 to 90, only one of them can be varied for material balance control. $F_{4,MeOH}$ is the only manipulated variable available for the maintenance of the material balance of methanol. $r_{overall,MeOH}$ must be maintained by $F_{4,MeOH}$. Then, $F_{4,H2O}$ cannot be used in the material balance for water. In order to ensure $r_{overall,\ H2O}$ is zero at steady-state, $F_{1,H2O}$ must be used for feedback control. Note that the improved control structure shown in Figure 7-8 is consistent with the conclusion from the analysis on the material balance equations.

Material balance equations for both the scrubber and the distillation column must be developed in order to incorporating more details in the input-output viewpoint to expose all units in the entire plant (Figure 7-7).

Scrubber:

MB for H_2O: $r_{scrubber,\ H2O} = F_{1,H2O} + F_{5,H2O} - F_{6,H2O} - F_{3,H2O}$ [7-34]

MB for MeOH: $r_{scrubber,\ MeOH} = F_{2,MeOH} - F_{3,MeOH} - F_{5,MeOH}$ [7-35]

MB for N_2: $r_{scrubber,\ N2} = F_{2,N2} - F_{6,N2}$ [7-36]

Distillation Column:

MB for H_2O: $r_{distill,\ H2O} = F_{3,H2O} - F_{4,H2O} - F_{5,H2O}$ [7-37]

MB for MeOH: $r_{distill,\ MeOH} = F_{3,MeOH} - F_{4,MeOH} - F_{5,MeOH}$ [7-38]

(The amount of nitrogen present in the distillation column is negligible.)

The structural matrices in Table 7-13 have been developed for the material balances of water and methanol to assist the consistent selection of manipulated variables.

Table 7 - 13: Structural Representation of the Water and Methanol Balance Equations (Open-loop)

	$F_{1,H2O}$	$F_{6,H2O}$	$F_{3,H2O}$	$F_{5,H2O}$	$F_{4,H2O}$
H_2O scrubber	+1	-1	-1	+1	
H_2O distillation			+1	-1	-1
	$F_{2,MeOH}$	$F_{3,MeOH}$	$F_{5,MeOH}$	$F_{4,MeOH}$	
MeOH scrubber	+1	-1	+1		
MeOH distillation		+1	-1	-1	

Since the variables which appear in the material balances of water do not affect those for methanol, the control of the material balances of both components can be studied separately. Recall from our earlier analysis at the input-output level that $F_{1,H2O}$ and $F_{4,MeOH}$ should be used as manipulated variables, these choices would remain to be manipulated variables at the lower level as well (the details of the logic will be explained in Chapter 8). These two variables do not have direct influence on $r_{distill,H2O}$ and $r_{scrubber,MeOH}$ so there is no need to update the structural matrix to account for the closed-loop effects of using $F_{1,H2O}$ and $F_{4,MeOH}$ as primary manipulated variables. Due to the requirement on product purity, $F_{4,H2O}$ is not an available manipulation. $F_{2,MeOH}$ is assumed to be externally defined. For practical reason, $r_{distill,H2O}$ and $r_{scrubber,MeOH}$ will be controlled by either $F_{3,H2O}$ and $F_{3,MeOH}$ or by $F_{5,H2O}$ and $F_{5,MeOH}$. Either set of control strategies will require adjustment of the total flow rate of one flow stream only, making implementation of the control strategy a strict forward task. In order to decide which set of control strategies is a better alternative, the available manipulations have to be evaluated based on the design criteria discussed in Chapter 6. In general, for long-horizon control, it is desired to choose a manipulation that has a wide physical range of operation, like one with a large gain. For short-horizon control, the ability to bring the process to steady-state quickly is important. Judging from the fact that F_3 is the feed to a distillation column, a large dead-time will be associated with any attempt to adjust the level of accumulation at the bottoms by this feed. Hence, F_5 is probably a better alternative for short-horizon control for this plant.

Hence, via systematic analysis of the overall material balance equations for the plant, the following set of control strategies have identified and their feasibility have been confirmed:

1. $F_{1,H2O}$ must be varied to maintain zero accumulation of water in scrubber.
2. $F_{4,MeOH}$ must be varied to maintain zero accumulation of methanol in distillation.
3. $F_{5,H2O}$ must be varied to maintain zero accumulation of water in distillation.
4. $F_{5,MeOH}$ must be varied to maintain zero accumulation of methanol in scrubber.

By implementing a composition controller which fixes the composition of methanol in distillate as suggested by Downs (1992; 1993a), $F_{4,MeOH}$ is effectively being adjusted to compensate for changes in the amount of methanol entering the process. A feasible control structure for the methanol recovery process has been developed.

Case Study: Acetaldehyde Oxidation Process

Acetic acid (HOAc) is commonly produced by oxidation of acetaldehyde (HAc) according to the following reaction:

$$\text{HAc (liq)} + \tfrac{1}{2}\,O_2 \text{ (gas)} \rightarrow \text{HOAc (liq)}$$

A schematic of the partial acetaldehyde oxidation process given by Downs (1992) is shown in Figure 7-10. The oxidation is a liquid phase reaction using water as a diluent and heat sink. The reaction rate is first order with respect to acetaldehyde concentration in the liquid phase and first order with respect to oxygen partial pressure in the gas phase. The vapor stream leaving the reactor enters a water scrubber where acetic acid and some acetaldehyde are removed from the vapor stream before the stream leaves the process. The liquid product leaving the reactor is the feed to the low boiler (LB) removal column whose function is to recover the unreacted acetaldehyde. Acetaldehyde recovered is recycled to the oxidizer. Water leaving the scrubber is also recycled to the oxidizer to maintain a concentration of 0.6 mol fraction in the oxidizer. The acid product is further concentrated in the water column where the water and acid are separated into relatively pure product streams.

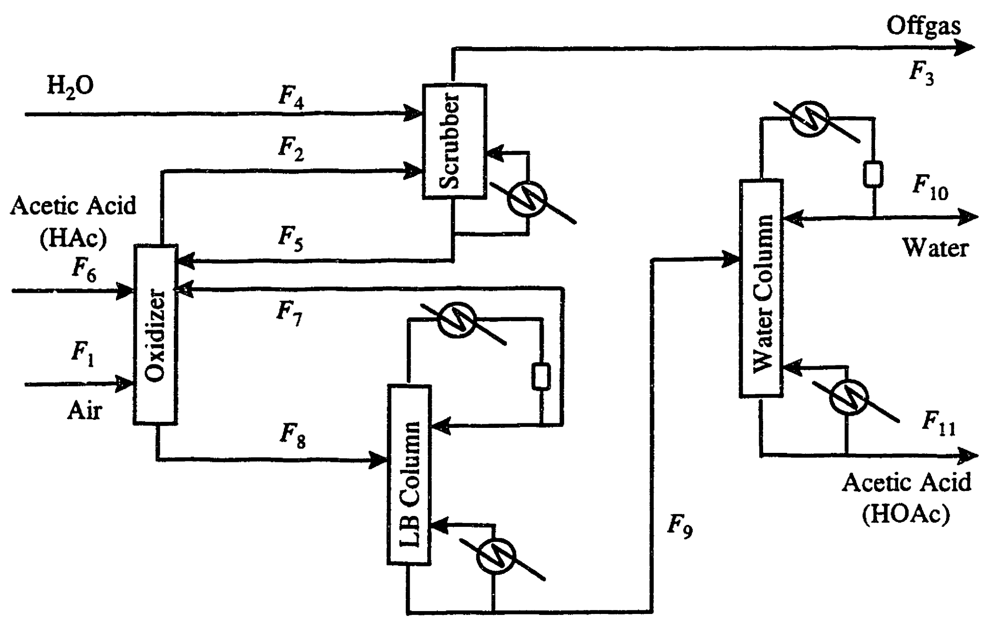


Figure 7 - 10: Acetaldehyde Oxidation Process (from Downs, 1992)

Downs (1992) has found that the control of the LB distillation column has a strong impact on the plant-wide control strategy. If the composition of the bottom product stream of the LB column is controlled via a temperature controller as shown in Figure 7-

11 (a), water will accumulate in the process. For an increase in the scrubber water feed, the inventory of water in the process will to rise in the oxidizer, increasing the amount of water in the system. As the feed to the LB column becomes richer in water, the bottoms of the LB column will also contain more water. However, the water to acid ratio is fixed in this control structure. Excess water in the feed has to be forced to the distillation stream and return back to the oxidizer. The concentration of water in the oxidizer then continues to rise. In practice, the water concentration becomes so high that the oxidation reaction is stopped and the plant has to be shut down.

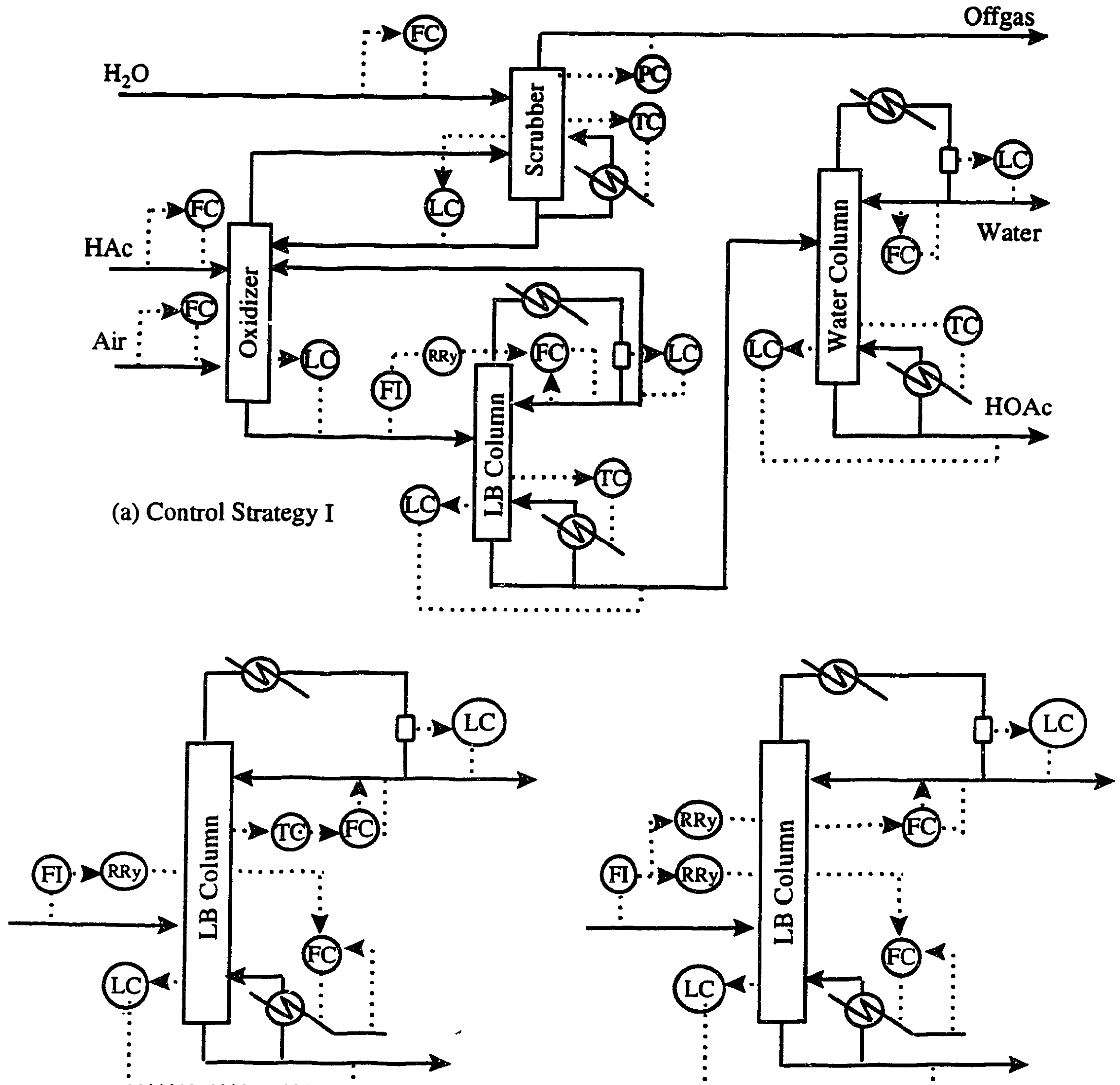


Figure 7 - 11: Acetaldehyde Oxidation Process Control Strategy (from Downs, 1992)

Downs (1992) has proposed two workable solutions as shown in Figure 7-11, both involve altering the LB control strategy. In control strategy II, the top composition of the LB column is controlled by means of the temperature control at the top of the column. By holding a relatively constant composition in the distillate stream that recycles back to the oxidizer, buildup up of water in the oxidizer is prevented. Control strategy III has no feedback control on the LB column. The reflux and the reboiler duty are simply ratioed to the feed rate. This strategy accounts for the changes but allows the top and bottom compositions to float.

Next, it will be shown that systematic analysis of the material balance equations in the modular multivariable framework leads to a control strategy that is similar to the workable solutions proposed by Downs (1992). There are 3 reactive components in this process (HAc, O_2, HOAc), 1 reaction and 2 inert materials (H_2O, N_2). According to equation [5-1], a total of 4 material balance equations are needed for each distributed inventories to completely described the overall material balance of the system. At the input-output level (Figure 7-12), the following material balance equations can be written:

MB of HAc:	$r_{\text{overall, HAc}} = F_{6,\text{HAc}} - F_{10,\text{HOAc}} - F_{3,\text{HAc}}$	[7-39]
MB of O_2:	$r_{\text{overall, O2}} = F_{1,\text{O2}} - \frac{1}{2} F_{10,\text{HOAc}} - F_{3,\text{O2}}$	[7-40]
MB of H_2O:	$r_{\text{overall, H2O}} = F_{4,\text{H2O}} - F_{3,\text{H2O}} - F_{11,\text{H2O}}$	[7-41]
MB of N_2:	$r_{\text{overall, N2}} = F_{1,\text{N2}} - F_{3,\text{N2}}$	[7-42]

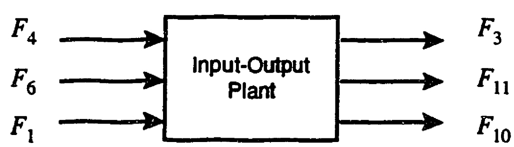


Figure 7 - 12: Input-Output Representation of the Acetaldehyde Oxidation Process

The open-loop gains of the residuals of the material balances have been computed based on the procedure described in Section 5.2.2 and they are shown in Table 7-14.

Using the open-loop gains, a control structure can be developed for this input-output representation in the modular multivariable framework as described in Chapter 6. For this simple case study, it will be assumed that there is no error in our open-loop model. Therefore, for long-horizon control, the size of the closed-loop gain (equation [6-13]) will be as the design criterion. Also, for the sake of illustration, it is assumed that the order of importance of the control objectives to be of the following order: $r_{\text{overall,HAc}} > r_{\text{overall,O2}} > r_{\text{overall,N2}} > r_{\text{overall,H2O}}$. The logic behind the ordering of control objectives will be detailed in Chapter 8.

Table 7 - 14: MMC analysis - Open and Closed-loop Gains of Material Balance Residuals at the Input-Output Level of the Acetaldehyde Oxidation Process

	Open-Loop Gains				Closed-Loop Gains			
	$r_{overall,HAc}$	$r_{overall,O2}$	$r_{overall,N2}$	$r_{overall,H2O}$	$r_{overall,HAc}$	$r_{overall,O2}$	$r_{overall,N2}$	$r_{overall,H2O}$
$F_{1,N2}$	0	0	0.96	0	0	0	0.96	0
$F_{3,N2}$	0	0	-0.96	0	0	0	-0.96	0
$F_{6,HAc}$	0.4	0	0	0	0.4	-0.2	0	0
$F_{10,HOAc}$	-0.39	-0.19	0	0	-0.39	0	0	0
$F_{3,HAc}$	-0.014	0	0	0	-0.014	0.0072	0	0
$F_{1,O2}$	0	0.24	0	0	0	0.24	0	0
$F_{3,O2}$	0	-0.047	0	0	0	-0.0472	0	0
$F_{4,H2O}$	0	0	0	0.0259	0	0	0	0.0259
$F_{3,H20}$	0	0	0	-0.0013	0	0	0	-0.0013
$F_{11,H2O}$	0	0	0	-0.025	0	0	0	-0.0246

Beginning from the most important objective, $r_{overall,HAc}$ a primary manipulated is selected from the set of available choices. It has been implicitly implied in Downs' (1992) study that F_1, F_4 and F_6 are not manipulatable. Then, $F_{10,HOAc}$ is the best primary for the maintenance of $r_{overall,HAc}$. Having chosen the primaries for $r_{overall,HAc}$, the closed-loop gains for $r_{overall,O2}$ from each of the available manipulations can be computed (see Table 7-14). Since F_1 and F_6 are not available choices, $F_{3,O2}$ is clearly the best primary for the next objective. Similarly, the primaries for $r_{overall,N2}$ and $r_{overall,H2O}$ have been selected to be respectively $F_{3,N2}$ and $F_{11,H2O}$. The associations of the manipulated variables with the control objectives are depicted in Figure 7-13. In a simplified plant representation of the input-output model allows us to identify the key material inventory control strategies for the long-horizon. Since all input streams are fixed externally, the outlet streams must be varied to ensure that there is a balance between the inputs and outputs.

Using an approach that is similar to the one which was used at the input-output level, a more elaborate control structure has been developed at a refined level (i.e. the complete plant) as shown in Figure 7-14. The following control strategies have been identified:

1. The material balance control of the gaseous materials (N_2 and O_2) should be maintained by adjusting the flows of F_2 and F_3.
2. The water balance control of the scrubber is maintained by varying the amount of water recycle.
3. The acetic acid balance control in the oxidizer must be accomplished through proper management of the outlet streams.
4. $F_{9,H2O}$ and $F_{9,HOAc}$ must vary independently to maintain the material balances of H_2O and HAc respectively.

5. The component inventories in the water column is maintained by varying the outlet streams.

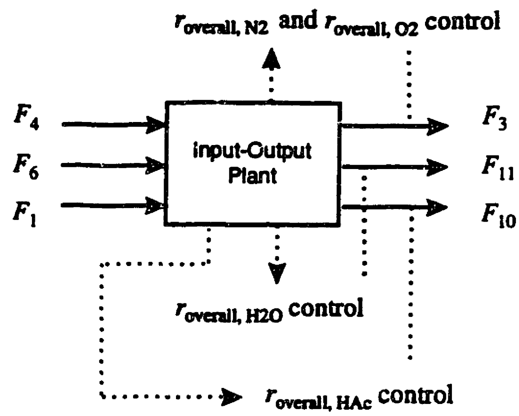


Figure 7 - 13: Control Structure for the Acetaldehyde Oxidation Process at the Input-Output level

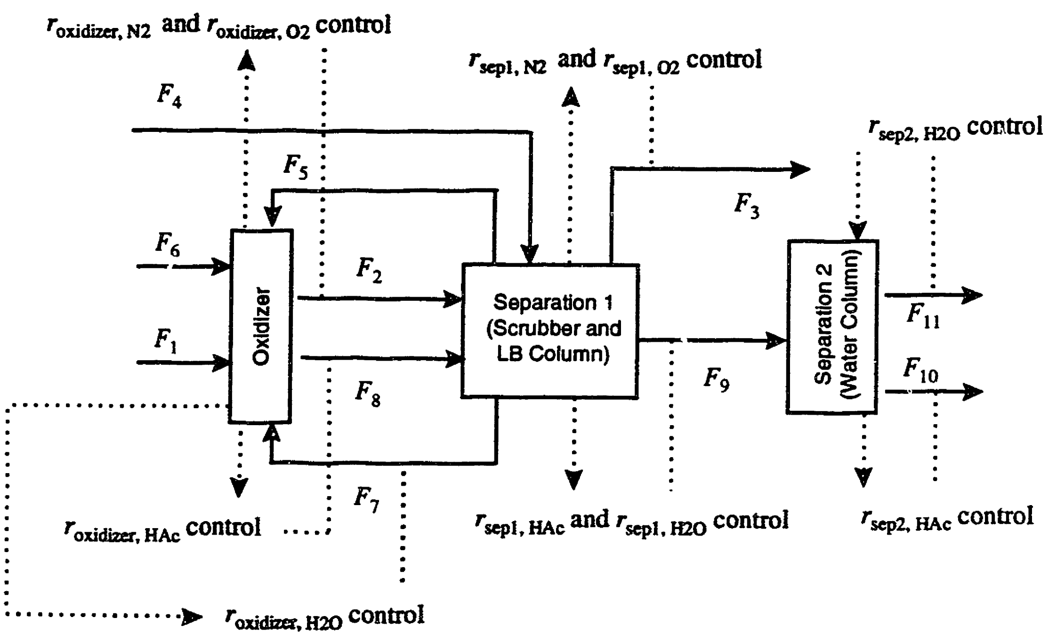


Figure 7 - 14: Control Structure for the Acetaldehyde Oxidation Process at the Refined Level

Thus, a composition controller which fixes the composition of acetic acid in F_9 as in control strategy I (Figure 7-11 (a)) would be incompatible with our fourth recommendation. Note also that the above control recommendations are consistent with the direction of flows of the main material streams in the two workable solutions proposed by Downs (1992) shown previously in Figures 7-11 (b) and (c).

This section has briefly demonstrated how control strategies which maintain both the overall material balance control and component inventory control can be systematically synthesized. By analyzing the individual material balance equations, and evaluating design alternatives in the modular multivariable control framework, the interaction generated under closed-loop control of plant objectives can be properly accounted for. This procedures ensures control strategies developed are internally consistent. Furthermore, in a methodical fashion, the pathways through which the major components must travel in order to prevent accumulation or depletion of materials in the plant have been identified.

7.3.4 Controlling Energy Accumulations

Similar to material inventories, energy inventories may be either self-regulating or integrating. The energy inventories of most non-reactive unit-operations are self-regulating. Most non-reactive processes do not generate or consume a significant amount of energy. Any difference between the amount of energy entering and leaving the process may be balanced by heat loss or gain through conduction, convection or radiation heat transfer.

For exothermic reactive systems, if the rate of heat generation exceeds that of the rate of heat being removed from the system, energy will accumulate in the reactor. For these systems, adequate reactor cooling facility must be provided to prevent reactor runaway. For endothermic reactive systems, if the rate of heat supply is not sufficient to sustain the reaction, the reaction will simply subside. This will of course result in loss of production.

For almost all unit-operations, control of unit energy balance simply requires adjustment of the heating or cooling system to maintain the unit at constant temperature and/or pressure. As the amount of energy inventories in most non-reactive unit-operations are self-regulating, the decision of whether the temperature or pressure should be controlled is simply a matter of whether deviation in the temperature or pressure is desirable or not.

In an integrated plant, not only do we need to ensure that no energy is being accumulated or depleted in the individual unit-operations, we must also ensure that energy does not accumulate or deplete in the global system as well. Accumulation or depletion of energy usually occurs in a plant via energy recycling, either through some material recycle streams or through explicit integration of heat sources and sinks in the plant by heat-exchangers. The use of qualitative simulations to identify energy accumulation through formal heat-integration has already been demonstrated in Section 7.2.3. Figure 7-15 gives an example of energy integration through a material recycle stream in the plant. Products from a highly exothermic reaction is separated from the raw materials in a distillation column. Raw materials recovered from the distillation is recycled back to the reactor. Using methods described in Section 4.2.3, a single-staged directed graph for this process has been constructed and is shown in Figure 7-16. See that an increase in enthalpy of F_1 (i.e. $H_1 = \sum_{i=1}^{n} F_{1,i}h_{1,i}$) would cause an increase in H_2 which increases H_3 through a highly exothermic reaction (Q_{rxn}). Assuming that there is little heat lost to the environment in the distillation operation, an increase in H_3 causes H_5 to increase as well. As F_5 is recycled and joined with the reactor feed, a positive feedback loop has been created. It is easy to see that the initial step change is being reinforced by the feedback effect, causing a bigger increase in temperature in the reactor. Even though there is no accumulation of energy *locally* in any units in the plant, the energy content of the recycle stream is *globally integrative*. The heat content somewhere in the loop formed by F_2-F_3-F_5 must be fixed to prevent reactor runaway from occurring. An obvious choice is to control the temperature of the reaction at some acceptable value by manipulating Q_{cw}. The phenomenon described here is similar to the case of accumulation of materials in the plant caused by the use of inconsistent local inventory control strategies that was discussed earlier in Section 7.3.1.

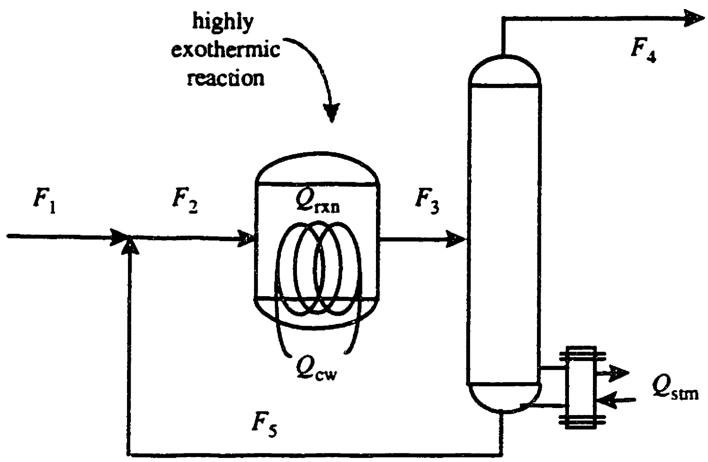


Figure 7 - 15: Recycling Energy Via a Material Recycle Stream

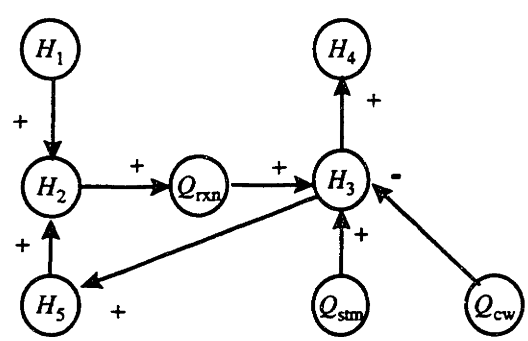


Figure 7 - 16: Single-staged Directed Graph for the Process in Figure 7-15

7.4 Managing Process Variations

It has been pointed out in Section 2.1 that operation of most real processes is affected by the continuously changing environment which give rise to variations in the plant. Due to the interactions that typically exist among process units in the plant, once variations have entered the process, they propagate through the plant in a complex and convoluted manner (Moore, 1993). Management of process variations plays a key role in quality improvements in the plant. Not only do process variations cause product variations, they can also impact the basic efficiency and productivity of the process units and affect how well the process operation can be studied.

The disturbance load paths in the plant can be systematically traced using the structural techniques presented in Section 4.2.2. Recall that the propagation of process variation could be altered by feedback control. The concept of transformation of process variation by feedback control have been summarized in Figure 4-8. Feedback control action reduces variation in the controlled variable by adjusting the manipulated variable to counter the effect of the incoming variation. In doing so, variation in the controlled variable is being transformed to the manipulated variable. Thus, the short-term focus of management of process variation entails deriving a set of control strategies which would minimize the impact of process variation on critical process variables. The next two sections illustrates how judicious selection of manipulated and/or controlled variables used in the control structure can divert process variations to less critical process outputs.

7.4.1 Transforming Process Variations in a Unit-operation

Case Study: A Liquid-liquid Extraction Process

A liquid-liquid extraction process studied by Downs (1993b) is shown in Figure 7-17. In this process, a solvent is used to extract acid from the acid-water mixture. The raffinate is mainly composed of water and a small amount of acid and solvent. The solvent-acid mixture is lighter so it floats on top of the aqueous phase. The level of the organic phase is controlled by a weir at top of the vessel so it is self-regulating. Extract leaves the tank by overflow. The interface level does not self-regulate and a feedback mechanism is required to maintain the level at an acceptable level. It is also desired to control the composition of acid in the extract at some fixed value.

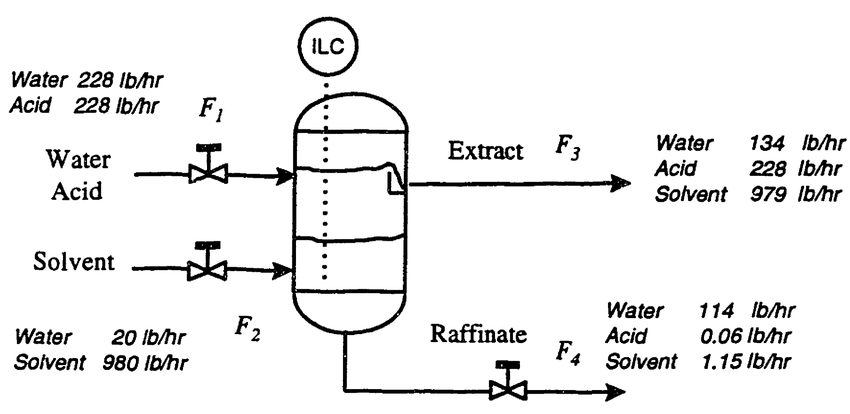
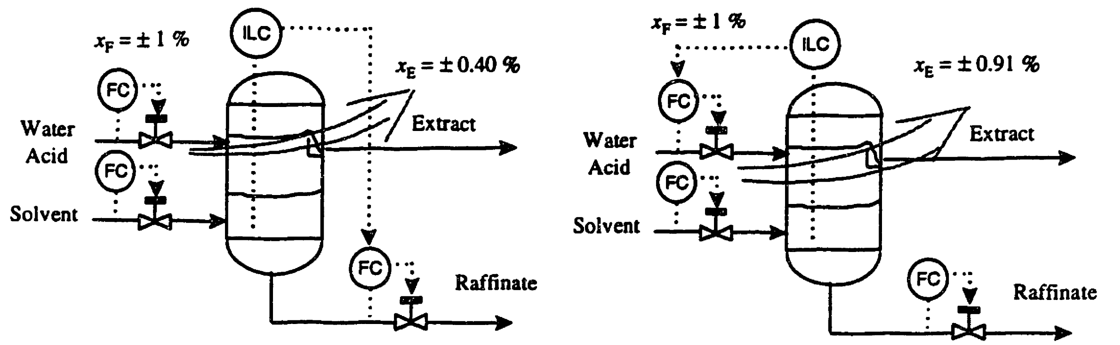


Figure 7 - 17: Liquid-liquid Extraction Process (Downs, 1993b)

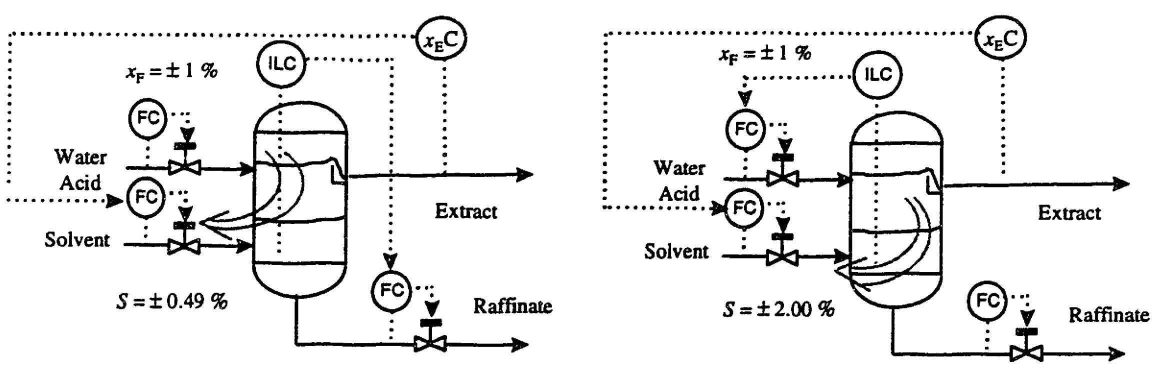
Figures 7-18 (a) and (b) compare how two different interface level control strategies transform the variation in the composition of acid in the feed mixture. Naturally, some of the feed composition variation will be transformed into flow variation of the manipulated variation. As the mass transfer rates are being altered by changes in the flows, the extend of extraction is also being affected, causing variation in the extract composition as well. Control strategy II has a bigger impact on the extract composition than control strategy I. To eliminate variation in the extract composition, Downs (1993b) proposed that the rate of solvent be adjusted accordingly. Figures 7-19 (a) and (b) compare the amounts of movements that are required in the solvent flow in order to eliminate the variation in extract composition initiated by the two different level control schemes. As shown, control strategy I appears to be the superior of the two. Not only is extract composition less sensitive to changes in the raffinate rate, but this control strategy also requires less changes in the solvent rate to eliminate variation in extract composition.



(a) Control Strategy I: manipulate raffinate

(b) Control Strategy II: manipulate water-acid feed

Figure 7 - 18: Controlling the Interface level in the Liquid-Liquid Extraction Tower (Downs, 1993b)



(a) Control Strategy I: manipulate raffinate to control interface level

(b) Control Strategy II: manipulate water-acid feed to control interface level

Figure 7 - 19: Controlling the Interface Level and Extract Composition in the Liquid-Liquid Extraction Tower. (Downs, 1993b)

Downs' example (1993b) has demonstrated that the feedback control system transforms both the direction in which process variation travels as well as the magnitude of the variation. Both control strategies are able to successfully insulate the interface level and the extract composition from a relatively small amount of variation in the acid composition in the water-acid mixture. Notice that the second control strategy requires a much bigger change in the solvent flow. Hence, it is more likely for the solvent flow to reach its saturation limits when a large feed composition disturbance is encountered. Thus, it is important to consider to where process variations are being diverted and by how much the manipulated variables must vary to eliminate the expected variation. How the more resilient control strategy (i.e. control strategy I) can be systematically derived by evaluating the alternatives quantitatively will be illustrated next.

There are two control objectives in this simple unit. First, and of higher priority, the interface level must be maintained at an acceptable level. Second, the composition of acid in the extract must be kept constant. The level of the interface is an integrating variable. It has been demonstrated in Section 5.3.1 that the size of the integrator gain is a good measure of the effectiveness of input as a manipulated variable for dynamic control. For liquid levels, the size of the integrator gain is simply the rate of change of the liquid level for a unit change of the manipulated variable. At steady-state, for every 228 lb of water entering the tank, approximately 114 lb of water leaves the tank as raffinate. If raffinate flow is fixed, we can assume that roughly half of the water entering the tank will accumulated in the aqueous phase, which contributes to a rise in the level of the interface. As the water-acid feed is made up of water and acid in a roughly 1 to 1 ratio (according to the base case), every pound entering from the feed would contribute to 0.25 lb increase in the accumulation of water in the bottom phase. For the raffinate, since its flow originates from the aqueous phase in the tank, we would expect that every pound that leaves the process as raffinate, there is a pound lost in the aqueous phase in the tank. Base on the above observation, we can claim that the magnitude of the integrator gain of the interface level caused by a unit change of the water-acid feed or extract flow must be a quarter of the magnitude of the integrator gain caused by a unit change in the raffinate. Since solvent does not accumulate in the aqueous phase, the corresponding integrator gain should be close to zero. Table 7-15 summarizes the estimated relative integrator gains. Based on the design criteria for dynamic control, clearly raffinate is the best manipulated variable.

Table 7 - 15: Integrator Gain for the interface level

Input	Estimated relative integrator gain
Water-acid Feed	x
Solvent	~ 0
Raffinate	$-4x$

To select the best manipulated variable for the control of the second objective, i.e. the extract composition, the effect of the closed-loop control of the interface level must be taken into account (recall Chapter 6). The closed-loop gain of extract composition to a unit change of solvent flow rate is 0.8 when raffinate is being used to control the interface level and 0.46 when water-acid feed is being used to control the level (data estimated based on Downs' (1993b) sensitivity analysis). Due to lack of additional dynamic information, selection will have to be made based on the magnitude of the closed-loop gain. As the size of the closed-loop gain is larger when raffinate is being used to maintain the level, less changes will be required of the solvent flow to adjust deviation in the extract composition. Through a systematic quantitative analysis, we can conclude that control strategy I is a superior design.

For this simple process, there are three non-reactive components so three independent material balance equations are needed to describe the flow of all the components in the system. These equations are:

$$r_{H2O} = F_{1,H2O} + F_{2,H2O} - F_{3,H2O} - F_{4,H2O} \qquad [7\text{-}43]$$

$$r_{acid} = F_{1,acid} - F_{3,acid} - F_{4,acid} \qquad [7\text{-}44]$$

$$r_{solvent} = F_{2,solvent} - F_{3,solvent} - F_{4,solvent} \qquad [7\text{-}45]$$

The gains of r_{H2O} by different manipulations have been estimated and complied in Table 7-16.

Table 7 - 16: Open-loop gain of r_{H2O}

	$F_{1,H2O}$	$F_{2,H2O}$	$F_{4,H2O}$
r_{H2O}	2.28	0.2	-1.14

Since F_3 is not a manipulatable input, $F_{3,H2O}$ is also not manipulatable. Based on the size of the gain alone, $F_{1,H2O}$ is the best manipulated variable for the control of the water inventory. Since the height of the interface level is a strong function of the amount of water inventory in the system, our control strategy suggests that $F_{1,H2O}$ should be used to maintain the interface level. However, $F_{1,H2O}$ cannot be physically manipulated without changing $F_{1,acid}$ as well. If $F_{1,acid}$ is changed, $F_{3,acid}$ must change to maintain r_{acid} at zero (note the size of $F_{4,acid}$ is negligible). When we consider how this feedback control strategy transforms the propagation of the composition variation, $F_{1,H2O}$ does not appear to be a good candidate anymore. The next best input is $F_{4,H2O}$. Since F_4 is largely made up of water, moving F_4 has the least effect on the inventory of other components in the system. F_4 is therefore the best manipulated variable for the maintenance of water inventory in the system if it is desire to minimize the variation of acid in extract.

The concept of variation transformation through single unit-operations and the importance of the proper use of feedback control strategy have been demonstrated in the previous study. Feedback control shifts the variation from a controlled output to the associated manipulated variable. Furthermore, a feed back control strategy may also attenuate or amplify variation in other process variables as a result of process interaction in a multivariable system. The design of control strategy must consider the effect of the feedback control on other critical areas in the plant. An ideal control strategy should ensure that the critical process variables in the plant are resilient to process variation from the surroundings. The implication of process variation in a plant-wide setting will be further demonstrated in the next case study.

7.4.2 Transforming Process Variation in a Plant with Recycles

Material recycles are commonly found in chemical processes for economical and practical reasons. The use of recycles adds a level of complexity to the control problem as recycles provide a means for the downstream units to interact (both statically and dynamically) with the units upstream. External feedback effects in the interconnected system are created as a result of the material recycles, permitting a wide range of possible feedback phenomena. From a steady-state control point of view, recycle streams provide additional degrees of freedom in the process by acting as buffers for the inventories of unreacted raw materials, by-products and inert. A process can have various steady-states for different sizes of the recycle. Once the sizes of the equipment in the plant have been fixed, the magnitude of the recycle flow that is closely related to the process operating conditions in the plant. Consequently, a recycle stream can act as disturbance sink where external variations can be divert. This gives the designer an additional degree of freedom to modify the process behavior. The next case study illustrates the importance of understanding how process variations can be shifted within an interconnected plant.

Case Study: Snowball Effect in a Reaction/Distillation Process

Luyben (1993a, 1993b, 1993c, 1994) and Tyreus (1993c) conducted a series of studies on recycle systems and have illustrated how ill-chosen plant control systems may amplify feedback effects in the plant. The simplest possible recycle system that is considered by Papadourakis (1987) is shown in Figure 7-20. In the continuous stirred-tank reactor (CSTR) a single irreversible, first-order reaction A $\rightarrow$ B takes place. Unreacted A is separated from the product B in a binary distillation column is recycled back to the reactor. The purified product B leaves the plant through the bottoms of the distillation column where unreacted A is concentrated in the distillate. The steady-state operating conditions for this plant are compiled in Table 7-17. At steady-state, the following relationships are true:

Overall balance:

$$F_o = B \qquad [7\text{-}46]$$

$$F_o z_o = B x_B + V_R k z \qquad [7\text{-}47]$$

Reactor balance:

$$F_o + D = F \qquad [7\text{-}48]$$

$$F_o z_o + D x_D = F z + V_R k z \qquad [7\text{-}49]$$

Combining Equations [7-46] and [7-47] yields:

$$z = \frac{F_o(z_o - x_B)}{kV_R} \qquad [7\text{-}50]$$

which shows how the reactor holdup, reactor composition and fresh feed flowrate are interrelated at steady-state.

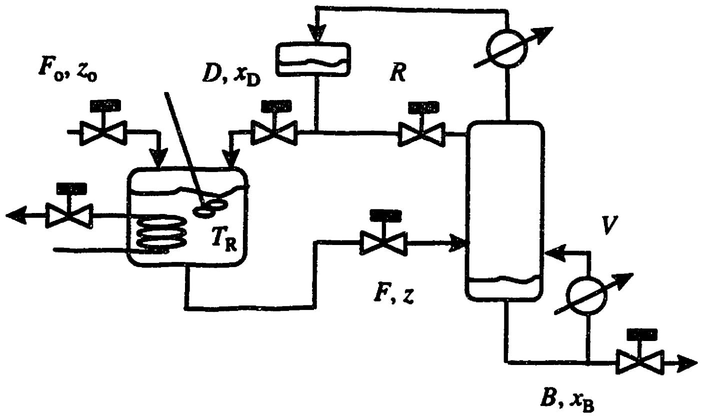


Figure 7 - 20: Reaction/Distillation Process (from Papadourakis, 1987)

Table 7 - 17: Operating conditions for the reaction/distillation process

Fresh feed A, F_o = 239.5 lb mol/hr
Mole fraction of A in feed, z_o = 0.9
Reactor volume, V_R = 1250 lb moles
Reactor composition, z = 0.5
Distillation feed, F = 500 lb mol/hr
Recycle flow, D = 260.5 lb mol/hr
Mole fraction of A in distillation bottoms, x_B = 0.0105
Mole fraction of A in recycle, x_D = 0.95
Reactor temperature, T_R = 617.32°R
1st order kinetic rate constant, k = 0.34086 hr^{-1}
Activation energy, E = 30841.77 Btu/lb mol
Pre-exponential factor, $k_o = 2.829 \times 10^{10}$

Luyben (1994) proposed two control structures for this process and they are shown in Figure 7-21 (a) and (b). Figure 7-21 (a) is what Luyben (1994) called a conventional control structure in which all liquid inventories are controlled by outlet flows and a two-point distillation control structure is employed. Figure 7-21 (b) shows an alternate control structure. In this control scheme, the reactor volume is allowed to vary according to the production rate. The feed to distillation column is flow controlled.

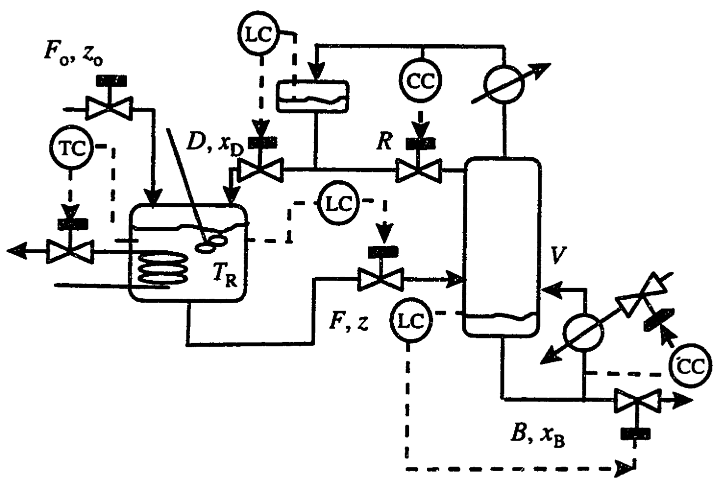
Luyben (1994) has found that when the plant is being controlled with a conventional control structure (i.e. 7-21 (a)), the recycle flow rate at steady-state depends strongly on the fresh feed flow and feed composition according to the following relationship:

$$D = \frac{F_o - \beta x_B}{\beta x_D / F_o - 1} \qquad [7\text{-}51]$$

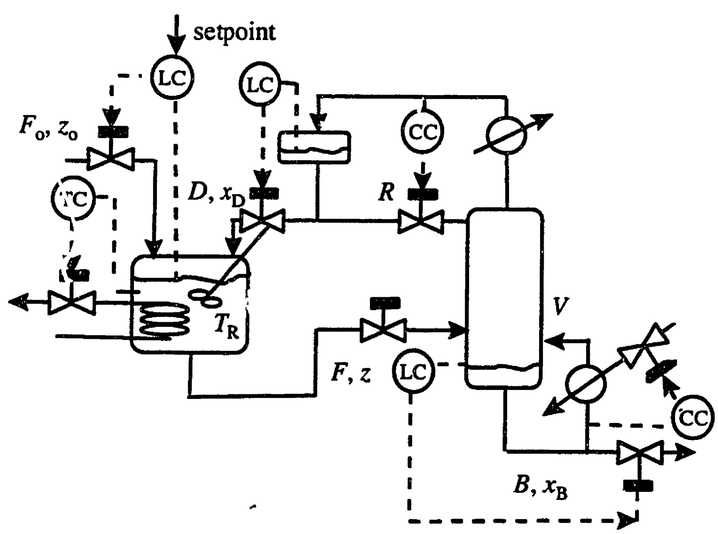
where:

$$\beta \equiv \frac{kV_R}{z_o - x_B}$$

With F fixed as a constant in the alternate control structure and V_R a variable, it had been shown by Luyben (1994) via material balance equations (Equations [7-46] to [7-49]) that the closed-loop plant would vary according to the following relationships:



(a) Conventional control structure



(b) Variable reactor volume control structure
proposed by Luyben (1994)

Figure 7 - 21: Control structures for the reaction/distillation process

$$D = F - F_o \qquad [7\text{-}52]$$

$$kV_R = \frac{FF_o(z_o - x_B)}{Fx_D - F_o(x_D - x_B)} \qquad [7\text{-}53]$$

Recycle rate D is directly proportional to fresh feed flow. Reactor holdup V_R is affected by both fresh feed flow rate and fresh feed composition change. Table 7-18 compares the relative changes in the key variables to step changes in fresh feed flow and fresh feed composition under to the two proposed schemes based on data computed by Luyben (1994). As shown, in order to bring the process to the new production rate (set by the fresh feed) and to eliminate variation in the feed composition using the conventional control structure, big changes in the recycle flow is required. Furthermore, if fresh feed was increased to 300 lb mol/hr, the recycle flow must increase by more than two folds to deliver the required change. The process exhibit what Luyben calls the *snowball effect* in recycle when the conventional control structure is used (Luyben, 1994). In the alternate control structure, by keeping the flow of feed at fixed value and allowing the reactor holdup to vary, recycle flow is much less sensitive to changes in the fresh feed.

Table 7 - 18: Comparison of relative change in plant conditions to step changes under conventional and Luyben's alternate control structures

	F_o set at 250 lb mol/hr		z_o set at 0.96	
	Conventional Fixed V_R	Alternate Varied V_R	Conventional Fixed V_R	Alternate Varied V_R
$z/z_{nominal}$	1.042	0.96	1.064	1
$D/D_{nominal}$	1.15	0.96	1.15	0.998
$V_R/V_{Rnominal}$	1	1.088	1	1.064

Luyben's studies (1993a, 1993b, 1993c, 1994) illustrate how different control strategies transform the variations in the fresh feed stream differently. Under the conventional control structure, these variations are mainly absorbed by the recycle flow while Luyben's variable reactor volume control structure (Figure 7-21 (b)) transforms the variations to the reactor holdup.

In a process which consists of units that are interconnected by forward and recycle streams, there are multiple opportunities for transformation of variation. As process variables are usually constrained within some physical limits, different control strategies may affect the range of closed-loop operability of the plant. Thus, it is important to systematically study different ways to transformed process variation in order to synthesize desirable control strategies.

The fundamental static behavior of this simple system can be captured in the structural representation shown in Table 7-19.

Table 7 - 19: Structural Representation of the Reactor/Distillation process

Potential Manipulated Variables						Production Obj.		Externally Defined	
V_R	k	z	x_D	D	F	x_B	B	F_o	z_o
							×	×	
×	×	×				×	×	×	×
				×	×			×	
×	×	×	×	×	×			×	×

Assuming that F_o has been reserved to maintain the production rate in the plant (an implicit assumption in Luyben's study (1994)), both F_o and z_o are externally defined variables and are not degrees of freedom in the design. Plant operation requires the maintenance of B and x_B at specific levels so these are our production objectives. The remaining variables are potential degrees of freedom in our static design. Three of the rows in the first section of the matrix have not been fully specified so there are three degrees of freedom (6 - 3 = 3) in the design. Tables 7-20 and 7-21 display the degrees of freedom that correspond to the conventional and the variable reactor volume control structures respectively. The symbol "⊗" signifies that variable to be the output of the controller, i.e. the chosen manipulated variables. All remaining variables must be pre-defined.

Table 7 - 20: Structural Representation of the Reactor/Distillation process controlled by the conventional control structure

Potential Manipulated Variables						Production Obj.		Externally Defined	
V_R	k	z	x_D	D	F	x_B	B	F_o	z_o
							×	×	
×	×	⊗				×	×	×	×
				⊗	×			×	
×	×	×	×	×	⊗			×	×

Table 7 - 21: Structural Representation of the Reactor/Distillation process controlled by the variable reactor volume control structure

Potential Manipulated Variables						Production Obj.		Externally Defined	
V_R	k	z	x_D	D	F	x_B	B	F_o	z_o
							×	×	
⊗	×	×				×	×	×	×
				⊗	×			×	
×	×	⊗	×	×	×			×	×

The conventional design sets the values of V_R , k and z while allowing z, D and F to vary. Luyben's variable reactor volume control structure (Luyben, 1994) allows V_R, z and D to vary. By pre-setting F at a fixed value, Luyben's variable reactor volume control structure has insulated the recycle stream from exhibiting snowball effect. However, the effect of external variation has not been eliminated from the system. The variable reactor volume control structure has *merely transformed* the variation to V_R. Several possible control strategies are summarized in Table 7-22. The choice of control strategy is in part related to the selection of controlled variables. The best control structure should be one which transforms external process variations to locations where effects variations are relatively harmless and one which allows the biggest tolerance of potential process variations.

Table 7 - 22: Possible Control Strategies for the Reactor/Distillation process

	Control Strategies	Manipulated Variables	Pre-defined Variables
1	Conventional	z, D and F	V_R , x_D and k
2	Variable reactor volume	V_R, z and D	F, x_D and k
3	Variable reactor temp (ie k)	k, D and F	V_R , x_D and z
4	Variable reactor volume II	V_R, D and F	k , x_D and z
5	Variable reactor volume III	V_R, x_D and D	F, z and k

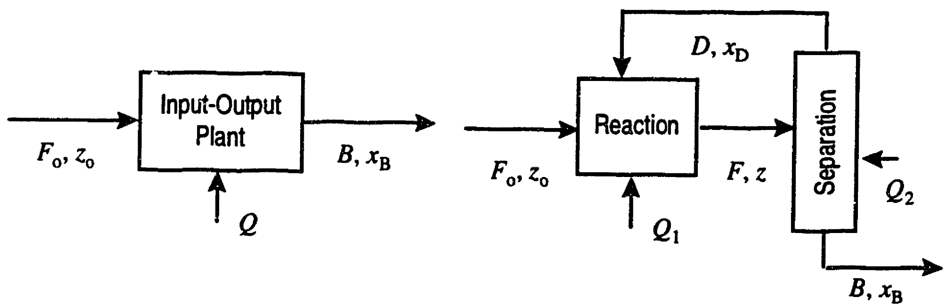
A Goal-driven approach to defining Control objectives

The abstract view of the plant as shown in Figure 7-22 (a). The overall production objectives that are observable from this level are summarized in Table 7-23.

Table 7 - 23: Control Objectives at the Input-Output Level

	Input-Output Representation
1	Maintain material balance of A.
2	Maintain production rate.
3	Maintain purity of B in product stream.
4	Maintain purity of B in product stream.

Figure 7-22 (b) shows the recycle structure of this process, which is the next level in the hierarchy of process representations. All the details of the reactor system are exposed at this stage. In Section 3.3.2, it was explained that control objectives used at the previous level should be updated to reflect the added details at this new level. The material balance objective is global in nature and it applies to both the reaction and separation sections. Production rate and product purity are specific objectives which will be translated directly to the sub-block for which they apply (i.e. the separation block). The cost optimization objective is a global one as well. It will be translated to both the reaction and distillation blocks. The updated control objectives are shown in Table 7-24.



(a) Input-Output representation (b) Recycle representation

Figure 7 - 22: Hierarchical Viewing of the Reactor/Distillation Process

Table 7 - 24: Initial Control Objectives at the Recycle Level

	Reaction	Distillation
1	Material Balance of A	Material Balance of A
2		Production Rate
3		Purity of B in product
4	Cost Minimization	Cost Minimization

With the initial control objectives defined, the next step is to look for opportunities to spawn new objectives and to refine the lumped objectives into more specific objectives. Consider a cause-and-effect network diagram for the process as shown in Figure 7-23.

Expected variations in F_o and z_o ultimately affect x_B and B. The efforts that are required in the minimization of variation in x_B and B can be reduced if additional objective(s) in the reaction block can be found which would help to divert some of the disturbances from the distillation section. One possible strategy is to minimize variation in z. As the distillation column has been designed for a specific operating region, the operability of the distillation column is preserved by maintaining z to be maintained at its nominal steady-state value. Note that z is also influenced by x_D. Even though there is no immediate cost savings by imposing a high recovery of A (since the amount of A leaving the process is defined by $1-x_B$), minimization of variation of x_D will reduce variation in the reaction area caused by the recycle stream. Hence, two new objectives will be spawned. The final set of control objectives at the recycle level are shown in Table 7-25.

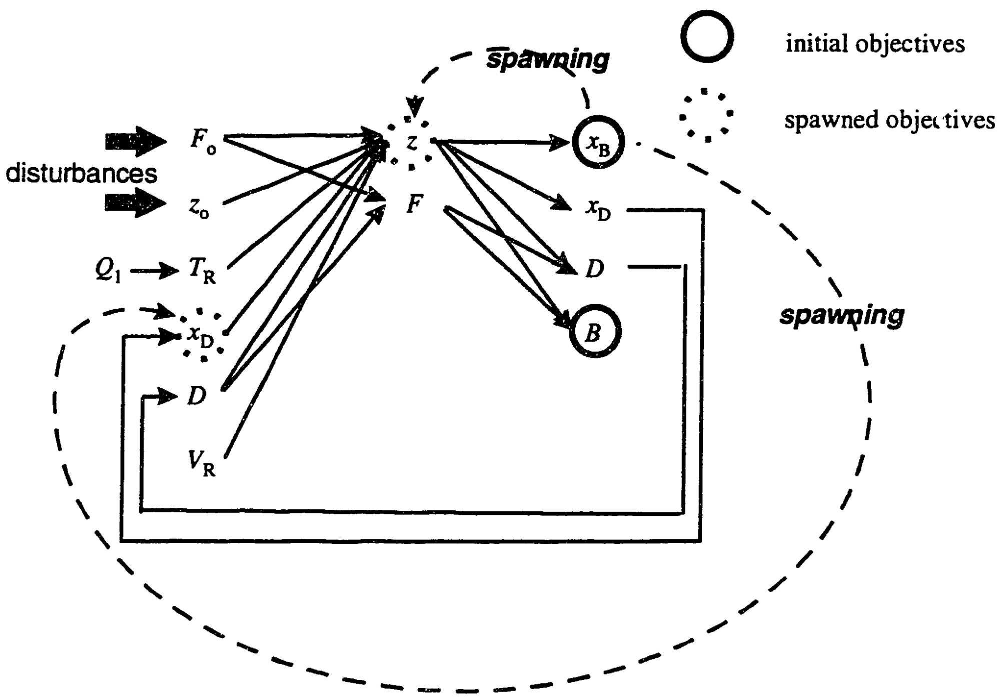


Figure 7 - 23: Causal Pathway Network for the Reactor/Distillation Process

Table 7 - 25: Final Control Objectives at the Recycle Level

	Reaction	Distillation
1	Material Balance of A	Material Balance of A
2		Production Rate
3		Purity of B in product
5	Maintain z	
		Maintain x_D
4	Cost Minimization	Cost Minimization

The above analysis suggests that B, x_B, x_D and z are suitable control objectives for this process and controlling these process variables will allow attainment of the production objectives stated in Table 7-23. Base on the structural matrix shown in Table 7-19, either {D, F and V_R} or {D, F and k} must vary to obtain a new steady state for changes in F_o or z_o. Implicitly assumed in the study is that F_o is varied to obtained the desired production rate, B. Both the variable reactor temperature strategy or the variable reactor volume strategy II in Table 7-33 are control structures which are consistent with the overall production objectives. The choice of the control strategy will ultimately depend on how the designer would like to transform the process variation and whether it is more harmful to divert variation to the reactor holdup or the reaction constant.

Most exothermic CSTRs are equipped with cooling water coils and agitators to ensure reactor materials are well-mixed. Large changes in the reactor holdup may have an impact on how much of the cooling water coil or agitator is being exposed in the reactor. If the volume is too low, not the entire cooling water coil may be submerged in the reacting mixture and the rate of heat transfer is affected by the decrease in surface area. If the volume is too large, the ability to transport heat to the mixture and the ability to maintain a well-mixed condition will be adversely affected. Since it is costly to overdesign the capacity of the reactor, there is not a large range of manipulation in the reactor holdup. On the other hand, reaction rate constant k is a strong function of the reactor temperature. Thus, k can be easily adjusted by manipulating the heat flow to the reactor. Using the cooling water as the ultimate manipulated variable, variations in F_o and z_o are can be quickly diverted to the external environment. Provided that the variation in reactor temperature does not severely alter the nature of the reaction kinetics, the variable reactor temperature control structure (see Figure 7-24) is a superior strategy over the others that we have considered in this case study.

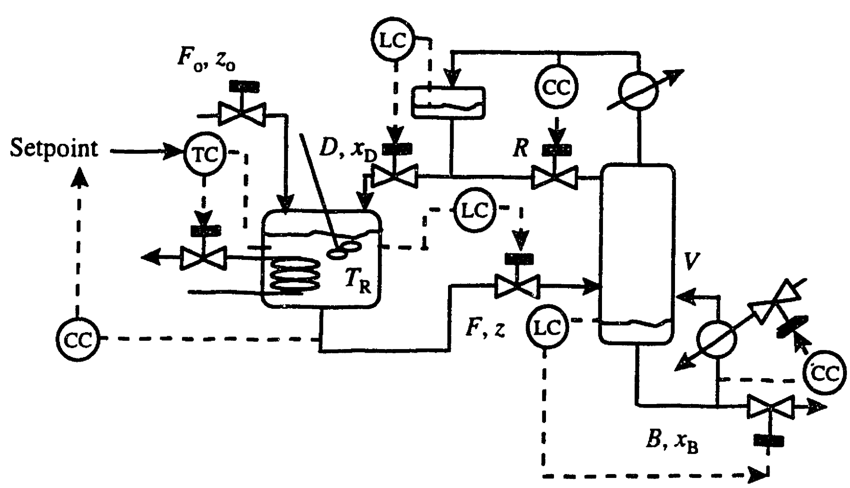


Figure 7 - 24: Variable reactor temperature control structure

Table 7-26 compares the relative changes in the static plant conditions to step changes in feed under the variable reactor temperature and Luyben's variable reactor volume control structures. We see that not only have we diverted the variation to the cooling water by adjusting the reactor temperature instead of the reactor holdup, the resulting closed-loop plant is also more robust to process variations. The results are more dramatic in the case where we set the production rate to 300 lb mol /hr. A variable reactor volume control strategy would require the holdup to increase by 60%. The equivalent change can be attained by a slight adjustment of the reactor temperature with the use of the variable reactor temperature control strategy.

Table 7 - 26: Comparison of relative change in plant conditions to step changes under variable reactor temperature and Luyben's variable reactor volume control structures

	F_0 set at 250 lb mol/hr		F_0 set at 300 lb mol/hr	
	Temperature varied Fixed z	Alternate Varied V_R Fixed F	Temperature varied Fixed z	Alternate Varied V_R Fixed F
$z/z_{nominal}$	1	0.96	1	0.7
$D/D_{nominal}$	1.044	0.96	1.2572	0.78
$V_R/V_{R,nominal}$	1	1.088	1	1.6
$T_R/T_{R,nominal}$	1.0018	1	1.0091	1

Under control-loop control, process disturbances are essentially diverted to the plant's manipulated variable. The structural representation of the plant (Table 7-19) clearly indicates that the choice of control objectives in effect determines the set of available manipulated variables. Consequently, the selection of process control objectives in the plant is closely related to the allocation of disturbance sinks. The goal-driven approach to the generation of specific control objectives demonstrated that a conscientious choice of control objectives allows not only the synthesis of a control structure that is consistent with the overall objective of the plan, but also a control structure that transforms disturbances to the most non-critical locations in the plant.

Chapter 8
Design Methodology for the Synthesis of Plant-wide Control Structures

8.1 Introduction

The design techniques presented in Chapters 4 through 6 have been shown to be useful for addressing a number of aspects of the plant-wide design problem in Chapter 7. In this chapter, the integration of the design techniques into the hierarchical framework introduced in Chapter 3 will be described. Particularly, a formal and systematic methodology for the synthesis of plant-wide control structures is presented in a step-wise fashion.

8.2. Preliminary Analysis

During the preliminary analysis, the designer should seek understanding of the process, identify production goals, process constraints, sources of process variations and examine flexibility of the operation. Familiarization of the process and the plant is essential for the development of a control structure which suits the needs of the operation.

8.2.1 Examine the Open-loop Stability of the Process Plant

One of the first steps of the design is to determine if the process is open-loop stable. The principal cause of operational instability in chemical plants has been discussed in Section 7.2. Furthermore, it has been illustrated that simple structural methods can help to determine if material or energy integration introduce process instability in the system.

The stabilization of process dynamics should be the first step in the design of a plant-wide control system because an unstable plant, when perturbed, will not attain a new steady-state on its own. Without the implementation of a sufficient process control strategy, the material and/or energy accumulation or equivalently the levels, concentration, temperature of pressure of a part of the plant might build up which might eventually cause violations of the operational and safety limits and lead to a plant runaway. Feedback control action must be introduced to prevent the process runaway. Another reason which makes process stabilization an important issue is related to the multilayer framework being employed in the proposed methodology. At the top levels of the hierarchy framework, design decisions are made based on abstractions of the process. In an abstract viewpoint of the plant, only the long-horizon characteristics can be observed (refer to Appendix A for details). However, because of (1), the open-loop characteristics of an unstable plant cannot be defined in the long-horizon. Thus, any decisions made with regard to the long-horizon process trend is only meaningful under the assumption that the unstable dynamics in the plant has been stabilized. This idea is depicted in Figure 8-1.

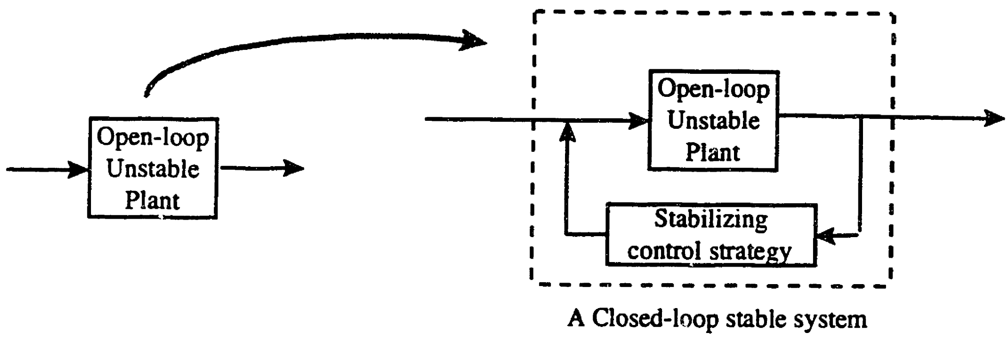


Figure 8 - 1: Stabilizing Control Strategy for an Open-loop Unstable Plant

Synthesizing a Process Stabilization Control Strategy

Depending on the source of process instability, the stabilization control scheme could be handled by a simple control routine, such as a PID control loop, or a more sophisticated control algorithm, such as a variant of a model predictive controller. For example, if the instability is caused by energy recycle due to heat-integration, often, one or more temperatures are needed to be maintained at fixed values. In such cases, simple PID temperature control loops may suffice and comprehensive process modeling of the open-loop system would not be required. In other cases where instability is caused by the present of an inherently unstable operating unit, such as the complex dynamics in a reactor. Then, a special reactor control strategy may be required to stabilize the system and one may need to develop a model that is appropriate for the required control strategy. In general, the initiation of the unstable process trend is usually manifested in the rapid rise or fall of one or more key process variables. These variables should be controlled so as to maintain the stability of the process. Suitable manipulated variable(s) should be identified using systematic procedure such as the modular multivariable design framework introduced in Chapter 6. Short-horizon design criteria should be employed since unstable modes exhibit very fast process dynamics. Open-loop plant tests in an open-loop unstable plant is forbidden. To develop a model for control purposes, one would have to either perform closed-loop plant experiments or develop a mechanistic model which captures the relevant unstable process dynamics. Methods for the modeling and control of reactive systems in the unstable operating region can be found in Hoo and Kantor (1985), Georgiou et al. (1989), Limqueco and Kantor (1990), Gobin et al. (1994).

Once a stabilizing feedback control strategy has been developed, we can proceed to the synthesis of plant control strategies in the hierarchical framework.

8.2.2 Prioritize Production Objectives

In the goal-driven design approach, it is important to acquire understanding of the plant production objectives and correctly prioritize control objectives into an order which reflects the operation goals in the overall production plan. This aspect of plant-wide design has been emphasized in Chapters 3 and 6. The specific ranking of objectives is based on our understanding of their functionalities in the plant. The prioritization of control objectives in a typical process plant is summarized below:

1. Process Stability
2. Material and Energy Balances
3. Production Goals
4. Operational Objectives
5. Plant Optimization

The above prioritization has been obtained through a paired comparison method (refer to Chapter 6) and the logic behind the prioritization is as follows:

1. As explained in the previous section, maintenance of process stability is the most important plant objective for an open-loop unstable plant. Furthermore, an unstable plant has no steady-state meaning. Any long-horizon analysis on the plant must assume that the plant's unstable mode are under closed-loop feedback control.
2. Unbalanced materials and energy flows induce accumulation or depletion of material or energy inventories in the plant. Control strategies which ensure that these balances are maintained should be one of the first goals of plant-wide control.
3. Production goals, such as production rate or product quality, are of the next level of importance. As these goals are closely associated with the purpose of the production unit, they are of high priorities.
4. Operational objectives are related to the operability of the process. These objectives assist the operation of the process and ensure that the process is being maintained at the safe operating region.
5. Optimization objectives should only be considered when all other objectives have been satisfied.

Prioritization of Material and Energy Balance Controls

The inventories of materials and energy within each block in a process viewpoint must be maintained at desirable levels by balancing the inflows and the outflows. In general, except for the case of rapid exothermic reactions, accumulation of energy in the process is relatively slow when compared to accumulation of materials in the process. Furthermore, disturbances which affect the energy balances can usually be localized by adjusting the nearby utility flows. Thus, the maintenance of material balances should be of higher priority then the maintenance of energy balances. However, if a certain energy balance is associated with an unstable exothermic reactor or if it belongs to a critical part of an unstable heat-integration loop, its maintenance is of the highest priority for obvious reason.

As most processes contain multiple number of components which require maintenance of a multiple number of material inventories, material balance controls should be prioritized as well. Since each process plant has its own specific production requirements and is being operated in its unique environment, a complete set of rules that will guide the designer to prioritize material balance controls for all processes cannot be defined. The prioritization of objectives should be evaluated on a case by case basis, drawing from the understanding of the nature of the process and the production needs. The criteria which are used to rank material balance controls include:

1. The expected rate of change of the material as indicated by the expected amount/frequency of variation of the inventory of that material caused by external process disturbances or setpoint changes. If the rate at which a certain chemical component is expected to vary either by a large amount or at a high frequency, it is expected that the balance of that component will be upset by the same amount/frequency. The maintenance of such a component is therefore more important.
2. The expected rate of change relative to the total capacitance of the inventory of that material in the system. A 10 mol/hr change of a material that has a large inventory in the plant does not affect the corresponding material balance as severely as a 10 mol/hr change of a material that has a small inventory. The inventory of the material is indicated by the amount of the material present in the internal material streams and in the process vessels.
3. The criticality of that material to the reactions. The maintenance of material balances of components which do not participate in the main reactions (such as carrier solvents, diluent, other inert or impurities) are not as crucial as those are that involved in the reactions.

The applications of these rules will be illustrated in the case studies in the chapters that follow.

8.3 Phase I: Long-Horizon Analysis

Following the hierarchical framework proposed in Chapter 3, the complexity of the design is reduced by decomposing a process plant vertically into a hierarchy of process representations to form a multistrata system. As explained in Chapter 3, each representation captures a certain level of details about the actual process. Such decomposition separates the plant dynamics, the impact of external variations at different frequencies and control objectives of various areal scopes. During Phase I of the design, the process plant is analyzed based on coarse viewpoints and the goal of this design phase is to develop control strategies which are suitable for maintaining production objectives which are relevant to the process over a relatively longer time-horizon.

8.3.1 Synthesize Control Structure For the Input-Output Plant

Development of plant-wide control strategies begins at the input-output level of the hierarchy of process representations. Based on the overall production plan, the control objectives and specifications that are relevant at the coarsest viewpoint (i.e. the input-output representation) can be completely specified. Control strategies at the coarse process representations are primarily driven by the maintenance of material and energy flows in the plant.

Before the input-ouput plant can be analyzed, the material and energy balance model for the input-ouput viewpoint be constructed. The number of independent material balances that are required to fully describe the overall system can determined via Equation [5-1]. At each level of the hierarchical framework, the focus is on the aspect of the pant that is relevant to that particular representation. This means, only objectives which are observable form the process streams crossing the system boundary and objectives which are related to the global plant will apply to that representation. Specifically, at the input-output level, objectives of interest are those which are related to the maintenance of material and energy balances (global objectives), the optimization objectives and those specific objectives which are localized to streams crossing the system boundary. The control objectives relevant to this level should be ranked in such a way that is consistent with the ranking established for all known production objectives during the preliminary analysis. Before proceeding in the design, it should be verified that the set of control objectives are indeed feasible by examining if the control specification violates any constraints imposed by stoichiometry.

With the model constructed, control objectives defined and prioritized, a control structure suitable for the time-scale represented by this process abstraction can be synthesized using the modular multivariable design framework (Chapter 6). At a coarse representation, only the slowest dynamics are relevant. Design criteria for static considerations should be employed. Furthermore, the way in which process variations are being transformed by the control strategies (recall Section 7.4) and the cost associated with the usage of the individual manipulated variables should play a role in the selection of primary manipulated variables. The details of the mechanics involved in the assignment of primary manipulated variables to objectives associated with material and energy balance controls have been demonstrated in the cases study on acetaldehyde oxidation process in Section 7.3.3. More involved examples concerning larger chemical processes will be illustrated in the case studies in the chapters to follow. The next section give details on the synthesis of control strategy for optimization control objectives in Phase I of the design.

8.3.2 Synthesis of Control Strategy for Optimization Control Objectives in Phase I

Once primary manipulated variables have been assigned to the non-optimizational production objectives, if there are excess degrees of freedom left (i.e. unassigned manipulated variables), one can explore opportunities for achieving the optimizational goal(s) for the process plant. During Phase I of the design, many of the process variables which are involved in the constraints governing the cost optimization are not observable. Thus, the purpose of this analysis is to determine if any key driving forces which may contribute to the cost optimization. The procedure in which one can identify optimization opportunities is best illustrated using an example.

EXAMPLE 8-1

Consider a hypothetical process in which A combines with B to produce C. The input-output representation of this process is shown in Figure 8-2. D is an inert in the system. It is expected to see random variation in the composition of A in F_1. The plant is open-loop stable. The molar flows of each components at the nominal steady-state is also given in the diagram. The prioritized control goals (see procedures in Section 8.2.1) at this level are summarized below:

1. Maintain the material balance of A (r_A).
2. Maintain the material balance of B (r_B).
3. Maintain the material balance of D (r_D).
4. Maintain the overall energy balance in the plant (e).
5. Maintain the production of C at 10, 000 lbmol/day (P).
6. Minimize production cost.

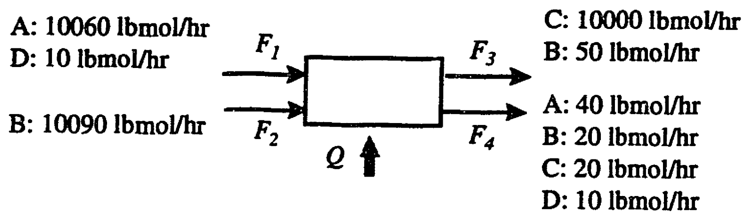


Figure 8 - 2: Input-Output Plant of the A + B → C Process

The maintenance of r_A is of the highest priority as it is expected that composition of A in F_1 to vary. D is an inert so r_D is less important than r_B.

The following set of control strategies for goals 1 through 5 have been derived using the modular multivariable framework described in Chapter 6:

1. F_1 is assigned to r_A.
2. F_2 is assigned to r_B.
3. $F_{4,D}$ is assigned to r_D.
4. Q is assigned to e.
5. $F_{3,C}$ is assigned to P.

Once primary manipulated inputs have been assigned to objectives 1 through 5, one can investigate if a control strategy which maintains the process at a low operational cost can be determined at this stage of the design. The cost function for this process as follows:

$$\begin{aligned}\Phi &\equiv \text{cost of raw materials} + \text{cost due loss of unrecoverable products} \\ &= c_1 F_{1,A} + c_2 F_{2,B} + c_3 F_{4,C}\end{aligned} \qquad [8\text{-}1]$$

where c_i (i = 1, 2, 3) are the coefficients of the corresponding variables. Thus, the optimization can be written as:

$$
\begin{aligned}
\min \Phi &= c_1F_{1,A} + c_2F_{2,B} + c_3F_{4,C} && [8\text{-}2]\\
\text{s.t.}\quad F_{1,A} &= F_{3,C} + F_{4,C} + F_{4,A} \quad \text{(maintain Goal 1)}\\
F_{2,B} &= F_{3,C} + F_{4,C} + F_{4,B} + F_{3,B} \quad \text{(maintain Goal 2)}\\
F_{4,D} &= F_{1,D} \text{ (maintain Goal 3)}\\
0 &= H_1 + H_2 - H_3 - H_4 + Q \quad \text{(maintain Goal 4)}
\end{aligned}
$$

Note that other constraints which define the physico-chemical behavior of the process is not observable at this level of representation. Since $F_{1,A}$, $F_{2,B}$ and $F_{3,C}$ have been selected to be primary manipulated variables for Goals 1, 2 and 3, these three variables are not our degrees of freedom in the optimization. In fact, the constraints can be substituted into Φ to eliminate $F_{1,A}$ and $F_{2,B}$. Then, the optimization simply becomes:

$$
\begin{aligned}
\min \Phi &= (c_1 + c_2)\,F_{3,C} + (c_1 + c_2 + c_3)\,F_{4,C} + c_1F_{4,A} && [8\text{-}3]\\
&\qquad + c_2F_{3,B} + c_2F_{4,B}\\
\text{s.t.}\quad F_{4,D} &= F_{1,D} \text{ (maintain Goal 3)}\\
0 &= H_1 + H_2 - H_3 - H_4 + Q \quad \text{(maintain Goal 4)}
\end{aligned}
$$

Since $F_{3,C}$ is related to the pre-specified production rate, its value can be considered fixed and therefore we can rewrite the optimization as follows:

$$
\begin{aligned}
\min \Phi' &= (c_1 + c_2 + c_3)\,F_{4,C} + c_1F_{4,A} + c_2F_{3,B} + c_2F_{4,B} && [8\text{-}4]\\
\text{s.t.}\quad F_{4,D} &= F_{1,D} \text{ (maintain Goal 3)}\\
0 &= H_1 + H_2 - H_3 - H_4 + Q \quad \text{(maintain Goal 4)}
\end{aligned}
$$

The sensitivity of Φ' to changes in $F_{4,C}$, $F_{4,A}$ and $c_2F_{3,B}$ is directly related to their corresponding coefficients. Clearly, $(c_1 + c_2 + c_3) > c_1 > c_2$. So reducing $F_{4,C}$ should result in the biggest savings. Decreasing $F_{4,A}$ and $F_{3,B}$ would also reduce the cost of production, although with less dramatic results.

Note that $F_{4,C}$, $F_{4,A}$, $F_{3,B}$ and $F_{4,B}$ are in fact related through some thermodynamic relationships governing some separation process which exists in the process. The degrees of freedom in the optimization can be further reduced by taking this into account. Suppose that some fictitious reaction product stream F_* exists and is being separated into a gas stream contain C and B in F_3 and a liquid stream containing A, C and D in F_4. The following relationships can be written:

$$F_{*,i} = F_{3,i} + F_{4,i} \quad \text{for each component } i \text{ in the process} \qquad [8\text{-}5]$$

$$\frac{F_{3,i}}{\sum F_{3,i}} = K^{i}_{3,4}(P_*,T_*)\frac{F_{4,i}}{\sum F_{4,i}} \quad \text{for each component } i \text{ in the process} \qquad [8\text{-}6]$$

Combining Equations [8-5] and [8-6], we obtain two generic relationships for each component:

$$f_1(F_*, F_{3,i}, F_{4,i}) = 0 \quad [8\text{-}7]$$
$$f_2(F_*, F_{3,i}, F_{4,i}) = 0 \quad [8\text{-}8]$$

An initial *component table* containing information about the relevant streams can be set up as in Table 8-1 (F_* is not observable and therefore will not be included). Components that are controlled objectives and components which have zero or minimal flows have been labeled with "specified" and "0" respectively.

Table 8 - 1: Initial Component Table

	F_3	F_4
A	0	
B		
C	Specified	
D	0	

Based on Equations [8-7] and [8-8], one can say that for each component, no more than one variable from the set $\{F_{3,i}$ and $F_{4,i}\}$ can be fixed. A value of a variable is fixed if it has be specified in a control objective, used as a manipulated variable in some control strategy, or if the amount of flow is virtually zero under all conditions. Since the values of $F_{3,A}$, $F_{3,C}$ and $F_{3,D}$ have been fixed, the flows of $F_{4,A}$, $F_{4,C}$ and $F_{4,D}$ are defined through Equations [8-7] and [8-8]. These variables are not degrees of freedom in the optimization so they are marked as "n/a" in the final component table (Table 8-2). Both $F_{3,B}$ and $F_{4,B}$ are free to vary. Since the flow of $F_{3,B}$ is bigger, $F_{3,B}$ will be selected to be the variable for optimization (marked as "√") and $F_{4,B}$ can be written as $f(F_{3,B})$, i.e. a function of $F_{3,B}$.

Table 8 - 2: Final Component Table

	F_3	F_4
A	0	n/a
B	√	
C	Specified	n/a
D	0	n/a

Eliminating $F_{4,C}$, $F_{4,A}$ from Φ', the simplified optimization becomes:

$$\min \Phi'' = c_2 (F_{3,B} + f(F_{3,B})) \quad [8\text{-}9]$$
$$\text{s.t.} \quad F_{4,D} = F_{1,D} \text{ (maintain Goal 3)}$$
$$0 = H_1 + H_2 - H_3 - H_4 + Q \text{ (maintain Goal 4)}$$

Since $(F_{3,B} + f(F_{3,B}))$ is essentially the amount of B leaving the process, then, reducing the amount of B leaving the process as much as possible without degrading the levels of achievements of other more important objectives will reduce the cost of operation.

The set of control strategies developed for Level 1 together form a control structure that is suitable for the input-output process representation. Due to lack of information about the process at the input-output level, what have been synthesized was a set of notional associations which define the directions of material and energy flows in the plant that assist the attainment of the overall production plan. Note that at this point in the analysis, the control structure is mainly made up of associations of generalized control objectives with primary manipulated variables. These control strategies will have to be further refined for direct implementation.

8.4 Maintaining Consistency in Control Structure Synthesis During Phase I

In the hierarchical framework, sets of control strategies are to be developed at various level of process representations. Once the plant has been analyzed at a certain viewpoint and a control structure has been developed for that viewpoint, we migrate down the hierarchy and re-analyze the plant at a finer scale. To maintain internal consistency among the different control structures which we develop at different levels of details, the viewpoint, the models which we use for analysis and the control objectives at a lower level must be consistent with those at all the levels above. Furthermore, control structures developed at a lower level should be upwardly consistent with those developed at the higher levels. In this section, the peculiarities pertaining to the refinement of process representations for the design of control structures at a finer process viewpoint will be presented.

8.4.1 Process Definition at the Refined Viewpoint

During refinement of process representations, the amount of details about the plant to be incorporated to the new representation is to be defined. The input-output viewpoint of the plant is to be refined into two or more sub-blocks, each captures certain specific aspect about the process. Each sub-block in a particular representation signifies a group of operating-units in the plant. A functional-based decomposition will be employed. Johnston, J.E. (1991) has stated the following advantages in a functional-based decomposition: (1) similar units are likely to have similar control objectives, thus the number of control tasks associated with a given sub-block in the viewpoint is minimized; (2) local control objectives for a plant typically are associated with one sub-block or the other, and not on both at the same time.

Once the scope of the new viewpoint has been defined, information about the process utilized at the previous level must be consistently utilized at the new levels. Mechanisms which ensures this consistency is maintained are discussed next.

Defining and Ranking Control Objectives at the Refined Viewpoint

As we progress from one viewpoint to a more detailed one, the control objectives associated with the previous level must be updated to reflect the added details in the new viewpoint. The following guidelines have been developed to assist the allocation of control objectives from the previous to the refined level.

1. Explicitly defined process objectives are local in nature. These objectives are allocated to the sub-blocks in which they can be observed.
2. Implicitly defined objectives at the previous level which are *separable* are refined into a number a new objectives in the various sub-blocks at the new level to reflect the added details of the representation. Examples of separable implicit objectives are objectives that are associated with the maintenance of material balance and energy balance controls. Those non-separable implicitly defined objectives at the previous level will remain to be a global objective in the new representation. These control objectives are allocated to all sub-blocks at the lower level.

The definition of a separable implicit objective is given below.

Definition 8-1: Separable implicit objectives

Given $Y_{A,n}$ to be an implicit objective associated with sub-lock $U_{A,n}$ at Level n and can be defined by variables associated with sub-block A only. At Level (n+1), block U_A is refined into sub-blocks $U_{B,n+1}$ and $U_{C,n+i}$. Then, $Y_{A,n}$ is separable if and only if

$$Y_{A,n} = Y_{B,n+1} + Y_{C,n+1}$$

such that $Y_{B,n+1}$ is an implicit objective associated with sub-block $U_{B,n+1}$ at Level (n+1) an can be defined by variables associated with sub-block $U_{B,n+1}$ only; $Y_{C,n+1}$ is an implicit objective associated with sub-block $U_{C,n+1}$ at Level (n+1) an can be defined by variables associated with sub-block $U_{C,n+1}$ only.

Once we have allocated objectives from the previous level to the new representation, we should examined if new objectivês can be further refined or spawned from the initial objectives to assist the attainment of process goals, using procedures described in Section 3.3.2.

The prioritization of control objectives at the refined level is driven by the ranking determined during the preliminary analysis and must be consistent with all prior levels. Implicit objectives which are separable are refined into multiple number of objectives at the refined level. Each of these refined objectives should be of equal importance at the new level. For example, an objective associated with the overall material balance control of material X at the input-output level is being refined into objectives associated with the material balance control of material X in the sub-blocks at the reaction-separation level. Since the overall material balance control of X in the plant can only be maintained through simultaneous balance of material X in both the sub-blocks, it is meaningless to compare the importance of the two new objectives at the refined level. The control of material balance of X in either sub-block are equally important.

The material and energy balance models which describe the inventory control objectives at the previous level should be expanded to reflect the added details and the new exposed structure of the plant. While expanding the models, we must ensure that the models at the refined level are consistent with those developed at the previous levels.

8.4.2 Maintaining Upward Compatibility of Control Structures

A control structure developed at Level (n+1) should be upwardly compatible with the control structure at Level n. In other words, when one abstracts the control structure at Level (n+1) into a structure corresponding to the viewpoint at Level n, the abstracted control structure should be either equivalent to the structure synthesized for Level n or be in a superset of the structure synthesized at Level n (details will be explained later). Some logistic regarding the relationships between sets of consistent control structures at different viewpoints will be presented in this section.

Maintaining Consistent Disturbance Propagation Pathways

Suppose it is required to maintain the accumulation of material X in a single component process at the input-output level for the generic system shown in Figure 8-3 (a). The accumulation of material X at the input-output level of the generic process can be described by the following material balance model:

$$F_1 + F_2 - F_3 - F_4 - r_{I/O} = 0 \qquad [8\text{-}10]$$

where $r_{I/O}$ symbolizes the residuals of X in the block. The corresponding directed graph corresponding to the process is shown in Figure 8-3 (b). To show the topology of the propagation of process disturbances, edges entering the node represent inputs of the material balance equation and the edge coming out of a node represent the output of the equation.

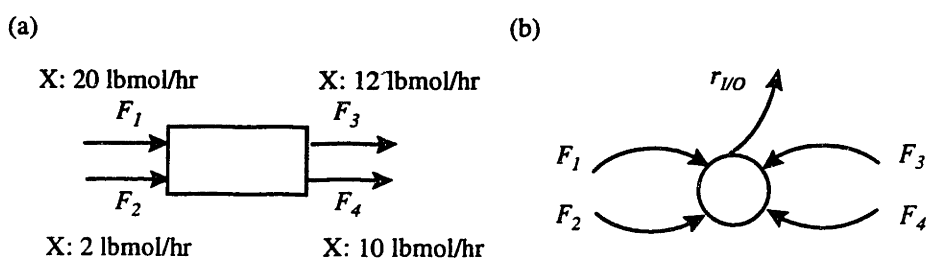


Figure 8 - 3: The Input-Output Level of a Generic Single component process (a) Process Viewpoint; (b) Directed Graph of the Process at this Viewpoint

The accumulation of material X at the input-output level of the generic process can be described by the following material balance model:

$$F_1 + F_2 - F_3 - F_4 - r_{I/O} = 0 \qquad [8\text{-}10]$$

where $r_{I/O}$ symbolizes the residuals of X in the block. In an open-loop system, given the flowrates of F_1, F_2, F_3 and F_4, rate of accumulation of X (i.e. $r_{I/O}$) within the unit can be computed according to equation [5-17]. Supposed the following relationships among the rates of accumulation of X by various inputs is true:

$$\left|dr_{I/O,F_1}\right| > \left|dr_{I/O,F_2}\right| > \left|dr_{I/O,F_3}\right| > \left|dr_{I/O,F_4}\right| \qquad [8\text{-}11]$$

where: $dr_{I/O,k}$ = rate of change residual of material X for a unit change of manipulation k

Based on the size of the gains, F_1 is chosen to be the primary manipulated variable for the maintenance of X at the input-output level. The corresponding control structure is shown in Figure 8-4 (a). As F_1 is used to maintain $r_{I/O}$ at a zero, the control system alters the direction of flow of information in the plant to a topology as shown in Figure 8-4 (b). The pathway indicated in Figure 8-4 (b) represents the most effective path for eliminating variation in $r_{I/O}$.

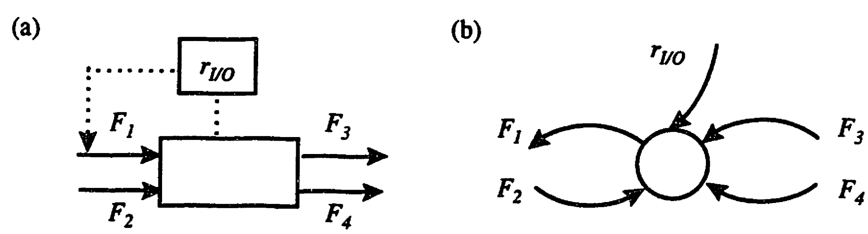


Figure 8 - 4: Controlled Process at the Input-Output Viewpoint (a) Control structure at the Input-Output Viewpoint; (b) Directed Graph of Viewpoint shown in Figure 8-3, under the Influence of Control Strategy in (a)

At Level n+1, the refined viewpoint is shown in Figure 8-5 (a) and the corresponding directed graph of the refined representation in Figure 8-5 (b). The model can be described by the following equations:

$$F_1 + F_2 + F_5 - F_6 - r_A = 0 \qquad [8\text{-}12]$$

$$F_6 - F_5 - F_3 - F_4 - r_B = 0 \qquad [8\text{-}13]$$

$$r_A + r_B - r_{I/O} = 0 \qquad [8\text{-}14]$$

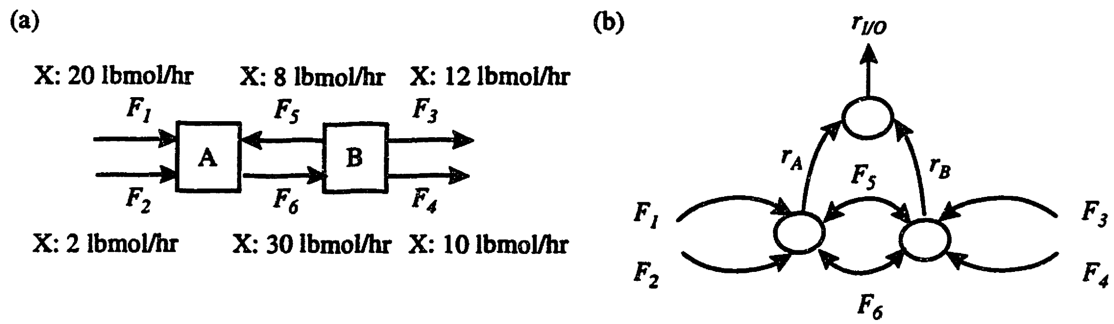


Figure 8 - 5: Refined Representation of the Generic Process (a) Process representation; (b) Directed-graph

Since

$$| dr_{I/O} | = | dr_A + dr_B | \qquad [8\text{-}15]$$

and

$$\left|dr_{I/O,F_1}\right| > \left|dr_{I/O,F_i}\right| \ , \ \forall i = 2,\ 3,\ 4 \qquad [8\text{-}16]$$

The following property about the system at Level (n+1) is true:

$$\left|dr_A + dr_B\right|_{F_1} > \left|dr_A + dr_B\right|_{F_i} \ , \ \forall i = 2,\ 3,\ 4 \qquad [8\text{-}17]$$

Hence, P_1:$r_{I/O} \Rightarrow r_A \Rightarrow F_1$; P_2: $r_{I/O} \Rightarrow r_B \Rightarrow F_5 \Rightarrow F_1$; P_3: $r_{I/O} \Rightarrow r_B \Rightarrow F_6 \Rightarrow F_1$ are the preferred pathways for the maintenance of inventory of material X in the overall system.

In a separable system as in the case for accumulations of materials and energy in the plant, the law of distribution holds and Equation [8-17] can be rewritten as follows:

$$\left|(dr_A)_{F_1} + (dr_B)_{F_1}\right| > \left|(dr_A)_{F_i} + (dr_B)_{F_i}\right| , \ \forall i = 2,\ 3,\ 4 \qquad [8\text{-}18]$$

In the shorter-range of analysis at Level (n+1),

$$(dr_B)_{F_1} = 0 \,;\ (dr_B)_{F_2} = 0 \,;\ (dr_A)_{F_3} = 0 \,;\ (dr_A)_{F_4} = 0$$

The pathways which have *immediate* effects on r_A include P_4: $r \Rightarrow r_A \Rightarrow F_1$; P_5: $r \Rightarrow r_A \Rightarrow F_5$; P_6: $r \Rightarrow r_A \Rightarrow F_6$; P_7: $r \Rightarrow r_A \Rightarrow F_2$; P_8: $r \Rightarrow r_A \Rightarrow F_5 \Rightarrow F_3$ or F_4 ; P_9: $r \Rightarrow r_A \Rightarrow F_6 \Rightarrow F_3$ or F_4. These pathways have been drawn in Figure 8-6. Based on the analysis at Level n, the following relation is true:

$$\left|dr_{A,F_1}\right| > \left|dr_{A,F_2}\right| \qquad [8\text{-}19]$$

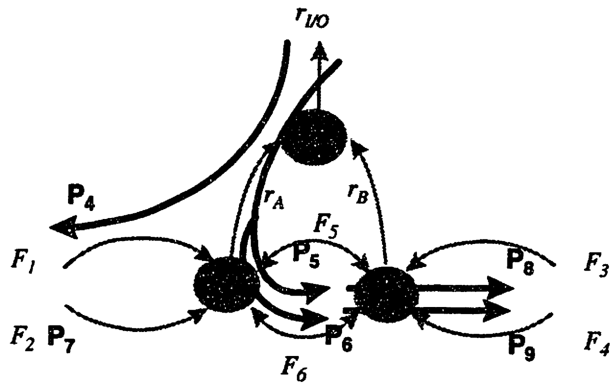


Figure 8 - 6: Possible Pathways to Divert Disturbances Affecting r_A

and F_1 (path P_4) is the best choice among manipulated variables F_2 (path P_7), F_3 and F_4 (paths P_8 or P_9). However, no statements about the relative sizes of $|dr_{A,F_1}|$ and $|dr_{A,F_i}|$; i = 5,6 (which form paths P_5 and P_6) can be made. Then, the best manipulated variable for the maintenance of the level of accumulation of material X in sub-block A must be a member of the set $\{F_1, F_5, F_6\}$. In other words, at Level (n+1) the designer can focus our analysis on the *new* manipulations which are directly linked to sub-block A and the best manipulated variable determined at the previous level.

Consistency Logic 1 for selection of manipulated variables

As we move from Level n to (n+1) we refine a separable control objective k to k_1, $k_2,\ldots, k_w$ where k_p ($1 \leq p \leq w$) indicates the objective is observable in sub-block U_p. The best manipulated variable m to control objective k at Level n is a member of the set of potential manipulated variables to control k_j at Level (n+1) where U_j ($1 \leq j \leq w$) is the sub-block in which m can be directly observed at Level (n+1).

The pathways along which r_B can be maintained are: P_{10}: $r \Rightarrow r_B \Rightarrow F_3$; P_{11}: $r \Rightarrow r_B \Rightarrow F_4$; P_{12}: $r \Rightarrow r_B \Rightarrow F_5$; P_{13}: $r \Rightarrow r_B \Rightarrow F_6$; P_{14}: $r \Rightarrow r_B \Rightarrow F_5 \Rightarrow F_1$ or F_2 ; P_{15}: $r \Rightarrow r_B \Rightarrow F_6 \Rightarrow F_1$ or F_2. Our analysis (conclusion) at Level n does not allow us to make any statements about the quality of any of the above pathways. The following generalization can be made:

Consistency Logic 2 for selection of manipulated variables

As we move from Level n to (n+1) we refine a separable control objective k to k_1, $k_2,\ldots, k_w$ where k_p ($1 \leq p \leq w$) indicates the objective is observable in sub-block U_p. The best manipulated variable m to control objective k at Level n can be directly observed from sub-block U_j at Level (n+1). Then, any manipulated variables can be the best manipulated variable for the maintenance of sub-goals k_i (where $i \neq j$) at Level (n+1).

Generating upwardly compatible control structures

Since F_1 is the best manipulated variable for the maintenance of the inventory of material X at the input-output level of the generic process (Figure 8-4 (a)). Based on *Consistency Logic 1*, the best manipulated variables for the control of r_A at Level (n+1) must be a member of the set $\{F_1, F_5, F_6\}$. Table 8-3 gives the structural representation of the system of equations at Level (n+1). The conventions here is that "+1" is used for an incoming process streams, "-1" is used for an outgoing process streams.

Table 8 - 3: Structural Representation of the process at Level (n+1)

F_1	F_2	F_3	F_4	F_5	F_6	r	r_A	r_B
1	1			1	-1		-1	
		-1	-1	-1	1			-1
						-1	1	1

From Section 8.4.1, both r_A and r_B are of equal importance. For the sake of illustration, it will be assumed in the rest of the discussion that that r_A is of higher priority than r_B. The method by which we synthesize control structure when there are objectives of equal importance will be discussed in Section 8.4.3.

Beginning from the most important objective r_A, a manipulated variable is to be chosen. Suppose F_6 is found to be the best manipulated variable for this objective, then, the matrix in Table 8-3 must be updated to reflect the feedback control association of this assignment. The updated matrix is given in Table 8-4.

Table 8 - 4: Updated Structural Representation of the process at Level (n+1)

F_1	F_2	F_3	F_4	F_5	F_6	r	r_A	r_B
1	1	-1	-1	0			-1	-1
						-1	1	1

The updated matrix indicates that through the assignment for of F_6 to r_A, F_1 and F_2 become directly related to r_B. If we select F_3 to be the manipulated variable for r_B, the control structure at Level (n+1) is will assign F_6 to maintain r_A and F_3 to maintain r_B. The corresponding control structure and directed graph of the closed-loop system are shown in Figures 8-7 (a) and (b) respectively. With this control configuration, disturbances entering through F_1, F_2, F_4 or r leave the process via F_3. Note this is a feasible control structure. F_3 is a valid manipulated variable as indicated by the structural matrix in Table 8-4. The control structure provides an outlet for disturbances entering the plant to leave the system through an external stream.

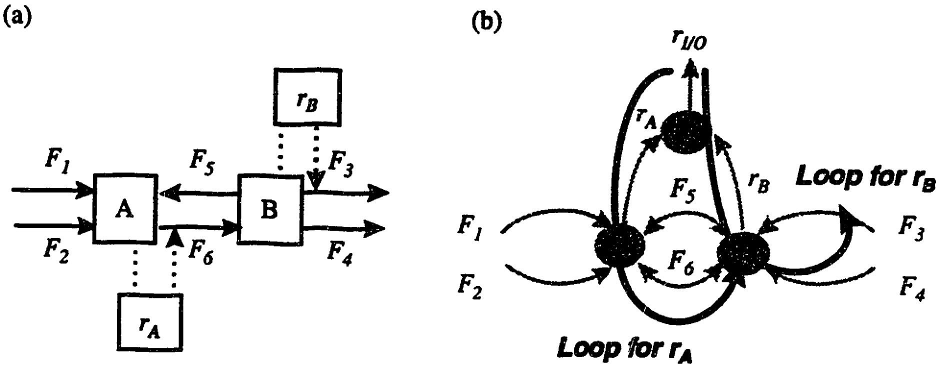


Figure 8 - 7: Control structure for the Generic Process at Level (n+1) (a) Control Structure; (b) Directed Graph of the Closed-loop System

However, if the control structure developed at Level (n+1) is abstracted to a viewpoint that is equivalent to the one at Level n, the structure shown in Figure 8-8 where r is being controlled by F_3. This structure is not equivalent to the one which was developed at Level n (shown previously in Figure 8-4 (a)). There is an inconsistency in the hierarchy of control structures. The control structure developed at Level (n+1) is not upwardly compatible with the structure at a higher level. In fact, the analysis at the higher level indicates that the structure which uses F_3 to control r is inferior to the structure developed earlier in Figure 8-4 (a). Based on this observation, the following consistency logic can be established:

Consistency Logic 3 for the selection of manipulated variables

To maintain upward compatibility, the best manipulated variable m for objective k at Level n should also be among the set of manipulated variables to control objectives $k_1, k_2, \ldots, k_w$ where k_p ($1 \le p \le j$) indicates the objective is observable in sub-block U_p at Level (n+1).

The application of the consistency logic rules to the synthesis of control structures at the refined levels will be illustrated in the chapters to follow.

Contraction of Control Structure

So far, in the discussion, it has been assumed that each sub-block in the process representation is a integrating material capacitor. In some cases, as one moves from a coarse level to a refined level, one may discover that some sub-blocks are solely made up of self-regulating units. Self-regulating units do not require intervention by a control system. In such cases, the set of consistency logic still holds, but in a modified sense.

In the above example, the viewpoint at Level n (Figure 8-3 (a)) is refined the viewpoint at Level (n+1) (Figure 8-5 (a)). If the sub-block A at Level (n+1) is a self-regulating process, there is no need to derive a control scheme for r_A. According to *Consistency Logic 2*, all manipulated variables are potential candidates for r_B. Suppose F_6 is found to be the best primary manipulated variable to maintain r_B at zero. Direct abstraction of this control structure to Level n would result in one which has no visible manipulated variable (F_6 is not visible from Level n). However, sub-block A is a self-regulating unit. As F_6 is varied to maintain r_B at zero, r_A is affected. By its self-regulating nature, other streams in sub-block A would have to move to drive r_A to zero. Thus, the following are scenarios possible:

1. If F_6 can be directly manipulated, then, the self-regulating mechanism would move either F_1 or F_2 or both accordingly.
2. When it has been determined that F_6 cannot be directly manipulated (either at Level (n+1) or at later levels when more information about the plant is available). *Spawn* flowrate of F_6 as a new objective (see Sections 2.4.1 and 3.3.2) and choose a manipulated variable to control its flow. Since F_1 has been determined to be an effective manipulated variable at Level n, according to *Consistency Logic 1* and the *Consistency Logic 3*, F_1 is a promising candidate.

Elaboration of Control Structure at the Refined level

Suppose at a refined level such as Level (n+1) of the generic process (Figure 8-5 (a)), F_1 is to maintain r_A external streams like F_3 or F_4 has been chosen to maintain r_B based on the size of their gains. One motivation for this selection is that using either F_3 or F_4 to maintain variation in r_B would allow variations to be quickly diverted to the environment. This is a valid argument. Figure 8-8 shows the pathway of such a control structure at Level (n+1) in a digraph. If such a strategy is used, the abstraction of the control structure at Level (n+1) would lead to a two inputs (F_1 and F_3) one output (r) control structure at Level n (see Figure 8-9). The abstracted control structure is potentially better than the original one as we have allocated more inputs to accomplish the control. By reserving F_1 to be the manipulated variable in the block to which it is directly linked and by considering diversion of disturbances in the plant at Level (n+1), we have opened the opportunity to *elaborate* the overall control structure. This control structure is a *superset* of the one developed at Level n.

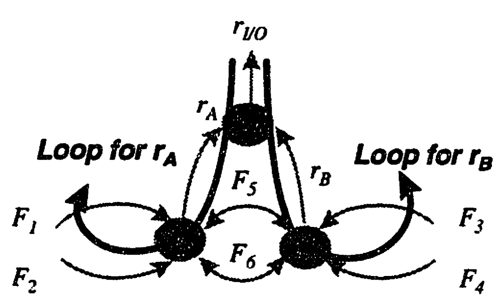


Figure 8 - 8: Directed Graph of the Generic Process Controlled by F_1 and F_3

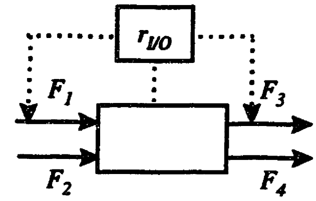


Figure 8 - 9: An Elaborated Overall Control Structure

Consistency Logic Map

Based on the discussions in the this sections, the following *consistency logic map* can be constructed:

1. Disturbances entering the plant must be diverted to the environment. If the overall control scheme contains disturbances in the plant, either materials or energy (depending on the nature of the disturbances) will accumulate in the plant, making some process variables integrative. In order to divert the incoming disturbances out of the process, at least one input/output stream must be used as manipulated variable.
2. If something has been chosen to be the best manipulated variable at Level n, by *Consistency Logic 3*, it is also going to be one of the best manipulated variables at each of the refined levels below Level n.
3. Suppose m is the best manipulated variable for block k at Level n. At Level $(n+1)$, we refine sub-block k into k_1, k_2, ... k_w where k_p symbolizes a goal observable in sub-block p $(1 \leq p \leq w)$. If manipulated variable m belongs in k_j, then, the following statements are true:
   - Manipulated variable m is in the set of potential manipulated variables for the refined objective in sub-block k_j. This set consists of m and all new manipulated variables attached to sub-block k_j which become observable at Level $(n+1)$.
   - No generalization can be made about sub-blocks k_i, where $i \neq j$.

8.4.3 Synthesize Control Structure at a Refined Level during Phase I

Once we have updated the input-output process representation to incorporate more information about the plant into the viewpoint, the control structure must also be updated to reflect the added details at the refined level. We will employ long-horizon design criteria to determine a set of control strategies for the representation as long as significant process dynamics is not observable in the representation.

For most chemical process, it is typical that control of material and energy balances are required in all the sub-blocks at the refined level. The material balances in all the sub-blocks of the same component will be assigned the same order of priority (recall Section 8.4.1). In the next example, the application of the mulitobjective design framework discussed in Chapter 6 to such a situation will be demonstrated.

EXAMPLE 8-2

The generalized reaction-separation system for A + B $\rightarrow$ C process studied in Example 8-1 is shown in Figure 8-10. At this level, the individual material accumulations of A, B, and

D as well as the energy accumulation must be maintained in both the reaction section and the separation section. The set of prioritized control objectives for this level is summarized in Table 8-5.

Table 8 - 5: Prioritized Control Objectives of the A+B $\rightarrow$ C Process at the Generalized Reaction-Separation Level

	Generalized Reaction	Generalized Separation
1	Maintain $r_{A\text{-}reaction}$ at zero	Maintain $r_{A\text{-}separation}$ at zero
2	Maintain $r_{B\text{-}reaction}$ at zero	Maintain $r_{B\text{-}separation}$ at zero
3	Maintain $r_{D\text{-}reaction}$ at zero	Maintain $r_{D\text{-}separation}$ at zero
4	Maintain $e_{\text{-}reaction}$ at zero	Maintain $e_{\text{-}separation}$ at zero
5		Production of C at 10,000 lbmol/day
6	Minimize Production Cost	

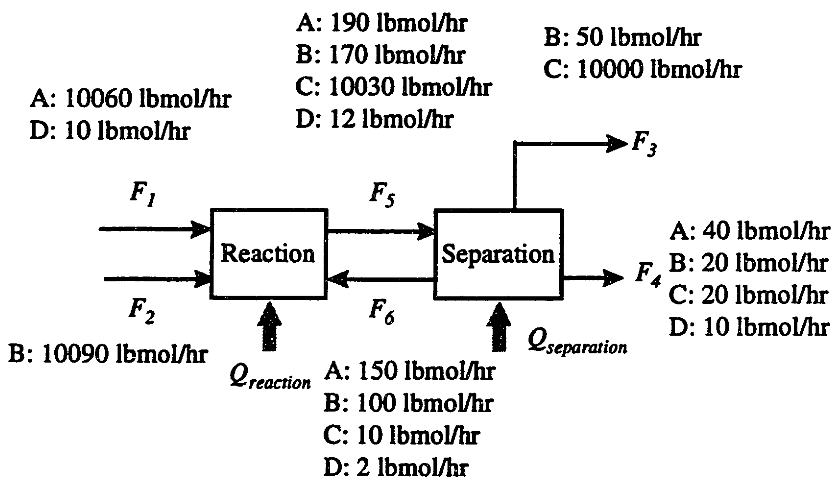


Figure 8 - 10: The Generalized Reaction-Separation System of the A + B $\rightarrow$ C Process

The material and energy balances which are suitable for this level of process representation are:

$$r_{A\text{-}reaction} = F_{1,A} + F_{6,A} + F_{6,C} - F_{5,C} - F_{5,A} \quad [8\text{-}20]$$

$$r_{A\text{-}separation} = F_{5,C} + F_{5,A} - F_{3,C} - F_{4,A} - F_{4,C} - F_{6,A} - F_{6,C} \quad [8\text{-}21]$$

$$r_{B\text{-}reaction} = F_{2,B} + F_{6,B} + F_{6,C} - F_{5,C} - F_{5,B} \quad [8\text{-}22]$$

$$r_{B\text{-}separation} = F_{5,C} + F_{5,B} - F_{3,C} - F_{3,B} - F_{4,C} - F_{5,B} - F_{6,B} - F_{6,C} \quad [8\text{-}23]$$

$$r_{D\text{-}reaction} = F_{1,D} + F_{6,D} - F_{5,D} \quad [8\text{-}24]$$

$$r_{D\text{-}separation} = F_{5,D} - F_{4,D} - F_{6,D} \quad [8\text{-}25]$$

$$e_{reaction} = H_1 + H_6 + H_2 - H_5 + Q_{reaction} \qquad [8\text{-}26]$$
$$e_{separation} = H_5 - H_6 - H_3 - H_4 + Q_{separation} \qquad [8\text{-}27]$$

Note that $r_{i\text{-}reaction} + r_{i\text{-}separation} = r_i$ for i = {A, B, D} and $e_{reaction} + e_{separation} = e$.

Some of the gains of the material residuals have been computed and are summarized in Table 8-6. Notice that by assuming that none of the sub-blocks in the representation are self-regulating units, with feedback control, the flowrate of the output streams of a sub-block are not dependent on the flowrate of the input streams. Hence, long range effect such as the effect of a change of F_1 on $r_{A\text{-}separation}$ is zero.

The control structure for this level control structure can be synthesized starting from the most important objective. It is required to develop a control strategy to maintain the overall material balance of A by maintaining zero accumulation in $r_{A\text{-}reaction}$ and $r_{A\text{-}separation}$. Since the maintenance of $r_{A\text{-}reaction}$ and $r_{A\text{-}separation}$ are of equal importance, the *open-loop gains* of both objectives will be studied and the best inputs for maintaining both of them at their desired values will be selected. Earlier at Level 1 (recall data in Example 8-1), we assigned F_1 to maintain the overall material balance of A. Then, based on the *Consistency Logic Map* developed in Section 8.4.2, the following statements can be made:

1. F_1 is a member of the set of potential manipulated input for the maintenance of $r_{A\text{-}reaction}$ since it is observable from the reaction sub-block. Other potential manipulated inputs are the new manipulated variables observable from the new level (Consistency Logic 1).
2. Any manipulated variable could be the best manipulated variable for the maintenance of
$r_{A\text{-}separation}$ (Consistency Logic 2)
3. F_1 should be a member of the set of best manipulated inputs to maintain both $r_{A\text{-}reaction}$ and $r_{A\text{-}separation}$ (Consistency Logic 3).

These statements allow one to conclude that the sets of potential manipulated variables to maintain $r_{A\text{-}reaction}$ and $r_{A\text{-}separation}$ are:

1. $r_{A\text{-}reaction}$: {F_1 and component flows in F_5 and F_6}
2. $r_{A\text{-}separation}$: {any manipulated variables}

Judging from the size of the gains in Table 8-6, F_1 and $F_{5,C}$ are the best manipulated inputs for the maintenance of $r_{A\text{-}reaction}$ and $r_{A\text{-}separation}$ respectively. Once the manipulations have been selected, the next step is to verify that the selections are feasible under closed-loop control. By assuming $r_{A\text{-}reaction}$ is of higher priority for a moment, the closed-loop feasibility is checked by computing the closed-loop gains of $r_{A\text{-}separation}$ while $r_{A\text{-}reaction}$ is under closed-loop control by F_1. As shown in Column 2 of Table 8-7, the gain of $F_{5,C}$ is not zero and it remains to be the best input for $r_{A\text{-}separation}$. $F_{5,C}$ is a feasible choice for the maintenance of $r_{A\text{-}separation}$.

Table 8 - 6: Open-loop gains at the Refined Level

	$r_{A\text{-}reaction}$	$r_{A\text{-}separation}$	$r_{B\text{-}reaction}$	$r_{B\text{-}separation}$
F_1	100.6	0	0	0
F_2	0	0	100.9	0
$F_{5,A}$	-1.9	1.9	0	0
$F_{5,B}$	0	0	-1.7	1.7
$F_{5,C}$	-100.3	100.3	-100.3	100.3
$F_{5,D}$	0	0	0	0
$F_{6,A}$	1.5	-1.5	0	0
$F_{6,B}$	0	0	1	-1
$F_{6,C}$	0.1	-0.1	0.1	-0.1
$F_{6,D}$	0	0	0	0
$F_{3,B}$	0	0	0	-0.5
$F_{3,C}$	0	-100	0	-100
$F_{4,A}$	0	-0.4	0	0
$F_{4,B}$	0	0	0	-0.2
$F_{4,C}$	0	-0.2	0	-0.2
$F_{4,D}$	0	0	0	0

Before we move on to the selection of inputs to maintain $r_{B\text{-}reaction}$ and $r_{B\text{-}separation}$, the gain estimates must be updated to reflect the control strategies selected for the pervious objectives. These are shown in Columns 3 and 4 of Table 8-7. Using similar reasoning as those for $r_{A\text{-}reaction}$ and $r_{B\text{-}separation}$, F_2 and $F_{5,B}$ are selected to be the inputs for $r_{B\text{-}reaction}$ and $r_{B\text{-}separation}$ respectively (conforming also to the Consistency Logic map). One must verify that these selections do not create conflict under closed-loop control. The gains for $r_{B\text{-}separation}$ while $r_{B\text{-}reaction}$ is under closed-loop control by F_2 are shown in Column 5 off Table 8-7. See that the gain of $F_{5,B}$ is not zero. The assignments are therefore valid.

The rest of the control structure for the generalized reaction-separation system can be developed in similar manner. Notice that abstraction of the control strategies for the maintenance of material balance of both A and B return the control strategies developed for the input-output representation. The control strategies at this level are upwardly compatible with those developed at the pervious level.

Table 8 - 7: Closed-loop gains at the Refined Level

	$r_{A\text{-reaction}}$	$r_{A\text{-separation}}$ closed-loop	$r_{B\text{-reaction}}$	$r_{B\text{-separation}}$	$r_{B\text{-separation}}$ closed-loop
F_1	**100.6**	0	0	0	0
F_2	0	0	**100.9**	0	0
$F_{5,A}$	-1.9	1.9	1.9	-1.9	-1.9
$F_{5,B}$	0	0	-1.7	**1.7**	**1.7**
$F_{5,C}$	-100.3	**100.3**	0	0	0
$F_{5,D}$	0	0	0	0	0
$F_{6,A}$	1.5	-1.5	-1.5	1.5	1.5
$F_{6,B}$	0	0	1.0	-1.0	-1.0
$F_{6,C}$	0.1	-0.1	0	0	0
$F_{6,D}$	0	0	0	0	0
$F_{3,B}$	0	0	0	-0.5	-0.5
$F_{3,C}$	0	-100	-100	0	0
$F_{4,A}$	0	-0.4	-0.4	0.4	0.4
$F_{4,B}$	0	0	0	-0.2	-0.2
$F_{4,C}$	0	-0.2	-0.2	0	0
$F_{4,D}$	0	0	0	0	0

At each refined viewpoint, long-horizon analysis is used to develop a more elaborate control structure which addresses the aspects of the overall production plan observable from that new level. The process viewpoint is further refined and the analysis is repeated, until a level whose process dynamics become significant is arrived. At that level, one begins Phase II of the design and carry out short-horizon analysis to develop a control structure that is suitable for dynamic process regulation of the controlled variables. The mechanics involved at Phase II of the design is discussed next.

8.5 Phase II: Short-horizon Analysis

In the second phase of the design, control structures are synthesized by evaluating the dynamic performance provided by the various manipulated variables. Long-horizon analysis is always performed at the coarsest viewpoint (i.e. Level 1) while short-horizon analysis is always performed at the most detailed viewpoint, say level N of the plant. Somewhere between Level 1 and Level N, the following criteria is satisfied:

Criterion for switching from long-horizon analysis to short-analysis

Let $\tau_1 \cdots \tau_w$ be the overall time constants of sub-blocks 1 to w at Level K. If the following condition holds for *all* of the sub-blocks at level K:

$$\tau_\delta \approx \min(\tau_\delta^a, \cdots, \tau_\delta^m) \quad \forall \alpha = 1, \cdots, w$$

where τ_δ^β = time constant in sub-block β at level K+1 and sub-block β is refined from sub-block δ at level K. Then, Phase II short-horizon analysis should be performed at Level K.

In other words, if the dynamics observable from all sub-blocks at Level K are similar to the dynamics observable at Level K+1. This criterion is consistent with a well known fact from control theory that hierarchically nested servo loops tend to suffer instability unless the band-width of the control loops differ by about an order of magnitude (Albus, 1991).

8.5.1 Generating and Ranking Specific Controlled Variables

During short-horizon analysis, the goal is to develop feedback control strategies for direct process regulation. Thus, at the level where the analysis is switched to Phase II, the objectives related to the maintenance of material and energy flows must be transformed into some specific process controlled variables that are easily measurable and are related to the levels of accumulations of the materials or energy in the sub-systems. After the relevant material and energy balances have been allocated to appropriate sub-blocks in the viewpoint, the procedure described next can be used for the generation of specific process controlled variables.

Step 1

For each sub-system observable at the level, determine if it is a material capacitor or energy capacitor. If the unit is not a material capacitor, material accumulation will always be zero and material balances associated with this sub-block can be dropped. If the sub-system is not an energy capacitor, energy accumulation will always be zero and the corresponding energy balance can be dropped.

Step 2

Residuals of all material balances of each sub-system form a group. For each group, identify a process variable that is easily measurable and indicates the levels of material accumulations in the sub-systems. The following rules can be used to examine each group of material balance residuals:

1. Do the materials involved present in the gas phase, liquid phase, solid phase or all of those?
2. If some materials exist in liquid phase, *collapse* (similar residuals are collapsed into a lumped residual if the lumped residual can be easily accessed or measured) and refine this group of objectives to the level(s) of the total amount of liquid in the sub-system

(the number of levels should be the same as the number of miscible liquid phases in the sub-system multiplied by the number of distributed accumulations in the sub-system)

- Is the level of the liquid integrating (study the structure of the sub-system) ?
  - If it is, this is a pure capacitor. Feedback control must be applied.
  - If it is not integrative and if variation of the level is acceptable, *demote* this objective.
- If the level of the liquid is related to the stabilization strategy, *promote* this objective.

3. If some materials exist in the gas phase as well, also *collapse* and refine this group of objectives to the pressure of the gas in the sub-system.
   - Is the pressure integrating (study the structure of the sub-system) ?
     - If it is, this is a pure capacitor. Feedback control must be applied.
       - Is the pressure linked to other sub-systems?
         - If it is, control only one pressure from all these sub-systems. Choose the most appropriate one to apply feedback control.
     - If it is not integrative and if variation of the level is acceptable, *demote* this objective.
   - If the pressure is related to the stabilization strategy, *promote* this objective.
4. If some materials exist in solid phase as well, also *collapse* and refine this group of objectives to the level of solid in the sub-system.
   - Is the level of solid integrating (study the structure of the sub-system)?
     - If it is, this is a pure capacitor. Feedback control must be applied.
     - If it is not integrative and if variation of the level is acceptable, *demote* this objective.
   - If the level of solid is related to the stabilization strategy, *promote* this objective.

Step 3

For each residual of energy balance, identify a process variable that is easily measurable and indicates the level of accumulations of the amount of energy in the sub-systems. The following rules can be used to examine each group of material balance residuals:

- Identify the key indicator of build-up of energy residual in the sub-system. Energy build-up is usually manifested in the temperature of the system. For sub-systems with gaseous materials, energy may also manifest in the pressure of the system.
  - Is this variable integrating (study the structure of the system) ?
    - If it is, this is a pure capacitor, feedback control must be applied.
    - If it is not integrative and if variation of the level is acceptable, *demote* this objective.
  - If this variable is related to the stabilization strategy, *promote* this objective.

Note that if there are alternative process variables that are related to the material or energy balances, choose the process variable based its accessibility; ability to detect presence of disturbances and relation to the overall objectives.

Ranking Specific Controlled Objectives

In general, material or energy balance equations may be refined into objectives that have been previously been selected to be used in feedback control of the plant for stabilization purposes. These objectives are promoted to first priorities. Self-regulating objectives are less critical than the integrating objectives so they are demoted to lower priorities. Self-regulating material residuals are demoted to priorities lower than all other integrative material residuals. As accumulation of energy usually produce localized effect in the plant, self-regulating energy residuals can be demoted to priorities lower than objectives related to product specifications.

8.5.2 Synthesize Control Structures for Short-horizon Control

During Phase II of the design, set of design criteria for short-horizon control described in Section 6.3.2 will be employed to generate a control structure for the process. The goal of this phase is to develop a set of control strategies for fast dynamic regulation of the process and minimize the effect of the fast varying disturbances on critical process variables. Again, during the selection of primary manipulated variable, transformation of process variation by the control strategies should also be taken into account, as well as the costs associated with the usage of the manipulations. The assignment of control inputs to process objectives and the development of a control structure has been demonstrated in Example 6-1. Application of the design method presented in Section 6.3.2 requires the knowledge of the dynamic feedback stabilization control strategy which maintains the stability of the system for an open-loop unstable process (determined during preliminary analysis); dynamic process models relating process inputs with controlled variables, quantifying the effects of deadtime, time constants, right-half plane zeros, etc. in the process; model uncertainty associated with the dynamic models and rangeability of the process inputs.

For most chemical plants, the maintenance of the overall material balance control entails the monitoring and control of levels of liquid accumulations in various vessels in the process which are usually integrative. Integrative objectives are of the top priorities in the hierarchy of control objectives. Strictly stable step models of other control objectives are usually only obtainable when the process integrators are under closed-loop control. Thus, a strategy in the synthesis of control structure for short-horizon control is to divide the model development into to stages. In the first stage, models for all process integrators are developed. Using the modular multivariable design framework, a set of control strategies which will maintain the overall material balance in the plant by keeping all process integrators at steady-state can be established. Then, in the second stage, stable step models of the rest of the control objectives can be developed while process integrators are under closed-loop control using the partial control structure developed during the first stage of the design. Such a two part approach conforms to the modular multiobjective design framework as strategies for the non-integrative control objectives are synthesized using models describing the plan dynamics when all other more important ones (such as the integrative variables) are under closed-loop control.

The control structures developed during Phase II of the design are based on criteria which are different from those employed during Phase I. Thus, abstraction of the control structure developed during Phase II does not necessarily produce a similar control structure as those identified during Phase I.

8.5.3 Refinement of Process Representations In Phase II

If further refinement opportunities exists in Phase II, the control objectives and control structure synthesized at the first level of Phase II will have to be updated to reflect the added details in the new representations. In general, two cases are possible:

1. If more detailed, higher order dynamics is revealed at the refined level, control decisions which are valid at the longer time-horizon of the previous level may not be valid in the shorter-horizon represented by the new representation. Control assignments must be re-established for the new level.
2. For the case where process dynamics at the refined level is not significantly different from the dynamics at the previous level, the control structure synthesized at the previous level only need to be updated if there are more control objectives at the refined level or if there are more available manipulated variables at the refined level.

If the second case is true, the procedure below can be followed to update the control structure for the new process representation.

At Level K

If the criterion for short-horizon analysis is met, short-horizon analysis will be performed. At this level, a set of manipulated variables M^K is available for selection.

Level K+1

The control structure derived at Level K has to be refined to reflect the added details at Level K+1. If the dynamics observable at Level K+1 is similar to dynamics observable at Level K, the control structure is adjusted because either (a) there are more control objectives at the refined level or (b) there are more available manipulated variables at the refined level is true. If *only* (a) is true, there is a new set of objectives J, then the control structure has to be refined starting from the level of priority corresponding to the highest priority level in set J. If (b) is true, there is a new set of manipulated variables M^{K+1} available for selection. Then, starting from the objective of the highest priority, evaluate if the availability of set M^{K+1} would generate a better control structure.

8.6 Developing a Multi-Horizon Control System

Following the framework introduced in Chapter 3, the proposed design methodology allow the generation of a set of control structures for the process plant. Each control structure has its relevance at a certain time-horizon that characterizes the process viewpoint associated with that control structure. The set of control structures can be integrated to produce a multi-horizon control system for the process plant. The generation of the multi-horizon control system consists of two steps. In the first step, detailed control the structure developed at the most detailed level is partition into different segments. In the second steps, control strategies developed at the coarser levels are integrated to the detailed control structure.

8.6.1 Partitioning the Detailed Control Structure

Based on observability in the time-resolution, the control structure developed at the most detailed level during Phase II can be partitioned into different sets, each set is related to a specific level of plant representation. A general rule is to associate each control objective with a time-scale corresponding to the level of representation from which it first becomes observable. Hence, each control objective should be regulated at a frequency related to the relevant time-horizon of that level of representation.

EXAMPLE 8-3

Figure 8-11 shows a hierarchy of control structures developed for a simple process plant. The functionality of each of the control structures is explained in Table 8-8. The control structure at Levels 1 and 2 have been developed using long-horizon design criteria, while that at Level 3 has been developed using short-horizon design criteria.

Table 8 - 8: Control Structures for Various Process Representations

	Control Structures for Various Process Representations	Relevant Time-horizon
Level 1	Maintain material balance of A using F_1	
	Maintain material balance of B using F_2	
	Maintain energy balance of the system using Q	
	Maintain production rate of C by adjusting $F_{4,C}$	
Level 2	Maintain material balance of A using $F_{6,A}$ and $F_{8,A}$	
	Maintain material balance of B using $F_{6,B}$ and $F_{8,B}$	
	Maintain energy balance of the system using Q_a and Q_b	
	Maintain production rate of C by adjusting $F_{4,C}$	
	Maintain composition of c adjusting $F_{7,c}$	
Level 3	Maintain liquid level in Unit *d* by F_9	Short
	Maintain liquid level in Unit *e* by F_7	Short
	Maintain liquid level in Unit *b* by F_4	Short
	Maintain production rate of C by F_2	Long
	Maintain composition of feed to sub-block *b* by adjusting Q_{cw1}	Intermediate

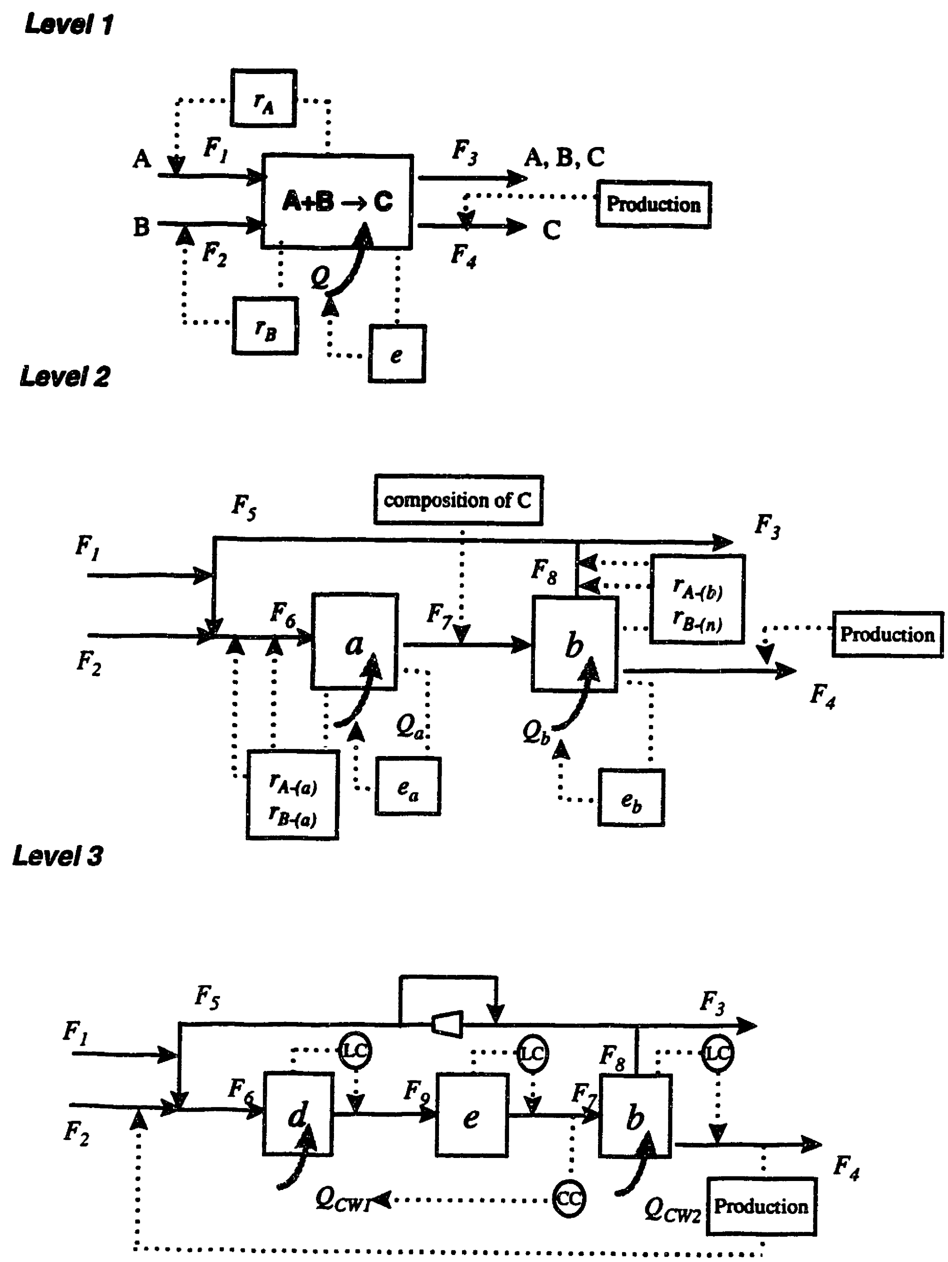


Figure 8 - 11: A Hierarchy of Control Structures for A Process Plant

The control structure at Level 3 is the most detailed control structure for the plant and it is the structure that can be implemented for direct process regulation. As shown in Table 8-8, the control structure at Level 3 is partitioned into three sets. The control strategies related to the maintenance of the liquid levels in Units *d*, *e* an *b* involve process variables and/or manipulated inputs which are first observable from the viewpoint at Level 3. These objectives are associated with dynamics which are observable from Level 3 and short-horizon control would be required. The control strategy related to the maintenance of the composition of C in the feed to Unit *b* is observable from both Levels 2 and 3. Since it is first observable from Level 2, its dynamics is slower than the dynamics associated with the liquid levels. This objective can be controlled using an intermediate time-horizon. The objective associated with the production rate is observable from Level 1. It has a long time-span of operation and can be controlled with a relatively long time-horizon.

In Example 8-3, the process dynamics have been divided into three categories. For larger plants with many different levels of representations, a finer division is possible.

8.6.2 Integrating Control Strategies at Different time-horizons

Control strategies developed during Phase I are primarily concerned with the management of material and energy flows in the system. These control strategies provide insights as to what process variables should be maintained or adjusted to assist the overall material and energy management in the system. If there are excess degrees of freedom, manipulated variables can be assigned to additional control objectives. Objectives related to the material and energy balance controls have been refined into level, pressure, or temperature controls at the detailed level. Any additional control strategies generated from strategies developed during Phase I of the design serve to supplement the control structure at the detailed level and should have lower priorities than those which have been identified directly from translation, refinement and spawning. The two important items to look for include:

- If several component flows of an inlet stream to an abstract block have been chosen as "manipulated variables" at an abstract level, these are values to be adjusted for different product specifications. The compositions (design values) of these materials in the stream should be controlled to assist convergence of material balances during disturbance rejection.
- If several component flows of an outlet stream of an abstract block have been chosen as "manipulated variables" at an abstract level, it means that some compositions in this stream should normally be allowed to float since their levels depend on the type of disturbances influencing the plant as well as the product specifications. However, we should identify physical manipulations in which these chosen variables can be adjusted so that inventories of materials can be directly regulated when required.

EXAMPLE 8-4

The following additional control strategies for the process studied in Example 8-3 have been identified:

1. Since the component flows of A and B in F_6 have to be adjusted at Level 2 to maintain the overall material flows in the system, the compositions of either A or B in F_6 (this stream does not contain C) can be controlled to assist the convergence of the overall material balance.
2. Since the component flow of A and B in F_8 have to be adjusted at Level 2 to maintain the overall material flows in the system, we should develop control strategies which assist the variation of the compositions of either A, B or C in F_8 as process conditions change.

If there are excess manipulated variables, control strategies which address these objectives an be developed. These control objectives are observable from Level 2, they can be controlled at an intermediate time-horizon. Since these are supplementary control objectives, they are of lower priorities than those which have been identified earlier by direct translation, refinement and spawning. The final detailed control structure for this process is summarized in Table 8-9.

Table 8 - 9: Final Detailed Control Structure for process in Figure 8-11

Final Detailed Control Structure	Relevant Time-horizon
Maintain liquid level in Unit *d* by F_9	Short
Maintain liquid level in Unit *e* by F_7	Short
Maintain liquid level in Unit *b* by F_4	Short
Maintain production rate of C by F_2	Long
Maintain composition of feed to sub-block *b* by adjusting Q_{CW1}	Intermediate
Maintain composition of A in feed to Unit *d*	Intermediate
Maintain composition of C in F_8	Intermediate

Note that each time-scale in the multi-horizon control system developed in Examples 8-3 and 8-4, serves a unique purpose. Control strategies deployed with a long-time horizon focus on the long-term material and energy balances of the plant. The intermediate ones focus on the maintenance of secondary objectives which assist production. The primary focus of the short-horizon control strategies is on fast dynamic regulation of key process variables and insulate them from high frequency disturbances. The functionality of the multi-horizon control system is pictorially displayed in Figure 8-19. Each layer of the multi-horizon control system can be assumed to be relatively independent of other layers in the hierarchy.

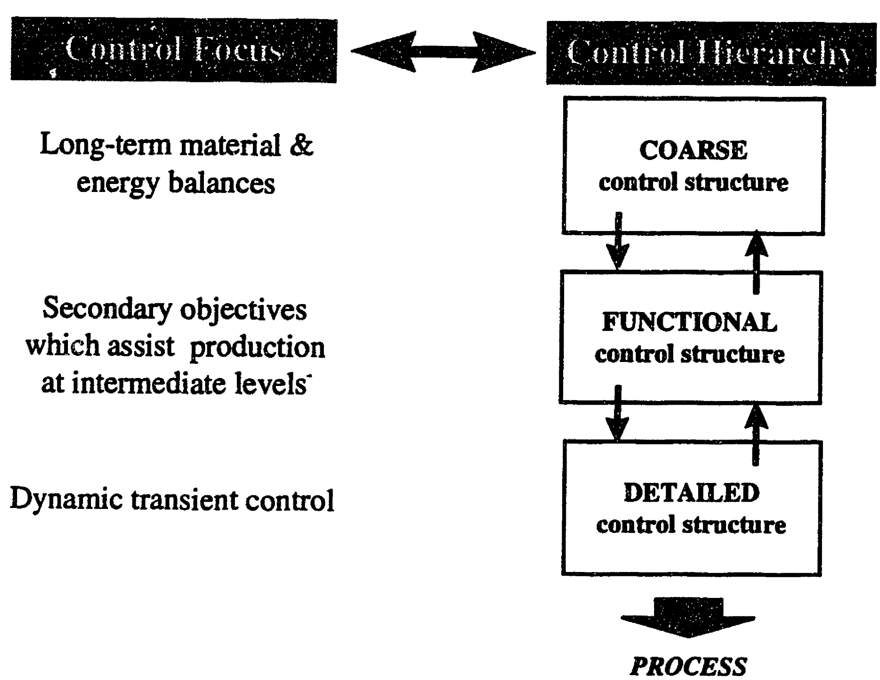


Figure 8 - 12: Functionality of a Multi-horizon Control System

8.7 Implementing the Plant-wide Control Structure

In general, the plant-wide control structure is to be implemented using a modular multivariable controller (MMC) (Meadowcroft, 1992; 1997) where the set of control inputs is solution to a series of minimization problems of the controlled objectives, in the order of their importance. The implementation of a MMC has been described in Section 6.5. Depending on the amount of interaction that exists among controlled variables and the availability of computational resources, the designer may wish to vary the complexity of the control structure and reduce a subset of the control system to SISO controls. An illustration of the implementation of a multi-horizon control system on an industrial process can be found in Chapter 11.

8.8 A Note on the Optimal Number of Hierarchical Levels

8.8.1 Suggested Number of Stratified Levels of Process Representations

In the proposed method, the process plant is being viewed in stages, from a coarse viewpoint which captures only the input-output process behavior to a detailed process viewpoint where all the interconnections in the plant are revealed. The purpose of the hierarchical stratification of the process plant is to reduce the complexity in the control structure synthesis and to provide representations which capture different ranges of process behavior. Since each level of process representation reveals some new information which is not observable from the previous level, the more gradual is the introduction of new information into the process viewpoint (i.e. higher the number of stratified levels), the easier it is for the designer to study the significance of the new information and manage the complexity of the design. However, analytical efforts are also required at each stratified level. The benefits of gradual introduction of new information into the process viewpoint is not free. Hence, optimally speaking, each new stratified level should satisfy the following two criteria:

1. Introduce an amount of new information that is manageable so that consistency in control objectives and control strategies can be easily maintained using guidelines developed in this chapter.
2. Introduce an amount of new information that warrants the effort of re-examination of the process plant.

8.8.2 Suggested Number of Layers in the Multi-horizon Control System

The multi-horizon control system proposed in Section 8.6 segregates the management of plant dynamics into different layers. Since the implementation of this control system assumes that the different layers behave relatively independently (such as in a cascaded control system), it is important that the relevant time-scale of the control objectives in one layer be at least 3 to 4 times larger than that of the layer immediately below. Ideally, the relevant time-scale of each layer should differ by roughly an order of magnitude (Albus, 1991). Thus, the optimal number of layers in the multi-horizon control system is a function of the degree of segregation and the range of dynamic phenomena that exist in the plant.

Ideally, the optimal number of layers in the multi-horizon control system can be determined by transforming the nonlinear mapping associated with the process plant into a series of summation of eigenfuctions. A nonlinear operator $f(y(t), u(t))$ can be transformed into a fourier series expansion of the following form:

$$f(y(t),u(t)) = \sum_j \alpha_j e^{i\omega_j t} \qquad [8\text{-}28]$$

In the fourier transform, the coefficients α_j in the expansion have values between $-\infty$ and ∞. These values are associated with the dynamics in the plant and hence the time-scales of operations in the process. In most physical systems, coefficients will not be evenly distributed over the axis, but are scattered into a number of groups. Wherever there is a group of coefficients which are of similar order of magnitudes, they represent similar process dynamics and a layer can be formed for these dynamics. Along the line, there will also be ranges where no coefficients exist. Creation of a layer would not be useful as no additional dynamics cannot be observed. Hence, the optimal number of layers can be determined by examining the ranges of values into which the coefficients fall.

In the proposed methodology, rather than determining the theoretical optimal number of levels for multi-horizon control using theoretical arguments, physical understanding of the process dynamics is used to guide the selection of the number of levels. It is believed that knowledge of the underlying dynamics governing the plant operations allows one to choose a number of levels that is close to the theoretical optimum.

Chapter 9
Synthesis of Plant Control Structure for the Hydrodealkylation of Toluene Plant

9.1 Introduction

The procedure formalized in Chapter 8 for the systematic generation of control structures for continuous process plant will be demonstrated on the Hydrodealkylation of Toluene Plant (HDA) shown previously in Chapter 2. The focus of this case study is on the decision-making process and mechanics that are involved in the long-horizon analysis for plant control. The key steps discussed in Chapter 8 will be followed closely.

9.2 Preliminary Analysis

During the preliminary analysis, the process, the overall production goals and the rank order of the set of production goals will be examined.

9.2.1 Understanding the HDA Process

The flowsheet of the HDA process (Douglas, 1988) is shown once again in Figure 9-1. The following reactions take place in the plug-flow reactor:

(R1) Toluene (T) + Hydrogen (H) $\rightarrow$ Benzene (B) + Methane (M)
(R2) 2Benzene (2B) $\rightarrow$ Diphenyl (D) + Hydrogen (H)

The letters in parenthesis are symbols that will be used to represent the various components in the system.

The overall production plan is to produce benzene at 265 mol/hour with a purity of 0.9997. This is the primary operation mode. The process is also constrained by several operational requirements:

- maintain the ratio of hydrogen/toluene in the reactor feed to be at 5 to prevent cooking in the reactor
- the reaction inlet temperature must be at least 1150°F for sufficient reaction rate

- the temperature of the reaction mixture should be kept below 1300°F to prevent cooking in the reactor
- the reactor effluent must be quenched to 1150°F in order to stop the reaction
- operational limits of the equipment, for example, inventories in the flash, distillation bottoms and distillation condensers must be maintained within acceptable equipment limits.

Base case values of the key process variables and the steady-state operating conditions can be found in Appendix A.1.

Process variations expected for the HDA plant include variation in: the temperature of cooling water according to ambient conditions; the temperatures and pressures of toluene and hydrogen according to ambient conditions as well as the upstream conditions; steam pressure and purity of hydrogen.

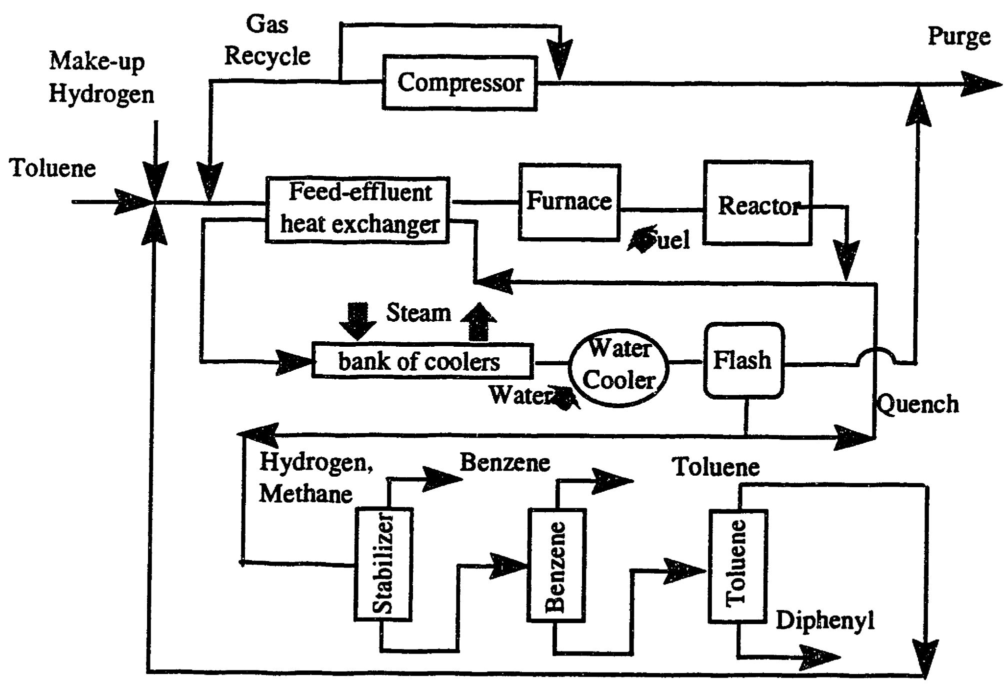


Figure 9 - 1: The Hydrodealkylation of Toluene Process

9.2.2 The Stability of the Open-loop Process

One of the first steps in the synthesis of plant-wide control structures is to determine if the plant is open-loop stable. First, in the HDA plant, the feed pre-heater, the furnace, the cooler, the phase-separator and the compressor are all inherently stable unit-operations. The reaction happens in an adiabatic tubular reactor. As internal stability is a result of backmixing, an *ideal* tubular reactor is always internally stable. Hence, a step change in the temperature of the inlet stream to the reactor will lead to a corresponding step change of the temperature of the outlet stream of the reactor. Next, possible instability caused by the unfortunate interconnection in the system is examined.

Instability induced by the Material Recycle Structure

The stability of the system caused by the pure material recycle effect can be quickly examined by performing a local numerical sensitivity analysis as described in Section 7.2.2. There are two material recycle loops in the HDA plant, one is rich in hydrogen and the other one is rich in toluene. The flow of materials in the plant has been simplified in Figure 9-2. The normalized molar flows with respect to the molar flow of toluene feed is shown in Figure 9-3 which are also given in row one of the chart shown in Table 9-1.

Our reactions are not autocatalytic; the ratio of { (toluene in feed to separation) / (toluene in mixed feed) } and { (benzene product) / (toluene in mixed feed) } can be assumed to stay roughly same. With this assumption, a simple local numerical sensitivity analysis can be performed to determine the pure material recycle effects. If toluene feed is increased from 1 unit to 2 units, the amount of toluene in the mixed feed increases. This produces more benzene, at the same time, there will also be an increase of toluene in the toluene recycle stream. The increased amount of recycle toluene further increases the amount of toluene in the mixed feed and more benzene is produced. However, the rate of increase of toluene in the recycle decreases in each round of the recycle loop. Eventually, the amount of increase stabilizes at a certain value. Hence, at steady state, a unit step increase in the toluene feed produces a finite step increase of benzene in the product stream (1.900-0.95 = 0.95). The rest of the toluene (1 - 0.95 = 0.05) has been converted to diphenyl, which is removed, and hydrogen through the side reaction.

A similar analysis can be performed on the hydrogen recycle. One will also find that under similar assumptions, the hydrogen recycle loop is stable to feed changes.

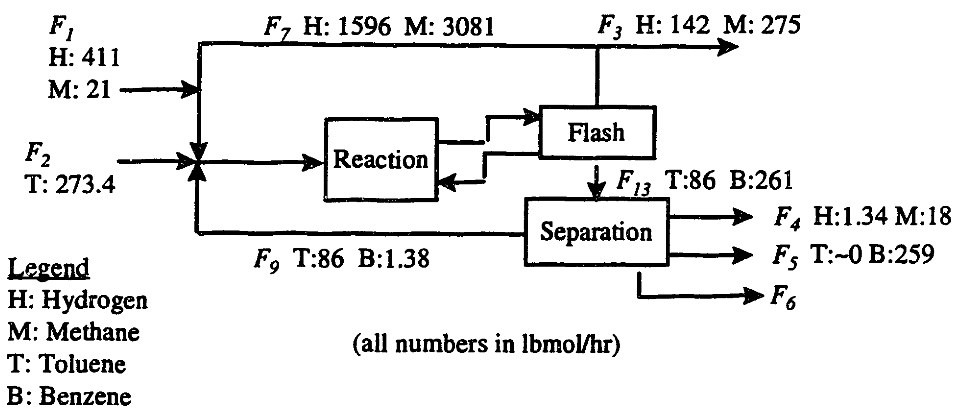
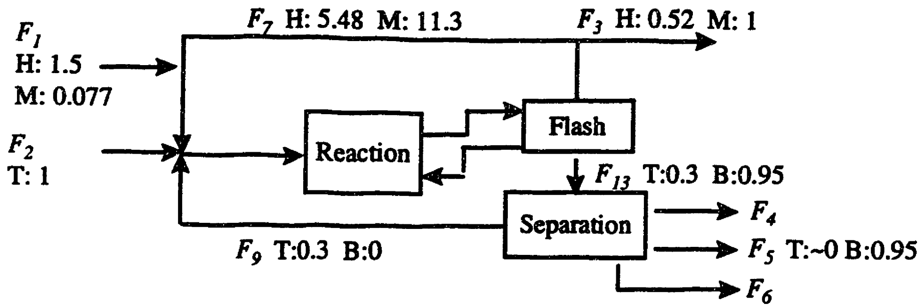


Figure 9 - 2: Isolated Material Recycles in the HDA Plant



(all numbers in unit molar flow)

Figure 9 - 3: Normalized flows for the Representation shown in Figure 9-2

Table 9 - 1: Local Numerical Simulation of the Toluene Recycle Loop of the HDA plant (all values in unit molar flow)

Stream Component	Feed T	Mixed Feed T	Feed to Sep T	Benzene B	Tol. Recycle T
steady-state	1	1.3	0.3	0.95	0.3
STEP UP					
1st round	2	2.3000	0.5308	1.6808	0.5308
2nd round	2	2.5308	0.5840	1.8494	0.5840
3rd round	2	2.5840	0.5963	1.8883	0.5963
4th round	2	2.5963	0.5991	1.8973	0.5991
5th round	2	2.5991	0.5998	1.8994	0.5998
6th round	2	2.5998	0.6000	1.8999	0.6000
7th round	2	2.6000	0.6000	1.9000	0.6000
8th round	2	2.6000	0.6000	1.9000	0.6000

Physical Relationships used:

T in Mixed Feed = T in Feed + T in Tol. Recycle

T in Feed to Separator = 0.3/1.3 * (T in Mixed Feed)

B in Benzene = (0.95/1.3) * T in Mixed Feed

T in Benzene = ~ 0

T in Tol. Recycle = T in Feed to Sep - T in Benzene

Instability Induced by the Energy Recycle Structure

In the HDA plant, material streams are interconnected in such a way that energy is being transferred from the hot streams to the cold streams in the process, forming a heat-integrated loop in the process. The heat-integrated loop has been isolated from the rest of the plant is displayed in Figure 9-4. To determine if the loop generates positive feedback in the system which destabilizes the system, a qualitative simulation using a signed causal model of the crucial portion of the plant is performed

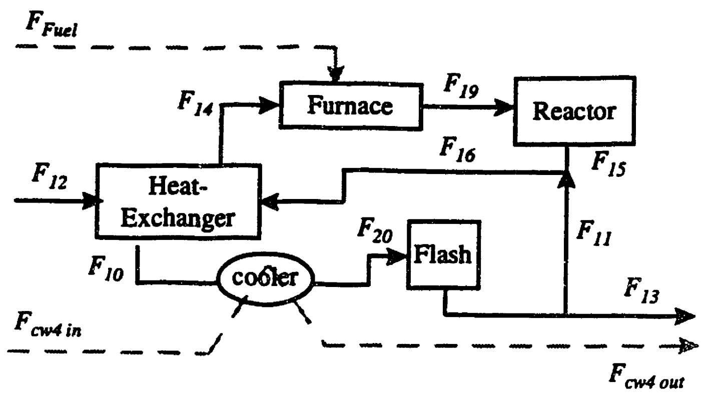


Figure 9 - 4: Isolated Heat-integrated loop in the HDA Plant

Choosing the level of Modeling Detail

The purpose of the simulation is to determine if heat accumulates in the integrated-loop when the heat content of the inlet streams changes. Heat content of F_{12} (mixed feed stream) is a function of both the flow rate and the temperature of the stream. Causal models which assume constant flows will be employed to simplify the analysis and avoid ambiguities. If it is found that the system is stable with respect to changes in T_{12} (temperature of F_{12}), Q_{Fuel} (heat supplied by fuel) and Q_{cw4} (heat supplied by coolant) the models will be expanded to include the influence of F_{12} on the system.

Constructing the Causal Models

1. Feed Pre-heater

The feed is pre-heated by transferring the energy from F_{16} to F_{12} in a counter-flow heat exchanger. The following relations describe the fundamental principles governing the unit:

$$H_{12} + Q_{ex} = H_{14} \qquad [9\text{-}1]$$

$$H_{16} = H_{10} + Q_{ex} \qquad [9\text{-}2]$$

$$Q_{ex} = UA\Delta T \qquad [9\text{-}3]$$

$$\Delta T = \frac{(T_{10} - T_{12}) - (T_{16} - T_{14})}{\ln\left(\dfrac{(T_{10} - T_{12})}{(T_{16} - T_{14})}\right)} \qquad [9\text{-}4]$$

where:

H_i = the rate of heat entering the system (enthalpy*mole flow) from stream i,

ΔT = the approach temperature of the streams involved in the feed pre-heater

U = heat-transfer coefficient

A = heat-transfer area

$R_h = 1/UA$ = resistance

The following causal interactions can be derived from Equations [9-1] to [9-4]:

$$H_{14} = f(+H_{12})$$
$$H_{10} = f(+H_{16})$$
$$\Delta T = f(-H_{12})$$
$$\Delta T = f(+H_{16})$$
$$Q_{ex} = f(+\Delta T)$$
$$H_{14} = f(+Q_{ex})$$
$$H_{10} = f(-Q_{ex})$$
$$Q_{ex} = f(-R_h)$$

Ignore fouling, R_h is constant at constant flows. Recall $A = f(+B)$ indicates that a positive change in B produces a positive change in A. Combining these causal interactions, a single-staged directed graph (SDG) describing the causal behavior of the system can be formed and it is shown in Figure 9-5.

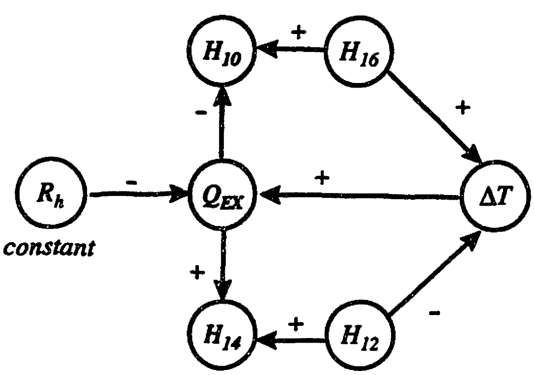


Figure 9 - 5: SDG of the of the Feed Pre-heater

2. Furnace

The following energy balance equation can be written for the furnace:

$$H_{14} + Q_{Fuel} = H_{19} \qquad [9\text{-}5]$$

which generates the following causal interactions:

$$H_{19} = f(+H_{14})$$
$$H_{19} = f(+Q_F)$$

3. Reactor

The reactor can be described by the following energy balance equations:

$$H_{19} + Q_{rxn} = H_{15} \quad [9\text{-}6]$$
$$Q_{rxn} = f(T_{19}) \quad [9\text{-}7]$$

where: Q_{rxn} = rate of heat generated from the reaction

These equations can be transformed to qualitative interactions:

$$H_{15} = f(+H_{19})$$
$$Q_{rxn} = f(+H_{19})$$

4. Mixer

The following quantitative equation can be written for the mixer:

$$H_{15} + H_{11} = H_{16} \quad [9\text{-}8]$$

which gives the following causal interactions:

$$H_{16} = f(+H_{11}) \quad [9\text{-}9]$$
$$H_{16} = f(+H_{15}) \quad [9\text{-}10]$$

5. Flash and Cooler

These units can be described by these quantitative equations:

$$H_{10} = H_{20} + Q_{cw4} \quad [9\text{-}11]$$
$$H_{20} = H_{11} + H_{13} + H_{8} \quad [9\text{-}12]$$

and these causal interactions:

$$H_{20} = f(+H_{10})$$
$$H_{10} = f(-Q_{cw4})$$
$$H_{11} = f(+H_{20})$$
$$H_{13} = f(+H_{20})$$
$$H_{18} = f(+H_{20})$$

The SDG for the entire system is shown in Figure 9-6.

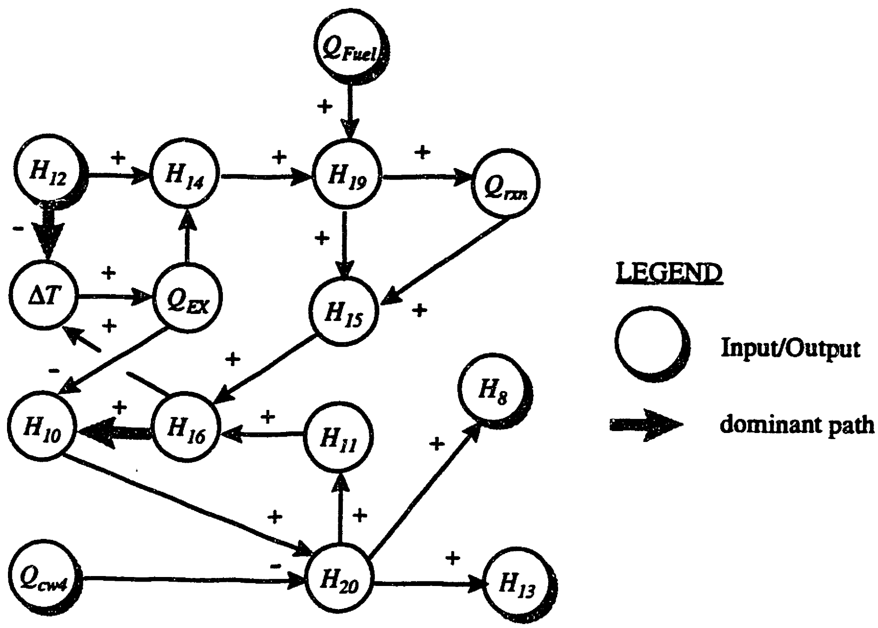


Figure 9 - 6: SDG for the Heat-integrated loop in the HDA Plant

Performing Qualitative Simulation

Case I: Increase T_{12}

At a constant F_{12}, increasing T_{12} increases H_{12}. As H_{12} is increased, there is a path which increases H_{14} and another path which decreases ΔT. Decreasing ΔT decreases Q_{ex} which decreases H_{14}. The two opposing forces make the ultimate response of H_{14} ambiguous. In order to resolve this conflict, quantitative sensitivity analysis about the nominal operating point must be performed (see Appendix A.2 for details). The results have been tabulated in Table 9-2.

Table 9 - 2: Results of Sensitivity Analysis on the Feed Pre-heater

Stream No.	T_{12}	T_{14}	T_{16}	T_{10}
Base Case (°F)	142.6	1140	1150	189.4
ΔT_{12} = +10F (°F)	152.6	1138	1150	193.65
ΔT_{16} = +20F (°F)	142.6	1159.53	1170	189.5

Hence, a step change in H_{12} (at a constant T_{16}) causes a small decrease in H_{14} and a moderate increase in H_{10}. A step change in H_{16} (at constant T_{12}) causes H_{14} to increase with a gain close to unity while H_{10} remains almost unchanged. As H_{12} increases, H_{14} decreases and H_{10} increases. As H_{10} increases, H_{20} increases which causes H_8, H_{13} and H_{11} to increase. Increasing H_{11} causes H_{16} to increase.

With the ambiguity resolved, the qualitative simulation can proceed. If H_{14} decreases, H_{19} decreases which causes H_{15} to decrease, which then causes H_{16} to decrease. Thus, there is another ambiguity at node H_{16}. If the resulting effect causes H_{16} to increase, it would cause H_{14} to increase. This causes H_{19} and H_{15} to increase. Increasing H_{15} causes H_{16} to increase further, making the loop unstable. If the two opposing forces cause H_{16} to decrease, the initial impact caused by a rise in H_{12} will be dampen and the loop will eventually stabilize at some new level. A sensitivity analysis (see Appendix A.2) indicates that H_{16} is insensitive to changes in the temperature of F_{11}. We can then conclude that the system is stable with respect to changes in T_{12}.

Case II: Increase Q_F

Increasing Q_F increases H_{19} which increases H_{15}. Increasing H_{19} also increases Q_{rxn} which reinforces the increase in H_{15}. As H_{15} increases, H_{16} increases which causes ΔT to increase as well. As ΔT increases, Q_{ex} increases and causes H_{14} to increase which reinforces the increase of H_{19} caused by changes in Q_F. With H_{16} increasing, our earlier analysis indicates that H_{10} would preferentially increase. This causes H_{20}, and therefore the output streams H_8 and H_{13}, to increase. Hence, the system is unstable unless a mechanism exists which maintains H_{19}, H_{15} or H_{16} at some fixed values.

Case III: Decrease Q_{cw4}

Decreasing Q_{cw4} causes H_{20} to increase. This in turns increases H_{11}. Our sensitivity analysis shows that H_{16} is insensitive to changes in T_{11}. Thus, at a constant F_{11}, we do not expect variation of Q_{cw4} to have a large effect on H_{16}. The system is stable with respect to changes in Q_{cw2}.

Developing the Stabilizing Control Strategy

Qualitative simulation indicates that the heat-integration loop is unstable with respect to unmonitored changes of the heat content of the fuel to furnace. If there is a step increase in the heat content of the fuel, the open-loop plant never stabilizes to a new steady-state by itself. In order to prevent runaway situations, a manipulated variable must be assigned to control the inventory of energy in the system somewhere in the loop. Fuel rate Q_{Fuel} is a function of the fuel rate F_{Fuel} and the heat contents of the materials which make up the fuel stream. In order to maintain the stability of the loop formed by nodes H_{14} - H_{19} - H_{15} - H_{16}, the heat contents of these nodes must be kept at some constant levels. The choices include:

1. Vary the flow of fuel to maintain T_{19} at constant value.
2. Vary the flow of F_{11} to maintain T_{16} at constant value.

Both options should be equally effective. In fact, it is part of the production objectives to maintain both T_{19} and T_{15} at fixed values. For plant stabilization, only one of the control strategy would suffice. Since fuel is an external stream while F_{11} is an internal stream, using F_{11} to maintain the stability of the loop will help to divert disturbance to the environment. The stability of the loop will be maintained using option one.

Note that even though the heat-integrated loop is open-loop unstable with respect to changes in Q_{Fuel}, the temperature of T_{19} to changes in Q_{Fuel} is an inherently stable process. It is the *interconnections* in the plant which introduces insatiability to the system. As long as there is a feedback mechanism to maintain the T_{19} at some fixed value, the loop is stable.

9.2.3 Prioritize Production Objectives

Based on the overall production plan, the operational requirements for the reaction and the other equipment constraints, overall plant production objectives have been prioritized as follows:

1. Maintain the levels of accumulations of materials and energy in the plant to be within their specified limits.
2. Produce benzene at 265 lbmol/hr.
3. Produce benzene at a purity of 0.9997.
4. Maintain reaction inlet temperature to be above 1150°F for sufficient reaction rate.
5. Maintain temperature of reacting mixture to be below 1300°F to prevent cooking in the reactor.
6. Maintain hydrogen/toluene ratio to be no less than 5 at reactor inlet to prevent cooking in the reactor.
7. Quench the reactor effluent to 1150°F in order to stop the reaction.
8. Minimize operating cost.

Objectives 1, 2, 3 and 8 are related to the entire plant and are observable objectives from the top of the hierarchy. Others are specific objectives which are related to unit-operations in the plant that are only visible at the refined levels. Objective 1 includes the process stabilization objective since it is associated with maintaining the energy content in the heat-integrated loop.

The order of the control objectives has been established by means of the paired comparison method (Section 6.2.2). The maintenance of the levels of accumulation of materials and energy and the stability of the energy integrated loop in the plant should precede all other operational requirements. Objectives which are related to the specifications of the products of the plant are of the next level of importance as they represent the purpose of the production unit. For the HDA process, the flow rate of the product is more important than that of the purity level because concentration of the product can usually be adjusted through blending. Then, the objectives which assist the plant operation will be considered. In the HDA plant, it is quite important to make sure that the reaction proceeds at a sufficient rate. Thus, the objective of maintaining the inlet temperature of the feed to be above 1150 °F is preferred to the constraints which exist to safeguard coking in the reactor. Since it is easier for coking to occur when the reaction mixture reaches a very high temperature than if we have a lower hydrogen/toluene ratio at the reactor inlet, it is of higher priority to make sure that the reaction mixture does not exceed the 1300 °F limit. Operational constraints which safeguard coking in the reactor are more important then the objective of quenching the reactor effluent to 1150 °F because whenever too much coke has been built-up in the reactor, it has to be decoked which may then affect production schedule. Cost optimization should only be considered after all product specifications and operational constraints have been satisfied.

9.3 Level 1: Input-Output Level

Synthesis of control structure begins with Phase I (see Chapter 8) in which long-horizon analysis is carried out. The input-output representation of the plant is shown in Figure 9-7. The goal of this phase of the design is to develop control strategies which will address the production objectives in Section 9.2.1. At Level 1, a set of long-horizon control strategies guided by the plant production objectives will be developed. It will be assumed in the discussion that the heat-integrated loop is being maintained at the desired level by manipulating the fuel. This assumption allows the long-horizon process behavior to be represented by general material and energy balance models, which have already been developed in Example 5-1.

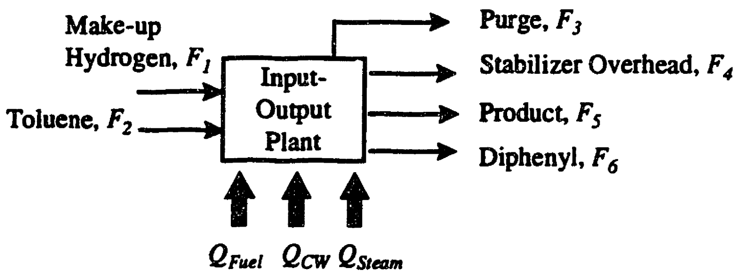


Figure 9 - 7: Level 1: Input-Output Plant Representation

Defining and Raking Control Objectives

At the input-output level, the focus is on the objectives which can be defined by variables observable from the process streams which cross the system boundary of the process representation in Figure 9-7. The objectives of relevant at this level, arranged in the order of importance determined during preliminary analysis, are:

1. Maintain the levels of accumulations of materials and energy in the plant to be within their specified limits.
2. Production of benzene at 265 lbmol/hr.
3. Purity of benzene at 0.9997.
4. Minimize operating cost.

Prioritizing Material and Energy Balance Controls

Material and energy balance controls will be prioritized using the guideline presented in Section 8.2.2, which is based on the expected process variations and the size of the inventory of individual materials in the system. Variations in the composition and the pressure (causes variations in flow) of the make-up hydrogen stream affect both the material balances of hydrogen and methane. Energy balance is affected by variations in the temperature of toluene, hydrogen and cooling water.

As noted in Section 8.2.2, changes which cause variation in the levels of accumulations of energy balance usually have localized effect. Energy balances are usually less important than material balance controls. In our case, variation in the heat content of fuel may destabilize the plant so it is of the highest priority to maintain the temperature of F_{19} at fixed value. Other temperature variations can be easily diverted away with some temperature control policy.

It has been assumed in the design that toluene feed is pure. Variations in the pressure of the make-up hydrogen can be eliminated by means of flow control. Then, the only source of material variations comes from the purity of the make-up hydrogen stream. A change in the purity level of this stream would introduce equal amounts of changes in the mole flows of both hydrogen and methane. At the input-output level, the information needed to determine the size of the capacitance of the inventories of hydrogen and methane [criterion 2 in Section 8.2.2] is not observable. However, methane is a by-product in the system and hydrogen is a necessary material in the creation of the product benzene. The maintenance of the inventory of hydrogen is therefore more important than that of methane [criterion 3 in Section 8.2.2]. Hence, the material balance of hydrogen in the plant is of the highest priority, followed the material balance of methane, which is followed by the material balance of toluene.

The set of objectives which are relevant at this level have been prioritized and summarized in Table 9-3. An objective that has been assigned priority level *i-j* means that it is an objective of priority *j* at level *i*.

Table 9 - 3: Prioritized Control Objectives at the Input-Output Level

1-1	Temperature of Stream 19 at fixed value (stabilizing strategy)
1-2	Maintain material balance control of H in the input-output plant (r_H)
1-3	Maintain material balance control of M in the input-output plant (r_M)
1-4	Maintain material balance control of T in the input-output plant (r_T)
1-5	Maintain energy balance control in the input-output plant (e)
1-6	Maintain benzene flow at the desired production level
1-7	Maintain benzene product purity
1-8	Minimize operating cost

Verify Feasibility of Control Objectives

Before proceeding with the synthesis, it should be verified that the control objectives in Table 9-3 do not violate any physical constraints. Material and energy balance equations at Level 1 can be generalized as follows:

$$
\begin{aligned}
&\frac{dr_H}{dt} = F_{1,H} + 0.5G_{R2} - (G_{R1} + G_{R2}) - F_{H,out} \\
&\frac{dr_M}{dt} = \alpha F_{1,H} + (G_{R1} + G_{R2}) - F_{M,out} \\
&\frac{dr_T}{dt} = F_{2,T} - (G_{R1} + G_{R2}) - F_{T,out} \\
&G_{R1} = F_{5,B} + F_{4,B} + F_{3,B} \\
&G_{R2} = 2F_{6,D} \\
&F_{H,out} = F_{3,H} + F_{4,H} \\
&F_{M,out} = F_{3,M} + F_{4,M} + F_{5,M} \\
&F_{T,out} = F_{3,T} + F_{5,T} + F_{6,T} \\
&F_5 = F_{5,T} + F_{5,B} \\
&\frac{de}{dt} = H_1 + H_2 + Q_{Fuel} + Q_{cw} + Q_{steam} - H_3 - H_4 - H_5 - H_6 \\
&H_i = \sum_j h_j(T) F_{i,j}
\end{aligned}
\qquad [9\text{-}13]
$$

where:

r_i = residual of material i

G_{Rj} = rate of generation of materials in reaction j

α = $F_{1,H} / (F_{1,H} + \alpha F_{1,H})$ equals purity of hydrogen in make-up hydrogen stream

e = residual of energy

α is an externally defined variable. For a fixed conversion, the selectivity S (defined as the ratio of modes of benzene at reactor outlet to model of toluene converted) is also fixed. A simple material balance (Douglas, 1988, pp. 102) will show that the following relationship is true:

$$
\frac{G_{R1}}{\frac{1}{2}G_{R2}} = \frac{Sx}{\frac{1}{2}(1-S)x} = \frac{S}{\frac{1}{2}(1-S)}
$$

where x is the conversion of toluene in the reactor. Since $F_{5,B} >> F_{3,B} + F_{4,B}$, the following relationship must hold at steady-state:

$$
\frac{F_{5,B}}{2F_{6,D}} = \frac{S}{(1-S)} \qquad [9\text{-}14]
$$

Hence, $F_{5,B}$ and $F_{6,D}$ cannot both be chosen as control objectives at the same time, although both can be used as manipulated variables. The control specifications at this level do not violate this constraint.

Quantifying the Long-horizon Process Behavior

During Phase I of the design, all flow components in the streams that cross the system boundary are considered to be manipulated variables, with the exception of the feed streams. Compositions in the feed stream are defined externally. Manipulation of component flows are therefore not feasible in feed streams.

The open-loop gains of the residuals of the material balance equations have been computed using the procedure described in Section 5.2.2 and are compiled in Table 9-4. Since flow valves information is not available, the best gain estimates can be obtained by perturbing each manipulated input by 1% of its nominal steady-state flow.

For the HDA plant, it is assumed that the base case is the sole operating point expected for the plant. During Phase I of the design, gains of the residuals of material balance equations are estimated from the principle of conservation and can therefore be assumed to be accurate for the operating point of interest.

Table 9 - 4: Open-loop gains of residuals at the Input-Output Level

Input	r_H	r_M	r_T	Input	r_H	r_M	r_T
F_1	4.1196	0.2168	0	$F_{4,M}$	0	-0.1893	0
F_2	0	0	2.7340	$F_{4,H}$	-0.0134	0	0
$F_{3,T}$	0	0	-0.0039	$F_{5,T}$	0	0	-0.0008
$F_{3,B}$	-0.0327	0.0327	-0.0327	$F_{5,B}$	-2.5919	2.592	-2.592
$F_{3,M}$	0	-2.7525	0	$F_{5,M}$	0	-0.0007	0
$F_{3,H}$	-1.426	0	0	$F_{6,T}$	0	0	-0.0024
$F_{4,B}$	-0.009	0.009	-0.009	$F_{6,D}$	-0.0466	0.0932	-0.0932

Synthesize Control Structure for the Input-Output Plant

A control structure that is suitable for maintaining the plant in the long-horizon at the nominal steady-state will be synthesized within the modular multiobjective design framework described in Chapter 6. Primary manipulated variables are assigned to the hierarchy of process objectives, sequentially, starting from the most important one. Fuel has been reserved to maintain the temperature in F_{19}, the most important objective in the process. The assignment for the rest of the control objectives will be illustrated in this section.

Goal 1-2: Maintain material balance control of Hydrogen (r_H)

From Table 9-4, F_1 has the largest open-loop gain on r_H and will therefore be able to maintain variation in the residual with the minimal change. Since it is also an input stream, assigning F_1 to Goal 1-2 will allow disturbances to be diverted to the external environment quickly. F_1 is therefore the best choice.

Goal 1-3: Maintain material balance control of Methane (r_M)

Once F_1 has been selected to be the primary manipulated variable for the maintenance of r_H, we evaluate the remaining manipulation for the control of r_M assuming that Goal 1-2 is under closed-loop control by F_1. The closed-loop gains for r_M while r_H is maintained by F_1 have been computed using the procedure described in Section 6.3.1 and are complied in Table 9-5. For an example of the mechanics involved in the computation, refer to Section 7.3.1. Inputs $F_{5,B}$, $F_{3,M}$ are promising candidates. If $F_{5,B}$ is assigned to control r_M, any variation in the level of accumulation of methane in the system would have a direct effect on the production and purity of benzene in the product. It is desired that disturbances be diverted from these objectives. Since the size of the gains of $F_{3,M}$ and $F_{5,B}$ are comparable, $F_{3,M}$ is assigned to control r_M.

Goal 1-4: Maintain material balance control of Toluene (r_T)

The closed-loop gains of r_T for changes in the remaining available manipulated variables are also complied in Table 9-5. Again, the preference is to divert disturbances away from the plant's production objectives. The gain of F_2 is comparable to that of $F_{5,B}$. Since F_2 is an input stream, assigning F_2 to this goal would allow disturbances to be quickly diverted to the environment upstream.

Table 9 - 5: Closed-loop gains of residuals at the Input-Output Level

Input	r_H	r_M	r_T	Input	r_H	r_M	r_T
F_1	4.1196	*assigned*	0	$F_{4,M}$	0	-0.1893	0
F_2	0	0	2.7340	$F_{4,H}$	-0.0134	0.0007	0
$F_{3,T}$	0	0	-0.0039	$F_{5,T}$	0	0	-0.0008
$F_{3,B}$	-0.0327	0.0344	-0.0327	$F_{5,B}$	-2.5919	2.7284	-2.592
$F_{3,M}$	0	-2.7525	*assigned*	$F_{5,M}$	0	-0.0007	0
$F_{3,H}$	-1.426	0.075	0	$F_{6,T}$	0	0	-0.0024
$F_{4,B}$	-0.009	0.0095	-0.009	$F_{6,D}$	-0.0466	0.0957	-0.0932

Goal 1-5: Maintain Energy balance control (e)

The energy balance equation indicates that Q_{Fuel}, Q_{CW} and Q_{Steam} are potential manipulated variables. Fuel has been used to maintain the stability of the heat-integrated loop of the plant. At this level, it cannot be determined if Q_{Fuel} alone is sufficient for maintaining the energy balance of the entire plant. Specifically, we do not know if the effects of adjusting Q_{Fuel} are confined to some subset of the plant (like the heat-integration loop). Without additional information about the system, it will be assumed that Q_{Fuel} is sufficient for this control.

Goal 1-6: Production Rate

F_5 has the most direct effect on the production rate and F_5 can be adjusted to meet the specified production.

Goal 1-7: Benzene Purity

At a fixed product flow (Goal 1-6), varying $F_{5,B}$ changes the level of purity in the product.

Note that the control polices for Goal 1-6 and 1-7 are "notional" control assignments which will be refined into specific control strategies at a later stage of the design.

Goal 1-8: Cost Minimization

Once all of the more important objectives (or goals) have been satisfied, one can proceed to optimize the plant for minimum operating cost using the procedure illustrated in Example 8-1. In general, objective function of the cost optimization problem of a process plant can be defined as follows:

$$\begin{aligned}\text{(Operating Cost) } \Phi = \ & \text{cost of usage of raw materials} \\ & - \text{resale/fuel values of materials leaving the plant} \\ & + \text{ cost due to lost of non-recovered products} + \text{cost of utilities}\end{aligned} \qquad [9\text{-}15]$$

Specifically, for the HDA plant, the following cost optimization can be written :

$$\min \Phi = \begin{Bmatrix} c_T F_2 + c_H F_1 - v_H F_{3,H} - v_M F_{3,M} - v_B F_{3,B} - v_T F_{3,T} - v_H F_{4,H} - v_M F_{4,M} \\ - v_B F_{4,B} - v_T F_{6,T} - v_D F_{6,D} + p_B F_{3,B} + p_B F_{4,B} + c_{Fuel} F_{Fuel} + c_{cw} F_{cw} \\ + c_{Steam} F_{Steam} + c_{compressor} \end{Bmatrix} \qquad [9\text{-}16]$$

s.t.:

1. maintain stability by maintaining T_{19} at desired level
2. maintain accumulation of hydrogen at desired level
3. maintain accumulation of methane at desired level
4. maintain accumulation of toluene at desired level
5. maintain accumulation of energy at desired level
6. F_5 = production rate
7. $F_{5,B}$ = product purity
8. other constraints not visible at this level

where: c_i = cost of material i or utility i
v_i = fuel or resale values of material i
p_B = market value of benzene
F_{CW} = total flow of cooling water
F_{Steam} = total flow of steam

Note that constraints 1 to 7 are control objectives which have been assigned primary manipulations (Fuel, F_1, $F_{3,M}$, F_2, F_5 and $F_{5,B}$) by the control associations identified earlier. For instance, F_1 has been assigned to r_H such that, at steady state, F_1 should move according to:

$$F_1 = (F_{4,B} + F_{5,B} + F_{3,B} + F_{6,D} + F_{3,H} + F_{4,H}) \,/\, x_{1,H} \qquad [9\text{-}17]$$

Similarly, to maintain r_M, $F_{3,M}$ moves according to the following strategy:

$$F_{3,M} = F_{1,M} + F_{3,B} + F_{4,B} + F_{5,B} + 2F_{6,D} - F_{4,M} \qquad [9\text{-}18]$$

and F_2 moves to maintain r_T in the following manner:

$$F_2 = F_{3,B} + F_{4,B} + F_{5,B} + 2F_{6,D} + F_{3,T} + F_{5,T} + F_{6,T} \qquad [9\text{-}19]$$

Fuel has been assigned to maintain the stability of the heat-integrated loop by maintaining the temperature of the stream to reactor at some fixed temperature. Once that has been fixed, we can assume at this point that the energy accumulation in the process is largely self-regulating.

Since $F_{5,B}$ and F_5 have been fixed by control specifications (i.e. they can be considered to be constant in the optimization) and F_5 is mainly made up of $F_{5,B}$ and $F_{5,T}$, the value of $F_{5,T}$ is fixed as well. Purity of hydrogen make-up, $x_{1,H}$, is an externally defined variable.

Substituting the material balance relationships [9-17] to [9-19] into Φ, we get:

$$\begin{aligned}\Phi = {} & (c_T + c_{H*} + p_B - v_M - v_B)\, F_{3,B} + (c_T + c_{H*} + p_B - v_M - v_B)\, F_{4,B} \\ & + (2c_T + c_{H*} - 2v_M - v_D)\, F_{6,D} + (c_T - v_T)\, F_{3,T} + (c_T - v_T)\, F_{6,T} \\ & + (c_{H*} - v_H)\, F_{4,H} + (c_{H*} - v_H)\, F_{3,H} - v_M F_{1,M} - 2v_M F_{4,M} \\ & + c_{cw} F_{cw} + c_{stm} F_{stm} + c_{compressor} + c_H F_{5,B} / X_{1,H} + c_T (F_{5,B} + F_{5,T}) - v_M F_{5,B}\end{aligned} \qquad [9\text{-}20]$$

where $c_{H*} = c_H / x_{1,H}$ and $x_{1,H}$ is an externally defined disturbance.

The constraints in the optimization have been eliminated by substitution. Dropping the constants $\{c_H F_{5,B} / X_{1,H} + c_T (F_{5,B} + F_{5,T}) - v_M F_{5,B} - v_M F_{1,M}\}$ in the objective function, the optimization minimizes:

$$\begin{aligned}\min \Phi = {} & (c_T + c_{H*} + p_B - v_M - v_B)\, F_{3,B} + (c_T + c_{H*} + p_B - v_M - v_B)\, F_{4,B} \\ & + (2c_T + c_{H*} - 2v_M - v_D)\, F_{6,D} + (c_T - v_T)\, F_{3,T} + (c_T - v_T)\, F_{6,T} \\ & + (c_{H*} - v_H)\, F_{4,H} + (c_{H*} - v_H)\, F_{3,H} - 2v_M F_{4,M} \\ & + c_{cw} F_{cw} + c_{stm} F_{stm} + c_{compressor}\end{aligned} \qquad [9\text{-}21]$$

The minimum operating cost can be found by searching over the feasible operating range of all unused or unspecified variables (which are the design degrees of freedom) that are observable from the input-output level.

By substituting the constraints and control specifications into the optimization, the degrees of freedom in the optimization has been reduced. The rest of the constraints which are still applicable to the optimization are not visible at this level (constraint set 7). These constraints are primarily constraints which govern the stoichiometry of reactions in the reactor and thermodynamic relationships which govern the distribution of flows of materials in the output streams. It is possible to further reduce the degrees of freedom in the design by studying these relationships.

Stoichiometry :

Equation [9-14] was derived earlier based on stoichiometry and it is a constraint on the system.

Thermodynamic Relations :

The distribution of materials in the outlet streams is accomplished in a downstream separation section which is not visible at Level 1. With F_3 being a vapor stream and F_4, F_5 and F_6 being liquid streams, there exists a pseudo phase-separation in the plant which can be generalized to a generic flash unit as shown in Figure 9-8. F_* is a fictitious stream which represents a mixture of products and raw materials that are to be separated. At equilibrium, the following materials balances and thermodynamic relationships governing the separation are true:

$$F_{*,i} = F_{3,i} + (F_{4,i} + F_{5,i} + F_{6,i}) \quad \forall\, i = \mathrm{T, B, H, M, D} \qquad [9\text{-}22]$$

Let

$$F_{4,i} + F_{5,i} + F_{6,i} = F_{liq,i} \quad \forall\, i = \mathrm{T, B, H, M, D} \qquad [9\text{-}23]$$

Then, the following thermodynamic relation for component i can be written:

$$\frac{F_{3,i}}{\sum F_{3,i}} = K^{i}_{3,liq}(P_*, T_*)\frac{F_{liq,i}}{\sum F_{liq,i}} \quad \forall\, i = \mathrm{T, B, H, M, D} \qquad [9\text{-}24]$$

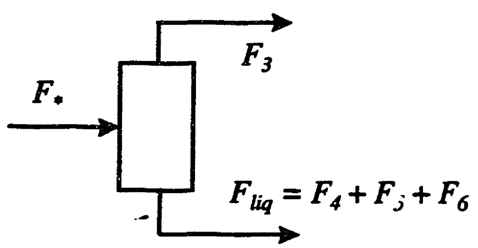


Figure 9 - 8: A Pseudo Separation System in the Input-Output Structure

Equations [9-22], [9-23] and [9-24] can be represented by two constraints in the following generic form at a constant P_* and T_*:

$$f_1(F_{*,i}, F_{3,i}, F_{liq,i}) = 0 \quad \forall\, i = \mathrm{T, B, H, M, D} \qquad [9\text{-}25]$$

$$f_2(F_{*,i}, F_{3,i}, F_{liq,i}) = 0 \quad \forall\, i = \mathrm{T, B, H, M, D} \qquad [9\text{-}26]$$

Then, from Equations [9-25] and [9-26], for each component i, there are 3 unknowns and 2 equations related to the separation section. Thus, the designer has the freedom to define only one variable in the set $\{F_{*,i}, F_{3,i}, F_{liq,i}\}$. At Level 1, $F_{*,i}$ is not a visible variable so it will not enter into the consideration. $F_{3,i}$ and $F_{liq,i}$ are inter-related through a thermodynamic relationship. Each component pair $\{F_{3,i}\ ,\ F_{liq,i}\ \}$ will be examined to identify the degrees of freedom for optimization. Also, from Equation [9-23], no more than 3 variables in the set $\{F_{liq,i}\ , F_{4,i}\ , F_{5,i}\ , F_{6,i}\}$ can have either fixed values, be defined as a manipulated variables or being chosen as degrees of freedom.

The initial component table for the generic separation unit has been constructed in Table 9-6. At level one, the most relevant streams are F_3 and F_{liq}. Since F_{liq} is a fictitious stream and ultimately, we wish to identify degrees of freedom which are observable at Level 1. So, F_4, F_5 and F_6 are also relevant streams. In this table, the following variables have been marked off:

1. Variables which have been selected as manipulated variables (indicated by "MV").
2. Variables which are control objectives with a specified value (indicated by "specified").
3. Variables whose flow rates at steady-state are either zero or insignificant compared to the other component flows in that stream (indicated by "~0").

Table 9 - 6: Initial Component Table for the Input-Output Level

	F_3	F_{liq}	F_4	F_5	F_6
H				0	0
M	MV			0	0
T			0	~0	
B				Specified	0
D	0		0	0	

<u>Degrees of Freedom Analysis</u> :

A variable has a *fixed* value if its flow is either very small or insignificant, or that its value is defined by a control objective. A variable becomes *unavailable* as a variable for optimization if its flow is fixed by a known relationship. The term "*degree of freedom for optimization*" and "*design variable*" will be used inter-changeably. Hence:

1. Either $F_{3,H}$ or $F_{liq,H}$ can be a degree of freedom in the optimization since both are related through Equations [9-25] and [9-26]. The flows of $F_{5,H}$ and $F_{6,H}$ are insignificant, $F_{4,H} = F_{liq,H}$. Then $F_{3,H}$ or $F_{liq,H}$ can be used as a degree of freedom in the optimization. $F_{3,H}$ is selected to be the design variable since it has a larger flow than $F_{4,H}$. Then, $F_{4,H} = f(F_{3,H})$ (i.e. $F_{4,H}$ is a function of $F_{3,H}$). We mark $F_{3,H}$ with a "√".
2. $F_{3,M}$ has been chosen to be the manipulated variable. $F_{liq,M}$ is therefore fixed and is not available as a degree of freedom in the optimization. We mark $F_{liq,M}$ with a "n/a" sign in the table. With the values of three of the variables in the set $\{F_{liq,M}\ ,\ F_{4,M}\ ,\ F_{5,M}\ ,\ F_{6,M}\}$ being fixed, $F_{4,M}$ is therefore unavailable as well.

3. Similarly to (1), either $F_{3,T}$ or $F_{liq,T}$ can be a degree of freedom in optimization and they are related through Equations [9-25] and [9-26]. With the flows of $F_{4,T}$ and $F_{5,T}$ being insignificant, $F_{6,T} = F_{liq,T}$. Hence, we can choose one variable from the set $\{F_{3,T}, F_{6,T}\}$ as degree of freedom in the optimization. Since $F_{3,T}$ has a bigger flow, $F_{3,T}$ can be varied to reduce the operating cost. Then, $F_{6,T}=f(F_{3,T})$. We mark $F_{3,T}$ with a "√".
4. $F_{5,B}$ is a control objective so its value has been pre-specified. $F_{6,B}$ is insignificant so $F_{4,B} = F_{liq,B} - F_{5,B}$. Either $F_{3,B}$ or $F_{4,B}$ can be used as a degree of freedom for optimization. Since $F_{3,B}$ has a larger flow, it will be used as a variable in the optimization. Then, $F_{4,B}=f(F_{3,B})$. We mark $F_{3,B}$ with a "√".
5. Since $F_{3,D}$ is insignificant, All diphenyl in $F_{*,i}$ passes to $F_{liq,D}$, making $F_{liq,D}$ not a degree of freedom in the optimization . With the flows of $F_{4,D}$ and $F_{5,D}$ be insignificant as well, $F_{6,D}$ is also unavailable for optimization. We mark $F_{liq,D}$ and $F_{6,D}$ with "n/a" in the table.

Results are summarized in the Table 9-7.

Table 9 - 7: Final Component Table for the Input-Output Level

	F_3	F_{liq}	F_4	F_5	F_6
H	√			0	0
M	MV	n/a	n/a	0	0
T	√		0	~0	
B	√			Specified*	0
D	0	n/a	0	0	n/a

Incorporating the above decisions into the optimization, the following unconstrained non-linear minimization can be written:

$$\begin{aligned}\min\ \Phi = {} & (c_T + c_{H^*} + p_B - v_M - v_B)(F_{3,B} + f(F_{3,B})) \\ & + (c_T - v_T)(F_{3,T} + f(F_{3,T})) + (c_{H^*} - v_H) f(F_{3,H}) \\ & + (c_{H^*} - v_H) F_{3,H} + c_{cw} F_{cw} + c_{stm} F_{stm} + c_{compressor}\end{aligned} \qquad [9\text{-}27]$$

Note that $F_{1,M}$ is an externally defined disturbance and $c_{H^*} = c_{H^*}/x_{1,H}$.

Since $c_T >> v_T$; $c_{H^*} >> v_H$; $p_B >> v_B$; and v_M is small, then:

$$(c_T + c_{H^*} + p_B - v_M - v_B) > 0 \qquad [9\text{-}28]$$

$$(c_T - v_T) > 0 \qquad [9\text{-}29]$$

$$(c_{H^*} - v_H) > 0 \qquad [9\text{-}30]$$

Coefficients of all the terms in Φ are positive. $\{F_{3,B} + f(F_{3,B})\}$ is the amount of loss of benzene. $\{F_{3,T} + f(F_{3,T})\}$ and $\{F_{3,H} + f(F_{3,H})\}$ are amounts of raw materials that the plant is losing to the environment. Hence, Φ can be minimized if we:

1. Reduce the amount of benzene leaving the process (i.e. $\{F_{3,B} + f(F_{3,B})\}$).
2. Reduce the loss of raw materials from the process (i.e. $\{F_{3,T} + f(F_{3,T})\}$ and $\{F_{3,H} + f(F_{3,H})\}$).

The second optimization strategy is equivalent to saying maximizing the recovery of raw materials. The cost minimization objective has been *spawned* into two more refined objectives.

The above strategies have resulted from tentative conclusion of the process based on information available at the input-output level only. These are control strategies which may help minimizing the plant's production cost. As details of the plant are being revealed at the refined levels, these strategies may have to be modified.

Control Structure at Level 1

The control structure at the input-output level (Level 1) is summarized in Table 9-8 and the control configuration is drawn in Figure 9-9. Control objectives are being maintained by adjusting variables which are observable from the streams that cross the system boundary defining this level. These control associations are notional in nature and will be refined into more specific control strategies later in the design.

Table 9 - 8: Control Structure at the Input-Output Level

Control Objectives		Assignment Input-Output Plant
1-1	Temperature of F_{19}	Q_{Fuel}
1-2	r_H	F_1
1-3	r_M	$F_{3,M}$
1-4	r_T	F_2
1-5	e	Q_{Fuel}
1-6	Production Level	F_5
1-7	Product Purity	$F_{5,B}$
1-8	Minimum Cost	minimize loss of benzene minimize loss of raw materials

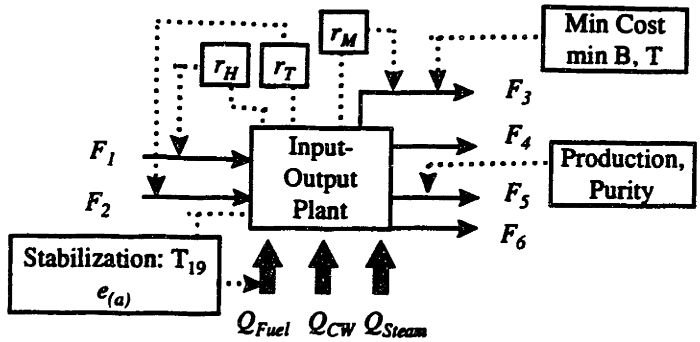


Figure 9 - 9: Control Structure for the Input-Output Representation of the HDA Plant

9.4 Level 2: Generalized Reaction-Separation System

Moving down the hierarchy of representations, more details about the plant are incorporated to the model at Level 2. A control structure that is suitable for the new representation is to be developed. At Level 2, the plant is segregated into a generalized reaction section (sub-block *a*) and a generalized separation section (sub-block *b*) as shown in Figure 9-10. Since the dominant time constants of the sub-blocks are much slower than the faster dynamics within the sub-blocks, long-horizon design criteria will be used to synthesize the control structure for this level. The material and energy balance model corresponding to this level of representation can be found in Appendix A.3.

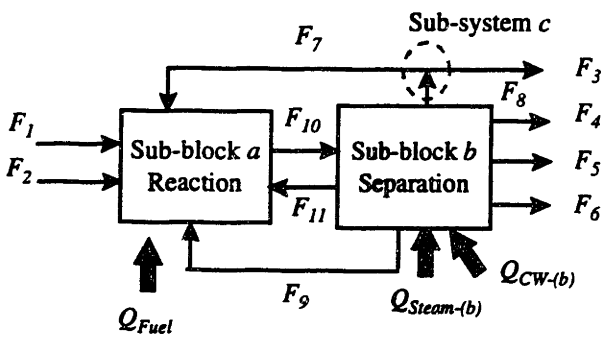


Figure 9 - 10: Process Representation at the Generalized Reaction-Separation Level (Level 2)

Progressive Generation of Control Objectives

The control objectives from the previous level which are associated with the overall production plan are have been used to define control objectives at the refined level as shown in Table 9-9. Note that the symbol $r_{i\text{-}(j)}$ is used to denote a material balance control objective for component *i* in sub-system *j*; $e_{(j)}$ to denote an energy balance control objective for sub-system *j*. Specific objectives which are observable from process streams at the input-output level are also allocated directly to the corresponding process streams at the lower level. Each objective related to material or energy balance control has been *translated* and *refined* into two separable control objectives. Note that it is not required to monitor the accumulation of materials and energy at the tee-junction (defined by system boundary *c*) as no accumulation of inventories of any kind is possible. Sub-block *c* is a self-regulating physical construction so material and energy balance controls are only required in sub-blocks *a* and *b*. For reasons explained in Section 8.4.1, the priorities of the maintenance of material balance of a component are of equal importance. A similar argument can be made about the energy balance control. The cost minimization objective is not a separable problem so we have maintained the global nature of the objective and it will be studied further when assignments have been made to other more important objectives. No new objective from the list given in Section 9.2 has become observable at this level. The prioritization of the control objectives developed at the earlier stages has been maintained.

At this level, objectives can only be defined in terms of the variables in the process streams which cross the system boundary, further refinement of these objectives, except for the cost optimization objective, is not possible. No spawning opportunities have been identified.

Table 9 - 9: Prioritized Control Objectives at the Generalized Reaction-Separation Level

	Reaction Sub-block *a*	Separation Sub-block *b*
2-1	Temperature of F_{19}	
2-2	$r_{H\text{-}(a)}$	$r_{H\text{-}(b)}$
2-3	$r_{M\text{-}(a)}$	$r_{M\text{-}(b)}$
2-4	$r_{T\text{-}(a)}$	$r_{T\text{-}(b)}$
2-5	$e_{(a)}$	$e_{(b)}$
2-6		Production Level
2-7		Product Purity
2-8	Minimize Cost	

Verify Feasibility of Control Objectives

At the more refined level, similar material balances (such as those used in Section 9.3.1) around the reaction block will show that:

$$G_{R1} = F_{10,B} - F_{11,B} - F_{7,B} - F_{9,B} \qquad [9\text{-}31]$$

$$G_{R2} = 2F_{10,D} - 2F_{11,D} - 2F_{9,D} \qquad [9\text{-}32]$$

Comparing to the other variables, $F_{7,B}$, $F_{9,B}$, $F_{9,D}$ are relatively small so we can say that :

$$\frac{F_{10,B} - F_{11,B}}{2F_{10,D} - 2F_{11,D}} \cong \frac{S}{1-S} \qquad [9\text{-}33]$$

The four variables above cannot be simultaneously chosen as control objectives. Our specifications of control objectives at this level have not violated constraints imposed by stoichiometry.

Quantifying the Long-Horizon Process Behavior at Level 2

The open-loop gains of the material accumulations caused by a 1% change in various feed flows or component flows observable at Level 2 have been computed and summarized in Table 9-10. Again, since there is only one known operating point, the gains can be assumed to be precise and there is no model uncertainty caused by a change in operating region.

Table 9 - 10: Open-loop gains of material accumulations at Level 2

Input	$r_{H\text{-}(a)}$	$r_{H\text{-}(b)}$	$r_{M\text{-}(a)}$	$r_{M\text{-}(b)}$	$r_{T\text{-}(a)}$	$r_{T\text{-}(b)}$	Input	$r_{H\text{-}(a)}$	$r_{H\text{-}(b)}$	$r_{M\text{-}(a)}$	$r_{M\text{-}(b)}$	$r_{T\text{-}(a)}$	$r_{T\text{-}(b)}$
F_1	4.12	0	0.2168	0	0	0	$F_{8,T}$	0	0	0	0	0	-0.0471
F_2	0	0	0	0	2.7340	0	$F_{8,B}$	0	-0.3989	0	0	0	-0.3989
$F_{3,T}$	0	0	0	0	0	0	$F_{8,M}$	0	0	0	-33.56	0	0
$F_{3,B}$	0	0	0.0327	0	0	0	$F_{8,H}$	0	-17.38	0	0	0	0
$F_{3,M}$	0	0	0	0	0	0	$F_{9,T}$	0	0	0	0	0.8586	-0.8586
$F_{3,H}$	0	0	0	0	0	0	$F_{9,B}$	0.0138	-0.0138	0	0	0.0138	-0.0138
$F_{4,B}$	0	-0.0090	0.0090	0	0	-0.0090	$F_{9,D}$	0.0003	-0.0003	0	0	0.0005	-0.0005
$F_{4,M}$	0	0	0	-0.1893	0	0	$F_{10,T}$	0	0	0	0	-1.1160	1.1160
$F_{4,H}$	0	-0.0134	0	0	0	0	$F_{10,B}$	-3.7770	3.7770	0	0	-3.7780	3.7780
$F_{5,T}$	0	0	0	0	0	-0.0008	$F_{10,D}$	-0.1211	0.1211	0	0	-0.1211	0.1211
$F_{5,B}$	0	-2.59	2.59	0	0	-2.59	$F_{10,M}$	0	0	-33.81	33.81	0	0
$F_{5,M}$	0	0	0	-0.0007	0	0	$F_{10,H}$	-17.40	17.40	0	0	0	0
$F_{6,T}$	0	0	0	0	0	-0.0025	$F_{11,T}$	0	0	0	0	0.2580	-0.2580
$F_{6,D}$	0	-0.0932	0.0932	0	0	-0.0932	$F_{11,B}$	0.76	-0.76	0	0	0.7640	-0.7640
$F_{7,T}$	0	0	0	0	0.0432	0	$F_{11,D}$	0.0274	-0.0274	0	0	0.0274	-0.0274
$F_{7,B}$	0.3663	0	0	0	0.3662	0	$F_{11,M}$	0	0	0.0560	-0.0560	0	0
$F_{7,M}$	0	0	30.82	0	0	0	$F_{11,H}$	0.0039	-0.0039	0	0	0	0
$F_{7,H}$	15.96	0	0	0	0	0							

Synthesize Control Structure for the Generalized Reaction-Separation System

The importance of maintaining upward compatibility of the control structure at Level 2 with the one developed at the previous level has been emphasized in Section 8.4.2. The *Consistency Logic Map* discussed in the previous chapter will be followed throughout the development. All component flows, except those in the feed streams, are potential manipulated variables. Again, fuel is used to maintain the temperature of F_{19} at a steady value. The control structure synthesis will proceed with the assignment of manipulated variables to Goal 2-2.

Goal 2-2: Maintain material balance control of Hydrogen

Previously at Level 1, F_1 has been assigned to be the manipulated variable for the maintenance of the overall balance of hydrogen in the system. Since F_1 is observable from sub-block *a*, it is expected that F_1 to be among the set of best possible manipulated variables for the maintenance of $r_{H\text{-}(a)}$, based on *Consistency Logic 1* (refer to Section 8.4.2). Other potential manipulated variable for the control of $r_{H\text{-}(a)}$ would come from the new manipulated variables observable at this level. According to *Consistency Logic 2*, any manipulated variables are potential candidate for the control of $r_{H\text{-}(b)}$. The new manipulated variables at this level are component flows in F_7, F_8, F_9, F_{11} and F_{10}. Hence, sets of best manipulated variables are:

1. $r_{H\text{-}(a)}$: { component flows of F_1, F_7, F_9, F_{10}, F_{11} }
2. $r_{H\text{-}(b)}$: { all manipulated variables }

Columns 1 and 2 of Table 9-11, show the open-loop gains of $r_{H\text{-}(a)}$ and $r_{H\text{-}(b)}$. Potential choices based on the magnitudes of the gains in order of significance are:

1. $r_{H\text{-}(a)}$: { $F_{10,H}$, $F_{7,H}$, F_1 }
2. $r_{H\text{-}(b)}$: { $F_{10,H}$, $F_{8,H}$ }

F_1 is indeed one of the best manipulated variable for $r_{H\text{-}(a)}$, which is consistent with *Consistency Logic 1*. Based on the size of the gains, $F_{10,H}$ and $F_{7,H}$ are more effective manipulations for the control of $r_{H\text{-}(a)}$ than F_1. However, it is highly desirable to divert disturbances to the environment as soon as possible. Therefore, F_1 is the best choice for $r_{H\text{-}(a)}$. Similarly, $F_{8,H}$, being close to the purge stream, can be used to divert the variations of the inventory of hydrogen in sub-block *b* away from the rest of the plant and is the best choice for $r_{H\text{-}(b)}$. In column 3, we have computed the closed-loop gain of $r_{H\text{-}(b)}$ while $r_{H\text{-}(a)}$ is being controlled by F_1. See that our assignments do not create any conflict under closed-loop control.

Goal 2-3: Maintain Material Balance Control of Methane

$F_{3,M}$ has been found to be the best manipulated variable for r_M at Level 1. Since system boundary *c* is not a material capacitor, changing F_3 would require direct changes in F_8 and/or F_7. F_7 can be associated with sub-block *a* while F_8 can be associated with sub-block *b*. Hence, the sets of potential manipulated variables are:

1. $r_{M\text{-}(a)}$: { component flows in F_7, F_9, F_{10}, F_{11}}
2. $r_{M\text{-}(b)}$: {component flows in F_8, F_9, F_{10}, F_{11}}

The closed-loop gains of $r_{M\text{-}(a)}$ and $r_{M\text{-}(a)}$ when $r_{H\text{-}(a)}$ and $r_{H\text{-}(b)}$ are being simultaneously maintained by F_1 and $F_{8,H}$ can be found in columns 4 and 5 of Table 9-11. The best choices in order of the magnitudes of the gains are:

1. $r_{M\text{-}(a)}$: { $F_{10,M}$, $F_{7,M}$ }
2. $r_{M\text{-}(b)}$: { $F_{10,M}$, $F_{8,M}$ }

$F_{7,M}$ and $F_{8,M}$ are indeed one of the best manipulated variables. Since the gains are in fact all of the same order of magnitude, decisions will be made based on the ability of the manipulated variables to divert disturbances to the external environment. Clearly, it is of our best interest to assign $F_{7,M}$ to $r_{M\text{-}(a)}$ and $F_{8,M}$ to $r_{M\text{-}(b)}$. Both of these streams are directly linked to the environment through the tee-junction defined by system boundary *c*. In column 6 of Table 9-12, we verified that such an assignment will not create any problems under closed-loop situations.

Goal 2-4: Maintain Material Balance Control of Toluene

F_2 has been identified at Level 1 to be the best manipulated variable for this objective. At a refined level, the sets of best choices are the component flows of:

1. $r_{T\text{-}(a)}$: {component flows in F_2, F_7, F_9, F_{10}, F_{11}}
2. $r_{T\text{-}(b)}$: {all manipulated variables}

Columns 7 and 8 of Table 9-12 show the closed-loop gains of $r_{T\text{-}(a)}$ and $r_{T\text{-}(b)}$ while Goals 2-2 and 2-3 are under closed-loop control. The best choices in order of importance are:

1. $r_{T\text{-}(a)}$: { $F_{10,B}$, F_2 }
2. $r_{T\text{-}(b)}$: { $F_{10,B}$, $F_{5,B}$}

Note that F_2 is indeed one of the best input for $r_{T\text{-}(a)}$. The size of the gain of $r_{T\text{-}(a)}$ by a unit change of F_2 is only slightly smaller than that from $F_{10,B}$. As we would like to divert disturbances to the environment, we will control $r_{T\text{-}(a)}$ by F_2. As for $r_{T\text{-}(b)}$, variations in $F_{5,B}$ would have direct impact on the production rate as well as the product purity. Thus, $F_{10,B}$ is assigned to $r_{T\text{-}(b)}$.

Goal 2-5: Maintain Energy Balance Control

At Level 2, with a refined structure, we see that the control policy for process stabilization (Goal 1) also maintains the energy balance of the reaction block of the plant. We have reserved Q_{Fuel} to do that. For $e_{(b)}$, we will use $Q_{cw\text{-}(b)}$ because this is the most economical utility.

Goal 2-6: Production Level

F_5 remains to be the best input to maintain the production level of the process.

Goal 2-7: Benzene Purity

At this point, $F_{5,B}$ is still the best manipulated variable for the maintenance of the level of purity in the product stream.

Control strategies for Goals 2-6 and 2-7 are still "notional" loops which will be refined later to more specific control policies using manipulated variables that can be physically implemented.

Table 9 - 11: Closed-loop gains of material accumulations at Level 2

Input	$r_{H-(a)}$	$r_{H-(b)}$	$r_{H-(b)}$ $r_{H-(a)}$ closed	$r_{M-(a)}$	$r_{M-(b)}$	$r_{M-(b)}$ $r_{M-(a)}$ closed	$r_{T-(a)}$	$r_{T-(b)}$	$r_{T-(b)}$ $r_{T-(a)}$ closed
F_1	4.1196	0	0	0	0	0	0	0	0
F_2	0	0	0	0	0	0	2.73	0	0
$F_{3,T}$	0	0	0	0	0	0	0	0	0
$F_{3,B}$	0	0	0	0.03	0	0	0	0	0
$F_{3,M}$	0	0	0	0	0	0	0	0	0
$F_{3,H}$	0	0	0	0	0	0	0	0	0
$F_{4,B}$	0	-0.01	-0.01	0.009	0	0	0	-0.01	-0.01
$F_{4,M}$	0	0	0	0	-0.19	-0.19	0	0	0
$F_{4,H}$	0	-0.01	-0.0134	0	0	0	0	0	0
$F_{5,T}$	0	0	0	0	0	0	0	0.00	0.00
$F_{5,B}$	0	-2.59	-2.59	2.59	0	0	0	-2.59	-2.59
$F_{5,M}$	0	0	0	0	-0.0007	-0.0007	0	0	0
$F_{6,T}$	0	0	0	0	0	0	0	-0.0024	-0.0024
$F_{6,D}$	0	-0.09	-0.0932	0.0932	0	0	0	-0.0932	-0.0932
$F_{7,T}$	0	0	0	0	0	0	0.0432	0	0
$F_{7,B}$	0.37	0	0	-0.0193	0	0	0.3662	0	0
$F_{7,M}$	0	0	0	30.82	0	0	0	0	0
$F_{7,H}$	15.96	0	0	-0.84	0	0	0	0	0
$F_{8,T}$	0	0	0	0	0	0	0	-0.0471	-0.0471
$F_{8,B}$	0	-0.40	-0.40	0	0	0	0	-0.3989	-0.3989
$F_{8,M}$	0	0	0	0	-33.56	-33.56	0	0	0
$F_{8,H}$	0	-17.38	-17.38	0	0	0	0	0	0
$F_{9,T}$	0	0	0	0	0	0	0.8586	-0.8586	-0.8586
$F_{9,B}$	0.0138	-0.0138	-0.0138	-0.0007	0	0	0.0138	-0.0138	-0.0138
$F_{9,D}$	0.0003	-0.0003	-0.0003	0	0	0	0.0005	-0.0005	-0.0005
$F_{10,T}$	0	0	0	0	0	0	-1.12	1.12	1.12
$F_{10,B}$	-3.78	3.78	3.78	0.20	0	0	-3.78	3.78	3.78
$F_{10,D}$	-0.12	0.12	0.12	0.01	0	0	-0.12	0.12	0.12
$F_{10,M}$	0	0	0	-33.81	33.81	33.81	0	0	0
$F_{10,H}$	-17.4	17.4	17.4	0.9157	0	0	0	0	0
$F_{11,T}$	0	0	0	0	0	0	0.26	-0.26	-0.26
$F_{11,B}$	0.76	-0.76	-0.76	-0.04	0	0	0.76	-0.76	-0.76
$F_{11,D}$	0.0274	-0.0274	-0.0274	0.00	0	0	0.0274	-0.0274	-0.0274
$F_{11,M}$	0	0	0	0.056	-0.056	-0.056	0	0	0
$F_{11,H}$	0.0039	-0.0039	-0.0039	-0.0002	0	0	0	0	0

Goal 2-8: Cost Minimization

At this level, the cost optimization is described as follows:

$$\min \Phi = \begin{Bmatrix} c_T F_2 + c_H F_1 - v_H F_{3,H} - v_M F_{3,M} - v_B F_{3,B} - v_T F_{3,T} - v_H F_{4,H} - v_M F_{4,M} \\ - v_B F_{4,B} - v_T F_{6,T} - v_D F_{6,D} + p_B F_{3,B} + p_B F_{4,B} + c_{Fuel} F_{Fuel} + c_{cw} F_{cw-b} \\ + c_{steam} F_{steam-b} + c_{compressor} \end{Bmatrix} \quad [9\text{-}34]$$

s.t.

1. Maintain stability
2. Maintain accumulation of hydrogen at desired level
3. Maintain accumulation of methane at desired level
4. Maintain accumulation of toluene at desired level
5. Maintain accumulation of energy at desired level
6. F_5 = production rate
7. $x_{5,B}$ = product purity
8. Other constraints related to the reaction and separation blocks which are not visible at this level

where:
c_i = cost of materials
v_i = fuel or resale values of materials
p_i = market value of product
$F_{cw\text{-}(b)}$ = flow of cooling water in the utility system of sub-block b
$F_{Steam\text{-}(b)}$ = flow of steam in the utility system of sub-block b

Control objectives (or equivalently, the constraints) with the assigned manipulated variables reduce the number of degrees of freedom in the optimization. Although sub-block c is not a material or energy capacitor, by its self-regulating nature, the material and energy balance will always be maintained at steady state, i.e.:

$$F_{7,i} + F_{3,i} = F_{8,i} \quad [9\text{-}35]$$

Introducing the control strategies, the material balances around sub-block c and the specifications on the product stream into the variables in the objective function, Φ is transformed into:

$$\begin{aligned}\Phi = & (c_T - v_T)\,F_{3,T} + (c_T + c_{H^*} + p_B - v_B)\,F_{3,B} + (2c_T + c_{H^*})\,F_{3,D} + c_{H^*}F_{8,T} \\ & + c_{H^*}F_{8,D} - c_{H^*}F_{7,H} + (c_T + c_{H^*})F_{6,T} + (2c_T + 2c_{H^*} - v_H)F_{6,D} \\ & + (c_T + c_{H^*} + p_B - v_B)\,F_{4,B} + c_{H^*}F_{10,H} - c_{H^*}F_{10,T} \\ & - 2c_{H^*}\,F_{10,D} + c_{H^*}\,(F_{9,D} + F_{9,T}) - c_{H^*}\,F_{9,H} \\ & + c_{H^*}\,(\,F_{11,D} + F_{11,T}) - c_{H^*}\,F_{11,H} - v_H\,F_{3,H} - v_M\,F_{3,M} \\ & - v_H\,F_{4,H} - v_M\,F_{4,M} - v_T F_{6,T} + c_{Steam}F_{Steam\text{-}(b)} + c_{compressor}\end{aligned} \qquad [9\text{-}36]$$

and c_{H^*} has been defined previous to be $c_H / x_{1,H}$.

The number of degrees of freedom in the optimization can be further reduced through the application of the stoichiometric and thermodynamic relationships.

<u>Stoichiometry</u> :

Earlier, the following relationship that is observable from Level 2 was identified:

$$\frac{F_{10,B} - F_{11,B}}{2F_{10,D} - 2F_{11,D}} \equiv \frac{S}{1-S} \qquad [9\text{-}33]$$

<u>Material Balances around Sub-system c</u> :

$$F_{3,i} + F_{7,i} = F_{8,i} \qquad [9\text{-}35]$$

<u>Thermodynamics</u> :

The separation system can be assumed to contain a unit as shown in Figure 9-11 which distributes a fictitious stream $F_{\neq}$ into a vapor stream F_8 and liquid stream F_{liq2} that is composed of F_4, F_5, F_6 and F_9. The following generic relationships can be formed by combining the component balances and thermodynamic relationships related to the fictitious separation unit:

$$f_1(F_{\neq i}, F_{8,i}, F_{liq2,i}) = 0 \qquad [9\text{-}37]$$

$$f_2(F_{\neq i}, F_{8,i}, F_{liq2,i}) = 0 \qquad [9\text{-}38]$$

where:

$$F_{liq2,i} = F_{4,i} + F_{5,i} + F_{6,i} + F_{9,i} \qquad [9\text{-}39]$$

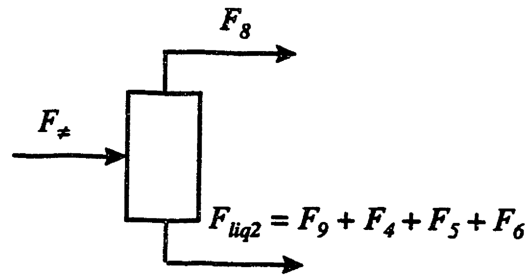


Figure 9 - 11: Pseudo Separation System in the Generalized Separation Block

Since $F_{\neq}$ in Equations [9-37] and [9-38] are from the pseudo-separation system and so they not visible at this level. These are not degrees of freedom in the optimization. The remaining variables, $F_{8,i}$ and $F_{liq2,i}$, are inter-related through the thermodynamic relationships. Then, for each component i, only one variable in the set $\{F_{8,i}, F_{liq2,i}\}$ can be used as a design variable. When one of the variable has been defined by either a control strategy or have been chosen to be a degree of freedom in the optimization, the value other variable is fixed through Equations [9-37] and [9-38]. Also, from Equation [9-39], no more than four variables from the set $\{F_{liq2,i}, F_{4,i}, F_{5,i}, F_{6,i}, F_{9,i}\}$ can have fixed values and from Equation [9-35], no more than two variables from the set $\{F_{3,i}, F_{7,i}, F_{8,i}\}$ can have fixed values.

The initial component table has been set up in Table 9-12 for the relevant streams (i.e. $F_{3,i}$, $F_{7,i}$, $F_{8,i}$, $F_{liq2,i}$, $F_{4,i}$, $F_{5,i}$, $F_{6,i}$ and $F_{9,i}$) at this level. We have used symbols "MV", "Specified" and "~0" to indicate component flows which have been assigned as manipulated variables, specified as controlled variables and have insignificant quantity at nominal steady-state respectively. At this level, we have introduced "small" to indicate component flows which are relatively small but not entirely insignificant. A degrees of freedom analysis similar to the one used in Level 1 (Section 9.3.1) can be used to further reduce the variables in the optimization.

Table 9 - 12: Initial Component Table for the Generalized Reaction-Separation System

component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{liq2,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H			MV			0	0	0
M		MV	MV			0	0	0
T					0	~0	small	
B						Specified	0	
D	0	0	0		0	0		small

Degrees of Freedom Analysis :

Based on the above statements, degrees of freedom in the optimization can be reduced systematically as shown below:

1. Since $F_{8,H}$ is a MV, $F_{liq2,H}$ is not available as a design variable. The values of $F_{5,H}$, $F_{6,H}$ and $F_{9,H}$ are small as well, so $F_{4,H}$ is essentially the same as $F_{liq2,H}$ and it is also not available as a design variable. Either $F_{3,H}$ or $F_{7,H}$ can be used as the degree of freedom in the optimization. Since the flow of $F_{7,H}$ is much larger than that of $F_{3,H}$, we will select $F_{7,H}$ to be the design variable. Then, $F_{3,H} = f(F_{7,H})$.
2. Both $F_{7,M}$ and $F_{8,M}$ have been chosen as manipulated variables. Then, constrained by Equation [9-35], $F_{3,M}$ is not available as a design variable. Also, when $F_{8,M}$ is fixed (by the control relationship), $F_{liq2,M}$ is automatically defined as a result of Equations [9-38] and [9-39]. With the flows of $F_{5,M}$, $F_{6,M}$ and $F_{9,M}$ being insignificant, $F_{4,M} = F_{liq2,M}$. Then, $F_{4,M}$ is also not available.
3. Either $F_{8,T}$ or $F_{liq2,T}$ can be chosen as a design variable. Since the flows of $F_{4,T}$ and $F_{5,T}$ are insignificant, then, $F_{9,T} + F_{6,T} = F_{liq2,T}$. With $F_{9,T}$ being a much larger flow than $F_{6,T}$ and $F_{8,T}$, we will select $F_{9,T}$ to be the design variable. Then, $F_{8,T} = f\ (F_{9,T})$. and $F_{6,T}=f'(F_{9,T})$. Among $F_{8,T}$, $F_{7,T}$ and $F_{3,T}$, only two can be degrees of freedom. Because $F_{3,T}$ appears directly in Φ, we will focus on $F_{3,T}$. Then, $F_{7,T} = f(F_{3,T}\ , f(F_{9,T}))$.
4. Either $F_{8,B}$ or $F_{liq2,B}$ can be chosen as design variable. $F_{8,B}$ is large. Focus on $F_{8,B}$ in the optimization. Then, among the gas streams, either $F_{3,B}$ or $F_{7,B}$ can be a degree of freedom. Because $F_{3,B}$ directly appears in Φ, we will focus on $F_{3,B}$. Then, $F_{7,B} = f(F_{3,B}, F_{8,B})$. In the $F_{liq2,B}$ portion, $F_{5,B}$ is a control objective so it is not a variable available for optimization. With $F_{6,B}$ being small, only one from the set $\{F_{4,B}, F_{9,B}\}$ can be a degree of freedom. Since $F_{4,B}$ is larger, we will assign $F_{4,B}$ to be the design variable. Then, $F_{9,B} = f(F_{4,B})$.
5. Similar to the previous level, virtually all diphenyl in $F_{\neq}$ ends up in $F_{liq2,D}$. With $F_{4,D}$, $F_{5,D}$ being insignificant and $F_{9,D}$ being small, $F_{liq2,D} = F_{6,D} + F_{9,D}$. Then, we assign $F_{6,D}$ to be the manipulated variable and $F_{9,D}=f(F_{6,D})$.

The final component table for the generalized reaction-separation system is setup as in Table 9-13.

Table 9 - 13: Final Component Table for the Generalized Reaction-Separation System

component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{liq2,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H		√	MV	n/a	n/a	0	0	0
M	n/a	MV	MV	n/a	n/a	0	0	0
T	√				0	~0	small	√
B	√		√		√	Specified	0	
D	0	0	0		0	0	√	small

Incorporating the above decisions into the optimization, the optimization can be written as:

$$
\begin{aligned}
\min\ \Phi = {} & (c_T - v_T)\, F_{3,T} + (c_T + c_{H^*} + p_B - v_B)\, F_{3,B} \\
& + (c_T + c_{H^*} + p_B - v_B) F_{4,B} + (2c_T + 2c_{H^*} - v_H) F_{6,D} \\
& + c_{H^*} f(F_{6,D}) + (c_T + c_{H^*} - v_T)\, f'(F_{9,T}) + c_{H^*} F_{9,T} \\
& + c_{H^*} f(F_{9,T}) - v_M f(F_{7,H}) - c_{H^*} F_{7,H} + c_{H^*} F_{10,H} \\
& - c_{H^*} F_{10,T} - c_{H^*} F_{10,D} - c_{H^*} F_{11,H} + c_{H^*} F_{11,T} + c_{H^*} F_{11,D} \\
& + c_{Steam} F_{Steam\text{-}(b)} + c_{compressor}
\end{aligned}
\qquad [9\text{-}40]
$$

s.t.:

$$F_{3,i} + F_{7,i} = F_{8,i}$$

and constraints imposed by the compressor

Note that $c_T >> v_T$; $c_{H^*} >> v_H$; $p_B >> v_B$; v_M, v_H and v_T are small. Then, $(c_T + c_{H^*} + p_B - v_B) > 0$, $(2c_T + 2c_{H^*} - v_H) > 0$. Then, $(F_{3,B} + F_{4,B})$ is the amount of loss of benzene from the process. Minimizing this amount can help to reduce the operating cost. Note that $f(F_{7,H}) = F_{3,H}$. $F_{3,H}$ is small compared to $F_{7,H}$. Increasing $F_{7,H}$ would help to reduce the cost as well (since $c_{H^*} F_{7,H}$ is positive and $v_M f(F_{7,H}) << c_{H^*} F_{7,H}$). So we want to maximize the recovery of hydrogen. Reducing $F_{3,T}$ would also help to lower the cost. The term ($F_{6,D} + f(F_{6,D})$) refers to the amount of diphenyl being produced in the process. Decreasing the production of diphenyl reduces the cost. Note that the amount of diphenyl being produced is strongly dependent on the one-pass conversion of toluene in the reactor. No conclusive statements can be made about F_9, F_{10} and F_{11}. Then, tentatively, the cost function Φ can be minimized if we:

1. reduce the amount of benzene leaving the process.
2. reduce the loss of raw materials from the process.

These conclusions are the same as those that we arrived at Level 1.

Control Structure at Level 2

The control structure that is suitable for the process representation at Level 2 is shown in Figure 9-12 and the control strategies are being summarized in Table 9-14. Abstraction of the control strategies for the maintenance of hydrogen and toluene at this level produces the control strategies at Level 1. Due to the self-regulating nature of sub-system c, changing a component in F_7 and F_8 would require a change of the component in F_3 as well. When $F_{7,M}$ and $F_{8,M}$ are both specified in the control strategy for the material balance control of methane, the methane control strategy at Level 1 has effectively been imposed at Level 2. Control strategies developed at this level are upwardly compatible with decisions made at Level 1.

Table 9 - 14: Control Structure at the Generalized Reaction-Separation level

Control Objectives		Assignment	
		Reaction Sub-block *a*	Separation Sub-block *b*
2-1	Temperature in F_{19}	Q_{fuel}	
2-2	$r_{H\text{-}(a)}$ and $r_{H\text{-}(b)}$	F_1	$F_{8,H}$
2-3	$r_{M\text{-}(a)}$ and $r_{M\text{-}(b)}$	$F_{7,M}$	$F_{8,M}$
2-4	$r_{T\text{-}(a)}$ and $r_{T\text{-}(b)}$	F_2	$F_{10,B}$
2-5	$e_{(a)}$ and $e_{(b)}$	Q_{fuel}	$Q_{CW\text{-}(b)}$
2-6	Production Level		F_5
2-7	Product Purity		$F_{5,B}$
2-8	Minimum Cost	minimize loss of benzene minimize loss of raw materials	

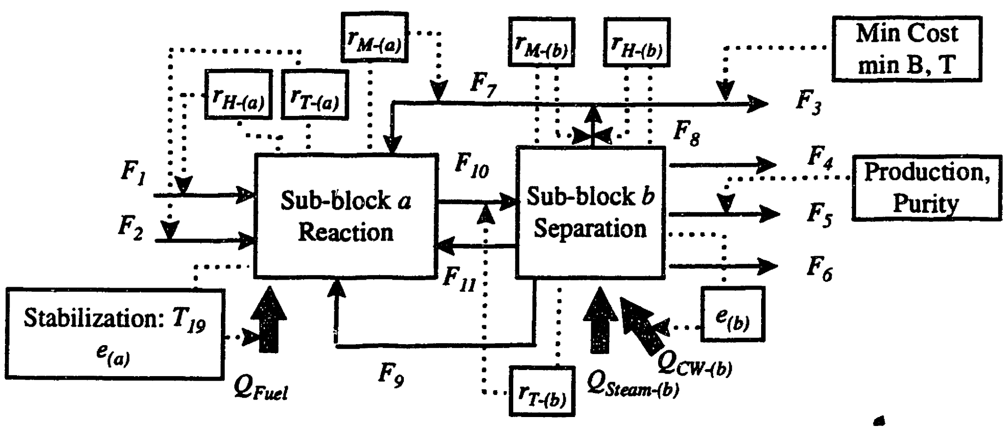


Figure 9 - 12: Control Structure for the Generalized Reaction-Separation System

9.5 Level 3a: Generalized Reaction - Expanded Separation System

The process representation for Level 3a is shown in Figure 9-13. At this level, generalized separation block is further refined into a generalized phase separation block and a product recovery section. The generalized reaction block is unchanged. The flow to the product recovery section, F_{13}, is the only additional manipulation. The reaction sub-block and the product recovery sub-block are still abstract view of the actual process. The dominant time-constants in these sections are greater than the dominant time constants within the sections. Long-horizon design criteria will be employed for the development of control structure at this level.

Progressive Generation of Control Objectives

Control objectives relevant at this level will be defined based on those at the previous level using the same principles employed at the previous level. No new objectives have become observable at this level. No other new objectives can be spawned or refined into more specific ones at this point. The prioritized control objectives at Level 3a are summarized in Table 9-15. Material and energy balances associated with sub-system *d* and *e* can be found in Appendix A.3.

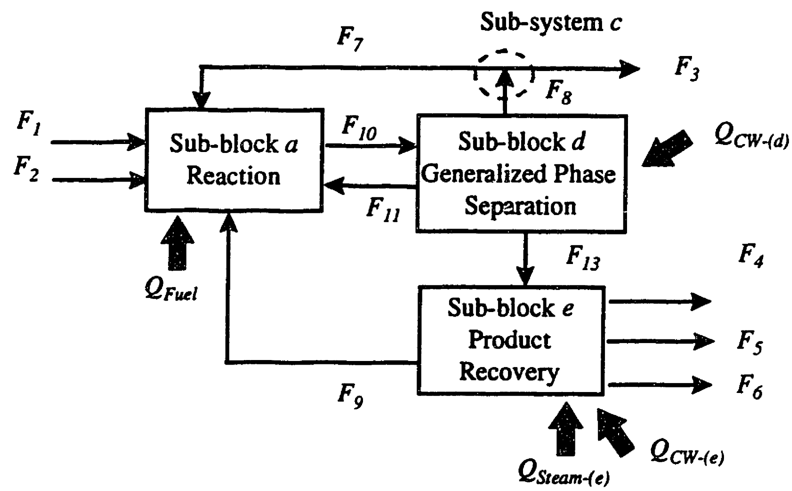


Figure 9 - 13: Process Representation the Generalized Reaction - Expanded Separation System (Level 3a)

Table 9 - 15: Prioritized Control Objectives at the Generalized Reaction - Expanded Separation Level

	Reaction	Separation	
	Sub-block *a*	Sub-block *d*	Sub-block *e*
3a-1	Temperature of F_{19}		
3a-2	$r_{H\text{-}(a)}$	$r_{H\text{-}(d)}$	$r_{H\text{-}(e)}$
3a-3	$r_{M\text{-}(a)}$	$r_{M\text{-}(d)}$	$r_{M\text{-}(e)}$
3a-4	$r_{T\text{-}(a)}$	$r_{T\text{-}(d)}$	$r_{T\text{-}(e)}$
3a-5	$e_{(a)}$	$e_{(d)}$	$e_{(e)}$
3a-6			Production Level
3a-7			Product Purity
3a-8	minimize operating cost		

Verify Feasibility of Control Objectives

At this level, no further refinement has been made on the reactor section. It can be easily verified that the specification of control objective do not violate constraints developed in Section 9.3 and 9.4.

Quantifying Process Behavior and Level 3a

The open-loop gains for the objectives associated with this level are complied in Table 9-16.

Synthesize Control Structure at the Generalized Reaction - Expanded Separation Level

As process refinement from the previously level has been confined to the generalized separation section, the modification of control structure will occur in the separation area. Goal 3a-1, temperature of F_{19}, is associated with the stabilization control strategy and will be maintained by adjusting Q_{Fuel}. The decisions we have to make concerning other control objectives are described below.

Table 9 - 16: Open-loop Gains of the Material Balance residuals at the Generalized Reaction - Expanded Separation Level

Input	$r_{H\text{-}(a)}$	$r_{H\text{-}(d)}$	$r_{H\text{-}(e)}$	$r_{M\text{-}(a)}$	$r_{M\text{-}(d)}$	$r_{M\text{-}(e)}$	$r_{T\text{-}(a)}$	$r_{T\text{-}(d)}$	$r_{T\text{-}(e)}$
F_1	4.1196	0	0	0.2168	0	0	0	0	0
F_2	0	0	0	0	0	0	2.734	0	0
$F_{3,T}$	0	0	0	0	0	0	0	0	0
$F_{3,B}$	0	0	0	0	0	0	0	0	0
$F_{3,M}$	0	0	0	0	0	0	0	0	0
$F_{3,H}$	0	0	0	0	0	0	0	0	0
$F_{4,B}$	0	0	-0.009	0	0	0.009	0	0	-0.009
$F_{4,M}$	0	0	0	0	0	-0.1893	0	0	0
$F_{4,H}$	0	0	-0.0134	0	0	0	0	0	0
$F_{5,T}$	0	0	0	0	0	0	0	0	-0.0008
$F_{5,B}$	0	0	-2.5919	0	0	2.592	0	0	-2.592
$F_{5,M}$	0	0	0	0	0	-0.0007	0	0	0
$F_{6,T}$	0	0	0	0	0	0	0	0	-0.0025
$F_{6,D}$	0	0	-0.0466	0	0	0.0932	0	0	-0.0932
$F_{7,T}$	0	0	0	0	0	0	0.0432	0	0
$F_{7,B}$	0.36625	0	0	-0.36625	0	0	0.3662	0	0
$F_{7,M}$	0	0	0	30.82	0	0	0	0	0
$F_{7,H}$	15.9614	0	0	0	0	0	0	0	0
$F_{8,T}$	0	0	0	0	0	0	0	-0.0471	0
$F_{8,B}$	0	-0.3989	0	0	0.399	0	0	-0.3989	0
$F_{8,M}$	0	0	0	0	-33.56	0	0	0	0
$F_{8,H}$	0	-17.38	0	0	0	0	0	0	0
$F_{9,T}$	0	0	0	0	0	0	0.8586	0	-0.8586
$F_{9,B}$	0.0138	0	-0.0138	-0.0138	0	0.0138	0.0138	0	-0.0138
$F_{9,D}$	0.0001	0	-0.0001	-0.0005	0	0.0005	0.0005	0	-0.0005
$F_{10,T}$	0	0	0	0	0	0	-1.12	1.12	0
$F_{10,B}$	-3.777	3.777	0	3.77665	-3.77665	0	-3.78	3.78	0
$F_{10,D}$	-0.0606	0.0606	0	0.1211	-0.1211	0	-0.1211	0.1211	0
$F_{10,M}$	0	0	0	-33.81	33.81	0	0	0	0
$F_{10,H}$	-17.4	17.4	0	0	0	0	0	0	0
$F_{11,T}$	0	0	0	0	0	0	0.258	-0.258	0
$F_{11,B}$	0.7639	-0.7639	0	-0.764	0.764	0	0.764	-0.764	0
$F_{11,D}$	0.0137	-0.0137	0	-0.0274	0.0274	0	0.0274	-0.0274	0
$F_{11,M}$	0	0	0	0.056	-0.056	0	0	0	0
$F_{11,H}$	0.00392	-0.00392	0	0	0	0	0	0	0
$F_{13,T}$	0	-0.0134	0.0134	0	0	0	0	-0.862	0.862
$F_{13,B}$	0	-2.6147	2.6147	0	-2.615	2.615	0	-2.6147	2.6147
$F_{13,D}$	0	-0.0469	0.0469	0	-0.09372	0.09372	0	-0.09374	0.09374
$F_{13,M}$	0	0	0	0	0.19	-0.19	0	0	0
$F_{13,H}$	0	0	0	0	0	0	0	0	0

Goal 3a-2: Maintain material balance control of hydrogen

Since the reaction blocked has remained unchanged and there are no new manipulated variables directly linked to this block, the control strategies associated with the control objectives in this block will remain the same. The new manipulated variables at this level are the component flows in F_{13}. At the previous level, F_1 and $F_{8,H}$ have been assigned to be the manipulated variables for $r_{H\text{-}(a)}$ and $r_{H\text{-}(b)}$ respectively. Then, the sets of best manipulated variables are:

1. $r_{H\text{-}(a)}$: $\{F_1\}$
2. $r_{H\text{-}(d)}$: $\{F_{8,H}$ and component flows in $F_{13}\}$
3. $r_{H\text{-}(e)}$: {all manipulated variables streams}

Table 9-17 (a) column 1 gives the open-loop gain of $r_{H\text{-}(a)}$ by all component flows. F_1 is indeed the best choice given that we would like to divert the disturbances away from the plant as early as possible. Columns 2 and 3 of Table 9-17 show the open-loop gains of $r_{H\text{-}(d)}$ and $r_{H\text{-}(d)}$. The best choices are:

1. $r_{H\text{-}(d)}$: $\{F_{8,H}\}$
2. $r_{H\text{-}(e)}$: $\{F_{13,B}, F_{5,B}\}$

Note that $F_{8,H}$ is indeed the better choice for controlling $r_{H\text{-}(d)}$. The magnitudes of the gains for $F_{13,B}$ and $F_{5,B}$ are similar. It is preferred that disturbances be diverted away from $F_{5,B}$, so $F_{13,B}$ is assigned to $r_{H\text{-}(e)}$. For $r_{H\text{-}(e)}$, $F_{8,H}$ is the better choice because we can quickly divert the variations to the environment through the purge stream. The closed-loop gains of $r_{H\text{-}(d)}$ and $r_{H\text{-}(e)}$ have been computed in columns 4 and 5 to verify that there is no conflict when all three objectives are under closed-loop control.

Goal 3a-3: Maintain material balance control of methane

$F_{8,M}$ and $F_{7,M}$ have been found to be the best manipulated variables for the maintenance of the material balance of methane. Thus, based on the Consistency Logic Map, we expect the sets of best manipulated variables at this level to be:

1. $r_{M\text{-}(a)}$: $\{F_{7,M}\}$
2. $r_{M\text{-}(d)}$: $\{F_{8,M}$ and component flows in $F_{13}\}$
3. $r_{M\text{-}(e)}$: {all manipulated variables streams}

The closed-loop gains of $r_{M\text{-}(a)}$, $r_{M\text{-}(d)}$ and $r_{M\text{-}(e)}$ while $r_{H\text{-}(a)}$, $r_{H\text{-}(d)}$. $r_{H\text{-}(e)}$ are under controlled by the previously selected manipulated variables have been computed and tabulated in columns 1, 2 and 3 of Table 9-17 (b). The best choices are:

1. $r_{M\text{-}(a)}$: $\{F_{7,M}\}$
2. $r_{M\text{-}(d)}$: $\{F_{8,M}\}$
3. $r_{M\text{-}(e)}$: $\{F_{4,M}, F_{13,M}, F_{5,B}\}$

Table 9 - 17 (a) : Closed-loop Gains of the Material Balance residuals at the Generalized Reaction - Expanded Separation Level

Input	$r_{H\text{-}(a)}$	$r_{H\text{-}(d)}$	$r_{H\text{-}(e)}$	$r_{H\text{-}(d)}$ closed-loop	$r_{H\text{-}(e)}$ closed-loop
F_1	4.1196	0	0	0	0
F_2	0	0	0	0	0
$F_{3,T}$	0	0	0	0	0
$F_{3,B}$	0	0	0	0	0
$F_{3,M}$	0	0	0	0	0
$F_{3,H}$	0	0	0	0	0
$F_{4,B}$	0	0	-0.009	0	-0.009
$F_{4,M}$	0	0	0	0	0
$F_{4,H}$	0	0	-0.0134	0	-0.0134
$F_{5,T}$	0	0	0	0	0
$F_{5,B}$	0	0	-2.591929	0	-2.5919
$F_{5,M}$	0	0	0	0	0
$F_{6,T}$	0	0	0	0	0
$F_{6,D}$	0	0	-0.0466	0	-0.0466
$F_{7,T}$	0	0	0	0	0
$F_{7,B}$	0.36625	0	0	0	0
$F_{7,M}$	0	0	0	0	0
$F_{7,H}$	15.9614	0	0	0	0
$F_{8,T}$	0	0	0	0	0
$F_{8,B}$	0	-0.3989	0	-0.3989	0
$F_{8,M}$	0	0	0	0	0
$F_{8,H}$	0	-17.38	0	-17.38	0
$F_{9,T}$	0	0	0	0	0
$F_{9,B}$	0.01383	0	-0.01383	0	-0.0138
$F_{9,D}$	0.0001309	0	-0.000131	0	-0.0001
$F_{10,T}$	0	0	0	0	0
$F_{10,B}$	-3.777	3.777	0	3.777	0
$F_{10,D}$	-0.06056	0.06056	0	0.0606	0
$F_{10,M}$	0	0	0	0	0
$F_{10,H}$	-17.4	17.4	0	17.4	0
$F_{11,T}$	0	0	0	0	0
$F_{11,B}$	0.7639	-0.7639	0	-0.7639	0
$F_{11,D}$	0.0137	-0.0137	0	-0.0137	0
$F_{11,M}$	0	0	0	0	0
$F_{11,H}$	0.00392	-0.00392	0	-0.0039	0
$F_{13,T}$	0	-0.01341	0.01341	-0.0134	0.0134
$F_{13,B}$	0	-2.6147	2.6147	-2.6147	2.6147
$F_{13,D}$	0	-0.04687	0.04687	-0.0469	0.0469
$F_{13,M}$	0	0	0	0	0
$F_{13,H}$	0	0	0	0	0

The best inputs for $r_{M\text{-}(a)}$ is indeed $F_{7,M}$ as expected. The new manipulated variable (component flows in F_{13}) at this level is not superior than our pervious choice, so $F_{8,M}$ is again assigned to $r_{M\text{-}(d)}$. For $r_{M\text{-}(e)}$, even though $F_{5,B}$ has the largest gain, it is our preference that variations be kept away from this variable as much as possible. Since the inventory of methane in sub-block e is expected to be insignificant, selection will be confined to $F_{4,M}$ and $F_{13,M}$. $F_{4,M}$ will be assigned to this objective as it is more able to divert disturbances to the environment sooner than $F_{13,M}$. The closed-loop gains of $r_{M\text{-}(d)}$ and $r_{M\text{-}(e)}$ have been computed and listed in columns 4 and 5 of Table 9-17 (b) to verify that we will not have any problem under closed-loop control.

Goal 3a-4: Maintain material balance control of toluene

At Level 2, we selected F_2 and $F_{10,B}$ to maintain the level of accumulation of toluene in the plant. F_2 should still be the best choice for $r_{T\text{-}(a)}$. The potential best manipulated variables for the rest of the objectives are:

1. $r_{T\text{-}(a)}$: { F_2 }
2. $r_{T\text{-}(d)}$: { $F_{10,B}$ }
3. $r_{T\text{-}(e)}$: { all manipulated variables }

The closed-loop gains of $r_{T\text{-}(a)}$, $r_{T\text{-}(d)}$ and $r_{T\text{-}(d)}$ are listed in columns 6 to 8 of Table 9-17 (b). Note that the best choices are :

1. $r_{T\text{-}(a)}$: { F_2 }
2. $r_{T\text{-}(d)}$: { $F_{10,B}$, $F_{5,B}$ }
3. $r_{T\text{-}(e)}$: { $F_{9,T}$, $F_{13,T}$ }

F_2 and $F_{10,B}$ are still the best choice for $r_{T\text{-}(a)}$ and $r_{T\text{-}(d)}$. As for $r_{T\text{-}(e)}$, the gains of $F_{9,T}$ and $F_{13,T}$ are similar. Because F_9 is a recycle stream so it is related to the feed streams to the reaction section. Thus, variations in the process can be passed to the environment via F_9 and the feed streams. $F_{9,T}$ will be assign to $r_{T\text{-}(e)}$. Alternatively, one can keep both options open. The closed-loop gains of $r_{T\text{-}(d)}$ and $r_{T\text{-}(e)}$ have been computed and tabulated in columns 9 and 10 to verify that the proposed control strategy is feasible.

Goal 3a-5: Maintain energy balance control

As in Level 2, maintaining Goal 3a-1 implicitly maintains $e_{(a)}$. Q_{Fuel} has already been reserved for this purpose. For $e_{(d)}$, $Q_{CW\text{-}(d)}$ is the only candidate. $Q_{CW\text{-}(e)}$ is a relatively cheaper resource than $Q_{Steam\text{-}(e)}$ so we will assign this manipulation to $e_{(d)}$ as well.

Goal 3a-6: Production Rate

Adjusting F_5 is still the best way to maintain the production level of the process.

Goal 3a-7: Purity in Benzene Product

$F_{5,B}$ will be used to maintain the level of purity in benzene.

Table 9-17 (b): Closed-loop Gains of the Material Balance residuals at the Generalized Reaction - Expanded Separation Level

Input	$r_{M\text{-}(a)}$	$r_{M\text{-}(d)}$	$r_{M\text{-}(e)}$	$r_{M\text{-}(d)}$ closed-loop	$r_{M\text{-}(e)}$ closed-loop	$r_{T\text{-}(a)}$	$r_{T\text{-}(d)}$	$r_{T\text{-}(e)}$	$r_{T\text{-}(d)}$ closed-loop	$r_{T\text{-}(e)}$ closed-loop
F_1	0	0	0	0	0	0	0	0	0	0
F_2	0	0	0	0	0	2.734	0	0	0	0
$F_{3,T}$	0	0	0	0	0	0	0	0	0	0
$F_{3,B}$	0	0	0	0	0	0	0	0	0	0
$F_{3,M}$	0	0	0	0	0	0	0	0	0	0
$F_{3,H}$	0	0	0	0	0	0	0	0	0	0
$F_{4,B}$	0	-0.009	0.018	-0.009	0.018	0	-0.009	0	-0.009	0
$F_{4,M}$	0	0	-0.1893	0	-0.1893	0	0	0	0	0
$F_{4,H}$	0	-0.0134	0.0134	-0.0134	0.0134	0	-0.0134	0.0134	-0.0134	0.0134
$F_{5,T}$	0	0	0	0	0	0	0	-0.0008	0	-0.0008
$F_{5,B}$	0	-2.5922	5.1842	-2.5922	5.1842	0	-2.5919	-0.0001	-2.5919	-0.0001
$F_{5,M}$	0	0	-0.0007	0	-0.0007	0	0	0	0	0
$F_{6,T}$	0	0	0	0	0	0	0	-0.0024	0	-0.0024
$F_{6,D}$	0	-0.0466	0.1398	-0.0466	0.1398	0	-0.0466	-0.0466	-0.0466	-0.0466
$F_{7,T}$	0	0	0	0	0	0.0432	0	0	0	0
$F_{7,B}$	-0.3855	0	0	0	0	0.3662	0	0	0	0
$F_{7,M}$	30.82	0	0	0	0	0	0	0	0	0
$F_{7,H}$	-0.84	0	0	0	0	0	0	0	0	0
$F_{8,T}$	0	0	0	0	0	0	-0.0471	0	-0.0471	0
$F_{8,B}$	0	0.399	0	0.399	0	0	-0.3989	0	-0.3989	0
$F_{8,M}$	0	-33.56	0	-33.56	0	0	0	0	0	0
$F_{8,H}$	0	0	0	0	0	0	0	0	0	0
$F_{9,T}$	0	0	0	0	0	0.8586	0	-0.8586	0	-0.8586
$F_{9,B}$	-0.0145	-0.0138	0.0277	-0.0138	0.0277	0.0138	-0.0138	0	-0.0138	0
$F_{9,D}$	-0.0005	-0.0001	0.0007	-0.0001	0.0007	0.0005	-0.0001	-0.0004	-0.0001	-0.0004
$F_{10,T}$	0	0	0	0	0	-1.116	1.116	0	1.116	0
$F_{10,B}$	3.9754	-3.7766	0	-3.7766	0	-3.778	3.778	0	3.778	0
$F_{10,D}$	0.1243	-0.1211	0	-0.1211	0	-0.1211	0.1211	0	0.1211	0
$F_{10,M}$	-33.81	33.81	0	33.81	0	0	0	0	0	0
$F_{10,H}$	0.9157	0	0	0	0	0	0	0	0	0
$F_{11,T}$	0	0	0	0	0	0.258	-0.258	0	-0.258	0
$F_{11,B}$	-0.8042	0.764	0	0.764	0	0.764	-0.764	0	-0.764	0
$F_{11,D}$	-0.0281	0.0274	0	0.0274	0	0.0274	-0.0274	0	-0.0274	0
$F_{11,M}$	0.056	-0.056	0	-0.056	0	0	0	0	0	0
$F_{11,H}$	-0.0002	0	0	0	0	0	0	0	0	0
$F_{13,T}$	0	0.0134	-0.0134	0.0134	-0.0134	0	-0.8486	0.8486	-0.8486	0.8436
$F_{13,B}$	0	0	0	0	0	0	0	0	0	0
$F_{13,D}$	0	-0.0468	0.0468	-0.0468	0.0468	0	-0.0469	0.0469	-0.0469	0.0469
$F_{13,M}$	0	0.19	-0.19	0.19	-0.19	0	0	0	0	0
$F_{13,H}$	0	0	0	0	0	0	0	0	0	0

Goal 3a-8: Cost Minimization

At this level, the cost optimization is described as follows:

$$\min \Phi = \begin{Bmatrix} c_T F_2 + c_H F_1 - v_H F_{3,H} - v_M F_{3,M} - v_B F_{3,B} - v_T F_{3,T} - v_H F_{4,H} - v_M F_{4,M} \\ - v_B F_{4,B} - v_T F_{6,T} - v_D F_{6,D} + p_B F_{3,B} + p_B F_{4,B} + c_{Fuel} F_{Fuel} + c_{cw} F_{cw-(d)} \\ + c_{cw} F_{cw-(e)} + c_{steam} F_{steam-(e)} + c_{compressor} \end{Bmatrix} \qquad [9\text{-}41]$$

s.t.:

1. Maintain temperature of F_{19}
2. Maintain accumulation of hydrogen at desired level
3. Maintain accumulation of methane at desired level
4. Maintain accumulation of toluene at desired level
5. Maintain accumulation of energy at desired level
6. F_5 = production rate
7. $x_{5,B}$ = product purity
8. Other constraints related to the reaction and the expanded separation blocks which are not visible at this level

where:

c_i = cost of materials

v_i = fuel or resale value of materials

p_i = market value of product

Substituting the control strategies, the product specifications into to objective function and the material balance relationships associated with sub-block c produce the following objective function:

$$\begin{aligned} \Phi = {} & F_{3,T}(c_T + c_{H^*} - v_T) + F_{3,B}(c_T + c_{H^*} + p_B - v_B) - F_{3,H} v_H - F_{3,M} v_M \\ & + F_{4,H}(c_{H^*} - v_H + v_M) + F_{4,B}(c_T + c_{H^*} + p_B - v_B) \\ & - F_{6,B} v_M + F_{6,D}(c_T + c_{H^*} - v_M - v_D) + F_{6,T}(c_T - v_T) \\ & - F_{7,H} c_{H^*} + F_{8,T} c_{H^*} + F_{9,H} v_M + F_{9,B} v_M \\ & + F_{9,D}(c_T + c_{H^*} - v_M) + F_{10,H} c_{H^*} - F_{10,D} c_{H^*} - F_{10,T} c_{H^*} \\ & - F_{11,H} c_{H^*} + F_{11,D} c_{H^*} + F_{11,T} c_{H^*} \\ & + F_{13,T} c_{H^*} + F_{13,D}(c_{H^*} + v_M) - F_{13,M} v_M - F_{13,H}(c_{H^*} + v_M) \\ & + c_{stm} F_{stm-(e)} + c_{compressor} \end{aligned} \qquad [9\text{-}42]$$

The degrees of freedom in the design can be further reduced by considering the following relationships:

<u>Stoichiometry</u> :

There are no new constraints from stoichiometry at this level. Equation [9-33] still apply.

Material Balances around Sub-system c and the product recovery section :

$$F_{3,i} + F_{7,i} = F_{8,i} \quad [9\text{-}35]$$

$$F_{13,i} = F_{4,i} + F_{5,i} + F_{6,i} + F_{9,i} \quad [9\text{-}43]$$

Thermodynamics :

At this level, a fictitious stream $F_{\neq}$ is being distributed into a vapor stream F_8 and a liquid stream F_{13} as shown in Figure 9-14. F_{13} is equivalent to F_{liq2} at Level 2 which is being further distributed into F_4, F_5, F_6 and F_9. Hence, the following *new* generic relations exist:

$$f_1(F_{\neq,i}\, , F_{8,i}, F_{13,i}) = 0 \quad [9\text{-}44]$$

$$f_2(F_{\neq,i}\, , F_{8,i}, F_{13,i}) = 0 \quad [9\text{-}45]$$

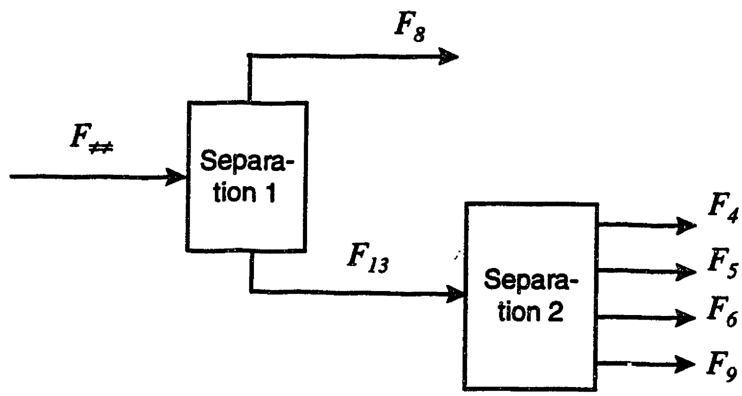


Figure 9 - 14: Pseudo-Separation Systems in the Expanded Separation Sub-block

At this level, we cannot observe $F_{\neq}$ in the generalized phase-separation section so we will assume that their values are fixed. Hence, based on Equation [9-44] and [9-45], $F_{8,i}$ and $F_{13,i}$ are constrained by some thermodynamic relationships. From Equation [9-35], we know that no more than two variables from the set $\{F_{3,i}, F_{7,i}\, , F_{8,i}\}$ can have fixed values. Also, from Equation [9-45], we know that no more than four variables from the set $\{F_{13,i}, F_{4,i}\, , F_{5,i}, F_{6,i}\, , F_{9,i}\ \}$ can have fixed values.

The initial component table corresponding to the process representation at this level has been set up in Table 9-18, using "MV", "specified" and "0" , "~0" or "small" to indicate components which are assigned to be manipulated variables, specified as controlled variables or that the amount at steady-state relatively small.

Table 9 - 18: Initial component table for the Generalized Reaction-Expanded Separation System

component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{13,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H			MV			0	0	0
M		MV	MV		MV	0	0	0
T					0	~0	small	MV
B				MV		specified	0	
D	0	0	0		0	0		small

<u>Degrees of Freedom Analysis</u> :

The opportunities for reduction of design degrees of freedom are listed below:

1. $F_{8,H}$ is a manipulated variable so the value of $F_{13,H}$ is fixed by the control relation and by Equations [9-44] and [9-45]. With the flows of $F_{5,H}$, $F_{6,H}$ and $F_{9,H}$ being insignificant, $F_{4,H} = F_{13,H}$ so $F_{4,H}$ is also not available as a degree of freedom. Either $F_{3,H}$ or $F_{7,H}$ can be used as the design variable in the optimization. Since the flow of $F_{7,H}$ is larger, we will use $F_{7,H}$ as the degree of freedom. Then, $F_{3,H} = f(F_{7,H})$.
2. $F_{7,M}$, $F_{8,M}$ and $F_{4,M}$ have been chosen to be manipulated variables. With the value of $F_{8,M}$ fixed by the control relation, $F_{13,M}$ is also fixed. Since the value of $F_{7,M}$, is also fixed by the control relation, the value of $F_{3,M}$ is then constrained by Equation [9-35] so it is not available for optimization.
3. Either $F_{13,T}$ or $F_{8,T}$ can be used as a degree of freedom. As toluene goes preferentially to the liquid stream, $F_{13,T}$ will be used as the design variable. $F_{9,T}$ has been selected to be a manipulated variable and both $F_{4,T}$ and $F_{5,T}$ are insignificant, $F_{6,T} = f(F_{13,T})$. Either $F_{3,T}$ or $F_{7,T}$ can be used as the design variable in the optimization. Since the effects of $F_{3,T}$ on Φ can be directly observed, $F_{3,T}$ would be our choice. Then, $F_{7,T} = f(F_{3,T})$.
4. $F_{13,B}$ is a manipulated variable. Then, $F_{8,B}$ becomes unavailable. Either $F_{3,B}$ or $F_{7,B}$ can be chosen as a degree of freedom. Focus on $F_{3,B}$ because its effect on Φ can be directly observed. Then, $F_{7,B} = f(F_{3,B})$. Three of the values in the set $\{F_{4,B}, F_{5,B}, F_{6,B}, F_{9,B}\}$ can be fixed. Since $F_{5,B}$ is a control objective and the value of $F_{6,B}$ is small, we can choose only one variable from the set $\{F_{4,B}, F_{9,B}\}$ to be the design variable. As $F_{4,B}$ is larger, we will select F [illegible] B as the design degree of freedom. Then, $F_{9,B} = f(F_{4,B})$.
5. All diphenyl in F [illegible] passes to F_{13} and then to F_6. $F_{9,D}$ is small, $F_{5,D}$ and $F_{4,D}$ are both insignificant. Thus, either $F_{13,D}$ or $F_{6,D}$ can be used as a design variable. To conform with the strategies defined at the pervious level, we will maintain $F_{6,D}$ to be the degree of freedom. Then, $F_{13,D} = f(F_{6,D})$.

The final component table for Level 3a is summarized in Table 9-19.

Table 9 - 19: Final component table for the Generalized Reaction-Expanded Separation System

Component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{13,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H		√	MV	n/a	n/a	0	0	0
M	n/a	MV	MV	n/a	MV	0	0	0
T	√		n/a	√	0	~0	small	MV
B	√		n/a	MV	√	Specified	0	
D	0	0	0		0	0	√	small

Implementing the above specifications reduces the optimization to:

$$
\begin{aligned}
\min\ \Phi = {} & F_{3,T}\,(c_T + c_{H*} - v_T) + F_{3,B}\,(c_T + c_{H*} + p_B - v_B) - f(F_{7,H})\, v_H \\
& + F_{4,B}\,(c_T + c_{H*} + p_B - v_B) + f(F_{4,B})\, v_M - F_{7,H}\, c_{H*} \\
& + F_{6,D}\,(c_T + c_{H*} - v_M - v_D) + f(F_{6,D})(c_{H*} + v_M) \\
& + F_{10,H}\, c_{H*} - F_{10,D}\, c_{H*} - F_{10,T}\, c_{H*} \\
& - F_{11,H}\, c_{H*} + F_{11,D}\, c_{H*} + F_{11,T}\, c_{H*} \\
& + F_{13,T}\, c_{H*} + f(F_{13,T})(c_T - v_T) \\
& + c_{stm} F_{stm\text{-}(e)} + c_{compressor}
\end{aligned}
\qquad [9\text{-}46]
$$

s.t.:

$$F_{3,i} + F_{7,i} = F_{8,i}$$

Constraints imposed by the compressor

Note that all c_i and v_i are greater than zero. Also, $c_T >> v_T$; $c_{H*} >> v_T$; v_B v_M and v_H are small. Then,

$(c_T + c_{H*} + p_B - v_B) > 0$. Then, it can be seen that $(F_{3,B} + F_{4,B})$ is the amount of loss of benzene from the process. Minimizing this amount can help to reduce the operating cost. Note that $f(F_{7,H}) = F_{3,H}$. $F_{3,H}$ is small compared to $F_{7,H}$. Increasing $F_{7,H}$ and lowering $F_{3,T}$ would help to reduce the cost as well (since $c_{H*}\, F_{7,H}$ is positive and $v_M\, f(F_{7,H}) << c_{H*}\, F_{7,H}$). So we want to maximize the recovery of raw materials. $(F_{6,D} + f(F_{6,D}))$ refers to the amount of diphenyl being produced in the process. Decreasing the production of diphenyl reduces the cost as well. Note that the amount of diphenyl being produced is strongly dependent on the one-pass conversion of toluene in the reactor. No conclusive statements can be made about F_6, F_{10}, F_{11} and F_{13}. Hence at this level, we can again tentatively say that Φ can be minimized if we:

1. Reduce the amount of benzene leaving the process.
2. Reduce the loss of raw materials from the process.

These conclusions are the same as those that we determined at the previous levels.

Control Structure at Level 3a

The control structure at this level is being displayed in Figure 9-15 and the set of the control strategies are summarized in Table 9-20. Note that abstraction of the control structure returns hydrogen and toluene material balance control policies which are identical to those developed at Level 2. For methane, and energy balance control, additional inputs at Level 3a are being used. The added details of the representation at this level allows the development of a control structure that is more elaborate than the one identified at Level 2. An *elaborated control structure* is potentially more beneficial as more degrees of freedom have been assigned to the objectives. The additional degrees of freedom have been added to modify certain plant behavior. In this case, more outlet streams have been selected to enhance the diversion of variations to the environment.

Table 9 - 20: Control Structure at the Generalized Reaction - Expanded Separation Level

Control Objectives		Assignment		
		Reaction Sub-block *a*	Gen. Phase-Separator Sub-block *d*	Product Recovery Sub-block *e*
3a-1	Temperature of F_{19}	Q_{Fuel}		
3a-2	$r_{H\text{-}(a)}$, $r_{H\text{-}(d)}$, $r_{H\text{-}(e)}$	F_1	$F_{8,H}$	$F_{13,B}$
3a-3	$r_{M\text{-}(a)}$, $r_{M\text{-}(d)}$, $r_{M\text{-}(e)}$	$F_{7,M}$	$F_{8,M}$	$F_{4,M}$
3a-4	$r_{T\text{-}(a)}$, $r_{T\text{-}(d)}$, $r_{T\text{-}(e)}$	F_2	$F_{10,B}$	$F_{9,T}$
3a-5	$e_{(a)}$, $e_{(d)}$, $e_{(e)}$	Q_{Fuel}	$Q_{CW\text{-}(d)}$	$Q_{CW\text{-}(e)}$
3a-6	Production Level			F_5
3a-7	Product Purity			$F_{5,B}$
3a-8	Minimum Cost	minimize loss of benzene minimize loss of raw materials		

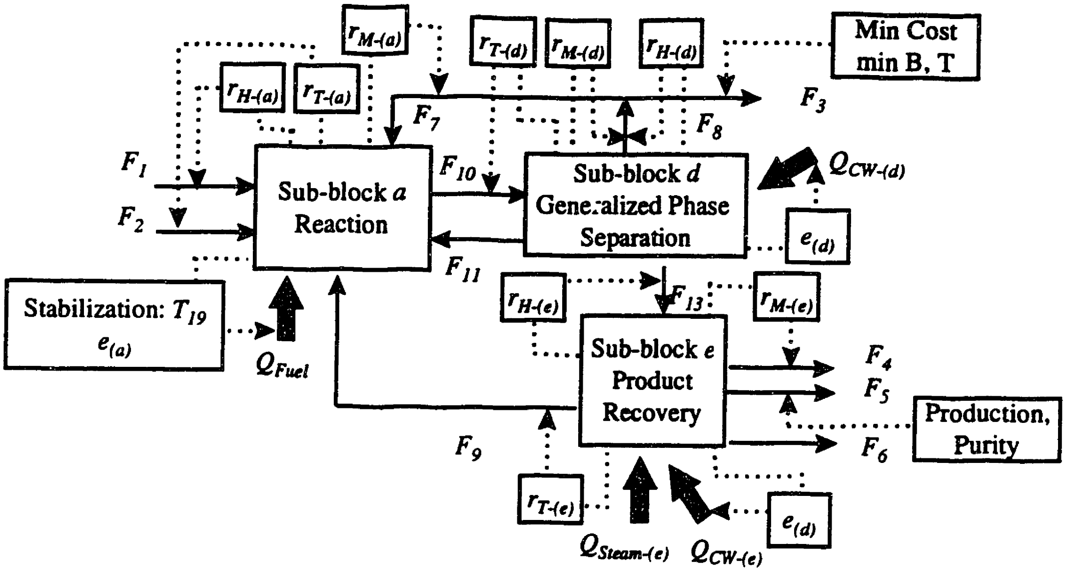


Figure 9 - 15: Control Structure for the Generalized Reaction - Expanded Separation System

9.6 Level 3b: Detailed Reaction-Expanded Separation System

At Level 3b, the reaction section is further refined to expose details of the operating units the generalized reaction section. The process representation is shown in Figure 9-16. The generalized phase-separation and product recovery section have not been modified. In this viewpoint, Sub-block *d* and *e* are still abstraction of the plant. Long-horizon design criteria still apply at this level.

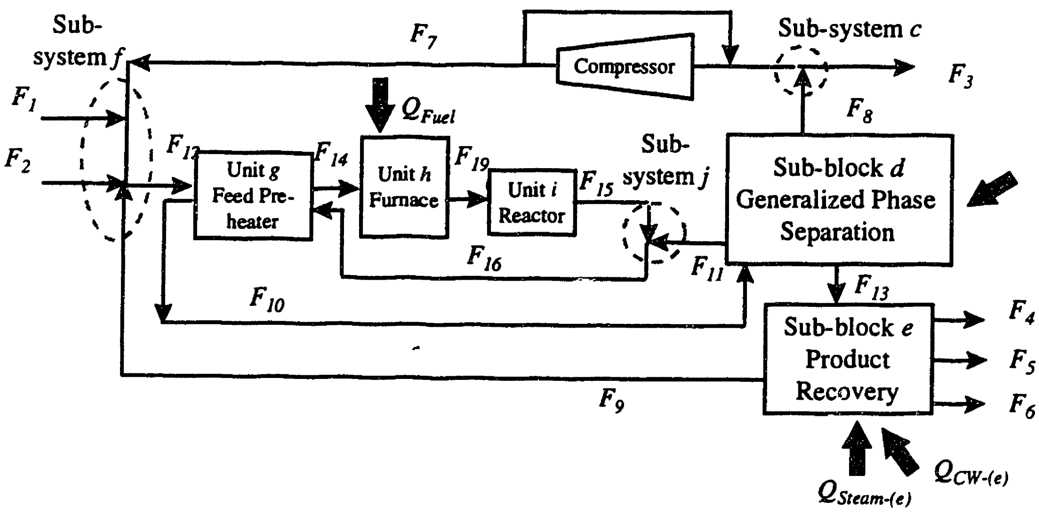


Figure 9 - 16: Process Representation of the Detailed Reaction-Expanded Separation System (Level 3b)

Progressive Generation of Control Objectives

The control objectives which correspond to the level of details observable at this level are summarized in Table 9-21. The stabilization control strategy has been *allocated* to unit h, the unit in which the control policy lies. The material and energy balance equations have been *translated* and *refined* directly from the reaction block in the previous level to describe the individual unit-operations in the reaction section.

Notice that units g, h, i (respectively feed pre-heater, furnace, reactor) and the mixers defined by system boundaries f and j are not material capacitors. Only the material accumulations in sub-blocks d and e require feedback control. Units g, h and i and the mixers at f and j are also not energy capacitors so it is not required to control energy accumulations in them. There are also no objectives that are specific to these unit-operations. Since the entire generalized reactor section (sub-block a at Levels 2 and 3a) is not a material or energy capacitor, the material and energy balance controls around system boundaries f, g, h, i and j can be dropped. The material and energy balances for the plant will be described by those which have been used for sub-block d and e at the previous level. As the abstract reaction block does not contain any material and energy capacitors, those control policies which have been developed for the reactor section at Levels 2 and 3a can be dropped.

At this level, with the revelation of the detailed structure of the reaction section, four new specific objectives have become observable. In fact, at this level, all the overall objectives of the production listed in Section 9.2 can be directly accessed.

Verify Feasibility of Control Objectives

At this level, G_{R1} and G_{R2} can be defined as:

$$G_{R1} = F_{20,B} - F_{19,B} \qquad [9\text{-}47]$$

$$G_{R2} = 2F_{20,D} - 2F_{19,D} \qquad [9\text{-}48]$$

which gives:

$$\frac{F_{20,B} - F_{19,B}}{2F_{20,D} - 2F_{19,D}} = \frac{S}{1-S} \qquad [9\text{-}49]$$

Table 9 - 21: Prioritized Control Objectives at the Detailed Reaction - Expanded Separation Level

	Furnace Unit *h*	Reactor Unit *i*	Generalized Phase-Separator Sub-block *d*	Product Recovery Sub-block *e*
3b-1	Temperature of F_{19}			
3b-2			$r_{H\text{-}(d)}$	$r_{H\text{-}(e)}$
3b-3			$r_{M\text{-}(d)}$	$r_{M\text{-}(e)}$
3b-4			$r_{T\text{-}(d)}$	$r_{T\text{-}(e)}$
3b-5			$e_{(d)}$	$e_{(e)}$
3b-6				Production Level
3b-7				Product Purity
3b-8	$T_{19} > 1150$ °F			
3b-9		Reacting mixture < 1300 °F		
3b-10		$F_{19,H}/F_{19,T} \geq 5$		
3b-11		reactor effluent ≤ 1150 °F		
3b-12	minimize operating cost			

Not all variables in Equation [9-49] can be specified to be controlled objectives. It can be easily verified that the control problem is properly posed. Our specifications at this level do not violate constraints arose from stoichiometry (from this or any levels above).

Synthesize Control Structure at the Detailed Reaction - Expanded Separation Level

At this level, sub-blocks *d* and *e* have not been refined. Hence, those manipulations selected to maintain the levels of accumulation of materials and energy in sub-blocks *d* and *e* will remain to be the best choices. This will be verified below. Open-loop gains have been previously given in Table 9-16.

Goal 3b-1: Temperature of F_{19}

The stabilization control policy has now been confined to Unit *h*. The *only* suitable manipulated variable is the fuel to furnace.

Goal 3b-2: Material balance control of hydrogen

Since there are no new observable manipulations available in sub-blocks *d* and *e*, the assignments that we identified at the previous level would remain to be the best choices.

1. $r_{H\text{-}(d)}$: { $F_{8,H}$ }
2. $r_{H\text{-}(e)}$: { $F_{13,B}$ }

Columns 1 and 2 of Table 9-22 gives the open-loop gains of these two sub-goals. $F_{8,H}$ and $F_{13,B}$ are indeed the best manipulated variables for the remaining sub-goals. The closed-loop gains of $r_{H\text{-}(f)}$ have been computed in column 3. These assignments do not create any conflicts under closed-loop situation.

Goal 3b-3: Material balance control of methane

Again, the assignments to $r_{H\text{-}(d)}$ and $r_{H\text{-}(e)}$ would remain the same:

1. $r_{M\text{-}(d)}$: { $F_{8,M}$ }
2. $r_{M\text{-}(e)}$: { $F_{4,M}$ }

Columns 4 and 5 in Table 9-22 show the closed-loop gains of these objectives with the material balance of hydrogen being maintained by the manipulations selected in the previous section. $F_{8,M}$ and $F_{4,M}$ remain to be the best ones for $r_{H\text{-}(d)}$ and $r_{H\text{-}(e)}$. The closed-loop gains of $r_{H\text{-}(e)}$ are shown in column 6. The chosen control structure is conflict-free.

Goal 3b-4: Material balance control of toluene

For this goal, have verified that the following are the best assignments:

1. $r_{T\text{-}(d)}$: { $F_{10,B}$ }
2. $r_{T\text{-}(e)}$: { $F_{9,T}$ }

Columns 7 and 8 in Table 9-22 show the closed-loop gains of these sub-goals while r_H and r_M are under closed-loop control. $F_{10,B}$ and $F_{9,T}$ are indeed the best manipulations for sub-blocks f and g. Closed-loop gains of sub-block g are tabulated in column 9. The control strategies are conflict-free.

Goal 3b-5: Energy balance control

To maintain the overall level of accumulation of energy in the system, two sub-goals must be simultaneously satisfied. The best manipulations are again the cooling water streams going into those blocks.

Goal 3b-6: Production Level

In the long-horizon analysis, adjusting the flow of F_5 is still the best choice to maintain the production rate at the specified value.

Goal 3b-7: Purity of Benzene

We will adjust the purity level by manipulating the flow of $F_{5,B}$.

Goal 3b-8: T_{19} > 1150 °F

This objective is equivalent to Goal 3b-1 so it has already been considered. Merging this objective with Goal 3b-1, T_{19} is to be fixed at some value that is above 1150 °F by Q_{Fuel}.

Goal 3b-9: Reacting mixture < 1300 °F

Goal 3b-9 can be accomplished by lowering T_{19} or by decreasing the conversion of toluene in the reactor. If T_{19} is being maintained at 1150 °F (the lower limit for inception of reactions), then, the only way to prevent the temperature of the reacting mixture from exceeding 1300 °F is by decreasing the feed rate which thereby reduces the total amount of heat generated in the reactor from the adiabatic exothermic reaction. This is an *override* control policy.

Goal 3b-10: $F_{19,H}/F_{19,T} \geq 5$

$F_{19,H}$ and $F_{19,T}$ are natural choices for this objective. We will assign $F_{19,H}$ to Goal 3b-10.

Goal 3b-11: Temperature of reactor effluent ≤ 1150 °F

This goal has been allocated to Unit *i* but the variable is in fact observable from the tee-junction defined by system boundary *j* defined in Figure 9-16. F_{11} (quench flow rate) is clearly the only choice here.

Table 9 - 22: Closed-loop gains of residuals of material balances at the Detailed Reaction - Expanded Separation Level

Input	$r_{H\text{-}(d)}$	$r_{H\text{-}(e)}$	$r_{H\text{-}(e)}$ closed-loop	$r_{M\text{-}(d)}$	$r_{M\text{-}(e)}$	$r_{M\text{-}(e)}$ closed-loop	$r_{T\text{-}(d)}$	$r_{T\text{-}(e)}$	$r_{T\text{-}(e)}$ closed-loop
F_1	0	0	0	0	0	0	0	0	0
F_2	0	0	0	0	0	0	0	0	0
$F_{3,T}$	0	0	0	0	0	0	0	0	0
$F_{3,B}$	0	0	0	0	0	0	0	0	0
$F_{3,M}$	0	0	0	0	0	0	0	0	0
$F_{3,H}$	0	0	0	0	0	0	0	0	0
$F_{4,B}$	0	-0.009	-0.009	-0.009	0.018	0.018	-0.009	0	0
$F_{4,M}$	0	0	0	0	-0.1893	-0.1893	0	0	0
$F_{4,H}$	0	-0.0134	-0.0134	-0.0134	0.0134	0.0134	-0.0134	0.0134	0.0134
$F_{5,T}$	0	0	0	0	0	0	0	-0.0008	-0.0008
$F_{5,B}$	0	-2.5919	-2.5919	-2.5922	5.1842	5.1842	-2.5919	-0.0001	-0.0001
$F_{5,M}$	0	0	0	0	-0.0007	-0.0007	0	0	0
$F_{6,T}$	0	0	0	0	0	0	0	-0.0025	-0.0024
$F_{6,D}$	0	-0.0466	-0.0466	-0.0466	0.1398	0.1398	-0.0466	-0.0466	-0.0466
$F_{7,T}$	0	0	0	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0	0	0	0
$F_{7,M}$	0	0	0	0	0	0	0	0	0
$F_{7,H}$	0	0	0	0	0	0	0	0	0
$F_{8,T}$	0	0	0	0	0	0	-0.0471	0	0
$F_{8,B}$	-0.3989	0	0	0.399	0	0	-0.3989	0	0
$F_{8,M}$	0	0	0	-33.56	0	0	0	0	0
$F_{8,H}$	-17.38	0	0	0	0	0	0	0	0
$F_{9,T}$	0	0	0	0	0	0	0	-0.8586	-0.8586
$F_{9,B}$	0	-0.0138	-0.0138	-0.0138	0.0277	0.0277	-0.0138	0	0
$F_{9,D}$	0	-0.0001	-0.0001	-0.0001	0.0007	0.0007	-0.0001	-0.0004	-0.0004
$F_{10,T}$	0	0	0	0	0	0	1.116	0	0
$F_{10,B}$	3.777	0	0	-3.7767	0	0	3.778	0	0
$F_{10,D}$	0.0606	0	0	-0.1211	0	0	0.1211	0	0
$F_{10,M}$	0	0	0	33.81	0	0	0	0	0
$F_{10,H}$	17.4	0	0	0	0	0	0	0	0
$F_{11,T}$	0	0	0	0	0	0	-0.258	0	0
$F_{11,B}$	-0.7639	0	0	0.764	0	0	-0.764	0	0
$F_{11,D}$	-0.0137	0	0	0.0274	0	0	-0.0274	0	0
$F_{11,M}$	0	0	0	-0.056	0	0	0	0	0
$F_{11,H}$	-0.0039	0	0	0	0	0	0	0	0
$F_{13,T}$	-0.0134	0.0134	0.0134	0.0134	-0.0134	-0.0134	-0.8486	0.8486	0.8486
$F_{13,B}$	-2.6147	2.6147	2.6147	0	0	0	0	0	0
$F_{13,D}$	-0.0469	0.0469	0.0469	-0.0468	0.0468	0.0468	-0.0469	0.0469	0.0469
$F_{13,M}$	0	0	0	0.19	-0.19	-0.19	0	0	0
$F_{13,H}$	0	0	0	0	0	0	0	0	0

Goal 3b-12: Minimization of Operating Cost

At this level, the cost optimization is described as follows:

$$\min\Phi = \begin{Bmatrix} c_T F_2 + c_H F_1 - v_H F_{3,H} - v_M F_{3,M} - v_B F_{3,B} - v_T F_{3,T} - v_H F_{4,H} - v_M F_{4,M} \\ - v_B F_{4,B} - v_T F_{6,T} - v_D F_{6,D} + p_B F_{3,B} + p_B F_{4,B} + c_{Fuel} F_{Fuel-i} + c_{cw} F_{cw-f} \\ + c_{cw} F_{cw-(g)} + c_{steam} F_{steam-(g)} + c_{compressor} \end{Bmatrix} \qquad [9\text{-}50]$$

s.t.:

1. $T_{19} = 1150$ °F
2. maintain accumulation of hydrogen at desired level
3. maintain accumulation of methane at desired level
4. maintain accumulation of toluene at desired level
5. maintain accumulation of energy at desired level
6. F_5 = production rate
7. $x_{5,B}$ = product purity
8. Reacting mixture < 1300 °F
9. $F_{19,H}/F_{19,T} \geq 5$
10. Temperature of reactor effluent ≤ 1150 °F
11. constraints related to the reaction section
12. other constraints related to the expanded separation blocks which are not visible at this level

where: c_i = cost of materials
v_i = fuel or resale values of materials
p_i = market value of product

The reactor block is not a capacitor of material or energy. Hence, only *Fuel*, F_5, $F_{5,B}$, $F_{8,H}$, $F_{13,B}$, $F_{8,M}$, $F_{4,M}$, $F_{10,B}$, $F_{9,T}$ and the cooling water are being used at this level. After substituting the control strategies and the product specifications into the objective functions, we have reduced Φ to:

$$\begin{aligned}\Phi = {} & c_T F_2 + c_H F_1 - v_H F_{3,H} - v_M F_{3,M} + (p_B - v_B) F_{3,B} - v_T F_{3,T} \\ & + (v_M - v_H) F_{4,H} + 2 v_M F_{4,D} + (p_B - v_B) F_{4,B} \\ & - (v_M + v_D) F_{6,D} - v_M F_{6,B} - v_T F_{6,T} \\ & + v_M F_{9,M} + v_M F_{9,H} - v_M F_{9,D} \\ & + v_M F_{13,D} - v_M F_{13,M} - v_M F_{13,H} \\ & + c_{Steam} F_{Steam-(e)} + c_{compressor}\end{aligned} \qquad [9\text{-}51]$$

Additional constraints which will help reduce the degrees of freedom in the optimization include:

Stoichiometry :

$$\frac{F_{20,B} - F_{19,B}}{2F_{20,D} - 2F_{19,D}} = \frac{S}{1-S} \tag{9-49}$$

Material Balances around Sub-system *c*, Sub-system *j* and the reaction section :
The following relationships for the self-regulating sub-systems are true:

$$F_{3,i} + F_{7,i} = F_{8,i} \tag{9-35}$$

$$F_{15,k} + F_{11,k} = F_{16,k} \tag{9-52}$$

$$F_{1,i} + F_{2,i} + F_{7,i} + F_{9,i} + F_{11,i} = F_{10,i} \tag{9-53}$$

Thermodynamics :
The separation section has not been further refined at this level. The constraints stated in the discussion of the previous level are still valid at this level.

The initial component table for the detailed reaction - expanded separation system which lists the status of each of the components in the relevant stream is shown in Table 9-23.

Table 9 - 23: Initial Component Table for the Detailed Reaction - Expanded Separation System

component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{13,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H			MV			0	0	0
M			MV		MV	0	0	0
T					0	~0	small	MV
B				MV		Specified	0	
D	0	0	0		0	0		small

Degrees of freedom Analysis :
Since only difference between the initial component table at this level and the initial component table at the previous level is that $F_{7,M}$ is not a manipulated at this level, the statements about components H, T, B and D at the previous level are still valid. Only row for methane in the Table 9-19 require an update.

With $F_{7,M}$ not being a manipulated variable, either $F_{3,M}$ or $F_{7,M}$ can be a degree of freedom in the optimization. Since $F_{3,M}$ can be directly observed in Φ, we will focus on $F_{3,M}$. Then, $F_{7,M} = f(F_{3,M})$. The status of the rest of the components in the plant has not changed from the previous level. The final component table for the relevant streams at this level is shown in Table 9-24.

Table 9 - 24: Final Component Table for the Detailed Reaction - Expanded Separation System

Component	$F_{3,i}$	$F_{7,i}$	$F_{8,i}$	$F_{13,i}$	$F_{4,i}$	$F_{5,i}$	$F_{6,i}$	$F_{9,i}$
H		√	MV	n/a	n/a	0	0	0
M	√		MV	n/a	MV	0	0	0
T	√	n/a	n/a	√	0	~0	small	MV
B	√		n/a	MV	√	Specified	0	
D	0	0	0		0	0	√	small

Implementing the above specifications gives the following optimization problem:

$$\begin{aligned}\min\ \Phi = {} & c_T F_2 + c_H F_1 - v_H f(F_{7,H}) - v_M F_{3,M} + (p_B - v_B) F_{3,B} - v_T F_{3,T} \\ & + (p_B - v_B) F_{4,B} - (v_M + v_D) F_{6,D} + v_M f(F_{6,D}) - v_T F_{6,T} \\ & + c_{stm} F_{stm\text{-}(e)} + c_{compressor}\end{aligned} \qquad [9\text{-}54]$$

s.t. :

1. $F_{3,i} + F_{7,i} = F_{8,i}$
2. $F_{15,k} + F_{11,k} = F_{16,k}$
3. $F_{1,i} + F_{2,i} + F_{7,i} + F_{9,i} + F_{11,i} = F_{10,i}$
4. Constraints imposed by the compressor and other units in the reactor section

Note that all c_i and v_i are greater than zero. Also, $c_T >> v_T$; $c_{H*} >> v_T$; v_B v_M and v_H are small. Then,

$(p_B - v_B) > 0$. Again, $(F_{3,B} + F_{4,B})$ is the amount of loss of benzene from the process. Minimizing this amount can help to reduce the operating cost. Reducing the usage of F_1 and F_2 minimizes the cost. This can be achieved by minimizing the loss of raw materials in the system, or equivalently, maximizes the recovery of raw materials. Since $f(F_{6,D}) = F_{9,D}$ which is much smaller in magnitude than $F_{6,D}$, then, $v_M f(F_{6,D}) - (v_M + v_D) F_{6,D} < 0$. Increasing the recovery of diphenyl would increase the fuel/resale revenue. As the reactor is exposed, conversion becomes a visible variable for optimization (see the description of a spawning opportunity below). Once the conversion is fixed, the amount of diphenyl generated in the process is no longer a variable. Then, we simply try to recover the by-product from the process to generate fuel/resale revenue. Based on these observations, we can say that Φ can be minimized if we:

1. Reduce the amount of benzene leaving the process.
2. Reduce the loss of raw materials from the process.

At this level, the detailed structure of the entire reaction block is revealed. During process design, the cost optimal conversion in the reactor has been determined to be 0.75. During operation, the actual conversion in the reactor is a function of composition in the feed streams, feed flowrates, reactor inlet temperature and the amount of built-up of coke in the reactor (which changes the reactor volume). At a fixed reactor inlet temperature, the amount of coke in the reactor has a particularly strong effect on the one-pass conversion as it changes the effective reactor volume. Conversion should be maintained at roughly the same level by adjusting the reactor inlet temperature.

In summary, Φ can be minimized if we:

1. Reduce the amount of benzene leaving the process.
2. Reduce the loss of raw materials from the process.
3. Maintain reactor conversion at ~0.75 (*spawning*).

As the internal variables associated with the reactor become observable at this level, a new cost saving opportunity has been identified.

Control Structure at Level 3b

We have summarized the control structure at this level in Table 9-25 and Figure 9-17 and it can be easily verify that it is upwardly compatible with the control structures developed at the earlier levels.

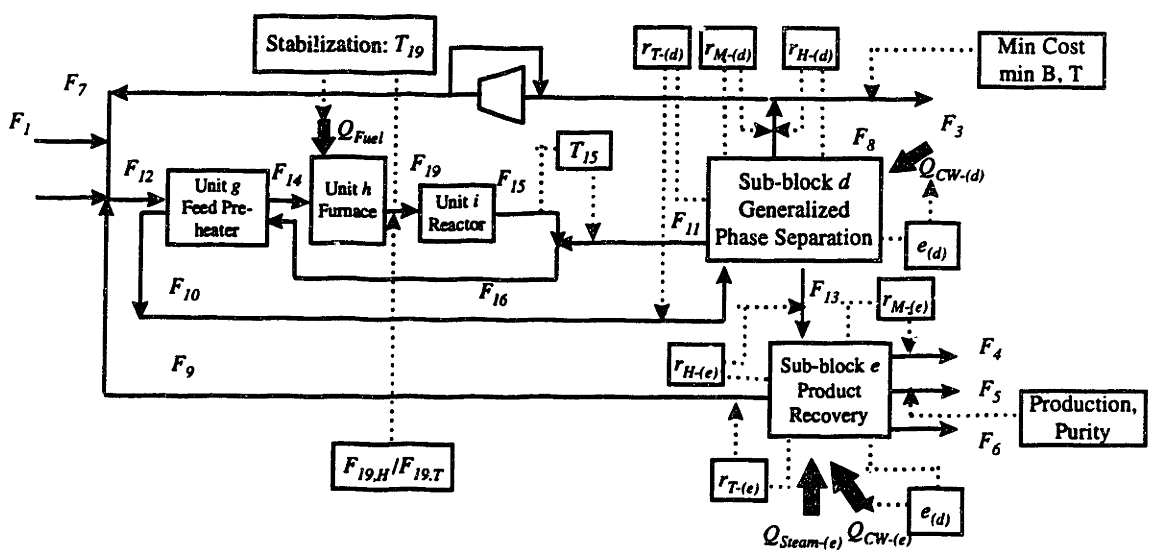


Figure 9 - 17: Control Structure at the Detailed Reaction - Expanded Separation Level

Table 9 - 25: Control Structure at the Detailed Reaction - Expanded Separation Level

Control Objectives		Assignment			
		Furnace Unit *h*	Reactor Unit *i*	Phase-Separator Sub-block *d*	Separation Sub-block *e*
3b-1	T_{19} fixed at 1150 °F or above	Q_{Fuel}			
3b-2	$r_{H\text{-}(d)}$, $r_{H\text{-}(e)}$			$F_{8,H}$	$F_{13,B}$
3b-3	$r_{M\text{-}(d)}$, $r_{M\text{-}(e)}$			$F_{8,M}$	$F_{4,M}$
3b-4	$r_{T\text{-}(d)}$, $r_{T\text{-}(e)}$			$F_{10,P}$	$F_{9,T}$
3b-5	$e_{(d)}$, $e_{(e)}$			$Q_{CW\text{-}(d)}$	$Q_{CW\text{-}(e)}$
3b-6	Production Level				F_5
3b-7	Product Purity				$F_{5,B}$
3b-8	$T_{19} > 1150$ °F	Q_{Fuel}			
3b-9	Reaction mixture < 1300°F		Feeds (override)		
3b-10	$F_{19,H} / F_{19,T} \geq 5$		$F_{19,H}$		
3b-11	Reactor effluent ≤ 1150°F		F_{11}		
3b-12	Minimum Cost		minimize loss of benzene, minimize loss of raw materials, keep conversion of toluene at 0.75		

9.7 Level 3c: Detailed Reaction - Augmented Separation System

At this level, the generalized phase-separation system has been augmented into a phase separator unit and a vapor recovery unit as shown in Figure 9-18. Notice that only a small amount of new information has been revealed in this level. According to the rules developed in Section 8.8.1, re-examination of the process plant may not be warranted. Nevertheless, analysis which must be carried out for the viewpoint shown in Figure 9-18 will be demonstrated. The objectives from the previous level have been allocated to the appropriate units at this level as shown in Table 9-26. The vapor recovery unit (Unit *l*) is not a material capacitor (in fact, a functional unit for vapor recovery is absent in the HDA plant) and sub-system *m* is just a stream divider. The overall material balance control is accomplished by maintaining the levels of material accumulations in Sub-block *k* and Sub-block *e*.

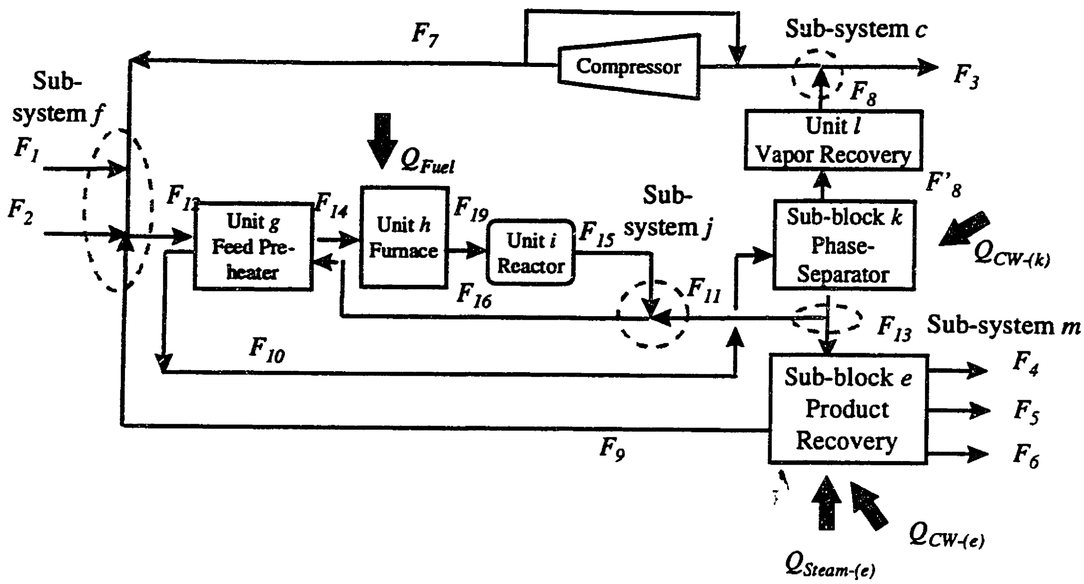


Figure 9 - 18: Process Representation of the Detailed Reaction - Augmented Separation System (Level 3c)

Table 9 - 26: Prioritized Control Objectives at the Detailed-Reaction - Augmented Separation System

	Furnace	Reactor	Phase-Separator	Vapor Recovery	Product Recovery
	Unit h	Unit i	Sub-block k	Unit l	Sub-block e
3c-1	T_{19} fixed at 1150°F or above				
3c-2			$r_{H\text{-}(k)}$		$r_{H\text{-}(e)}$
3c-3			$r_{M\text{-}(k)}$		$r_{M\text{-}(e)}$
3c-4			$r_{T\text{-}(k)}$		$r_{T\text{-}(e)}$
3c-5			$e_{(k)}$		$e_{(e)}$
3c-6					Production Level
3c-7					Product Purity
3c-8	$T_{19} > 1150$ °F (same as 3c-1)				
3c-9		Reacting mixture < 1300 °F			
3c-10		$F_{19,H}/F_{19,T} \geq 5$			
3c-11		reactor effluent ≤ 1150 °F			
3c-12	minimize operating cost				

Verify Feasibility of Control Objectives

At this level, no further refinement has been made on the reactor section but the generalized phase separation has been refined to expose the phase separator in the plant. Although the detailed structure of the phase separator block is not revealed, it is known that vapor-liquid separation is the only process taking place in that area. Hence, the following chemical thermodynamics equilibrium relationships hold:

$$T_8 = T_{11} = T_{13} \qquad [9\text{-}55]$$

$$P_8 = P_{11} = P_{13} \qquad [9\text{-}56]$$

$$y_{8,i} = k^i_{11,13}(P_8, T_8)\, x_{11,i} = k^i_{11,13}(P_8, T_8)\, x_{13,i}$$

i.e. $$\frac{F_{8,i}}{F_8} = k^i_{11,13}(P_8,T_8)\frac{F_{11,i}}{F_{11}} = k^i_{11,13}(P_8,T_8)\frac{F_{13,i}}{F_{13}} \quad [9\text{-}57]$$

These relationships further reduce the degrees of freedom to specify control objectives in the phase separation section. It can be easily verify that our specification of control objective do not violate these constraints.

Synthesize Control Structure at the Detailed Reaction - Augmented Separation Level

The augmentation of the vapor-liquid separation system at this level has resulted in the spun off of a unit which is neither a material nor energy capacitor. F_8 is essentially identical to F_8'. Control assignments for sub-block *d* at the previous level are also the best assignments for Sub-block *k* at this level. Other control assignments should be identical to those developed at Level 3b.

At this level, the vapor-liquid separation block has been refined into a phase-separator and a vapor-recovery unit. The only difference between this level and the previous level is the revelation of the phase-separator. As the control assignments for the plant at this level of representation is essentially identical to the one developed for Level 3b, the modified cost function Φ after substituting the known material balance relationships should be identical to the one given in Equation [9-51]. Additional thermodynamic relationships concerning the phase split such as Equations [9-55], [9-56] and [9-57] apply. Combining these equations with the component balances relating the feed stream and the outlet streams of the phase-separator unit, the following generic thermodynamic relations exist for the phase-separator:

$$f_1(F_{10,i}, (F_{11,i} + F_{13,i}), F_{8,i}) = 0 \quad [9\text{-}58]$$

$$f_2(F_{10,i}, (F_{11,i} + F_{13,i}), F_{8,i}) = 0 \quad [9\text{-}59]$$

$F_{10,i}$, $F_{11,i}$ and $F_{8,i}$ do not appear the objective function Φ defined in [9-53]. Including Equations [9-55], [9-56], [9-58] and [9-59] as additional constraints in the optimization, the new cost-optimization is given by:

$$\min\ \Phi = c_T F_2 + c_H F_1 - v_H f(F_{7,H}) - v_M F_{3,M} + (p_B - v_B) F_{3,B} - v_T F_{3,T} \quad [9\text{-}60]$$
$$+ (p_B - v_B) F_{4,B} - (v_M + v_D) F_{6,D} + v_M f(F_{6,D}) - v_T F_{6,T}$$
$$+ c_{stm} F_{stm\text{-}(e)} + c_{compressor}$$

s.t.:

1. $F_{3,i} + F_{7,i} = F_{8,i}$
2. $F_{15,k} + F_{11,k} = F_{16,k}$
3. $F_{1,i} + F_{2,i} + F_{7,i} + F_{9,i} + F_{11,i} = F_{10,i}$
4. $T_8 = T_{11} = T_{13}$
5. $P_8 = P_{11} = P_{13}$
6. $f_1(F_{10,i}, (F_{11,i} + F_{13,i}), F_{8,i}) = 0$
7. $f_2(F_{10,i}, (F_{11,i} + F_{13,i}), F_{8,i}) = 0$
8. Constraints imposed by the compressor and other units in the reactor section

The process representation as this level shows that the reactor effluent is split into a phase that is rich in light materials (hydrogen, methane) and a phase that is rich in heavy materials (toluene, benzene, diphenyl). The light materials do not undergo further separation in the vapor-recovery block while the heavy materials undergo further processing which allows the recovery of toluene in F_9. To minimize loss of toluene and benzene in the purge, it is advantageous to condense as much heavy materials in the phase-separator as possible until some physical constraints is hit. For cost minimization, the phase separation should be operated at the coldest possible temperature. The temperature of cooling water is expected to vary with the ambient temperature and it is undesirable to pass the variation in the temperature of the coolant to the composition in the feed to the separation section. To minimize composition variation, the phase-separation should be controlled at some low temperature that can always be satisfied by the available coolant (*spawn* a supplementary objective).

In summary, the cost function Φ can be minimized if we:

- reduce the amount of benzene leaving the process
- reduce the loss of raw materials from the process
- maintain reactor conversion at ~0.75 (*spawning*)
- minimize phase separation temperature (*spawning*)

As the temperature and pressure of the phase-separator become visible at this level, we have identified an additional a cost saving opportunity.

Control Structure at Level 3c

The control structure at the detailed reaction-augmented separation level is summarized in Table 9-27 and Figure 9-19. The vapor recovery unit has not been drawn in Figure 9-19 as it does not physically exist in the HDA plant. The control structure at this level is essentially identical to the one developed at the previously level as only a small amount of details has been added to the new representation.

Table 9 - 27: Control Structure at the Detailed Reaction - Augmented Separation Level

	Control Objectives	Assignment: Furnace Unit h	Reactor Unit i	Phase-Separator Unit k	Vapor Recovery Unit l	Separation Sub-block e
3c-1	T_{19} fixed at 1150°F or above	Q_{Fuel}				
3c-2	$r_{H\text{-}(k)}$, $r_{H\text{-}(e)}$			$F_{8,H}$		$F_{13,B}$
3c-3	$r_{M\text{-}(k)}$, $r_{M\text{-}(e)}$			$F_{8,M}$		$F_{4,M}$
3c-4	$r_{T\text{-}(k)}$, $r_{T\text{-}(e)}$			$F_{10,B}$		$F_{9,T}$
3c-5	$e_{(k)}$, $e_{(e)}$			$Q_{CW\text{-}(k)}$		$Q_{CW\text{-}(e)}$
3c-6	Production Level					F_5
3c-7	Product Purity					$F_{5,B}$
3c-8	$T_{19} > 1150$ °F	Q_{Fuel}				
3c-9	Reaction mixture < 1300 °F		Feeds (override)			
3c-10	$F_{19,H} / F_{19,T} \geq 5$		$F_{19,H}$			
3c-11	Reactor effluent ≤ 1150 °F		F_{11}			
3c-12	Minimum Cost	minimize loss of benzene, minimize loss of raw materials, optimize phase separation temperature, keep conversion of toluene at 0.75				

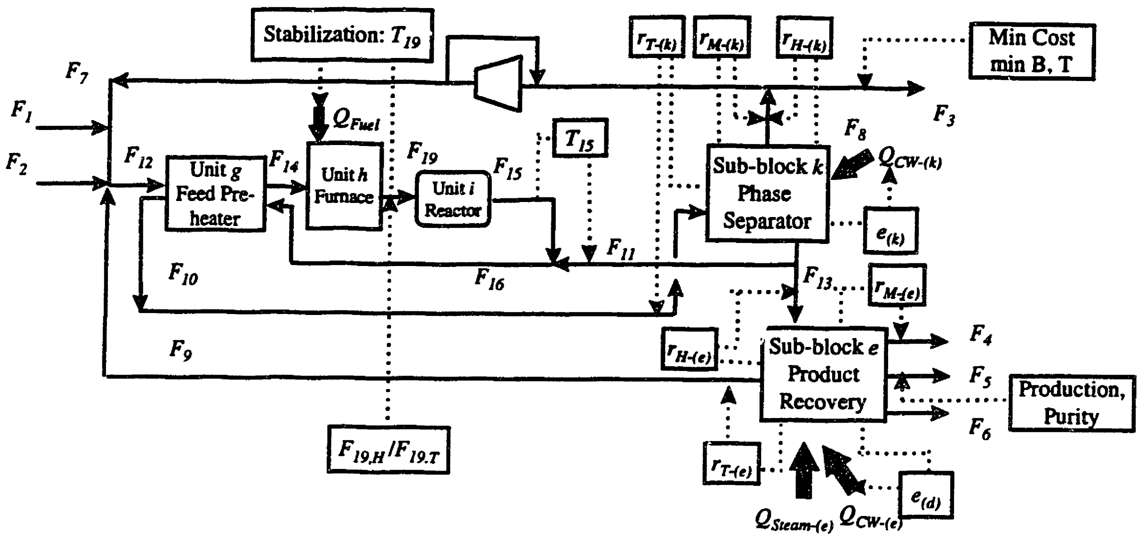


Figure 9 - 19: Control Structure at the Detailed Reaction - Augmented Separation Level

9.8 Level 4: Detailed Plant

As the final step of process refinement, the vapor-liquid separation system and product recovery system are expanded to reveal all the details in the plant. At the detailed level, all the sub-blocks have been refined into specific unit-operations. The final representation is identical to the flowsheet displayed in Figure [9-1]. The control objectives at the previous level are allocated to the appropriate process units and are prioritized in Table 9-28.

At this level, the dominant time constant in each sub-block is essentially the same as the dominant time constant of the unit inside that sub-block, the criterion in Section 8.5 has been met. The dynamics of the process must be incorporated in the analysis and begin Phase II of the design. Short-horizon design criteria discussed in Section 6.3.2 should be employed for the synthesis of the control structure for dynamic process regulation.

Table 9 - 28: Prioritized Control Objectives at the Detailed Level

	Furnace	Reactor	Water Cooler	Flash	Stabilizer	Benzene	Toluene
	Unit *h*	Unit *i*	Unit *n*	Unit *o*	Unit *p*	Unit *q*	Unit *r*
4-1	T_{19} fixed at 1150°F or above						
4-2				$r_{H\text{-}(n)}$	$r_{H\text{-}(o)}$	$r_{H\text{-}(p)}$	$r_{H\text{-}(q)}$
4-3				$r_{M\text{-}(n)}$	$r_{M\text{-}(o)}$	$r_{M\text{-}(p)}$	$r_{M\text{-}(q)}$
4-4				$r_{T\text{-}(n)}$	$r_{T\text{-}(o)}$	$r_{T\text{-}(p)}$	$r_{T\text{-}(q)}$
4-5			$e_{(m)}$		$e_{(o)}$	$e_{(p)}$	$e_{(q)}$
4-6						Production	
4-7						Purity	
4-8	$T_{19} >$ 1150°F						
4-9		Reaction mixture < 1300°F					
4-10		$F_{19,H}/F_{19,T} \geq 5$					
4-11		reactor effluent ≤ 1150°F					
4-12	minimization of operating cost						

9.9 Summary

In this case study the mechanics that are involved in Phase I has been demonstrated. Techniques presented in Chapter 4 to 6 have been applied to synthesize strategies for long-horizon control. It has been identified during Phase I of the design how the key material should flow in the process. From the control structure at Level 3c, maintenance of material balances in the separation area is crucial.

The application of these techniques will be demonstrated once again in the expanded William-Otto plant in Chapter 10. Further development of the control structure at Level 4 of the HDA process for dynamic regulation of specific process outputs must be developed within Phase II of the methodology. The procedure for Phase II of the design will be demonstrated on the Tennessee Eastman Challenge Problem presented in Chapter 11.

Chapter 10
Synthesis of Plant Control Structure for the Expanded William-Otto Plant

10.1 Introduction

In the previous chapter, the details of the mechanics involved during Phase I of methodology for the synthesis of plant-wide control structure have been demonstrated on the HDA plant. In this chapter, the methodology will be demonstrated again on the expanded Williams-Otto Plant (Johnston, R.D., 1985). The key decisions that are made during the synthesis will be explained.

10.2 Preliminary Analysis

10.2.1 Understanding the expanded Williams-Otto Plant

This case study is based on a process flowsheet developed by Johnston, R.D. (1985) which is an expansion of the Williams-Otto (WO) plant (Williams and Otto, 1960). The process flow diagram of the test plant is shown in Figure 10-1. This plant has the same unit operations as the original Williams-Otto plant but with considerably more heat integration and recycle. In this process, hypothetical raw materials A and B combine and react according to the following irreversible and exothermic reactions :

$$\text{(R1) } A+B \rightarrow C$$
$$\text{(R2) } C+B \rightarrow P+E$$
$$\text{(R3) } P+C \rightarrow G$$

G is a heavy oily material which must be disposed of as fuel oil. C and E are by-products and are being processed in a downstream plant (not shown in Figure 1).

The raw material streams F_A and F_B are fed to the water-cooled Reactor 1, together with a recycle from Column 2 which is rich in component B. This reactor operates at 350 °K where C, P, E and G are formed. The hot reactor product is cooled to 311 °K at which temperature the reactor product separates into two layers, the heavy layer being 50% w/w

B and 50% w/w G. All heavy material G passes into the lower layer, which is separated in Decanter 1. The upper layer undergoes further reaction at 360 °K in the steam-heated Reactor 2, with the hot reactor product providing the heating medium for the reboiler of Column 2. This stream is further cooled to 311 °K before passing to Decanter 2 where the heavy material G plus entrained B pass out as a lower layer. The upper layer of Decanter 2 passes to Column 1, the top product of which is 98% w/w P with 60% recovery of P. The separation of product P from the mixture is relatively easy. The base product from Column 1 is, in part, recycled to Reactor 2, with the remainder going to a downstream plant where by-products C and E are being processed. The heavy material from both decanters are combined and fed to Column 2, the purpose of which is to recover component B. The top product of this column (98% w/w B with 95% recovery of B) is combined with pure B feed before passing to Reactor 1. The hot base product from Column 2 is cooled by heat exchange with the distillate before passing to storage (Johnston, R.D.,1985). The steady-state flow rates and temperatures of all streams can be found in Appendix B.1 which have been determined by Johnston, R.D. (1985).

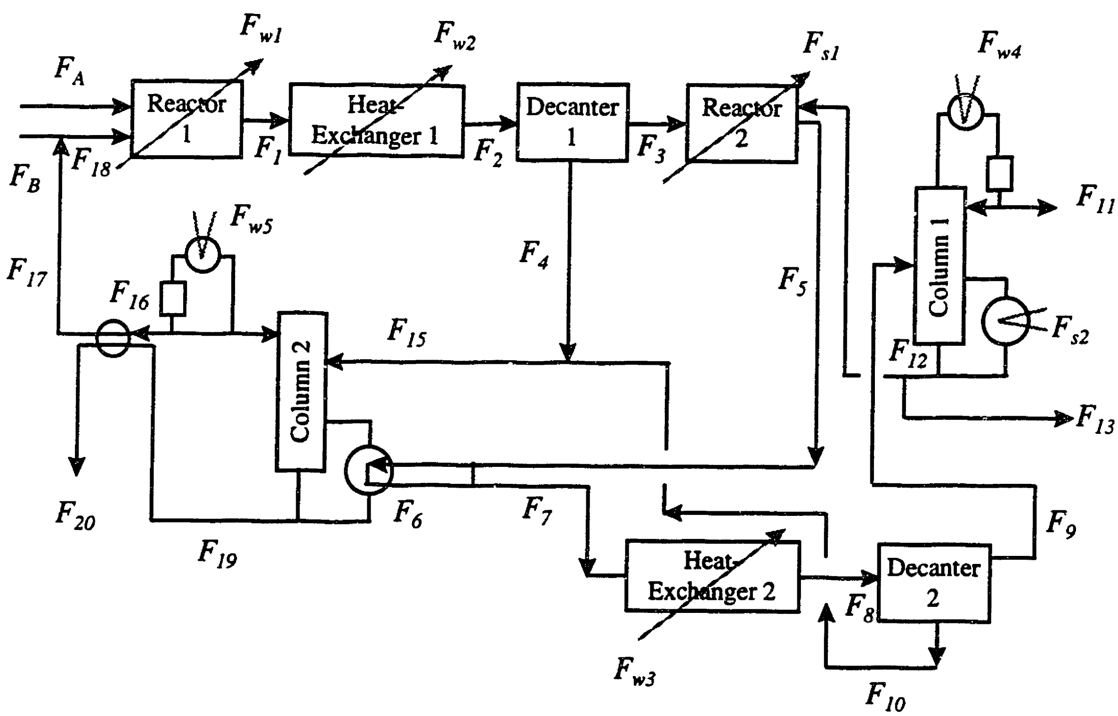


Figure 10 - 1: Process Flowsheet of the Expanded Williams-Otto Plant

The overall objective of the plant is to produce 20,000 tonnes per annum of a high grade (98% pure) product P, with pure A and pure B as the raw materials. There is an operational constraint on the temperatures of the inlet streams of the decanters. For operational feasibility, the temperatures of these streams must be below 100 F (311 °K). The following are some known process disturbances:

1. Wide variations in the condenser cooling water temperature. This limits the capacity of the distillation column in the original plant (Williams and Otto, 1960).
2. Variations in the temperatures of Feeds A and B.

3. Flow variations in Feed A.

10.2.2 The Stability of the Open-loop Process

In the expanded WO plant, The heat-exchangers and decanters in the plant are inherently stable operations. Since the separation of product P from the mixture is easy (Williams and Otto, 1960), the operation of Column 1 should also be stable. Due to lack of information, it will be assumed that B and G are non-azeotropic so that the distillation Column 2 can be assumed to be a stable operation.

The isothermal CSTRs may or may not be stable. The exact nature of this operation can only be detected by means of numerical analysis on the reactor systems. In this case study, for the sake of illustrating the decision making process in control structure synthesis, it will be assumed that the reactors are equipped with sufficient heating and cooling capacities such that they are always internally stable. It was shown in Chapters 7 and 9 that if the reaction is non-autocatlytic, pure material recycle effects will not induce instability in the plant. Thus, it is more interesting to study the instability induced by energy recycle in the interconnected system

Instability Induced by the Energy Recycle Structure

The SDG of the two energy recycle loops in the plant has been drawn in Figure 10-2. H_i refers the rate of heat entering or leaving the system through stream *i*. Consider an increase in H_5 caused by an increase in Q_{s1} (due to increase in the steam temperature). In the open-loop situation, the disturbance causes a chain of events to occur:

1. Increasing H_5 causes an increase in H_6 and H_7. Increase of H_7 increases H_8 and decreases the approach temperature between F_7 and F_{w3} which decreases H_8. Analysis of the pre-heater in Section 9.2.1 indicates that the latter path is indeed the dominant path. Hence, increasing H_7 decreases H_8 and H_9 and H_{14}. Steam F_{14} is recycled back to Reactor 2 and so it causes the temperature of Reactor 2 to decrease. This returns a stabilizing effect to the original increase in temperature. Then, the heat-integrated loop is stable.
2. Increasing H_5 also causes an increase in H_{19}. Since F_{19}, being a hot fluid, always transfer heat to the cold fluid F_{16}. Hence, an increase in H_{19} increases H_{17} which increases H_{18} and eventually causes an increase in H_5. Thus, the original perturbation is reinforced. A positive feedback is created in the heat-integrated loop.

Whether the energy-integration in the plant poses stability problem depends on the relative extents of the effects in the above two cases, as well as how sensitive is the heat of reaction to changes in reaction temperature. Note that one of the operational requirement is to maintain F_2 to be below 311 °K. Once F_2 is maintained at a fixed temperature, the heat-integration loop will always remain stable at all operating state. F_{w2} would naturally be the choice of manipulated variable for this control objective. Without performing a quantitative analysis, we can there assume that the stability of the heat-integrated loop will not pose a problem during dynamic operation of the plant.

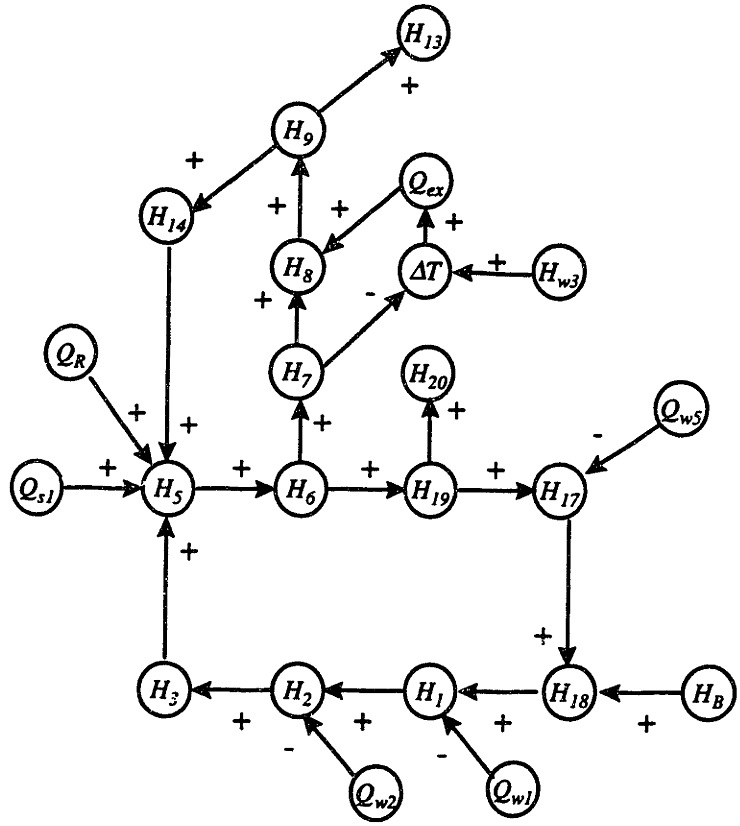


Figure 10 - 2: SDG of the heat-integrated loops in the expanded WO plant

10.2.3 Prioritize Production Objectives

Based on the overall production plan and the operational requirement, the hierarchy of production objectives for this plant are:

1. Maintain the accumulation of materials and energy to be within their specified limits.
2. Maintain the purity of P at or above 98%.
3. Produce P at 20,000 tonnes per annum.
4. Maintain F_2 and F_8 to be below 311 °K.

The logic of the prioritization follows those in Section 9.2.3. The purity of the product is a more important objective for the expanded WO plant because it was specified in the problem statement that high grade material must be produced.

10.3 Level 1: Input-Output Plant

The input-output representation of the expanded WO plant is shown in Figure 10-3. The goal of this stage of the design is to identify a set of control strategies which address control issues observable from the time-horizon corresponding to the representation. Long-horizon design criteria will be employed. The general material and energy balance models have been developed in Appendix B.2. For this plant, there are 6 reactive components (A, B, C, E, P and G), 3 reactions and no inert material. Three independent material balances are required to completely describe the material flows in each block.

Writing material balances for components A, B and P and energy balances will completely define the system.

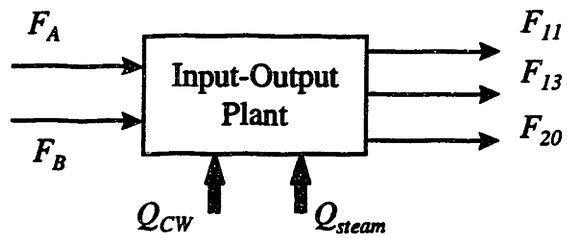


Figure 10 - 3: Input-Output Representation of the Expanded Williams-Otto Plant

Defining and Raking Control Objectives

At the input-output level, the focus is on the objectives which can be defined by variables observable from the process streams which cross the system boundary of the process representation in Figure 10-3. The objectives of relevant at this level, arranged in the order of importance determined during preliminary analysis, are:

1. Maintain the accumulation of materials and energy to be within their specified limits.
2. Maintain the purity of P at or above 98%.
3. Produce P at 20,000 tonnes per annum.

Prioritizing Material and Energy Balance Controls

Recall that the external disturbances coming into the plant are mainly:

- variations in temperatures of coolants and feed streams
- variations in the flowrate of A

The flowrate of F_A is not manipulatable. Since A is the limiting reagent, its variations will have a large impact on the operation of the plant. Thus, the maintenance of the inventory of A-based materials is the most important objective. Then, the maintenance of the inventory of B-based materials should follow as these materials are present in the entire plant. The set of objectives which are relevant at this level have been prioritized and summarized in Table 10-1. An objective that has been assigned priority level *i-j* means that it is an objective of priority *j* at level *i*.

Table 10 - 1: Prioritized Control Objectives at the Input-Output Level

1-1	Maintain material balance control of A in the input-output plant (r_A)
1-2	Maintain material balance control of B in the input-output plant (r_B)
1-3	Maintain material balance control of P in the input-output plant (r_P)
1-4	Maintain energy balance control in the input-output plant (e)
1-5	Maintain product purity at or above 0.98
1-6	Maintain P flow at the desired production level

Verify Feasibility of Control Objectives

In this process, the flowrate of F_A is not manipulatable. Then, at a fixed conversion, reaction selectivity, and the degree of product purification, the amount of P is fixed (for reason similar to the methanol system studied in Section 7.3.3 whose feeds are also not manipulatable). It is expected that there may be problem in trying to satisfy objective 1-6

Quantify the Long-horizon Process Behavior

During Phase I of the design, all flow components in the streams that cross the system boundary are considered to be manipulated variables, with the exception of those in the feed streams. Compositions in the feed stream are defined externally. Manipulation of component flows are therefore not feasible in feed streams. In addition, F_A is not manipulatable. The open-loop gains of the residuals of the material balance equations have been computed using the procedure described in Section 5.2.2 and are compiled in Table 10-2. Since flow valves information is not available, the gain estimates can be obtained by perturbing each manipulated input by 1% of its nominal steady-state flow.

For the this plant, it is assumed that the base case is the sole operating point expected for the plant. During Phase I of the design, gains of the residuals of material balance equations are estimated from the principle of conservation and can therefore be assumed to be accurate for the operating point of interest.

Table 10 - 2: Open-loop Gains of Residuals at the Input-Output Level

	r_A	r_B	r_P
$F_{11,A}$	-0.0054	0	0
$F_{11,C}$	0	0	0
$F_{11,E}$	0	0	0
$F_{11,G}$	0	0	0
$F_{13,A}$	-0.0854	0	0
$F_{13,C}$	-0.0083	-0.0083	0
$F_{13,E}$	-0.4511	-0.9022	0.4511
$F_{13,G}$	0	0	0
$F_{20,A}$	0	0	0
$F_{20,C}$	0	0	0
$F_{20,E}$	0	0	0
$F_{20,G}$	-0.1074	-0.1074	-0.1074
F_B	0	1.4	0
$F_{11,B}$	0	0	0
$F_{13,B}$	0	-0.3655	0
$F_{20,B}$	0	-0.0164	0
$F_{11,P}$	0	0	-0.2644
$F_{13,P}$	0	0	-0.0793
$F_{20,P}$	0	0	0

Synthesize Control Structure for the Input-Output Plant

A control structure that is suitable for maintaining the plant in the long-horizon at the nominal steady-state will be synthesized within the modular multiobjective design framework described in Chapter 6. Primary manipulated variables are assigned to the hierarchy of process objectives, sequentially, starting from the most important one.

Goal 1-1: Maintain r_A

Based on the size of the gains, $F_{13,E}$ is clearly the best choice (F_{13} is the by-product stream).

Goal 1-2: Maintain r_B

The closed-loop gain of r_B with r_A being maintained by $F_{13,E}$ are shown in Table 10-4. F_B, the feed stream to the system, is the best manipulated variable for the control of the inventory of B in the system.

Goal 1-3: Maintain r_P

From Table 10-4, both $F_{11,P}$ and $F_{20,G}$ have very large gains. However, using $F_{11,P}$ will divert variations to the purity of the product P. $F_{20,G}$ is the best choice.

Goal 1-4: Maintain e

Anyone of the utility stream can be used to maintain the energy accumulation of the plant at constant level. Since cooling water is a cheaper utility than steam, Q_{cw} is assigned to maintain *e*.

Goal 1-5: Maintain the purity of P at or above 98%.

Varying $F_{11,P}$ changes the purity of P in the product stream.

Goal 1-6: Produce P at 20,000 tonnes per annum

As mentioned in the previous section, with F_A, the limiting raw material, being a non-manipulatable variable, the production rate of the process cannot be fixed at arbitrary value. In order to maintain production rate at the desired level, internal variables such as reactor conversion, reaction temperature or reaction volume, must be adjusted so as to minimize the deviation of F_{11} from the desired value. None of the aforementioned variables are observable from the input-output representation. Thus, a control strategy cannot be developed at this point.

Table 10 - 3: Closed-loop Gains of Residuals at the Input-Output Level

	r_A	r_B	r_P
$F_{11,A}$	-0.0054	0.0108	-0.0054
$F_{11,C}$	0	0	0
$F_{11,E}$	0	0	0
$F_{11,G}$	0	0	0
$F_{13,A}$	-0.0854	0.1707	-0.0853
$F_{13,C}$	-0.0083	0.0083	-0.0083
$F_{13,E}$	-0.4511	0	0
$F_{13,G}$	0	0	0
$F_{20,A}$	0	0	0
$F_{20,C}$	0	0	0
$F_{20,E}$	0	0	0
$F_{20,G}$	-0.1074	0.1074	-0.2149
F_B	0	1.4	0
$F_{11,B}$	0	0	0
$F_{13,B}$	0	-0.3655	0
$F_{20,B}$	0	-0.0164	0
$F_{11,P}$	0	0	-0.2644
$F_{13,P}$	0	0	-0.0793
$F_{20,P}$	0	0	0

Control Structure at Level 1

The control structure at the input-output level (Level 1) is summarized in Table 10-5 and the control configuration is drawn in Figure 10-4. Control objectives are being maintained by adjusting variables which are observable from the streams that cross the system boundary defining this level. These control associations are notional in nature and will be refined into more specific control strategies later in the design.

Table 10 - 4: Control Structure at the Input-Output Level

Control Objectives		Assignment Input-Output Plant
1-1	r_A	$F_{13,E}$
1-2	r_B	F_B
1-3	r_P	$F_{20,G}$
1-4	e	F_{w3}
1-5	Product Purity	$F_{11,P}$
1-6	Production Level	*Cannot be determined*

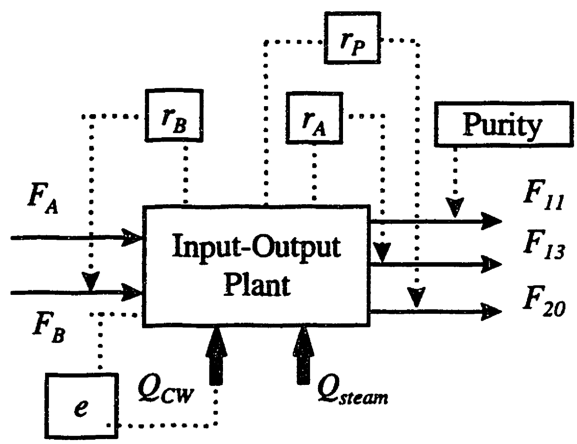


Figure 10 - 4: Control Structure of the Expanded WO plant at Level 1

10.4 Level 2: Generalized Reaction-Separation System

Moving down to Level 2 of the hierarchy of representations, more details about the plant are incorporated. A control structure that is suitable for the new representation is to be developed. The representation at Level 2 is shown in Figure 10-5. The plant is segregated into a generalized reaction section (sub-block *a*) and a generalized separation section (sub-block *b*). Since the dominant time constants of the sub-blocks are much slower than the faster dynamics within the sub-blocks, long-horizon design criteria will be used to synthesize the control structure for this level. The material and energy balance model corresponding to this level of representation can be found in Appendix B.2.

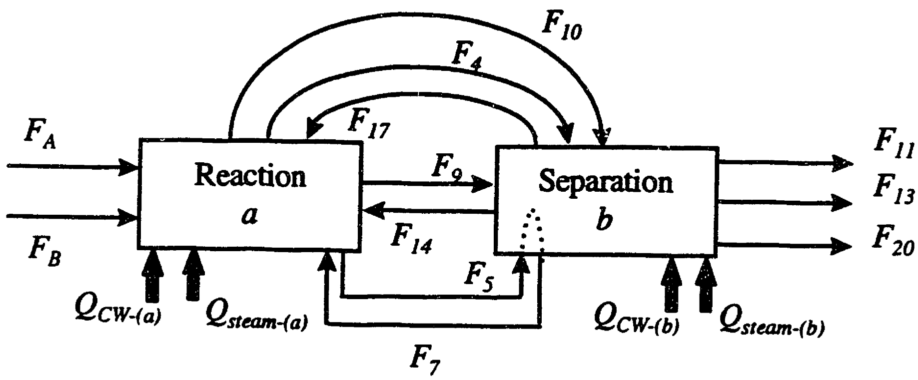


Figure 10 - 5: Level 2: Generalized Reaction-Separation System

Progressive Generation of Control Objectives

The control objectives from the previous level which are associated with the overall production plan are have been used to define control objectives at the refined level as shown in Table 10-5. The symbol $r_{i\text{-}(j)}$ is used to denote a material balance control objective for component i in sub-system j; $e_{(j)}$ to denote an energy balance control objective for sub-system j. Specific objectives which are observable from process streams at the input-output level are also allocated directly to the corresponding process streams at the lower level. Each objective related to material or energy balance control has been *translated* and *refined* into two separable control objectives. The priorities of the maintenance of material balance of a component are of equal importance. No new objective from the list given in Section 10.2 has become observable at this level. The prioritization of the control objectives developed at the earlier stages has been maintained.

At this level, objectives can only be defined in terms of the variables in the process streams which cross the system boundary, further refinement of these objectives, except for the cost optimization objective, is not possible. No spawning opportunities have been identified.

Table 10 - 5: Prioritized Control Objectives at the Generalized Reaction-Separation Level

	Reaction Sub-block *a*	Separation Sub-block *b*
2-1	$r_{A\text{-}(a)}$	$r_{A\text{-}(b)}$
2-2	$r_{B\text{-}(a)}$	$r_{B\text{-}(b)}$
2-3	$r_{P\text{-}(a)}$	$r_{P\text{-}(b)}$
2-4	$e_{(a)}$	$e_{(b)}$
2-5		Product Purity
2-6		Production Level

Verify Feasibility of Control Objectives

Again, as flowrate of F_A is not manipulatable the inability to maintain the production level at any pre-specified value will be carried to Level 2.

Quantifying the Long-Horizon Process Behavior at Level 2

The open-loop gains of the material accumulations caused by a 1% change in various feed flows or component flows observable at Level 2 have been computed and summarized in Table 10-6. Again, since there is only one known operating point, the gains can be assumed to be precise and there is no model uncertainty caused by a change in operating region.

Table 10 - 6: Open-loop Gains or Residuals At Level 2

	$r_{A-(a)}$	$r_{A-(b)}$	$r_{B-(a)}$	$r_{B-(b)}$	$r_{P-(a)}$	$r_{P-(b)}$
$F_{11,A}$	0	-0.0054	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{13,A}$	0	-0.0854	0	0	0	0
$F_{13,C}$	0	-0.0083	0	-0.0083	0	0
$F_{13,E}$	0	-0.4511	0	-0.9022	0	0.4511
$F_{13,G}$	0	0	0	0	0	0
$F_{20,A}$	0	0	0	0	0	0
$F_{20,C}$	0	0	0	0	0	0
$F_{20,E}$	0	0	0	0	0	0
$F_{20,G}$	0	-0.1074	0	-0.1074	0	-0.1074
F_{B}	0	0	1.4	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{13,B}$	0	0	0	-0.3655	0	0
$F_{20,B}$	0	0	0	-0.0164	0	0
$F_{11,P}$	0	0	0	0	0	-0.2644
$F_{13,P}$	0	0	0	0	0	-0.0793
$F_{20,P}$	0	0	0	0	0	0
$F_{9,A}$	-0.1951	0.1951	0	0	0	0
$F_{9,C}$	-0.0185	0.0185	-0.0185	0.0185	0	0
$F_{9,E}$	-1.0025	1.0025	-2.0050	2.0050	1.0025	-1.0025
$F_{9,G}$	0	0	0	0	0	0
$F_{4,A}$	0	0	0	0	0	0
$F_{4,C}$	0	0	0	0	0	0
$F_{4,E}$	0	0	0	0	0	0
$F_{4,G}$	-0.0635	0.0635	-0.0635	0.0635	-0.0635	0.0635
$F_{14,A}$	0.1043	-0.1043	0	0	0	0
$F_{14,C}$	0.0102	-0.0102	0.0102	-0.0102	0	0
$F_{14,E}$	0.5513	-0.5513	1.1027	-1.1027	-0.5513	0.5513
$F_{14,G}$	0	0	0	0	0	0
$F_{17,A}$	0	0	0	0	0	0
$F_{17,C}$	0	0	0	0	0	0
$F_{17,E}$	0	0	0	0	0	0
$F_{17,G}$	0.0021	-0.0021	0.0021	-0.0021	0.0021	-0.0021
$F_{9,B}$	0	0	-0.8121	0.8121	0	0
$F_{4,B}$	0	0	-0.1906	0.1906	0	0
$F_{14,B}$	0	0	0.4467	-0.4467	0	0
$F_{17,B}$	0	0	0.3122	-0.3122	0	0
$F_{9,P}$	0	0	0	0	-0.4408	0.4408
$F_{4,P}$	0	0	0	0	0	0
$F_{14,P}$	0	0	0	0	0.0969	-0.0969
$F_{17,P}$	0	0	0	0	0	0
$F_{10,A}$	0	0	0	0	0	0
$F_{10,C}$	0	0	0	0	0	0
$F_{10,E}$	0	0	0	0	0	0
$F_{10,G}$	-0.0460	0.0460	-0.0460	0.0460	-0.0460	0.0460
$F_{10,B}$	0	0	-0.1381	0.1381	0	0
$F_{10,P}$	0	0	0	0	0	0

Synthesize Control Structure for the Generalized Reaction-Separation System

The *Consistency Logic Map* discussed in the previous chapter will be followed throughout the development. All component flows, except those in the feed streams, are potential manipulated variables. F_A is not a manipulatable variable.

Goal 2-1: Maintain material balance control of A

At the previous level, $F_{13,E}$ was assigned to maintain the overall material balance of A in the process. This manipulated variable is observable from sub-block b at Level 2. Then, based on the *Consistency Logic Map* (Chapter 8), $F_{13,E}$ and the newly available manipulated variables such as the component flows in F_9, F_{14}, F_{17}, F_4 and F_{10} are possible primary manipulated variable for the maintenance of $r_{A\text{-}(b)}$. F_5 and F_7 are merely involved in heat-integration with no material transfer. Component flows in these streams have no real impact on the material balances in the two sub-block. For $r_{A\text{-}(a)}$, any inputs are potential manipulated variables. In other words:

1. $r_{A\text{-}(a)}$: {all manipulated variables}
2. $r_{A\text{-}(b)}$: {component flows of F_{13}, F_9, F_5, F_7, F_{14}, F_{17}, F_4 and F_{10}}

Based on the open-loop gains for the two residuals in Table 10-6, $F_{9,E}$, with the largest gain, is the best manipulated variable for $r_{A\text{-}(a)}$. For $r_{A\text{-}(b)}$, both $F_{14,E}$ and $F_{13,E}$ are potential inputs. However, with $F_{13,E}$ being an outlet stream, disturbances can be quickly diverted to the environment if $F_{13,E}$ is used to maintain $r_{A\text{-}(b)}$. Thus, $F_{13,E}$ is the preferred choice. It can be easily verified that our assignments do not have any conflict under closed-loop control.

Goal 2-2: Maintain material balance control of B

The closed-loop gains of $r_{B\text{-}(a)}$ and $r_{B\text{-}(b)}$ while $r_{A\text{-}(a)}$ and $r_{A\text{-}(b)}$ are under closed-loop control have been computed and shown in Columns 1 and 2 of Table 10-7. F_B was assigned to r_B at Level 1. The sets of possible manipulated variables are:

1. $r_{B\text{-}(a)}$: { component flows of F_B, F_9, F_{14}, F_{17}, F_4 and F_{10}}
2. $r_{B\text{-}(b)}$: { all manipulated variables }

Based on the gains in Table 10-7, F_B is clearly the best choice for $r_{B\text{-}(a)}$. For $r_{B\text{-}(b)}$, $F_{9,B}$ has the largest gain, followed by $F_{14,B}$ and $F_{9,A}$. Since none of these inputs serve the purpose of transferring disturbances directly to the environment, we will assign $r_{B\text{-}(b)}$ to an input with the biggest gain, i.e. $F_{9,B}$. Column 3 in Table 10-7 verifies that this assignment is feasible under closed-loop control.

Goal 2-3: Maintain material balance control of P

The closed-loop gain of $r_{P\text{-}(a)}$ and $r_{P\text{-}(b)}$ are shown in Columns 4 and 5 of Table 10-7. $F_{11,P}$ was assigned to r_P at Level 1The sets of potential manipulated variables are:

1. $r_{P\text{-}(a)}$: {all manipulated variables}
2. $r_{P\text{-}(b)}$: {component flows of F_{20}, F_9, F_{14}, F_{17}, F_4 and F_{10}}

Clearly, $F_{9,P}$ is the best choice for $r_{P\text{-}(a)}$ and $F_{20,G}$ the best choice for $r_{P\text{-}(b)}$. The feasibility of these assignments are verified in Column 6 of Table 10-7.

Goal 2-4: Maintain energy balance control

Again, anyone of the utility stream can be used to maintain the energy accumulation of the plant at constant level. $Q_{cw\text{-}(a)}$ will be assigned to maintain $e_{(a)}$ and $Q_{cw\text{-}(b)}$ to $e_{(b)}$.

Goal 2-5: Maintain the purity of P at or above 98%.

Varying $F_{11,P}$ changes the purity of P in the product stream.

Goal 2-6: Produce P at 20,000 tonnes per annum

As concluded at Level 1, with F_A, the limiting raw material, being a non-manipulatable variable, the production rate of the process cannot be fixed at arbitrary value. It cannot be determined at this point how internal variables, such as reactor conversion, can be adjusted to minimize deviation from the desired production level.

Table 10 - 7: Closed-loop Gains of Residuals At Level 2

	$r_{B\text{-}(a)}$	$r_{B\text{-}(b)}$	$r_{B\text{-}(b)}$ closed-loop	$r_{P\text{-}(a)}$	$r_{P\text{-}(b)}$	$r_{P\text{-}(b)}$ closed-loop
$F_{11,A}$	0	0.0108	0.0108	0	-0.0054	-0.0054
$F_{11,C}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{13,A}$	0	0.1707	0.1707	0	-0.0854	-0.0854
$F_{13,C}$	0	0.0083	0.0083	0	-0.0083	-0.0083
$F_{13,E}$	0	0	0	0	0	0
$F_{13,G}$	0	0	0	0	0	0
$F_{20,A}$	0	0	0	0	0	0
$F_{20,C}$	0	0	0	0	0	0
$F_{20,E}$	0	0	0	0	0	0
$F_{20,G}$	0	0.1074	0.1074	0	-0.2149	-0.2149
F_{B}	1.4	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{13,B}$	0	-0.3655	-0.3655	0	0	0
$F_{20,B}$	0	-0.0164	-0.0164	0	0	0
$F_{11,P}$	0	0	0	0	-0.2644	-0.2644
$F_{13,P}$	0	0	0	0	-0.0793	-0.0793
$F_{20,P}$	0	0	0	0	0	0
$F_{9,A}$	0.3902	-0.3902	-0.3902	-0.1951	0.1951	0
$F_{9,C}$	0.0185	-0.0185	-0.0185	-0.0185	0.0185	0
$F_{9,E}$	0	0	0	0	0	0
$F_{9,G}$	0	0	0	0	0	0
$F_{4,A}$	0	0	0	0	0	0
$F_{4,C}$	0	0	0	0	0	0
$F_{4,E}$	0	0	0	0	0	0
$F_{4,G}$	0.0635	-0.0635	-0.0635	-0.1271	0.1271	0
$F_{14,A}$	-0.2086	0.2086	0.2086	0.1043	-0.1043	0
$F_{14,C}$	-0.0102	0.0102	0.0102	0.0102	-0.0102	0
$F_{14,E}$	0	0	0	0	0	0
$F_{14,G}$	0	0	0	0	0	0
$F_{17,A}$	0	0	0	0	0	0
$F_{17,C}$	0	0	0	0	0	0
$F_{17,E}$	0	0	0	0	0	0
$F_{17,G}$	-0.0021	0.0021	0.0021	0.0042	-0.0042	0
$F_{9,B}$	-0.8121	0.8121	0.8121	0	0	0
$F_{4,B}$	-0.1906	0.1906	0.1906	0	0	0
$F_{14,B}$	0.4467	-0.4467	-0.4467	0	0	0
$F_{17,B}$	0.3122	-0.3122	-0.3122	0	0	0
$F_{9,P}$	0	0	0	-0.4408	0.4408	0
$F_{4,P}$	0	0	0	0	0	0
$F_{14,P}$	0	0	0	0.0969	-0.0969	0
$F_{17,P}$	0	0	0	0	0	0
$F_{10,A}$	0	0	0	0	0	0
$F_{10,C}$	0	0	0	0	0	0
$F_{10,E}$	0	0	0	0	0	0
$F_{10,G}$	0.046	-0.046	-0.046	-0.0921	0.0921	0
$F_{10,B}$	-0.1381	0.1381	0.1381	0	0	0
$F_{10,P}$	0	0	0	0	0	0

Control Structure at Level 2

The control structure that is suitable for the process representation at Level 2 is shown in Figure 10-6 and the control strategies are being summarized in Table 10-8. Abstraction of the control strategies produces the control strategies at Level 1. Control strategies developed at this level are upwardly compatible with decisions made at Level 1.

Table 10 - 8: Control Structure at the Generalized Reaction-Separation level

Control Objectives		Assignment	
		Reaction Sub-block *a*	Separation Sub-block *b*
2-1	$r_{A\text{-}(a)}$ and $r_{A\text{-}(b)}$	$F_{9,E}$	$F_{13,E}$
2-2	$r_{B\text{-}(a)}$ and $r_{B\text{-}(b)}$	F_B	$F_{9,B}$
2-3	$r_{P\text{-}(a)}$ and $r_{P\text{-}(b)}$	$F_{9,P}$	$F_{20,G}$
2-4	$e_{(a)}$ and $e_{(b)}$	$Q_{cw\text{-}(a)}$	$Q_{cw\text{-}(b)}$
2-5	Product Purity		$F_{11,P}$
2-6	Production Level		*cannot be determined*

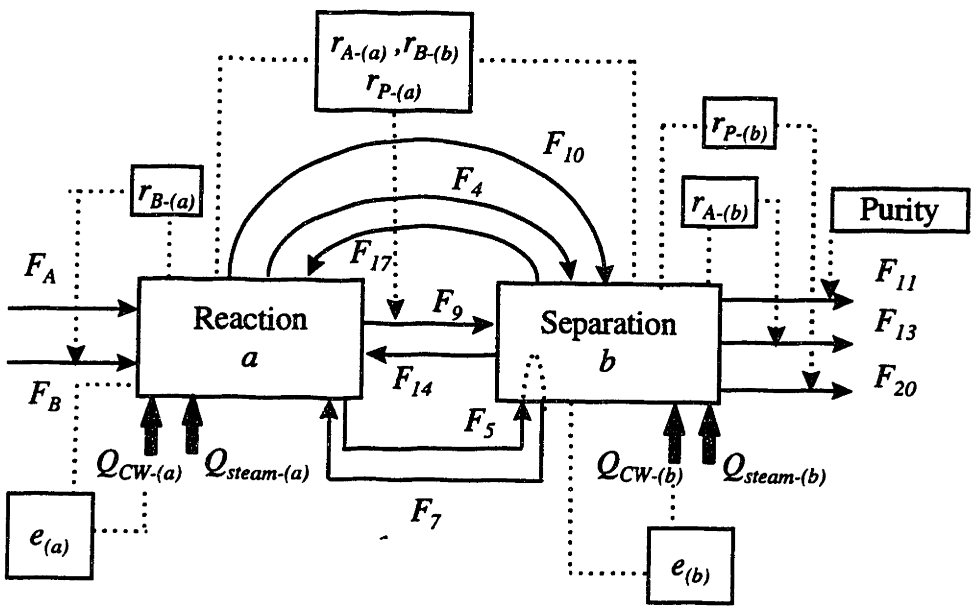


Figure 10 - 6: Control Structure at Level 2

10.5 Level 3: Expanded Generalized Reaction-Separation System

Moving down to Level 3 of the hierarchy of representations, the generalized reaction block is divided into to two reaction blocks (sub-blocks *d* and *e*) as shown in Figure 10-7. The mixer in sub-block *c* does not allow material or energy to accumulate. Feedback control is not required in that block. Since the dominant time constants of the sub-blocks are much slower than the faster dynamics within the sub-blocks, long-horizon design criteria will be used to synthesize the control structure for this level. The material and energy balance model corresponding to this level of representation can be found in Appendix B.2.

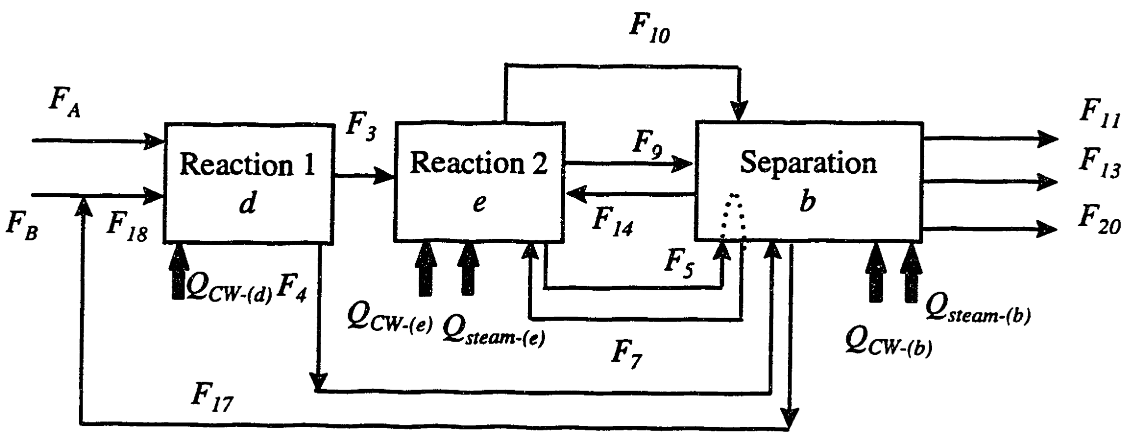


Figure 10 - 7: Level 3: Expanded Generalized Reaction-Separation System

Progressive Generation of Control Objectives

The control objectives from the previous level which are associated with the overall production plan are have been used to define control objectives at the refined level as shown in Table 10-9. Specific objectives which are observable from process streams at the input-output level are also allocated directly to the corresponding process streams at the lower level. Each objective related to material or energy balance control has been *translated* and *refined* into two separable control objectives. The priorities of the maintenance of material balance of a component are of equal importance. No new objectives from the list given in Section 10.2 have become observable at this level. The prioritization of the control objectives developed at the earlier stages has been maintained.

Table 10 - 9: Prioritized Control Objectives at the Generalized Reaction-Separation Level

	Reaction 1 Sub-block *d*	Reaction 1 Sub-block *e*	Separation Sub-block *b*
3-1	$r_{A\text{-}(a)}$	$r_{A\text{-}(e)}$	$r_{A\text{-}(b)}$
3-2	$r_{B\text{-}(a)}$	$r_{B\text{-}(e)}$	$r_{B\text{-}(b)}$
3-3	$r_{P\text{-}(a)}$	$r_{P\text{-}(e)}$	$r_{P\text{-}(b)}$
3-4	$e_{(a)}$	$e_{(e)}$	$e_{(b)}$
3-5			Product Purity
3-6			Production Level

At this level, objectives can only be defined in terms of the variables in the process streams which cross the system boundary, further refinement of these objectives is not possible. No spawning opportunities have been identified.

Verify Feasibility of Control Objectives

Again, as flowrate of F_A is not manipulatable the inability to maintain the production level at pre-specified value will be carried to Level 3.

Quantifying the Long-Horizon Process Behavior at Level 3

The open-loop gains of the material accumulations caused by a 1% change in various feed flows or component flows observable at Level 2 have been computed and summarized in Table 10-10. Again, since there is only one known operating point, the gains can be assumed to be precise and there is no model uncertainty caused by a change in operating region.

Synthesize Control Structure at the Expanded Generalized Reaction - Separation Level

As process refinement from the previously level has been confined to the generalized reaction section, the modification of control structure will occur in the reaction area.

Goal 3-1: Maintain material balance of A

At Level 2, we assigned $F_{9,E}$ and $F_{13,E}$ to $r_{A\text{-}(a)}$ and $r_{A\text{-}(b)}$ respectively. Since sub-block *b* has not undergone any refinement, it is expected that $F_{13,E}$ will remain to be the best choice for $r_{A\text{-}(b)}$. For the sub-blocks in the reaction area, since $F_{9,E}$ is directly linked to sub-block *e*, it is expected that $F_{9,E}$ will be among the best manipulated variable for that sub-block, along with other new observable manipulated variables, such as F_3.

1. $r_{A\text{-}(d)}$: {all manipulated variables}
2. $r_{A\text{-}(e)}$: { component flows in F_9, F_3}

3. $r_{A\text{-}(b)}$: $\{F_{13,E}\}$

Judging from Column 1 in Table 10-10, $F_{3,E}$ and $F_{3,A}$ are both promising candidates for the maintenance of $r_{A\text{-}(d)}$. Since the gain of $F_{3,E}$ is bigger so we assign this manipulated variable to $r_{A\text{-}(d)}$. $F_{9,E}$ and $F_{13,E}$ are clearly the best inputs for $r_{A\text{-}(e)}$ and $r_{A\text{-}(b)}$ respectively. It can be easily verified that these selections are feasible under closed-loop control.

Table 10 - 10: Open-loop gains of residuals at Level 3

	$r_{A-(d)}$	$r_{A-(e)}$	$r_{A-(b)}$	$r_{B-(d)}$	$r_{B-(e)}$	$r_{B-(b)}$	$r_{P-(d)}$	$r_{P-(e)}$	$r_{P-(b)}$
$F_{11,A}$	0	0	-0.0054	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0	0	0	0
$F_{13,A}$	0	0	-0.0854	0	0	0	0	0	0
$F_{13,C}$	0	0	-0.0083	0	0	-0.0083	0	0	0
$F_{13,E}$	0	0	-0.4511	0	0	-0.9022	0	0	0.4511
$F_{13,G}$	0	0	0	0	0	0	0	0	0
$F_{20,A}$	0	0	0	0	0	0	0	0	0
$F_{20,C}$	0	0	0	0	0	0	0	0	0
$F_{20,E}$	0	0	0	0	0	0	0	0	0
$F_{20,G}$	0	0	-0.1074	0	0	-0.1074	0	0	-0.1074
F_{B}	0	0	0	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0	0	0	0
$F_{13,B}$	0	0	0	0	0	-0.3655	0	0	0
$F_{20,B}$	0	0	0	0	0	-0.0164	0	0	0
$F_{11,P}$	0	0	0	0	0	0	0	0	-0.2644
$F_{13,P}$	0	0	0	0	0	0	0	0	-0.0793
$F_{20,P}$	0	0	0	0	0	0	0	0	0
$F_{9,A}$	0	-0.1951	0.1951	0	0	0	0	0	0
$F_{9,C}$	0	-0.0185	0.0185	0	-0.0185	0.0185	0	0	0
$F_{9,E}$	0	-1.0025	1.0025	0	-2.0050	2.0050	0	1.0025	-1.0025
$F_{9,G}$	0	0	0	0	0	0	0	0	0
$F_{4,A}$	0	0	0	0	0	0	0	0	0
$F_{4,C}$	0	0	0	0	0	0	0	0	0
$F_{4,E}$	0	0	0	0	0	0	0	0	0
$F_{4,G}$	-0.0635	0	0.0635	-0.0635	0	0.0635	-0.0635	0	0.0635
$F_{14,A}$	0	0.1043	-0.1043	0	0	0	0	0	0
$F_{14,C}$	0	0.0102	-0.0102	0	0.0102	-0.0102	0	0	0
$F_{14,E}$	0	0.5513	-0.5513	0	1.1027	-1.1027	0	-0.5513	0.5513
$F_{14,G}$	0	0	0	0	0	0	0	0	0
$F_{17,A}$	0	0	0	0	0	0	0	0	0
$F_{17,C}$	0	0	0	0	0	0	0	0	0
$F_{17,E}$	0	0	0	0	0	0	0	0	0
$F_{17,G}$	0	0	-0.0021	0	0	-0.0021	0	0	-0.0021
$F_{9,B}$	0	0	0	0	-0.8121	0.8121	0	0	0
$F_{4,B}$	0	0	0	-0.1906	0	0.1906	0	0	0
$F_{14,B}$	0	0	0	0	0.4467	-0.4467	0	0	0
$F_{17,B}$	0	0	0	0	0	-0.3122	0	0	0
$F_{9,P}$	0	0	0	0	0	0	0	-0.4408	0.4408
$F_{4,P}$	0	0	0	0	0	0	0	0	0
$F_{14,P}$	0	0	0	0	0	0	0	0.0969	-0.0969
$F_{17,P}$	0	0	0	0	0	0	0	0	0
$F_{10,A}$	0	0	0	0	0	0	0	0	0
$F_{10,C}$	0	0	0	0	0	0	0	0	0
$F_{10,E}$	0	0	0	0	0	0	0	0	0
$F_{10,G}$	0	-0.0460	0.0460	0	-0.0460	0.0460	0	-0.0460	0.0460
$F_{10,B}$	0	0	0	0	-0.1381	0.1381	0	0	0
$F_{10,P}$	0	0	0	0	0	0	0	0	0
$F_{18,A}$	0	0	0	0	0	0	0	0	0
$F_{18,C}$	0	0	0	0	0	0	0	0	0
$F_{18,E}$	0	0	0	0	0	0	0	0	0
$F_{18,G}$	0.0021	0	0	0.0021	0	0	0.0021	0	0
$F_{18,B}$	0	0	0	1.712261	0	0	0	0	0
$F_{18,P}$	0	0	0	0	0	0	0	0	0
$F_{3,A}$	-0.2396	0.2396	0	0	0	0	0	0	0
$F_{3,C}$	-0.0255	0.0255	0	-0.0255	0.0255	0	0	0	0
$F_{3,E}$	-0.3311	0.3311	0	-0.6621	0.6621	0	0.3311	-0.3311	0
$F_{3,G}$	0	0	0	0	0	0	0	0	0
$F_{3,B}$	0	0	0	-0.7727	0.7727	0	0	0	0
$F_{3,P}$	0	0	0	0	0	0	-0.2695	0.2695	0

Goal 3-2: Maintain material balance of B

At Level 2, F_B and $F_{9,B}$ are used to maintain the material balance of B. At this level, F_B is not directly linked to any of the sub-blocks in the reactor area. However, since sub-block *c* is self-regulating. Changing F_B must necessarily change F_{18}. Hence, F_{18} is a potential manipulated variable for the maintenance of $r_{B\text{-}(d)}$, along with the component flows in F_3 (the new manipulated variable observable at this level). Since no refined has occurred in the separation block, $F_{9,B}$ should remain to be the best choice for $r_{B\text{-}(b)}$.

1. $r_{B\text{-}(d)}$: { component flows in F_{18}, F_3}
2. $r_{B\text{-}(e)}$: { all manipulated variables }
3. $r_{B\text{-}(b)}$: {$F_{9,B}$}

The gains of the material residuals while the material balance of A is under closed-loop control have been computed and summarized in Columns 1 to 3 in Table 10-11. See that $F_{18,B}$ and $F_{9,B}$ are indeed the best manipulated variable for the maintenance of $r_{B\text{-}(d)}$ and $r_{B\text{-}(b)}$ respectively. For $r_{B\text{-}(e)}$, $F_{3,B}$ is the best choice.

Columns 4 and 5 in Table 10-11 verifies that these assignments are feasible.

Goal 3-3: Maintain material balance of P

$F_{9,P}$ and $F_{20,G}$ have been assigned to be the primary manipulated variables to maintain $r_{P\text{-}(a)}$ and $r_{P\text{-}(b)}$ respectively. Hence, for the same reason as before, we expect $F_{20,G}$ to remain to be the best manipulated variable for $r_{P\text{-}(b)}$. Since $F_{9,P}$ is observable from $r_{P\text{-}(e)}$ and not $r_{P\text{-}(d)}$, it is expected that $F_{9,P}$ would be among the best manipulated variable for the maintenance of $r_{P\text{-}(e)}$.

1. $r_{P\text{-}(d)}$: { all manipulated variables }
2. $r_{P\text{-}(e)}$: { component flows in F_9, F_3}
3. $r_{P\text{-}(b)}$: {$F_{20,G}$}

Based on the closed-loop gains in Table 10-11, clearly it is logical to assign either $F_{3,A}$ or $F_{3,P}$ to $r_{P\text{-}(d)}$, $F_{9,P}$ to $r_{P\text{-}(e)}$ and $F_{20,G}$ to $r_{P\text{-}(d)}$. The feasibility of these assignments have been verified in Columns 9 and 10 of Table 10-11.

Goal 3-4: Maintain energy balance control

Again, anyone of the utility stream can be used to maintain the energy accumulation of the plant at constant level. Since cooling water is a cheaper utility than steam, assign $Q_{cw\text{-}(b)}$ to maintain $e_{(b)}$, $Q_{cw\text{-}(d)}$ to maintain $e_{(d)}$ and $Q_{cw\text{-}(e)}$ to maintain $e_{(e)}$.

Goal 3-5: Maintain the purity of P at or above 98%.

Varying $F_{11,P}$ changes the purity of P in the product stream.

Goal 3-6: Produce P at 20,000 tonnes per annum

As concluded at Level 1 and Level 2, with F_A, the limiting raw material, being a non-manipulatable variable, the production rate of the process cannot be fixed at arbitrary value. The control strategy cannot be determined.

Table 10 - 11: Closed-loop gains of residuals at Level 3

	$r_{B-(d)}$	$r_{B-(e)}$	$r_{B-(b)}$	$r_{B-(e)}$ (CL)	$r_{B-(b)}$ (CL)	$r_{P-(d)}$	$r_{P-(e)}$	$r_{P-(b)}$	$r_{P-(e)}$ (CL)	$r_{P-(b)}$ (CL)
$F_{11,A}$	0	0	0.0108	0	0.0108	0	0	-0.0054	0	-0.0054
$F_{11,C}$	0	0	0	0	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0	0	0	0	0
$F_{13,A}$	0	0	0.1707	0	0.1707	0	0	-0.0853	0	-0.0853
$F_{13,C}$	0	0	0.0083	0	0.0083	0	0	-0.0083	0	-0.0083
$F_{13,E}$	0	0	0	0	0	0	0	0	0	0
$F_{13,G}$	0	0	0	0	0	0	0	0	0	0
$F_{20,A}$	0	0	0	0	0	0	0	0	0	0
$F_{20,C}$	0	0	0	0	0	0	0	0	0	0
$F_{20,E}$	0	0	0	0	0	0	0	0	0	0
$F_{20,G}$	0	0	0.1074	0	0.1074	0	0	-0.2149	0	-0.2149
F_B	0	0	0	0	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0	0	0	0	0
$F_{13,B}$	0	0	-0.3655	0	-0.3655	0	0	0	0	0
$F_{20,B}$	0	0	-0.0164	0	-0.0164	0	0	0	0	0
$F_{11,P}$	0	0	0	0	0	0	0	-0.2644	0	-0.2644
$F_{13,P}$	0	0	0	0	0	0	0	-0.0793	0	-0.0793
$F_{20,P}$	0	0	0	0	0	0	0	0	0	0
$F_{9,A}$	0	0.3902	-0.3902	0.3902	-0.3902	0	-0.1951	0.1951	-0.1951	0
$F_{9,C}$	0	0.0185	-0.0185	0.0185	-0.0185	0	-0.0185	0.0185	-0.0185	0
$F_{9,E}$	0	0	0	0	0	0	0	0	0	0
$F_{9,G}$	0	0	0	0	0	0	0	0	0	0
$F_{4,A}$	0	0	0	0	0	0	0	0	0	0
$F_{4,C}$	0	0	0	0	0	0	0	0	0	0
$F_{4,E}$	0	0	0	0	0	0	0	0	0	0
$F_{4,G}$	0.0635	0	-0.0635	0	-0.0635	-0.1271	0	0.1271	-0.1271	0
$F_{14,A}$	0	-0.2086	0.2086	-0.2086	0.2086	0	0.1043	-0.1043	0.1043	0
$F_{14,C}$	0	-0.0102	0.0102	-0.0102	0.0102	0	0.0102	-0.0102	0.0102	0
$F_{14,E}$	0	0	0	0	0	0	0	0	0	0
$F_{14,G}$	0	0	0	0	0	0	0	0	0	0
$F_{17,A}$	0	0	0	0	0	0	0	0	0	0
$F_{17,C}$	0	0	0	0	0	0	0	0	0	0
$F_{17,E}$	0	0	0	0	0	0	0	0	0	0
$F_{17,G}$	0	0	0.0021	0	0.0021	0	0	-0.0042	0	-0.0042
$F_{9,B}$	0	-0.8121	0.8121	-0.8121	0.8121	0	0	0	0	0
$F_{4,B}$	-0.1906	0	0.1906	0	0.1906	0	0	0	0	0
$F_{14,B}$	0	0.4467	-0.4467	0.4467	-0.4467	0	0	0	0	0
$F_{17,B}$	0	0	-0.3123	0	-0.3123	0	0	0	0	0
$F_{9,P}$	0	0	0	0	0	0	-0.4408	0.4408	-0.4408	0
$F_{4,P}$	0	0	0	0	0	0	0	0	0	0
$F_{14,P}$	0	0	0	0	0	0	0.0969	-0.0969	0.0969	0
$F_{17,P}$	0	0	0	0	0	0	0	0	0	0
$F_{10,A}$	0	0	0	0	0	0	0	0	0	0
$F_{10,C}$	0	0	0	0	0	0	0	0	0	0
$F_{10,E}$	0	0	0	0	0	0	0	0	0	0
$F_{10,G}$	0	0.046	-0.046	0.046	-0.046	0	-0.0921	0.0921	-0.0921	0
$F_{10,B}$	0	-0.1381	0.1381	-0.1381	0.1381	0	0	0	0	0
$F_{10,P}$	0	0	0	0	0	0	0	0	0	0
$F_{18,A}$	0	0	0	0	0	0	0	0	0	0
$F_{18,C}$	0	0	0	0	0	0	0	0	0	0
$F_{18,E}$	0	0	0	0	0	0	0	0	0	0
$F_{18,G}$	-0.0021	0	0	0	0	0.0042	0	0	0.0042	0.0042
$F_{18,B}$	1.7123	0	0	0	0	0	0	0	0	0
$F_{18,P}$	0	0	0	0	0	0	0	0	0	0
$F_{3,A}$	0.4792	-0.4792	0	-0.4792	0	-0.2396	0.2396	0	0	0
$F_{3,C}$	0.0255	-0.0255	0	-0.0255	0	-0.0255	0.0255	0	0	0
$F_{3,E}$	0	0	0	0	0	0	0	0	0	0
$F_{3,G}$	0	0	0	0	0	0	0	0	0	0
$F_{3,B}$	-0.7727	0.7727	0	0.7727	0	0	0	0	0	0
$F_{3,P}$	0	0	0	0	0	-0.2695	0.2695	0	0	0

Control Structure at Level 3

The set of control strategies suitable for Level 3 are drawn in Figure 10-8 and the strategies are summarized in Table 10-12. Due to the self-regulatory nature of sub-block c, manipulating $F_{18,B}$ to maintain $r_{B\text{-}(d)}$ would require a change in F_B. Hence, abstraction of the control structure at this level will return the one developed at Level 2, maintaining the internal consistency of the development.

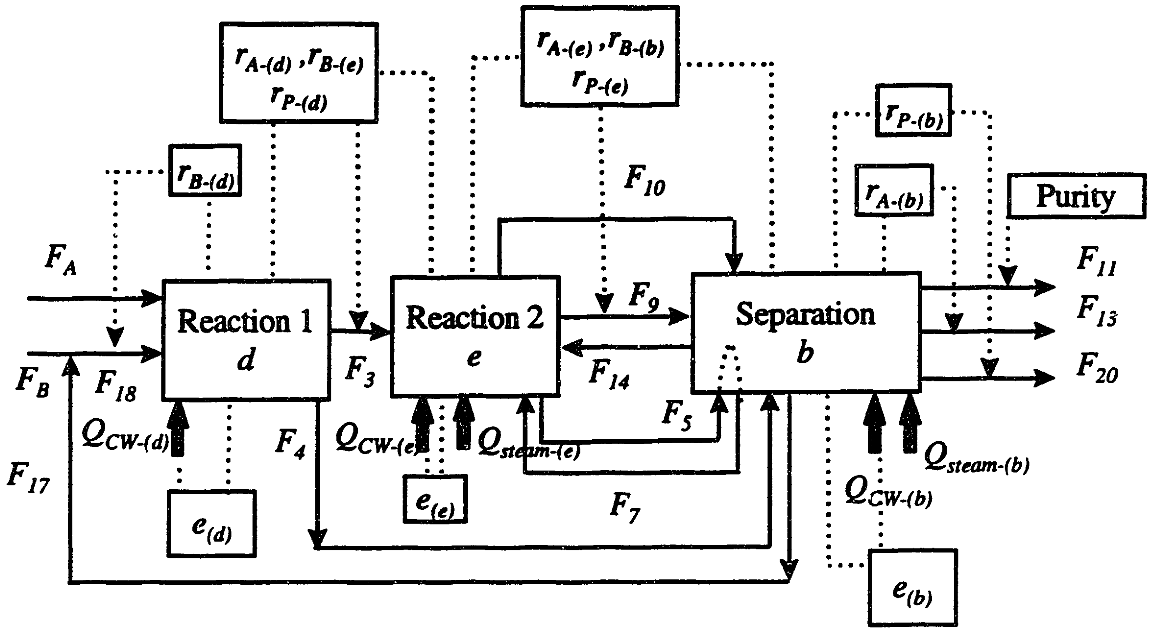


Figure 10 - 8: Control structure at Level 3

Table 10 - 12: Control Structure at the Expanded Generalized Reaction-Separation level

Control Objectives		Assignment: Reaction 1 Sub-block d	Assignment: Reaction 2 Sub-block e	Assignment: Separation Sub-block b
3-1	$r_{A\text{-}(d)}$, $r_{A\text{-}(e)}$, $r_{A\text{-}(b)}$	$F_{3,E}$	$F_{9,E}$	$F_{13,E}$
3-2	$r_{B\text{-}(d)}$, $r_{B\text{-}(e)}$, $r_{B\text{-}(b)}$	$F_{18,B}$	$F_{3,B}$	$F_{9,B}$
3-3	$r_{P\text{-}(d)}$, $r_{P\text{-}(e)}$, $r_{P\text{-}(b)}$	$F_{3,A}$ or $F_{3,P}$	$F_{9,P}$	$F_{20,G}$
3-4	$e_{(d)}$, $e_{(e)}$, $e_{(b)}$	F_{w1} or F_{w2}	F_{w3}	F_{w4} or F_{w5}
3-5	Product Purity			$F_{11,P}$
3-6	Production Level			

10.6 Level 4: Detailed Process Representation

The next level of presentation reveals all the details in the plant (see Figure 10-1). At this level, the dominant time constant in each sub-block is essentially the same as the dominant time constant of the unit inside that sub-block, the criterion in Section 8.5 has been met. The dynamics of the process must be incorporated in the analysis and begin Phase II of the design. Short-horizon design criteria discussed in Section 6.3.2 should be employed for the synthesis of the control structure for dynamic process regulation.

10.7 Summary

In this case study, the key pathways in which materials should flow in the plant to ensure that there is a balance between the inlet and outlet streams have been identified. It is found that the plant throughput cannot be set at any value. Such restriction was not identified in Johnston, R.D.'s (1985) study.

In this and in the previous chapter, the mechanics that are involved in Phase I of the methodology for the synthesis of plant-wide control structures has been demonstrated. Specifically, the systematic identification of:

- the stability of the open-loop system
- a control strategy for process stabilization
- a set of control objectives which have been generated based upon the overall production plan
- a set of notional control strategies which indicate the directions of material and energy flows that can best maintain the material and energy balances in the plant
- a set of upwardly compatible control structures for different time-scales of operation
- refinement and spawning of control objectives which assist the cost optimization objective

have been illustrated. Further development of the control structure at the detailed level for dynamic regulation of specific process outputs must be developed within Phase II of the methodology. The procedure for Phase II of the design will be demonstrated on the Tennessee Eastman Challenge Problem presented in Chapter 11.

Chapter 11
Synthesis of Plant Control Structure for the Tennessee Eastman Problem

11.1 Introduction

In this chapter, the synthesis of complete plant-wide control structure for the Tennessee Eastman challenge problem (TEC) proposed by Downs and Vogel (1993) will be demonstrated.

11.2 Preliminary Analysis

11.2.1 Understanding the TEC Process

Figure 11-1 gives the process flowsheet of the Tennessee Eastman Problem (Downs and Vogel, 1993). There are four primary gaseous raw material streams: Feed A, Feed D, Feed E and Feed C. The first three streams are primarily made up of reactants A, D and E respectively. Feed C is a mixture of A and C. All raw material streams contain some impurities which are mainly B and F. B is an inert. Feed streams A, D and E combine with the recycle stream (which is the main source of C for the reaction) enter a continuous stirred-tank reactor. At the specified operating temperature and pressure, the reaction mixture exists in a gas-liquid phase equilibrium. The gaseous raw materials react exothermically and irreversibly to form denser products G and H:

$$\text{(R1)}\quad A\,(g) + C\,(g) + D\,(g) \rightarrow G\,(l)$$
$$\text{(R2)}\quad A\,(g) + C\,(g) + E\,(g) \rightarrow H\,(l)$$
$$\text{(R3)}\quad A\,(g) + E\,(g) \rightarrow F\,(l)$$
$$\text{(R4)}\quad 3\,D\,(g) \rightarrow 2\,F\,(l)$$

The reactions are catalyzed by a non-volatile catalyst dissolved in the liquid phase. The reactor effluent is cooled and is subsequently flashed. The vent of the flash is rich in raw materials. Part of this vent is returned to the reactor through the recycle stream while the rest of the vent is purged. The liquid portion of the flashed material is rich in products. Products in the stream are being further concentrated in a stripper before they exit the plant through the product stream (stream 11). Products G and H are separated in a downstream refining section which is not included in this problem. Stripping is done by Feed C which also contains key components for the reactions and it enters the reactor through the gas recycle system.

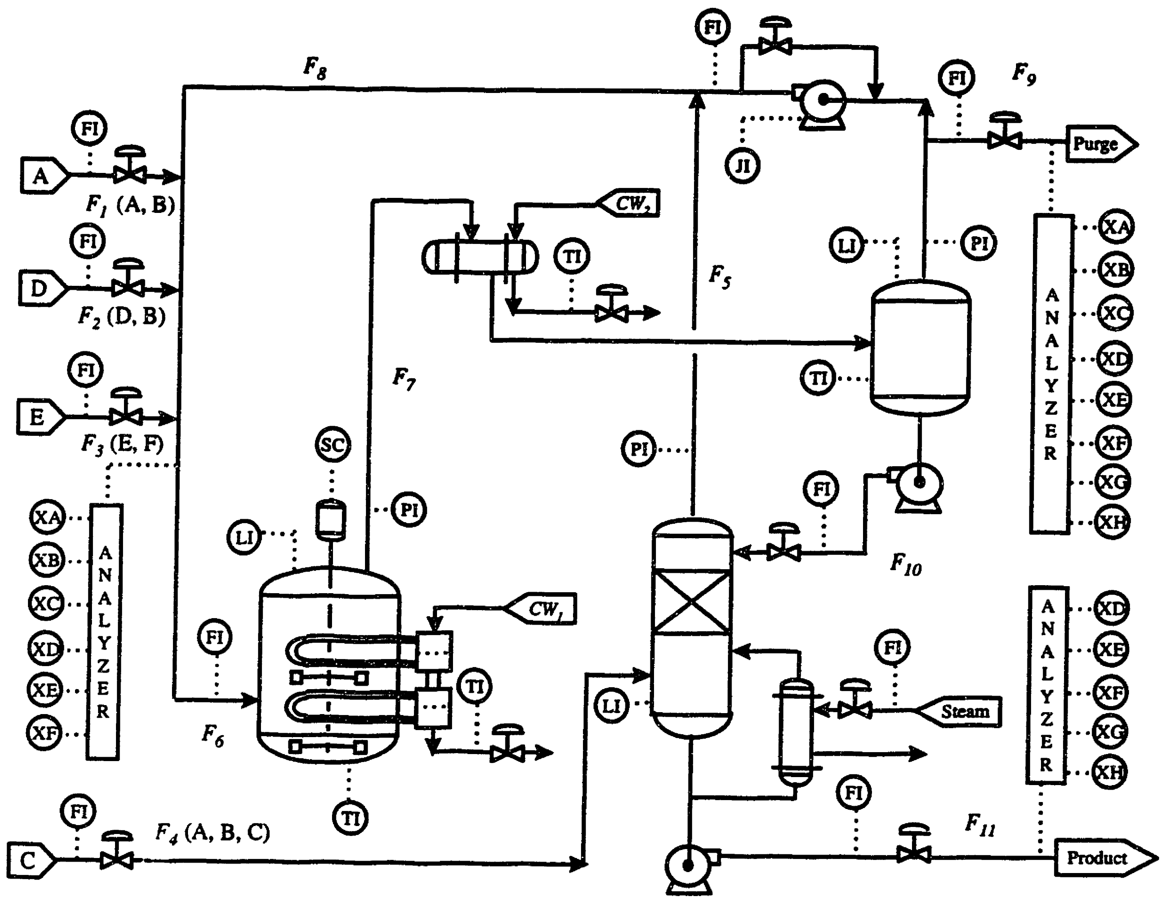


Figure 11 - 1: Schematic of the Tennessee Eastman challenge (TEC) Process (Downs and Vogel, 1993)

It is required to develop a plant-wide control system to assist plant operation to attain the following production objectives:

- Maintain process variables at desired values (at the primary operating mode, the plant is to produce combined G and H at a rate of 14076 kg/hr with a 50/50 mass ratio of product mix in the product stream).
- Keep process operating conditions within equipment constraints.
- Minimize variability of product rate and product quality during disturbances.
- Minimize movement of valves which affect other processes.
- Recover quickly and smoothly from disturbances, production rate changes, or product mix changes.

There are a total of 12 manipulated variables in the process.

The plant primarily produces the product at 14076 kg/hr with a 50/50 mass ratio of G/H. Due to market demand or capacity limitation, it is anticipated that the product mix specification, as well as the production rate, to vary. The base case (Mode 1) and five other *known* operating modes are listed in Table 11-1. The cost-optimal steady-state operating point for each mode of operations have been determined by Ricker (1995) and they are compiled in Appendix C.1.

The operational constraints on the equipment used in the plant are listed in Table 11-2. The normal operating limits exist to protect equipment operation. The high and low shutdown limits are part of the process interlock strategy and are used to shut down the process in the event the process conditions get out of hand.

Table 11 - 1: Operation Modes of the TEC process

Mode	G/H Mass Ratio	Production Rate (stream 11)
Base Case (1)	50/50	7038 kg/hr G and 7038 kg/hr H
2	10/90	1408 kg/hr G and 12669 kg/hr H
3	90/10	10000 kg/hr G and 1111 kg/hr H
4	50/50	maximum production rate
5	10/90	maximum production rate
6	90/10	maximum production rate

Table 11 - 2: Process Operating Constraints

Process Variables	Normal Operating Limits		Normal Operating Limits	
	Low Limit	High Limit	Low Limit	High Limit
Reactor Pressure	none	2895 kPa	none	3000 kPa
Reactor Level	50 %	100 %	8.5 %	112 %
Reactor Temperature	none	150 °C	none	175 °C
Product Separator Level	30 %	100 %	10 %	133 %
Stripper base Level	30 %	100 %	10 %	133 %

The four feed streams are products of other production facilities within the plant complex. Significant holdup is available for Feed E, however, less holdup is available for Feed A and Feed D, and very little holdup is available for Feed C. For feeds which have little holdup, changes in their feed rates to this process are product demand changes to the processes which produce those components. As a results, there are additional flow variability is of concern, particular for stream 4.

A list of the sources and frequencies process disturbances expected for the plant is shown in Table 11-3. The plant control system should attempt to minimize any anticipated effects of these disturbances on the flow and quality of the products.

Table 11 - 3: Expected Process Disturbances

Disturbance Type	Process Variable	Frequency/Type of Variation
1	A/C Feed Ratio, B Composition Constant (Stream 4)	Step
2	B Composition, A/C Ratio Constant (Stream 4)	Step
3	D Feed Temperature (Stream 2)	Step
4	Reactor Cooling Water Inlet Temperature	Step
5	Condenser Cooling Water Inlet Temperature	Step
6	A Feed Loss (Stream 1)	Step
7	C Header Pressure Loss - Reduced Availability (Stream 4)	Step
8	A, B, C Feed Composition (Stream 4)	Random Variation
9	D Feed Temperature (Stream 2)	Random Variation
10	C Feed Temperature (Stream 4)	Random Variation
11	Reactor Cooling Water Inlet Temperature	Random Variation
12	Condenser Cooling Water Inlet Temperature	Random Variation
13	Reaction Kinetics	Slow Drift
14	Reaction Cooling Water Valve	Sticking
15	Condenser Cooling Water Valve	Sticking
16 - 20	Unknown	Unknown

11.2.2 The Stability of the Open-loop Process

In this process, both the separator and stripper in the process are inherently stable unit-operations. The reactor is a two-phase CSTR and it is known that it is open loop unstable. With the presence of an unstable reactor in the plant, it is highly unlikely that the overall plant is in fact stable due to some fortunate choice of interconnection. Numerical simulations using the software supplied by Downs and Vogel (1993) confirmed that the plant is indeed unstable for the entire operating region. Step changes cause the plant to enter into oscillatory modes with increasing amplitudes of oscillations. This suggests the presence of complex eigenvalues in the right-half plane in the plant. There is no formal heat integration in the system. Energy is being recycled in the plant through the material recycle streams, which has been found to be unstable.

Developing the Stabilizing Control Strategy

Since the plant is open-loop unstable, a stabilizing feedback control strategy is required. Run-away behavior in the reactor is induced by fluctuation in the reaction conditions, the reactor can be stabilized by maintaining the reaction rates at some constant level. The rates are functions of the temperature, pressure, gaseous reaction volume (gas volume equals total vessel volume less liquid level) and the mole flows of reactants. A degree of freedom analysis indicates that at a fixed number of moles of reactants in the reactor, controlling either temperature, pressure or level would lead to self-regulation of the third variable.

Reactor Temperature Control Policy

Reactor cooling water (CW_I) is in close vicinity with the reactor temperature. A small deadtime is expected. Assigning reactor cooling water to control reactor temperature also helps to divert variation of coolant temperature to the environment through the coolant outlet and completely eliminate the effects reactor temperature variation on the process.

Reactor Level Control Policy

Maintaining the level of the reactor at some comfortable level is desirable because control of temperature depends on the coverage of the cooling water coil by the liquid phase in the reactor. The ability to control temperature is lost when the level goes below 40%. Reactor level is associated with the process unstable modes which exhibits fast process dynamics. Manipulated variables for the control of reactor level should be selected based on short-horizon design criteria. The dynamics of the reactor level to step changes of various manipulated inputs have been modeled as a integrator plus deadtime process as shown in Table 11-4. These models have obtained from plant tests with the reactor temperature under feedback control. The essential data are shown in Table 11-4.

Table 11 - 4: Process Model - Reactor Level

Inputs	Deadtime	Integrator Gain					
	all modes	**Base**	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	8 min	3	1.37	0	2.121	1.32	0
Product	40 min	0.00087	-0.00388	-0.004	-0.00468	0.00648	0.00278
Steam	30 min	0.36198	0.31178	0	0.22625	0.34517	0
Cond. CW	10 min	-6.198	-6.1521	0	-7.33	-5.81	0
Recycle	2 min	3.5	3.25	3.47	3.784	3.36	4.301
Separator Bot	8 min	2.26	3.05	3.928	3.49	3.235	4.716

For process stabilization, the manipulated variable should be one that is able to response quickly to any changes in the process dynamics. Thus, manipulated inputs which have variation constraints (such as the feed streams) are not being considered. Agitator must be kept at full speed to maintain the well-mixed condition. Reactor cooling water is also not an available manipulated variable as it has already been assigned to control reactor temperature. The ability of the remaining manipulated variable to reject disturbances acting on the reactor level can be evaluated using the design criteria developed for short-horizon control. Specifically, they will be judged by the size of the integrator gains (Equation [6-14], data shown in Table 10-4), the size of the deadtime (Equation [6-15], data shown in Table 10-4) and their rangeability (Equation [6-19], data shown in Appendix C.1). According to Equation [6-32], the performance index V_j for input j can be evaluated according to the following performance index:

$$V_j = w_{integrator}\left|\frac{V_{integrator,j}}{N_{integrator}}\right| + w_{deadtime}\left|\frac{V_{deadtime,j}}{N_{deadtime}}\right| + w_{rangeability}\left|\frac{V_{rangeability,j}}{N_{rangeability}}\right| \qquad [11\text{-}1]$$

The normalization factors N_i (i = integrator, deadtime or rangeability) in Equation 11-1 are chosen in such a way that all $V_{i,j} / N_i$ is are of roughly the same order of magnitude. The following weights have been chosen: $w_{integrator} = 3$; $w_{deadtime} = 1$; $w_{rangeability} = 0.4$. A heavier emphasis is placed on the size of the integrator gain because the size of the integrator gain predicts both the speed and magnitude of the changes in the output. The weight on the deadtime is heavier than that of the rangeability because deadtime limits the achievable performance of the system. The details of the computation can be found in Appendix C.2.

Table 11-5 summarizes the performance indexes of all available inputs for the control of reactor level at all possible operating modes. For modes 1, 2, 4 and 5, condenser cooling water (CW_2) is the best manipulated variable because it has the smallest performance index, indicating that deviation in the reactor level can be quickly eliminated. At modes 3 and 6, condenser cooling water is at saturation so recycle flow or separator bottom flow become the best choices at those two operating modes. When condenser cooling water is adjusted to control reactor level, the amount of materials that are being recycled back to the reactor is essentially controlled by altering the phase-equilibrium in the flash. Thus, both the condenser cooling water and recycle flow function in very much the same way. The reactor level control policy uses condenser cooling water for the maintenance of reactor level at operating modes 1, 2, 4 and 5 and recycle flow for the maintenance of reactor level at operating modes 3 and 6. The two control strategies are like mirrors to one another.

Table 11 - 5: Performance Indexes of Inputs for the control of Reactor Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	67.13	127.34	infinity	86.05	131.51	infinity
Product	178910.6	40888.21	39663.19	33908.83	24499.87	57049.53
Steam	630.26	infinity	infinity	892.91	651.58	infinity
Condenser CW	**48.64**	**48.35**	infinity	**36.19**	**48.79**	infinity
Recycle	209.74	213.22	**54.93**	206.34	211.62	**44.48**
Separator Bot	82.48	64.50	**53.92**	57.37	61.33	**46.57**

11.2.3 Prioritize Production Objectives

Based on the overall production plan, the process operating constraints, the prioritized overall plant production objectives are:

1. Maintain the levels of accumulations of materials and energy in the plant to be within their specified limits.
2. Maintain mass ratio of G/H in the product stream at the desired value.
3. Maintain production rate at the desired level.
4. Keep constrained process variables (reactor pressure, temperature, reactor level, separator level and stripper level) to be within their respective equipment limits.
5. Maximize production rate if required.
6. Minimize operating cost.

Note that objectives 1, 2, 3, 5 and 6 are related to the entire plant and are observable objectives from the start of our analysis. Objective 4 is related to variables in specific unit operations in the plant. These variables are only visible at the refined levels. Objective 1 encompasses the stability stipulation.

The production objectives have been ranked according to rules discussed in Section 8.2.2. Paired comparison of the two production objectives demonstrate that it is more important to have a tight control of the G/H ratio in the product stream than a tight control of the production rate. As the product stream is sent to a downstream refining section for further procession, variation of the composition in the product stream is a more severe disturbance to the refining unit than variation of the flow. From the range of operation in the plant (Modes 1 to 6), it is also expected that there will be a considerable amount of variation in the production rate during the course of its operation, while the product ratio remain to be at several specific values. Hence, the control of the product ratio to be of higher priority.

11.3 Phase I: Long-horizon Analysis

Control structure synthesis begins with the examination of the coarser viewpoint of the plant which characterize the long-horizon behavior of the process.

11.3.1 Level 1: Input-Output Level

The input-output representation of the process is shown in Figure 11-2. A set of long-horizon control strategies guided by the plant production objectives is to be synthesized. There are 7 reactive components ($N_C = 7$) in the plant (A, C, D, E, F, G, H) , 1 inert material B ($N_I = 1$) and 4 independent reactions ($N_R = 4$). According to Equation [5-1], four independent material balances (components A, C, E and D) are needed to completely describe the flow of materials in the process. These balances and the overall energy balances are summarized in Appendix C.3.

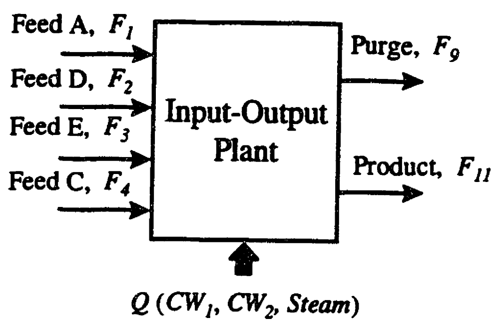


Figure 11 - 2: Input-Output Representation of the TEC process

Defining and Ranking Control Objectives

Focusing on only variables observable from Figure 11-2, the hierarchy of production objectives of relevance at the input-output level is:

1. Maintain process stability.
2. Maintain levels of accumulations of material and energy in the plant.
3. Maintain the mass ratio G/H in the product stream at the desired value.
4. Maintain production rate at the desired value.
5. Maximize production rate (Modes 4, 5 and 6).
6. Minimize operating cost.

The maintenance of the various accumulations of components and energy in the plant must be ranked according their levels of importance (see Section 8.2.2). External disturbances expected for the plant (see Table 11-3) can be classified into the following categories:

- Variation in the temperatures of coolants (related to energy balances)
- Variation in the compositions of A, B sand C in Feed C (related to material balances)
- Variation in the temperatures of Feeds D and C (related to energy balances)
- Loss of Feed A (related to material balances)

For this process, variation in temperatures can be easily localized through the implementation of temperature control schemes. For example, variations of the temperatures of feed streams are diverted to the reactor cooling water by means of the reactor temperature control policy (also the stabilizing control policy). For material accumulations, variations in the inventories of A and C appear to have the most significant impact on the plant. Both A and C are reactive materials and the expected amounts of variations in both components are similar ($\delta x_{A,4} = \delta x_{C,4} = 0.03$). Since C enters the plant through Feed C only while A enters the plant through both Feed A and Feed C, there is only one degree of freedom to maintain the inventory of C. The maintenance of the inventory of C should therefore of higher priority. Although the plant may experience the loss of Feed A, it is a severe disturbance and one which should not occur on a regular basis. This disturbance will be treated as a special case. The rate of accumulation of inert B in the plant is expected to be slow so the control of the inventory of inert is the least important one. The set of prioritized control objectives at the input-output level are shown in Table 11-6. Priority level *i-j* to indicate a goal which is of priority *j* at level *i*.

Table 11 - 6: Prioritized Control Objectives at the Input-Output Level

1-1	Reactor temperature (stabilization strategy)
1-2	Reactor level (stabilization strategy)
1-3	Maintain material balance control of C in the input-output plant (r_C)
1-4	Maintain material balance control of A in the input-output plant (r_A)
1-5	Maintain material balance control of E in the input-output plant (r_E)
1-6	Maintain material balance control of B in the input-output plant (r_B)
1-7	Maintain energy balance control in the input-output plant (e)
1-8	Maintain the G/H ratio in the product stream at desired value
1-9	Maintain production rate at the desired value
1-10	Maximize production rate (for modes 4, 5 and 6 only)
1-11	Minimize operating cost

Verify Feasibility of Control Objectives

To verify the feasibility of control objectives, the following material balance equations (see Appendix C.3) can be written:

$$
\begin{aligned}
r_A &= F_{1,A} + F_{4,A} - (G_{R1} + G_{R2} + G_{R3}) - F_{9,A} - F_{11,A} \\
r_C &= F_{4,C} - (G_{R1} + G_{R2}) - F_{9,C} - F_{11,C} \\
r_E &= F_{3,E} - (G_{R2} + G_{R3}) - F_{9,E} - F_{11,E}
\end{aligned}
\qquad [11\text{-}2]
$$

where G_{R1} , G_{R2} and G_{R3} are the rates of generation of materials in reactions R1, R2 and R3 respectively. They are defined as:

$$
\begin{aligned}
G_{R1} &= F_{9,G} + F_{11,G} \\
G_{R2} &= F_{9,H} + F_{11,H} \\
G_{R3} &= F_9 x_{9,F} + F_{11} x_{11,F} - F_3 x_{3,F} - 2/3\, F_2 x_{2,D} \\
&\quad + 2/3\,(F_9 x_{9,D} + F_{11} x_{11,D}) + 2/3\,(F_9 x_{9,G} + F_{11} x_{11,G})
\end{aligned}
\qquad [11\text{-}3]
$$

The following approximation had been found to be applicable for all operation modes at steady-states:

$$(G_{R1} + G_{R2} + G_{R3}) / (G_{R1} + G_{R2}) \approx 1 \qquad [11\text{-}4]$$

Then, $G_{R3} \rightarrow 0$. Now, let

$$\frac{G_{R1} + G_{R2}}{G_{R2} + G_{R3}} \approx \frac{G_{R1} + G_{R2}}{G_{R2}} \equiv \beta \qquad [11\text{-}5]$$

Then,

$$G_{R1} / G_{R2} = (\beta\text{-}1) \qquad [11\text{-}6]$$

The value of β at each of the operating modes have been computed and shown in Table 11-7.

Table 11 - 7: β at each Operating Mode

Operating Modes	β	G_{R1} / G_{R2}	$(F_{11,G} / F_{11,H})$ by mass
Base, 4	2.2	1.2	1
2, 5	1.1	0.12	0.11
3, 6	11	10.89	9

It can be seen from Table 11-7, β is related to the G/H mass ratio in the product stream F_{11}. The fact that $F_{9,G}$ and $F_{9,H}$ are relatively small, we can allows the following approximation to be made:

$$G_{R1}/G_{R2} \approx F_{11,G} / F_{11,H} = (\beta\text{-}1) \qquad [11\text{-}7]$$

which is related to the G/H ratio. Since this ratio is fixed, we cannot specify values for both $F_{11,G}$ and $F_{11,H}$. None of the objectives in Table 11-6 violates the constraint specified by Equation [11-7].

Quantifying Long-horizon Process Behavior

The material and energy balance model for this process can be found in Appendix C.3. At Level 1, long-horizon design criteria such as gains and static model uncertainty give good indication of the effectiveness of the use of the various inputs for control. The open-loop gain of the residual of a balance equation can be estimated as described in Section 5.2.2. Since the rangeability varies from stream to stream, for a fair comparison, the perturbation $\delta F_{i,j}$ are scaled to reflect the changes in the outputs which are equivalent to a 1% change of the stream valves. For those streams which cannot be directly manipulated by process valves, the gains are perturbed by 1% of the estimated "maximum flows". These open-loop gains are compiled in Appendix C.4.

Accounting for Process Nonlinearity and Model Uncertainty

In the long-horizon analysis at steady-state, residuals of the accumulations terms of the material and energy balance equations are estimated from the principal of conversation and so they can be assumed to be precise and contain little model error. The rate of change of the residuals will, however, depend on the operating region as well as linearity of the system. The process is primarily being operated at the base case (Mode 1), but the steady-state is expected to vary to meet different product specifications. It is expected that the cost-optimal operating point to vary nonlinearly as the specification of G/H and the production rate changes. Hence, it is best to quantify model uncertainty by determining how the process gains may change as the operating point is being varied from the base case to other possible operating regions.

The robustness measure C_g (Equation [6-9]) is used to quantify model uncertainty. Computation of C_g requires determination of the range of variation expected in the process models. In this case study, as the process is being transferred from one mode to another, the set of gains describing the process move from one set to another simultaneously. The uncertainty in the gains is structured and combination of gains measured at different modes will most likely not occur. Rather than computing the C_g corresponding to the worst case scenario by assuming the gain perturbation to be uncorrelated (which may be too conservative and impractical), C_g can be determined by simply computing the ratio of the maximum to the minimum vales among the six possible ones at the six anticipated operating regions. The C_g for the worst case scenario can be used to help discriminate the various options if there are more than one choice suitable for assignment.

Synthesize control structure at the input-output level

At the input output levels, the goal is to develop *notional* control strategies that can be implemented to assist the achievement of the overall production plan. All flow components in the plant, with the exceptions of those associated with feed streams, are considered as possible manipulated variables. The compositions in the feed streams are fixed by external environment, component flow variation is not possible in feed streams. Although component flows are not variables that can be physically adjusted, it will become clear later on how these manipulations are replaced by other equivalents which can be physically realized.

In the modular multivariable design framework, primary manipulated variables will be assigned to maintain each of the control objectives, sequentially, starting from the most important one. The first two objectives listed in Table 11-6 are related to the process stabilizing strategy. Reactor cooling water and condenser cooling water have already been assigned for that purpose. The assignments for the rest of the objectives are discussed below.

Goal 1-3: Maintain material balance control of C

The open-loop gains of the residuals of the material balance of C (i.e. r_C) in the input-output plant for a 1% change in the component flows have been compiled in Table 11-8, along with the values of the robustness measures. The data indicates that F_4 (Feed C), and $F_{11,G}$ (the flow of G in the product stream) have the greatest impact on the level of accumulations of C in the system. However, judging from the size of the C_g, the impact of process nonlinearity on the closed-loop system by $F_{11,G}$ will be much more significant than that of F_4. For F_4, the C_g is close to unity so the impact of uncertainty on the variation is minimal. F_4 will be assigned to maintain the material balance of component C in the system.

Goal 1-4: Maintain material balance control of A

The primary manipulated variable to maintain the material balance of A will be selected based on the closed-loop gains of r_A , i.e. the gains of the residuals of the material balance of A while the material balance of C is being maintained by F_4. The closed-loop gains of r_A be as demonstrated in the example in Section 7.3.1. These values are complied in Table 11-9.

The size of the gains cause by changes in F_2 (Feed D) is the largest with the C_g closest to unity. This is obviously the best choice. Feed D, being the limiting reagent, is operating at its saturation limit at Mode 4 and 6 (refer to data in Appendix C.1). When Feed D is at saturation, a secondary manipulated variable must be chosen to maintain the objective. F_1 (Feed A) is the next best choice for this objective. Hence, the decision is to assign Feed D to maintain r_A at operating modes 1, 2, 3 and 5; assign Feed A to maintain r_A at operating modes 4 and 5.

The employment of two different control strategies depending on the mode at which the plant is being operated, a *variable control structure* design has been initiated for the plant. For ease of maintenance, it is most desirable to utilize a control strategy that will enable the plant to operate in the entire operating region. However, such an approach is not feasible given that the available degrees of freedom change from operating mode to operating mode.

Table 11 - 8: Open-loop Gains of r_C at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	C_g
F_1	0	0	0	0	0	0	
F_4	3.47	3.47	3.47	3.47	3.47	3.47	1.00
F_3	0	0	0	0	0	0	
F_2	0	0	0	0	0	0	
$F_{9,A}$	0	0	0	0	0	0	
$F_{9,B}$	0	0	0	0	0	0	
$F_{9,C}$	-4.79E-02	-5.32E-02	-3.77E-02	-6.64E-02	-5.29E-02	-4.05E-02	1.76
$F_{9,D}$	0	0	0	0	0	0	
$F_{9,E}$	0	0	0	0	0	0	
$F_{9,F}$	0	0	0	0	0	0	
$F_{9,G}$	-2.27E-02	-4.80E-03	-3.84E-02	-1.63E-02	-4.59E-03	-3.63E-02	8.37
$F_{9,H}$	-1.18E-02	-2.10E-02	-2.04E-03	-7.70E-03	-2.01E-02	-1.91E-03	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	-1.13E-01	-4.58E-02	-5.45E-02	-4.45E-02	-4.57E-02	-4.52E-02	2.55
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	-2.41	-0.53	-4.09	-2.38	-0.53	-4.08	7.75
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37	10.51

Table 11 - 9: Closed-loop Gains of r_A at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	C_g
F_1	0.45	0.45	0.45	0.45	0.45	0.45	1.00
F_4	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	
F_3	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	1.01
F_2	1.21	1.21	1.21	1.21	1.21	1.21	1.00
$F_{9,A}$	-0.1205	-0.1332	-0.1138	-0.1733	-0.1337	-0.1187	1.52
$F_{9,B}$	0	0	0	0	0	0	
$F_{9,C}$	4.56E-02	5.05E-02	3.58E-02	6.31E-02	5.03E-02	3.85E-02	1.76
$F_{9,D}$	-0.0022	-0.0003	-0.0059	-0.0019	-0.0003	-0.0058	18.56
$F_{9,E}$	0	0	0	0	0	0	
$F_{9,F}$	-0.0197	-0.0268	-0.0074	-0.0242	-0.0271	-0.0079	3.65
$F_{9,G}$	-1.62E-02	-3.40E-03	-2.75E-02	-1.17E-02	-3.30E-03	-2.60E-02	8.36
$F_{9,H}$	-6.00E-04	-1.00E-03	-1.00E-04	-4.00E-04	-1.00E-03	-1.00E-04	11.20
$F_{11,A}$	-0.0885	-0.0217	-0.0215	-0.0267	-0.0272	-0.0215	4.12
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	1.08E-01	4.35E-02	5.19E-02	4.24E-02	4.34E-02	4.30E-02	2.55
$F_{11,D}$	-0.0003	0	-0.0009	-0.0006	0	-0.0009	30.33
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	-0.0086	-0.0132	-0.0032	-0.0196	-0.0145	-0.0036	6.16
$F_{11,G}$	-1.72	-0.38	-2.93	-1.70	-0.38	-2.92	7.75
$F_{11,H}$	-0.09	-0.19	-0.02	-0.10	-0.19	-0.02	10.69

Goal 1-5: Maintain material balance control of E

At the previous decision point, the generation of control structure diverged into two paths. Objective r_A is being controlled by two different control systems, depending on the operating mode. The closed-loop gains of r_E at Modes 1, 2, 3 and 5 by the various inputs will have to be determined separately from those for Modes 4 and 6. The corresponding closed-loop gains are complied in Table 11-10.

- For Modes 1, 2, 3 and 5, the size of the gains of F_3 (Feed E) and $F_{11,H}$ are the largest. Since F_3 has a C_g that is close to unity, F_3 is a better alternative. However, at Mode 5, F_3 is again at its saturation. We must choose a secondary manipulated variable for the maintenance of r_E at Mode 5. $F_{11,H}$ is the next best alternative. Note that when $F_{11,H}$ is adjusted, there will be direct impact on the G/H ratio in the product stream. Our objective is to divert disturbances away from important plant objectives as early as possible. Then, the next best choice, i.e. F_1 (Feed A) will be assigned to maintain r_E at this level.
- For Modes 4 and 6, F_3 is the best choice for these two operating modes.

So, at this level, F_3 will be assigned to Modes 1, 2, 3, 4 and 6; F_1 will be assigned to Mode 5.

Table 11 - 10: Closed-loop Gains of r_E at the Input-Output Level

Input	Base	Mode 2	Mode 3	Mode 5	C_g	Input	Mode 4	Mode 6	C_g
F_1	-0.45	-0.45	-0.45	-0.45	1.00	F_1	*assigned*	*assigned*	
F_4	*assigned*	*assigned*	*assigned*	*assigned*		F_4	*assigned*	*assigned*	
F_3	1.82	1.81	1.82	1.82	1.00	F_3	1.82	1.82	1.00
F_2	*assigned*	*assigned*	*assigned*	*assigned*		F_2	1.21	1.21	1.00
$F_{9,A}$	1.21E-01	1.33E-01	1.14E-01	1.34E-01	1.17	$F_{9,A}$	0	0	
$F_{9,B}$	0	0	0	0		$F_{9,B}$	0	0	
$F_{9,C}$	-4.56E-02	-5.05E-02	-3.58E-02	-5.03E-02	1.41	$F_{9,C}$	0	0	
$F_{9,D}$	0	0	0	0		$F_{9,D}$	-1.90E-03	-5.80E-03	3.05
$F_{9,E}$	-5.92E-02	-8.13E-02	-1.61E-02	-8.35E-02	5.19	$F_{9,E}$	-6.52E-02	-1.66E-02	3.93
$F_{9,F}$	0	0	0	0		$F_{9,F}$	-2.42E-02	-7.90E-03	3.06
$F_{9,G}$	1.10E-03	2.00E-04	1.90E-03	2.00E-04	9.50	$F_{9,G}$	-1.09E-02	-2.42E-02	2.22
$F_{9,H}$	-1.12E-02	-2.00E-02	-1.90E-03	-1.91E-02	10.53	$F_{9,H}$	-7.70E-03	-1.90E-03	4.05
$F_{11,A}$	8.85E-02	2.17E-02	2.15E-02	2.72E-02	4.12	$F_{11,A}$	0	0	
$F_{11,B}$	0	0	0	0		$F_{11,B}$	0	0	
$F_{11,C}$	-1.08E-01	-4.35E-02	-5.19E-02	-4.34E-02	2.49	$F_{11,C}$	0	0	
$F_{11,D}$	0	0	0	0		$F_{11,D}$	-6.00E-04	-9.00E-04	1.50
$F_{11,E}$	-2.72E-02	-4.18E-02	-7.30E-03	-4.58E-02	6.27	$F_{11,E}$	-5.39E-02	-8.20E-03	6.57
$F_{11,F}$	0	0	0	0		$F_{11,F}$	-1.96E-02	-3.60E-03	5.44
$F_{11,G}$	1.18E-01	2.64E-02	2.00E-01	2.59E-02	7.71	$F_{11,G}$	-1.58	-2.72	1.72
$F_{11,H}$	-1.81	-3.69	-0.35	-3.69	10.46	$F_{11,H}$	-1.94	-0.37	5.24

Goal 1-6: Maintain material balance control of B

Similarly, base on the size of the gains and the size of the robustness measure (see Table 11-11), $F_{9,B}$ is the best manipulated variable for the control of r_B at any operating mode.

Goal 1-7: Maintain energy balance control at the Input-Output Level

Reactor cooling water, condenser cooling water and steam are manipulations which can be used directly for energy balance control at this level. Both of the coolants have been assigned to the plant's stabilization strategy. These control assignments implicitly maintains the energy balance of the plant.

Goal 1-8: Maintain the G/H ratio in the Product stream at Desired Value

The ratio $F_{11,G}/F_{11,H}$ has the most direct influence on the mass ratio in the product stream. Keep in mind that the assignments at the input-output level are strictly notional will be further refined into associations which can be directly implemented.

Goal 1-9: Maintain Production Rate at the Desired Level

Similarly, the flow of F_{11} has the most direct effect on the production rate and will be assigned to this goal at all operating modes.

Goal 1-10: Maximize the Production rate (Modes 4, 5 and 6)

Production can be maximized by maximizing the use of the limiting raw materials until we hit some constraints in the plant. Feed D (F_2) is the limiting raw materials for Modes 4 and 6 while Feed E (F_3) is the limiting raw material for Mode 5. Maximizing the use of these material streams within the process constraints maximizes the plant's throughputs.

Table 11 - 11: Closed-loop Gains of r_B at the input-output level

Input	Base	Mode 2	Mode 3	C_g	Input	Mode 4	Mode 6	C_g	Input	Mode 5
F_1	-2.28E-05	-4.20E-05	-2.28E-05	1.84	F_1	*assigned*	*assigned*		F_1	*assigned*
F_4	*assigned*	*assigned*	*assigned*		F_4	*assigned*	*assigned*		F_4	*assigned*
F_3	*assigned*	*assigned*	*assigned*		F_3	*assigned*	*assigned*		F_3	-9.15E-05
F_2	*assigned*	*assigned*	*assigned*		F_2	1.82E-03	1.82E-03	1.00	F_2	*assigned*
$F_{9,A}$	1.81E-05	2.56E-05	1.71E-05	1.50	$F_{9,A}$	1.73E-05	1.19E-05	1.46	$F_{9,A}$	1.34E-05
$F_{9,B}$	-8.05E-02	-4.28E-02	-1.84E-01	4.30	$F_{9,B}$	-6.73E-02	-1.84E-01	2.74	$F_{9,B}$	-4.18E-02
$F_{9,C}$	4.52E-04	5.12E-04	3.64E-04	1.41	$F_{9,C}$	6.44E-04	3.93E-04	1.64	$F_{9,C}$	5.13E-04
$F_{9,D}$	3.29E-07	6.16E-08	8.93E-07	14.50	$F_{9,D}$	1.92E-07	5.77E-07	3.01	$F_{9,D}$	4.81E-08
$F_{9,E}$	-8.92E-10	-1.56E-09	-2.42E-10	6.45	$F_{9,E}$	-6.49E-10	-2.00E-10	3.25	$F_{9,E}$	4.20E-06
$F_{9,F}$	2.96E-06	5.16E-06	1.12E-06	4.62	$F_{9,F}$	2.42E-06	7.91E-07	3.06	$F_{9,F}$	4.07E-06
$F_{9,G}$	2.19E-04	4.77E-05	3.80E-04	7.97	$F_{9,G}$	1.61E-04	3.59E-04	2.23	$F_{9,G}$	4.55E-05
$F_{9,H}$	1.13E-04	2.07E-04	2.00E-05	10.32	$F_{9,H}$	7.55E-05	1.87E-05	4.03	$F_{9,H}$	1.98E-04
$F_{11,A}$	1.33E-05	4.19E-06	3.24E-06	4.11	$F_{11,A}$	2.67E-06	2.15E-06	1.24	$F_{11,A}$	2.72E-06
$F_{11,B}$	-4.50E-07	-2.27E-02	-4.54E-03	50444	$F_{11,B}$	-3.90E-04	-4.00E-04	1.03	$F_{11,B}$	-2.27E-03
$F_{11,C}$	1.07E-03	4.40E-04	5.27E-04	2.43	$F_{11,C}$	4.32E-04	4.39E-04	1.01	$F_{11,C}$	4.43E-04
$F_{11,D}$	4.51E-08	5.78E-09	1.37E-07	23.69	$F_{11,D}$	5.89E-08	9.09E-08	1.54	$F_{11,D}$	4.50E-09
$F_{11,E}$	-4.11E-10	-8.03E-10	-1.10E-10	7.33	$F_{11,E}$	-5.37E-10	-1.00E-10	5.37	$F_{11,E}$	2.30E-06
$F_{11,F}$	1.30E-06	2.53E-06	4.78E-07	5.30	$F_{11,F}$	1.96E-06	3.63E-07	5.40	$F_{11,F}$	2.18E-06
$F_{11,G}$	2.33E-02	5.26E-03	4.06E-02	7.71	$F_{11,G}$	2.35E-02	4.03E-02	1.72	$F_{11,G}$	5.23E-03
$F_{11,H}$	1.83E-02	3.81E-02	3.64E-03	10.47	$F_{11,H}$	1.90E-02	3.63E-03	5.24	$F_{11,H}$	3.82E-02

Goal 1-11: Minimize Operating Cost

Once all of the more important objectives have been satisfied, the plant can be optimized for minimum operating cost. The objective function for cost minimization has been defined by Downs (Downs et al., 1993) as follows:

$$\begin{aligned} \textit{Operating Cost } (\Phi) &= (C_{purge})*(\textit{purge rate}) + (C_{prod})*(\textit{product rate}) \\ &\quad + (C_{compress})*(\textit{compressor work}) + (C_{steam})*(\textit{Steam rate}) \end{aligned} \qquad [11\text{-}8]$$

where:

C_{purge} = molar cost of lost of raw materials and products in purge

C_{prod} = molar cost of lost of raw materials in product stream

$C_{compress}$ = compressor cost

C_{steam} = steam cost

such that:

$$C_{purge} = C_A x_{9,A} + C_C x_{9,C} + C_D x_{9,D} + C_E x_{9,E} + C_F x_{9,F} + C_G x_{9,G} + C_H x_{9,H} \qquad [11\text{-}9]$$

$$\begin{aligned} C_{purge} F_9 &= C_A F_{9,A} + C_C F_{9,C} + C_D F_{9,D} + C_E F_{9,E} + C_F F_{9,F} + C_G F_{9,G} \\ &\quad + C_H F_{9,H} \end{aligned} \qquad [11\text{-}10]$$

$$C_{prod} = C_D x_{11,D} + C_E x_{11,E} + C_F x_{11,F} \qquad [11\text{-}11]$$

$$C_{prod} F_{11} = C_D F_{11,D} + C_E F_{11,E} + C_F F_{11,F} \qquad [11\text{-}12]$$

C_i, i = A, B, … H are cost per kgmol of each component, $x_{i,j}$ is the molar composition of j in stream i. The market of each component as well as the steam and compressor cost are complied in Table 11-12.

Table 11 - 12: Market value of Materials, Compressor and Steam costs

C_A = 2.206 \$/kgmol	C_E = 14.56 \$/kgmol	C_H = 22.94 \$/kgmol
C_A = 2.206 \$/kgmol	C_F = 17.89 \$/kgmol	$C_{compress}$ = 0.0536 \$/kW-hour (constant)
C_D = 22.06 \$/kgmol	C_G = 30.44 \$/kgmol	C_{steam} = 0.0318 \$/kg (constant)

Substituting Equations [11-9] to [11-12] into the objective function Φ, the optimization can be written as:

$$\text{Min } \Phi = c_A F_{9,A} + c_C F_{9,C} + c_D F_{9,D} + c_E F_{9,E} + c_F F_{9,F} + c_G F_{9,G} + c_H F_{9,H} + c_D F_{11,D} + c_G F_{11,G} + c_F F_{11,F} + C_{compress} W + C_{steam} F_{steam} \quad [11\text{-}13]$$

s.t.:

1. Maintain reactor temperature at the desired level
2. Maintain reactor level at the desired level
3. Maintain accumulation of C at the desired level
4. Maintain accumulation of A at the desired level
5. Maintain accumulation of E at the desired level
6. Maintain accumulation of B at the desired level
7. Maintain accumulation of energy in the system
8. $F_{11,G} / F_{11,H}$ at the pre-specified value
9. F_{11} at the pre-specified value for modes 1, 2 and 3
10. Maximized production rate for modes 4, 5 and 6

The governing principle of the optimization can be extracted using similar procedure as presented in Example 8-1. Other constraints which govern the process include:

Stoichiometry :

Earlier, the following relationship based on stoichiometry has been identified:

$$G_{R1}/G_{R2} \approx F_{11,G} / F_{11,H} = (\beta\text{-}1) \quad [11\text{-}7]$$

Thermodynamic Relations :

Notice that F_9 is a vapor stream while F_{11} is a liquid stream. Hence, a phase separation has taken place. The distribution of materials in the outlet streams are accomplished through some separation system that is not yet observable. A pseudo separation system such as the one shown in Figure 11-3 is assumed to present within the input-output structure. At equilibrium, the following relationships around the structure in Figure 11-3 are true:

Material balances:

$$F_{*,i} = F_{9,i} + F_{11,i} \quad \forall\, i = \text{A, B, C, D, E, F, G, H} \quad [11\text{-}14]$$

Thermodynamic relations:

$$\frac{F_{9,i}}{\sum F_{9,i}} = K_{9,11}(P^*,T^*)\frac{F_{11,i}}{\sum F_{11,i}} \quad [11\text{-}15]$$

where $K_{9,11}(P^*,T^*)$ is a pseudo equilibrium constant governing the separation. Combining the two relationships, at constant P^* and T^*, the following generic constraints exist:

$$f_1(F_{*,i}, F_{9,i}, F_{11,i}) = 0 \qquad [11\text{-}16]$$
$$f_2(F_{*,i}, F_{9,i}, F_{11,i}) = 0 \qquad [11\text{-}17]$$

There are 3 unknowns and 2 equations. For each component i, one variable from the set $\{F_{*,i}, F_{9,i}, F_{11,i}\}$ can be specified. At Level 1, $F_{*,i}$, P^* and T^* are not visible variables so they are not degrees of freedom available. $F_{9,i}$ and $F_{11,i}$ are inter-related through a thermodynamic relationship. We will examine each component to identify the degrees of freedom for optimization.

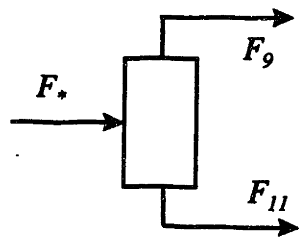


Figure 11 - 3: A Pseudo Separation System in the Input-Output Structure

The initial component table for the generic separation is shown in Table 11-13. At the input-output level, the most relevant streams are F_9, F_{11} and F_*. F_* is not observable and therefore will not be relevant in the analysis. Variables which have been selected as manipulated variables are indicated by "MV"; those that are control objectives with a specified value are indicated by "specified"; those whose flow rates at steady-state are either zero or insignificant compared to the other component flows in that stream are indicated by "~0".

Table 11 - 13: Initial Component Table for the Input-Output Level

Component	F_9	F_{11} specified
A		~0
B	MV	~0
C		~0
D		~0
E		~0
F		~0
G		
H		

Degrees of Freedom Analysis :

Again, the term "degrees of freedom for optimization" and "design variables" interchangeably. A variable has a fixed value if its flow is either very small or insignificant, or that its value is defined by a control objective. A variable becomes unavailable as a variable for optimization if its flow is fixed by either the material balance controls (as manipulated variables), thermodynamic relations or stoichiometric constraints. The following statement can be made:

1. With F_{11} and the product ratio being chosen as control objectives, the flow of $F_{11,G}$ and $F_{11,H}$ are no longer degrees of freedom in our design. There values are marked "n/a" in Table 11-14.
2. Furthermore, $F_{9,G}$ and $F_{9,H}$ are related to $F_{11,G}$ and $F_{11,H}$ through thermodynamic relationships. Hence, $F_{9,G}$ and $F_{9,H}$ are also not degrees of freedom in our design.
3. For similar reasons, $F_{9,B}$ has been chosen to be a manipulated variable. Through the thermodynamic relationships, $F_{11,B}$ is not a design degrees of freedom.
4. Then, the remaining variables are potential degrees of freedom in our cost optimization. However, $F_{11,A}$, $F_{11,C}$, $F_{11,D}$, $F_{11,E}$ and $F_{11,F}$ are relatively small, so only $F_{9,A}$, $F_{9,C}$, $F_{9,D}$, $F_{9,E}$ and $F_{9,F}$ will be considered as design variables in the optimization. These variables are marked "√" in Table 11-14.

Table 11 - 14: Final Component Table for the Input-Output Level

Component	F_9	F_{11} specified
A	√	~0
B	MV	n/a
C	√	~0
D	√	~0
E	√	~0
F	√	~0
G	n/a	n/a
H	n/a	n/a

By eliminating variables which have been chosen to be manipulated variables, and by incorporating thermodynamic restrictions on the distribution of materials in the plant, the optimization is reduced to:

$$\text{Min } \Phi = c_A F_{9,A} + c_C F_{9,C} + c_D F_{9,D} + c_E F_{9,E} + c_F F_{9,F} + C_{compress} W + C_{steam} F_{steam} \quad [11\text{-}18]$$

s.t.

1. maintain reactor temperature at the desired level
2. maintain reactor level at the desired level
3. maintain accumulation of C at the desired level
4. maintain accumulation of A at the desired level
5. maintain accumulation of E at the desired level
6. maintain accumulation of B at the desired level
7. maintain accumulation of energy in the system
8. $F_{11,G} / F_{11,H}$ at the pre-specified value
9. F_{11} at the pre-specified value for modes 1, 2 and 3
10. maximized production rate for modes 4, 5 and 6

The cost breakdown for Mode 1, the base case, at steady-state is shown in Table 11-15. Steam cost is negligible. Compressor work can also be assumed to stay at a roughly constant value. Purge cost is the largest component in the cost function. The purge stream is primary made up of the raw materials in the process, operating cost can be minimized by minimizing the loss of raw materials in purge.

Table 11 - 15: Cost breakdown for Mode 1

Purge cost:	\$ 73.75 $\Rightarrow C_{purge} = \$7.83$
Product cost:	\$ 25.46 $\Rightarrow C_{prod} = \$\,0.12$
Compressor:	\$ 14.95
Steam:	\$ 0.15
Total:	\$ 114.31

Control Structures at Level 1

The sets of control strategies for all operating modes at Level 1 is summarized in Table 11-16. All control objectives are maintained by adjusting some variables observable from the streams which cross the boundaries of the system. The primary goal of the case study is to develop a set of control strategies that would be suitable for the base case (Mode 1) and account for nonlinearity in the system. By computing the robustness measure using data from the entire operating range, the control strategies which are suitable at other operating point as well have also been identified. Due the saturation limits that exist at some operating modes and due to nonlinearity induced by the changes in the G/H specifications in the product stream, the control structure must change from one mode to another. Saturation limits and model uncertainty have all contributed to a *variable control structure* for this plant. Such type of a control structure arise naturally in the synthesis with no *a priori* stipulation.

Table 11 - 16: Summary of control structure at Level 1 for all operation modes

	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
	F_5 at saturation	F_5 at saturation	CW_2 at saturation	F_5, F_2 at saturation	F_5, F_3 at saturation	F_2, CW_2 at saturation
Stability: Reactor Temp.	CW_1	CW_1	CW_1	CW_1	CW_1	CW_1
Stability: Reactor Level	CW_2	CW_2	F_5 [1]	CW_2	CW_2	F_5 [1]
Maintain Balance of C	F_4	F_4	F_4	F_4	F_4	F_4
Maintain Balance of A	F_2	F_2	F_2	F_1 [2]	F_2	F_1 [2]
Maintain Balance of E	F_3	F_3	F_3	F_3	F_1 [2]	F_3
Maintain Balance of B	$F_{9,B}$	$F_{9,B}$	$F_{9,B}$	$F_{9,B}$	$F_{9,B}$	$F_{9,B}$
Energy Balance	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2
G/H	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$
Production	F_{11}	F_{11}	F_{11}			
Max. Production				F_2	F_3 [2]	F_2
Minimize Cost	minimize loss of raw materials in purge stream					

[1] Change of control structure due to the specification on G/H.
[2] Change of control structure due to saturation of limiting reactant.

The control structure for the base case (Mode 1) is shown in Figure 11-4. At this level, some of the associations, such as the manipulations of specific component flow rates, are notional and will be refined to strategies which are more specific later in the design.

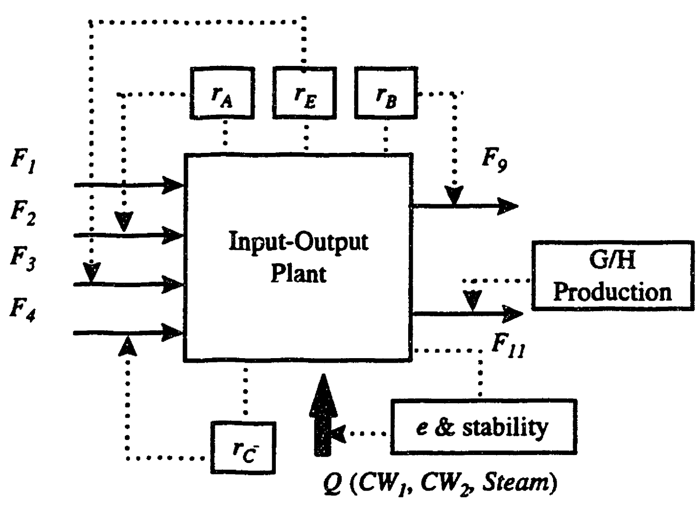


Figure 11 - 4: Control Structure for the Input-Output Level (Base Case)

11.3.2 Level 2: Generalized Reaction-Separation System

The next level of representation in the hierarchy exposes the generalized reaction and separation systems in the plant as shown in Figure 11-5. At this level, the sub-blocks in the process are still abstract and none of the details in the plant have been exposed. The dominant time constant of the generalized separation system is expected to be larger than that of the individual separation units in the plant. Design criteria for long-horizon will be used to develop a control structure that is suitable for this level of representation. The material and energy balance model can be found in Appendix C.3.

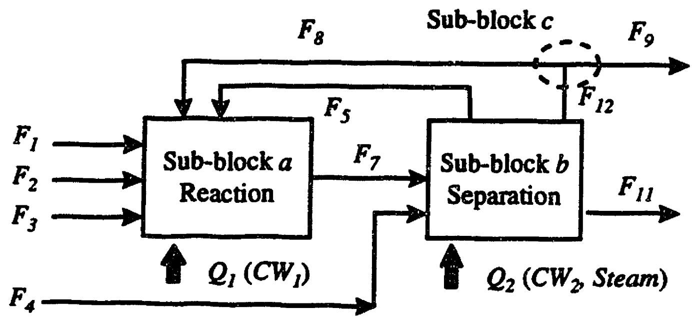


Figure 11 - 5: Process Representation of the Generalized Reaction-Separation System (Level 2)

Progressive Generation of Control Objectives

Control objectives at the input-output level are assigned to the appropriate sub-block(s) at this level as shown in Table 11-17. "$r_{i-(j)}$" refers to the maintenance of the material balance of component i in sub-block j; "$e_{(j)}$" refers to the maintenance of the energy balance in sub-block j.

The process stabilization objectives *allocated* to sub-block a where the sources of the unstable modes in the plant are located. The material and energy balance equations have been *translated* and *refined* directly from the input-output block to sub-blocks a and b generated from the previous level. It is not required to maintain the material and energy balances at the tee junction (defined by system boundary c) as no accumulation is possible. The maintenance of each components in both sub-blocks should be of the same priority. The specific control objectives related to production specifications can be directly observed from the product streams and so these objectives have been assigned to the generalized separation block. Optimization objectives such as goals 10 and 11 are applicable to the entire plant and remain to be global objectives. No new objectives become observable at this level. The prioritization for the control objectives developed at the earlier stages of the designed has been maintained. No further refinement or spawning opportunities cannot be identified. Refinement of optimization objectives will only be studied after we have assigned manipulations to all other more important ones.

Table 11 - 17: Prioritized Control Objectives at the Generalized Reaction-Separation Level

	Reaction Block sub-block *a*	Separation Block sub-block *b*
2-1	Reactor Temperature	
2-2	Reactor Level	
2-3	$r_{C\text{-}(a)}$	$r_{C\text{-}(b)}$
2-4	$r_{A\text{-}(a)}$	$r_{A\text{-}(b)}$
2-5	$r_{E\text{-}(a)}$	$r_{E\text{-}(b)}$
2-6	$r_{B\text{-}(a)}$	$r_{B\text{-}(b)}$
2-7	$e_{(a)}$	$e_{(b)}$
2-8		G/H ratio
2-9		Production (modes 1,2,3)
2-10	Maximize Production (modes 4, 5 and 6)	
2-11	Minimize Cost	

Verify Feasibility of Control Objectives

At this refined level, material balances around sub-block *a* gives the following refined definition of G_{R1} and G_{R2}:

$$G_{R1} = F_{7,G} - F_{8,G} - F_{5,G} \qquad [11\text{-}19]$$

$$G_{R2} = F_{7,H} - F_{8,H} - F_{5,H} \qquad [11\text{-}20]$$

Then, according to Equation [11-7], we cannot simultaneously specify all of the variables in the following equation:

$$(F_{7,G} - F_{8,G} - F_{5,G}) / (F_{7,H} - F_{8,H} - F_{5,H}) = \beta - 1 \qquad [11\text{-}21]$$

The choice of control objectives must not cause [11-7] and [11-21] to be overspecified.

Quantifying Process Behavior at Level 2

The open-loop gains of each of the material accumulations in the system caused by a 1% change in the flow perturbation have been estimated and compiled in Appendix C.4. The impact of model uncertainty in on the process gains will be computed based on the variation of the gain over the entire operating region.

Synthesize Control Structure at the Generalized Reaction-Separation Level

The goal at this level is to identify the notional control associations for the achievement of control objectives observable from the representation shown in Figure 11-5. Again, changes of all flow components except those of the feed streams will be considered as potential manipulated variables. Control structure at this level can be synthesized using long-horizon design criteria. The Consistency Logic Map (Section 8.4.2) will be followed throughout the development. The stabilization control strategy associated with Goal 2-1 and Goal 2-2 of our hierarchy of control objectives in Table 11-17 is still valid. Synthesis will proceed with Goal 2-3.

Goal 2-3: Maintain material balance control of C

At Level 1, F_4 (Feed C) was assigned to maintain the overall material balance control of C. According to *Consistency Logic 3*, F_4 should be among the best manipulated variables at this level as well. Furthermore, F_4 is observable from sub-block *b*, F_4 is expected to be among one of the best possible manipulations for maintaining the material balance of C in that sub-block (*Consistency Logic 1*). The other potential candidates would come from newly observable manipulations, such as component flows in F_5, F_{12} and F_7. According to *Consistency Logic 2*, any manipulated variables are potential candidates for maintaining the material balance in sub-block *a*. In summary, the primary manipulated variables for each sub-block will be selected from the following sets:

1. $r_{C\text{-}(a)}$: {all manipulated variables}
2. $r_{C\text{-}(b)}$: {component flows in F_4, F_5, F_{12} and F_7 }

The open-loop gains of $r_{C\text{-}(a)}$ and $r_{C\text{-}(b)}$ are complied Tables 11-18 and 11-19 respectively. Judging from the magnitudes of the gains and the size of the robustness measure, F_4 is a good candidate for the control of $r_{C\text{-}(b)}$. Note that the best manipulated variables are indeed the flow of C in F_4, F_5, F_{12} and F_7. F_{11}, a manipulation found to be unsatisfactory for the control of r_C at Level 1 is indeed the worst manipulation at this Level. The observation is consistent with *Consistency Logic 1*. $F_{5,C}$ is equally effective for the control of $r_{C\text{-}(b)}$ and $r_{C\text{-}(a)}$. Since the goal is to divert disturbances to the environment as early as possible, F_4 is assigned to $r_{C\text{-}(b)}$ and $F_{5,C}$ to $r_{C\text{-}(a)}$. Assuming $r_{C\text{-}(a)}$ is of higher priority, it can be easily verified (by computing the closed-loop gains) that F_4 would remain to be the best candidate for the control of $r_{C\text{-}(b)}$ while $F_{5,C}$ is being used to $r_{C\text{-}(a)}$.

Goal 2-4: Maintain material balance control of A

At Level 1, F_2 (Feed D) was assigned to Modes 1, 2, 3 and 5; F_1 (Feed A) was assigned to Modes 4 and 6. According to the consistency logic developed earlier, the potential manipulated variables for each sub-goal would come from the following sets:

1. $r_{A\text{-}(a)}$: { component flows in F_2, F_8, F_5 and F_7 } - Modes 1, 2, 3 and 5
   { component flows in F_1, F_8, F_5 and F_7 } - Modes 4 and 6
2. $r_{A\text{-}(b)}$: { all manipulated variables }

The closed-loop gains of the two sub-goals are shown in Tables 11-20 and 11-21. For $r_{A\text{-}(a)}$, $F_{7,A}$, $F_{5,A}$, $F_{8,A}$ and F_2 are good candidates. Although the gains of $F_{7,A}$, $F_{5,A}$ and $F_{8,A}$ are greater than that of F_1 and F_2, varying $F_{7,A}$ and $F_{5,A}$ would divert disturbances to downstream operation. It is our preference to divert disturbances to the environment as soon as possible. We will keep F_2 (modes 1, 2, 3 and 5) and F_1 (modes 4 and 6) be the manipulated variables for $r_{A\text{-}(a)}$.

For $r_{A\text{-}(b)}$, $F_{7,A}$, $F_{5,A}$ and $F_{12,A}$ are good choices. Variation in any of these flows would affect both the downstream and upstream operation. Again, it is desirable to divert disturbances to the environment as soon as possible. Since the gains of $F_{12,A}$ are the largest and this stream is closest to the vent of the process, we will assign $F_{12,A}$ to $r_{A\text{-}(b)}$. The chosen assignment do not have conflict under closed-loop control.

Goal 2-5: Maintain material balance control of E

At Level 1, F_3 (Feed E) was assigned to control r_E at Modes 1, 2, 3, 4 and 6; F_1 (Feed A) at mode 5. Then, the potential manipulated variables are:

1. $r_{E\text{-}(a)}$: {component flows in F_3, F_8, F_5, F_7 } - Modes 1, 2, 3, 4 and 6
   {component flows in F_1, F_8, F_5, F_7 } - Mode 5
2. $r_{E\text{-}(b)}$: {all manipulated variables}

The closed-loop gains can be found Tables 11-22 and 11-23. The ability to divert disturbances to the environment as soon as possible makes F_3 an attractive candidate for the maintenance of $r_{E\text{-}(a)}$ at Modes 1, 2, 3, 4 and 6; F_1 an attractive candidate for the maintenance of $r_{E\text{-}(a)}$ at Mode 5. For $r_{E\text{-}(b)}$, $F_{7,E}$, $F_{7,G}$ and $F_{12,E}$ are the best manipulated variables. Since E is associated with reaction R3 which produces liquid products G and H, we should therefore divert variation in the inventory of E to the heavier streams such as F_7 or F_{11}. $F_{7,E}$ appears to be the best choice for Modes 1, 2, 4 and 5 while $F_{7,G}$ appears to be the best for Modes 3 and 6. Since Modes 3 and 6 operate at an extreme G/H ratio, a different manipulated variable is required to maintain the inventory. The chosen assignment do not have conflict under closed-loop control.

Goal 2-6: Maintain material balance control of B

$F_{9,B}$ had been chosen at the previous level to maintain r_B. Since $F_{9,B}$ is related to $F_{12,B}$ and $F_{8,B}$ by the material balance around system boundary *c* , the potential variables are:

1. $r_{B\text{-}(a)}$: { component flows in F_8, F_5, F_7}
2. $r_{B\text{-}(b)}$: { component flows in F_{12}, F_5, F_7}

$F_{7,B}$, $F_{8,B}$ and $F_{12,B}$ are clearly the best manipulated variables (see Tables 11-24 and 11-25). To ensure fast diversion of disturbances to the environment, $F_{8,B}$ and $F_{12,B}$ will be assigned to $r_{B\text{-}(a)}$ and $r_{B\text{-}(b)}$ respectively. The chosen assignment do not have conflict under closed-loop control.

Goal 2-7: Maintain Energy balance control

Both of the coolants have already been assigned to maintain the stability of the plant. These control assignments implicitly maintain the energy balance of the plant.

Goal 2-8: G/H ratio in product stream

The ratio $F_{11,G} / F_{11,H}$ has the most direct influence on the ratio in the product stream.

Table 11 - 18: Open-loop Gains of $r_{C-(a)}$ at the Generalized Reaction-Separation Level

	Base	Mode2	Mode 3	Mode4	Mode 5	Mode6	C_g
F_1	0	0	0	0	0	0	
F_4	0	0	0	0	0	0	
F_3	0	0	0	0	0	0	
F_2	0	0	0	0	0	0	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	3.39	3.44	3.44	3.44	3.45	3.48	1.03
$F_{5,D}$	0	0	0	0	0	0	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0	0	0	0	0	0	
$F_{5,G}$	0.21	0.03	0.25	0.09	0.03	0.28	11.1
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	-2.92	-3.26	-3.82	-2.98	-3.20	-3.28	1.31
$F_{7,D}$	0	0	0	0	0	0	
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	0	0	0	0	0	0	
$F_{7,G}$	-3.29	-0.67	-12.01	-3.40	-0.66	-10.2	18.1
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79	5.03
$F_{8,A}$	0	0	0	0	0	0	
$F_{8,B}$	0	0	0	0	0	0	
$F_{8,C}$	1.93	2.09	3.62	2.07	2.05	2.94	1.87
$F_{8,D}$	0	0	0	0	0	0	
$F_{8,E}$	0	0	0	0	0	0	
$F_{8,F}$	0	0	0	0	0	0	
$F_{8,G}$	0.90	0.19	3.69	0.51	0.18	2.64	20.8
$F_{8,H}$	0.47	0.83	0.20	0.24	0.78	0.14	5.97
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 19: Open-loop Gains of $r_{C\text{-}(b)}$ at the Generalized Reaction-Separation Level

	Base	Mode2	Mode 3	Mode 4	Mode 5	Mode6	C_g
F_1	0	0	0	0	0	0	
F_4	3.47	3.47	3.47	3.47	3.47	3.47	1.00
F_3	0	0	0	0	0	0	
F_2	0	0	0	0	0	0	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	-0.11	-0.05	-0.05	-0.04	-0.05	-0.05	2.55
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	-2.41	-0.53	-4.09	-2.38	-0.53	-4.08	7.75
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37	10.6
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	-3.39	-3.44	-3.44	-3.44	-3.45	-3.48	1.03
$F_{5,D}$	0	0	0	0	0	0	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0	0	0	0	0	0	
$F_{5,G}$	-0.21	-0.03	-0.25	-0.09	-0.03	-0.28	11.1
$F_{5,H}$	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	2.92	3.26	3.82	2.98	3.20	3.28	1.31
$F_{7,D}$	0	0	0	0	0	0	
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	0	0	0	0	0	0	
$F_{7,G}$	3.29	0.67	12.01	3.40	0.66	10.20	18.1
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79	5.03
$F_{8,A}$	0	0	0	0	0	0	
$F_{8,B}$	0	0	0	0	0	0	
$F_{8,C}$	0	0	0	0	0	0	
$F_{8,D}$	0	0	0	0	0	0	
$F_{8,E}$	0	0	0	0	0	0	
$F_{8,F}$	0	0	0	0	0	0	
$F_{8,G}$	0	0	0	0	0	0	
$F_{8,H}$	0	0	0	0	0	0	
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	-1.95	-2.14	-3.66	-2.13	-2.10	-2.98	1.88
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	-0.92	-0.19	-3.73	-0.52	-0.18	-2.68	20.5
$F_{12,H}$	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14	6.03

Table 11 - 20: Closed-loop Gains of $r_{A\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode2	Mode 3	Mode4	Mode 5	Mode6	C_g
F_1	0.45	0.45	0.45	0.45	0.45	0.45	1.00
F_4	0	0	0	0	0	0	
F_3	2.00E-04	2.00E-04	2.00E-04	2.00E-04	2.00E-04	2.00E-04	1.01
F_2	1.21	1.21	1.21	1.21	1.21	1.21	1.00
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	3.24	3.29	3.29	3.28	3.28	3.42	1.06
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	3.50E-03	0.00E+00	9.20E-03	2.60E-03	1.00E-04	1.40E-02	Inf
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0.13	0.19	0.05	0.19	0.20	0.06	4.15
$F_{5,G}$	0.35	0.05	0.41	0.15	0.04	0.47	11.14
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01	9.34
$F_{7,A}$	-7.32	-8.16	-11.49	-7.78	-8.06	-9.61	1.57
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	0	0	0	0	0	0	
$F_{7,D}$	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49	32.59
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76	2.39
$F_{7,G}$	-5.49	-1.12	-20.02	-5.66	-1.11	-17.00	18.09
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79	5.04
$F_{8,A}$	4.78	5.24	10.93	5.40	5.18	8.63	2.29
$F_{8,B}$	0	0	0	0	0	0	
$F_{8,C}$	0	0	0	0	0	0	
$F_{8,D}$	0.09	0.01	0.57	0.06	0.01	0.42	46.66
$F_{8,E}$	0	0	0	0	0	0	
$F_{8,F}$	0.78	1.05	0.71	0.75	1.05	0.58	1.83
$F_{8,G}$	1.50	0.31	6.15	0.85	0.30	4.40	20.76
$F_{8,H}$	0.47	0.83	0.20	0.24	0.78	0.14	5.97
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 21: Closed-loop Gains of $r_{A-(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	C_g
F_1	0	0	0	0	0	0	
F_4	0	0	0	0	0	0	
F_3	0	0	0	0	0	0	
F_2	0	0	0	0	0	0	
$F_{11,A}$	-0.09	-0.02	-0.02	-0.03	-0.03	-0.02	4.12
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	1.08E-01	4.35E-02	5.19E-02	4.24E-02	4.34E-02	4.30E-02	2.55
$F_{11,D}$	-3.00E-04	0.00E+00	-9.00E-04	-6.00E-04	0.00E+00	-9.00E-04	30.33
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	-8.60E-03	-1.32E-02	-3.20E-03	-1.96E-02	-1.45E-02	-3.60E-03	6.16
$F_{11,G}$	-1.72	-0.38	-2.93	-1.70	-0.38	-2.92	7.75
$F_{11,H}$	-9.34E-02	-1.94E-01	-1.81E-02	-9.51E-02	-1.90E-01	-1.81E-02	10.69
$F_{5,A}$	-3.2365	-3.2857	-3.2852	-3.283	-3.2844	-3.4173	1.06
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	-3.50E-03	0.00E+00	-9.20E-03	-2.60E-03	-1.00E-04	-1.40E-02	Inf
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	-1.32E-01	-1.95E-01	-4.86E-02	-1.91E-01	-2.02E-01	-6.23E-02	4.15
$F_{5,G}$	-0.35	-0.05	-0.41	-0.15	-0.04	-0.47	11.14
$F_{5,H}$	-0.1108	-0.1226	-0.0131	-0.0429	-0.1103	-0.0148	9.34
$F_{7,A}$	7.32	8.16	11.49	7.78	8.06	9.61	1.57
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	0	0	0	0	0	0	2.66
$F_{7,D}$	1.37E-01	1.93E-02	6.23E-01	9.04E-02	1.91E-02	4.86E-01	32.58
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	1.33	1.82	0.87	1.37	1.83	0.76	2.39
$F_{7,G}$	5.49	1.12	20.02	5.66	1.11	17.00	18.09
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79	5.04
$F_{8,A}$	0	0	0	0	0	0	
$F_{8,B}$	0	0	0	0	0	0	
$F_{8,C}$	-1.84	-1.99	-3.44	-1.97	-1.95	-2.80	1.87
$F_{8,D}$	0	0	0	0	0	0	
$F_{8,E}$	0	0	0	0	0	0	
$F_{8,F}$	0	0	0	0	0	0	
$F_{8,G}$	-0.86	-0.18	-3.51	-0.48	-0.17	-2.51	20.76
$F_{8,H}$	-0.45	-0.79	-0.19	-0.23	-0.74	-0.13	5.96
$F_{12,A}$	-4.90	-5.37	-11.05	-5.57	-5.31	-8.75	2.25
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	1.85	2.04	3.48	2.03	2.00	2.84	1.88
$F_{12,D}$	-0.09	-0.01	-0.58	-0.06	-0.01	-0.43	45.96
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	-0.80	-1.08	-0.72	-0.78	-1.08	-0.58	1.85
$F_{12,G}$	-0.66	-0.14	-2.67	-0.37	-0.13	-1.92	20.44
$F_{12,H}$	-2.35E-02	-4.23E-02	-9.70E-03	-1.21E-02	-3.91E-02	-6.90E-03	6.13

Table 11 - 22: Closed-loop Gains of $r_{E\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 5	C_g	Mode 4	Mode 6	C_g
F_1	-0.45	-0.45	-0.45	-0.45	1.00	0	0	
F_4	0	0	0	0		0	0	
F_3	1.82	1.81	1.82	1.82	1.00	1.82	1.82	1.00
F_2	0	0	0	0		1.21	1.21	1.00
$F_{11,A}$	0	0	0	0		0	0	
$F_{11,B}$	0	0	0	0		0	0	
$F_{11,C}$	0	0	0	0		0	0	
$F_{11,D}$	0	0	0	0		0	0	
$F_{11,E}$	0	0	0	0		0	0	
$F_{11,F}$	0	0	0	0		0	0	
$F_{11,G}$	0	0	0	0		0	0	
$F_{11,H}$	0	0	0	0		0	0	
$F_{5,A}$	-3.24	-3.29	-3.29	-3.28	1.02	0	0	
$F_{5,B}$	0	0	0	0		0	0	
$F_{5,C}$	0	0	0	0		0	0	
$F_{5,D}$	0	0	0	0		2.60E-03	1.40E-02	5.38
$F_{5,E}$	0.40	0.58	0.11	0.62	5.77	0.52	0.13	3.97
$F_{5,F}$	0	0	0	0		0.19	0.06	3.07
$F_{5,G}$	-0.21	-0.03	-0.25	-0.03	9.79	6.05E-02	1.87E-01	3.10
$F_{5,H}$	0	0	0	0		4.29E-02	1.48E-02	2.90
$F_{7,A}$	7.32	8.16	11.49	8.06	1.57	0	0	
$F_{7,B}$	0	0	0	0		0	0	
$F_{7,C}$	0	0	0	0		0	0	
$F_{7,D}$	0	0	0	0		-0.09	-0.49	5.38
$F_{7,E}$	-3.99	-5.52	-1.89	-5.62	2.97	-3.70	-1.60	2.32
$F_{7,F}$	0	0	0	2.00E-04		-1.37	-0.76	1.80
$F_{7,G}$	3.29	0.67	12.01	0.66	18.08	-2.26	-6.80	3.00
$F_{7,H}$	0	0	0	3.00E-04		-2.48	-0.79	3.13
$F_{8,A}$	-4.78	-5.24	-10.93	-5.18	2.29	0	0	
$F_{8,B}$	0	0	0	0		0	0	
$F_{8,C}$	0	0	0	0		0	0	
$F_{8,D}$	0	0	0	0		0.06	0.42	7.04
$F_{8,E}$	2.35	3.20	1.55	3.23	2.09	2.03	1.21	1.68
$F_{8,F}$	0	0	0	-1.0E-04	0.00	0.75	0.58	1.31
$F_{8,G}$	-0.90	-0.19	-3.69	-0.18	20.76	0.34	1.76	5.21
$F_{8,H}$	0	0	0	-1.0E-04		0.24	0.14	1.73
$F_{12,A}$	0	0	0	0		0	0	
$F_{12,B}$	0	0	0	0		0	0	
$F_{12,C}$	0	0	0	0		0	0	
$F_{12,D}$	0	0	0	0		0	0	
$F_{12,E}$	0	0	0	0		0	0	
$F_{12,F}$	0	0	0	0		0	0	
$F_{12,G}$	0	0	0	0		0	0	
$F_{12,H}$	0	0	0	0		0	0	

Table 11 - 23: Closed-loop Gains of $r_{E\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 5	C_g	Mode 4	Mode 6	C_g
F_1	0	0	0	0		0	0	
F_4	0	0	0	0		0	0	
F_3	0	0	0	0		0	0	
F_2	0	0	0	0		0	0	
$F_{11,A}$	0	0	0	0		0	0	
$F_{11,B}$	0	0	0	0		0	0	
$F_{11,C}$	0	0	0	0		0	0	
$F_{11,D}$	-3.00E-04	0	-9.00E-04	0		-6.00E-04	-9.00E-04	1.50
$F_{11,E}$	-2.72E-02	-4.18E-02	-7.30E-03	-4.58E-02	6.27	-5.39E-02	-8.20E-03	6.57
$F_{11,F}$	-8.60E-03	-1.32E-02	-3.20E-03	-1.45E-02	4.53	-1.96E-02	-3.60E-03	5.44
$F_{11,G}$	-1.60	-0.35	-2.73	-0.35	7.75	-1.58	-2.72	1.72
$F_{11,H}$	-1.91	-3.89	-0.37	-3.88	10.47	-1.94	-0.37	5.24
$F_{5,A}$	0	0	0	0		0	0	
$F_{5,B}$	0	0	0	0		0	0	
$F_{5,C}$	0	0	0	0		0	0	
$F_{5,D}$	-3.50E-03	0	-9.20E-03	-1.00E-04		-2.60E-03	-1.40E-02	5.38
$F_{5,E}$	-0.40	-0.58	-0.11	-0.62	5.77	-0.52	-0.13	3.97
$F_{5,F}$	-0.13	-0.19	-0.05	-0.20	4.15	-0.19	-0.06	3.07
$F_{5,G}$	-0.14	-0.02	-0.16	-0.02	9.79	-0.06	-0.19	3.10
$F_{5,H}$	-0.11	-0.12	-0.01	-0.11	9.36	-0.04	-0.01	2.90
$F_{7,A}$	0	0	0	0		0	0	
$F_{7,B}$	0	0	0	0		0	0	
$F_{7,C}$	0	0	0	0		0	0	
$F_{7,D}$	0.14	0.02	0.62	0.02	32.62	0.09	0.49	5.38
$F_{7,E}$	3.99	5.52	1.89	5.62	2.97	3.70	1.60	2.32
$F_{7,F}$	1.33	1.82	0.87	1.83	2.09	1.37	0.76	1.80
$F_{7,G}$	2.19	0.45	8.01	0.44	18.09	2.26	6.80	3.00
$F_{7,H}$	2.18	3.99	0.92	3.99	4.33	2.48	0.79	3.13
$F_{8,A}$	0	0	0	0		0	0	
$F_{8,B}$	0	0	0	0		0	0	
$F_{8,C}$	0	0	0	0		0	0	
$F_{8,D}$	0	0	0	0		0	0	
$F_{8,E}$	0	0	0	0		0	0	
$F_{8,F}$	0	0	0	0		0	0	
$F_{8,G}$	0	0	0	0		0	0	
$F_{8,H}$	0	0	0	0		0	0	
$F_{12,A}$	0	0	0	0		0	0	
$F_{12,B}$	0	0	0	0		0	0	
$F_{12,C}$	0	0	0	0		0	0	
$F_{12,D}$	-0.09	-0.01	-0.58	-0.01	46.10	-0.06	-0.43	6.90
$F_{12,E}$	-2.41	-3.28	-1.56	-3.32	2.12	-2.10	-1.22	1.71
$F_{12,F}$	-0.80	-1.08	-0.72	-1.08	1.50	-0.78	-0.58	1.33
$F_{12,G}$	-0.61	-0.13	-2.48	-0.12	20.45	-0.35	-1.79	5.11
$F_{12,H}$	-0.48	-0.85	-0.20	-0.80	4.28	-0.25	-0.14	1.76

Table 11 - 24: Closed-loop Gains of $r_{B\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	C_g	Mode 3	Mode 6	C_g	Mode 4	Mode 5
F_1	-2.28E-05	-4.20E-05	1.84	0	0		0	0
F_4	0	0		0	0		0	0
F_3	0	0		0	0		0	-9.15E-05
F_2	0	0		0	6.11E-05	inf	1.00E-04	0
$F_{11,A}$	0	0		0	0		0	0
$F_{11,B}$	0	0		0	0		0	0
$F_{11,C}$	0	0		0	0		0	0
$F_{11,D}$	-4.52E-12	-5.80E-13	7.79	0	2.27E-07	inf	0	1.51E-09
$F_{11,E}$	-4.11E-10	-8.03E-10	1.96	0	2.04E-06	inf	0	2.30E-06
$F_{11,F}$	-1.30E-10	-2.53E-10	1.95	0	9.07E-07	inf	0	7.30E-07
$F_{11,G}$	-2.42E-08	-6.78E-09	3.56	1.00E-03	6.80E-04	1.47	0	1.77E-05
$F_{11,H}$	-2.87E-08	-7.47E-08	2.60	1.00E-04	9.24E-05	1.08	0	1.95E-04
$F_{5,A}$	-4.87E-04	-6.33E-04	1.30	-5.00E-04	-3.41E-04	1.46	-3.00E-04	-3.28E-04
$F_{5,B}$	3.67E-02	3.13E-02	1.17	3.14E-02	2.41E-01	7.68	3.40E-02	3.31E-02
$F_{5,C}$	0	0		0	0		0	0
$F_{5,D}$	-5.26E-07	0		0	2.10E-06	inf	0	-8.45E-09
$F_{5,E}$	2.00E-14	9.00E-14	4.50	0	3.24E-05	inf	0	8.97E-11
$F_{5,F}$	-1.99E-05	-3.75E-05	1.88	0	9.34E-06	inf	0	-2.02E-05
$F_{5,G}$	-5.33E-05	-8.97E-06	5.94	0	-8.17E-10	inf	0	-4.20E-06
$F_{5,H}$	-1.67E-05	-2.36E-05	1.42	0	2.21E-06	inf	0	-1.10E-05
$F_{7,A}$	1.10E-03	1.60E-03	1.45	1.70E-03	9.60E-04	1.77	8.00E-04	8.06E-04
$F_{7,B}$	-4.90	-2.63	1.86	-18.59	-14.93	1.25	-3.02	-2.52
$F_{7,C}$	0	0		0	0		0	0
$F_{7,D}$	0	0		-1.00E-04	-7.28E-05	1.37	0	1.912E-06
$F_{7,E}$	0	0		-7.00E-04	-3.99E-04	1.76	0	0
$F_{7,F}$	2.00E-04	4.00E-04	2.00	-2.00E-04	-1.14E-04	1.75	1.00E-04	1.83E-04
$F_{7,G}$	8.00E-04	2.00E-04	4.00	0	0		6.00E-04	1.11E-04
$F_{7,H}$	3.00E-04	8.00E-04	2.67	-2.00E-04	-1.19E-04	1.68	2.00E-04	3.99E-04
$F_{8,A}$	-7.00E-04	-1.00E-03	0.70	-1.60E-03	-8.62E-04	1.86	-5.00E-04	-5.18E-04
$F_{8,B}$	3.17	1.68	1.88	17.69	13.39	1.32	2.10	1.62
$F_{8,C}$	0	0		0	0		0	0
$F_{8,D}$	0	0		-1.00E-04	-4.2E-05	2.38	0	-1.84E-06
$F_{8,E}$	0	0		0	1.209E-08	inf	0	-1.63E-04
$F_{8,F}$	-1.00E-04	-2.00E-04	2.00	-1.00E-04	-5.75E-05	1.74	-1.00E-04	-1.58E-04
$F_{8,G}$	-2.00E-04	-1.00E-04	2.00	-9.00E-04	-4.00E-04	2.05	-1.00E-04	-3.56E-05
$F_{8,H}$	-1.00E-04	-2.00E-04	2.00	0	-1.39E-05		0	-1.17E-04
$F_{12,A}$	0	0		0	0		0	0
$F_{12,B}$	0	0		0	0		0	0
$F_{12,C}$	0	0		0	0		0	0
$F_{12,D}$	-1.34E-09	-2.44E-10	5.51	2.00E-04	1.06E-04	1.88	0	6.32E-07
$F_{12,E}$	-3.63E-08	-6.30E-08	1.74	6.00E-04	3.05E-04	1.96	0	1.67E-04
$F_{12,F}$	-1.21E-08	-2.08E-08	1.72	3.00E-04	1.46E-04	2.06	0	5.42E-05
$F_{12,G}$	-9.26E-09	-2.48E-09	3.74	9.00E-04	4.46E-04	2.02	0	6.12E-06
$F_{12,H}$	-7.24E-09	-1.63E-08	2.25	1.00E-04	3.51E-05	2.85	0	4.01E-05

Table 11 - 25: Closed-loop Gains of $r_{B\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	C_g	Mode 3	Mode 6	C_g	Mode 4	Mode 5
F_1	0	0		0	0		0	0
F_4	0	0		0	0		0	0
F_3	0	0		0	0		0	0
F_2	0	0		0	0		0	0
$F_{11,A}$	0	0		0	0		0	0
$F_{11,B}$	-4.50E-07	-2.27E-02	50444	-4.50E-03	-4.00E-04	11.25	-4.00E-04	-2.27E-03
$F_{11,C}$	1.09E-03	4.49E-04	2.42	5.00E-04	4.43E-04	1.13	4.00E-04	4.48E-04
$F_{11,D}$	0	0		0	-1.86E-11		0	0
$F_{11,E}$	0	0		0	-1.66E-10		0	0
$F_{11,F}$	0	0		0	-7.4E-11		0	0
$F_{11,G}$	2.3E-02	5.19E-03	4.44	4.01E-02	4.00E-02	1.00	2.33E-02	5.17E-03
$F_{11,H}$	1.82E-02	3.81E-02	2.09	3.60E-03	3.63E-03	1.01	1.90E-02	3.80E-02
$F_{5,A}$	0	0		0	0		0	0
$F_{5,B}$	-3.67E-02	-3.13E-02	1.17	-3.14E-02	-2.41E-01	7.68	-3.40E-02	-3.31E-02
$F_{5,C}$	0	0		0	0		0	0
$F_{5,D}$	0	0		0	-2.86E-10		0	0
$F_{5,E}$	0	0		0	-2.65E-09		0	0
$F_{5,F}$	0	0		0	-1.27E-09		0	0
$F_{5,G}$	3.53E-08	-1.98E-08	-1.8	0	4.362E-08		0	3.90E-08
$F_{5,H}$	-1.11E-08	4.83E-08	-4.3	0	-3.84E-10		0	4.81E-08
$F_{7,A}$	0	0		0	0		0	0
$F_{7,B}$	4.90	2.63	1.86	18.59	14.93	1.25	3.02	2.52
$F_{7,C}$	3.16E-08	5.78E-08	1.83	0	-3.06E-08	0.00	0	-2.18E-08
$F_{7,D}$	0	0		0	9.91E-09		0	0
$F_{7,E}$	0	0		0	3.26E-08		0	0
$F_{7,F}$	0	0		0	1.56E-08		0	0
$F_{7,G}$	4.64E-08	2.34E-08	1.98	0	0		0	1.55E-08
$F_{7,H}$	-1.71E-08	2.28E-08	-1.3	0	-8.8E-09		0	8.30E-08
$F_{8,A}$	0	0		0	0		0	0
$F_{8,B}$	0	0		0	0		0	0
$F_{8,C}$	-1.85E-02	-2.05E-02	1.11	-3.55E-02	-2.89E-02	1.23	-2.03E-02	-2.01E-02
$F_{8,D}$	0	0		0	0		0	0
$F_{8,E}$	0	0		0	0		0	0
$F_{8,F}$	0	0		0	0		0	0
$F_{8,G}$	-0.01	0.00	4.78	-0.04	-0.03	1.40	-5.00E-03	-1.74E-03
$F_{8,H}$	0.00	-0.01	1.80	0.00	0.00	1.40	-2.40E-03	-7.62E-03
$F_{12,A}$	0	0		0	0		0	0
$F_{12,B}$	-3.28	-1.73	1.90	-17.87	-13.58	1.32	-2.16	-1.66
$F_{12,C}$	1.87E-02	2.10E-02	1.12	3.58E-02	2.93E-02	1.22	2.09E-02	2.06E-02
$F_{12,D}$	0	0		0	-8.69E-09		0	0
$F_{12,E}$	0	0		0	-2.49E-08		0	0
$F_{12,F}$	0	0		0	-1.19E-08		0	0
$F_{12,G}$	8.80E-03	1.90E-03	4.63	3.65E-02	2.63E-02	1.39	5.10E-03	1.79E-03
$F_{12,H}$	4.60E-03	8.30E-03	1.80	1.90E-03	1.38E-03	1.38	2.40E-03	7.81E-03

Goal 2-9: Production rate (Modes 1, 2 and 3 only)

The flow of F_{11} has the most direct effect on the production rate.

Goal 2-10: Maximize Production Rate (Modes 4, 5 and 6)

Production can be maximized by maximizing the use of the limiting raw materials. Feed D (F_2) is the limiting raw materials for Modes 4 and 6 and Feed E (F_3) is the limiting raw material for Mode 5. Maximizing the use of these material streams within the process constraints maximizes the plant's throughput.

Goal 2-11: Minimize Production Cost

The objectives function for the cost optimization in Equation [11-13] applies to this level as well. The cost optimization can be written as:

$$\begin{aligned}\text{Min } \Phi = {} & c_A F_{9,A} + c_C F_{9,C} + c_D F_{9,D} + c_E F_{9,E} + c_F F_{9,F} + c_G F_{9,G} + c_H F_{9,H} \\ & + c_D F_{11,D} + c_G F_{11,G} + c_F F_{11,F} + C_{compress}\, W + C_{steam} F_{steam}\end{aligned}$$

s.t.

1. maintain reactor temperature at the desired level
2. maintain reactor level at the desired level
3. maintain accumulation of C at the desired level
4. maintain accumulation of A at the desired level
5. maintain accumulation of E at the desired level
6. maintain accumulation of B at the desired level
7. maintain energy balance control
8. $F_{11,G} / F_{11,H}$ at the pre-specified value
9. F_{11} at the pre-specified value for Modes 1, 2 and 3
10. maximize production rate for Modes 4, 5 and 6

Constraints 1 to 10 correspond to the control objectives relevant at this level. The degrees of freedom in the optimization can be further reduced by considering the relationships below.

<u>Stoichiometry</u> :

The following relationship identified earlier is a constraint as a result of the specification in the product stream.

$$(F_{7,G} - F_{8,G} - F_{5,G}) / (F_{7,H} - F_{8,H} - F_{5,H}) = \beta - 1 \qquad [11\text{-}21]$$

Material Balances around the splitter :

The following equations are related to the component balances around system boundary *c*. These balances are not under closed-loop control as materials do not accumulate in this sub-system.

$$F_{12,i} = F_{8,i} + F_{9,i} \qquad [11\text{-}22]$$

$$F_{9,j}/F_{12,j} = F_{9,i}/F_{12,i} \text{ for all } j \neq i \qquad [11\text{-}23]$$

Thermodynamic Relations :

At this level, one may visualize the separation system as a unit which distributes a fictitious steam F_+ into a vapor stream F_{vap} ($= F_5 + F_{12}$) and a liquid stream F_{11} as shown in Figures 11-6. Using similar logic as those employed at Level 1, the following generic relationships exist for this fictitious separation unit:

$$f_1 (F_{+,i}, F_{vap,i}, F_{11,i}) = 0 \qquad [11\text{-}24]$$

$$f_2 (F_{+,i}, F_{vap,i}, F_{11,i}) = 0 \qquad [11\text{-}25]$$

where: $F_{vap,i} = F_{5,i} + F_{12,i}$

F_+ , P_+ and T_+ of sub-block *b* are not visible at this level so they are not degrees of freedom in the optimization. The remaining variables ($F_{vap,i}$ and $F_{11,i}$) are inter-related through thermodynamics relationships.

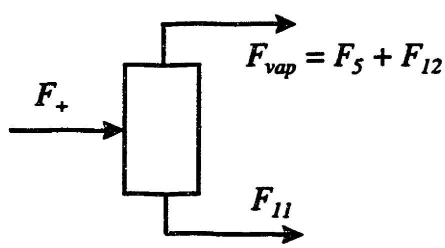


Figure 11 - 6: Pseudo Separation System in the Generalized Separation Block at Level 2

The initial component table for the generalized reaction-separation system has been set up in Table 11-26. Component flows which have been assigned to be the manipulated variables in the control system are indicated by "MV" in the table; small flows are marked "~0" and those which are associated with control objectives are indicated by "specified".

Table 11 - 26: Initial Component Table for the Generalized Reaction-Separation System

component	F_9	F_8	F_{12}	F_5	F_{11} (specified)
A			MV		~0
B			MV		~0
C				MV	~0
D					~0
E					~0
F					~0
G					
H					

<u>Degrees of Freedom Analysis</u> :

The following degrees of freedom analysis can be performed to reduce the design variables in the optimization. A variable becomes unavailable for optimization if its value is fixed by either the material balances, thermodynamic relations or stoichiometric constraints.

1. Similar to the previous level, with F_{11} and the product ratio being chosen as control objectives, the flow of $F_{11,G}$ and $F_{11,H}$ are no longer degrees of freedom. These variables have been marked "n/a" in Table 11-27.
2. as $F_{11,G}$ and $F_{11,H}$ are being fixed by the product specifications, with the thermodynamic relationships, $F_{vap,G}$ and $F_{vap,H}$ are fixed as well. This means $F_{12,G}$, $F_{12,H}$, $F_{5,G}$ and $F_{5,H}$ are not degrees of freedom in the optimization.
3. Since $F_{12,A}$, $F_{12,B}$ and $F_{5,C}$ have been chosen as manipulated variables, $F_{5,A}$, $F_{5,B}$ and $F_{12,C}$ are not available degrees of freedom.
4. At this level, with additional variables like F_8, F_{12} and F_5, we found that the thermodynamic relationships do not impose direct restrictions on the available degrees of freedom in F_9. All component flows in F_9 can be considered to be design variables and they are marked as " $\surd$ " in Table 11-27.

Table 11 - 27: Final Component Table for the Generalized Reaction-Separation System

component	F_9	F_8	F_{12}	F_5	F_{11} (specified)
A	√		MV	n/a	~0
B	√		MV	n/a	~0
C	√		n/a	MV	~0
D	√				~0
E	√				~0
F	√				~0
G	√		n/a	n/a	n/a
H	√		n/a	n/a	n/a

Then, the optimization becomes:

$$\text{Min } \Phi = c_A F_{9,A} + c_C F_{9,C} + c_D F_{9,D} + c_E F_{9,E} + c_F F_{9,F} + c_G F_{9,G} + c_H F_{9,H} + C_{compress} W + C_{steam} F_{steam} \quad [11\text{-}26]$$

s.t.:

1. maintain reactor temperature at the desired level
2. maintain reactor level at the desired level
3. maintain accumulation of C at the desired level
4. maintain accumulation of A at the desired level
5. maintain accumulation of E at the desired level
6. maintain accumulation of B at the desired level
7. maintain energy balance control
8. $F_{11,G} / F_{11,H}$ at the pre-specified value
9. F_{11} at the pre-specified value for Modes 1, 2 and 3
10. maximize production rate for Modes 4, 5 and 6
11. $F_{12,i} = F_{9,i} + F_{8,i}$
12. $F_{9,j} / F_{12,j} = F_{9,i} / F_{12,i}$ for all $j \neq i$

Constraints 11 and 12 are related to the material balances around system boundary *c*. Constraint 12 ensures that the mix in F_{12} are maintained in F_9 and F_8. Purge cost, which is primary made up of the raw materials in the process, is the largest component in the cost function. The operating cost can be minimized by minimizing the loss of raw materials in purge.

Control Structure at Level 2

The control structure at Level 2 is summarized in Table 11-28 and the structure for the base case is shown in Figure 11-7. Abstraction of the control strategy for the maintenance of material balances of C, A and E do produces the control structure at Level 1. Abstraction of the control strategy for the maintenance of material balance of B reduces to a the one developed at Level 1 as well if the self-regulating nature of material flows in sub-system *c* is taken into account. As $F_{8,B}$ and $F_{12,B}$ change, by the self-regulating nature, $F_{9,B}$ must vary accordingly to maintain a zero accumulation in this sub-system. Thus, all the control strategies that we have developed are compatible with those which we have synthesized at the earlier level. The control strategies developed at the previous level have facilitated the generation of control strategies that allow efficient diversion of process variations to the environment.

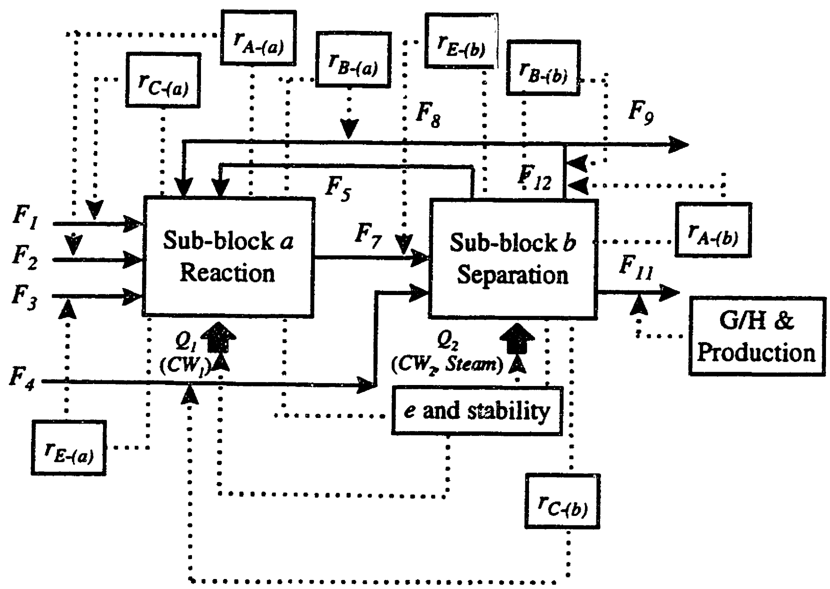


Figure 11 - 7: Control Structure for the Base Case at the Generalized Reaction-Separation Level

Table 11 - 28: Summary of Control Structure at Level 2 for all operation modes

	Base Case	**Mode 2**	**Mode 3**	**Mode 4**	**Mode 5**	**Mode 6**
	F_5 at saturation	F_5 at saturation	CW_2 at saturation	F_5, F_2 at saturation	F_5, F_3 at saturation	F_2, CW_2 at saturation
Reactor Temperature	CW_1	CW_1	CW_1	CW_1	CW_1	CW_1
Reactor Level	CW_2	CW_2	F_5 [1]	CW_2	CW_2	F_5 [1]
$r_{C\text{-}(a)}$	$F_{5,C}$	$F_{5,C}$	$F_{5,C}$	$F_{5,C}$	$F_{5,C}$	$F_{5,C}$
$r_{C\text{-}(b)}$	F_4	F_4	F_4	F_4	F_4	F_4
$r_{A\text{-}(a)}$	F_2	F_2	F_2	F_1 [2]	F_2	F_1 [2]
$r_{A\text{-}(b)}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$
$r_{E\text{-}(a)}$	F_3	F_3	F_3	F_3	F_1 [2]	F_3
$r_{E\text{-}(b)}$	$F_{7,E}$	$F_{7,E}$	$F_{7,G}$ [1]	$F_{7,E}$	$F_{7,E}$	$F_{7,G}$ [1]
$r_{B\text{-}(a)}$	$F_{8,B}$	$F_{8,B}$	$F_{8,B}$	$F_{8,B}$	$F_{8,B}$	$F_{8,B}$
$r_{B\text{-}(b)}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$
$e_{(a)}$ and $e_{(b)}$	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2
G/H	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$	$F_{11,G}/F_{11,H}$
Production	F_{11}	F_{11}	F_{11}			
Max. Production				F_2	F_3 [2]	F_2
Minimize Cost	minimize loss of raw materials in purge stream					

[1] Change of control structure due to the specification on G/H.

[2] Change of control structure due to saturation of limiting reactant.

11.3.3 Level 3: Detailed Reaction - Generalized Separation System

The process representation of the plant at Level 3 is shown in Figure 11-8. At this level, all the details of the reaction section has been revealed. The separation block remains unchanged. The additional manipulated variables are the component flows in F_6 and the agitator. As mentioned in Section 11.2, the agitator speed will be maintained at its maximum capacity to ensure the reactor is always at the perfectly mixed state. This new manipulated variable is therefore not a degree of freedom in our design. As the separation block is still an abstract view of the downstream separation, we will continue to use long-horizon design criteria at this stage of our analysis. Material balances corresponding to sub-system boundaries *d* and *e* can be found in Appendix C.3.

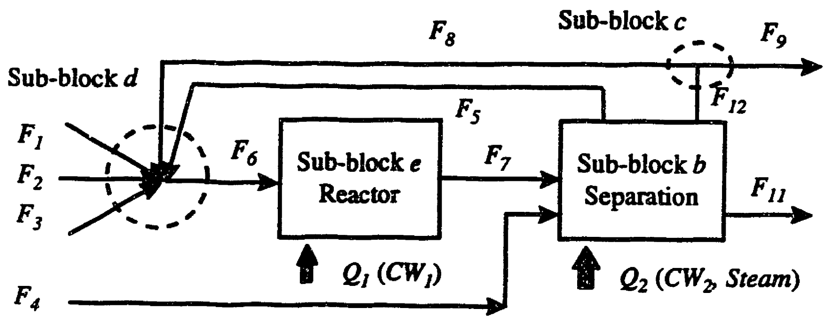


Figure 11 - 8: Process Representation of the Detailed reaction-Generalized Separation System (Level 3)

Progressive Generation of Control Objectives

Again, it is not required to maintain material and energy balances at the mixer (defined by system boundary *d*) since no accumulations is possible. The material and energy balance equations have been *translated* and *refined* directly from the reactor block to the reactor section. With the revelation of the detailed structure of the reactor, the operational constraints on the reactor temperature and pressure become visible control objectives. Since the control of reactor temperature is already involved in the process stabilization strategy, the operational constraint on reactor temperature is redundant. Only the management of reactor pressure will be considered in our design. Table 11-29 summarizes the control objectives at this level. See that we have retained the prioritization developed at the earlier levels.

Table 11 - 29: Prioritized Control Objectives at the Detailed Reaction - Generalized Separation Level

	Detailed Reactor *sub-block e*	Separation Block *sub-block b*
3-1	Reactor Temperature	
3-2	Reactor Level	
3-3	$r_{C\text{-}(e)}$	$r_{C\text{-}(b)}$
3-4	$r_{A\text{-}(e)}$	$r_{A\text{-}(b)}$
3-5	$r_{E\text{-}(e)}$	$r_{E\text{-}(b)}$
3-6	$r_{B\text{-}(e)}$	$r_{B\text{-}(b)}$
3-7	$e_{(e)}$	$e_{(b)}$
3-8		G/H ratio
3-9		Production (modes 1,2,3)
3-10	Reactor Pressure < 2895 kPa	
3-11	maximize production (modes 4, 5 and 6)	
3-12	minimize cost	

Verify Feasibility of Control Objectives

We must ensure that our control specifications do not violate any constraints imposed by stoichiometry.

At this level, G_{R1} and G_{R2} can be defined as:

$$G_{R1} = F_{7,G} - F_{6,G} \qquad [11\text{-}27]$$

$$G_{R2} = F_{7,H} - F_{6,H} \qquad [11\text{-}28]$$

Hence,

$$(F_{7,G} - F_{6,G}) / (F_{7,H} - F_{6,H}) = \beta - 1 \qquad [11\text{-}29]$$

Our control problem is properly posed as we have not simultaneously specifies all of the variables in Equation [11-29] in our design.

Quantify Process Behavior at Level 3

The open-loop gains for the objectives associated with the separation are not affected. The new manipulated variables (component flows in F_6 has no immediate impact on the control objectives in the separation level. Thus, the open-loop gains tabulated in Appendix C.4 still apply. The open-loop gains for $r_{C\text{-}(e)}$, $r_{A\text{-}(e)}$, $r_{E\text{-}(e)}$ and $r_{B\text{-}(e)}$ can be found in Appendix C.4. These data will be used to synthesize the control structure at this level.

Synthesize Control Structure at the Generalized Reaction-Separation Level

As process refinement from the previous level had been confined to the reaction section, we expect that modification of the control structure will centered in the reaction area as well. Synthesis begins at Goal 3.

Goal 3-3: Maintain material balance control of C

At the previous level, $F_{5,C}$ was assigned to maintain $r_{C\text{-}(a)}$ and F_4 was assigned to maintain $r_{C\text{-}(b)}$. Since sub-block *b* has not been further refined at this level, we expect F_4 to remain to be the best manipulated variable for $r_{C\text{-}(b)}$. For $r_{C\text{-}(e)}$, since the mixer at sub-block *d* is not a material capacitor, the influence of $F_{5,C}$ would directly affect $F_{6,C}$. If we look at the gains for $r_{C\text{-}(e)}$ in Table 11-30, $F_{6,C}$ is indeed the best manipulated variable in terms of the size of the gains, its C_g and also its ability to divert disturbances. Hence we will assign $F_{6,C}$ to $r_{C\text{-}(e)}$. This assignment is in agreement with the *Consistency Logic* developed in Chapter 8. It can be easily verified that the two assignments are compatible under closed-loop control.

Goal 3-4: Maintain material balance control of A

At Level 2, F_2 (and F_1 at Modes 4 and 6) was assigned to $r_{A\text{-}(a)}$. Varying F_2 and F_1 would directly affect compositions in F_6. Examination of the closed-loop gains for $r_{A\text{-}(e)}$ in Table 11-32 indicates that $F_{6,A}$ is the best choice. $F_{12,A}$ remains to be the best manipulated variable for $r_{A\text{-}(b)}$ (see data in Table 11-33). Our assignments are in agreement with the *Consistency Logic* and are compatible under closed-loop control.

Goal 3-5: Maintain material balance control of E

Previously, we have allocated F_3 (and F_1 at Modes 5) to $r_{E\text{-}(a)}$. Again, changing this stream has a direct impact on the component flows F_6. Data show that $F_{6,E}$ is the best manipulated variable for this objective. $F_{7,E}$ and $F_{7,G}$ remain to be the best choice for $r_{E\text{-}(b)}$ (see Tables 11-34 and 11-35).

Goal 3-6: Maintain material balance control of B

For the same reason as above, $F_{6,B}$ turned out to be the best choice for MB-B-(*e*). $F_{12,B}$ remains to be the manipulated variable for MB-B-(*b*) (see Tables 11-36 and 11-37).

Table 11 - 30: Open-loop gains of $r_{C\text{-}(e)}$

Input	Base	Mode2	Mode 3	Mode4	Mode 5	Mode 6	C_g
F_4	0	0	0	0	0	0	
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	4.90	5.06	9.08	5.56	11.59	7.88	2.37
$F_{7,D}$	0	0	0	0	0	0	
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	0	0	0	0	0	0	
$F_{6,G}$	1.26	0.26	3.36	0.61	0.08	2.55	39.63
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13	8.41
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	3.39	3.44	3.44	3.44	3.45	3.48	1.03
$F_{5,D}$	0	0	0	0	0	0	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0	0	0	0	0	0	
$F_{5,G}$	0.21	0.03	0.25	0.09	0.03	0.28	11.14
$F_{5,H}$	1.11E-01	1.23E-01	1.31E-02	4.29E-02	1.10E-01	1.48E-02	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	-2.92	-3.26	-3.82	-2.98	-3.20	-3.28	1.31
$F_{7,D}$	0	0	0	0	0	0	
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	0	0	0	0	0	0	
$F_{7,G}$	-3.3	-0.67	-12.01	-3.40	-0.66	-10.2	18.1
$F_{7,H}$	-2.2	-3.99	-0.92	-2.48	-3.99	-0.79	5.03
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 31: Open-loop gains of $r_{C\text{-}(b)}$

Input	Base	Mode2	Mode 3	Mode 4	Mode 5	Mode6	C_g
F_4	3.47	3.47	3.47	3.47	3.47	3.47	1.00
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	0	0	0	0	0	0	
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	0	0	0	0	0	0	
$F_{6,G}$	0	0	0	0	0	0	
$F_{6,H}$	0	0	0	0	0	0	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	-0.11	-0.05	-0.05	-0.04	-0.05	-0.05	2.55
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	-2.41	-0.53	-4.09	-2.38	-0.53	-4.08	7.75
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37	10.51
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	-3.39	-3.44	-3.44	-3.44	-3.45	-3.48	1.03
$F_{5,D}$	0	0	0	0	0	0	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0	0	0	0	0	0	
$F_{5,G}$	-0.21	-0.03	-0.25	-0.09	-0.03	-0.28	11.14
$F_{5,H}$	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	2.92	3.26	3.82	2.98	3.20	3.28	1.31
$F_{7,D}$	0	0	0	0	0	0	
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	0	0	0	0	0	0	
$F_{7,G}$	3.29	0.67	12.01	3.40	0.66	10.20	18.09
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79	5.03
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	-1.95	-2.14	-3.66	-2.13	-2.10	-2.98	1.88
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	-0.92	-0.19	-3.73	-0.52	-0.18	-2.68	20.45
$F_{12,H}$	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14	6.03

Table 11 - 32: Closed-loop gains of $r_{A\text{-}(e)}$

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	C_g
F_4	0	0	0	0	0	0	
$F_{6,A}$	8.41	9.07	14.88	9.05	11.03	12.56	1.77
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	1.05	0.21	4.27	1.32	0.00	3.69	15087
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	1.06	1.46	0.65	0.96	0.68	0.56	2.62
$F_{6,G}$	2.10	0.43	5.60	1.02	0.14	4.25	39.63
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13	8.41
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	3.24	3.29	3.29	3.28	3.28	3.42	1.06
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	3.50E-03	0.00E+00	9.19E-03	2.63E-03	8.43E-05	1.40E-02	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0.13	0.19	0.05	0.19	0.20	0.06	4.15
$F_{5,G}$	0.35	0.05	0.41	0.15	0.04	0.47	11.13
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01	9.34
$F_{7,A}$	-7.32	-8.16	-11.49	-7.78	-8.06	-9.61	1.57
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	0	0	0	0	0	0	
$F_{7,D}$	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49	32.59
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76	2.39
$F_{7,G}$	-5.49	-1.12	-20.02	-5.66	-1.11	-17.00	18.09
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79	5.04
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 33: Closed-loop gains of $r_{A-(b)}$

Input	Base	Mode2	Mode 3	Mode 4	Mode 5	Mode6	C_g
F_4	0	0	0	0	0	0	
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	0	0	0	0	0	0	
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	0	0	0	0	0	0	
$F_{6,G}$	0	0	0	0	0	0	
$F_{6,H}$	0	0	0	0	0	0	
$F_{11,A}$	-8.85E-02	-2.17E-02	-2.15E-02	-2.67E-02	-2.72E-02	-2.15E-02	4.12
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	1.08E-01	4.35E-02	5.19E-02	4.24E-02	4.34E-02	4.30E-02	2.55
$F_{11,D}$	-3.00E-04	0.00E+00	-9.00E-04	-6.00E-04	0.00E+00	-9.00E-04	30.33
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	-8.60E-03	-1.32E-02	-3.20E-03	-1.96E-02	-1.45E-02	-3.60E-03	6.16
$F_{11,G}$	-1.72	-0.38	-2.93	-1.70	-0.38	-2.92	7.75
$F_{11,H}$	-9.34E-02	-1.94E-01	-1.81E-02	-9.51E-02	-1.90E-01	-1.81E-02	10.69
$F_{5,A}$	-3.24	-3.29	-3.29	-3.28	-3.28	-3.42	1.06
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	3.22	3.27	3.27	3.27	3.28	3.31	1.03
$F_{5,D}$	-3.50E-03	0.00E+00	-9.20E-03	-2.60E-03	-1.00E-04	-1.40E-02	Inf
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	-1.32E-01	-1.95E-01	-4.86E-02	-1.91E-01	-2.02E-01	-6.23E-02	4.15
$F_{5,G}$	-1.52E-01	-2.00E-02	-1.77E-01	-6.50E-02	-1.80E-02	-2.01E-01	11.14
$F_{5,H}$	-5.40E-03	-6.10E-03	-6.00E-04	-2.10E-03	-5.40E-03	-7.00E-04	9.53
$F_{7,A}$	7.32	8.16	11.49	7.78	8.06	9.61	1.57
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	-2.77	-3.10	-3.63	-2.83	-3.04	-3.12	1.31
$F_{7,D}$	0.14	0.02	0.62	0.09	0.02	0.49	32.58
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	1.33	1.82	0.87	1.37	1.83	0.76	2.39
$F_{7,G}$	2.36	0.48	8.59	2.43	0.48	7.30	18.08
$F_{7,H}$	0.11	0.20	0.05	0.12	0.20	0.04	5.12
$F_{12,A}$	-4.90	-5.37	-11.05	-5.57	-5.31	-8.75	2.25
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	1.85	2.04	3.48	2.03	2.00	2.84	1.88
$F_{12,D}$	-0.09	-0.01	-0.58	-0.06	-0.01	-0.43	45.96
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	-0.80	-1.08	-0.72	-0.78	-1.08	-0.58	1.85
$F_{12,G}$	-0.66	-0.14	-2.67	-0.37	-0.13	-1.92	20.44
$F_{12,H}$	-2.35E-02	-4.23E-02	-9.70E-03	-1.21E-02	-3.91E-02	-6.90E-03	6.13

Table 11 - 34: Closed-loop gains of $r_{E\text{-}(e)}$

Input	Base	Mode2	Mode 3	Mode4	Mode 5	Mode6	C_R
F_4	0	0	0	0	0	0	
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	1.05	0.21	4.27	1.32	0.00	3.69	15087.60
$F_{6,E}$	4.36	6.64	1.95	4.23	2.07	1.64	4.05
$F_{6,F}$	1.06	1.46	0.65	0.96	0.68	0.56	2.62
$F_{6,G}$	0.84	0.17	2.24	0.41	0.06	1.70	39.63
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13	8.41
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	3.50E-03	0.00E+00	9.19E-03	2.63E-03	8.43E-05	1.40E-02	
$F_{5,E}$	0.40	0.58	0.11	0.52	0.62	0.13	5.77
$F_{5,F}$	0.13	0.19	0.05	0.19	0.20	0.06	4.15
$F_{5,G}$	0.14	0.02	0.16	0.06	0.02	0.19	11.13
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	0	0	0	0	0	0	
$F_{7,D}$	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49	32.59
$F_{7,E}$	-3.99	-5.52	-1.89	-3.70	-5.62	-1.60	3.52
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76	2.39
$F_{7,G}$	-2.19	-0.45	-8.01	-2.26	-0.44	-6.80	18.09
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79	5.04
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 35: Closed-loop gains of $r_{E\text{-}(b)}$

Input	Base	Mode2	Mode 3	Mode 4	Mode 5	Mode6	C_g
F_4	0	0	0	0	0	0	
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	0	0	0	0	0	0	
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	0	0	0	0	0	0	
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	0	0	0	0	0	0	
$F_{6,G}$	0	0	0	0	0	0	
$F_{6,H}$	0	0	0	0	0	0	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	-3.0E-04	0.0E+00	-9.0E-04	-6.0E-04	0.0E+00	-9.0E-04	30.33
$F_{11,E}$	-2.7E-02	-4.2E-02	-7.3E-03	-5.4E-02	-4.6E-02	-8.2E-03	7.41
$F_{11,F}$	-8.6E-03	-1.3E-02	-3.2E-03	-2.0E-02	-1.5E-02	-3.6E-03	6.16
$F_{11,G}$	-1.60	-0.35	-2.73	-1.58	-0.35	-2.72	7.75
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37	10.51
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0	0	0	0	0	0	
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	-3.5E-03	0.0E+00	-9.2E-03	-2.6E-03	-1.0E-04	-1.4E-02	Inf
$F_{5,E}$	-0.40	-0.58	-0.11	-0.52	-0.62	-0.13	5.77
$F_{5,F}$	-0.13	-0.19	-0.05	-0.19	-0.20	-0.06	4.15
$F_{5,G}$	-0.14	-0.02	-0.16	-0.06	-0.02	-0.19	11.13
$F_{5,H}$	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01	9.34
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	0	0	0	0	0	0	
$F_{7,C}$	0	0	0	0	0	0	
$F_{7,D}$	0.14	0.02	0.62	0.09	0.02	0.49	32.58
$F_{7,E}$	3.99	5.52	1.89	3.70	5.62	1.60	3.52
$F_{7,F}$	1.33	1.82	0.87	1.37	1.83	0.76	2.39
$F_{7,G}$	2.19	0.45	8.01	2.26	0.44	6.80	18.09
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79	5.04
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	-0.09	-0.01	-0.58	-0.06	-0.01	-0.43	45.96
$F_{12,E}$	-2.41	-3.28	-1.56	-2.10	-3.32	-1.22	2.71
$F_{12,F}$	-0.80	-1.08	-0.72	-0.78	-1.08	-0.58	1.85
$F_{12,G}$	-0.61	-0.13	-2.48	-0.35	-0.12	-1.79	20.45
$F_{12,H}$	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14	6.03

Table 11 - 36: Closed-loop gains of $r_{B-(e)}$

Input	Base	Mode2	Mode 3	Mode4	Mode 5	Mode6	C_g
F_4	0	0	0	0	0	0	
$F_{6,A}$	0	0	0	0	0	0	
$F_{6,B}$	3.90	2.13	14.01	2.18	0.11	11.03	126.06
$F_{6,C}$	0	0	0	0	0	0	
$F_{7,D}$	0	0	0	0	0	0	
$F_{6,E}$	0	0	0	0	0	0	
$F_{6,F}$	0	0	0	0	0	0	
$F_{6,G}$	0	0	0	0	0	0	
$F_{6,H}$	0	0	0	0	0	0	
$F_{11,A}$	0	0	0	0	0	0	
$F_{11,B}$	0	0	0	0	0	0	
$F_{11,C}$	0	0	0	0	0	0	
$F_{11,D}$	0	0	0	0	0	0	
$F_{11,E}$	0	0	0	0	0	0	
$F_{11,F}$	0	0	0	0	0	0	
$F_{11,G}$	0	0	0	0	0	0	
$F_{11,H}$	0	0	0	0	0	0	
$F_{5,A}$	0	0	0	0	0	0	
$F_{5,B}$	0.0367	0.0313	0.0314	0.034	0.0331	0.2413	7.70
$F_{5,C}$	0	0	0	0	0	0	
$F_{5,D}$	0	0	0	0	0	0	
$F_{5,E}$	0	0	0	0	0	0	
$F_{5,F}$	0	0	0	0	0	0	
$F_{5,G}$	0	0	0	0	0	0	
$F_{5,H}$	0	0	0	0	0	0	
$F_{7,A}$	0	0	0	0	0	0	
$F_{7,B}$	-4.90	-2.63	-18.59	-3.02	-2.52	-14.93	7.38
$F_{7,C}$	0	0	0	0	0	0	
$F_{7,D}$	0	0	0	0	0	0	
$F_{7,E}$	0	0	0	0	0	0	
$F_{7,F}$	0	0	0	0	0	0	
$F_{7,G}$	0	0	0	0	0	0	
$F_{7,H}$	0	0	0	0	0	0	
$F_{12,A}$	0	0	0	0	0	0	
$F_{12,B}$	0	0	0	0	0	0	
$F_{12,C}$	0	0	0	0	0	0	
$F_{12,D}$	0	0	0	0	0	0	
$F_{12,E}$	0	0	0	0	0	0	
$F_{12,F}$	0	0	0	0	0	0	
$F_{12,G}$	0	0	0	0	0	0	
$F_{12,H}$	0	0	0	0	0	0	

Table 11 - 37: Closed-loop gains of $r_{B\text{-}(b)}$

Input	Base	Mode2	Mode 4	Mode 5	C_g	Mode 3	Mode6	C_g
F_4	0	0	0	0		0	0	
$F_{6,A}$	0	0	0	0		0	0	
$F_{6,B}$	0	0	0	0		0	0	
$F_{6,C}$	0	0	0	0		0	0	
$F_{7,D}$	0	0	0	0		0	0	
$F_{6,E}$	0	0	0	0		0	0	
$F_{6,F}$	0	0	0	0		0	0	
$F_{6,G}$	0	0	0	0		0	0	
$F_{6,H}$	0	0	0	0		0	0	
$F_{11,A}$	0	0	0	0		0	0	
$F_{11,B}$	-4.5E-07	-2.3E-02	-3.9E-04	-2.3E-03	50444	-4.5E-03	-4.0E-04	11.35
$F_{11,C}$	1.1E-03	4.5E-04	4.4E-04	4.5E-04	2.49	5.3E-04	4.4E-04	1.21
$F_{11,D}$	0	0	0	0		-1.3E-05	-1.3E-05	1.00
$F_{11,E}$	0	0	0	0		-1.1E-04	-1.2E-04	1.12
$F_{11,F}$	0	0	0	0		-4.7E-05	-5.3E-05	1.14
$F_{11,G}$	2.3E-02	5.2E-03	2.3E-02	5.2E-03	4.50	1.1E-07	1.1E-07	1.00
$F_{11,H}$	1.8E-02	3.8E-02	1.9E-02	3.8E-02	2.09	-1.8E-03	-1.8E-03	1.00
$F_{5,A}$	0	0	0	0		0	0	
$F_{5,B}$	-3.7E-02	-3.1E-02	-3.4E-02	-3.3E-02	1.17	-3.1E-02	-2.4E-01	7.67
$F_{5,C}$	3.2E-02	3.4E-02	3.4E-02	3.4E-02	1.04	3.4E-02	3.4E-02	1.01
$F_{5,D}$	0	0	0	0		-1.4E-04	-2.1E-04	1.53
$F_{5,E}$	0	0	0	0		-1.6E-03	-1.9E-03	1.21
$F_{5,F}$	0	0	0	0		-7.1E-04	-9.2E-04	1.28
$F_{5,G}$	2.0E-03	2.7E-04	8.9E-04	2.5E-04	8.22	9.9E-08	9.9E-08	1.00
$F_{5,H}$	1.1E-03	1.2E-03	4.2E-04	1.1E-03	2.86	-6.4E-05	-7.2E-05	1.12
$F_{7,A}$	0	0	0	0		0	0	
$F_{7,B}$	4.90	2.63	3.02	2.52	1.94	18.59	14.93	1.25
$F_{7,C}$	-2.8E-02	-3.2E-02	-2.9E-02	-3.1E-02	1.15	-3.7E-02	-3.2E-02	1.17
$F_{7,D}$	0	0	0	0		9.2E-03	7.1E-03	1.28
$F_{7,E}$	0	0	0	0		2.8E-02	2.3E-02	1.19
$F_{7,F}$	0	0	0	0		1.3E-02	1.1E-02	1.14
$F_{7,G}$	-3.1E-02	-6.6E-03	-3.3E-02	-6.5E-03	5.12	0	0	
$F_{7,H}$	-2.1E-02	-3.9E-02	-2.4E-02	-3.9E-02	1.87	4.5E-03	3.9E-03	1.16
$F_{12,A}$	0	0	0	0		0	0	
$F_{12,B}$	-3.28	-1.73	-2.16	-1.66	1.97	-17.87	-13.58	1.32
$F_{12,C}$	1.9E-02	2.1E-02	2.1E-02	2.1E-02	1.13	3.6E-02	2.9E-02	1.23
$F_{12,D}$	0	0	0	0		-8.5E-03	-6.3E-03	1.35
$F_{12,E}$	0	0	0	0		-2.3E-02	-1.8E-02	1.28
$F_{12,F}$	0	0	0	0		-1.1E-02	-8.6E-03	1.24
$F_{12,G}$	8.8E-03	1.9E-03	5.1E-03	1.8E-03	4.94	5.7E-08	1.0E-07	1.82
$F_{12,H}$	4.6E-03	8.3E-03	2.4E-03	7.8E-03	3.43	-9.7E-04	-6.9E-04	1.41

Goal 3-7: Maintain Energy Balance Control

Both of the coolants have already been assigned to maintain the stability of the plant. These control assignments implicitly maintain the energy balance of the plant.

Goal 3-8: G/H ratio in product stream

The ratio $F_{11,G} / F_{11,H}$ is still the most direct influence on the ratio in the product stream.

Goal 3-9: Production rate (Modes 1, 2 and 3 only)

The flow of F_{11} has the most direct effect on the production rate.

Goal 3-10: Reactor Pressure < 2895 kPa

The manipulated variables that are directly linked to the reactor are the component flows of materials in F_6 and F_7. The pressure in the reactor is a function of the temperature, gas volume in the vessel (a function of the rector level) and the number of moles of gaseous materials in tank. The temperature and level of the reactor are under control for reactor stabilization. The major component flows of F_6 have already been used in the material balance control. The remaining degrees of freedom are the component flows of $F_{6,D}$, $F_{6,F}$, $F_{6,G}$ and $F_{6,H}$. D is the lightest component and is therefore more likely to be in the gas phase than other materials. We will adjust $F_{6,D}$ to control the reactor pressure.

Goal 3-11: Maximize production rate (modes 4, 5 and 6)

Again, similar to what was observed at the previous level, production can be maximized by maximizing the use of the limiting raw materials. Feed D (F_2) is the limiting raw materials for Modes 4 and 6 and Feed E (F_3) is the limiting raw material for Mode 5. Maximizing the use of these material streams within the process constraints maximizes the plant's throughput.

Goal 3-12: Minimize Production Cost

The optimization at this level can be described by:

$$\text{Min } \Phi = c_A F_{9,A} + c_C F_{9,C} + c_D F_{9,D} + c_E F_{9,E} + c_F F_{9,F} + c_G F_{9,G} \quad [11\text{-}30]$$
$$+ c_H F_{9,H} + c_D F_{11,D} + c_G F_{11,G} + c_F F_{11,F} + C_{compress} W$$
$$+ C_{steam} F_{steam}$$

s.t.:

1. maintain reactor temperature at the desired level
2. maintain reactor level at the desired level
3. maintain accumulation of C at the desired level
4. maintain accumulation of A at the desired level
5. maintain accumulation of E at the desired level
6. maintain accumulation of B at the desired level
7. maintain accumulation of energy at the desired level
8. $F_{11,G} / F_{11,H}$ at the pre-specified value
9. F_{11} at the pre-specified value for modes 1, 2 and 3
10. maximized production rate for modes 4, 5 and 6
11. Reactor Pressure < 2895 kPa
12. $F_{12,i} = F_{9,i} + F_{8,i}$
13. $F_{9,j} / F_{12,j} = F_{9,i} / F_{12,i}$ for all $j \neq i$
14. $F_{1,i} + F_{2,i} + F_{3,i} + F_{5,i} + F_{8,i} = F_{6,i}$

Constraints 1 to 11 correspond to the control objectives at this level. Constraints 12 to 14 are related to the self-regulating material capacitors at sub-systems *c* and *d*. The only refinement that took place when we moved from Level 2 to Level 3 was in the reactor section so any additional reduction in freedom for the cost optimization at this level will arise from reaction section.

Stoichiometry :

The following stoichiometric constraint was identified earlier:

$$(F_{7,G} - F_{6,G}) / (F_{7,H} - F_{6,H}) = \beta - 1 \quad [11\text{-}29]$$

The stoichiometric constrain does not impose any further restriction on the design variables in the optimization. Thus, at this level, the optimization is the same as the one at Level 2, but with more physical constraints (constraints 11 and 14).

Control Structure at Level 3

The control structure at Level 3 is summarized in Table 11-38 and is drawn in Figure 11-9. Notice that at this level, the control structure has become more uniform throughout the entire operating region. As the time-horizon becomes shorter and shorter, the impact of production limits on the base case control structure becomes less pronounced. Abstraction of the control structures at all operating modes return the control structures at the previous levels. The control structures at this level are compatible with those at higher levels.

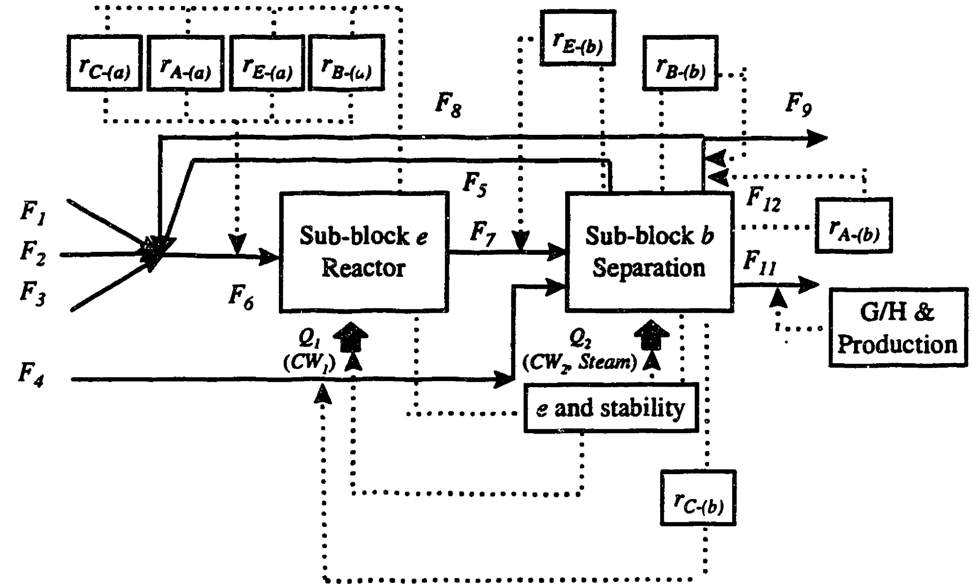


Figure 11 - 9: Control Structure for the Base Case at Level 3

Table 11 - 38: Summary of Control Structure at Level 3 for all operating modes

	Base Case F_5 at saturation	**Mode 2** F_5 at saturation	**Mode 3** CW_2 at saturation	**Mode 4** F_5, F_2 at saturation	**Mode 5** F_5, F_3 at saturation	**Mode 6** F_2, CW_2 at saturation
Reactor Temperature	CW_1	CW_1	CW_1	CW_1	CW_1	CW_1
Reactor Level	CW_2	CW_2	F_5 [1]	CW_2	CW_2	F_5 [1]
$r_{C\text{-}(e)}$	$F_{6,C}$	$F_{6,C}$	$F_{6,C}$	$F_{6,C}$	$F_{6,C}$	$F_{6,C}$
$r_{C\text{-}(b)}$	F_4	F_4	F_4	F_4	F_4	F_4
$r_{A\text{-}(e)}$	$F_{6,A}$	$F_{6,A}$	$F_{6,A}$	$F_{6,A}$	$F_{6,A}$	$F_{6,A}$
$r_{A\text{-}(b)}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$	$F_{12,A}$
$r_{E\text{-}(e)}$	$F_{6,E}$	$F_{6,E}$	$F_{6,E}$	$F_{6,E}$	$F_{6,E}$	$F_{6,E}$
$r_{E\text{-}(b)}$	$F_{7,E}$	$F_{7,E}$	$F_{7,G}$ [1]	$F_{7,E}$	$F_{7,E}$	$F_{7,G}$ [1]
$r_{B\text{-}(e)}$	$F_{6,B}$	$F_{6,B}$	$F_{6,B}$	$F_{6,B}$	$F_{6,B}$	$F_{6,B}$
$r_{B\text{-}(b)}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$	$F_{12,B}$
$e(e)$ and $e_{(e)}$	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2	CW_1 & CW_2
G/H	$F_{11,G}$ / $F_{11,H}$	$F_{11,G}$ / $F_{11,H}$	$F_{11,G}$ / $F_{11,H}$	$F_{11,G}$ / $F_{11,H}$	$F_{11,G}$ / $F_{11,H}$	$F_{11,G}$ / $F_{11,H}$
Production	F_{11}	F_{11}	F_{11}			
R_P < 2895 kPa	$F_{6,D}$	$F_{6,D}$	$F_{6,D}$	$F_{6,D}$	$F_{6,D}$	$F_{6,D}$
Max. Production				F_2	F_3 [2]	F_2
Minimize Cost	minimize loss of raw materials in purge stream					

[1] Change of control structure due to the specification on G/H.

[2] Change of control structure due to saturation of limiting reactant.

11.4 Phase II: Short-Horizon Analysis at Level 4 (Detailed Plant)

The representation of the process at Level 4 is equivalent to the process flowsheet shown earlier in Figure 11-1. At this level, the detailed structure of the entire plant is revealed. The expansion taken place centered about the separation section. The criteria for switching from long-horizon analysis to short-horizon analysis presented in Section 8.5 is met. Phase II of the design begins at this level.

11.4.1 Generating and Ranking Specific Controlled Objectives

The control objectives from Phase I have been *translated* and *refined* to the appropriate units at the detailed level (see Table 11-39). At this level, the constraints on the levels of the flash and stripper have become observable. These levels are non self-regulating, so maintaining these levels to be within their specified limits is more important than maintaining the reactor pressure (which is self-regulating) to be within its equipment limit. It is not possible to decide whether separator level or stripper level is more important so they will be treated as equally important objectives. The prioritization of the control objectives developed in Section 11.2 has been maintained.

Table 11 - 39: Control Objectives at Level 4 (Detailed Plant) Inherited from Phase I

	Reaction Section	Separation Section	
	Reactor Unit *e*	Separator Unit *f*	Stripper Unit *g*
1	Reactor Temperature		
2	Reactor Level		
3	$r_{C\text{-}(e)}$	$r_{C\text{-}(f)}$	$r_{C\text{-}(g)}$
4	$r_{A\text{-}(e)}$	$r_{A\text{-}(f)}$	$r_{A\text{-}(g)}$
5	$r_{E\text{-}(e)}$	$r_{E\text{-}(f)}$	$r_{E\text{-}(g)}$
6	$r_{B\text{-}(e)}$	$r_{B\text{-}(f)}$	$r_{B\text{-}(g)}$
7	$e_{(e)}$	$e_{(f)}$	$e_{(g)}$
8			G/H ratio
9			Production (Modes 1,2,3)
10		Separator Level	Stripper Level
11	Reactor Pressure < 2895 kPa		
12	Maximize production (Modes 4, 5 and 6) Minimize cost		

Generating of Specific Process Control Variables

In Phase II, the goal is to develop a control structure for direct process regulation. Control objectives associated with the material and energy balance control must be converted into some specific process variables using the method introduced in Section 8.4.1. Specific process controlled variables will be generated by studying groups of relevant material and energy balance control specifications.

Material balance controls around the reactor

The relevant control objectives are: $r_{C\text{-}(e)}$, $r_{A\text{-}(e)}$, $r_{E\text{-}(e)}$, $r_{B\text{-}(e)}$. Materials in the reactor exist both in the gas and liquid phases, according to Section 8.5.1, this group will be refined into the level and pressure of the reactor. Reactor level is already a variable under control by the stabilization strategy. It was pointed out earlier that when both reactor level and temperature are fixed, reactor pressure becomes self-regulating. However, because of the operational constraint on the reactor (objective 11), it is not desirable to allow reactor pressure to float freely. Both the reactor level and reactor pressure will be controlled. Due to its self-regulating nature, reactor pressure will be controlled at a lower priority (*demotion*).

Material balance controls around the Separator

Here, the relevant control objectives are: $r_{C\text{-}(f)}$, $r_{A\text{-}(f)}$, $r_{E\text{-}(f)}$, $r_{B\text{-}(f)}$. Materials in the separator exist in both the gas and liquid phases. This group will be refined into the separator level and pressure of the separator. Note that the pressure of the separator is linked to that of the reactor (and the stripper as well). The pressures of the three vessels attain some equilibrium values at steady-state and only one of the three pressures needs to be controlled. Since there is an operational constraint on the pressure of the reactor, it makes sense to control that one.

Material balance controls around the Stripper

Here, the relevant control objectives are: $r_{C\text{-}(f)}$, $r_{A\text{-}(f)}$, $r_{E\text{-}(f)}$, $r_{B\text{-}(f)}$. For the same reasons as above, this group will be refined into stripper level and pressure. Since stripper pressure is connected the other two pressures in the system, we do not need to exert control action on this one.

Energy balance control around the Reactor

We can refine the energy balance around the reactor ($e_{(e)}$) into the temperature of the reactor. It is needed to fix the value of this temperature for stabilization purposes, so it is *promoted* to priority 1.

Energy balance control around the Separator

The energy balance around the separator ($e_{(f)}$) can be refined into the temperature of the separator. This variable is self-regulating and the variation of temperature in this vessel is acceptable. In fact, in the stabilization strategy, the phase equilibrium condition in the separator is adjusted (by adjusting condenser cooling water) to control the amount of material being recycled back to the reactor. Hence, there is no need to control the temperature of the separator.

Energy balance control around the Stripper

Similarly, the energy balance around the stripper ($e_{(g)}$) can be refined into the temperature of the stripper. This is also a self-regulating variable. Note that we expect to see variations of Feed C by virtue of its control function as a manipulated variable (it is being used in all control structures at all levels at all operating modes). The variation of the flow of the stripping agent would likely cause variations in the level, temperature and the quality of the stripping process. The level of the stripper is a control objective. The stripper temperature can also be regulated to maintain the quality of the stripping process. This variable is self-regulating so it can be *demoted.*

Product ratio

The ratio of products is being explicitly controlled at this level. Since the product stream is mainly made up of G and H only, the mass ratio of G/H is a function of %G in the stream (a more directly measured variable). It can be easily verified that the density of the product stream is not very sensitive to the amount of G present. As long as the plant is being maintained closed to one of the pre-specified operating modes, the control of the G/H mass ratio can be accomplished by controlling directly the %G in the stream. This is an objective *refinement.*

Production (Modes 1, 2 and 3)

The production rate is also being explicitly controlled at this level. Note that when the ratio of G to H in the product stream stays at roughly the same value, the density of the material also stays roughly constant. Thus, one can control the production rate by maintaining the volumetric flow of the product stream (a directly measured variable). This is also an objective *refinement.*

Maximize Production (Modes 4, 5 and 6)

It has been determined that production throughput is maximized by increasing the flow of the limiting reagent until some plant constraints are hit. F_2 (Feed D) is the limiting raw material for Modes 4 and 6, while F_3 (Feed E) is the limiting reagent for Mode 5. These inputs are already being operated at their saturation limits (i.e. 100% valve position). Thus, our objective is to minimize the deviation of these flows from their saturation limits.

Cost Minimization

It has been determined at the previous levels that cost minimization can be achieved by recycling as much raw materials as possible. This objective can be *refined* to an objective which maximizes the recycle flow. Note that for the base case, as well as Modes 2, 4 and 5, recycle flow is already at its maximum. Hence, the objective is to minimize the deviation of recycle flow from its steady-state value.

The Hierarchy of Controlled Objectives

A hierarchy of specific controlled objectives (shown in Table 11-40) has been formed from the initial objectives shown earlier in Table 11-39. Reactor temperature and reactor level remain to be the two most important objectives as they are associated with the process stabilization strategy. The maintenance of separator and stripper levels should follow for they are related to the overall material balance control. It is not possible to determine if the control of the separator level or the stripper level is more important. Next, we will deal with the constraint on the reactor pressure. As indicated earlier, reactor pressure is a self-regulating variable once reactor temperature and reactor level are being fixed. However, due to the operational constraint, it is not desirable to allow the pressure level to float freely. Hence, we will derive a control structure which will guard against its violation. Control objectives 10 in Table 11-39 (i.e. separator and stripper level controls) are associated with the material balance control scheme for the plant so they have already been addressed. Stripper temperature is associated with the energy balance control of the stripper. Since this is a self-regulating variable, its priority has been demoted to 4-7. Once all the operational goals have been achieved, optimization possibilities will be investigated if there are excess degrees of freedom. No new constraints can be identified at this level.

Table 11 - 40: Initial Specific Control Objectives at Level 4 for Direct Regulation

	Reaction Section	Separation Section	
	Reactor Unit *e*	Separator Unit *f*	Stripper Unit *g*
4-1	Reactor Temperature		
4-2	Reactor Level		
4-3		Separator Level	Stripper Level
4-4	Reactor Pressure < 2895 kPa		
4-5			% G in Product
4-6			Product Flow (Modes 1,2,3)
4-7			Stripper Temperature
4-8	Maintain F_2 (Modes 4 and 6) or F_3 (Mode 5) at maximum		
4-9	Maintain recycle at maximum		

These control objectives do not violate stoichiometric constraints identified earlier in the design. We will be able to generate a feasible control structure with the above set of control objectives.

11.4.2 Synthesis of Control Structure for Short-Horizon Control

The goal of the design in Phase II is to develop a control structure that is suitable for direct regulation of the key process controlled objectives in the presence of frequently varying external process disturbances (either changing input conditions or setpoint changes on production specifications).

The implementation of the analysis described in Chapter 6 requires the availability of dynamic models of the plant which allows the quantification of the effect of deadtime, time constants, right-half plane zeros, etc. The plant is open-loop unstable. The open-loop transfer function model describing reactor temperature by reactor cooling water has been obtained by linearization:

$$G=\frac{-163(s+4.44)(s+0.028+0.09i)(s+0.028-0.09i)(s-0.00064)(s-0.00000016)(s+0.0626)}{(s+0.00325+0.0735i)(s+0.00326-0.0735i)(s+0.06257)(s-0.5998+6.2739i)(s-0.5998-6.2739i)(s-0.0000002)(s-0.007)} \quad [11\text{-}30]$$

The process model shown in Equation [11-30] is typical of all open-loop transfer functions of this plant. Note that all of the RHP zeros are very close to the origin. This factor alone will give very large of magnitudes in V_{RHP} (Equation [6-18]), a measure of the performance degradation as a result of the process RHP zeroes. Then, no logical assignments can be concluded from such analysis. In addition to that, some of the RHP poles are extremely close to the RHP zeros which suggests that the dynamics of the unstable modes are hard to control (Morari and Zafiriou, 1989). In order to stabilize the plant, inputs that can give very fast control actions with large magnitudes must be used.

The control structure at the detailed level will be synthesized in two stages. In the first stage, control strategies for the regulation of the plant's fast dynamics, including the unstable modes and the integrating modes will be developed. Next, control strategies for the relatively slower dynamics at the detailed level will be constructed.

Developing control structure for the unstable and integrating modes

Due to the nature of the unstable and integrating modes, manipulated variables used to control objectives associated with these process dynamics must be able to execute fast control actions. Recall that one of the overall production plan is to minimize the movements of gas feeds which affect other processes (Section 11.2). This would mean that Feeds A, D, E and C are not suitable for fast dynamic control of the fast modes in the process. Also, inputs which have their nominal values at saturation also cannot be relied upon for plant stabilization. Hence, at this stage of the design, the manipulated variables available for selection are:

1. Modes 1, 2, 4 and 5: purge (F_9), separator bottom flow (F_{10}), stripper bottom flow (F_{11}), reactor cooling water (CW_1) and condenser cooing water (CW_2).
2. Modes 3 and 6: recycle (F_8), purge, separator bottom flow, stripper bottom flow, reactor cooling water.

We have previously assigned reactor cooling water to control reactor temperature. This assignment was made based on the following reasons:

1. The input is in close vicinity with the output and we expect a small deadtime in the process.
2. The assignment of reactor cooling water to reactor temperature will force the variation of coolant temperature to leave the process through the coolant outlet and completely eliminate the effects of this disturbance on the process.

Furthermore, condenser cooling water has been selected to maintain the reactor level at the base case at Modes 2, 4 and 5; recycle flow to maintain this objective at Modes 3 and 6. The analysis was carried out using models which consist of integrator gain plus deadtime. The primary manipulated variables have been selected based on the performance indexes described by Equation [11-1]. Selection of primary manipulated variables for the rest of the control objectives at this stage of the design will employ a similar procedure. The details of the analysis in this section can be found in Appendix C.5. The key points of the assignments are summarized below.

Objective 4-3: Separator Level and Stripper Level

Both the control of separator level and stripper level are of equal importance. Both cases of ordering will be examined. We will proceed the analysis by assuming separator level is of higher priority. Analysis will be performed under the condition that reactor temperature and reactor level are under closed-loop control. The closed-loop process models of the separator level by each of the available process inputs are shown in Table 11-41. Using these data the performance indexes of each of the inputs for this objectives have been computed in Appendix C.5 and complied in Table 11-42.

Table 11 - 41: Closed-loop Process Model - Separator Level

Manipulation	Deadtime (min)		Integrator Gain					
	(1,2,4 ,5)	(3,6)	Mode 1	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	8	10	5.6045	2.5158	0	3.3769	2.3083	0
Product	40	50	-0.0038	-0.0068	-0.0008	-0.0092	0.0129	-0.0029
Steam	30	60	1.4648	1.4148	0	0.4942	0.731	0
Condenser CW	10	10	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	2	30	6.8649	6.3799	*assigned*	5.9773	6.3133	*assigned*
Separator Bot	0	0	-5.6847	-4.945	-7.2832	-2.9246	-4.6857	-6.9056

Table 11 - 42: Performance Indexes of Inputs for the control of Separator Level

Manipulations	Mode 1	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	52.51	95.16	*infinity*	73.63	102.36	*infinity*
Product	54941.25	30722.25	260816.5	22722.31	16215.49	71988.52
Steam	360.29	*infinity*	*infinity*	639.99	503.25	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	220.27	222.58	*assigned*	224.78	222.92	*assigned*
Separator Bot	**49.74**	**55.43**	**35.09**	**84.14**	**57.54**	**35.96**

The best manipulated variables are those which have small performance indexes. Both purge and separator bottom flows are possible manipulated variable for Modes 1, 2, 4 and 5. For Modes 3 and 6, separator bottom flows is the only candidate. It is desirable to employ a uniform control structure for the entire operating region, if possible. We will assign separator bottom flows to the control of separator level.

Next, the manipulated variable for controlling the stripper level is to be selected. The closed-loop models for the stripper level are summarized in Table 11-43. The performance indexes for each of the inputs are computed and shown in Table 11-44. As shown, stripper level can be best controlled by manipulating the product flowrate.

Table 11 - 43: Closed-loop process Model - Stripper Level

Manipulation	Deadtime (min) (1,2,4,5)	Deadtime (min) (3,6)	Integrator Gain Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	20	18.3	12.1573	12.4896	0	39.3769	5.4185	0
Product	0	0	-11.1267	-11.9902	-10.3144	-10.9987	-11.9155	-10.3044
Steam	15	15	2.8369	6.5765	0	5.5258	1.4515	0
Condenser CW	20	18.3	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	55	55	14.9539	31.5332	*assigned*	60.2983	14.2778	*assigned*
Separator Bot	0	0	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

Table 11 - 44: Performance Indexes of Inputs for the control of Stripper Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	81.19	76.82	*infinity*	40.43	145.41	*infinity*
Product	**63.09**	**59.17**	**68.45**	**66.98**	**59.35**	**68.01**
Steam	427.73	*infinity*	*infinity*	314.73	649.37	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	279.56	256.40	*assigned*	246.44	281.65	*assigned*
Separator Bot	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

It has been verified that reversing the order of importance of separator level and stripper level does not affect the assignment. Hence, we will assign separator bottom flow to separator level and product flow to stripper level.

Objective 4-4: Reactor Pressure

The closed-loop process models for reactor pressure are complied in Table 11-45 and the associated performance indexes are shown in Table 11-46. Purge flow is the best input for the maintenance of reactor pressure. Purge flow of this process is very small. Since reactor pressure is operating at a point that is much closer to the high limit than the low limit, it is important to identify a manipulated variable that can be used to prevent reactor shut-down as a result of over-pressurization in the reactor vessel. Recycle can be relaxed from its 1% limit at Modes 1, 2, 4 and 5 to alleviate pressure build-up.

Table 11 - 45: Closed-loop process Model - Pressure Level

Manipulation	Deadtime (min) (1,2,4,5)	(3,6)	Integrator Gain Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	5	5	-2.042	-6.1267	0	-7.3751	-5.0826	0
Product	40	40	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*
Steam	0	0	1.1102	1.7601	2.15	0.6572	1.2068	2.1
Condenser CW	15	15	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	0	5	3.9848	7.3821	*assigned*	3.27	8.5063	*assigned*
Separator Bot	30	30	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

Table 11 - 46: Performance Indexes of Inputs for the control of Pressure Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	**24.62**	**13.00**	**77.04**	**11.92**	**13.74**	**159.39**
Product	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*
Steam	177.20	*infinity*	*infinity*	194.60	175.18	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	158.99	155.76	*assigned*	160.53	155.25	*assigned*
Separator Bot	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

The control structure for the unstable and integrating modes is summarized in Table 10-47. At the detailed level, the control structure has become more uniform.

Table 11 - 47: Summary of Control Structure for Unstable and Integrating Modes at Level 4

	Base Case F_5 at saturation	**Mode 2** F_5 at saturation	**Mode 3** CW_2 at saturation	**Mode 4** F_5, F_2 at saturation	**Mode 5** F_5, F_3 at saturation	**Mode 6** F_2, CW_2 at saturation
Reactor Temperature	CW_1	CW_1	CW_1	CW_1	CW_1	CW_1
Reactor Level	CW_2	CW_2	F_5 [1]	CW_2	CW_2	F_5 [1]
Separator Level	F_{10}	F_{10}	F_{10}	F_{10}	F_{10}	F_{10}
Stripper Level	F_{11}	F_{11}	F_{11}	F_{11}	F_{11}	F_{11}
Reactor Pressure	F_9	F_9	F_9	F_9	F_9	F_9

Developing Control Structure to Maintain Product Specifications and other Production Objectives

The remaining free manipulated variables are:

- Modes 1, 2, 4 and 5: Feeds A, D, E, C, recycle and steam flow.
- Modes 3 and 6: Feeds A, D, E, C, condenser cooling water and steam flow.

Once the control structure for the process unstable and integrating modes is implemented, step tests can then be performed on the plant to allow the generation of process models which will assist synthesis of the control structure to maintain product specifications and other production objectives. Each operating mode has its specific needs as far as product specifications are concerned. At some modes, the limiting feed is also at saturation so as to maximize the throughput of the plant. Due to the nonlinearity expected for the plant, models for the remaining objectives should be determined at each mode and assignment selected on a mode by mode basis. The analysis will proceed for the primary operating mode.

Objectives 4-5 and 4-6: %G in product stream and product flow

The process models of %G in product stream (Objective 5) and product flow (Objective 6) by all four feed streams are summarized in Table 11-48. These models represent the change of the output for a 1% change in the input when the process unstable and integrating modes are under closed-loop control. Recycle flow and steam flow are at saturation so these inputs will not be considered for the control of operational objectives.

Table 11 - 48: Closed-loop Process model for %G in product and product flow

	Feed A	Feed C	Feed D	Feed E
%G in Product	Deadtime > 20 hours	Deadtime > 20 hours	$\frac{0.5036e^{-1.48s}}{0.343s+1}$ $\lvert\varepsilon\rvert=1.0204$	$\frac{-0.3202e^{-0.33s}}{2.7126s+1}$ $\lvert\varepsilon\rvert=0.9025$
Product Flow (m^3hr^{-1})	Deadtime > 20 hours	Deadtime > 20 hours	$\frac{0.0752e^{-0.05s}}{0.344s+1}$ $\lvert\varepsilon\rvert=1.2073$	$\frac{0.0788e^{0.0s}}{0.2139s+1}$ $\lvert\varepsilon\rvert=1.3362$

Feed A and Feed C have virtually little effects on the objectives so these two manipulations can be eliminated in our design. The next step is to decide how the control objectives should be associated with Feed D and Feed E. The performance measures applicable to these control outputs include the size of the deadtime (given by Equation [6-15], data shown in Table 11-48); the size of the dominant time constant (given by Equation [6-16], data shown in Table 11-48); rangeability (given by Equation [6-19], data shown in Appendix C.1 and model uncertainty (given by Equation [6-32], data shown in Table 11-48). The performance index V_j for input j is then given by:

$$V_j = w_{deadtime}\left|\frac{V_{deadtime,j}}{N_{deadtime}}\right| + w_{dominant}\left|\frac{V_{dominanat,j}}{N_{dominant}}\right| + w_{rangeability}\left|\frac{V_{rangeability,j}}{N_{rangeability}}\right| + w_{uncertainty}\left|\frac{V_{uncertainty,j}}{N_{uncertainty}}\right| \qquad [11\text{-}31]$$

and N_i (i = deadtime, dominant, rangeability and uncertainty) is chosen so that all $V_{i,j}/N_i$ are of roughly the same order of magnitudes. The following weights have been chosen: $w_{deadtime} = 1$; $w_{rangeability} = 1$; $w_{dominant} = 2.5$; $w_{uncertainty} = 2$. The rationale behind the choice of the weights is as follows. The nominal steady-state values of both inputs are roughly 50%, so a heavy weight on rangeability will not differentiate any differences between the two. The dynamic of these control objectives are also relatively slow, so the size of the deadtime also does not play a heavy role in the performance. As will be shown later in Section 11.5, for these control objectives, the size of the deadtime will have little impact on the closed-loop performance. Then, the dominant time constant and the size of the model uncertainty are therefore the key determining factors. Their weights should be heavier so as to amplify the differences of the different model aspects on the closed-loop performance. Using these weights, the performance index for Feed D on %G in product is computed to be 4.92 and that of Feed E computed to be 6.85. These values appear to be not very sensitive to the choice of both the absolute sizes and relative sizes of $w_{dominant}$ and $w_{uncertainty}$. We can therefore assign Feed D to control %G in the product stream. Feed E will then be available for the maintenance of the product flow rate.

Objective 7: Stripper Temperature

Stripper temperature can be easily maintained by adjusting the steam flow. This also allows disturbances to be diverted to the environment Although steam flow is at saturation (100%) for all operating modes, this is a low priority objective so we are satisfied with a one-direction control.

Control Structure at the Detailed Level

The control structure for the maintenance of product specifications and other operational objectives at the detailed level is summarized in Table 11-49. The control structure synthesized at this level is drawn in Figure 11-10.

Table 11 - 49: Summary of Control Structure for Production and Operational Objectives

Objectives	**Base Case** F_5 at saturation
%G in Product	F_2
Product Flow	F_3
Stripper Temperature	Steam
Minimize Cost	Keep F_5 close to 0%

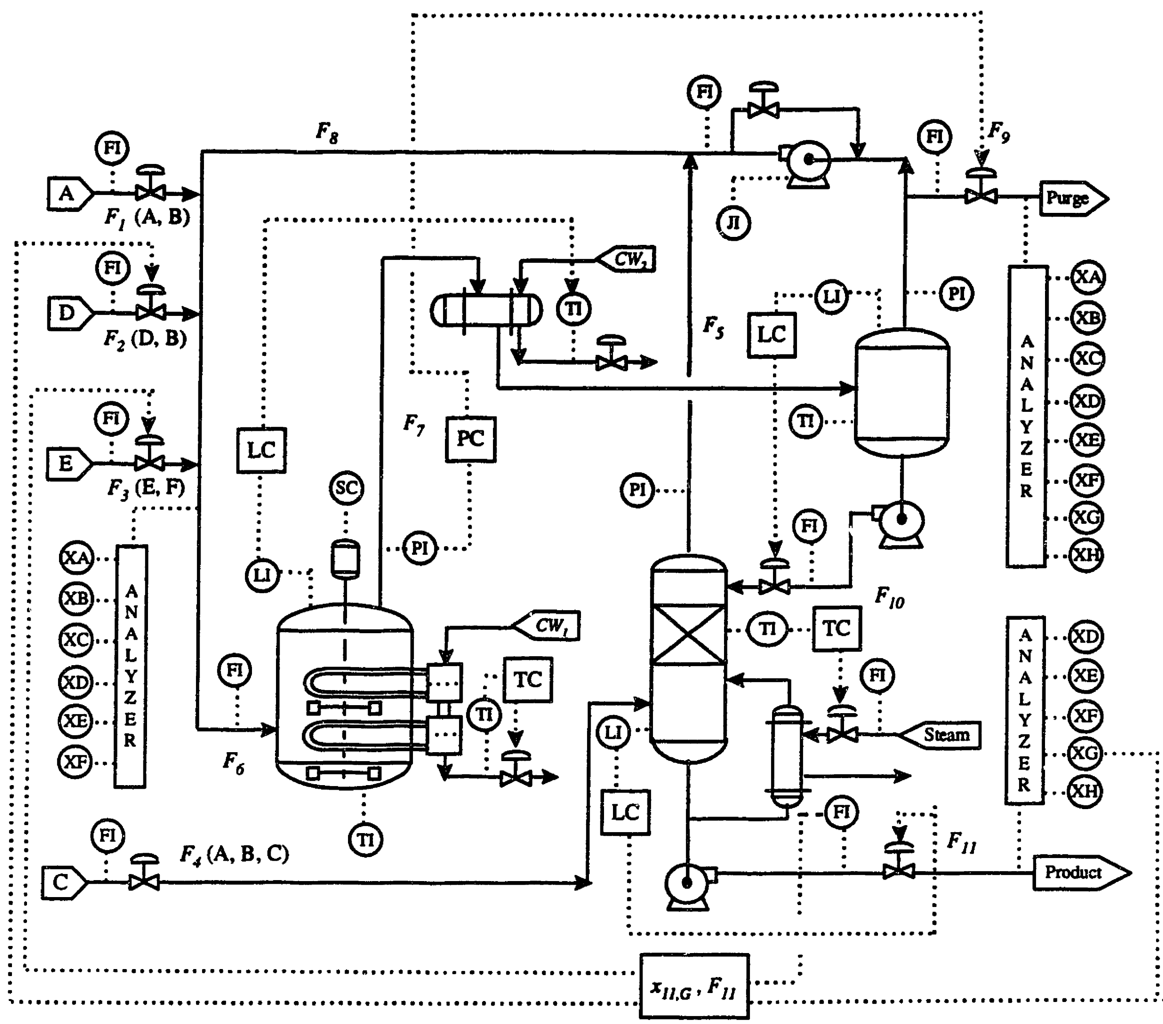


Figure 11 - 10: Control Structure for the Detailed Level

11.5 Multi-horizon Control System

Schematics of the control strategies that we have synthesized for each of process representations have been shown in Figures 11-4, 11-7, 11-9 and 11-10. Each level of process representation is associated with a relevant time-horizon which is related to the response time of the manipulated variables on the outputs observable from that representation. The set of control structures can be integrated as described in Section 8.6 to generate a multi-horizon control system.

11.5.1 Partitioning Control Strategies at the Detailed level

The control structure developed for the detailed level has been partitioned into different sets, each set is related to a specific level of representation of the plant. The partitioned detailed control structure which maintains objectives of relevance to this operation is shown in Table 11-50. Objectives 4-1 through 4-4 and objective 4-7 are only observable at Level 4, the detailed process representation. These controlled objectives are associated with the fastest time-scale of operation and should be under short-interval of feedback control. Objectives 4-5 and 4-6 are related to the product specifications. These objectives are first observable from the input-output level. Furthermore, the detailed control structure employs inputs (F_2 and F_3) which are first observable from the input-output level. Thus, essentially, this set of controlled objectives are related to the slowest time-scale of operation and can be controlled with a longer interval of feedback control. To minimize operating cost, the recycle flow is maximized by keeping F_5 as close to the 0% valve position as close as possible, without violating any other operational constraints. Since F_5 is first observable from Level 2, the rate of movement of F_5 can be associated with an immediate interval of feedback control.

Table 11 - 50: Partitioned Detailed Control Structure at Level 4

	Controlled Objectives	Relevant Time-horizon	Level of Representation
4-1	Reactor Temperature	Short	Level 4
4-2	Reactor Level	Short	Level 4
4-3	Separator Level	Short	Level 4
	Stripper Level	Short	Level 4
4-4	Reactor Pressure < 2895 kPa	Short	Level 4
4-5	% G in Product	Long	Level 1
4-6	Product Flow (Modes 1,2,3)	Long	Level 1
4-7	Stripper Temperature	Short	Level 4
4-9	Minimize Cost: Keep F_5 at 0%	Immediate	Level 2

11.5.2 Integrating Control Strategies at Different Levels

The primary control objectives at Levels 1, 2 and 3 are the maintenance of material and energy flows in the system and maintenance of products at the required specifications. Objectives related to the material and energy balance controls have been refined into reactor level, separator level, stripper level, reactor pressure, reactor temperature and stripper temperature. Thus, any additional specific control strategies generated based on control strategies developed at the abstract levels will serve to supplement the control strategies at the detailed level to meet the overall production goals, i.e. no increase of level of accumulation of materials and energy in the plant. The following additional control opportunities exist:

1. At Level 3, the detailed reaction/generalized separation level, the inventory of different components in the reaction section are being maintained by adjusting the compositions of several components in the reactor feed. Since the inventories of components A and C subject to frequent variations due to variations of compositions of Feed C (see Table 11-3), the compositions of A and C in reactor feed are objectives that can be *spawned* at Level 3 to supplement the control.
2. It was identified at Level 2, the generalized reaction-separation level, that $F_{12,A}$ and $F_{12,B}$ should be adjusted to maintain the inventories of A and B in the separation block.

The exact values of %A and %B in F_{12} is a function of the compositions of A and B in the various feed streams and other conditions in the reactor area. B is an inert. If there is build-up of B in the system, the excess amount should be purged. A physically manipulated variable must be available to indirectly adjust the compositions of B in the gas recycle system. Note that adjusting $F_{12,B}$ is equivalent to adjusting $F_{9,B}$ or %B in purge. A is a raw material so the build-up of A is not detrimental to the operation of the system. Also, the build-up of A (or any other gaseous material) is being partly controlled by means of the reactor pressure control policy as well as the maintenance of %A in reactor feed.

The excess degrees of freedom in our design are Feed C (F_4), Feed A (F_1) and recycle flow (F_5) if we are willing to sacrifice the cost minimization objective. The newly identified control objectives based on control strategies developed at the abstract levels include %A in reactor feed, %C in reactor feed and %B in purge. These objectives are supplementary in nature, their priorities would be lower than those which have been identified earlier but higher than the cost minimization objectives. The cost minimization objective is hence demoted to rank 4-11. The maintenance of materials of C is of higher priority than that of A, which is of higher priority than that of B, the new objectives will also be ranked accordingly.

Objectives 4-8 and 4-9: Maintain %C and %A in reactor feed to be at their steady-state values

The free manipulated variable include F_4 (Feed C), F_1 (Feed A) and F_5 (recycle). F_5 is a its saturation limit and therefore unsuitable for the maintenance of compositions in reactor feed, which is expected to be subject to random process variations.

Notice that we have consistently assigned F_4 to maintain the level of accumulation of C in the system at all levels analyzed during Phase I. This suggests that F_4 is the best input for this objective at long and intermediate horizon. We will verify that F_4 is also best primary manipulated variable for this objective at short-horizon as well by performing an analysis using short-horizon design criteria. The closed-loop models for %C in reactor feed and %A in reactor feed by F_4 and F_1 while objectives 4-1 through 4-7 are under closed-loop control have been developed and are shown in Table 11-51. Using the same selection method for Objectives 4-5 and 4-6 (%G in product stream and product flow) described in Section 11.4.2 and the same weights for the different dynamic aspects, the performance index for %C in reactor feed by Feed C is determined to be 5.3 while that by Feed A is 5.6. Hence, Feed C is a slightly better manipulated variable for the control %C of in reactor feed. We will assign Feed C to maintain %C in reactor feed and Feed A to maintain %A in reactor feed.

Table 11 - 51: Closed-loop models for %C and %A in Reactor Feed

	Feed C	Feed A
%C in Feed	$\dfrac{6.2233e^{-0.28s}}{7.99s+1}$ $\lvert\varepsilon\rvert = 0.7730$	$\dfrac{-0.754e^{-0.03s}}{19.5565s+1}$ $\lvert\varepsilon\rvert = 0.7009$
%A in Feed	$\dfrac{1.7641e^{-0.10s}}{6.7493s+1}$ $\lvert\varepsilon\rvert = 0.6981$	$\dfrac{1.4355e^{-0.13s}}{15.6362s+1}$ $\lvert\varepsilon\rvert = 0.7073$

Objective 4-10: %B in Purge

The recycle flow is the free manipulation available to us and its nominal value at the cost-optimal steady-state is at saturation, consistent with the cost optimization control strategy. We have demoted the cost-optimization objective to rank 4-11. Thus, recycle flow can be relaxed from the saturation limit (to purge more and recycle less gaseous materials) if it is required to lower the amount of build-up of B in the system and can be used to control the inventory of B in the system.

The final multi-horizon control system is summarized in Table 11-52 and a schematic of the final control system is shown in Figure 11-11. One should be cautioned that the associations drawn in the figure by no means imply that the control structure consists of a set of SISO loops. Each association merely signifies that a certain manipulated variable has been reserved to be the primary manipulated variable for the maintenance of a certain controlled objective in the plant.

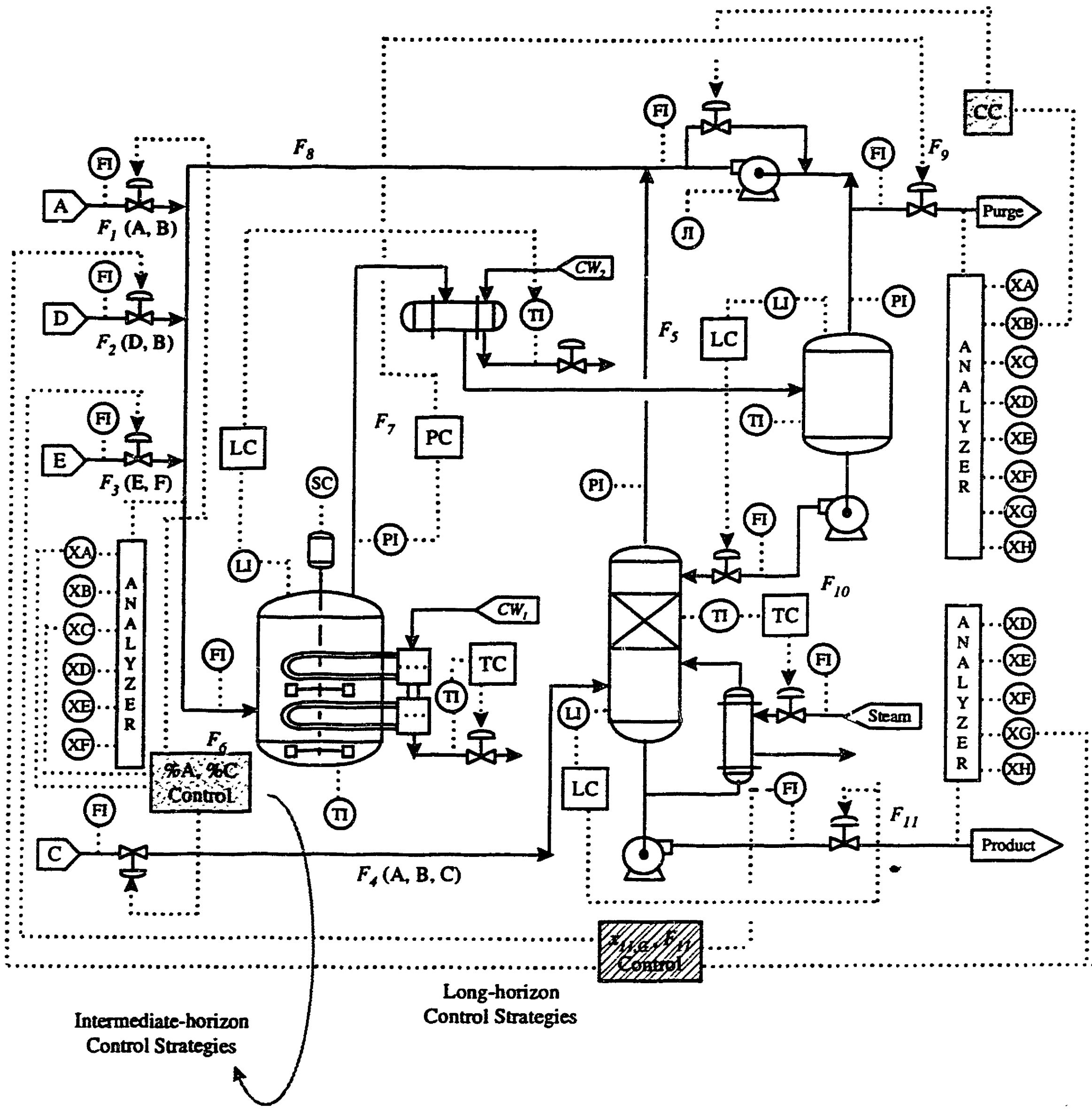


Figure 11 - 11: A Multi-horizon Control System for the TEC Process

Table 11 - 52: Multi-horizon Control System for the Tennessee Eastman Challenge Problem (Base Case Design)

	Controlled Objectives	Relevant Time-horizon	Primary Manipulated Var.
4-1	Reactor Temperature	Short (Level 4)	Reactor CW
4-2	Reactor Level	Short (Level 4)	Condenser CW
4-3	Separator Level	Short (Level 4)	F_{10}
	Stripper Level	Short (Level 4)	F_{11}
4-4	Reactor Pressure < 2895 kPa	Short (Level 4)	F_9
4-5	% G in Product	Long (Level 1)	F_2
4-6	Product Flow (Modes 1,2,3)	Long (Level 1)	F_3
4-7	Stripper Temperature	Short (Level 4)	Steam
4-8	%C in Reactor Feed	Immediate (Level 3)	F_4
4-9	%A in Reactor Feed	Immediate (Level 3)	F_1
4-10	%B in Purge	Immediate (Level 2)	F_5
4-11	Minimize Cost: Keep F_5 at 0%	Immediate (Level 2)	Keep F_5 close to 0%

11.6 Implementation

The synthesis of the control structure for the plant has been driven by sequential satisfaction of the hierarchy of production objectives in the plant. Theoretically, to fully reproduce the expected impact of the design on the plant, one may be required to implement the control structure in a full-scale multiobjective framework. However, for a plant with over ten levels of priorities, implementation of a full-blown multivariable-multiobjective controller algorithm may be impractical. Simplifications can be made to the controller design while maintaining the multivariable-multiobjective flavor in the control algorithm.

11.6.1 Application of the Notion of Preemptive Priorities

The notion of preemptive priorities was introduced in Section 6.2.2. The use of preemptive priorities is a means to facilitate the practical application of multiobjective optimization. One should always attempt to reduce the number of priority levels to a minimum that is consistent with the true representation of the actual problem under consideration.

In the Tennessee Eastman plant, the ordered set of objectives can be assigned to the preemptive priorities at shown in Table 11-53. The 12 original priority levels has been reduced to 8 preemptive priorities. Reactor temperature is of the highest preemptive priority as it is associated with the process stabilization objective. Reactor level is associated with the stabilization objective as well, but is also closely related to the overall material balance control in the plant. Hence, we group the maintenance of all vessel level to the same priority level. Reactor pressure is a self-regulating variable once objectives 1 through 3 are being maintained at steady-state so it is not as important as the control of the levels in the vessels. Next, the maintenance of %G and production rate can be grouped together, and so are the objectives concerning the feed compositions. Controlled objectives of the same preemptive priorities are of equal importance.

Table 11 - 53: Preemptive Priorities of the Controlled Objectives

	Controlled Objectives	Relevant Time-horizon	Preemptive Priorities
1	Reactor Temperature	Short (Level 4)	I
2	Reactor Level	Short (Level 4)	II
3	Separator Level	Short (Level 4)	II
4	Stripper Level	Short (Level 4)	II
5	Reactor Pressure < 2895 kPa	Short (Level 4)	III
6	% G in Product	Long (Level 1)	IV
7	Product Flow (Modes 1,2,3)	Long (Level 1)	IV
8	Stripper Temperature	Short (Level 4)	V
9	%C in Reactor Feed	Immediate (Level 3)	VI
10	%A in Reactor Feed	Immediate (Level 3)	VI
11	%B in Purge	Immediate (Level 2)	VII
12	Minimize Cost: Keep F_5 at 0%	Immediate (Level 2)	VIII

11.6.2 Exploitation of the Multi-horizon Nature of Process Operation

The implementation of the control structure can be further simplified by taking advantage of the different time-scales of operation in the plant and examine the degree of interaction among the assigned parings. The Tennessee Eastman plant has two main tiers of dynamics. Some variables change rapidly upon changes of *any* manipulated variables. These are process variables that are associated with the reactor and the integrating elements. Thus, priorities I through III and V in Table 11-56 are associated with fast dynamics, priorities IV, VI, VII and VIII are associated with variables of much slower dynamics. Such differences in the process dynamics can be exploited to simplify the implementation.

Controlling variables of fast dynamics

Variables of very fast dynamics must be under close monitoring using high frequency application of control actions. Experience with the plant indicates that these variables should be controlled at a rate in the order of 0.01 hr^{-1}. At such rate, it would be more practical to make use of simple Proportional-Integral-Derivative control (PID) loops than to applied a full-scale multivariable-multiobjective controllers.

Furthermore, open-loop step tests indicate that the integrative elements in the plant would only attain their steady-state rates of change under perturbation of plant inputs if and only if the reactor temperature is under control by cooling water. This suggests that feedback control of reactor temperature alone by reactor cooling water provides some stabilizing effects. By controlling reactor temperature at a rate much greater than 0.01 hr^{-1}, say 0.002 hr^{-1}, one can implement the rest of the control structure assuming that the reactor temperature is fixed.

A relative gain array (RGA) analysis on the priority II objectives gives the following RGA (Bristol, 1966) matrix $\Lambda = [\lambda_{ij}]$:

$$\Lambda = \begin{bmatrix} 1.7729 & -0.7726 & -0.0003 \\ -0.7730 & 1.7720 & 0.0009 \\ 0 & 0.0006 & 0.9994 \end{bmatrix} \qquad [11\text{-}32]$$

where rows one, two and three represent the effects on reactor level, separator level and stripper level respectively and columns one, two and three represent the effect due to condenser cooling water, separator bottom flow and product flow respectively (the validity of the use of RGA for interaction analysis on integrating element had been proven by Arkun and Downs, 1990).

If all λ_{ii} (i = 1, 2, 3) in the matrix are close to unity, it would indicate that there is little interaction if we pair output i with input i. The matrix suggests that controlling the objectives set in Priority II as SISO loops, we should expect good control of stripper level while a small amount of interaction between the other two loops. This interaction can probably be counteracted by detuning one of the control loops. Thus, the implementation of control structure can be simplified by implementing these three objectives as SISO PID loops. Since these three objectives belong to the same preemptive priorities, there is no need to solve for the control action in a multiobjective framework as per the modular multivariable controller (Meadowcroft, 1992; 1997).

The dynamics of reactor pressure to changes in the process is also very fast. Thus, its control will be implemented as SISO PID loops as well. Variation in purge flow will interact with the control of reactor level. Since pressure is a less critical objective, this loop is detuned.

Stripper temperature, an objective of priority V, has a relatively fast dynamics to changes in Feed C, but our study on the plant has shown that changes in the primary manipulated variables of this objective (i.e. steam) has very little effect on the other more important objectives in the plant (refer to data in Appendix C.3). We will implement the control of stripper temperature with a PID as well.

Controlling Slower dynamics in the process

Objective sets in priorities IV and VI react much slower to changes in the process. These variables can be effectively controlled at a rate of the order of 10^{-1} hr^{-1}; we can take advantage of this fact to implement full-blown multivariable-multiobjective controller algorithms for the control of these variables. Since the control of priorities I, II, III and V are at a much faster rate (20 to 50 times faster), the control of the variables with slower dynamics can be implemented assuming that the temperature, levels and pressure are all being maintained to be within their desirable limits.

Note that the dynamics of %B in purge is also relatively slow compared to the pressures and levels in the plant. We expect that the recycle flow will only be used infrequently to purge excess B in the system. A PID loop will be sufficient for that purpose.

The practical implementation of the multi-horizon multiobjective control system is summarized in Table 11-54.

Table 11 - 54: A Practical Implementation of the Multi-horizon multiobjective Control System

Controlled Objectives	Controller Type	Control horizon
Short-horizon Control		
Reactor Temperature	PI	0.002 hr
Reactor Level	PI	0.01 hr
Separator Level	PI	0.01 hr
Stripper Level	PI	0.01 hr
Reactor Pressure	PI	0.01 hr
Stripper Temperature	PI	0.01 hr
Intermediate-horizon Control		
%C in Feed	MMC goal 1	0.2 hr
%A in Feed	MMC goal 2	0.2 hr
%B in Purge (if required)	PI	0.2 hr
Keep F5 at saturation	PI	0.2 hr
Long-horizon Control		
%G in Product	MMC goal 1	0.75 hr
Product Flow	MMC goal 2	0.75 hr

11.6.3 Modular Multivariable Controller Design

The MIMO control of the controlled objectives over the intermediate and long horizons can be accomplished with the used of a Modular Multivariable Controller (MMC; Mdeadowcroft, 1992; 1997) such that the implementation conforms to the multiobjective approach. A MMC is essentially a model predictive controller (MPC) that is being designed in the goal programming framework (discussed previously in Chapter 6).

The two 2x2 MMC controllers (one at the intermediate-horizon control level, one at the long-horizon control level) have been implemented using the linearized models of the plant of the following form:

$$\hat{y} = M\,u + C\,u_o \qquad [11\text{-}33]$$

where $\hat{y}$ = vector of predicted outputs (controlled objectives)
u = vector of future control actions
u_o = vector of past control inputs
M = impulse response matrix of output y by the future control action
C = matrix which describes the effect of past control actions on the future outputs

Matrices M and C can be computed using standard techniques described in Prett and Garcia (1988) based on process models tabulated in Tables 11-48 and 11-51.

The control actions for the two goals are computed through a series of linear programming (LP) optimizations. The objective functions are the 1-norm of the error of the predicted output from the setpoint r_i of goal i over some prediction horizon P, i.e. :

$$a_i = \|r_i - \hat{y}_i\|_1 \qquad [11\text{-}34]$$

where $\hat{y}_i(m)$ is the vector of predicted outputs over prediction horizon P. At time-step m ($m \leq P$) let $r_i(m) - y_i(m) = k_i^+(m) - k_i^-(m)$, where $k_i^+(m)$ and $k_i^-(m)$ are both greater than or equal to zero. Then, the objective function of goal i is simply:

$$a_i = \sum_{m=1}^{P} k_i^+(m) + k_i^-(m) \qquad [11\text{-}35]$$

The first optimization solves for the control actions for the first objective (one of the higher priority) as follows:

P1:

$$a_1^{(1)} = \min_{u_1, k_1^+, k_1^-} \sum_{m=1}^{P} k_1^+(m) + k_1^-(m) \qquad [11\text{-}36]$$

subject to:

$$M_{11}u_1 + k_i^+ - k_i^- = r_1 - C_{11}u_{o,1} + e_1$$
$$u_1(1+C) = \ldots = u_1(P) = u_1(C)$$
$$k_i^+(m) \geq 0 \ \forall \ m = 1 \text{ to } P,\ i = 1$$
$$k_i^-(m) \geq 0 \ \forall \ m = 1 \text{ to } P,\ i = 1$$

where M_{11} is the impulse response matrix of y_1 by u_1, C_{11} is the matrix of past control action of $u_{o,1}$ on $\hat{y}_1$. Vector e_1 is the model error in a standard MPC algorithm, defined as the difference between the measured output and the predicted output. C is the control horizon and P is the prediction horizon such that $C \leq P$. Optimization P1 computes the optimal value of $u_1^{(1)}$ for the control of y_1 over the horizon P. The achievement level of the first objective is simply $a_1^* = a_1^{(1)}$.

Having obtained the achievement level of the first objective (regardless of the achievement level of the second objective), we can re-compute the control actions for both objectives 1 and 2 by imposing the requirement that the incorporation of control actions for the second objective will not degrade the performance of the first objective, which is of higher priority.

P2: $$a_2^{(2)} = \min_{u_1,u_2,k_1^+,k_1^-,k_2^+,k_2^-} \sum_{m=1}^{P} k_2^+(m) + k_2^-(m) \qquad [11\text{-}37]$$

subject to:

$$\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} k_1^+ \\ k_2^+ \end{bmatrix} - \begin{bmatrix} k_1^- \\ k_2^- \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} - \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}\begin{bmatrix} u_{o,1} \\ u_{o,2} \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}$$

$$\sum_{m=1}^{P} k_1^+(m) + k_1^-(m) \le a_1^*$$

$$u_1(1+C) = \ldots = u_1(P) = u_1(C)$$

$$u_2(1+C) = \ldots = u_2(P) = u_2(C)$$

$$k_i^+(m) \ge 0 \ \forall\ m = 1 \text{ to } P$$

$$k_i^-(m) \ge 0 \ \forall\ m = 1 \text{ to } P$$

M_{ij} is the impulse response matrix of output i by u_j. C_{ij} is the matrix which describe the effect of $u_{o,j}$ on y_i. Vector e_2 is the model error in a standard MPC algorithm, defined as the difference between the measured output and the predicted output. P2 gives us the control actions u_1^* and u_2^* which will minimize the error in the outputs and give preference to the more important objective. Extension to a $n \times n$ MMC design is straight forward.

11.6.4 Specifications of Controllers

The specifications of the controllers used in this case study are summarized in this section. The tuning constants of the PI controllers are complied in Table 11-55. The specifications of the two MMC controllers are summarized in Table 11-56. Only control actions which are confined between 0% to 100% are allowed. As the main purpose of this exercise is to verify the applicability of the proposed methodology, these tuning constants have been obtained via a trial-and-error method and they are not necessarily the best tuning constants for this process. Nonetheless, these controller specifications, when implemented, provide satisfactory control performance (see Section 11.6.5).

Table 11 - 55: PI Controller tuning constants (sampling rate for reactor temperature is 0.002 hr, sampling rate for all other outputs is 0.01 hr)

Controlled Objectives	Manipulated Variables	Gain (appropriate units)	Integral Time Constant (min)
Reactor Temperature	Reactor cooling water	-4	10
Reactor Level	Condenser cooling water	-2	50
Separator Level	Separator Bottom Flow	-1.5	150
Stripper Level	Stripper bottoms	-0.1	300
Reactor Pressure	Purge	-2	10
Stripper Temperature	Steam	3	50
%B in Purge (if required)	Recycle	1	50

Table 11 - 56: Specifications for the MMC controllers

Controlled Objectives	Manipulated Variables	MMC Controller Specifications
Intermediate-horizon Control		
%C in Feed	Feed C	Sampling unit: 0.2 hr
%A in Feed	Feed A	MMC prediction horizon: 10 units
		MMC control horizon: 7 units
Long-horizon Control		
%G in Product	Feed D	Sampling unit: 0.75 hr
Product Flow	Feed E	MMC prediction horizon: 5 units
		MMC control horizon: 5 units

11.6.5 Performance of Proposed Multi-horizon Control System

The performance of the multi-horizon plant-wide control system developed for the Tennessee Eastman process has be evaluated via computer simulations.

Process Regulation in the presence of Disturbances

The ability of the proposed control structure to maintain the process objectives in the presence of external disturbances has been tested by applying all of the twenty possible disturbances (shown previous Table 11-3) expected for the plant in our simulation studies. The results of the tests are summarized below.

Our control structure can easily reject temperature variations in the feed stream or coolants (such as disturbance types 3, 4, 5, 9, 10, 11 and 12 in Table 11-3). Figure 11-12 shows the responses of some of the key process variables, when the process is subject to a step change in the reactor cooling water (disturbance types 4). Notice that we are able to maintain the product ratio G/H to a be at 1 and the flow of G in the product stream to be at 7038 kg/hr. The variations of both outputs are within the specified limits. We are able to maintain a very tight control of the reactor pressure and level. Control actions in the feed streams were not required, avoiding any demand changes in the upstream process (one of the production objectives)

Our process could also be subjected to frequent changes in the compositions of A, B and/or C in F_4 (such as disturbance types 1, 2, 8 and 7). Figure 11-13 shows the output response of some key process variables and key process inputs when there are random variations of A, B and C compositions in F_4 (disturbance type 8). As shown, we are able to maintain the product ratio at the specified value. There is a larger amount of variation of the product flow of G compare to the effect of temperature variation in the input streams. However, the extend of the variability is within the specified limits. Reactor level and pressure react to changes in the feed composition but we are able to maintain the stability of the reactor under tight control. Feed A and Feed C are used to maintain %A and %C in reactor feed. These inputs must vary as the composition of A, B and C changes in F_4. Feed D and Feed E are not needed to compensate for such variations. In Figure 11-14, we see the effect of changes in B composition in F_4 on the plant (disturbance type 2) . Very tight control can be accomplished by our control structure. Figure 11-15 shows the output responses when there is a loss in the header pressure for Feed C (disturbance type 7). The flow control implementation of our design quickly eliminate such a disturbance.

Figure 11-16 shows the changes in the key process variations when the plant is subject to an unknown disturbance (type 16). Our control structure is able to maintain the process at the desired setpoints.

Setpoint changes of process variables

The ability of the control structure to bring the process to a new steady-state has been tested by performing setpoint changes in ratio of products from 50/50 (by mass) to 40/60 (by mass); lower production rate by 15% and increase composition of B in purge by 1%. The time responses of the process to these tests are shown in Figures 11-17 through 11-19. Our control structure can successfully effect the required changes in production specifications (1 and 2) while maintaining the stability of the process (Figure 11-17 and 11-18). Although there were large upset in the reactor level and reactor pressure during the transient, we were able to maintain the stability of the reactor at all times. All four feeds had to move to adjust the plant to new product specifications. The change in Feed D and E were very gradual since they were controlling the plant at a long time-horizon. The ability of the chosen control structure to purge inert out of the system is demonstrated in Figure 11-19 where we increase the composition of B in the purge stream. Our control structure is able to maintain the product specifications while bringing such a change.

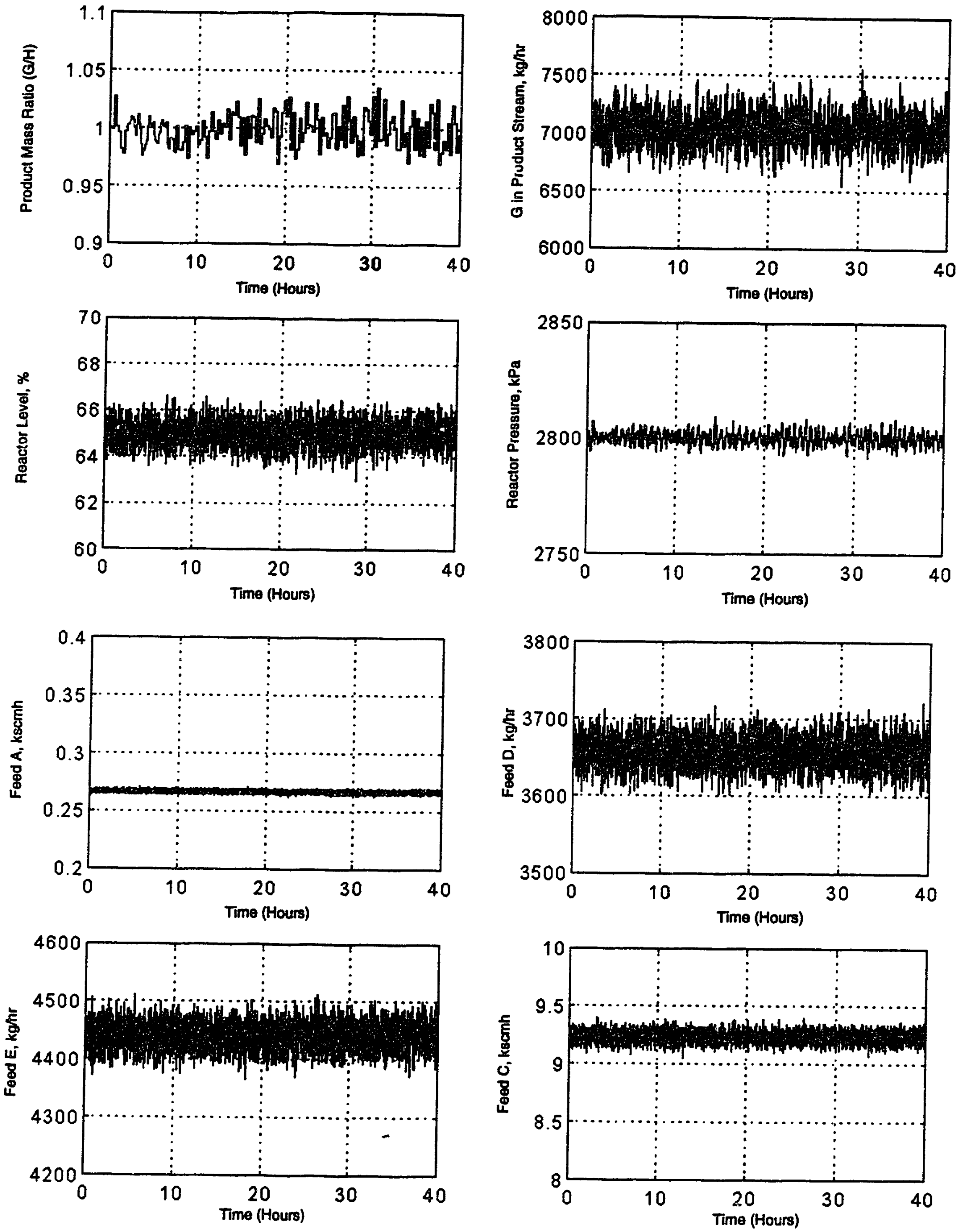


Figure 11 - 12: Effect of a Step Change in Temperature of Reactor Cooling Water

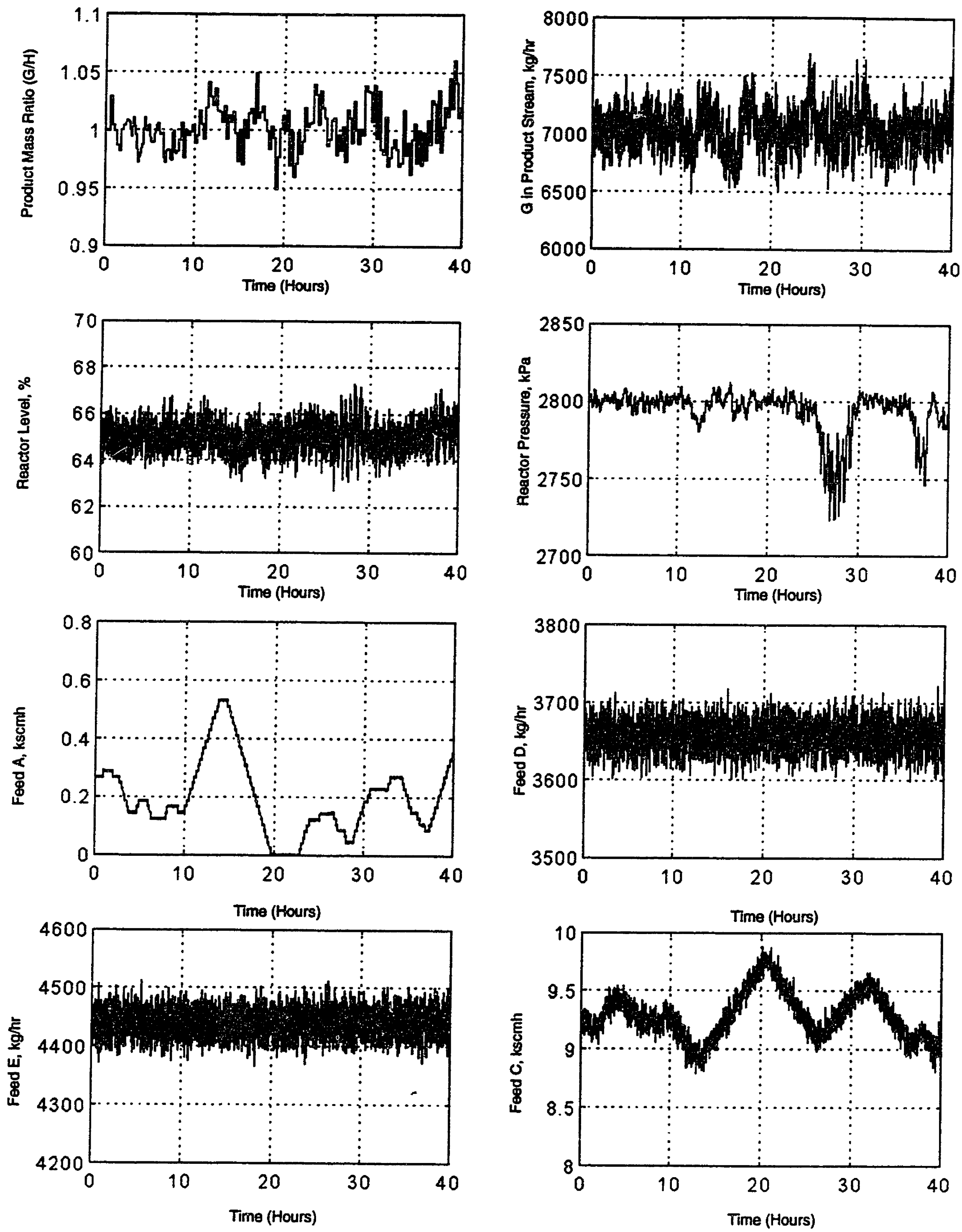


Figure 11 - 13: Effect of random variations of A, B, and C composition in F_4

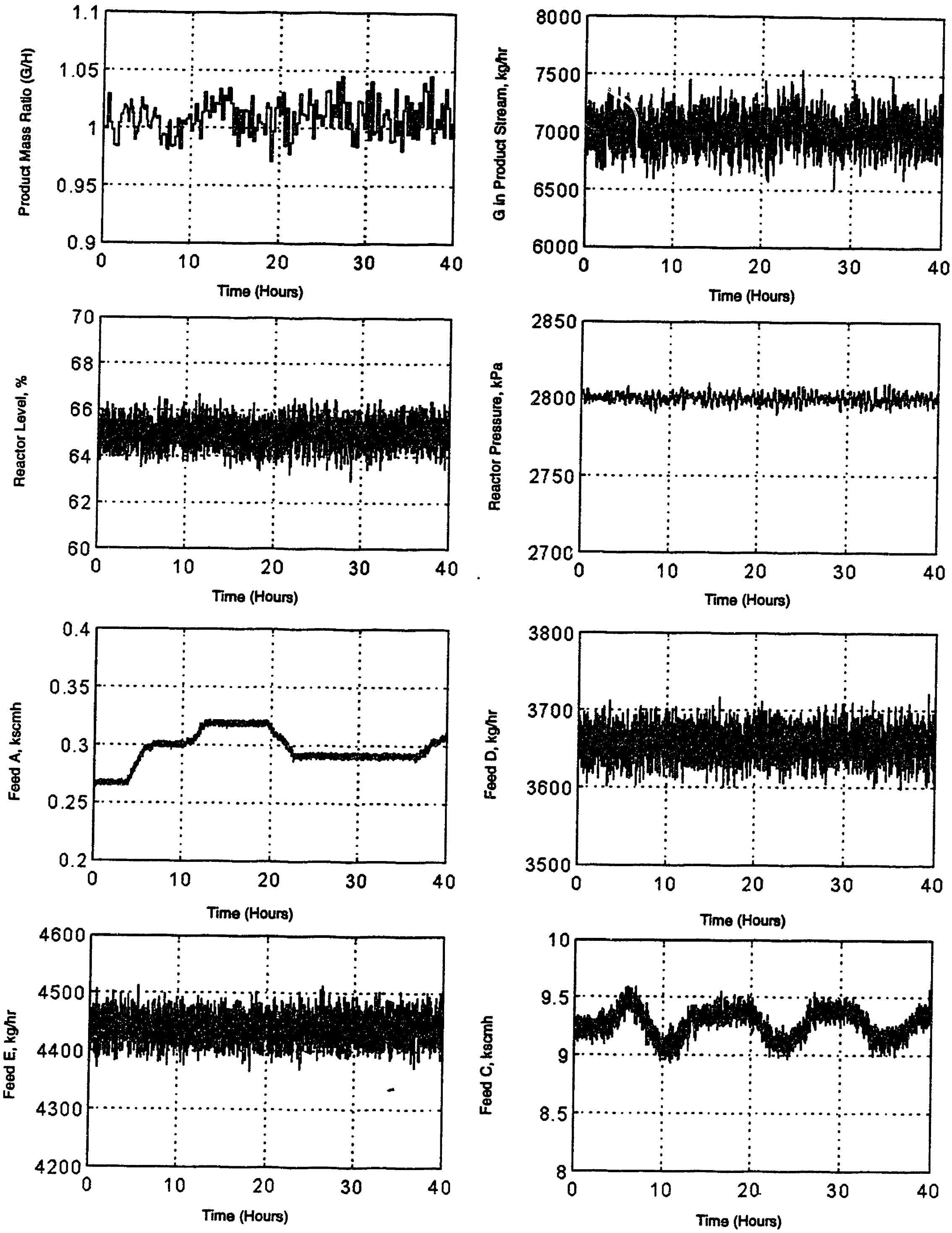


Figure 11 - 14: Effect of Changes in B Composition in F_4

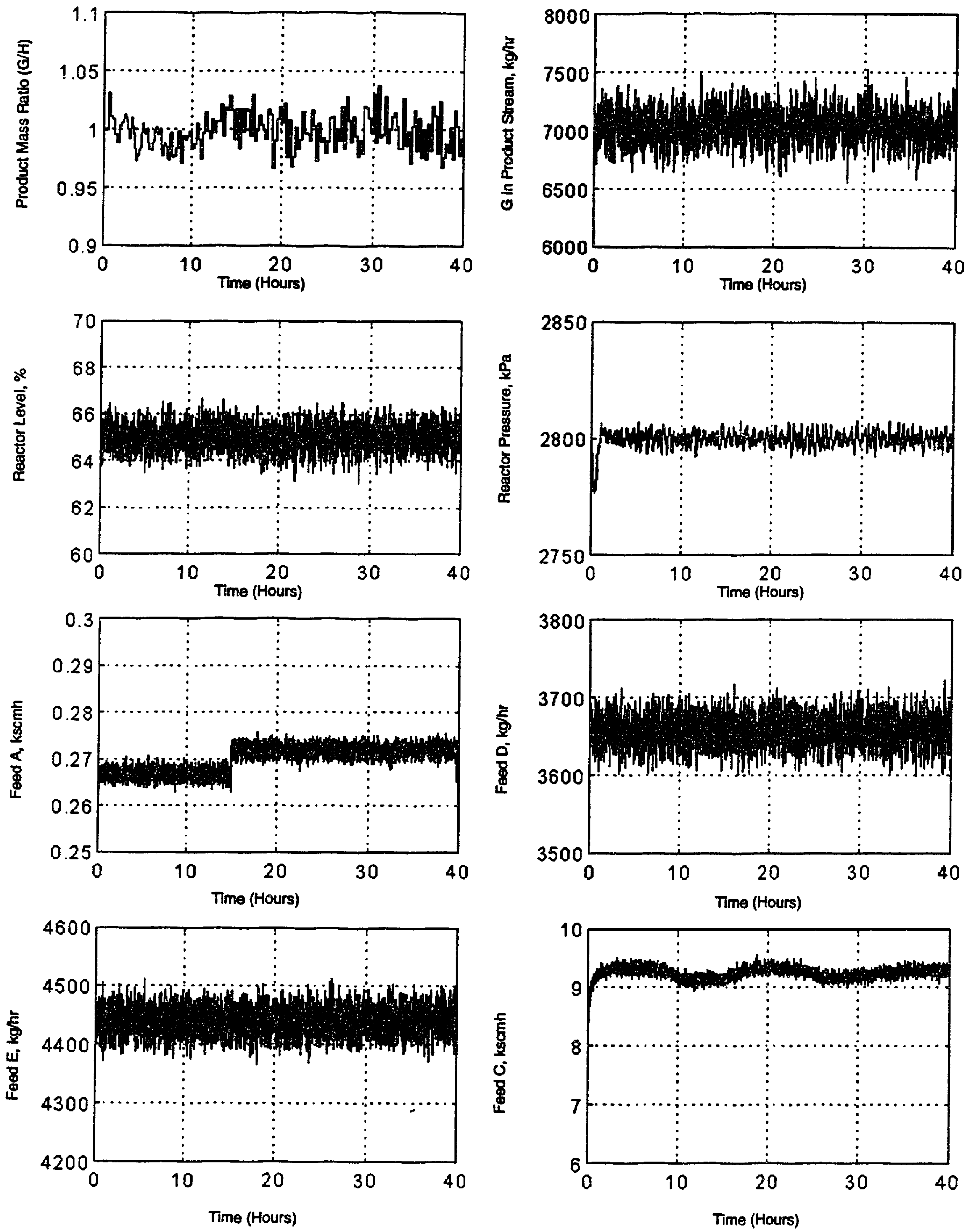


Figure 11 - 15: Effect of Loss in the Header Pressure of Feed C

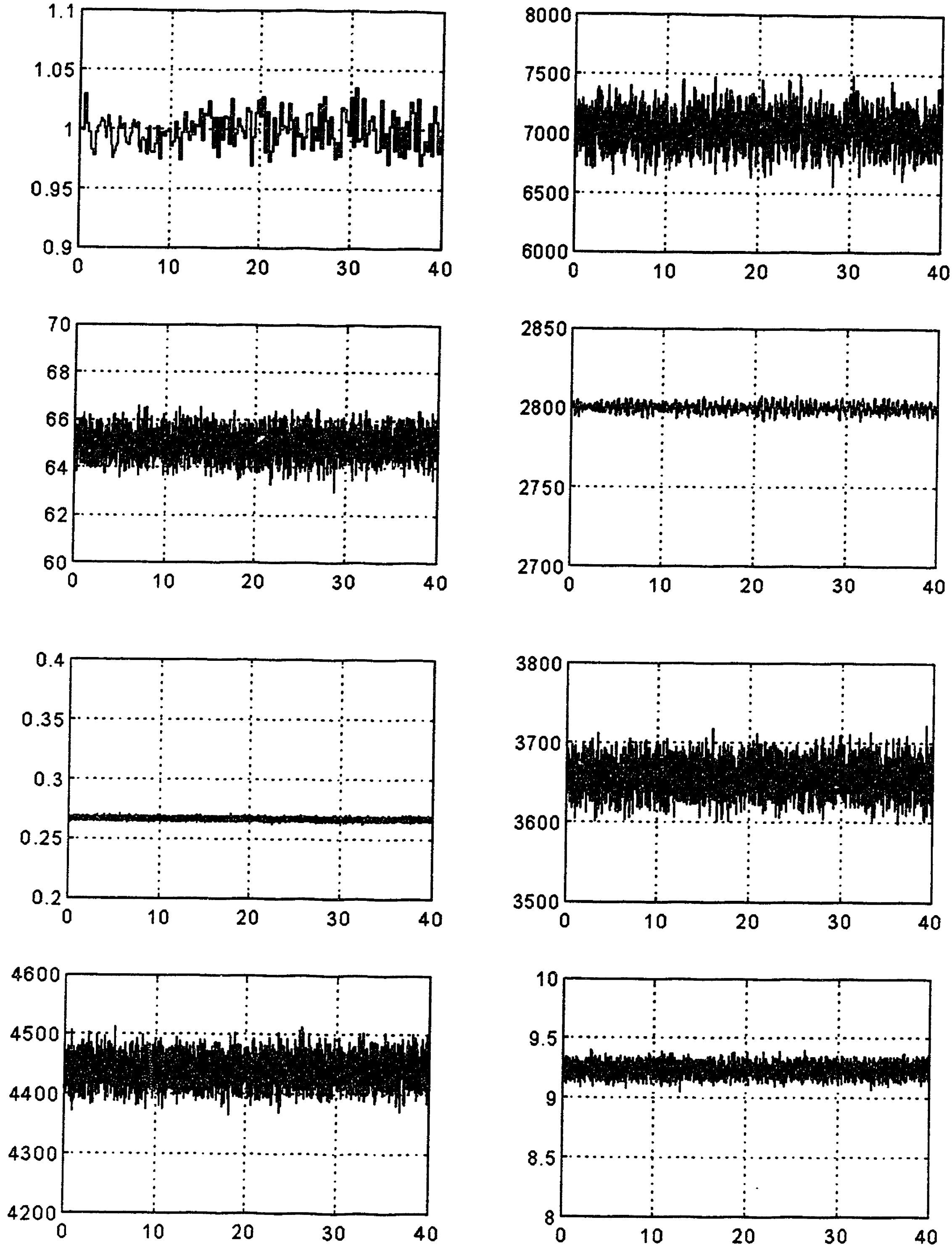


Figure 11 - 16: Effect of an Unknown Disturbance

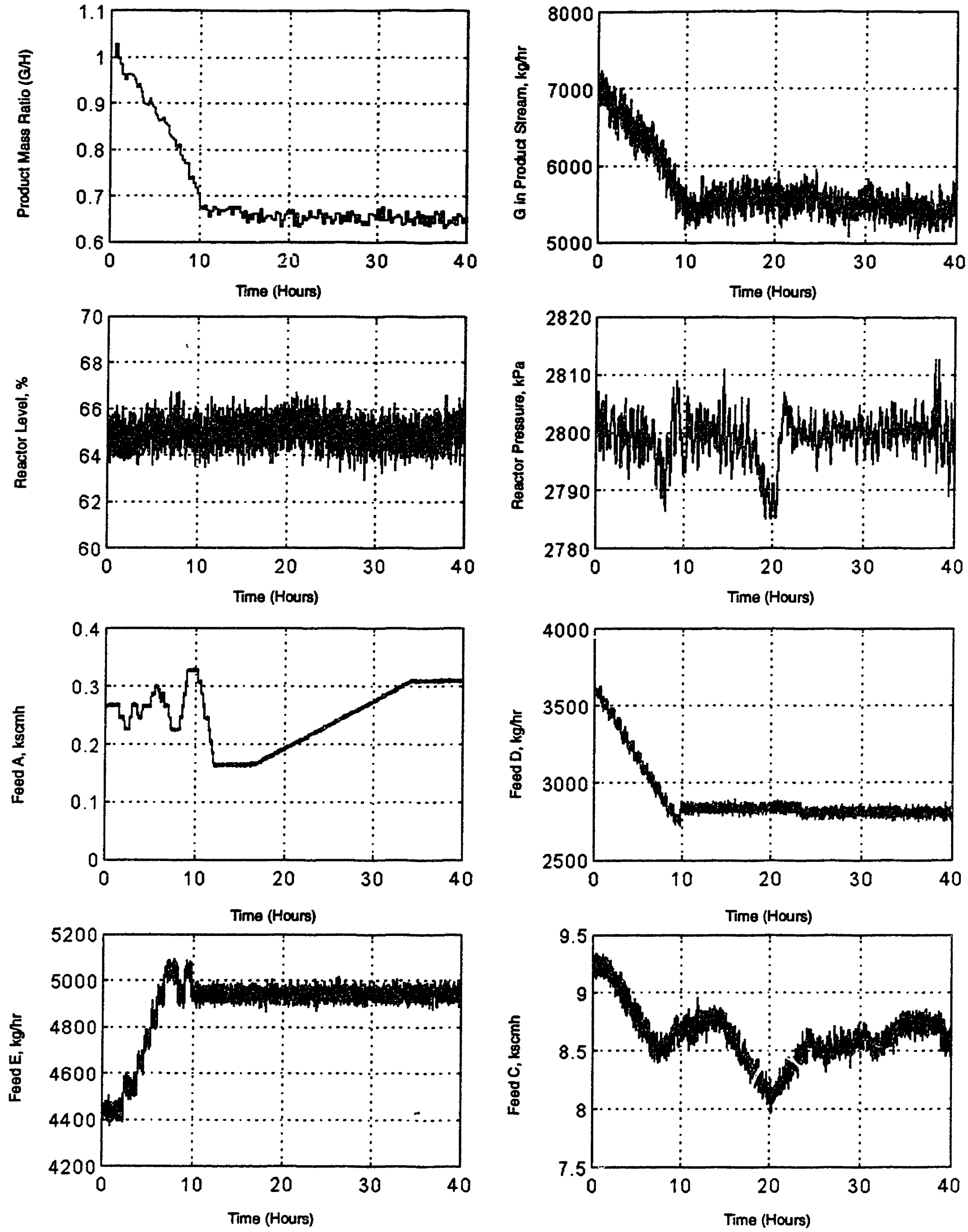


Figure 11 - 17: Effect of a Step Change in Product Ratio (new G/H = 0.66)

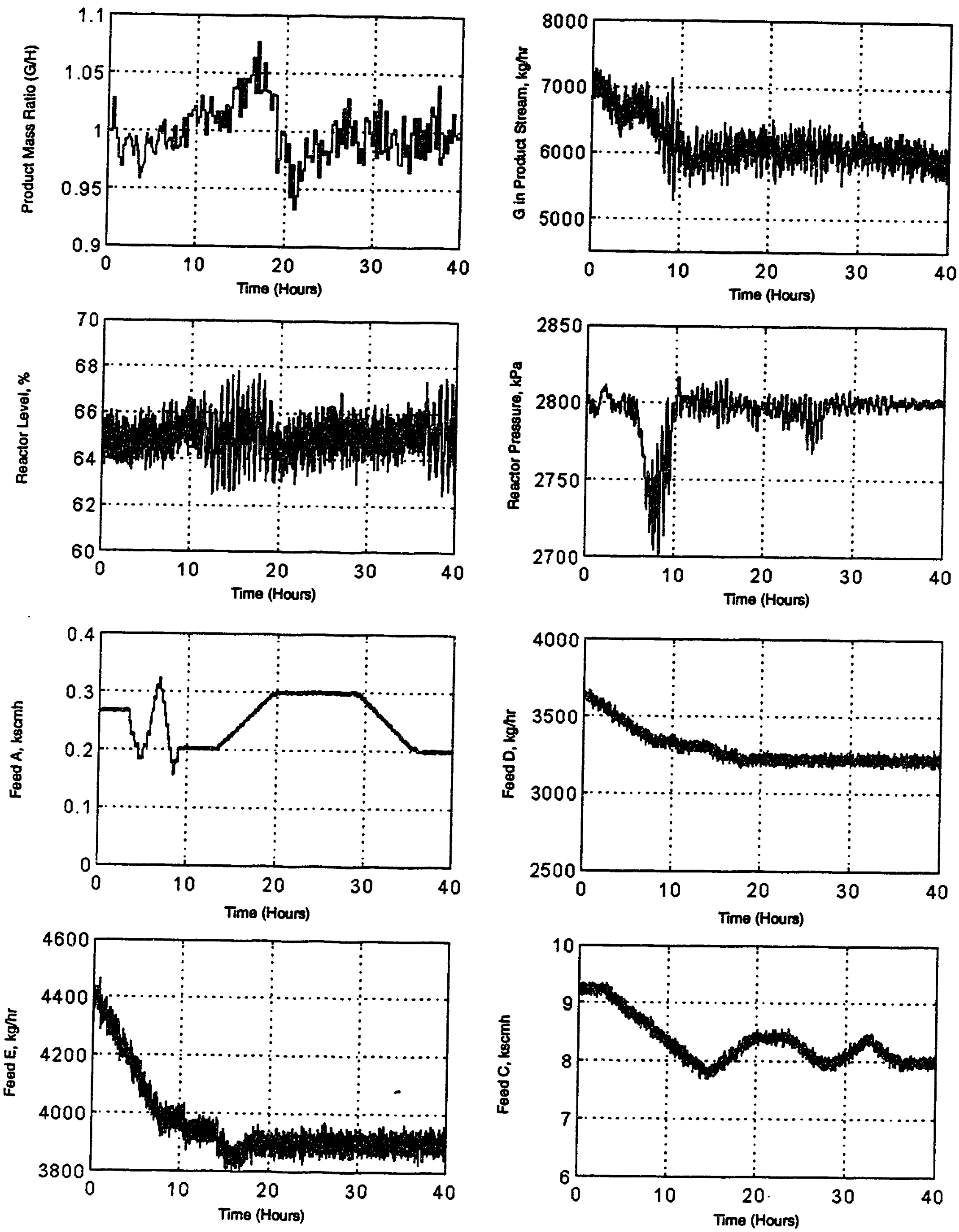


Figure 11 - 18: Effect of a Step Down in Production Rate by 15%

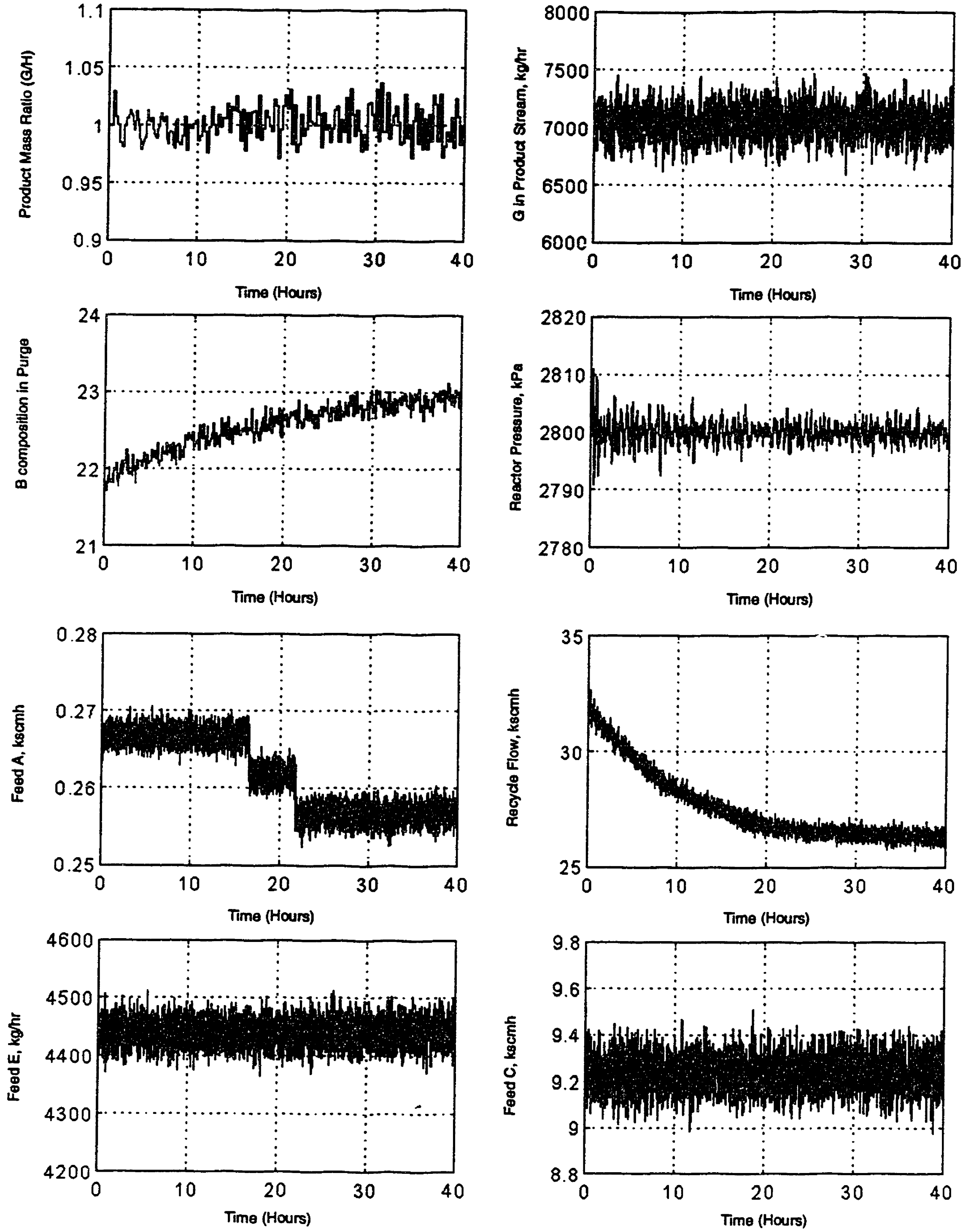


Figure 11 - 19: Effect of a Step Change in B in Purge by 1%

A Severe Process Upset

A more interesting disturbance is type 6 where the flow of feed A is temporarily lost. This is a very severe disturbance and one that is not expected to happened on a regular basis. Rather than sacrificing the performance of the whole control system to anticipate disturbance 6, a special control strategy has been developed to handle the loss of feed A. Steady-state analysis indicates that product specifications can be maintained by increasing the gas holdup in the process to allow for accumulation of unreacted gases. Also, Feed C should be raised to increase the amount of A entering to the process. As soon as disturbance 6 occurs, the control system puts Feed C on manual and increases its flow to 9.8 kscmh. Also, reactor level is lowered 60%, separator and stripper levels are both lowered to 10%. Reactor pressure setpoint is changed to 2850 kPa. Figure 11-20 shows the dynamic responses of a few key variables in the process during such an occurrence. Notice that by increasing the volume of gas hold-up in the process via judicious adjustments of the setpoints of the pressure and liquid levels in the plant, the control system is able to maintain the products at the required specifications for 40 hours or more. Due to process limitation, it is not able to keep reactor pressure under 2895 kPa (the high limit, not the shut-down limit) and reactor pressure alarm will be triggered during the loss of feed A. A similar set of steady-state operating set-points for handling disturbance 6 has been used by Ricker and Lee (1995b).

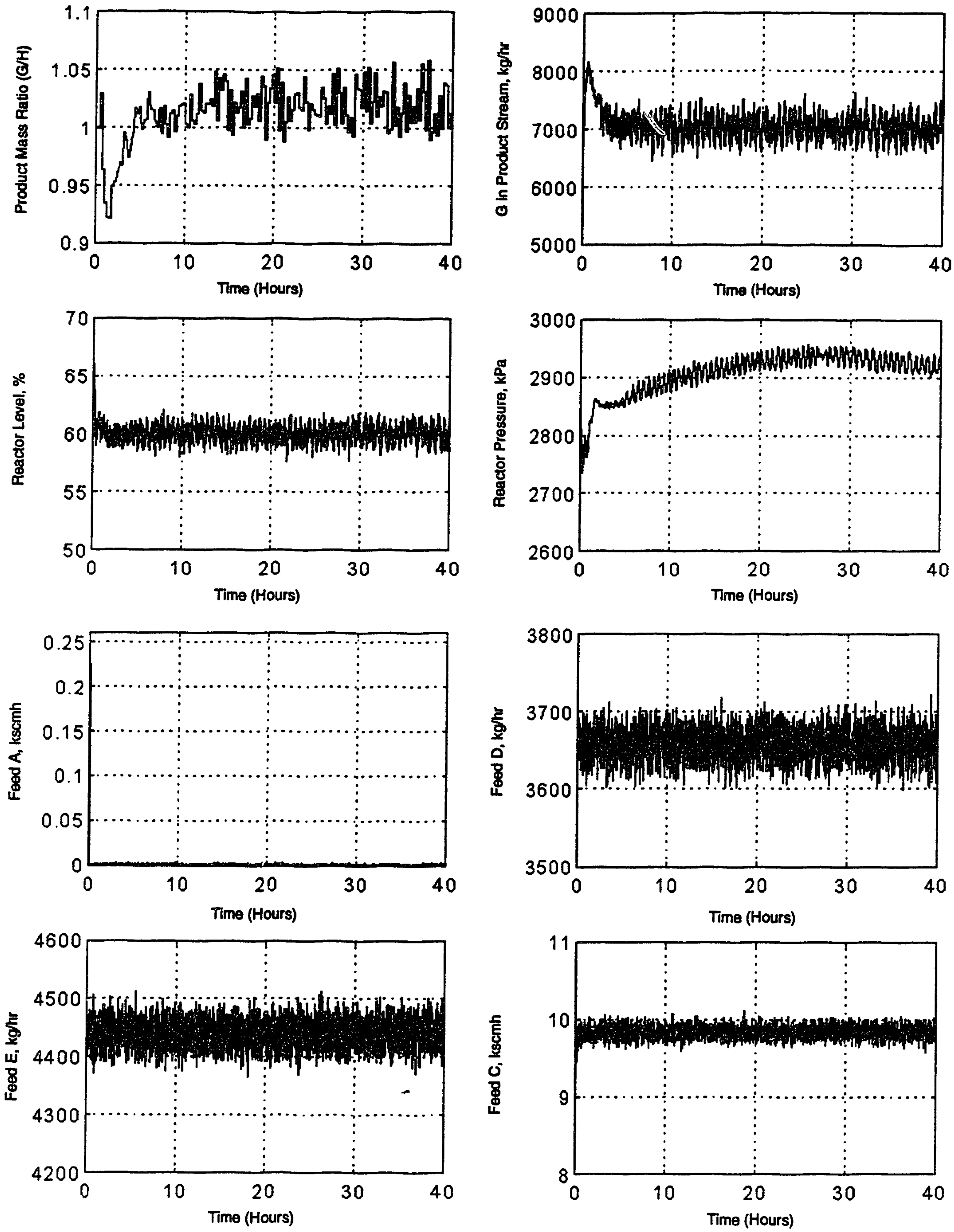


Figure 11 - 20: Effect of Loss of Feed A

11.7 Comparison of Proposed Control Structure with those Developed by Others

The proposed control structure is able to maintain the product ratio and production rate to be at their specifications (G/H ratio at 1 and flow of G at 7038 kg/hr) in the presence of all 20 different types of disturbances. Table 11-55 summarizes the cost of operation during the course of 40 hours of operation and the operating cost at the new steady-states for all cases of process changes studied for this work. The operating costs complied by Lyman (1995) for their proposed design are also included for comparison. Using the cost-optimal steady-state conditions as the starting point of analysis, the plant can be operated at a lower cost than similar case studies which have been reported by others (such as Lyman and Georgakis, 1995).

Table 11 - 57: Summary of Operating Costs of the Tennessee Eastman Process under several changes in the plant

Type of Changes in the Plant	Operating cost for 40 hrs (Dollars) Lyman (1995)	Operating cost for 40 hrs (Dollars) This work	Average Operating cost at steady state (Dollars per hour) This work
Disturbance Type 1	6580	5172	127.74
Disturbance Type 2	11233	6729	163.69
Disturbance Type 3	6777	4576	114.41
Disturbance Type 4	6777	4577	114.31
Disturbance Type 5	6771	4575	114.23
Disturbance Type 6	11919	12484	324.53
Disturbance Type 7	6776	4551	113.77
Disturbance Type 8	6942	4614	113.62
Disturbance Type 9	6775	4576	114.28
Disturbance Type 10	6776	4582	114.47
Disturbance Type 11	6776	4578	114.67
Disturbance Types 12	6791	4706	122.43
Disturbance Type 13	6680	5227	148.46
Disturbance Type 14	n/a	4577	114.43
Disturbance Type 15	n/a	4670	116.46
Unknown Disturbances and 3	n/a	4576	114.41
Unknown Disturbances and 3	n/a	4587	114.48
Unknown Disturbances and 3	n/a	4623	115.07
Unknown Disturbances and 3	n/a	4576	114.46
Unknown Disturbances and 3	n/a	4619	117.24
Lower G/H product ratio	6713	5412	163.98
Lower production by 85%	5407	4429	86.64
Lower Reactor Pressure	6047	5792	135.46
Increase B in purge	6769	5942	119.86

Almost all control structures which have been proposed for the TEC plant (McAvoy and Ye, 1994; Lyman and Georgakis, 1995; Banerjee and Arkun, 1995; Ricker and Lee, 1995) use the separator flow to and stripper flow to maintain the levels in separator and stripper. Reactor cooling water is used to control the reactor temperature. The control strategies which are used to maintain reactor level, reactor pressure, production and product ratio vary from one proposal to the other.

Closed-loop process simulations indicate that roughly 10 hours is needed to bring the plant to a new production rate or new product ratio using the proposed control structure in this work. This is length of time was also observed by others who have studied this process (McAvoy and Ye, 1994; Lyman and Georgakis, 1995; Banerjee and Arkun, 1995; Ricker and Lee, 1995). The systematic methodology proposed in this research allows the generation of a satisfactory control structure for the TEC plant in one trial. Other researchers (such as Lyman and Georgakis, 1995) obtained a satisfactory control structure by first generating several candidates structures and then testing each of the candidates using computer simulations to determine which one would give satisfactory results. Almost all researchers who have worked on this case study (McAvoy and Ye, 1994; Lyman and Georgakis, 1995; Ricker and Lee, 1995) have ignored the constraints imposed on feed rate variability stated in the original problem (Downs and Vogel, 1993). With the exception of the work proposed by Banerjee and Arkun (1995) who treated the plant-wide design problem as a monolithic multivariable control design problem, all other researchers have arrived at a satisfactory control structure via *ad hoc* and heuristics guidance. A formal and systematic method which can be applied to other process plants has not been proposed by these researchers (McAvoy and Ye, 1994; Lyman and Georgakis, 1995; Ricker and Lee, 1995).

Chapter 12
Interaction of Design and Control

12.1 Introduction

In Chapter 8, a systematic methodology for the synthesis of plant-wide control structures for chemical process plants was described. The assumption used throughout the discussion is that the plant control structure is developed based on a fixed flowsheet. This logic follows the traditional approach to the design of a new process plant which begins with the synthesis of the *design-optimal* process flowsheet at the desired steady-state conditions. Criteria used in the selection of process flowsheets are usually driven by *economics*, with little considerations given to the inherent transient behavior of the final process. Once the detailed process flowsheet has been fixed, a plant control system is to be developed so that the process can achieve some desired closed-loop characteristics.

The relationship between process design and process controllability was first pointed out by Ziegler and Nichols (1943). By "controllability", Ziegler and Nichols (1943) referred to the ability of the process to achieve and maintain the desired equilibrium value. In a typical schematic of a closed-loop system shown in Figure 12-1, the controller and the process form a unit. Thus, the quality of the closed-loop control of output y by inputs $\boldsymbol{m}$ is a function of the control strategies employed; the level of sophistication of the controller (such as a proportional-integral-derivative controller or a variant of a model predictive controller), as well as the tuning parameters; modelability of the process (i.e. whether a model can be developed for control purposes); and the process itself (i.e. the size and interconnection of units in the process). If a process itself is inherently hard to control, even with the best control strategies, the most sophisticated controller algorithm and the most accurate process model, control performance may still be unsatisfactory. If is determined that the control performance specification cannot be met even with the best control strategies, the only way to improve control performance is through modification of the flowsheet and/or re-sizing of process equipment.

The subject of interaction between process design and control is one which has caught the interests of the academic community in recent years. An extensive review can be found in Morari and Perkins (1994). Research effort has been focused on generating process flowsheets with economics and controllability in mind (Narraway and Perkins, 1993a, 1993b; Georgiou and Floudas, 1989; Luyben and Floudas, 1992, 1994). In this study, the focus is on the issues related to *plant revamp* for improvement of process control. Particularly, the opportunities for plant revamp will be studied within the modular multivariable control (MMC) framework presented in Chapters 3 and 6.

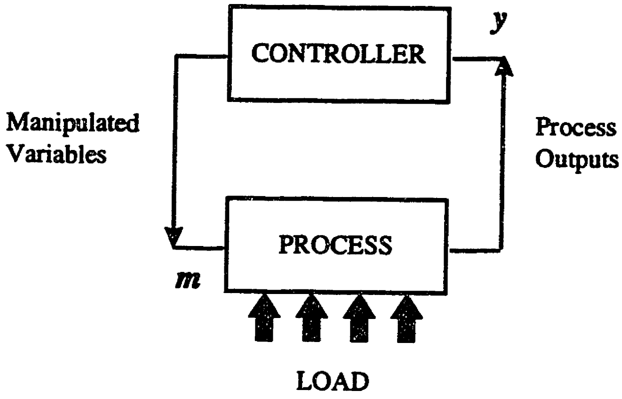


Figure 12 - 1: Closed-loop Control of a Process

12.2 Study of Process Revamp Opportunities in the Modular Multivariable Control Synthesis Framework

The essential feature of the methodology for control structure synthesis described in Chapter 8 is the use of a modular multivariable controller (MMC) design framework for the generation of control assignments (Chapters 3 and 6). The control structure is developed by associating primary manipulated variables to the set of control objectives, sequentially, starting from the most important control objectives. Consider a simple 2×2 system:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} + \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \qquad [12\text{-}1]$$

where y_1 and y_2 are control objectives, m_1 and m_2 are process manipulated variables, d_1 and d_2 are process disturbances and a, b, c and d are frequency-dependent elements in the transfer function matrix. The dependence on frequency will be omitted in the rest of the discussion for brevity. Suppose y_1 is a more important objective for this control system. It has also been determined that m_1 is a superior control input for the maintenance of y_1. Then, the MMC design methodology described in Section 6.3 leads to the following closed-loop description of the plant:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = G_+ F \begin{bmatrix} y_{1,sp} - d_1 \\ y_{2,sp} - d_2 \end{bmatrix} \qquad [12\text{-}2]$$

The matrix F in Equation [12-2] is a filter that is used to add robustness to the control system. It generally has the form:

$$F = \begin{bmatrix} \frac{1}{(\lambda_1 s+1)^{n_1}} & 0 \\ 0 & \frac{1}{(\lambda_2 s+1)^{n_2}} \end{bmatrix} \qquad [12\text{-}3]$$

where λ_1 and λ_2 are the filter constants, n_1 and n_2 are the order of the filter that is necessary to make the controller proper. G_+ in Equation [12-2] is a triangularly decoupled matrix:

$$G_+ = \begin{bmatrix} a_+ & 0 \\ c(a_-)^{-1}(1-G_{2+}f_2) & G_{2+} \end{bmatrix} \qquad [12\text{-}4]$$

such that:

$$G_2 = (d-ca^{-1}b) = (d-ca^{-1}b)_+(d-ca^{-1}b)_- = G_{2+}G_{2-} \qquad [12\text{-}5]$$

The transfer function a_+ is the non-invertible element in a (while a_- is the invertible element in a). Provided that there are no input constraints, the control performance of y_1 and y_2 are strictly determined by G_+. The closer is G_+F to the identity matrix, the better the expected control performance.

The control action required to accomplish the output profile in [12-2] is given by:

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = G_-^{-1}F\begin{bmatrix} y_{1,sp}-d_1 \\ y_{2,sp}-d_2 \end{bmatrix} \qquad [12\text{-}6]$$

where:

$$G = G_+G_- \qquad [12\text{-}7]$$

For the specific control assignments in the system in [12-1], the optimal MMC profiles of the control inputs are:

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \frac{\begin{bmatrix} da_+ - bca^{-1}(1-G_{2+}f_2) & -bG_{2+} \\ -ca_+ + aca^{-1}(1-G_{2+}f_2) & aG_{2+} \end{bmatrix}}{ad-cb}\begin{bmatrix} y_{1,sp}-d_1 \\ y_{2,sp}-d_2 \end{bmatrix} \qquad [12\text{-}8]$$

If G_+ and F can be set to the identity matrix, and if the control action recommended in [12-8] can be executed, perfect MMC closed-loop transient control can be achieved. The inherent process limitations to perfect control is therefore captured by the non-invertible elements in the process and the physical limits on $\boldsymbol{m}$. Any modification in the plant which results in less severe non-invertible elements in G_+ and expanded range of operation of $\boldsymbol{m}$ would result in improved control performance. In the rest of the discussion, the term $G_-^{-1}(s)F(s)$ will be referred to as the *perfect MMC controller*, with no restrictions on the inputs.

When the process is being controlled according to the MMC assignments such that m_1 is the manipulated variables for y_1 and m_2 is the manipulated variable for y_2, the following statements are true:

1. According to [12-4], control performance of y_1 can be improved by reducing the impact of the non-invertible elements in the transfer function a.
2. According to [12-4], control performance of y_2 can be improved by reducing the impact of the non-invertible elements in G_2 and by making the term $c(a_-)^{-1}(1-G_{2+}f_2)$ as close to zero as possible. Obviously, if G_{2+} can be set to unity, $c(a_-)^{-1}(1-G_{2+}f_2)$ approaches zero quickly if a filter with a small filter constant is sufficient to add robustness in the system.
3. According to [12-8], the profile of the inputs is affected by all transfer functions in the matrix which describes the process dynamics. This is expected. Although in the MMC framework, through the association of individual inputs to distinct control objectives, G_+ is a triangularly decoupled matrix, the controller itself is a full scale multivariable controller which accounts for the interaction in the system. Thus, variation of any process dynamics in the system will affect the profiles of the control inputs.

The above statements define the *pathways* which are being established in the system during control structure synthesis. These pathways link control performance of individual outputs to certain elements in the transfer function matrix. For larger systems, simply replace [12-1] by [6-20] and [6-21]. The relationships between control performance of individual outputs and the various elements in the transfer function matrix is analogous to the presentation above.

The focus of this chapter is on how plant revamp opportunities for individual control objectives can be selectively identified in the MMC framework described above. As the interplay between process design and control is quite an involved subject, a complete understanding of the intricate relationship between the two aspects of plant operation is not possible in a brief investigation. The intent of the current study is to identify key issues and to perhaps suggest a framework in which opportunities for control performance improvement can be formally studied. The scope this study is limited to systems which have good linear approximations and systems whose impact of model uncertainty on control performance is negligible.

12.3 Mapping between Control Performance and Process Characteristics

In the previous section, we have pointed out the how plant revamp opportunities for individual control objectives can be selectively identified in the MMC framework. In this section, the goal is to summarize how unsatisfactory control performance is related to the inherent process characteristics. Understanding of such relationships will assist the identification of opportunities for improvement in control performance of individual control objectives (see Section 12.2).

The description of the inherent process characteristics by G_+ as well as the characteristics of the perfect controller have been exploited to develop guidelines for the synthesis of control structures (Chapters 5 and 6). In a *reversed* manner, unsatisfactory closed-loop characteristics can also be traced back to the inherent process characteristics which limits performance and suggest changes that can be made in the process to improve the quality of the closed-loop response.

As any changes in the process involves cost, once a plant has been built, design modifications should only be introduced if the desired closed-loop static and dynamic characteristics cannot be met even with the best control system. As in the case for control structure synthesis (see Chapter 6), the approach to plant revamp should also be a goal driven one. The control performance of the existing system is to determine if the specifications on closed-loop performance (defined by production objectives) can be met even with the best set of process control strategies. Unacceptable control performance is than traced back to physical factors of the inherent process dynamics which limit the performance. Once the limitations have been identified, design changes which will result in improved control performance can be proposed. Such proposal must be based on understanding of the fundamental principles governing the process. A cost-benefit analysis must then be carried out to determine if there is a positive return of investment from the proposed process revamp. This idea is depicted in Figure 12-2. In this section, the knowledge required in the INHERENT PROCESS LIMITATIONS IDENTIFIER in Figure 12-2 will be summarized. This identifier consists of a mapping between unsatisfactory control performance to factors related to process design.

Skogestad (1994) has generalized the ability to achieve acceptable control performance as the *input-output* controllability of the system. Typical desirable closed-loop static and dynamic characteristics include: no offset or input saturation at steady-state; the ability to react to process changes and the ability to insulate process from high frequency process variations. The performance of the control system is judged by how well the above specific objectives can be attained with the best possible control system and is solely a function of the inherent process characteristics. If the control performance is unacceptable, even with the best control configuration, the only way to improve process performance is by changing the inherent process characteristics. The link between typical undesirable closed-loop static and dynamic characteristics and the physical parameters governing the process will be summarized in the next few sections.

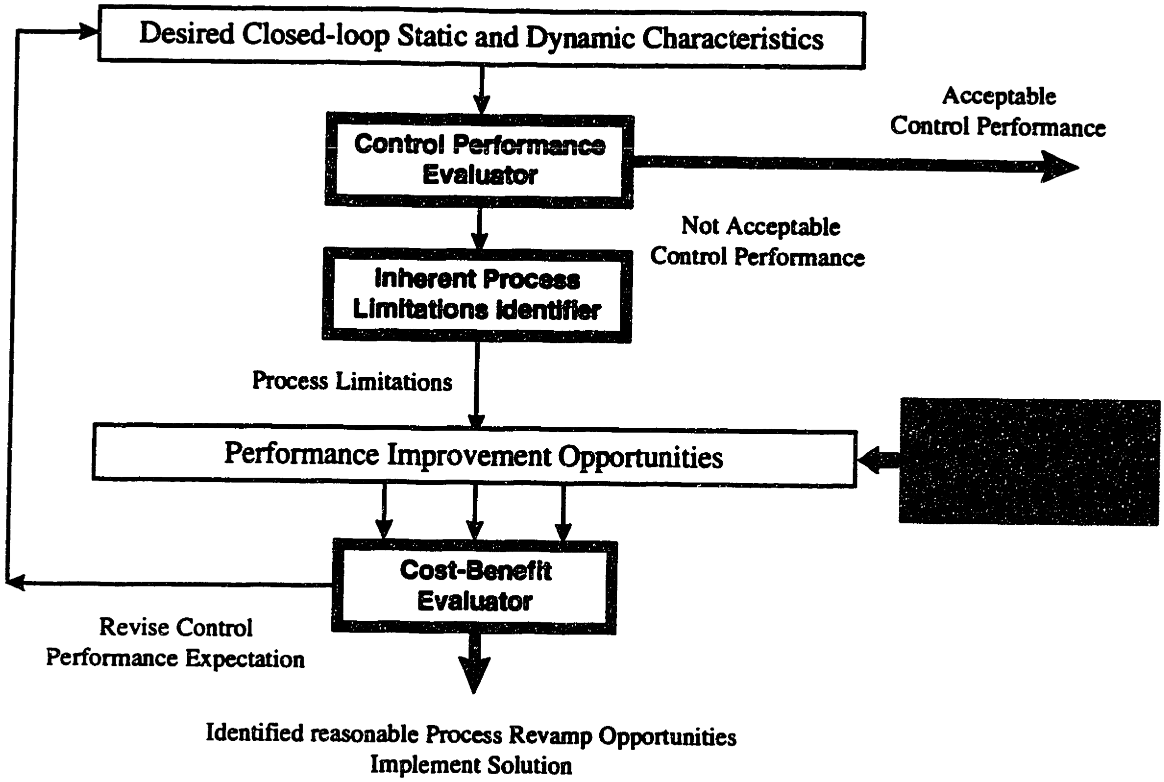


Figure 12 - 2: From Closed-loop Process Characteristics to Process Improvement Opportunities

12.3.1 Steady-state Offset and Input Saturation at Steady-State

Steady-state offset is related to the ability to attain the desired steady-state in the presence of persistent process disturbances. For steady-state control, G_+ in Equation [12-2] is necessarily an identity matrix. Thus, the quality of the control is strictly determined by the rangeability of the inputs and the size of the gain. For a single-input, single-output (SISO) system, the process is simply described by:

$$y_{ss} = Km_{ss} + d_{ss} \qquad [12\text{-}9]$$

where y_{ss} and m_{ss} are respectively values of the output and input at steady-state, K is the gain of the output for a step change in the input and d_{ss} is the persistent disturbance acting on the process at steady-state. In a physical system, the control action must be confined to within its physical limits:

$$m_{lower} < m < m_{upper} \qquad [12\text{-}10]$$

The attainable outputs are confined to a range defined by:

$$Km_{lower} + d < y < Km_{upper} + d \quad \text{for } K > 0 \qquad [12\text{-}11]$$

or

$$Km_{upper} + d < y < Km_{lower} + d \quad \text{for } K < 0 \qquad [12\text{-}12]$$

If the desired steady-state value of y is outside the feasible range, steady-state offset will be observed, with the input at one of the saturation limits. Furthermore, unless the process is being operated at its maximum throughput, saturation of key inputs at steady-state usually means loss of degrees of freedom. The ability of the process to react to unexpected changes in the process or environment is limited. It has been pointed out in Section 6.3.1 that the control performance at steady-state is limited by the rangeability of the control input and the magnitude of the process gain. The error at steady-state can be corrected by altering the gain of the system, or by expanding the range of operation of the input.

For a multi-input, multi-output (MIMO) system given by:

$$\boldsymbol{y} = \boldsymbol{Km} + \boldsymbol{d} \qquad [12\text{-}13]$$

where $\boldsymbol{K}$ is the steady-state gain matrix and K_{ij} is the steady-state gain of output i to a unit change of input j, steady-state offset in output y_i is a function of a multiple number of gains K_{ij}, the ranges of operation of a multiple number of inputs m_j, as well as the relative importance of the outputs assumed in the multivariable controller.

Following the lexicographic goal programming philosophy in MMC framework (Chapter 6), control objectives are satisfied sequentially, starting from the most important one. Control action for the maintenance of an objective of a lower priority is introduced without degrading the achievable performance of the objectives which are of higher priority. Hence, any steady-state offset in the multivariable system is a function of the rank order of the control objectives. In a multivariable system, changes in one open-loop gain in the steady-state matrix $\boldsymbol{K}$ may affect the solution of one or more outputs. Care must be taken so that any changes in the design for the improvement of the control performance of a particular output does not degrade any attainable performance of the higher objectives in the original design.

EXAMPLE 12-1

A 2×2 system is given by:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 6 & 2 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} + \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \qquad [12\text{-}14]$$

at steady-state. It is desired to maintain both y_1 and y_2 to be at 70 and 60 respectively. The maximum expected magnitudes of the disturbance $d_{1,max}$ and $d_{2,max}$ have been found to be -10 and -20 respectively. Objective y_1 is of higher priority. The inputs m_1 and m_2 must both be confined to the range between -10 and 10. It can be easily verified that the steady-state solution of the 2×2 system when disturbances have maximum impact on the plant is given by:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 10.9091 \\ 7.2727 \end{bmatrix} \quad [12\text{-}15]$$

which is infeasible (since $u_1 > 10$). Several possible feasible implementations of the control system are summarized in Table 12-1. Case 1 corresponds to the MMC implementation where introduction of additional control action for y_2 does not degrade the achievable control performance of y_1, the more important objective. Case 2 is a similar MMC implementation but with y_2 being more important than y_1. Case 3 corresponds to a solution to some weighted multiobjective steady-state optimization with y_1 being slightly more important than y_2 but not in an absolute sense. Thus, we see that in a multivariable system, the control performance is a function of the relative importance of the objectives assumed in the controller design.

Table 12 - 1: Possible Implementation of the 2×2 System

	u_1	u_2	y_1	y_2	error in y_1	error in y_2
1	10	10	70	70	0	10
2	10	8	66	60	-4	0
3	10	9	68	65	-2	5

Similar to the SISO case, control performance can again be improved by expanding the ranges of operation of the inputs or by altering the steady-state process gains. However, since zero offset is possible for y_1 in the original design, any changes in the design to reduce steady-state offset in y_2 must not degrade the original achievement level of the more important objective. Several alternative designs based on altering steady-state gains are summarized in Table 12-2. Cases 4 and 5 are acceptable ways to improve the existing system. The steady-state offset in y_2 is reduced without degrading the control performance attainable for y_1 in the original design. Case 6 is inferior to the original design as a steady-state offset in y_1 is generated even though offset in y_2 is eliminated.

Table 12 - 2: Possible Alternative Designs of the 2×2 System

	K	u_1	u_2	y_1	y_2	error in y_1	error in y_2
4	$\begin{bmatrix} 6 & 2 \\ 4 & 3.8 \end{bmatrix}$	10	10	70	58	0	-2
5	$\begin{bmatrix} 6 & 3 \\ 4 & 6 \end{bmatrix}$	10	6.667	70	60	0	0
6	$\begin{bmatrix} 5.7 & 2 \\ 4 & 4 \end{bmatrix}$	10	10	67	60	-3	0

Process Revamp to Alleviate Steady-State Offset or Input Saturation

The presence of steady-state offset in the system suggests that the process has not been properly designed to meet the expected range of production specifications or that the magnitude of the persistent process disturbances have been underestimated during process design. Alteration of the process static gains or the ranges of operation of the inputs are the only ways to eliminate steady-state offset.

For a SISO system with a positive gain K, the upper limit of the input is simply:

$$m_{\text{upper}} \geq (y_{\text{sp}}\text{-}d)_{\max} / K \qquad [12\text{-}16]$$

For a $n \times n$ MIMO system, the limit of input j must satisfy the following relation.

$$r = \begin{bmatrix} y_{sp,1} - d_1 \\ \vdots \\ y_{sp,n} - d_n \end{bmatrix}$$
$$m_j \geq \left| \, [c_{j1} \cdots c_{jn}] \cdot r \right|_{\max} \quad \forall r \qquad [12\text{-}17]$$

where $[c_{ij}]$ is the (i,j) element in C, $C = K^{-1}$.

Increasing the ranges of operation of the critical inputs is the simplest and cheapest solution to the problem. However, changing the ranges of operation of the inputs may or may not always be possible as the usage of inputs may represent demands in other processes. There may also be bottlenecks in the plant which prevent the effect of the increase in the magnitude of the input to propagate to the concerned output. When the ranges of operation of the critical inputs cannot be expanded, offsets can only be eliminated by altering the process gains. Some process gains can be altered by changing the system parameters, others are associated with the fundamental property of the materials being employed in the system and cannot be changed. Examples include the gain in the temperature of a vessel for a step change in the temperature of coolant/steam or gain in the output of a mixing process are limited to unity. Changing one parameter in the physical system may affect the static gains of a number of element in the process gain matrix. Care must be taken so that the achievable performance of the more important objectives are not degraded as a result of the process revamp.

12.3.2 Input Saturation During Transient

If input reaches its saturation limit, the optimal control action from the perfect controller cannot be executed and closed-loop control must necessarily be sub-optimal. Additional time must be passed before the disturbances can be eliminated or the new setpoint can be reached. From Equation [12-6], it can be deduced that a process with a large time constant would demand more severe control action by the perfect MMC controller (see Section 12.2) in order to eliminate error in the output. By expanding the range of operation of the concerned input or by modifying the parameters which govern the transient behavior, this situation can be alleviated.

Input saturation during transient is an indication of the process not being able to respond fast enough to changes in the manipulated variable. The time that is required to eliminate error in the output can be reduced if the physical system can be changed to reduce the size of one or more of the time constants.

Modifying the Process to change the Transient Characteristics

In general, for an invertible SISO system defined by:

$$g(s)=\frac{(a_1s+1)\cdots(a_js+1)}{(b_1s+1)\cdots(b_ks+1)} \quad \text{for } k>j \text{ and } a_v>0 \quad \forall v \qquad [12\text{-}18]$$

The optimal control action to a step changes in (y_{sp}-d) is simply:

$$m(s)=\frac{(b_1s+1)\cdots(b_ks+1)}{(a_1s+1)\cdots(a_js+1)}\,\frac{1}{(\lambda s+1)^n}(y_{sp}-d) \quad \text{for } n\geq(k-j) \qquad [12\text{-}19]$$

where λ is the filter time constant. For a fixed λ, the severity of the optimal control profile $m(s)$ is governed by the sizes of the time constants b_q, q = 1 to k and the location of the process negative zeros a_v, v = 1 to j. Decreasing the size of any of the b_q or increasing the size of any of the a_v would reduce the severity of the required control action and hence reduce the time that is needed to eliminate output error if the range of operation of the input is limited.

For the most simplistic form of MIMO system defined by the following transfer function matrix $G(s)$ between inputs $[\, m_1(s) \;\; m_2(s)]^T$ and outputs $[\, y_1(s) \;\; y_2(s)]^T$:

$$G(s) = g(s)\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}$$

$$g(s) = \frac{(a_1 s+1)\cdots(a_j s+1)}{(b_1 s+1)\cdots(b_k s+1)} \quad \text{for } k > j \text{ and } a_v > 0 \quad \forall v \qquad [12\text{-}20]$$

In the MMC multiobjective framework, m_1 is the primary manipulated variable for y_1 and m_2 is that for y_2, y_1 being a more important control objective. Assuming $g(s)$ to be an invertible process, using Equation [12-4], $G_+(s)$ is simply given by:

$$G_+(s) = \begin{bmatrix} 1 & 0 \\ \frac{K_{21}}{K_{11}}(1-f_2) & 1 \end{bmatrix}$$

$$f_2(s) = \frac{1}{(\lambda_2 s+1)^n} \quad \text{for } n \geq (k-j) \qquad [12\text{-}21]$$

Even though the process is invertible, the MMC triangular factorization produces a lower triangular matrix. The non-zero elements $G_{+,ij}$, $j < i$, allow for dynamic interaction. These elements in fact approach zero very fast as f_k $\forall$ k are low-pass filters. Since $G_-^{-1}(s) = G^{-1}(s)G_+(s)$, the matrix $\left[G_-^{-1}(s)F(s)\right]$ which defines the H_2-optimal profiles of the inputs is given by Equations [12-6] and [12-8]:

$$G_-^{-1}(s)F(s) = \frac{g^{-1}(s)}{K_{11}K_{22} - K_{12}K_{21}} \begin{bmatrix} K_{22} - \frac{K_{12}K_{21}}{K_{11}}(1-f_2) & -K_{12} \\ -K_{21}f_2 & K_{11} \end{bmatrix} \begin{bmatrix} f_1 & 0 \\ 0 & f_2 \end{bmatrix} \qquad [12\text{-}22]$$

$$f_1(s) = \frac{1}{(\lambda_1 s+1)^n} \quad \text{for } n \geq (k-j)$$

Hence, the severity of the optimal control profile $m(s)$ is governed by the sizes of b_q, $q = 1$ to k and a_v, $v = 1$ to j. Decreasing the size of any of the b_q or increasing the size of any of the a_v would reduce the severity of the required control actions for both inputs and hence reduce the time that is needed to eliminate error of both outputs if the rangeability of the input is limited.

For a more general 2×2 MIMO system such as one whose transfer function matrix $G(s)$ is of the form given by:

$$G(s) = \begin{bmatrix} \frac{(a_{11}s+1)\cdots(a_{1j}s+1)}{(b_{11}s+1)\cdots(b_{1k}s+1)} & \frac{(a_{21}s+1)\cdots(a_{2j}s+1)}{(b_{21}s+1)\cdots(b_{2k}s+1)} \\ \frac{(a_{31}s+1)\cdots(a_{3j}s+1)}{(b_{31}s+1)\cdots(b_{3k}s+1)} & \frac{(a_{41}s+1)\cdots(a_{4j}s+1)}{(b_{41}s+1)\cdots(b_{4k}s+1)} \end{bmatrix} \qquad [12\text{-}23]$$

where all elements in the matrix are proper and invertible and $G(s)$ is invertible. The optimal profile of a particular input will be affected by each of the elements in $G(s)$ as shown in earlier in Equation [12-8]. The parameters which must be changed to alter the severity of the control action must be formulated on a case-by-case basis.

12.3.3 Inability to Quickly Eliminate Output Error

According to Equation [12-2], the output must necessarily deviate from the desired value for a certain period of time if the process contains non-invertible elements (such as deadtime and RHP zeros).

Modifying the Process to Reduce Effect of Process Deadtime

Under perfect feedback control, error in the output cannot be eliminated within a time horizon that is smaller than the process deadtime. For a SISO process given by $G(s) = g(s)e^{-t_d s}$, where $g(s)$ is an invertible element as previously defined in Equation [12-18] and t_d is the process deadtime. Then, the optimal profile of the output is simply:

$$y(s) = e^{-t_d s} F(s)(y_{sp} - d) \qquad [12\text{-}24]$$

$F(s)$ is a n^{th} order scalar filter, where n is greater than or equal to $(k\text{-}j)$, k and j define the order of the lag and lead elements in $g(s)$ respectively. Regardless of the choice of filter, $e^{-t_d s}$ quantifies the limiting control factor in the process. Any process modification that reduces the size of t_d would improve the control performance.

Deadtime is usually a result of transportation delay or response delay due to measurement lag or actuator lag. Apparent deadtime is caused by the presence of a large number of lag systems in series, commonly occurred in multi-staged processes such as distillation columns. The deadtime in a SISO process can be reduced by changing the piping system to reduce transportation delay, or by speeding up the measurement process. Apparent deadtime of a high order system can only be reduced by substantially modifying the design. For example, the apparent deadtime of a distillation column can be reduced by reducing the number of trays in the column. This may of course affect the separation ability of the system which will ultimately affect the static gain. Thus, there is a trade-off between the speed of the response and the flexibility of the operation at steady-state.

The above ideas can be easily extended to MIMO systems but care must be taken in the redesign to ensure that control performance of more important objectives is not sacrificed for the improvement of control performance of control objectives of lesser importance. The next few examples will illustrate this idea. The next example shows how control performance can be improved by *decreasing* the process deadtime.

EXAMPLE 12-2

Consider a 2 × 2 MIMO process dominated by the presence of deadtime. The transfer function matrix $\boldsymbol{G}(s)$ describes the open-loop response of outputs $y(s) = [y_1(s)\ y_2(s)]^T$ by inputs $\boldsymbol{m}(s) = [\,m_1(s)\ m_2(s)]^T$:

$$G(s)=\begin{bmatrix} e^{-5s} & e^{-7s} \\ e^{-8s} & e^{-6s} \end{bmatrix} \qquad [12\text{-}25]$$

Assigning m_1 to be the primary manipulated variable to control y_1 and m_2 to control y_2 in the MMC design, the following $G_+(s)$ for the closed-loop system ($F(s)=1$ is used) can be obtained from Equation [12-4] :

$$G_+(s)F(s)=\begin{bmatrix} e^{-5s} & 0 \\ e^{-8s}(1-e^{-6s}) & e^{-6s} \end{bmatrix} \qquad [12\text{-}26]$$

In Section 2.2, we noted that improvement of control performance in y_2 is possible if the deadtime in the second output by both m_1 and m_2 can be significantly reduced so that the modified process $G^*(s)$ is given by:

$$G^*(s)=\begin{bmatrix} e^{-5s} & e^{-7s} \\ e^{-2s} & e^{-3s} \end{bmatrix} \qquad [12\text{-}27]$$

The corresponding non-invertible part of the MMC design is ($F(s)=I$) :

$$G^*_+(s)F(s)=\begin{bmatrix} e^{-5s} & 0 \\ e^{-2s}(1-e^{-3s}) & e^{-3s} \end{bmatrix} \qquad [12\text{-}28]$$

The process modification resulted in improved control performance.

In terms of control performance, $G^*(s)$ is a better design than $G(s)$ since error in y_2 can be eliminated faster in the new design. Furthermore, $G^*(s)$ gives improved performance in y_2 without degrading the achievable performance of y_1 in the original design $G(s)$, conforming to the multi-objective design philosophy.

It has been noted by some researchers (Holt and Morari, 1985a) that it is possible to improve control performance in some systems by *increasing* the process deadtime. It will be shown in the next example that this type of process modification may not always produce the same benefits when dynamic interaction is allowed in the MMC framework.

EXAMPLE 12-3

Consider the following process studied by Holt and Morari (1985a):

$$G_1(s)=\begin{bmatrix} e^{-2s} & 0 \\ e^{-s} & e^{-4s} \end{bmatrix} \qquad [12\text{-}29]$$

The output response of a *dynamically decoupled* design is governed by the following non-invertible matrix ($F(s) = I$) :

$$G_{1+,\text{decoupled}}(s) = \begin{bmatrix} e^{-5s} & 0 \\ 0 & e^{-4s} \end{bmatrix} \qquad [12\text{-}30]$$

and the following physically realizable controller ($Q_{1,\text{decoupled}}$):

$$Q_{1,\text{decoupled}}(s) = G_{1-,\text{decoupled}}^{-1}(s) = \begin{bmatrix} e^{-3s} & 0 \\ -1 & 1 \end{bmatrix} \qquad [12\text{-}31]$$

Notice that in this system, y_2 response much faster to m_1 than m_2. To effect a setpoint change in y_1 while y_2 remains at the original value, m_2 must be used to cancel out the effect of m_1 on y_2. Since the delay between m_1 and y_2 is three units smaller than that between m_2 and y_2, the signal of m_1 by the controller must be delayed by three time units. Thus, the fastest that y_1 can response to a setpoint change is 5 time units. Two units from the delay between y_1 and m_1 and three units of added delay to allow m_2 to correct action on y_2 by m_1. It was suggested that increasing the time constant between m_1 and y_2 could improve control performance. In the modified plant where the deadtime between y_2 and m_1 has been increased to four time units:

$$G_2(s) = \begin{bmatrix} e^{-2s} & 0 \\ e^{-4s} & e^{-4s} \end{bmatrix} \qquad [12\text{-}32]$$

the non-invertible matrix that is equivalent to a dynamically decoupled design is:

$$G_{2+,\text{decoupled}}(s) = \begin{bmatrix} e^{-2s} & 0 \\ 0 & e^{-4s} \end{bmatrix} \qquad [12\text{-}33]$$

which is better than the one for the original design (see Equation [12-30]). The controller ($Q_{2,\text{decoupled}}$) is simply:

$$Q_{2,\text{decoupled}}(s) = G_{2-,\text{decoupled}}^{-1}(s) = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \qquad [12\text{-}34]$$

In the multiobjective design framework, priority is given to the more important control objectives. With y_1 being more important, MMC factorization gives the following *triangularly decoupled* and non-invertible matrix for the original design ($F(s) = I$) :

$$G_{1+,MMC}(s)=\begin{bmatrix} e^{-2s} & 0 \\ e^{-s}(1-e^{-4s}) & e^{-4s} \end{bmatrix} \quad [12\text{-}35]$$

and the following physically realizable controller ($Q_{1,MMC}$):

$$Q_{1,MMC}(s)=G^{-1}_{1-,MMC}(s)=\begin{bmatrix} 1 & 0 \\ -e^{-s} & 1 \end{bmatrix} \quad [12\text{-}36]$$

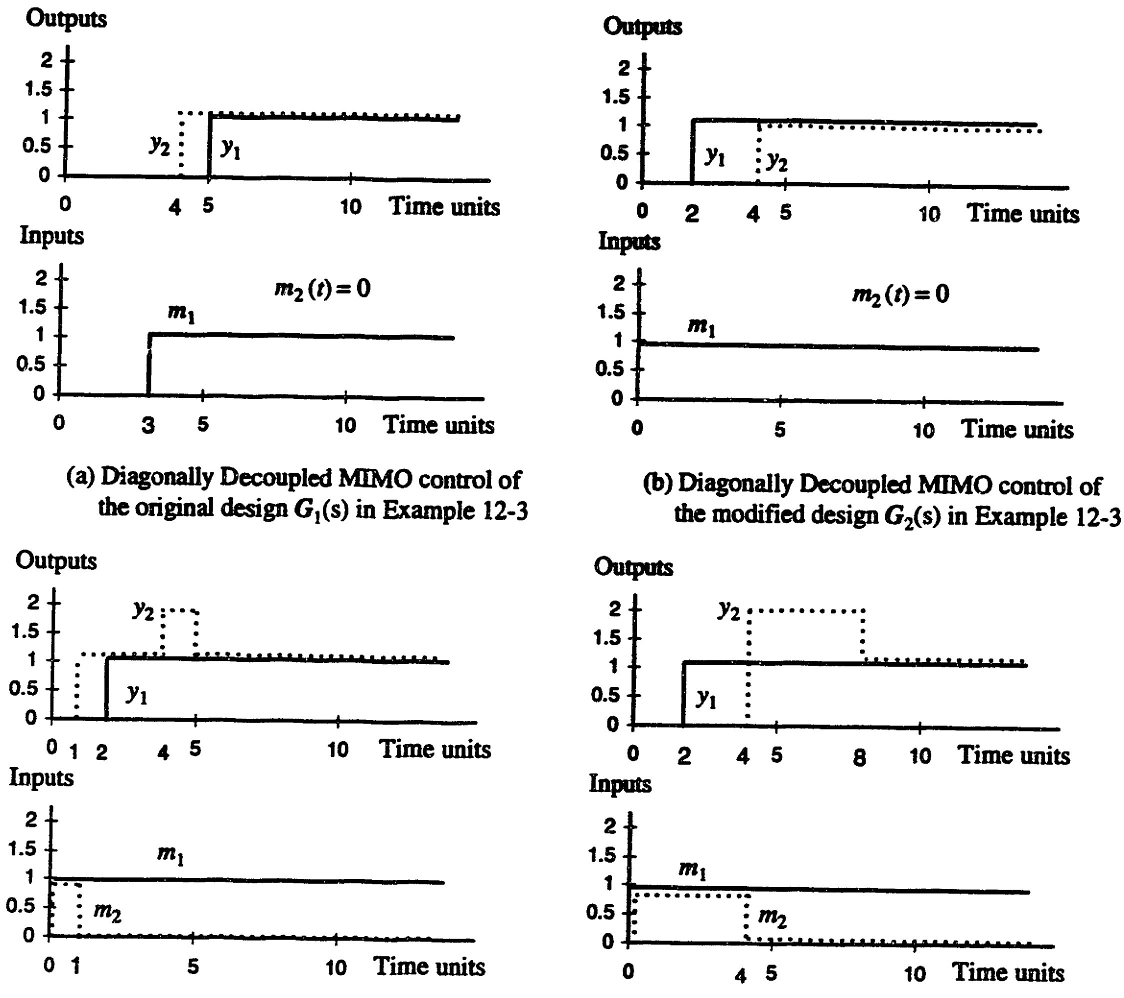
The price of improved control performance of y_1 is dynamic interaction in y_2 for changes in ($y_{1,sp}$ - d_1). The non-invertible matrix of the MMC design for the modified plant is given by:

$$G_{2+,MMC}(s)=\begin{bmatrix} e^{-2s} & 0 \\ e^{-4s}(1-e^{-4s}) & e^{-4s} \end{bmatrix} \quad [12\text{-}37]$$

which is worse than $G_{1+,MMC}(s)$. The MMC controller ($Q_{2,MMC}$) for the modified plant is:

$$Q_{2,MMC}(s)=G^{-1}_{2-,MMC}(s)=\begin{bmatrix} 1 & 0 \\ -e^{-4s} & 1 \end{bmatrix} \quad [12\text{-}38]$$

Figure 12-3 compares the output response of the original process (G_1) and the modified design (G_2), to a change of 1 unit in the setpoints of both y_1 and y_2, using both the fully decoupled controller and the triangularly decoupled MMC controller. The proposed process modification resulted in improved control performance of y_1 by the decoupled controller. In the goal driven MMC controller design, the error in y_1 is the same in both the original and modified process. However, the error of y_2 is higher in the modified system. Increasing the deadtime has not produced improved control performance when dynamic interaction is allowed in the MMC design framework.



(a) Diagonally Decoupled MIMO control of the original design $G_1(s)$ in Example 12-3

(b) Diagonally Decoupled MIMO control of the modified design $G_2(s)$ in Example 12-3

(c) MMC control of the original design $G_1(s)$ in Example 12-3

(d) MMC control of the modified design $G_2(s)$ in Example 12-3

Figure 12 - 3: Effect of Increasing deadtime in a MIMO system on Control Performance

Modifying the Process to Attenuate Inverse Response Behavior

Based on Equation [6-18], the closer is the RHP zero to the imaginary axis, the larger will be the integrated squared error in the optimal feedback output response, and a longer time is needed to bring the process to a new setpoint or eliminate process disturbances. Inverse response behavior is a result of the presence of two opposing mechanisms governing the dynamics of the system. For MIMO systems, it is the presence of RHP transmission (RHPT) zeros which makes the process non-invertible. Even if none of the elements in the transfer function matrix contain RHP zeros, inverse response behavior is still possible as a result of process interaction among variables.

Two common occurrence of inverse response behavior in chemical plants given by Ogunnaike and Ray (1994) are provided below:

1. *Level in a drum boiler*

   A drum boiler generates steam for the plant's utility system. The drum is normally filled with liquid material at boiling point whose total volume (or level) of liquid in the drum is a function of both the mass of the liquid in the drum as well as the volume of the bubbles. A positive step change in the cold feed material would ultimately cause an increase in the total volume of liquid in the drum. However, at the introduction of cold water, the temperature in the drum drops, causing liquid bubbles to collapse and immediately decreases the total liquid volume. The initial cooling effect will eventually be overridden by the rise in material flow to the system, producing an inverse response behavior.

2. *Exit temperature of a tubular catalytic reactor*

   The exit temperature of a certain tubular catalytic reactor exhibits inverse response to both step up and step down of the inlet temperature. This phenomena is a result of the competing processes governing the transport of temperature and concentration of reactants down the tubular reactor. A step increase in the inlet temperature produces two effects: a thermal effect which transport the heat down the length of the tubular reactor and a kinetic effects which increases the rate of reaction and thereby decreases the concentration of reactants down the length of the reactor. When the heat capacity of the catalyst is high, the concentration front travels much faster than the temperature front. Hence, the immediate effect of an increase in feed inlet temperature is that the concentration of the reactants decreases along the length of the reactor, decreasing the rate of the reaction and therefore a drop in the exit temperature. Eventually, when the temperature front catches up with the concentration front, the exit temperature will go up.

It can be easily seen from these examples that inverse response behavior is caused by a combination of physical factors. Deriving process modification opportunities which would eliminate (i.e. make the RHP zero disappear) or attenuate (i.e. move the RHP zero away from the origin) inverse response behavior a requires good understanding of the fundamental principles governing the phenomena. The inverse response behavior can be made less severe by dampening the process which opposes the ultimate process response. An example of such modification given by Tyreus (1993b) is shown next.

EXAMPLE 12-4

Tyreus (1993b) studied a tubular catalytic reactor which exhibits inverse response behavior in the exit temperature to rapid changes in the inlet temperature. Pinjala et al. (1988) have shown that when this type of reactors is being operated with a large Lewis number (Lewis number is the ratio between the propagation speed of the concentration and the temperature disturbance), the inverse response behavior is most severe for systems that have a large adiabatic temperature rise, low axial thermal conductivity, and where the kinetics and reactor design is such that the per pass conversion is nearly complete. Using a series of mixed tanks to model the tubular reactor, Tyreus (1993b) varied the axial mixing effect by varying the number of mixed tanks in the model. Figure 12-4 shows the open-loop response to a 5 °C step down in inlet temperature of several systems (all with Lewis number of 36) modeled by 10, 20 and 40 mixed tanks in series. Although the relationship between the Peclet number of a system and the number of stirred tanks is not obvious, one can assume that a large number of mixed tanks in series corresponds to a large Peclet number. Thus, a system with 10 tanks corresponds to the most axially dispersed reactor. As shown, axial dispersion significantly reduces the severity of the inverse response behavior. Note that the mixing effect also reduces the steady-state gain of the system. Consequently, there is again a trade-off between initial output error during transient and flexibility of the process at steady-state.

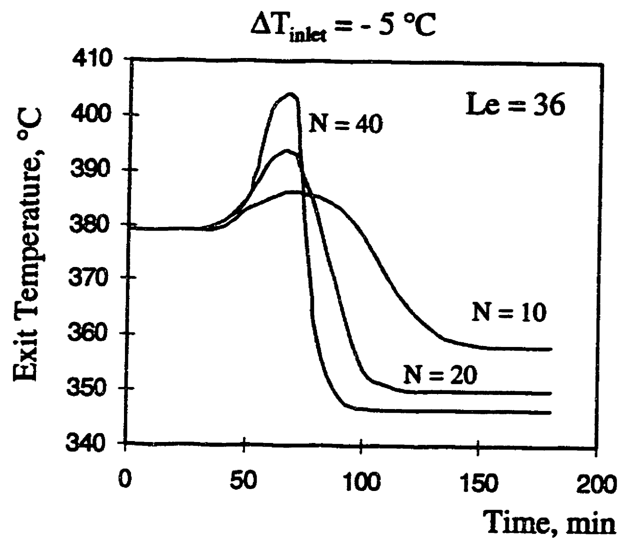


Figure 12 - 4: Inverse Response in a Tubular Catalytic Reactor (from Tyreus, 1993b)

As shown in the previous example, to attenuate the inverse response characteristics in the process, the thermal axial dispersion must be increased to reduce the severity of the inverse response behavior. Thus, a considerable modification in the reactor design is required in order to modify the process dynamics.

12.3.4 Inability to Handle Frequently Varying Disturbances or Setpoint Changes

Due to the limitation imposed by the dynamics of the process, even a physically realizable perfect controller may not be able to handle high frequency disturbance variation or setpoint changes. The ability to maintain the output at the desired value at all times is limited by the dynamics of the process as well as the rangeability of the input. Suppose the control action is limited by the follow constraint on the manipulated variable:

$$\|m\| \leq \|m\|_{max} \qquad [12\text{-}39]$$

Morari (1983) has shown that the maximum disturbance that can be handled by the system at each frequency is given by:

$$\left\| y_{sp} - d \right\| \le \left\| G(i\omega) \right\| \left\| m \right\|_{\max} \qquad [12\text{-}40]$$

where $G(i\omega)$ is the open-loop transfer function of the process. Normalizing m appropriately such that $\|m\|_{\max} = 1$, the amplitude ratio plot of $\|G(i\omega)\|$ is simply a plot of the maximum "disturbance" (y_{sp}-d) which can be handled by the closed-loop system using a perfect controller. A system with the larger static gain and the smaller time constant is better able to handle disturbance variation (see Figure 12-5). At frequencies above the inverse of the time constant, the amplitude ratio decreases rapidly, implying that $\|G(i\omega)^{-1}\|$ must be large and very large control action is required in order to quickly eliminate upset in the process. In practice, very large control action cannot be implemented and the input can at most be at its saturation limit. Hence, control performance degrades rapidly when the process is subject to high frequency upset. This fact explains why even for an invertible process, the output may be constantly drifting and never at its setpoint value if it is subject to disturbances which vary at a frequency larger than what it can physically handle.

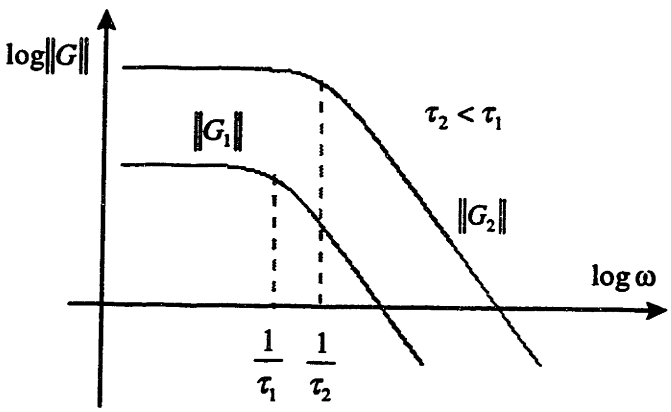


Figure 12 - 5: Comparison of the system and controller gains for two systems G_1 and G_2 (from Morari, 1983)

Extending this idea to MIMO systems, the maximum disturbance on output i that the process can handle at each frequency by a perfect controller must be confined to the region described by the following inequality:

$$\left\| y_{i,sp} - d_i \right\| \le \sigma_{\min}\left[G(i\omega) \right] \left\| m_{\min,i} \right\| \qquad [12\text{-}41]$$

where $m_{\min,i}$ is the input direction which gives y_i the minimum amplification and $\sigma_{\min}\,[G(i\omega)]$ is the minimum singular value. Equation [12-36] gives the upper bound of the allowable disturbance for a given process.

Modifying the Process to Reduce Output Variation

When a plant is subjected to disturbances that vary at a frequency that is too fast to be handled even by a perfect controller, variation in the process output could be large and the output may appear to be constantly drifting. Based on Figure 12-5, increasing the process gain, decreasing the time constant, increase the range of operation of the control input will improve the control performance. In addition, if the root cause of the disturbance is known and there is a way to eliminate or moderate the disturbance, control performance could also be improved. The next example demonstrates these ideas.

EXAMPLE 12-5

The following are the transfer functions corresponding to the simple process shown in Figure 12-6:

$$G(s)=\frac{1}{\tau s+1} \quad G_d(s)=1 \quad \tau=100 \text{ min}$$

During a 200 minutes of process operation, d varied from 1 to -1, then to 0 and then back to 2 at a frequency of 1/50 min^{-1}. With input constrained to -5 and 5, the performance of the control by a constrained MMC controller is shown in Figure 12-7 (A constrained MMC controller is used in lieu of the prefect MMC controller in this example because the constraints on the inputs make the control action from the perfect MMC controller physically unrealizable). Rapid variation of d and the limits on the control input prevent the controller to maintain the output reasonably close to the desired setpoint (y_{sp} = 0). The output appears to be constantly drifting and is almost never at its steady-state.

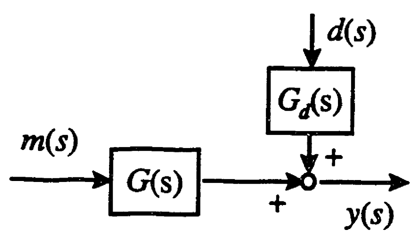


Figure 12 - 6: Schematic of a Process Subjected to Output Disturbances

Figure 12-6 suggests that the control action that is required to eliminate the error is drastically reduced if the inverse of the time constant could be increased to roughly the same frequency as the disturbance. Suppose it is possible to modify the plant so that the time constant of the process is reduced to 50 min. The closed-loop control of the process by the same controller is shown in Figure 12-8. With the same restrictions on the control input, a faster process allows faster attenuation of the disturbance.

By reducing the process time constant, error in the output is reduced. Further reduction in the time constant would obviously improve the control performance. However, major modification is usually required in order to scale down the process so that it the residence time is reduced by half. If this was a reactor, reducing the residence time by half would mean decreasing the reactor conversion and the recycle flow must necessarily increased.

Rather than changing the process $G(s)$ which could be quite costly, the effect of the disturbances acting on the process could be modified using buffer tanks. Installing a buffer tank in the process moderates the disturbances according to the following transfer function:

$$G_d(s) = \frac{1}{\tau_d s + 1} \quad \tau_d = 20\text{min}$$

The control performance of the plant with a buffer tank using the same controller is shown in Figure 12-9. With this process modification, we are able obtain nearly perfect control almost all the time and the error in the output is drastically reduced.

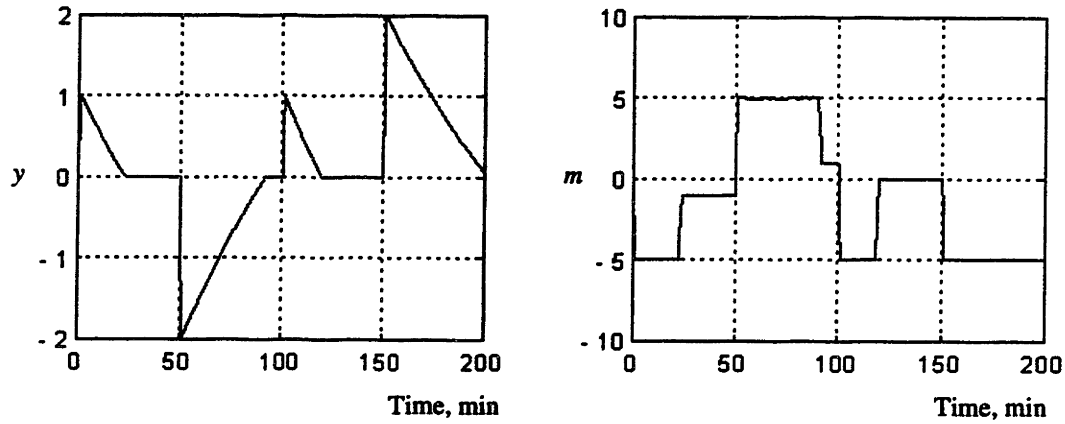


Figure 12 - 7: Control Performance of a Process subject to frequently varying step disturbance

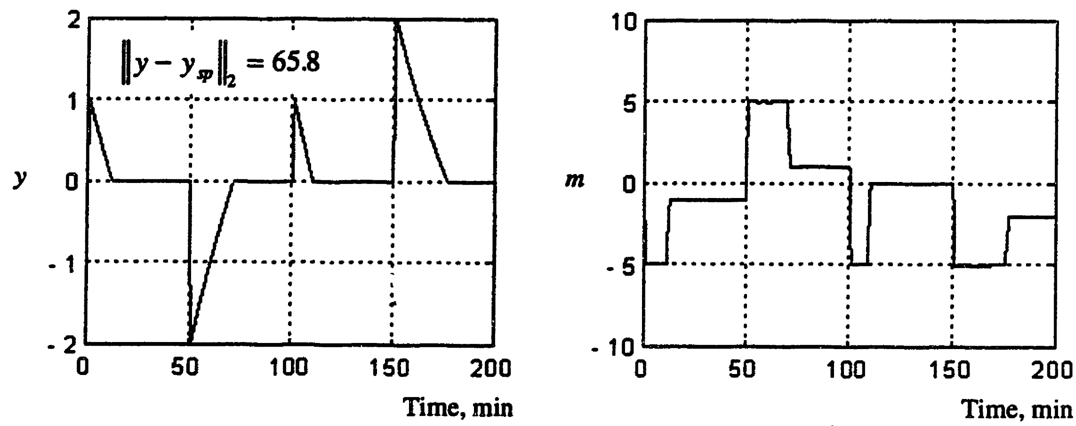


Figure 12 - 8: Control Performance of a Modified Process subject to frequently varying step disturbance

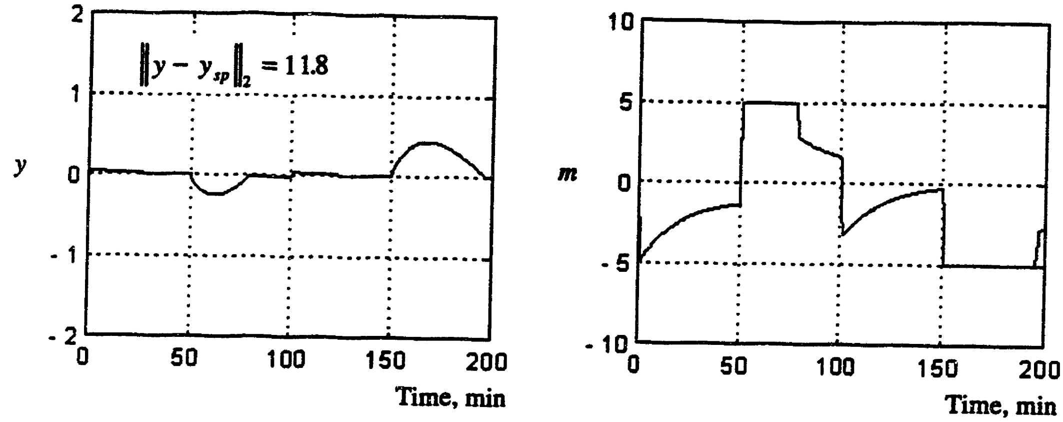


Figure 12 - 9: **Control Performance of a Modified Process subject to frequently varying step disturbance filtered by a buffer tank**

The previous example has demonstrated the various ways to improve the control performance of a process whose ranges of operation of the control action is limited. The best way to reduce output variation is to eliminate or modify the disturbances acting on the system. Given a process with constrained control action, a buffer tank could be added to the process so that all expected disturbances can be easily attenuated. The problem of determining the cost-optimal size and number of buffer tanks that would sufficiently attenuate process disturbances has been studied by Skogestad (1994).

12.4 Modifying the Process to Improve Control Performance

In Section 12.2, we have discuss how process revamp opportunities for individual control objectives can be selectively identified in the MMC framework. Assignments made during control structure synthesis establish pathways which link individual transfer functions to the control performance of specific control objectives. Once these elements have been identified the link between control performance and factors which govern the dynamics in the process should be used to pin down the inherent process limitations. Figure 12-10 summarizes the structure which exists in the INHERENT PROCESS LIMITATION IDENTIFIER proposed previously in Figure 12-2. Unsatisfactory control performance can be traced to parameters which describe the process in the frequency domain. The range of operation of the control input and the process gain are the most important factors governing the performance of the closed-loop control, followed by the process time constants of the process. Initial output error is a result of the presence of invertible elements and can only be relieved by changing the dead-time or RHP zeros in the system. Variation in the process output can also be reduced by modifying the impact of process disturbances on the system.

Once the parameters in the frequency model which limit control performance have been identified, they can be changed by altering physical parameters that define the process. A good understanding of the fundamental principles which govern the process is required to establish the link between parameters in the frequency models and the physical parameters of the system. Often, the process gain, process time constants and RHP zeros of a SISO pair are not entirely independent of one another. For example, changing a physical parameter in the design to affect the time constant may affect the process gain. For the MIMO case, changing one physical parameter in the design may affect the time constants or gains of several SISO pairs in the system.

Furthermore, due to the interactive nature of a MIMO system, care must be taken so that design modification to improve control performance of an output would not degrade the achievable control performance of the more important outputs in the original design. Specifically, to relieve the effects of non-invertible elements in the system the Principle 12-1 can be used.

Principle 12-1: Design Modification to reduce effects of Non-invertible elements in the Multiobjective Framework

Suppose $\boldsymbol{G}$ corresponds to the transfer function matrix for the first k^{th} objectives of the original plant design such that:

$$\begin{bmatrix} \boldsymbol{y} \\ y_k \end{bmatrix} = \boldsymbol{G}\begin{bmatrix} \boldsymbol{m} \\ m_k \end{bmatrix} + \begin{bmatrix} \boldsymbol{h} \\ h_k \end{bmatrix} \quad [12\text{-}42]$$

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{b} \\ \boldsymbol{c} & d \end{bmatrix} \quad [12\text{-}43]$$

where all the symbols have been previously defined in Chapter 6. The matrix has been arranged so that objectives in vector $\boldsymbol{y}$ are more important that that of y_k. In a multiobjective approach, the non-invertible part of the process from the MMC factorization is given by:

$$\boldsymbol{G}_+ = \begin{bmatrix} \boldsymbol{A}_+ & 0 \\ \boldsymbol{c}(\boldsymbol{A}_-)^{-1}(1 - G_{k+}\boldsymbol{f}_k) & G_{k+} \end{bmatrix} \quad [12\text{-}44]$$

such that :

$$G_k = (d - \boldsymbol{c}\boldsymbol{A}^{-1}\boldsymbol{b}) = (d - \boldsymbol{c}\boldsymbol{A}^{-1}\boldsymbol{b})_-(d - \boldsymbol{c}\boldsymbol{A}^{-1}\boldsymbol{b})_+ = G_{k-}G_{k+} \quad [12\text{-}45]$$

Suppose it is desired to introduce modification in the design to improve control performance in y_k. The design modification will change $\boldsymbol{G}$ to $\boldsymbol{G}^*$ which contains an non-invertible part of the following form:

$$\boldsymbol{G}^*_+ = \begin{bmatrix} \boldsymbol{A}^*_+ & 0 \\ \boldsymbol{c}^*(\boldsymbol{A}^*_-)^{-1}(1 - G^*_{k+}\boldsymbol{f}^*_k) & G^*_{k+} \end{bmatrix} \quad [12\text{-}46]$$

An acceptable design modification is one such that $\boldsymbol{A}^*_+$ does not contain more severe non-invertible elements than $\boldsymbol{A}_+$.

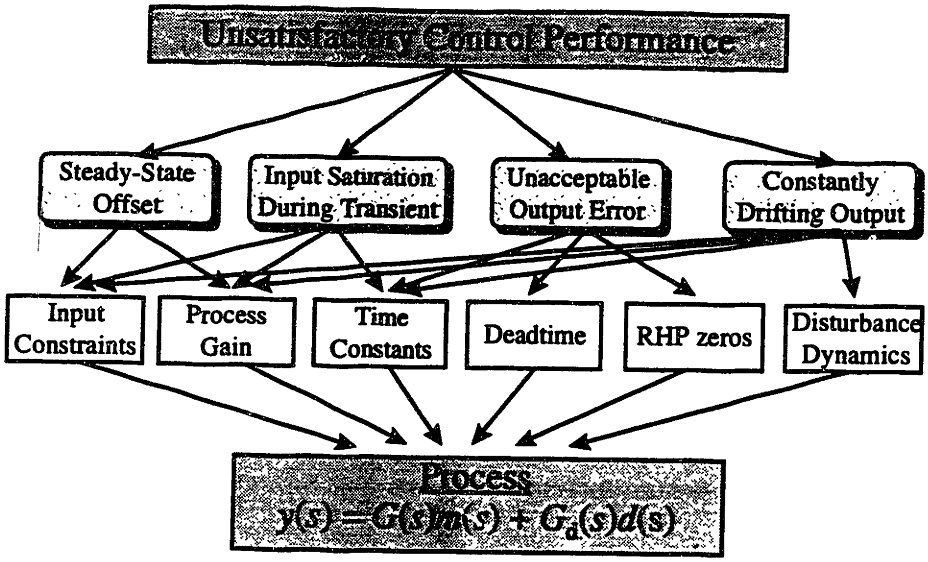


Figure 12 - 10: Structure of the Inherent Process Limitation Identifier

12.5 Case Study: Improving Control Performance of a Continuous-stirred Tank Reactor

A solution containing B (S_B) at various concentration levels and temperatures is to be delivered to various parts of a pharmaceutical complex. A schematic of the production of S_B is shown in Figure 12-11. B can be produced by isomerization of A, a readily available and stable compound, using a catalyst. The reaction is mildly exothermic. There is no restriction on the concentration of A in S_B.

A stirred-tank reactor, equipped with a cooling coil is being used to convert a solution contain A, S_A, to S_B at the desired concentration level and temperature using feedback control. Variables that can be manipulated are the concentration of A at the reactor inlet ($c_{A,i}$) and the flowrate of cooling water. S_A at the desired concentration can be accurately delivered using high-precision mass flow meters in the solution preparation area. It will be assumed in this study that the volume of the reaction material is under perfect feedback control by manipulating the flow of F so that F_i equals F at all times.

S_B is primarily being produced at a concentration of 0.8 lbmol/ft^3 and at a temperature of 600 °R. It is crucial for quality control of the products in the pharmaceutical complex that the concentration of B, c_B, in S_B to be kept within ± 0.01 lbmol/ft^3 of the desired value. Variation in the temperature of S_B should also be minimized. It is expected that the temperature of the coolant at the inlet to vary.

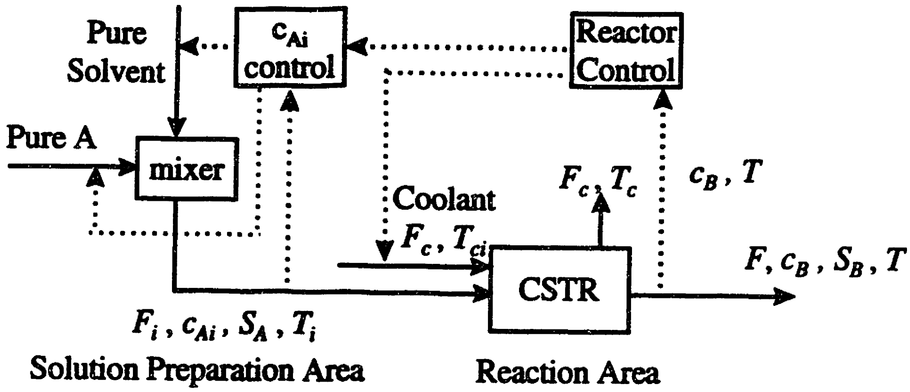


Figure 12 - 11: Schematic of the Production of S_B

12.5.1 Process Modeling

The process model used for our study is given below:

$$\frac{dc_B}{dt} = \frac{-1}{\tau} c_B - k_o e^{-E/RT} c_B + k_o e^{-E/RT} c_{Ai} \qquad [12\text{-}47]$$

$$\frac{dT}{dt} = \frac{1}{\tau}(T_i - T) + Jk_o e^{-E/RT}(c_{Ai} - c_B) - \frac{UA_t W_S}{\rho_S c_{P,S} V}(T - T_c) \qquad [12\text{-}48]$$

$$\frac{dT_c}{dt} = \frac{F_c}{T_c}(T_{ci} - T_c) + \frac{UA_t W_c}{\rho_c c_{P,c} V_c}(T - T_c) \qquad [12\text{-}49]$$

$$J = \frac{-\Delta H W_S}{\rho_S c_{P,S}} \qquad [12\text{-}50]$$

$$\tau = \frac{V}{F_i} \qquad [12\text{-}51]$$

where:
k_o = frequency factor of reaction rate constant, min^{-1}
E = activation energy, Btu/lbmol
R = ideal gas constant, Btu/lbmol/°R
T = reactor temperature, also temperature of S_B, °R
T_i = inlet temperature of S_A, °R
U = heat transfer coefficient, Btu/min/ft^2/°F
A_t = heat transfer area, ft^2
W_S = molecular weight of solution, lb/lbmol
W_c = molecular weight of coolant, lb/lbmol
ρ_S , $c_{p,S}$ = density (lb/ft^3) and heat capacity (Btu/lbmol/°F) of solution
ρ_c , $c_{p,c}$ = density (lb/ft^3) and heat capacity (Btu/lbmol/°F) of coolant
T_c = temperature of coolant in the jacket, °F

F_i = flow of S_A, ft^3/min
F_c = flow of coolant, ft^3/min
F = flow of S_B, ft^3/min
V = reactor volume, ft^3
V_c = volume of cooling jacket, ft^3
ΔH_r = heat of reaction, Btu/lbmol

The values of the physical parameters for the base case design are summarized in Table 12-3.

Table 12 - 3: Base case design of the CSTR

k_o = 16.96E+02 hr^{-1}	$c_{p,c} \approx c_{p,S}$ = 18 But/lbmol/ °F
E = 3.624E+04 Btu/lbmol	$\rho_c \approx \rho_S$ = 0.9941 g/cm^3
T = 600 °R	W_S = 33.4 lb/lbmol
F_i = 6.667 ft^3/min	W_c = 18 lb/lbmol
T_i = 580 °R	ΔH_r = -1200 Btu/lbmol ($550 \leq T \leq 620$)
T_{ci} = 519 °R	U = 130 Btu/hr/ft^2/°F
T_c = 594.0013 °R	A = 150 ft^2
V= 2000 ft^3	V_c = 150 ft^3
c_{Ai} = 0.95 lbmol/ft^3	F_c = 0.4197 ft^3/min
c_B = 0.8 lbmol/ft^3	$F_{c,max}$ = 2.5 ft^3/min, $c_{Ai,max}$ = 3 lbmol/ft^3

The rate of change of temperature of coolant in the cooling coil has been approximated with a lumped model with V_c being a pseudo volume of the cooling jacket. The following model in the frequency domain has been obtained by linearizing the differential equations at the design steady-state:

$$\begin{bmatrix} c_B \\ T \end{bmatrix} = G \begin{bmatrix} c_{Ai} \\ F_c \end{bmatrix} + G_d \begin{bmatrix} T_i \\ T_{ci} \end{bmatrix} \quad [12\text{-}52]$$

where:

$$G(s) = \frac{\begin{bmatrix} 0.0178(s+0.03)(s+0.016) & -3.289\times10^{-7} \\ 0.639(s+0.0378)(s+0.0033) & -0.0024(s+0.0211) \end{bmatrix}}{(s+0.0378)(s+0.0122+0.0027i)(s+0.0122-0.0027i)} \quad [12\text{-}53]$$

and

$$G_d(s) = \frac{\begin{bmatrix} 4.5032\times10^{-7}(s+0.0378) & 1.8404\times10^{-9} \\ 0.0033(s+0.0376)(s+0.0213) & 1.3623\times10^{-5}(s+0.0211) \end{bmatrix}}{(s+0.0378)(s+0.0122+0.0027i)(s+0.0122-0.0027i)} \quad [12\text{-}54]$$

The process is stable with poles at: -0.0378, -0.0122±0.0027i and there are no RHP transmission zeros.

12.5.2 Controller Design

The concentration of B in S_B is a more important objective. It has been determined that c_{Ai} is a much more effective manipulated variable than F_c. For this case study, c_{Ai} is assigned to c_B and F_c is assigned to T.

The (1,1) element in $G(s)$ corresponds to the transfer function between c_{Ai} and c_B. It is a completely invertible element. Then, MMC factorization produces the following lower triangular matrix that governs the quality of the control performance:

$$G_+(s) = \begin{bmatrix} 1 & 0 \\ \dfrac{0.639(s+0.0378)(s+0.0033)}{0.0178(s+0.03)(s+0.016)}(1-f_2(s)) & 1 \end{bmatrix} \quad [12\text{-}55]$$

$G_+(s)$ which must be multiplied by a filter of the following form to make the control action physically realizable:

$$F(s) = \begin{bmatrix} f_1(s) & 0 \\ 0 & f_2(s) \end{bmatrix} = \begin{bmatrix} \dfrac{1}{\lambda_1 s+1} & 0 \\ 0 & \dfrac{1}{(\lambda_2 s+1)^2} \end{bmatrix} \quad [12\text{-}56]$$

The perfect controller in the multiobjective design is simply given by Equation [12-6]. Note that $G_+(s)F(s)$ does not contain any non-invertible element and it is nearly an identity matrix except at high frequency. The (2,1) element accounts for the interaction in the system and shifts the attention to the more important output c_B. The output responses are also being moderated by the filter.

12.5.3 Evaluation of Control Performance

The control performance of the base case design will be evaluated at the most common operating conditions. The process is primarily being operated at c_B = 0.8 lbmol/ft^3 and at T = 600°R. Temperature setpoint is also expected to vary from T =597 °R to 603 °R. This is operating point A. The process under study also supplies S_B to another section in the pharmaceutical complex which requires S_B to have a concentration of 0.6 lbmol/ft^3 and at 585 °R. This is operating point B. When product demands are high, the process could be required to switch between operating points A and B at an interval of every 12 hours. The inlet temperature of S_A and F_c are outlet streams of other processes. The maximum magnitudes of the random variations in these temperatures have been found to be about ± 2 °R. However, at times, due to sudden process upset at upstream, T_{ci} may introduce significant step disturbances to the process.

The control performance of the base case design at the expected operating region will be evaluated using a perfect controller designed in the MMC framework (Equation [12-

55]), unless otherwise stated. The filter constants λ_1 and λ_2 have been chosen to be 5 min and 20 min respectively. These values have been chosen to add robustness to the controller to random variation in the T_i and T_{ci}. Since the size of the dominant time constant of the system is approximately 81 min (equivalent to the inverse of the real part of the pole closest to the origin), which is bigger than the size of the filter; the transient behavior will be governed by the pair of complex poles. As our study has been limited to linear systems with no model error, the effect of nonlinearity and model uncertainty in the closed-loop control will be ignored. Furthermore, it will be assumed that process is properly design such that there is no steady-state offset at all expected operating conditions.

The transient response of the process outputs to a step up and a step down in reactor temperature at operating point A is shown in Figures 12-12 and 12-13 respectively. The feedback control is accomplished by a perfect controller designed in the MMC framework (see Equation [12-50]). With c_B being a more important objective, the perfect MMC controller tries to maintain c_{Ai} very close to its desired value at all time and let T slowly move to the new setpoint. While the response of a step up in temperature is acceptable, due to saturation of F_c during step down, approximately 7 hours is required to bring T to a lower temperature. As indicated in the figures, the error in T during a step up in temperature is 3 times larger than the error during a temperature step down. The lower limit on the coolant flowrate prevents the perfect controller from bringing temperature to the new setpoint within an acceptable time horizon.

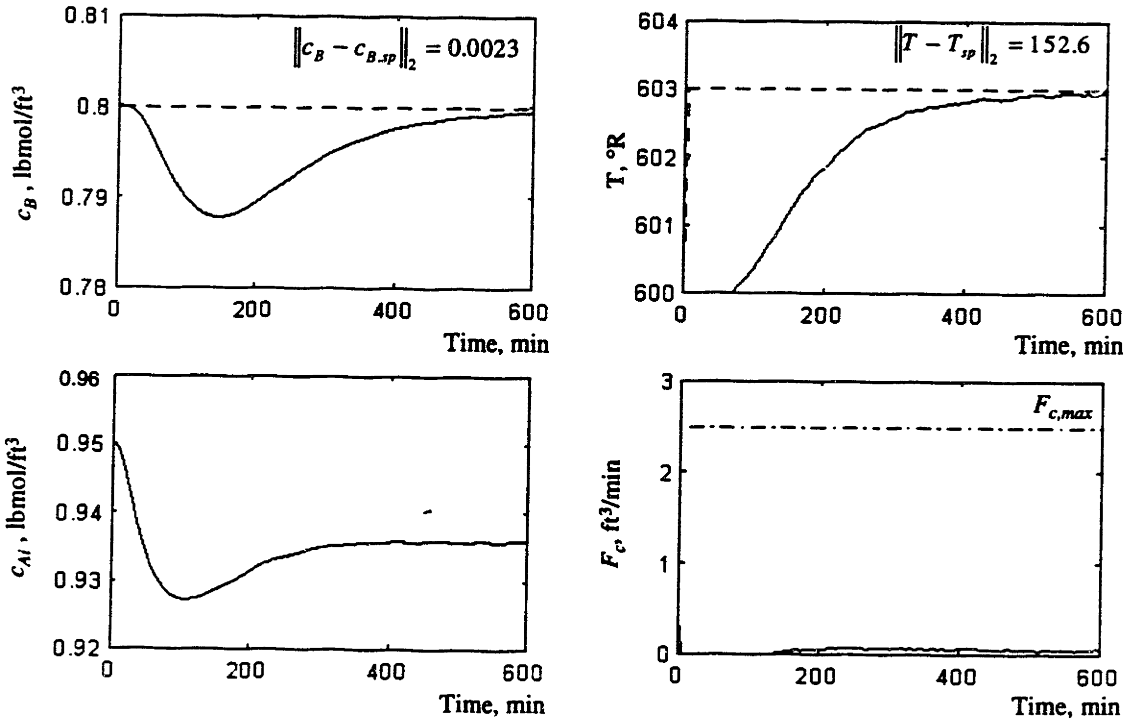


Figure 12 - 12: Process Response to a Step up in Reactor Outlet Temperature using a perfect controller

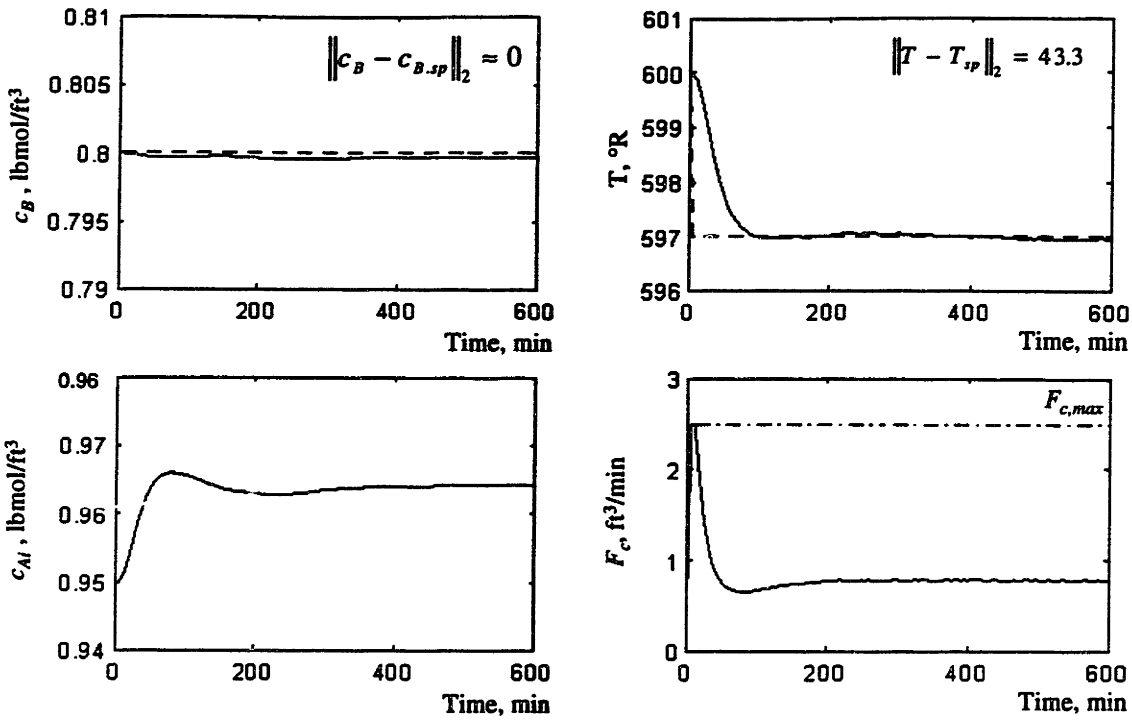
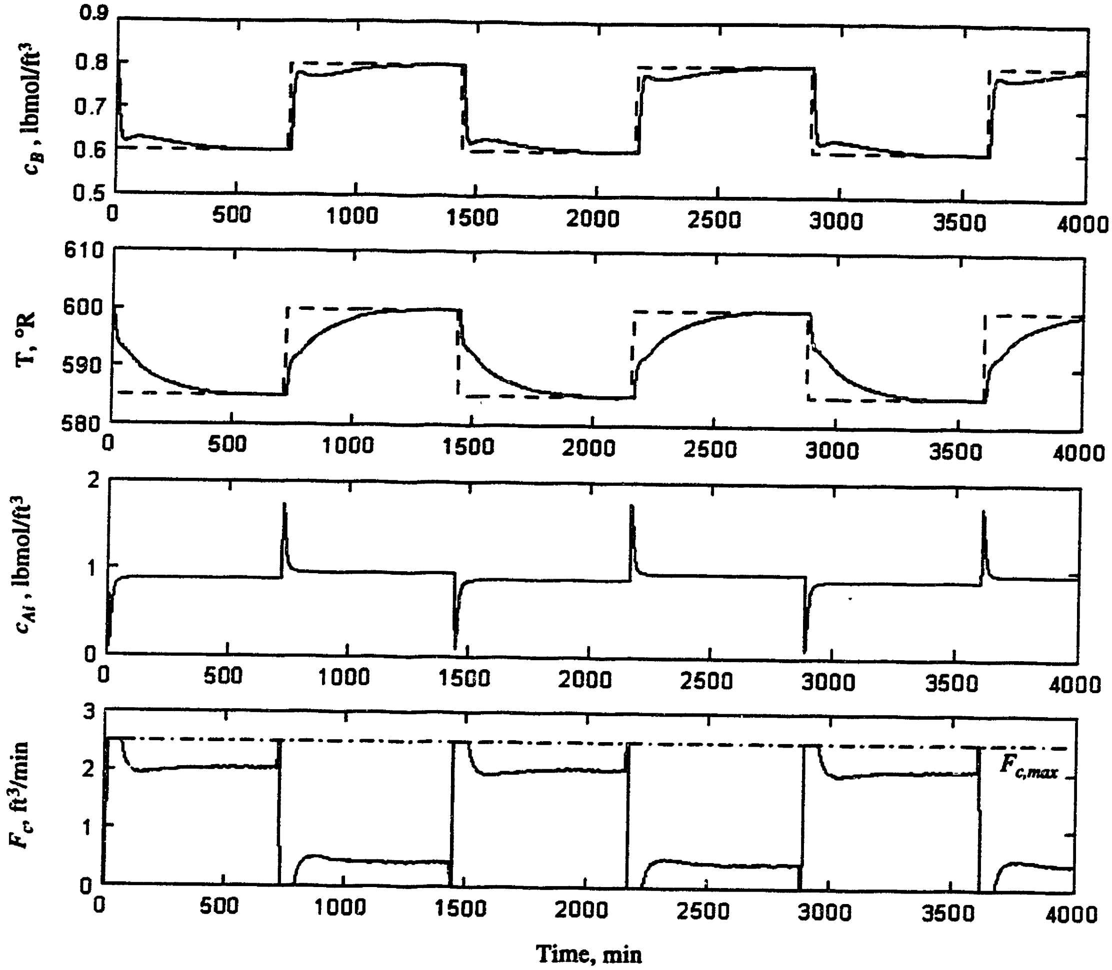


Figure 12 - 13: Process Response to a Step down in Reactor Outlet Temperature using a perfect controller

The control performance during the high demand period when the process must be changed from operating point A to operating point B every 12 hours is shown in Figure 12-14. Although c_B follows the setpoint trajectory fairly closely, approximately 8 hours is required for the reactor outlet temperature to reach the desired setpoint. The speed of the response is again limited by the range of operation of the coolant. The perfect controller requires a much larger control action in F_c than what is realizable. When operation requires setpoint of temperature to be changed as often as every 12 hours, a settling time of 8 hours is unacceptable.

Control performance could be improved if the input constraints are taken into consideration by employing a constrained MMC controller. Figure 12-15 shows the performance of the system under control by a constrained MMC controller. The errors in both c_B and T have been reduced when constraints on inputs are taken into account by the controller. In fact, the control of c_B is almost perfect. However, over 3 hours is still required to force the system to follow the setpoint trajectory of T. A settling time of 3 hours is quite a long considering that the setpoint is being changed again in another 8 hours after the new target has been reached.

The ability of the process to absorb disturbance shock is demonstrated in Figure 12-16. The process is subject to sudden and severe changes in T_{ci} at a 12 hours interval. The perfect controller is able to maintain both the outputs fairly close to the desired values at all times with no saturation in inputs.



$\left\| c_B - c_{B,sp} \right\|_2 = 0.7979$ $\left\| T - T_{sp} \right\|_2 = 1.26 \times 10^4$

Figure 12 - 14: Switching Process between Operating Point A and Operating Point B with a perfect controller

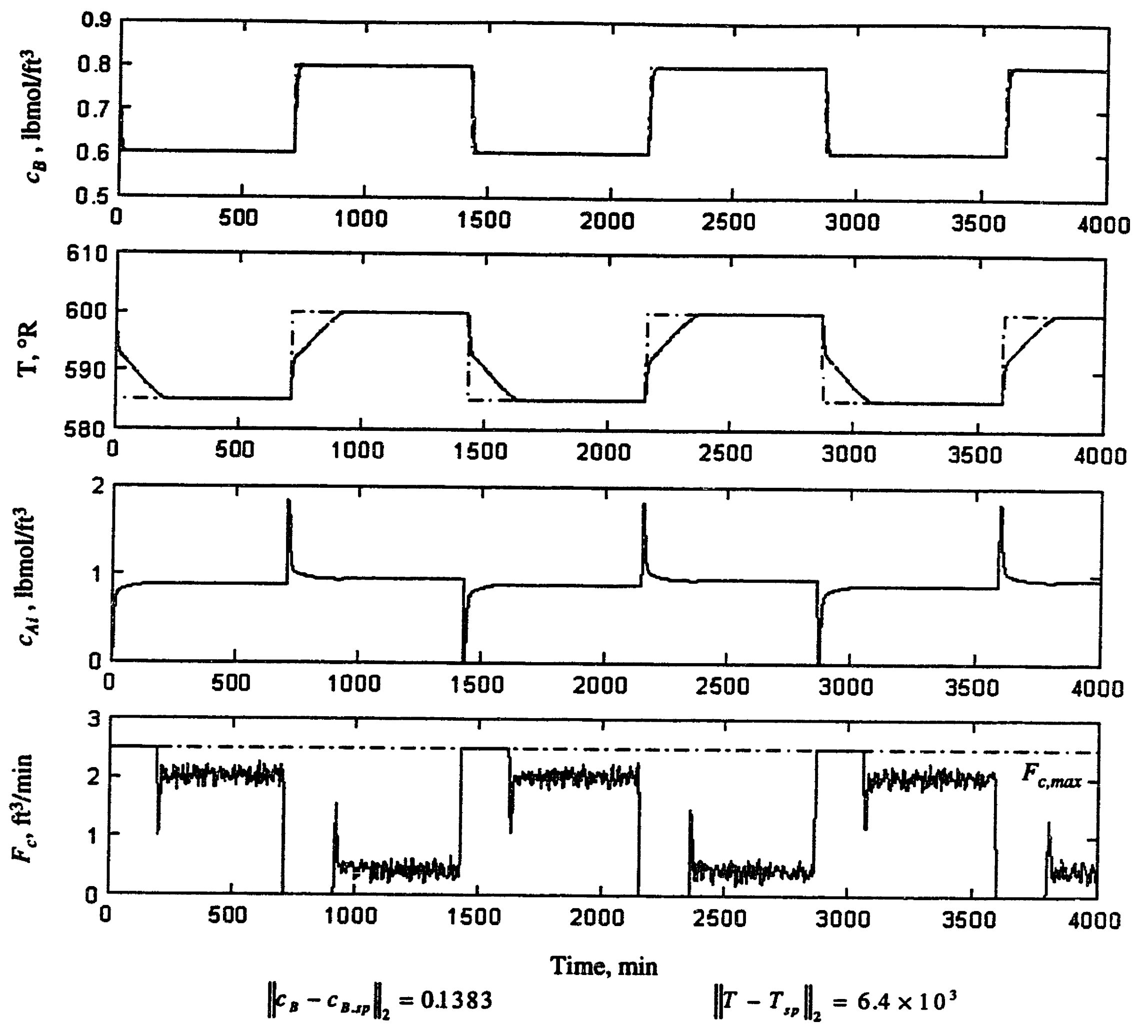
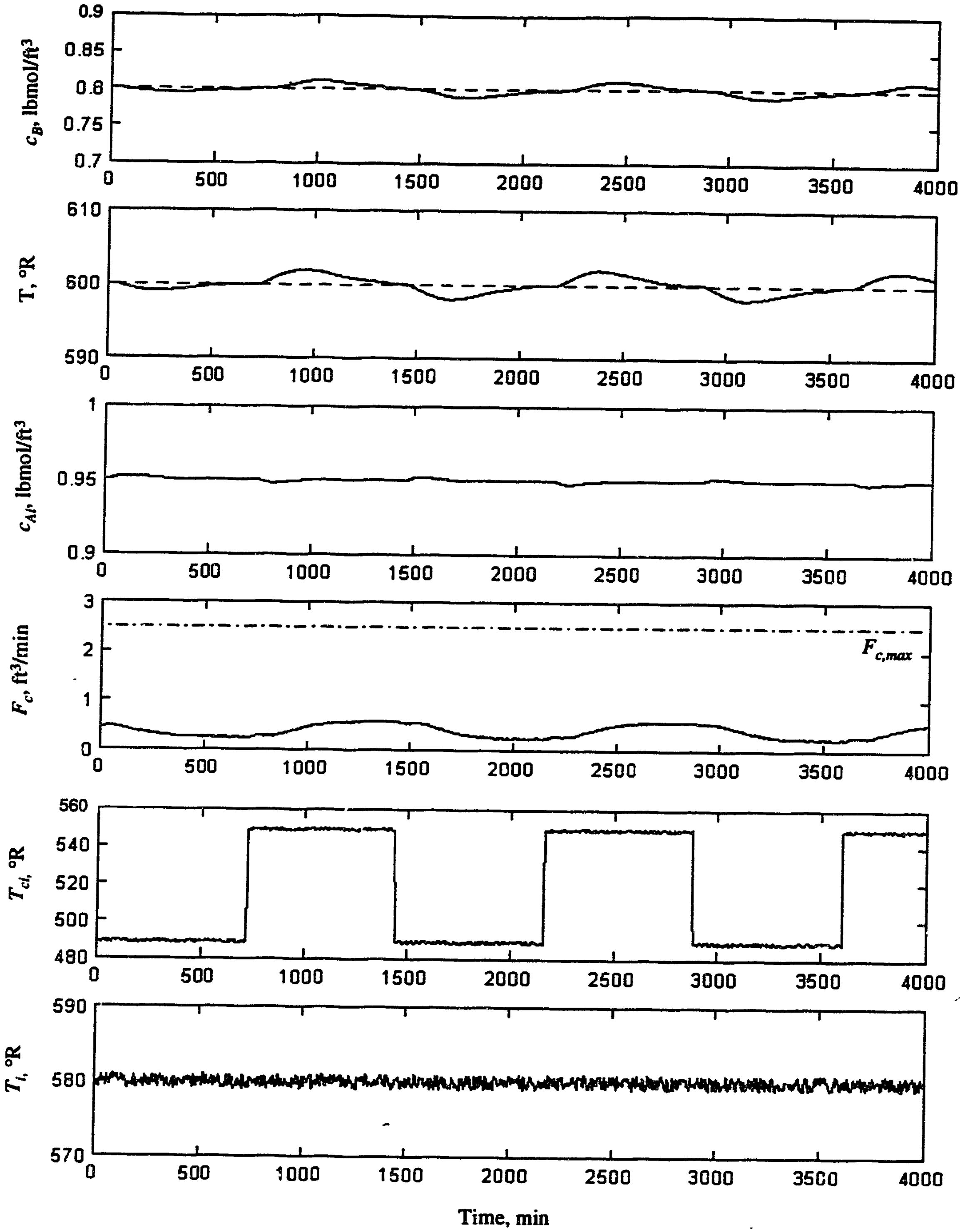


Figure 12 - 15: Switching Process between Operating Point A and Operating Point B using a constrained MMC



$\left\| c_B - c_{B,sp} \right\|_2 = 0.033$ $\left\| T - T_{sp} \right\|_2 = 963.9$

Figure 12 - 16: Control Performance of the Process subject to sudden and severe changes in T_{ci}

12.5.4 Modifying the Process to Improve Control Performance

The evaluation in the previous section shows that the process is able to follow very closely the setpoint trajectory of c_B and it is able to absorb sudden and severe changes in T_{ci}, but it is unable to respond fast enough to changes in the setpoint of T. The symptoms of unsatisfactory performance are mainly input saturation and constantly drifting reactor outlet temperature when the process is being switched between operating points A and B at a 12 hours interval. The control performance is limited by the range of operation of F_c. Figure 12-10 indicates that expanding the range of operation of F_c or reducing the dominant time constant of the process will help to improve the control performance.

Process simulations indicate that F_c always exceeds its saturation limits during setpoint changes of T. Expanding the range of operation of F_c would be a natural decision. However, F_c is an outlet stream from some other parts of the pharmaceutical complex, increasing the demand of F_c may have adverse effect on other parts of the plant. Furthermore, F_c cannot go below zero. Expanding the range of operation of F_c will only help cooling but the speed of the response during heating is unaffected. A cooler and a heater can also be added at the outlet of the reactor to correct temperature in S_B is a feasible but expensive alternative. This approach will only be used if no other feasible methods are available. Modifying the configuration of the reactor system may modify the time constants governing the system and hence speed up the response of the process to step changes in T. In this study, the possibility of changing the physical parameters which define the reactor system to improve control performance will be investigated.

This process is basically limited by a fairly large dominant time constant (80 min). The goal of the process revamp is to improve control performance of the second objective (i.e. T). Since it is completely invertible, according to the theory presented in Section 12.2, the limitation of the control performance comes from the invertible process dynamics (such as time constants) and the rangeability of the inputs. Then, according to Equation [12-48], rather than the non-invertible elements, all elements in the matrix $G(s)$ affect control performance. As explained earlier in Section 12.3, a process should be modified so that it will be governed by negative poles which are farther away from the origin than those in the original system. In a multivariable process, the poles of the system are governed by a number of parameters. A set of explicit equations which show how the poles move are not available. The change in the process poles must be computed for each set of design conditions.

It has been assumed in the study that no other heat transfer material is available besides the one that is being employed. Then, the only process parameters which are directly adjustable are the volume of the reactor and the area of heat transfer. Both of these alternatives will be examined.

Decrease Volume of Reactor

The reactor volume can be reduced by as much as 70% without exposing the cooling coil in the reactor. It is important that the cooling coil be submerged in the liquid so that no heat transfer area is lost as a result of operating the process with a smaller reactor volume. As the reactor volume is reduced, the conversion of A to B is also reduced. Then c_{Ai} must be increased to produce S_B with the same concentration of B. The process variables corresponding to the modified design at the primary operating point with the are summarized in Table 12-4. All other process variables not mentioned in Table 12-4 are not affected by the plant modification.

Table 12 - 4: Decrease Reactor Volume by 70%

$T_c = 594.0024$ °R
$V = 600$ ft^3
$F_c = 0.4196$ ft^3/hr
$c_{Ai} = 1.30$ lbmol/ft^3

The model in the frequency domain for the new design at the primary operating point has been found to be:

$$\begin{bmatrix} c_B \\ T \end{bmatrix} = G_1 \begin{bmatrix} c_{Ai} \\ F_c \end{bmatrix} + G_{1,d} \begin{bmatrix} T_i \\ T_{ci} \end{bmatrix} \qquad [12\text{-}57]$$

where:

$$G_1(s) = \frac{\begin{bmatrix} 0.0178(s+0.0326+0.0232i)(s+0.0326-0.0232i) & -3.654\times10^{-6} \\ 0.639(s+0.0378)(s+0.0111) & -0.0081(s+0.0289) \end{bmatrix}}{(s+0.0378)(s+0.02+0.00145i)(s+0.02-0.00145i)} \qquad [12\text{-}58]$$

and

$$G_{1,d}(s) = \frac{\begin{bmatrix} 5.0032\times10^{-6}(s+0.0378) & 2.0444\times10^{-8} \\ 0.0111(s+0.0373)(s+0.0293) & 4.5402\times10^{-5}(s+0.0289) \end{bmatrix}}{(s+0.0378)(s+0.02+0.00145i)(s+0.02-0.00145i)} \qquad [12\text{-}59]$$

In the new design, the pair of complex poles are farther away from the origin, reducing the dominant time constant to approximately 50 min which is smaller than the dominant time constant for the original design. The other system pole (-0.0378) has not been affected. Zeros in the systems have also been affected but the overall multivariable remain invertible. We expect the speed of the response would be improved as the dominant time constant is decreased. Since the poles of the system have been altered, we also expect that the speed of response of both process outputs to be faster.

The response of the process to a step up in reactor output temperature is shown in Figure 12-17. With the new design, we are able to shorten the settling time to roughly 3 hours using a perfect controller, compare to over 7 hours with the original design. Figure 12-18 shows the control performance of the process when it is being switched between operating points A and B at a 12 hours interval, using a perfect controller. The error in T is much lower in this case than in the original design. The settling time of T has been reduced to approximately 2.5 hours. There is still input saturation during transient but performance is much more acceptable than previous design. Using a constrained MMC which accounts of input constraints, we are able to reduce the settling time of T to roughly 1.5 hours (see Figure 12-19).

Simulations have shown that the proposed modification improves the control performance of T without degrading the achievable performance of c_B during setpoint changes, even at a 12 hours interval. As the process time constant is reduced, the poles of $G_{1,d}(s)$ are also faster than those in $G_d(s)$. Then, the ability of the process to act as a buffer to input disturbances, such as T_{ci} has been adversely affected (recall Section 12.3.4). The ability for the new design to handle sudden and severe changes in T_{ci} must be evaluated. The control performance of the process subject to the same type of disturbance upset as in Figure 12-16 is shown in Figure 12-20. The error in both outputs are larger. The new design is much more sensitive to variation in T_{ci}. This is the classic trade-off between control performance with respect to setpoint changes and sensitivity to disturbances.

Control performance to changes in T_{ci} can only be improved by eliminating the sudden variation such as by installing an additional buffer tank (Skogestad, 1994) or cooler/heater at the inlet of the reactor or a more sophisticated controller. The output response of the process that is under control by a constrained MMC is shown in 12-21. By accounting for the process variation as model uncertainty, the error in both outputs can be reduced to a more acceptable level.

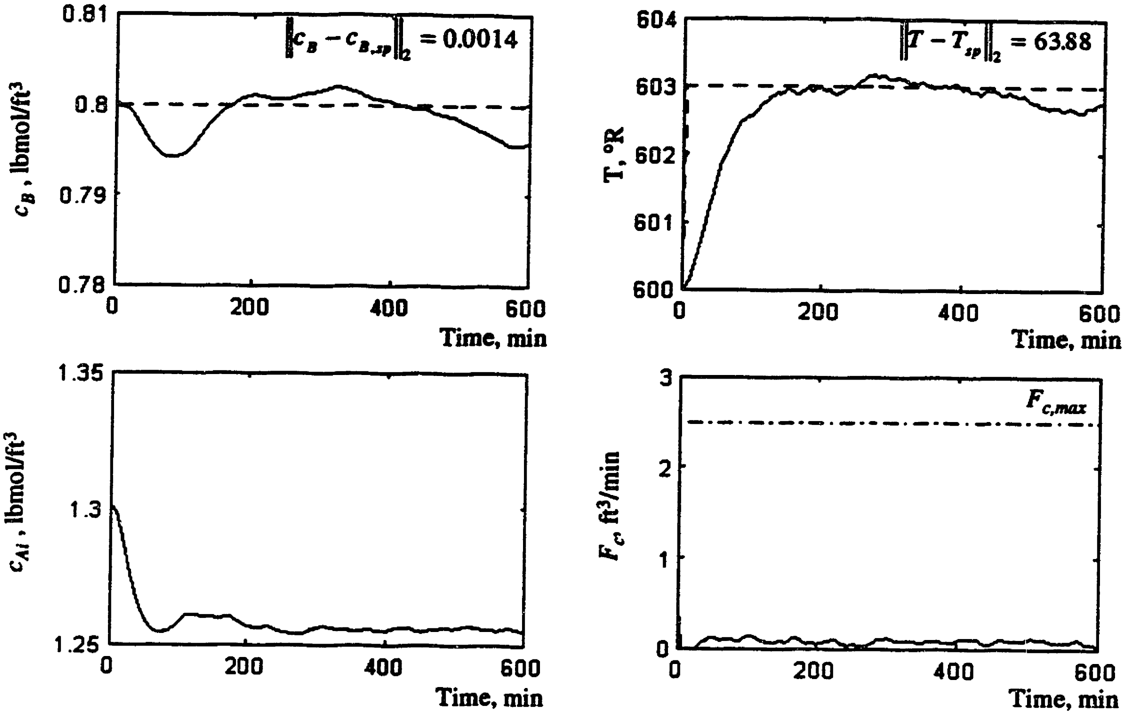
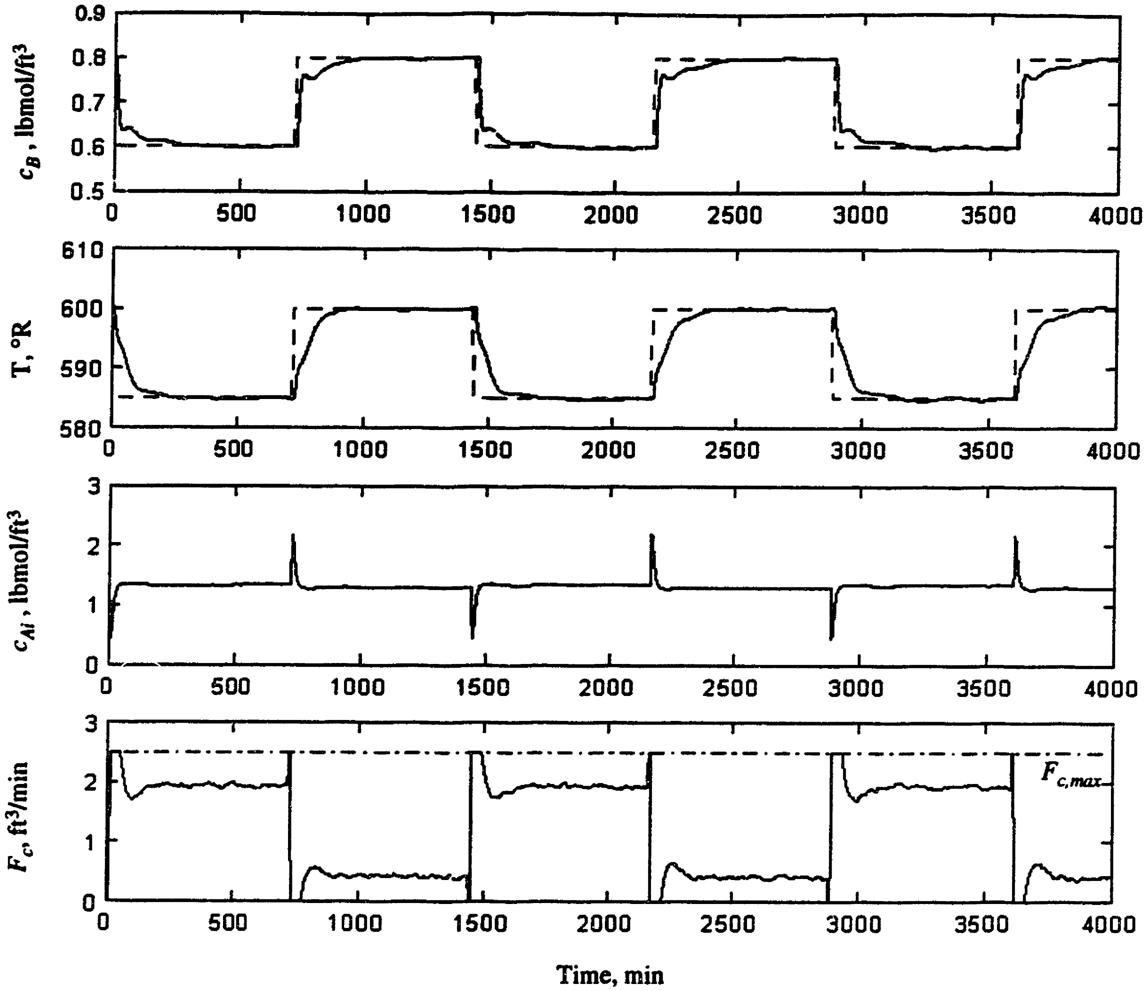
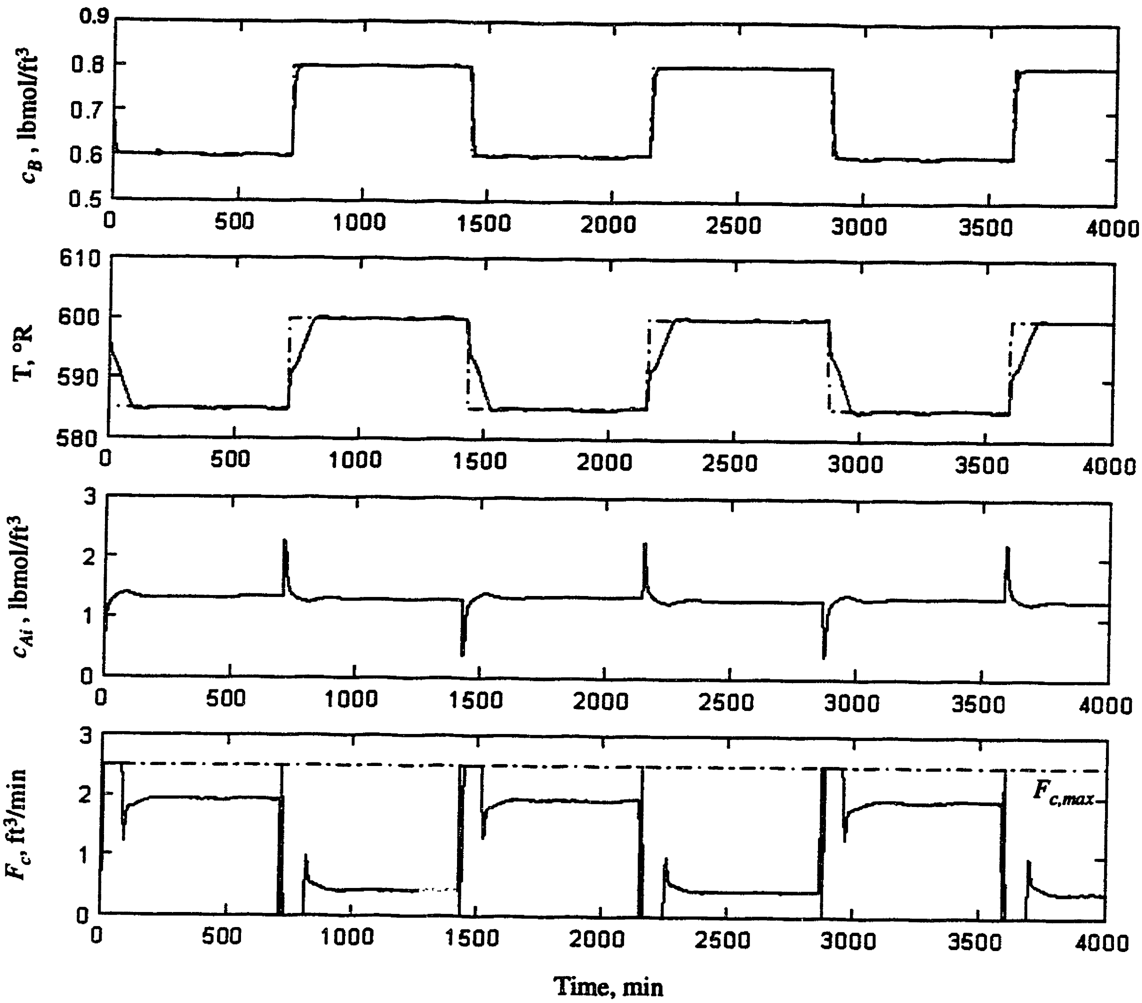


Figure 12 - 17: Process Response to a Step up in Reactor Outlet Temperature using a perfect controller, reactor volume = 600 ft^3



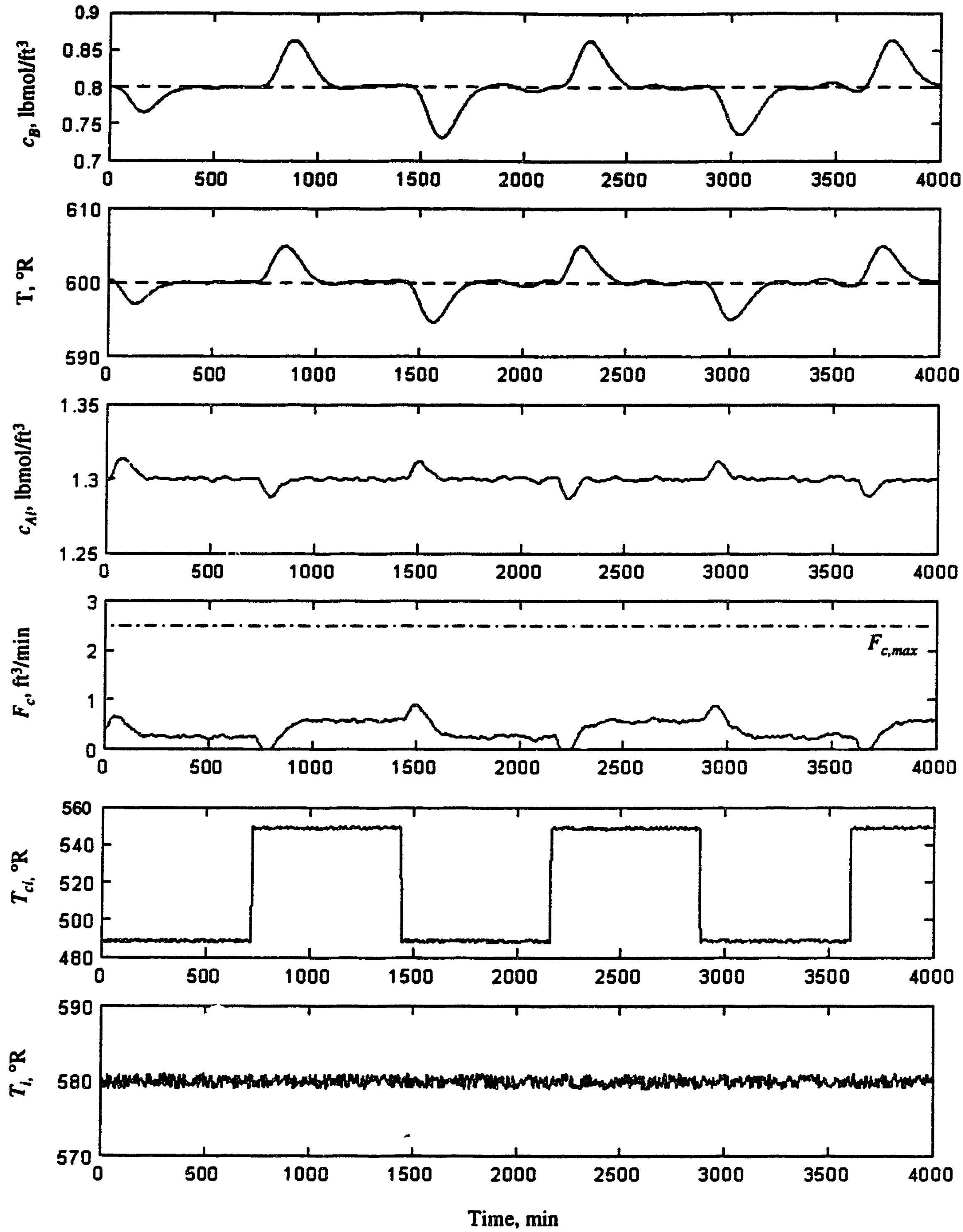
$\left\| c_B - c_{B,sp} \right\|_2 = 0.7878$ $\left\| T - T_{sp} \right\|_2 = 8.626 \times 10^3$

Figure 12 - 18: Switching Process between Operating Point A and Operating Point B using a perfect controller, reactor volume = 600 ft3



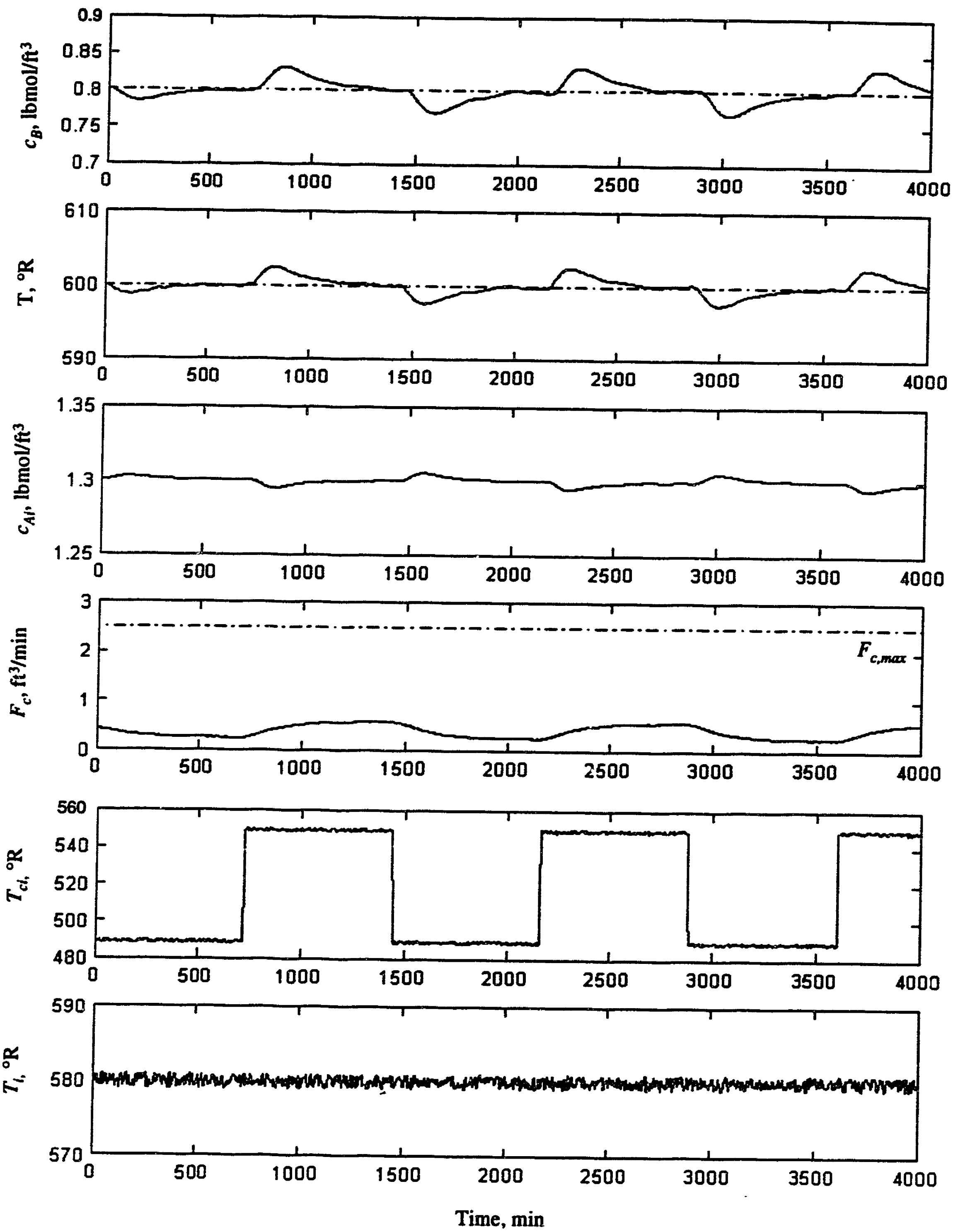
$\left\| c_B - c_{B,sp} \right\|_2 = 0.1328$ $\left\| T - T_{sp} \right\|_2 = 4.92 \times 10^3$

Figure 12 - 19: Switching Process between Operating Point A and Operating Point B using a constrained MMC controller, reactor volume = 600 ft^3



$\left\| c_B - c_{B,sp} \right\|_2 = 0.5244$ $\quad\quad$ $\left\| T - T_{sp} \right\|_2 = 2.93 \times 10^3$

Figure 12 - 20: Control Performance of the Process subject to sudden and sever changes in T_{ci} using a perfect controller, reactor volume = 600 ft^3



$\|c_B - c_{B,sp}\|_2 = 0.1752$ $\qquad$ $\|T - T_{sp}\|_2 = 1.02 \times 10^3$

Figure 12 - 21: Control Performance of the Process subject to sudden and sever changes in T_{ci} using a constrained MMC controller, reactor volume = 600 ft^3

Increase Heat Transfer Area

The response of the process can also be improved by increasing the heat transfer area and thereby improving the efficiency of heating and cooling. Increasing the heat transfer area requires redesigning of the cooling coil which could be costly. A design whose area is increased by a moderate factor, i.e. 1.5 of the original area, will be examined. The values of the process variables at the primary operating point which have been affected by the new design are summarized in Table 12-5.

Table 12 - 5: Increase Heat Transfer Area by 50%

$T_c = 596.00$ °R
$A = 225$ ft^2
$F_c = 0.4088$ ft^3/hr

The model in the frequency for the new design at the primary operating point has been found to be:

$$\begin{bmatrix} c_B \\ T \end{bmatrix} = G_2 \begin{bmatrix} c_{Ai} \\ F_c \end{bmatrix} + G_{2,d} \begin{bmatrix} T_i \\ T_{ci} \end{bmatrix} \qquad [12\text{-}60]$$

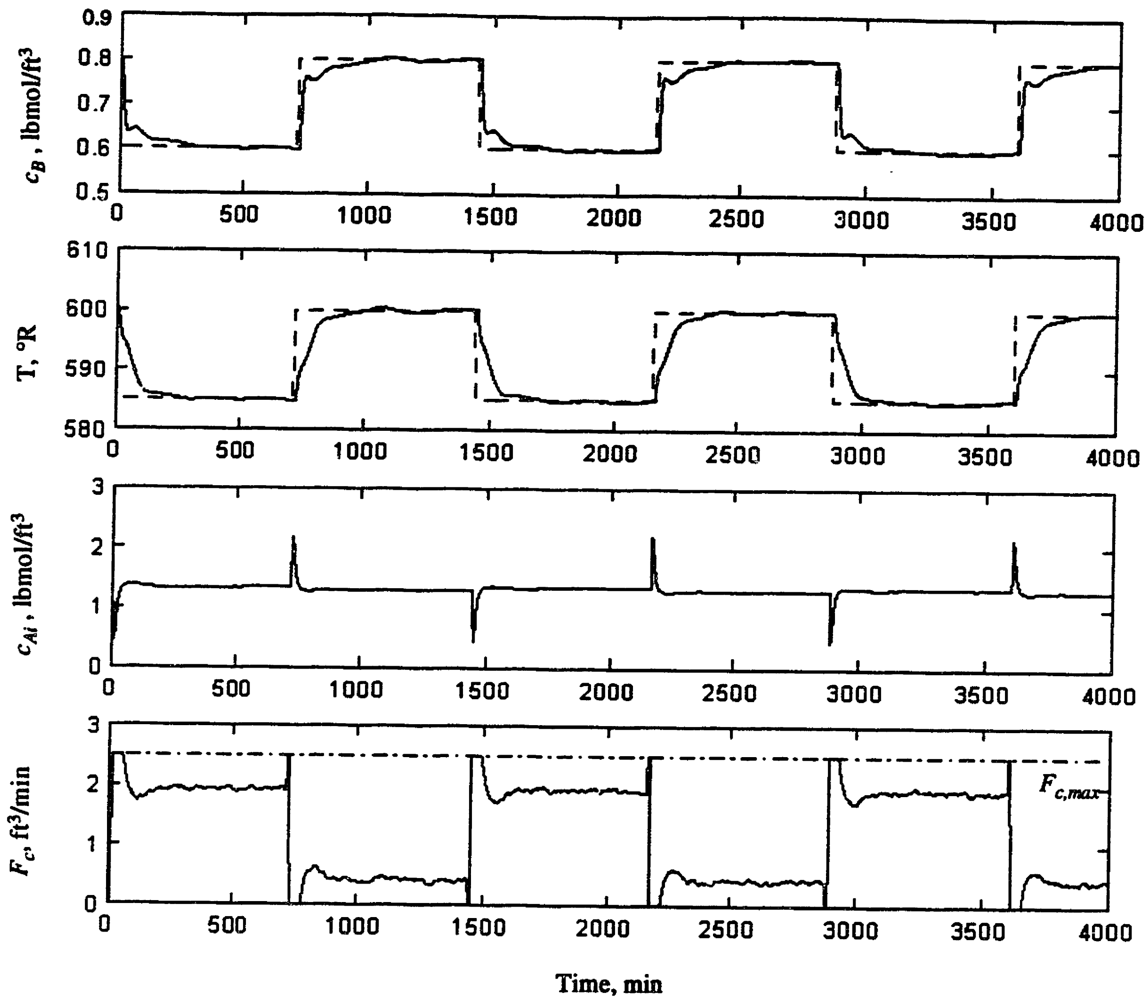
where:

$$G_2(s) = \frac{\begin{bmatrix} 0.0178(s+0.0436)(s+0.0233) & -5.0646\times10^{-7} \\ 0.639(s+0.0552)(s+0.0033) & -0.0037(s+0.0211) \end{bmatrix}}{(s+0.0552)(s+0.0134+0.0053i)(s+0.0134-0.0053i)} \qquad [12\text{-}61]$$

and

$$G_{2,d}(s) = \frac{\begin{bmatrix} 4.5032\times10^{-7}(s+0.0552) & 2.6889\times10^{-9} \\ 0.0033(s+0.0382+0.0238i)(s+0.0382-0.0238i) & 1.9904\times10^{-5}(s+0.0211) \end{bmatrix}}{(s+0.0552)(s+0.0134+0.0053i)(s+0.0134-0.0053i)} \qquad [12\text{-}62]$$

The system does not have any RHP transmission zero. Although this design has produced a pole that is much farther away from the origin than the fastest pole in the original design (-0.0552), the dominant time constant is controlled by the pole closer to the origin and it is about 76 min, just a fraction smaller than the dominant time constant in the original design. The new design is not expected to produce any appreciable improvement in control performance. Figure 12-22 shows the result of switching the process between operating points A and B at an interval of 12 hours. The errors of the outputs are roughly the same as that for the original design and over 6 hours is required to bring the reactor output temperature to a new setpoint. Alternative 1 is therefore a superior choice.



$\|c_B - c_{B,sp}\|_2 = 0.7443$ $\|T - T_{sp}\|_2 = 1.1132 \times 10^4$

Figure 12 - 22: Switching Process between Operating Point A and Operating Point B using a perfect controller, heat transfer area = 225 ft^2

It has been demonstrated in this case study process that improvement of control performance of the CSTR is possible, but there exists the classic trade-off between control performance with respect to setpoint changes and sensitivity to disturbances.

12.6 Summary and Further Investigation

Attempts have been made in this study to develop the link between control performance and plant design. Conforming to the methodology proposed for the synthesis of plant wide control strategies, it is recommended that opportunities for improvement of control performance of individual control objectives be carried out similarly in the modular multiobjective framework. Specifically, the assignments made during control structure synthesis establish some pathways which determine the control performance of certain output objectives. These pathways should be studied to determine the elements (i.e. the specific transfer functions) which influence process control. Once these elements have been identified, the INHERENT PROCESS LIMITATION IDENTIFIER established in

Figure 12-10 can be used to locate specific process parameters in the frequency domain model that should be modified for improvement of control performance.

In this study, the effects of process nonlinearity on a system controlled by a linear controller as well as effect of model uncertainty on the control system performance have been ignored. Future work should explore how unsatisfactory control performance can be traced to those factors and how modification in the process (by making the process less nonlinear or less susceptible to modeling error) can be made. In addition, the mapping in Figure 12-10 should be expanded to include the effects of the various form of process interconnections in an integrated plant on control performance.

Conforming to the mutliobjective design philosophy proposed in the synthesis of plant-wide control structures, process modification to improve control performance of a particular output is only recommended if the control performance of the more important control objectives are not affected adversely. A formal framework which allows the evaluation of the impact of a design modification on the multivariable system is required.

Chapter 13
Research Contributions and Future Research Directions

13.1 Summary of Research

In this research, the fundamental issues associated with the design of plant-wide control strategies for chemical processes have been identified and a design framework which is suitable for addressing these issues has been formalized. It has been found in this research that the a hierarchical approach which requires the decomposition of the process plant into a family of representations offers several attractive features for control system design. First, hierarchical decomposition reduces the complexity of the design problem by allowing the designer to focus on simpler plant representations such that the understanding of the plant production plan is clearer. In a progressive view of the chemical plant, specific control objectives which are consistent with the overall production plan can be generated. Second, the hierarchical framework decomposes the process behavior into a set of layers, each corresponds to a different time-scale of operations. Simpler process representations capture the plant behavior which are observable over longer time-horizons while more detailed process representations bring out the faster dynamics in the process. Hence, within the hierarchical framework, the range of process phenomena with which the designer is concerned have been divided according to their associated time-horizons, each of which is characterized by one of the representations in the hierarchy of plant stratification. Control strategies synthesized at each process representation form a control structure suitable for addressing objectives which are relevant for that representation. Sets of control strategies are combined to form a multi-horizon control system. Control actions are executed over various time-horizons to address disturbances which impact the process over different time-scales.

Systematic analytical aids which are needed to address issues at various stages of control system design have been formalized and integrated into the proposed methodology. Structural techniques are employed to examine the disturbance load paths in the plant which are important in the selection of controlled and manipulated variables. Qualitative simulation are employed to reason the plant behavior. For the synthesis of control strategies, techniques which quantify the effect of each of the manipulated variables on the control objectives both for over a long time-horizon and short time-horizon are used. Long horizon analysis is employed to develop control strategies for simpler process representations which capture the process behavior over a relatively long time-scale. Short-horizon analysis is employed to quantify the dynamic impact of manipulated inputs on relevant process outputs.

The plant control structure is synthesized in a goal-driven manner and within a multiobjective framework. The engineering preferences and design trade-offs are systematically expressed in the rank order of production objectives. The control structure is generated via a sequential assignment of primary manipulated variables to the control objectives, starting from the most important one. This approach allows the generation of formal associations among control objectives and manipulated variables which form a control structure that is relatively transparent.

The application of specific design techniques to tackle fundamental plant-wide control issues have been demonstrated on a number of processes studied by Downs (1992; 1993a; 1993b; 1993c), Luyben and co-workers (1993a; 1993b; 1993c; 1994) and Tyreus (1993c). It is shown that the various design techniques employed by the proposed methodology are useful for:

- studying the qualitative process behavior
- preventing the generation of infeasible control structures;
- generating feasible and promising candidate control structures;
- identifying process control objectives
- developing control strategies which take disturbances propagation into account.

It is shown that design techniques developed in the present research offers a systematic and analytical means to address issues which were resolved in a intuitive, heuristic or trial-and-error manner in the original studies.

The proposed methodology is broken into three distinct phases. In Phase I, long-horizon analysis is employed to develop suitable control strategies for maintaining the plant over a long time-scale of operation. In Phase II short-horizon analysis is employed to develop control strategies which are suitable for direct process regulations. Then, during the last phase, the control strategies developed in Phase I and Phase II of the design are integrated to form a multi-horizon control system. In a tutorial manner, the synthesis of complete plant control systems have been demonstrated on industrial processes such as the hydrodealkylation of toluene plant, the expanded Williams-Otto plant and the Tennessee Eastman process. The detailed mechanics involved in the Phase I of the design are the focus of the first two case studies while the details of Phase II of the design are illustrated in the third case study.

This research is concluded with a preliminary investigation into the interaction of design and control. Since the quality of closed-loop control is affected by both the control structure used as well as the plant itself, a goal-driven framework for the identification of process revamp opportunities to improve control performance is proposed. It is recommended that opportunities for improvement of control performance of individual control objectives be carried out in the modular multivariable control (MMC) framework. Specifically, the assignments made during control structure synthesis establish some pathways which determine the control performance of certain output objectives. These pathways should be studied to determine the elements (i.e. the specific transfer functions) which influence process control. Using a mapping which link unsatisfactory control performance to model parameters in the frequency domain, the inherent process limitations to control performance can be identified and process revamp recommendations can be made.

13.2 Contributions of Research

The main contributions of this research include:

1. the identification of key considerations arising in the synthesis of plant-wide control strategies;
2. the laying out of a conceptual hierarchical framework for studying the control relevant characteristics of process operations, and
3. the development of a systematic methodology for the design of plant-wide control structures.

Furthermore, techniques which address issues such as:

- identification of specific control tasks and control objectives which are consistent with the overall production plan
- verification of the feasibility of control strategies
- decision making in a multi-objective setting
- formulation of control schemes to meet long-range operational requirements and short-range dynamic control specifications
- generation of control strategies in a multivariate environment

have been formalized. These techniques form the basis of a comprehensive engineering solution to the design of plant-wide control strategies.

Research has also ventured into the natural extension of this work to study how design affects control performance and how specific process revamp opportunities can be determined within the modular multivariable control framework used in control structure synthesis. This study has set the road for someone to further develop the ideas in a PhD thesis.

Attractive Features of the Proposed Methodology

The methodology developed in this research overcomes several shortcomings that are present in the several existing methodologies. The shortcomings and weaknesses in the existing methods have been summarized in Section 2.4. Some of the shortcomings include the assumption of the availability of specific process control objectives, failure to address the multivariable and multiobjective nature of the design problem, lack of a systematic mechanism to help decision making and fight complexity, reliance on design heuristics and rule-of-thumb. The attractive features of the proposed methodology is summarized below:

- The proposed methodology does not assume the availability of a set of pre-defined control objectives. Instead, the specific controlled variables which are consistent with the overall production plan are derived during the generation of plant control structure.

- Since control strategies are developed based on quantitative analytical models and by considering the effect of interaction in a multivariable system, implicit in the design, control strategies are feasible and controllable.
- The engineering preferences and design trade-offs are systematically accounted for in a multiobjective decision making environment.
- The selection of process controlled objectives and manipulated variables is partly driven by the concept of diversion plant disturbances to less critical areas in the plant.
- The hierarchical framework formalized in this research is especially applicable to large chemical plants as this approach offers a means to fight complexity.
- Furthermore, the hierarchical framework naturally exploits the range of process phenomena at various time-scales of process operation.
- In the modular multivariable framework, control objectives are distinctively associated with manipulated variables one at a time, allowing the formation of a control structure that is relatively transparent and easily comphrensible, but at the same time, accounts for process interaction in the multivariable environment.

Hence, the methodology is systematic in a nature and is supported by control theory. Guidelines and techniques developed allow the use of an engineering approach the synthesis of plant-wide control structures in an unambiguous manner.

13.3 Future Research Directions

The methodology developed in this research is suitable for synthesizing a plant control structure which maintains the process at the desired steady-state(s) through regulation of controlled variables over several time-horizons, as shown previously in Figure 3-1. Most chemical processes are operated in a continuously changing environment, caused by either changes in ambient condition, quality or source of raw material or market demand. As illustrated in the Tennessee Eastman case study (Chapter 11), a control structure that is developed based on models for a certain range of process operation may not be optimal when the plant is being operated in a different operating regime. The proposed methodology suggests the use of a variable control structure to encompass the wide range of operating conditions. A method which assists the implementation of a pre-determined variable control structure is therefore needed.

The internal operation conditions of plant equipment generally undergo continuous changes. Fouling may occur in heat-exchanger, coke may build up in a furnace or a reactor. In unit-based control, this type of problems are usually solved by using an adaptive control algorithm which may entail the improvement of the process model used in the control. Extensive plant variation may also make an existing plant control structure sub-optimal or even infeasible. If that is the case, a new control structure must be adopted by the plant. Techniques which allow the detection of such circumstances as well as an online update of the plant control structure would be desirable. The modular multivariable controller design framework (Meadowcroft, 1992, 1997) offers an attractive framework for which such adaptive control strategies could be developed. The subject of online control structure adaptation is one which few researchers have explored and should be an area of research that will be required by the ever changing process operating environment.

The intricate relationship between process design and control was introduced in Chapter 12. The interaction of design and control has been briefly investigated in this study. The scope of the research covered a small class of processes, namely, those systems which have good linear approximations and systems whose impact of model uncertainty on control performance is negligible. The structure of the INHERENT PROCESS LIMITATION IDENTIFIER established in Figure 12-10 has been developed for a small class of systems. A more quantitative and extensive formalism for a more general class of multivariable systems is required. More comprehensive guidelines for the tracing of the pathways from individual control objectives to various elements (such as transfer functions in the process) affecting control performance should be expanded within the modular multivariable controller design framework. Furthermore, future work should explore how unsatisfactory control performance can be traced to model uncertainty and the representation of a nonlinear process by a linearized model. A systematic methodology which allows one to identify the effects of the various form of process interconnections in an integrated plant on control performance is also desirable.

Systematic approaches which address the aforementioned issues would improve the robustness of plant-wide control strategies to the various changes in process operation.

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Appendix A
Additional Data for the HDA Case Study

A.1 Optimal Base Case Design Variable for the HDA Process and Steady State Conditions

The following optimal base case design variables have been obtained from McKetta (1977).

Design Variables	Design Value
Reactor pressure	500 psia *
Reactor conversion	0.75 *
H_2 Purge composition	0.46
Benzene recovery in product	0.99
Reflux ratio in product column	1.2 R_m * (minimum reflux)
Toluene recovery in toluene column	0.986
Diphenyl recovery in toluene column	0.807
Recycle ratio of toluene from toluene column	1.0 *
Inlet temperature to partial condenser	428 K
Outlet temperature from partial condenser	311 K

Variables marked with (*) have been optimized during process design with respect to the total annualized cost and should be maintained to be at or close to their design values. Other variables are free to change for cost optimization.

The conditions of each process streams in the plant at the nominal stead-state have been obtained from a rigorous Aspen steady-state simulation (Park, 1995). Streams numbers shown below correspond to the labels of the process streams used in Figure 9-1.

Stream #	Stream name	Toluene	Benzene	Diphenyl	Methane	Hydrogen	Total	Phase	Temp	Pressure
				(mole flow of material in lb mol/hr)					°F	psia
2	Toluene	273.40	0.00	0.00	0.00	0.00	273.40	L	75	605
12	Mixed Feed	363.59	38.01	0.03	3103.25	2008.11	5512.98	L & V	142.6021	605
14	To feed heater	363.59	38.01	0.03	3103.25	2008.11	5512.98	V	1140	570
19	To reactor	363.59	38.01	0.03	3103.25	2008.11	5512.98	V	1150	500
15	From reactor	90.90	301.37	4.69	3375.89	1740.06	5512.90	V	1215.863	500
16	Quenched	116.08	377.77	6.06	3381.44	1740.45	5621.79	V	1150	490
10	Between H.X.	116.08	377.77	6.06	3381.39	1740.45	5621.74	L & v	189.411	455
20	To Phase Separator	116.08	377.77	6.06	3381.39	1740.45	5621.74	L & v	100	450
7	Separator Gas	4.32	36.62	0.00	3081.57	1596.14	4718.66	V	100	450
3	Purge Gas	0.39	3.27	0.00	275.26	142.58	421.49	V	100	450
1	Make-up H2	0.00	0.00	0.00	21.68	411.96	433.65	V	75	605
7+1	Recycle Gas	4.32	36.62	0.00	3103.25	2008.11	5152.31	V	143	605
11	Quench Oil	25.18	76.39	1.37	5.55	0.39	108.89	L	100	450
13	Stabilizer Feed	86.18	261.48	4.69	19.00	1.34	372.69	1%V	100	450
4	Stabilizer overhead	0.00	0.90	0.00	18.93	1.34	21.18	L	125	150
	Stabilizer bottoms	86.18	260.58	4.69	7.03E-02	1.99E-04	351.52	L	386	165
	Clay feed	86.18	260.58	4.69	7.03E-02	1.99E-04	351.52	L	450	315
17	Clay effluent	86.18	260.58	4.69	7.03E-02	1.99E-04	351.52	L	370	150
5	Benzene Product	0.08	259.19	0.00	7.03E-02	2.00E-04	259.34	L	145.1916	10
18	Benzene Bottoms	86.11	1.38	4.69	0.00	0.00	92.18	L	208	10
6	Fuel oil	0.25	0.00	4.66	0.00	0.00	4.91	L	436.1701	15
9	Recycle toluene	85.86	1.38	0.03	0.00	0.00	87.27	L	230.3113	15
8	Separator Vent	4.71	39.90	0.00	3356.83	1738.72	5140.15	V	100	450

A.2 Quantitative Sensitivity Analysis related to the Heat-integrated loop

Quantitative Sensitivity Analysis of the Feed pre-heater

At steady state, T_{12} = 142.6 °F, T_{14} = 1140 °F, T_{16} = 1150 °F, T_{10} = 189.4 °F. Since:

$$Q_{ex} = UA\Delta T \tag{9-3}$$

$$\Delta T = [(T_{10} - T_{12}) - (T_{16} - T_{14})] / \ln[(T_{10} - T_{12}) / (T_{16} - T_{14})] \tag{9-4}$$

Also,

$$Q_{ex} = K_F(T_{14} - T_{12}) = K_Q(T_{16} - T_{10}) \tag{A-1}$$

At constant flows, U, K_F and K_Q are constants. A = 5140 ft^2, U = 24 (h) * 60 Btu/h/ft^2/°F (from McKetta, 1977). Then, at steady state, ΔT = 23.8 °F. Substituting these values into [9-3] and equating [9-3] with [A-1], we obtain:

$$K_F = UA(23.8)/997.4\ ;\ K_Q = UA\ (23.8)/906.6 \tag{A-2}$$

Case I: Increase T_{12} from 142.6 °F to 152.6 °F

The new steady-state values are solutions to:

$$\frac{AU23.8}{997.4}(T_{14} - 152.6) = \frac{(T_{10} - 152.6) - (1150 - T_{14})}{\ln\left(\dfrac{T_{10} - 152.6}{1150 - T_{14}}\right)} \tag{A-3}$$

$$\frac{AU23.8}{960.6}(1150 - T_{10}) = \frac{(T_{10} - 152.6) - (1150 - T_{14})}{\ln\left(\dfrac{T_{10} - 152.6}{1150 - T_{14}}\right)} \tag{A-4}$$

Solving, we get: T_{14} = 1138 °F (cooler) and T_{10} = 193.65 °F (hotter).

Case II: Set T_{16} = 1170 °F, T_{12} remains at 142 °F

Using a similar method, we found that at the new steady state, T_{14} = 1159.53 °F (hotter) and T_{10} = 189.5 °F (essentially unchanged).

Quantitative Sensitivity Analysis of the Mixer (F_{15} + F_{11} = F_{16})

Base case data (from Aspen simulation):

Stream	F_{16}	F_{15}	F_{11}
Enthalpy (Btu/lbmol)	-2407.309	-2768.899	15861.04
Flow (lbmol/hr)	5621.19	5512.902	108.8872

The heat content of F_{16} is given by:

$$H_{16} = h_{16}F_{16} = h_{15}F_{15} + h_{11}F_{11} \tag{A-5}$$

where:

h_i = molar enthalpy of stream i
H_i = rate of heat flow of stream i

It is interested to determine changes in dH_{16} for a negative change in T_{15} and a positive change in T_{11}.

$$dH_{16} = \frac{\partial H_{16}}{\partial T_{11}} + \frac{\partial H_{16}}{\partial T_{15}} = \frac{\partial H_{16}}{\partial h_{11}}\frac{\partial h_{11}}{\partial T_{11}} + \frac{\partial H_{16}}{\partial h_{15}}\frac{\partial h_{15}}{\partial T_{15}} \qquad \text{[A-6]}$$

Assume that h_{11} is roughly proportional to T_{11}. Then for a 4°F rise in T_{10} (resulted from a 10°F increase in T_{12}), we assume there is a 4°F rise in T_{11}. Then,

$$h_{11}\ (@T_{11} = 104\ °F) = 15861.04 \times \frac{104}{100} = 16495.4816\ \text{Btu/lbmol} \qquad \text{[A-7]}$$

At constant h_{15}, F_{15} and F_{11}, we can compute the h_{16} at the new steady-state using the above relations:

$$h_{16}\ (@T_{11} = 104\ °F) = -2396.026\ \text{Btu/lbmol} \qquad \text{[A-8]}$$

Then,

$$\frac{dH_{16}}{H_{16}} = 4.68 \times 10^{-3} \qquad \text{[A-9]}$$

H_{16} is insensitive to changes in T_{11}. If T_{15} decreases, at constant F_{11}, we expect H_{16} to decrease.

A.3 Material and Energy Balance Models

Level 1: Input-Output Plant

The process representation at this level is shown in Figure 9-7. The following reactions occur in the HDA plant:

(R1) Toluene (T) + Hydrogen (H) → Benzene (B) + Methane (M)
(R2) 2Benzene (2B) → Diphenyl (D) + Hydrogen (H)

Let $F_{i,j}$ be the mol flow (lb mol/hr) of component j in stream i. The following material balance equations can be written:

Material Balance of Toluene

(Rate of T entering the plant) + (Rate of T being generated)
= (Rate of T consumed in R1) + (Rate of T consumed in R2) + (Rate of T leaving the plant)

$(F_{2,T}) + (0) = (F_{5,B} + F_{3,B} + F_{4,B}) + (2\ F_{6,D}) + (F_{3,T} + F_{5,T} + F_{6,T})$

Then, the rate of accumulation of toluene in the system as a result of an imbalance between the in flows and out flows is simply:

$$r_T = (F_{2,T}) + (0) - (F_{5,B} + F_{3,B} + F_{4,B}) - (2F_{6,D}) - (F_{3,T} + F_{5,T} + F_{6,T})$$

Material Balance of Hydrogen

(Rate of H entering the plant) + (Rate of H being generated)

= (Rate of H consumed in R1) + (Rate of H consumed in R2) + (Rate of H leaving the plant)

$$r_H = F_{1,H} + F_{6,H} - F_{4,B} - F_{5,B} - F_{3,B} - 2F_{6,D} - F_{3,H} - F_{4,H}$$

Material Balance of Methane

(Rate of M entering the plant) + (Rate of M being generated)

= (Rate of M consumed in R1) + (Rate of M consumed in R2) + (Rate of M leaving the plant)

$$r_M = F_{1,M} + F_{4,B} + F_{3,B} + 2F_{6,D} - F_{3,M} - F_{4,M} - F_{5,M}$$

Energy Balance

$$e = H_1 + H_2 - H_4 - H_5 - H_6 + Q_{fuel} + Q_{steam} + Q_{cw}$$

Level 2: Generalized Reaction-Separation System

The following material and energy balance equations describe the process representation shown in Figure 9-10. Each material is described by three material balance equations, each describing one sub-system in the process representation.

Material Balance of Toluene

$$r_{T\text{-}(a)} = F_{2,T} + F_{11,T} + F_{9,T} + F_{7,T} - F_{10,B} + F_{11,B} + F_{7,B} + F_{9,B} - 2F_{10,D} + 2F_{11,D} + 2F_{7,D} + 2F_{9,D} - F_{10,T}$$

$$r_{T\text{-}(b)} = F_{10,T} + F_{10,B} + 2F_{10,D} - F_{8,T} - F_{8,B} - 2F_{8,D} - F_{5,T} - F_{5,B} - 2F_{5,D} - F_{6,T} - F_{6,B} - 2F_{6,D} - F_{9,T} - F_{9,B} - 2F_{9,D} - F_{11,T} - F_{11,B} - 2F_{11,D} - F_{4,T} - F_{4,B} - 2F_{4,D}$$

$$r_{T\text{-}(c)} = F_{8,T} + F_{8,B} + 2F_{8,D} - F_{7,T} - F_{7,B} - 2F_{7,D} - F_{3,T} - F_{3,B} - 2F_{3,D}$$

Adding $r_{T\text{-}(a)}$, $r_{T\text{-}(b)}$ and $r_{T\text{-}(c)}$ returns the material balance of toluene at the input-output level, i.e. r_T.

Material Balance of Hydrogen

$$r_{H\text{-}(a)} = F_{1,H} + F_{7,H} + F_{7,B} + F_{7,D} + F_{11,H} + F_{11,B} + F_{11,D} + F_{9,H} + F_{9,B} + F_{9,D} - F_{10,H} - F_{10,B} - F_{10,D}$$

$$r_{H\text{-}(b)} = F_{10,H} + F_{10,B} + F_{10,D} - F_{11,H} - F_{11,B} - F_{11,D} - F_{8,H} - F_{8,B} - F_{8,D} - F_{5,H} - F_{5,B} - F_{5,D} - F_{6,H} - F_{6,B} - F_{6,D} - F_{4,H} - F_{4,B} - F_{4,D} - F_{9,H} - F_{9,B} - F_{9,D}$$

$$r_{H\text{-}(c)} = F_{8,H} + F_{8,B} + F_{8,D} - F_{7,H} - F_{7,B} - F_{7,D} - F_{3,H} - F_{3,B} - F_{3,D}$$

Adding $r_{H\text{-}(a)}$, $r_{H\text{-}(b)}$ and $r_{H\text{-}(c)}$ returns the material balance of toluene at the input-output level, i.e. r_H.

Material Balance of Methane

$$r_{M\text{-}(a)} = F_{1,M} + F_{11,M} - F_{11,B} - 2F_{11,D} + F_{7,M} - F_{7,B} - 2F_{7,D} + F_{9,M} - F_{9,B} - 2F_{9,D} - F_{10,M} + F_{10,B} + 2F_{10,D}$$

$$r_{M\text{-}(b)} = F_{10,M} - F_{10,B} - 2F_{10,D} - F_{11,M} + F_{11,B} + 2F_{11,D} - F_{9,M} + F_{9,B} + 2F_{9,D} - F_{8,M} + F_{8,B} + 2F_{8,D} - F_{4,M} + F_{4,B} + 2F_{4,D} - F_{5,M} + F_{5,B} + 2F_{5,D} - F_{6,M} + F_{6,B} + 2F_{6,D}$$

$$r_{M\text{-}(c)} = F_{8,M} - F_{8,B} - 2F_{8,D} - F_{7,M} + F_{7,B} + 2F_{7,D} - F_{3,M} + F_{3,B} + 2F_{3,D}$$

Adding $r_{M\text{-}(a)}$, $r_{M\text{-}(b)}$ and $r_{M\text{-}(c)}$ returns the material balance of toluene at the input-output level, i.e. r_M.

Energy Balance Model

$e_{(a)} = H_1 + H_2 + H_7 + H_{11} + H_9 - H_{10} + Q_{Fuel}$
$e_{(b)} = H_{10} - H_4 - H_5 - H_6 - H_8 - H_{11} - H_9 + Q_{Steam\text{-}(b)} + Q_{cw\text{-}(b)}$
$e_{(c)} = H_8 - H_3 - H_7$

Level 3a: Generalized Reaction-Expanded Separation Level

The representation of the process at this level is shown in Figure 9-13. The material and energy balances for sub-blocks *d* and *e* are shown next.

Material Balance of Toluene

$$r_{T\text{-}(d)} = F_{10,T} + F_{10,B} + 2F_{10,D} - F_{8,T} - F_{8,B} - 2F_{8,D} - F_{11,T} - F_{11,B} - 2F_{11,D} - F_{13,T} - F_{13,B} - 2F_{13,D}$$

$$r_{T\text{-}(e)} = F_{13,T} + F_{13,B} + 2F_{13,D} - F_{5,T} - F_{5,B} - 2F_{5,D} - F_{6,T} - F_{6,B} - 2F_{6,D} - F_{9,T} - F_{9,B} - 2F_{9,D} - F_{4,T} - F_{4,B} - 2F_{4,D}$$

Material Balance of Hydrogen

$$r_{H\text{-}(d)} = F_{10,H} + F_{10,B} + F_{10,D} - F_{11,H} - F_{11,B} - F_{11,D} - F_{8,H} - F_{8,B} - F_{8,D} - F_{13,H} - F_{13,B} - F_{13,D}$$

$$r_{H\text{-}(e)} = F_{13,H} + F_{13,B} + F_{13,D} - F_{5,H} - F_{5,B} - F_{5,D} - F_{6,H} - F_{6,B} - F_{6,D} - F_{4,H} - F_{4,B} - F_{4,D} - F_{9,H} - F_{9,B} - F_{9,D}$$

Material Balance of Methane

$$r_{M\text{-}(d)} = F_{10,M} - F_{10,B} - 2F_{10,D} - F_{11,M} + F_{11,B} + 2F_{11,D} - F_{13,M} + F_{13,B} + 2F_{13,D} - F_{8,M} + F_{8,B} + 2F_{8,D}$$

$$r_{M\text{-}(e)} = F_{13,M} - F_{13,B} - 2F_{13,D} - F_{9,M} + F_{9,B} + 2F_{9,D} - F_{4,M} + F_{4,B} + 2F_{4,D} - F_{5,M} + F_{5,B} + 2F_{5,D} - F_{6,M} + F_{6,B} + 2F_{6,D}$$

Energy Balance Model

$e_{(d)} = H_{10} - H_8 - H_{11} - H_{13} + Q_{cw\text{-}(d)}$
$e_{(e)} = H_{13} - H_4 - H_5 - H_6 - H_9 + Q_{Steam\text{-}(e)} + Q_{cw\text{-}(e)}$

Appendix B
Additional Data for the Expanded William-Otto Case Study

B.1 Steady State Operating Condition of the Expanded William-Otto Plant

The following data have been obtained from Johnston, R.D. (1985). The streams correspond to the label in Figure 10-1.

Stream	F_A	F_B	F_1	F_3	F_4	F_5
Temp (°K)	294.3	294.3	350	311	311	360
Flow (kg mol /hr)	65.76	140	189.262	163.8394	25.41467	265.2959
Mole fractions						
A	1	0	0.126556	0.14624	0	0.073534
B	0	1	0.508987	0.471598	0.75	0.35816
C	0	0	0.013497	0.015586	0	0.006956
E	0	0	0.174894	0.20207	0	0.377892
G	0	0	0.033564	0	0.25	0.017366
P	0	0	0.142501	0.164505	0	0.166091

Stream	F_6	F_9	F_{10}	F_{11}	F_{13}	F_{14}
Temp (°K)	340	311	311	306.5	311	311
Flow (kg mol /hr)	237.6195	246.8958	18.41	26.979	98.94974	120.9382
Mole fractions						
A	0.073534	0.079016	0	0.02	0.086256	0.086256
B	0.35816	0.328928	0.75	0	0.369334	0.369334
C	0.006956	0.007492	0	0	0.008421	0.008421
E	0.377892	0.406036	0	0	0.455883	0.455883
G	0.017366	0	0.25	0	0	0
P	0.166091	0.178529	0	0.98	0.080105	0.080105

Stream	F_{15}	F_{16}	F_{18}	F_{20}
Temp (°K)	311	305	299.1	330
Flow (kg mol /hr)	43.82467	31.43717	171.4381	12.38696
Mole fractions				
A	0	0	0	0
B	0.75	0.993243	0.998764	0.132634
C	0	0	0	0
E	0	0	0	0
G	0.25	0.006757	0.001236	0.867366
P	0	0	0	0

Note that $F_8 = F_7 = F_6$ and $F_{20} = F_{19}$. Also, $F_{12} = F_{13} + F_{14}$.

B.2 Material and Energy Balance Model for the expanded WO plant

The following reactions occur in expanded WO plant:

$$(R1)\ A + B \xrightarrow{k_1} C$$
$$(R2)\ C + B \xrightarrow{k_2} P + E$$
$$(R3)\ P + C \xrightarrow{k_3} G$$

Level 1: Input-Output Level

The process representation of this level is shown in Figure 10-3. $F_{i,j}$ will be used to refer to the molar flow of component j in stream i in the following equations.

Material Balance of A

F_A = (C produced in R1 not reacted in R2 or R3) + (C generated in R1, reacted in R2)
+ (C generated in R1, reacted in R3) + (unreacted A)

$$F_A = (F_{11,C} + F_{13,C} + F_{20,C}) + (F_{11,E} + F_{13,E} + F_{20,E}) + (F_{11,G} + F_{13,G} + F_{20,G}) + (F_{11,A} + F_{13,A} + F_{20,A})$$

Hence,

$$r_A = F_A - (F_{11,C} + F_{13,C} + F_{20,C}) - (F_{11,E} + F_{13,E} + F_{20,E}) - (F_{11,G} + F_{13,G} + F_{20,G}) - (F_{11,A} + F_{13,A} + F_{20,A})$$

Material Balance of B

F_B = (C produced in R1 not reacted in R2 or R3) + (C generated in R1, reacted in R2 and B reacted in R2) + (C generated in R1, reacted in R3) + (unreacted B)

$$F_B = (F_{11,C} + F_{13,C} + F_{20,C}) + 2*(F_{11,E} + F_{13,E} + F_{20,E}) + (F_{11,G} + F_{13,G} + F_{20,G}) + (F_{11,B} + F_{13,B} + F_{20,B})$$

Hence,

$$r_B = F_B - (F_{11,C} + F_{13,C} + F_{20,C}) - 2*(F_{11,E} + F_{13,E} + F_{20,E}) - (F_{11,G} + F_{13,G} + F_{20,G}) - (F_{11,A} + F_{13,A} + F_{20,A})$$

Material Balance of C

Amount of C generated $= F_A - F_{11,A} - F_{13,A} - F_{20,A}$
= Total amount of A reacted
$= (F_{11,C} + F_{13,C} + F_{20,C}) + (F_{11,E} + F_{13,E} + F_{20,E}) + (F_{11,G} + F_{13,G} + F_{20,G})$

Hence, $r_C = r_A$.

Material Balance of P

(Amount of P generated in R2) = (amount of P reacted in R3) + (amount of P leaving the process)

$$(F_{11,E} + F_{13,E} + F_{20,E}) = (F_{11,G} + F_{13,G} + F_{20,G}) + (F_{11,P} + F_{13,P} + F_{20,P})$$

Hence,

$$r_P = (F_{11,E} + F_{13,E} + F_{20,E}) - (F_{11,G} + F_{13,G} + F_{20,G}) - (F_{11,P} + F_{13,P} + F_{20,P})$$

Material Balance of E

$$(F_{11,E} + F_{13,E} + F_{20,E}) = (F_{11,E} + F_{13,E} + F_{20,E})$$

Material Balance of G

$$(F_{11,G} + F_{13,G} + F_{20,G}) = (F_{11,G} + F_{13,G} + F_{20,G})$$

Hence, the three unique material balances are those for A, B and P.

Energy Balance

$e = H_A + H_B - H_{13} - H_{11} - H_{20} + Q_{cw} + Q_{steam}$ where H_i refers to the molar energy flow into the unit.

Level 2: Generalized Reaction-Separation Section

The process representation of this level is shown in Figure 10-5.

Material Balance of A

$$r_{A\text{-}(a)} = F_A - (F_{9,C} + F_{9,E} + F_{9,G} + F_{9,A}) - (F_{4,C} + F_{4,E} + F_{4,G} + F_{4,A}) - (F_{10,C} + F_{10,E} + F_{10,G} + F_{10,A}) + (F_{14,C} + F_{14,E} + F_{14,G} + F_{14,A}) + (F_{17,C} + F_{17,E} + F_{17,G} + F_{17,A})$$

$$r_{A\text{-}(b)} = (F_{9,C} + F_{9,E} + F_{9,G} + F_{9,A}) + (F_{4,C} + F_{4,E} + F_{4,G} + F_{4,A}) + (F_{10,C} + F_{10,E} + F_{10,G} + F_{10,A}) - (F_{14,C} + F_{14,E} + F_{14,G} + F_{14,A}) - (F_{17,C} + F_{17,E} + F_{17,G} + F_{17,A}) - (F_{13,C} + F_{13,E} + F_{13,G} + F_{13,A}) - (F_{20,C} + F_{20,E} + F_{20,G} + F_{20,A})$$

F_5 and F_7 do not enter into the balance because it is known that it is merely an heat-integration loop with no real transfer of materials.

Note that $r_{A\text{-}(a)} + r_{A\text{-}(b)} = r_A$.

Material Balance of B

$$r_{B\text{-}(a)} = F_B - (F_{9,C} + 2F_{9,E} + F_{9,G} + F_{9,B}) - (F_{4,C} + 2F_{4,E} + F_{4,G} + F_{4,B}) - (F_{10,C} + 2F_{10,E} + F_{10,G} + F_{10,B}) + (F_{14,C} + 2F_{14,E} + F_{14,G} + F_{14,B}) + (F_{17,C} + 2F_{17,E} + F_{17,G} + F_{17,B})$$

$$r_{B\text{-}(b)} = (F_{9,C} + 2F_{9,E} + F_{9,G} + F_{9,B}) + (F_{4,C} + 2F_{4,E} + F_{4,G} + F_{4,B}) + (F_{10,C} + 2F_{10,E} + F_{10,G} + F_{10,B}) - (F_{14,C} + 2F_{14,E} + F_{14,G} + F_{14,B}) - (F_{17,C} + 2F_{17,E} + F_{17,G} + F_{17,B}) - (F_{13,C} + 2F_{13,E} + F_{13,G} + F_{13,B}) - (F_{20,C} + 2F_{20,E} + F_{20,G} + F_{20,B})$$

F_5 and F_7 do not enter into the balance because it is known that it is merely an heat-integration loop with no real transfer of materials.

Note that $r_{B\text{-}(a)} + r_{B\text{-}(b)} = r_B$.

Material Balance of P

$$r_{P\text{-}(a)} = F_{9,E} + F_{4,E} + F_{10,E} + F_{17,G} + F_{17,P} + F_{14,G} + F_{14,P} - F_{17,E} - F_{14,E} - F_{9,G} - F_{9,P} - F_{4,G} - F_{4,P} - F_{10,G} - F_{10,P}$$

$$r_{P\text{-}(b)} = F_{11,E} + F_{13,E} + F_{20,E} + F_{17,E} + F_{14,E} + F_{9,G} + F_{9,P} + F_{4,G} + F_{4,P} + F_{10,G} + F_{10,P} - F_{11,G} - F_{11,P} - F_{13,G} - F_{13,P} - F_{20,G} - F_{20,P} - F_{9,E} - F_{4,E} - F_{10,E} - F_{17,G} - F_{17,P} - F_{14,G} - F_{14,P}$$

F_5 and F_7 do not enter into the balance because it is known that it is merely an heat-integration loop with no real transfer of materials.

Note that $r_{P\text{-}(a)} + r_{P\text{-}(b)} = r_P$.

Energy Balance

$$e_{(a)} = H_A + H_B + H_{17} + H_{14} + H_7 + Q_{CW\text{-}(a)} + H_{Steam\text{-}(a)} - H_5 - H_9 - H_4 - H_{10}$$

$$e_{(b)} = H_5 + H_9 + H_4 + H_{10}\ Q_{CW\text{-}(b)} + H_{Steam\text{-}(b)} - H_{13} - H_{20} - H_{11} - H_{17} - H_{14} - H_7 +$$

Note that $e_{(a)} + e_{(b)} = e$.

Level 3: Expanded Generalized Reaction-Separation Level

The process representation for this level is shown in Figure 10-7. Since only sub-block a has been refined, balances around sub-block b remain valid at this level.

Material Balance of A

$$r_{A\text{-}(c)} = (F_{17,C} + F_{17,E} + F_{17,G} + F_{17,A}) - (F_{18,C} + F_{18,E} + F_{18,G} + F_{18,A})$$

$$r_{A\text{-}(d)} = F_A + (F_{18,C} + F_{18,E} + F_{18,G} + F_{18,A}) - (F_{3,C} + F_{3,E} + F_{3,G} + F_{3,A}) - (F_{4,C} + F_{4,E} + F_{4,G} + F_{4,A})$$

$$r_{A\text{-}(e)} = (F_{3,C} + F_{3,E} + F_{3,G} + F_{3,A}) + (F_{14,C} + F_{14,E} + F_{14,G} + F_{14,A}) - (F_{9,C} + F_{9,E} + F_{9,G} + F_{9,A}) - (F_{10,C} + F_{10,E} + F_{10,G} + F_{10,A})$$

$r_{A\text{-}(c)} + r_{A\text{-}(d)} + r_{A\text{-}(e)} = r_{A\text{-}(a)}$.

Material Balance of B

$$r_{B\text{-}(c)} = F_B + (F_{17,C} + 2F_{17,E} + F_{17,G} + F_{17,B}) - (F_{18,C} + 2F_{18,E} + F_{18,G} + F_{18,B})$$

$$r_{B\text{-}(d)} = (F_{18,C} + 2F_{18,E} + F_{18,G} + F_{18,B}) - (F_{3,C} + 2F_{3,E} + F_{3,G} + F_{3,B}) - (F_{4,C} + 2F_{4,E} + F_{4,G} + F_{4,B})$$

$$r_{B\text{-}(e)} = (F_{3,C} + 2F_{3,E} + F_{3,G} + F_{3,B}) + (F_{14,C} + 2F_{14,E} + F_{14,G} + F_{14,B}) - (F_{9,C} + 2F_{9,E} + F_{9,G} + F_{9,B}) - (F_{10,C} + 2F_{10,E} + F_{10,G} + F_{10,B})$$

$r_{B\text{-}(c)} + r_{B\text{-}(d)} + r_{B\text{-}(e)} = r_{B\text{-}(a)}$.

Material Balance of P

$$r_{P\text{-}(d)} = F_{18,E} + F_{17,G} + F_{17,P} - F_{17,E} - F_{18,G} - F_{18,P}$$

$$r_{P\text{-}(d)} = F_{3,E} + F_{4,E} + F_{18,G} + F_{18,P} - F_{4,G} - F_{4,P} - F_{18,E} - F_{3,G} - F_{3,P}$$

$$r_{P\text{-}(e)} = F_{9,E} + F_{10,E} + F_{3,G} + F_{3,P} + F_{14,G} + F_{14,G} - F_{3,E} - F_{9,G} - F_{9,P} - F_{14,E} - F_{10,G} - F_{10,P}$$

$r_{P\text{-}(c)} + r_{P\text{-}(d)} + r_{P\text{-}(e)} = r_{P\text{-}(a)}$.

Energy Balance

$$e_{(c)} = H_B + H_{17} - H_{18}$$

$$e_{(d)} = H_A + H_{18} + Q_{CW\text{-}(d)} + H_{Steam\text{-}(d)} - H_3 - H_4$$

$$e_{(e)} = H_3 + H_{17} + H_{14} + Q_{CW\text{-}(a)} + H_{Steam\text{-}(a)} - H_5 - H_9 - H_{10}$$

$e_{(c)} + e_{(d)} + e_{(e)} = e_{(a)}$.

Appendix C
Additional Data for the TEC Case Study

C.1 Optimal steady-states for the Tennessee Eastman Process (from Ricker, 1995)

Manipulated variables and measured outputs corresponding to the cost optimal steady-states of the base case and the other five operating modes are shown below.

	Manipulated Inputs	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
1	D Feed, %	**62.935**	12.637	89.130	100.00	13.098	100.000
2	E Feed, %	**53.147**	96.216	8.381	86.175	100.000	9.428
3	A Feed, %	**26.248**	30.412	19.114	49.477	32.009	21.543
4	A + C Feed, %	**60.566**	56.092	51.368	96.595	58.155	57.640
5	Recycle valve, %	**1.000**	1.000	77.621	1.000	1.000	71.166
6	Purge valve, %	**25.770**	44.347	6.501	48.742	47.095	10.654
7	Separator valve, %	**37.266**	35.799	29.146	60.960	37.422	32.685
8	Stripper valve, %	**46.444**	42.865	39.425	74.522	44.491	44.250
9	Steam valve, %	**1.000**	1.000	1.000	1.000	1.000	1.000
10	Reactor coolant, %	**35.992**	25.257	35.550	60.794	26.070	40.538
11	Condenser coolant, %	**12.431**	12.907	99.000	35.534	14.115	99.000
12	Agitator speed, %	**100.000**	100.000	100.000	100.000	100.000	100.000

Steady-state values of all measurable process variables at all operating modes.

	Measurements	Base Case (50/50)	Mode 2 (10/90)	Mode 3 (90/10)	Mode 4 (50/50)	Mode 5 (10/90)	Mode 6 (90/10)
1	A Feed, kscmh	**0.267**	0.309	0.194	0.503	0.325	0.219
2	D Feed, kg/h	**3657**	743	5179	5811	761	5811
3	E Feed, kg/h	**4440**	8038	700	7244	8354	788
4	A + C Feed, kscmh	**9.24**	8.55	7.83	14.73	8.87	8.79
5	Recycle flow, kscmh	**32.18**	31.69	19.67	29.22	31.27	10.08
6	Reactor feed, kscmh	**47.36**	46.08	32.09	53.76	46.24	34.02
7	Reactor pressure, kPa	**2800**	2800	2800	2800	2800	2800
8	Reactor level, %	**65.0**	65.0	65.0	65.0	65.0	65.0
9	Reactor temperature, °C	**122.9**	124.2	121.9	128.2	124.6	123.0
10	Purge rate, kscmh	**0.211**	0.361	0.087	0.462	0.384	0.099
11	Sep temperature, °C	**91.7**	90.3	83.4	74.1	88.9	80.9
12	Sep level, %	**50.0**	50.0	50.0	50.0	50.0	50.0
13	Sep pressure, kPa	**2706**	2705	2765	2699	2705	2761
14	Sep underflow, m^3/h	**25.28**	26.31	17.55	40.06	27.45	19.60
15	Stripper level, %	**50.0**	50.0	50.0	50.0	50.0	50.0
16	Stripper pressure, kPa	**3326**	3327	2996	3365	3330	3015
17	Stripper underflow, m^3/h	**22.89**	22.73	18.04	36.04	23.55	20.20
18	Stripper temperature, °C	**66.5**	65.4	62.3	51.5	63.9	60.5
19	Steam flow, kg/h	**4.74**	4.90	5.34	6.87	5.11	5.59
20	Compressor work, kW	**278.9**	274.7	272.6	263.2	271.7	293.2
21	React. cool temperature,°C	**102.4**	108.6	101.9	96.6	108.5	100.6
22	Cond. cool temperature,°C	**92.0**	91.6	45.0	73.5	89.8	45.7
23	Feed %A, mol %	**32.21**	34.82	29.46	26.40	34.78	29.99
24	Feed %B, mol %	**14.93**	8.18	27.74	8.78	7.85	26.34
25	Feed %C, mol %	**18.75**	19.43	17.97	22.36	19.54	18.80
26	Feed %D, mol %	**6.03**	1.20	12.68	7.95	1.24	13.23
27	Feed %E, mol %	**13.71**	25.47	3.86	17.01	26.03	3.91
28	Feed %F, mol %	**4.04**	5.60	1.29	3.88	5.60	1.33
29	Purge, %A, mol %	**32.73**	36.63	27.86	40.94	36.71	28.61
30	Purge, %B, mol %	**21.83**	11.77	45.07	15.90	11.47	44.41
31	Purge, %C, mol %	**13.11**	14.63	9.22	15.68	14.57	9.76
32	Purge, %D, mol %	**0.9**	0.13	2.18	0.68	0.13	2.09
33	Purge, %E, mol %	**16.19**	22.37	3.94	15.41	22.92	4.00
34	Purge, %F, mol %	**5.39**	7.37	1.82	5.72	7.44	1.91
35	Purge, %G, mol %	**6.62**	1.32	9.40	3.85	1.26	8.76
36	Purge, %H, mol %	**3.23**	5.79	0.50	1.82	5.51	0.46
37	Product, %D, mol%	**0.01**	0.00	0.03	0.02	0.00	0.03
38	Product, %E, mol%	**0.58**	0.92	0.16	1.21	1.01	0.18
39	Product, %F, mol%	**0.19**	0.29	0.07	0.04	0.32	0.08
40	Product, %G, mol%	**53.83**	11.66	90.09	53.35	11.65	90.07
41	Product, %H, mol%	**43.91**	85.64	8.17	43.52	85.53	8.16

C.2 Selection of Manipulated Variable for the Control of Reactor Level using Short-Horizon control design criteria

As the reactor level is associated with the unstable modes in the process, the best manipulated variable for the control of this output will be selected based on short-horizon control design criteria. The relevant dynamic process models are in Table 11-4. Using equations [6-14], [6-15] and [6-19], measures which indicate the contribution of different aspects of the model on the achievable performance of the control are computed below.

Measures of the effect of Deadtime ($V_{deadtime,j}$) on Reactor Level by each output at all operating modes

Inputs, j	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	8	8	8	8	8	8
Product	40	40	40	40	40	40
Steam	30	30	30	30	30	30
Cond. Water	10	10	10	10	10	10
Recycle	2	2	2	2	2	2
Sep Bot	8	8	8	8	8	8
$\bar{V}_{deadtime}$	16.33	16.33	16.33	16.33	16.33	16.33

Measures of the effect of Rangeability $V_{rangeability,j}$ on Reactor Level by each output at all operating modes

Inputs, j	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	0.0388048	0.0225494	0.1052521	0.0205162	0.0212337	0.0938615
Product	0.0215332	0.0234384	0.0253646	0.0392495	0.0224765	0.0225984
Steam	1	*infinity*	1	1	1	1
Cond. Water	0.0804441	0.0774773	1	0.0281421	0.0708466	1
Recycle	1	1	0.0446847	1	1	0.0346813
Sep Bot	0.0268341	0.0279337	0.03431	0.0256148	0.0267222	0.0305951
$\bar{V}_{reangeability}$	0.041904	0.0378497	0.0524029	0.0283806	0.0353197	0.045434

Measures of $V_{integrator,j}$ on Reactor Level by each output at all operating modes

Inputs, j	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	0.333	0.730	infinity	0.471	0.758	infinity
Product	1128.668	257.732	250.000	213.675	154.321	359.712
Steam	2.763	3.207	infinity	4.420	2.897	infinity
Cond. Water	0.161	0.163	infinity	0.136	-0.172	infinity
Recycle	0.286	0.308	0.288	0.264	0.298	0.233
Sep Bot	0.442	0.328	0.255	0.287	0.309	0.212
$\bar{V}_{integrator}$	0.306	0.382	0.271	0.290	0.384	0.222

The averages $\bar{V}_i$ (for i = deadtime, rangeability and integrator) have been computed by taking averages of the measures for each of the modes, excluding data which fall outside the normal order of magnitudes of the measures. For example, $\bar{V}_{integrator}$ for Modes 1, 2, 4 and 5 have been computed by excluding the data for product flow and steam as their values are much bigger than the rest of the inputs. Such large values automatically indicate that these inputs would not be suitable choices as manipulated variable. Thus, for fair comparison, these data will be excluded in the averages. The gross averages $\bar{\bar{V}}_i$ is simply the average $\bar{V}_{i,j}$ for all operating modes:

Gross averages of performance measures	$\bar{\bar{V}}_i$
$\bar{\bar{V}}_{deadtime}$	16.33
$\bar{\bar{V}}_{reangeability}$	0.04022
$\bar{\bar{V}}_{integrator}$	0.309

Hence, the data for rangeability and integrator gain can be adjusted to roughly the same order of magnitude as those for deadtime by multiplying the measures by an appropriately chosen normalization factor N_i :

$$N_i = \bar{\bar{V}}_i / \bar{\bar{V}}_{deadtime} \quad \text{for } i = \text{rangeability, integrator}$$

The normalized measures ($V_{i,j} / N_i$) are shown next:

Normalized Measures of the effect of deadtime ($V_{deadtime,j}$) on Reactor Level by each output at all operating modes

Inputs, j	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	8	8	8	8	8	8
Product	40	40	40	40	40	40
Steam	30	30	30	30	30	30
Cond. Water	10	10	10	10	10	10
Recycle	2	2	2	2	2	2
Sep Bot	8	8	8	8	8	8

Normalized measures of the effect of rangeability $V_{rangeability,j}$ on Reactor Level by each output at all operating modes

Inputs, j	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	15.760515	9.1584207	42.747972	8.3326183	8.6240255	38.12169
Product	8.7456607	9.5194769	10.3018	15.941145	9.1287785	9.1782894
Steam	406.14848	*infinity*	406.14848	406.14848	406.14848	406.14848
Cond. Water	32.672229	31.467303	406.14848	11.429855	28.774246	406.14848
Recycle	406.14848	406.14848	18.148643	406.14848	406.14848	14.085749
Sep Bot	10.898634	11.345247	13.934965	10.403393	10.853201	12.426143

Normalized measures of $V_{integrator,j}$ on Reactor Level by each output at all operating modes

Inputs, *j*	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	17.608477	38.558709	*infinity*	24.905909	40.019267	*infinity*
Product	59622.384	13614.802	13206.358	11287.485	8152.0728	19001.954
Steam	145.93467	169.43175	*infinity*	233.48257	153.04178	*infinity*
Cond. Water	8.5229803	8.5865691	*infinity*	7.2067438	9.092157	*infinity*
Recycle	15.092981	16.253979	15.223467	13.960209	15.721855	12.282128
Sep Bot	23.374085	17.319814	13.44843	15.136227	16.329345	11.201321

Once data have been normalized to roughly the same order of magnitude, a fair comparison can be made. The overall performance index for input *j* which accounts for all three measurable effects is simply given by:

$$V_j = w_{integrator}\left|\frac{V_{integrator,j}}{N_{integrator}}\right| + w_{deadtime}\left|\frac{V_{deadtime,j}}{N_{deadtime}}\right| + w_{rangeability}\left|\frac{V_{rangeability,j}}{N_{rangeability}}\right| \qquad [11\text{-}1]$$

Using $w_{integrator} = 3$; $w_{deadtime} = 1$; $w_{rangeability} = 0.4$ (the rationale behind the selection of their sizes have been discussed in Section 11.2.2), we obtain the following overall performance indexes for all operating modes:

Performance Indexes of Various Inputs for the control of Reactor Level

Manipulations	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	67.13	127.34	infinity	86.05	131.51	infinity
Product	178910.6	40888.21	39663.19	33908.83	24499.87	57049.53
Steam	630.26	infinity	infinity	892.91	651.58	infinity
Condenser CW	**48.64**	**48.35**	infinity	**36.19**	**48.79**	infinity
Recycle	209.74	213.22	**54.93**	206.34	211.62	**44.48**
Separator Bot	82.48	64.50	**53.92**	57.57	61.33	**46.57**

For modes 1, 2, 4 and 5, condenser cooling water (CW_2) is the best manipulated variable because it has the smallest performance index, indicating that deviation in the reactor level can be quickly eliminated. At modes 3 and 6, condenser cooling water is at saturation so recycle flow or separator bottom flow become the best choices at those two operating modes. When condenser cooling water is adjusted to control reactor level, the amount of materials that are being recycled back to the reactor is essentially controlled by altering the phase-equilibrium in the flash. Thus, both the condenser cooling water and recycle flow function in very much the same way. The reactor level control policy uses condenser cooling water for the maintenance of reactor level at operating modes 1, 2, 4 and 5 and recycle flow for the maintenance of reactor level at operating modes 3 and 6. The two control strategies are like mirrors to one another.

C.3: Material and Energy Balances

Level 1: Input-Output Level

The process presentation corresponding to Level 1 is shown in Figure 11-2. Reactions occurring in this process are:

(R1) A (g) + C (g) + D (g) $\rightarrow$ G (l)
(R2) A (g) + C (g) + E (g) $\rightarrow$ H (l)
(R3) A (g) + E (g) $\rightarrow$ F (l)
(R4) 3 D (g) $\rightarrow$ 2 F (l)

In the balance equations below, F_i refer to the flow rate of stream i (where the indexes correspond to the numbering system used in Figure 10-2), $x_{i,j}$ refer to the mole fraction of component j in stream i, r_j refer to the rate of accumulation of component of j in the system.

Material Balance of A

(Rate of A entering the plant) + (rate of A being generated) = (rate of unreacted A leaving)
+ (rate of A consumed in R1) + (rate of A consumed in R2) + (rate of A consumed in R3)

$$(F_1x_{1,A} + F_4x_{4,A}) + (0) = (F_9x_{9,A} + F_{11}x_{11,A}) + (F_9x_{9,G} + F_{11}x_{11,G}) + (F_9x_{9,H} + F_{11}x_{11,H}) + (F_9x_{9,F} + F_{11}x_{11,F} - F_3x_{3,F} - F_{F\ formed\ in\ R4})$$

The rate at which F is being formed in R4 can be obtained by writing material balance of D around the system:

(Rate of D entering the plant) + (rate of D being generated) = (rate of unreacted D leaving)
+ (rate of D consumed in R1) + (rate of D consumed in R4)

$$(F_2x_{2,D}) + (0) = (F_9x_{9,D} + F_{11}x_{11,D}) + (F_9x_{9,G} + F_{11}x_{11,G}) + 3/2\,(F_{F\ formed\ in\ R4})$$

Then, the material balance of A becomes:

$$F_1x_{1,A} + F_4x_{4,A} = F_9x_{9,A} + F_{11}x_{11,A} + F_9x_{9,G} + F_{11}x_{11,G} + F_9x_{9,H} + F_{11}x_{11,H} + F_9x_{9,F} + F_{11}x_{11,F} - F_3x_{3,F} - 2/3\,F_2x_{2,D} + 2/3\,(F_9x_{9,D} + F_{11}x_{11,D}) + 2/3\,(F_9x_{9,G} + F_{11}x_{11,G})$$

Or,

$$r_A = F_1x_{1,A} + F_4x_{4,A} - F_9x_{9,A} - F_{11}x_{11,A} - F_9x_{9,G} - F_{11}x_{11,G} - F_9x_{9,H} - F_{11}x_{11,H} - F_9x_{9,F} - F_{11}x_{11,F} + F_3x_{3,F} + 2/3\,F_2x_{2,D} - 2/3\,(F_9x_{9,D} + F_{11}x_{11,D}) - 2/3\,(F_9x_{9,G} + F_{11}x_{11,G})$$

Material Balance of C

(Rate of C entering the plant) + (rate of C being generated) = (rate of unreacted C leaving)
+ (rate of C consumed in R1) + (rate of C consumed in R2)

Then,

$$r_C = F_4x_{4,C} - F_9x_{9,C} - F_{11}x_{11,C} - F_9x_{9,G} - F_{11}x_{11,G} - F_9x_{9,H} - F_{11}x_{11,H}$$

Material Balance of E

(Rate of E entering the plant) = (rate of unreacted E leaving) + (rate of E consumed in R2) + (rate of E consumed in R3)

$$(F_3x_{3,E}) + (0) = (F_9x_{9,E} + F_{11}x_{11,E}) + (F_9x_{9,H} + F_{11}x_{11,H}) + (F_{F\,formed\,in\,R3})$$

The rate of F being formed from R3 can be obtained by writing material balance of F:

$$F_3x_{3,F} + F_{F\,formed\,in\,R3} + F_{F\,formed\,in\,R4} = F_9x_{9,F} + F_{11}x_{11,F}$$

Hence, the material balance of E is simply:

$$r_E = F_3x_{3,E} - F_9x_{9,E} - F_{11}x_{11,E} - F_9x_{9,H} - F_{11}x_{11,H} - F_9x_{9,F} - F_{11}x_{11,F} + F_3x_{3,F}$$
$$+ 2/3\,F_2x_{2,D} - 2/3\,(F_9x_{9,D} + F_{11}x_{11,D}) - 2/3\,(F_9x_{9,G} + F_{11}x_{11,G})$$

Material Balance of B

(Rate of B entering the plant) = (rate of unreacted B leaving)

So, $r_B = F_4x_{4,B} + F_1x_{1,B} + F_2x_{2,B} - F_9x_{9,B} - F_{11}x_{11,B}$

Energy Balance

Energy balances will be written in terms of the stream enthalpies and heat:

$$e = H_1 + H_2 + H_3 + H_4 - H_9 - H_{11} + Q$$

Level 2: Generalized Reaction-Separation System

The following material and energy balance model correspond to the process representation shown in Figure 11-5. For brevity, we will use $F_{i,j}$ to represent $F_ix_{i,j}$.

Material Balance of A

Material balance of A corresponding to sub-block *a*:

$$r_{A\text{-}(a)} = F_1x_{1,A} + F_3x_{3,F} + 2/3\,F_2x_{2,D} + F_{8,A} + F_{8,F} + F_{8,G} + F_{8,H} + 2/3\,F_{8,D} + 2/3\,F_{8,G}$$
$$+ F_{5,A} + F_{5,F} + F_{5,G} + F_{5,H} + 2/3\,F_{5,D} + 2/3\,F_{5,G} - F_{7,A} - F_{7,F} - F_{7,G} - F_{7,H} - 2/3\,F_{7,D} - 2/3\,F_{7,G}$$

Material balance of A corresponding to sub-block *b*:

$$r_{A\text{-}(b)} = F_4x_{4,A} + F_{7,A} + F_{7,F} + F_{7,G} + F_{7,H} + 2/3\,F_{7,D} + 2/3\,F_{7,G} - F_{5,A} - F_{5,F} - F_{5,G} - F_{5,H} - 2/3\,F_{5,D} - 2/3\,F_{5,G}$$
$$- F_{12,A} - F_{12,F} - F_{12,G} - F_{12,H} - 2/3\,F_{12,D} - 2/3\,F_{12,G} - F_{11,A} - F_{11,F} - F_{11,G} - F_{11,H} - 2/3\,F_{11,D} - 2/3\,F_{11,G}$$

Material balance of A corresponding to sub-block *b*:

$$r_{A\text{-}(c)} = F_{12,A} + F_{12,F} + F_{12,G} + F_{12,H} + 2/3\,F_{12,D} + 2/3\,F_{12,G} - F_{8,A} - F_{8,F} - F_{8,G} - F_{8,H} - 2/3\,F_{8,D} - 2/3\,F_{8,G}$$
$$- F_{9,A} - F_{9,F} - F_{9,G} - F_{9,H} - 2/3\,F_{9,D} - 2/3\,F_{9,G}$$

Note that $r_{A\text{-}(a)} + r_{A\text{-}(b)} + r_{A\text{-}(c)} = r_A$.

Material Balance of C

Material balance of C corresponding to sub-block *a*:

$$r_{C\text{-}(a)} = F_{8,G} + F_{8,H} + F_{8,C} + F_{5,G} + F_{5,H} + F_{5,C} - F_{7,G} - F_{7,H} - F_{7,C}$$

Material balance of C corresponding to sub-block *b*:

$$r_{C\text{-}(b)} = F_{7,G} + F_{7,H} + F_{7,C} + F_4x_{4,C} - F_{11,G} - F_{11,H} - F_{11,C} - F_{5,G} - F_{5,H} - F_{5,C} - F_{12,G} - F_{12,H} - F_{12,C}$$

Material balance of C corresponding to sub-block *c*:

$$r_{C\text{-}(c)} = F_{12,G} + F_{12,H} + F_{12,C} - F_{9,G} - F_{9,H} - F_{9,C} - F_{8,G} - F_{8,H} - F_{8,C}$$

Again, $r_{C\text{-}(a)} + r_{C\text{-}(b)} + r_{C\text{-}(c)} = r_C$.

Material Balance of E

Material balance of E corresponding to sub-block *a*:

$$r_{E\text{-}(a)} = F_3x_{3,E} + 2/3\ F_2x_{2,D} + F_{8,E} + F_{8,F} + F_{8,H} + 2/3\ F_{8,D} + 2/3\ F_{8,G} + F_{5,E} + F_{5,F} + F_{5,H} \\ +2/3\ F_{5,D} + 2/3\ F_{5,G} - F_{7,E} - F_{7,F} - F_{7,H} - 2/3\ F_{7,D} - 2/3\ F_{7,G}$$

Material balance of E corresponding to sub-block *b*:

$$r_{E\text{-}(b)} = F_{7,E} + F_{7,F} + F_{7,H} + 2/3\ F_{7,D} + 2/3\ F_{7,G} - F_{5,E} - F_{5,F} - F_{5,H} - 2/3\ F_{5,D} - 2/3\ F_{5,G} \\ - F_{12,E} - F_{12,F} - F_{12,H} - 2/3\ F_{12,D} - 2/3\ F_{12,G} - F_{11}x_{11,E} - F_{11}x_{11,H} - F_{11}x_{11,F} - 2/3\ F_{11}x_{11,D} - 2/3\ F_{11}x_{11,G}$$

Material balance of E corresponding to sub-block *c*:

$$r_{E\text{-}(c)} = F_{12,E} + F_{12,F} + F_{12,H} + 2/3\ F_{12,D} + 2/3\ F_{12,G} - F_{8,E} - F_{8,F} - F_{8,H} - 2/3\ F_{8,D} - 2/3\ F_{8,G} \\ - F_{9,E} - F_{9,F} - F_{9,H} - 2/3\ F_{9,D} - 2/3\ F_{9,G}$$

Again, $r_{E\text{-}(a)} + r_{E\text{-}(b)} + r_{E\text{-}(c)} = r_E$.

Material Balance of B

Material balance of B corresponding to sub-block *a*:

$$r_{B\text{-}(a)} = F_{1,B} + F_{2,B} + F_{5,B} + F_{8,B} - F_{7,B}$$

Material balance of B corresponding to sub-block *b*:

$$r_{B\text{-}(b)} = F_{4,B} + F_{7,B} - F_{5,B} - F_{12,B} - F_{11,B}$$

Material balance of B corresponding to sub-block *c*:

$$r_{B\text{-}(c)} = F_{12,B} - F_{8,B} - F_{9,B}$$

Again, $r_{B\text{-}(a)} + r_{B\text{-}(b)} + r_{B\text{-}(c)} = r_E$.

Energy Balance Model

The energy balances can be written as:

$$e_a = H_1 + H_2 + H_3 + H_8 + H_5 - H_7 + Q_a$$

$$e_b = H_4 + H_7 - H_{12} - H_5 - H_{11} + Q_b$$

$$e_c = H_{12} - H_8 - H_9$$

Note that $e_a + e_b + e_c = e$.

Level 3: Detailed Reaction-Separation System

At this level, we are required to expand the material and energy balance equations for sub-system a at Level 2 into systems d and e at this level. The material and energy balances for sub-system b do not need to be refined. The following material and energy balance model correspond to the process representation shown in Figure 10-9. Since sub-system d is a self-regulating unit, we will only show the material and energy balance equations for sub-system e.

Material Balance of A

$$r_{A\text{-}(e)} = F_{6,A} + F_{6,F} + F_{6,G} + F_{6,H} + 2/3\ F_{6,D} + 2/3\ F_{6,G} - F_{7,A} - F_{7,F} - F_{7,G} - F_{7,H} - 2/3\ F_{7,D} - 2/3\ F_{7,G}$$

Material Balance of C

$$r_{C\text{-}(e)} = F_{6,C} F_{6,G} + F_{6,H} - F_{7,C} - F_{7,G} - F_{7,H}$$

Material Balance of E

$$r_{E\text{-}(e)} = F_{6,E} + F_{6,F} + F_{6,H} + 2/3\ F_{6,D} + 2/3\ F_{6,G} - F_{7,E} - F_{7,F} - F_{7,H} - 2/3\ F_{7,D} - 2/3\ F_{7,G}$$

Material Balance of B

$$r_{B\text{-}(e)} = F_{6,B} - F_{7,B}$$

Energy Balance

$$e_e = H_6 - H_7 + Q_e$$

C.4 Open-Loop gains

Open-loop Gains of r_C at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	3.47	3.47	3.47	3.47	3.47	3.47
F_3	0	0	0	0	0	0
F_2	0	0	0	0	0	0
$F_{9,A}$	0	0	0	0	0	0
$F_{9,B}$	0	0	0	0	0	0
$F_{9,C}$	-4.79E-02	-5.32E-02	-3.77E-02	-6.64E-02	-5.29E-02	-4.05E-02
$F_{9,D}$	0	0	0	0	0	0
$F_{9,E}$	0	0	0	0	0	0
$F_{9,F}$	0	0	0	0	0	0
$F_{9,G}$	-2.27E-02	-4.80E-03	-3.84E-02	-1.63E-02	-4.59E-03	-3.63E-02
$F_{9,H}$	-1.18E-02	-2.10E-02	-2.04E-03	-7.70E-03	-2.01E-02	-1.91E-03

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	-1.13E-01	-4.58E-02	-5.45E-02	-4.45E-02	-4.57E-02	-4.52E-02
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	-2.41	-0.53	-4.09	-2.38	-0.53	-4.08
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37

Open-loop Gains of r_A at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0.45	0.45	0.45	0.45	0.45	0.45
F_4	3.30	3.30	3.30	3.30	3.30	3.30
F_3	1.82E-04	1.81E-04	1.82E-04	1.81E-04	1.82E-04	1.82E-04
F_2	1.21	1.21	1.21	1.21	1.21	1.21
$F_{9,A}$	-1.20E-01	-1.33E-01	-1.14E-01	-1.73E-01	-1.34E-01	-1.19E-01
$F_{9,B}$	0	0	0	0	0	0
$F_{9,C}$	0	0	0	0	0	0
$F_{9,D}$	-2.19E-03	-3.15E-04	-5.94E-03	-1.92E-03	-3.16E-04	-5.78E-03
$F_{9,E}$	0	0	0	0	0	0
$F_{9,F}$	-1.97E-02	-2.68E-02	-7.43E-03	-2.42E-02	-2.71E-02	-7.92E-03
$F_{9,G}$	-3.78E-02	-8.00E-03	-6.40E-02	-2.72E-02	-7.65E-03	-6.06E-02
$F_{9,H}$	-1.18E-02	-2.10E-02	-2.04E-03	-7.70E-03	-2.01E-02	-1.91E-03

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	-8.85E-02	-2.17E-02	-2.15E-02	-2.67E-02	-2.72E-02	-2.15E-02
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	-3.03E-04	-3.03E-05	-9.09E-04	-5.94E-04	-3.02E-05	-9.07E-04
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	-8.62E-03	-1.32E-02	-3.18E-03	-1.96E-02	-1.45E-02	-3.63E-03
$F_{11,G}$	-4.01	-0.88	-6.82	-3.96	-0.88	-6.80
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37

Open-loop Gains of r_E at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	0	0	0	0	0	0
F_3	1.82	1.81	1.82	1.82	1.82	1.82
F_2	1.21	1.21	1.21	1.21	1.21	1.21
$F_{9,A}$	0	0	0	0	0	0
$F_{9,B}$	0	0	0	0	0	0
$F_{9,C}$	0	0	0	0	0	0
$F_{9,D}$	-2.19E-03	-3.15E-04	-5.94E-03	-1.92E-03	-3.16E-04	-5.78E-03
$F_{9,E}$	-5.92E-02	-8.13E-02	-1.61E-02	-6.52E-02	-8.35E-02	-1.66E-02
$F_{9,F}$	-1.97E-02	-2.68E-02	-7.43E-03	-2.42E-02	-2.71E-02	-7.92E-03
$F_{9,G}$	-1.51E-02	-3.20E-03	-2.56E-02	-1.09E-02	-3.06E-03	-2.42E-02
$F_{9,H}$	-1.18E-02	-2.10E-02	-2.04E-03	-7.70E-03	-2.01E-02	-1.91E-03

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	-3.03E-04	-3.03E-05	-9.09E-04	-5.94E-04	-3.02E-05	-9.07E-04
$F_{11,E}$	-2.72E-02	-4.18E-02	-7.27E-03	-5.39E-02	-4.58E-02	-8.16E-03
$F_{11,F}$	-8.62E-03	-1.32E-02	-3.18E-03	-1.96E-02	-1.45E-02	-3.63E-03
$F_{11,G}$	-1.60	-0.35	-2.73	-1.58	-0.35	-2.72
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37

Open-loop Gains of r_B at the input-output level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	4.55E-05	4.54E-05	4.54E-05	4.54E-05	4.54E-05	4.54E-05
F_4	3.32E-02	3.40E-02	3.40E-02	3.40E-02	3.40E-02	3.40E-02
F_3	0	0	0	0	0	0
F_2	1.82E-04	2.33E-04	1.82E-04	1.82E-04	1.82E-04	1.82E-04
$F_{9,A}$	0	0	0	0	0	0
$F_{9,B}$	-8.05E-02	-4.28E-02	-1.84E-01	-6.73E-02	-4.18E-02	-1.84E-01
$F_{9,C}$	0	0	0	0	0	0
$F_{9,D}$	0	0	0	0	0	0
$F_{9,E}$	0	0	0	0	0	0
$F_{9,F}$	0	0	0	0	0	0
$F_{9,G}$	0	0	0	0	0	0
$F_{9,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	-4.54E-07	-2.27E-02	-4.54E-03	-3.91E-04	-2.27E-03	-4.03E-04
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{C\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	0	0	0	0	0	0
F_3	0	0	0	0	0	0
F_2	0	0	0	0	0	0
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	3.39	3.44	3.44	3.44	3.45	3.48
$F_{5,D}$	0	0	0	0	0	0
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0	0	0	0	0	0
$F_{5,G}$	0.21	0.03	0.25	0.09	0.03	0.28
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	-2.92	-3.26	-3.82	-2.98	-3.20	-3.28
$F_{7,D}$	0	0	0	0	0	0
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	0	0	0	0	0	0
$F_{7,G}$	-3.29	-0.67	-12.01	-3.40	-0.66	-10.20
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	0	0	0	0	0	0
$F_{8,B}$	0	0	0	0	0	0
$F_{8,C}$	1.93	2.09	3.62	2.07	2.05	2.94
$F_{8,D}$	0	0	0	0	0	0
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0	0	0	0	0	0
$F_{8,G}$	0.90	0.19	3.69	0.51	0.18	2.64
$F_{8,H}$	0.47	0.83	0.20	0.24	0.78	0.14
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{C\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	3.47	3.47	3.47	3.47	3.47	3.47
F_3	0	0	0	0	0	0
F_2	0	0	0	0	0	0
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	-0.11	-0.05	-0.05	-0.04	-0.05	-0.05
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	-2.41	-0.53	-4.09	-2.38	-0.53	-4.08
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	-3.39	-3.44	-3.44	-3.44	-3.45	-3.48
$F_{5,D}$	0	0	0	0	0	0
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0	0	0	0	0	0
$F_{5,G}$	-0.21	-0.03	-0.25	-0.09	-0.03	-0.28
$F_{5,H}$	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	2.92	3.26	3.82	2.98	3.20	3.28
$F_{7,D}$	0	0	0	0	0	0
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	0	0	0	0	0	0
$F_{7,G}$	3.29	0.67	12.01	3.40	0.66	10.20
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	0	0	0	0	0	0
$F_{8,B}$	0	0	0	0	0	0
$F_{8,C}$	0	0	0	0	0	0
$F_{8,D}$	0	0	0	0	0	0
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0	0	0	0	0	0
$F_{8,G}$	0	0	0	0	0	0
$F_{8,H}$	0	0	0	0	0	0
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	-1.95	-2.14	-3.66	-2.13	-2.10	-2.98
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	-0.92	-0.19	-3.73	-0.52	-0.18	-2.68
$F_{12,H}$	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14

Open-loop Gains of $r_{A\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0.45	0.45	0.45	0.45	0.45	0.45
F_4	0	0	0	0	0	0
F_3	1.82 E-04	1.81 E-04	1.82 E-04	1.81 E-04	1.82 E-04	1.82 E-04
F_2	1.21	1.21	1.21	1.21	1.21	1.21
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	3.24	3.29	3.29	3.28	3.28	3.42
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	3.50 E-03	0.00 E+00	9.19 E-03	2.63 E-03	8.43 E-05	1.40 E-02
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	1.32 E-01	1.95 E-01	4.86 E-02	1.91 E-01	2.02 E-01	6.23 E-02
$F_{5,G}$	0.35	0.05	0.41	0.15	0.04	0.47
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01
$F_{7,A}$	-7.32	-8.16	-11.49	-7.78	-8.06	-9.61
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	-1.37 E-01	-1.93 E-02	-6.23 E-01	-9.04 E-02	-1.91 E-02	-4.86 E-01
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76
$F_{7,G}$	-5.49	-1.12	-20.02	-5.66	-1.11	-17.00
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	4.78	5.24	10.93	5.40	5.18	8.63
$F_{8,B}$	0	0	0	0	0	0
$F_{8,C}$	0	0	0	0	0	0
$F_{8,D}$	8.70 E-02	1.24 E-02	5.70 E-01	5.97 E-02	1.22 E-02	4.20 E-01
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0.78	1.05	0.71	0.75	1.05	0.58
$F_{8,G}$	1.50	0.31	6.15	0.85	0.30	4.40
$F_{8,H}$	0.47	0.83	0.20	0.24	0.78	0.14
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{A\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0	F_{5A}	-3.24	-3.29	-3.29	-3.28	-3.28	-3.42	F_{8A}	0	0	0	0	0	0
F_4	3.30	3.30	3.30	3.30	3.30	3.30	F_{5B}	0	0	0	0	0	0	F_{8B}	0	0	0	0	0	0
F_3	0	0	0	0	0	0	F_{5C}	0	0	0	0	0	0	F_{8C}	0	0	0	0	0	0
F_2	0	0	0	0	0	0	F_{5D}	-3.50 E-03	0.00 E+00	-9.19 E-03	-2.63 E-03	-8.43 E-05	-1.40 E-02	F_{8D}	0	0	0	0	0	0
F_{11A}	-0.09	-0.02	-0.02	-0.03	-0.03	-0.02	F_{5E}	0	0	0	0	0	0	F_{8E}	0	0	0	0	0	0
F_{11B}	0	0	0	0	0	0	F_{5F}	-0.13	-0.19	-0.05	-0.19	-0.20	-0.06	F_{8F}	0	0	0	0	0	0
F_{11C}	0	0	0	0	0	0	F_{5G}	-0.35	-0.05	-0.41	-0.15	-0.04	-0.47	F_{8G}	0	0	0	0	0	0
F_{11D}	-3.03 E-04	-3.03 E-05	-9.09 E-04	-5.94 E-04	-3.02 E-05	-9.07 E-04	F_{5H}	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01	F_{8H}	0	0	0	0	0	0
F_{11E}	0	0	0	0	0	0	F_{7A}	7.32	8.16	11.49	7.78	8.06	9.61	F_{12A}	-4.90	-5.37	-11.05	-5.57	-5.31	-8.75
F_{11F}	-8.62 E-03	-1.32 E-02	-3.18 E-03	-1.96 E-02	-1.45 E-02	-3.63 E-03	F_{7B}	0	0	0	0	0	0	F_{12B}	0	0	0	0	0	0
F_{11G}	-4.01	-0.88	-6.82	-3.96	-0.88	-6.80	F_{7C}	0	0	0	0	0	0	F_{12C}	0	0	0	0	0	0
F_{11H}	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37	F_{7D}	0.14	0.02	0.62	0.09	0.02	0.49	F_{12D}	-0.09	-0.01	-0.58	-0.06	-0.01	-0.43
							F_{7E}	0	0	0	0	0	0	F_{12E}	0	0	0	0	0	0
							F_{7F}	1.33	1.82	0.87	1.37	1.83	0.76	F_{12F}	-0.80	-1.08	-0.72	-0.78	-1.08	-0.58
							F_{7G}	5.49	1.12	20.02	5.66	1.11	17.00	F_{12G}	-1.54	-0.32	-6.21	-0.87	-0.30	-4.46
							F_{7H}	2.18	3.99	0.92	2.48	3.99	0.79	F_{12H}	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14

Open-loop Gains of $r_{E\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0	F_{5A}	0	0	0	0	0	0	F_{8A}	0	0	0	0	0	0
F_4	0	0	0	0	0	0	F_{5B}	0	0	0	0	0	0	F_{8B}	0	0	0	0	0	0
F_3	1.82	1.81	1.82	1.82	1.82	1.82	F_{5C}	0	0	0	0	0	0	F_{8C}	0	0	0	0	0	0
F_2	1.21	1.21	1.21	1.21	1.21	1.21	F_{5D}	3.50 E-03	0.00 E+00	9.19 E-03	2.63 E-03	8.43 E-05	1.40 E-02	F_{8D}	8.70 E-02	1.24 E-02	5.70 E-01	5.97 L-02	1.22 E-02	4.20 E-01
F_{11A}	0	0	0	0	0	0	F_{5E}	0.40	0.58	0.11	0.52	0.62	0.13	F_{8E}	2.35	3.20	1.55	2.03	3.23	1.21
F_{11B}	0	0	0	0	0	0	F_{5F}	0.13	0.19	0.05	0.19	0.20	0.06	F_{8F}	0.78	1.05	0.71	0.75	1.05	0.58
F_{11C}	0	0	0	0	0	0	F_{5G}	0.14	0.02	0.16	0.06	0.02	0.19	F_{8G}	0.60	0.13	2.46	0.34	0.12	1.76
F_{11D}	0	0	0	0	0	0	F_{5H}	0.11	0.12	0.01	0.04	0.11	0.01	F_{8H}	0.47	0.83	0.20	0.24	0.78	0.14
F_{11E}	0	0	0	0	0	0	F_{7A}	0	0	0	0	0	0	F_{12A}	0	0	0	0	0	0
F_{11F}	0	0	0	0	0	0	F_{7B}	0	0	0	0	0	0	F_{12B}	0	0	0	0	0	0
F_{11G}	0	0	0	0	0	0	F_{7C}	0	0	0	0	0	0	F_{12C}	0	0	0	0	0	0
F_{11H}	0	0	0	0	0	0	F_{7D}	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49	F_{12D}	0	0	0	0	0	0
							F_{7E}	-3.99	-5.52	-1.89	-3.70	-5.62	-1.60	F_{12E}	0	0	0	0	0	0
							F_{7F}	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76	F_{12F}	0	0	0	0	0	0
							F_{7G}	-2.19	-0.45	-8.01	-2.26	-0.44	-6.80	F_{12G}	0	0	0	0	0	0
							F_{7H}	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79	F_{12H}	0	0	0	0	0	0

Open-loop Gains of $r_{E\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	0	0	0	0	0	0
F_3	0	0	0	0	0	0
F_2	0	0	0	0	0	0
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	-3.03 E-04	-3.03 E-05	-9.09 E-04	-5.94 E-04	-3.02 E-05	-9.07 E-04
$F_{11,E}$	-2.72 E-02	-4.18 E-02	-7.27 E-03	-5.39 E-02	-4.58 E-02	-8.16 E-03
$F_{11,F}$	-8.62 E-03	-1.32 E-02	-3.18 E-03	-1.96 E-02	-1.45 E-02	-3.63 E-03
$F_{11,G}$	-1.60	-0.35	-2.73	-1.58	-0.35	-2.72
$F_{11,H}$	-1.91	-3.89	-0.37	-1.94	-3.88	-0.37

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	-3.50 E-03	0.00 E+00	-9.19 E-03	-2.63 E-03	-8.43 E-05	-1.40 E-02
$F_{5,E}$	-0.40	-0.58	-0.11	-0.52	-0.62	-0.13
$F_{5,F}$	-0.13	-0.19	-0.05	-0.19	-0.20	-0.06
$F_{5,G}$	-0.14	-0.02	-0.16	-0.06	-0.02	-0.19
$F_{5,H}$	-0.11	-0.12	-0.01	-0.04	-0.11	-0.01
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	1.37 E-01	1.93 E-02	6.23 E-01	9.04 E-02	1.91 E-02	4.86 E-01
$F_{7,E}$	3.99	5.52	1.89	3.70	5.62	1.60
$F_{7,F}$	1.33	1.82	0.87	1.37	1.83	0.76
$F_{7,G}$	2.19	0.45	8.01	2.26	0.44	6.80
$F_{7,H}$	2.18	3.99	0.92	2.48	3.99	0.79

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	0	0	0	0	0	0
$F_{8,B}$	0	0	0	0	0	0
$F_{8,C}$	0	0	0	0	0	0
$F_{8,D}$	0	0	0	0	0	0
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0	0	0	0	0	0
$F_{8,G}$	0	0	0	0	0	0
$F_{8,H}$	0	0	0	0	0	0
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	-8.92 E-02	-1.27 E-02	-5.76 E-01	-6.17 E-02	-1.25 E-02	-4.26 E-01
$F_{12,E}$	-2.41	-3.28	-1.56	-2.10	-3.32	-1.22
$F_{12,F}$	-0.80	-1.08	-0.72	-0.78	-1.08	-0.58
$F_{12,G}$	-0.61	-0.13	-2.48	-0.35	-0.12	-1.79
$F_{12,H}$	-0.48	-0.85	-0.20	-0.25	-0.80	-0.14

Open-loop Gains of $r_{B\text{-}(a)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	4.55 E-05	4.54 E-05	4.54 E-05	4.54 E-05	4.54 E-05	4.54 E-05
F_4	0	0	0	0	0	0
F_3	0	0	0	0	0	0
F_2	1.82 E-04	2.33 E-04	1.82 E-04	1.82 E-04	1.82 E-04	1.82 E-04
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	3.67 E-02	3.13 E-02	3.14 E-02	3.40 E-02	3.31 E-02	2.41 E-01
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	0	0	0	0	0	0
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0	0	0	0	0	0
$F_{5,G}$	0	0	0	0	0	0
$F_{5,H}$	0	0	0	0	0	0
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	-4.90	-2.63	-18.59	-3.02	-2.52	-14.93
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	0	0	0	0	0	0
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	0	0	0	0	0	0
$F_{7,G}$	0	0	0	0	0	0
$F_{7,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	0	0	0	0	0	0
$F_{8,B}$	3.17	1.68	17.69	2.10	1.62	13.39
$F_{8,C}$	0	0	0	0	0	0
$F_{8,D}$	0	0	0	0	0	0
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0	0	0	0	0	0
$F_{8,G}$	0	0	0	0	0	0
$F_{8,H}$	0	0	0	0	0	0
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{B\text{-}(b)}$ at the Generalized Reaction-Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_1	0	0	0	0	0	0
F_4	3.32 E-02	3.40 E-02	3.40 E-02	3.40 E-02	3.40 E-02	3.40 E-02
F_3	0	0	0	0	0	0
F_2	0	0	0	0	0	0
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	-4.54 E-07	-2.27 E-02	-4.54 E-03	-3.91 E-04	-2.27 E-03	-4.03 E-04
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	-3.67 E-02	-3.13 E-02	-3.14 E-02	-3.40 E-02	-3.31 E-02	-2.41 E-01
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	0	0	0	0	0	0
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0	0	0	0	0	0
$F_{5,G}$	0	0	0	0	0	0
$F_{5,H}$	0	0	0	0	0	0
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	4.90	2.63	18.59	3.02	2.52	14.93
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	0	0	0	0	0	0
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	0	0	0	0	0	0
$F_{7,G}$	0	0	0	0	0	0
$F_{7,H}$	0	0	0	0	0	0

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{8,A}$	0	0	0	0	0	0
$F_{8,B}$	0	0	0	0	0	0
$F_{8,C}$	0	0	0	0	0	0
$F_{8,D}$	0	0	0	0	0	0
$F_{8,E}$	0	0	0	0	0	0
$F_{8,F}$	0	0	0	0	0	0
$F_{8,G}$	0	0	0	0	0	0
$F_{8,H}$	0	0	0	0	0	0
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	-3.28	-1.73	-17.87	-2.16	-1.66	-13.58
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{C\text{-}(e)}$ at the Detailed Reaction - Generalized Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_4	0	0	0	0	0	0
$F_{6,A}$	0	0	0	0	0	0
$F_{6,B}$	0	0	0	0	0	0
$F_{6,C}$	4.90	5.06	9.08	5.56	11.59	7.88
$F_{7,D}$	0	0	0	0	0	0
$F_{6,E}$	0	0	0	0	0	0
$F_{6,F}$	0	0	0	0	0	0
$F_{6,G}$	1.26	0.26	3.36	0.61	0.08	2.55
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	3.39	3.44	3.44	3.44	3.45	3.48
$F_{5,D}$	0	0	0	0	0	0
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0	0	0	0	0	0
$F_{5,G}$	0.21	0.03	0.25	0.09	0.03	0.28
$F_{5,H}$	1.11 E-01	1.23 E-01	1.31 E-02	4.29 E-02	1.10 E-01	1.48 E-02

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	-2.92	-3.26	-3.82	-2.98	-3.20	-3.28
$F_{7,D}$	0	0	0	0	0	0
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	0	0	0	0	0	0
$F_{7,G}$	-3.29	-0.67	-12.01	-3.40	-0.66	-10.20
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{A\text{-}(e)}$ at the Detailed Reaction - Generalized Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_4	0	0	0	0	0	0
$F_{6,A}$	8.41	9.07	14.88	9.05	11.03	12.56
$F_{6,B}$	0	0	0	0	0	0
$F_{6,C}$	0	0	0	0	0	0
$F_{7,D}$	1.05	0.21	4.27	1.32	0.00	3.69
$F_{6,E}$	0	0	0	0	0	0
$F_{6,F}$	1.06	1.46	0.65	0.96	0.68	0.56
$F_{6,G}$	2.10	0.43	5.60	1.02	0.14	4.25
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0
$F_{5,A}$	3.24	3.29	3.29	3.28	3.28	3.42
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	3.50E-03	0.00E+00	9.19E-03	2.63E-03	8.43E-05	1.40E-02
$F_{5,E}$	0	0	0	0	0	0
$F_{5,F}$	0.13	0.19	0.05	0.19	0.20	0.06
$F_{5,G}$	0.35	0.05	0.41	0.15	0.04	0.47
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{7,A}$	-7.32	-8.16	-11.49	-7.78	-8.06	-9.61
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49
$F_{7,E}$	0	0	0	0	0	0
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76
$F_{7,G}$	-5.49	-1.12	-20.02	-5.66	-1.11	-17.00
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{E\text{-}(e)}$ at the Detailed Reaction - Generalized Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_4	0	0	0	0	0	0
$F_{6,A}$	0	0	0	0	0	0
$F_{6,B}$	0	0	0	0	0	0
$F_{6,C}$	0	0	0	0	0	0
$F_{7,D}$	1.05	0.21	4.27	1.32	0.00	3.69
$F_{6,E}$	4.36	6.64	1.95	4.23	2.07	1.64
$F_{6,F}$	1.06	1.46	0.65	0.96	0.68	0.56
$F_{6,G}$	0.84	0.17	2.24	0.41	0.06	1.70
$F_{6,H}$	0.66	1.12	0.18	0.29	0.37	0.13

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{11,A}$	0	0	0	0	0	0
$F_{11,B}$	0	0	0	0	0	0
$F_{11,C}$	0	0	0	0	0	0
$F_{11,D}$	0	0	0	0	0	0
$F_{11,E}$	0	0	0	0	0	0
$F_{11,F}$	0	0	0	0	0	0
$F_{11,G}$	0	0	0	0	0	0
$F_{11,H}$	0	0	0	0	0	0
$F_{5,A}$	0	0	0	0	0	0
$F_{5,B}$	0	0	0	0	0	0
$F_{5,C}$	0	0	0	0	0	0
$F_{5,D}$	3.50 E-03	0.00 E+00	9.19 E-03	2.63 E-03	8.43 E-05	1.40 E-02
$F_{5,E}$	0.40	0.58	0.11	0.52	0.62	0.13
$F_{5,F}$	0.13	0.19	0.05	0.19	0.20	0.06
$F_{5,G}$	0.14	0.02	0.16	0.06	0.02	0.19
$F_{5,H}$	0.11	0.12	0.01	0.04	0.11	0.01

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
$F_{7,A}$	0	0	0	0	0	0
$F_{7,B}$	0	0	0	0	0	0
$F_{7,C}$	0	0	0	0	0	0
$F_{7,D}$	-0.14	-0.02	-0.62	-0.09	-0.02	-0.49
$F_{7,E}$	-3.99	-5.52	-1.89	-3.70	-5.62	-1.60
$F_{7,F}$	-1.33	-1.82	-0.87	-1.37	-1.83	-0.76
$F_{7,G}$	-2.19	-0.45	-8.01	-2.26	-0.44	-6.80
$F_{7,H}$	-2.18	-3.99	-0.92	-2.48	-3.99	-0.79
$F_{12,A}$	0	0	0	0	0	0
$F_{12,B}$	0	0	0	0	0	0
$F_{12,C}$	0	0	0	0	0	0
$F_{12,D}$	0	0	0	0	0	0
$F_{12,E}$	0	0	0	0	0	0
$F_{12,F}$	0	0	0	0	0	0
$F_{12,G}$	0	0	0	0	0	0
$F_{12,H}$	0	0	0	0	0	0

Open-loop Gains of $r_{B\text{-}(e)}$ at the Detailed Reaction - Generalized Separation Level

Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6	Input	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
F_4	0	0	0	0	0	0	$F_{11,A}$	0	0	0	0	0	0	$F_{7,A}$	0	0	0	0	0	0
$F_{6,A}$	0	0	0	0	0	0	$F_{11,B}$	0	0	0	0	0	0	$F_{7,B}$	-4.90	-2.63	-18.59	-3.02	-2.52	-14.93
$F_{6,B}$	3.90	2.13	14.01	2.18	0.11	11.03	$F_{11,C}$	0	0	0	0	0	0	$F_{7,C}$	0	0	0	0	0	0
$F_{6,C}$	0	0	0	0	0	0	$F_{11,D}$	0	0	0	0	0	0	$F_{7,D}$	0	0	0	0	0	0
$F_{7,D}$	0	0	0	0	0	0	$F_{11,E}$	0	0	0	0	0	0	$F_{7,E}$	0	0	0	0	0	0
$F_{6,E}$	0	0	0	0	0	0	$F_{11,F}$	0	0	0	0	0	0	$F_{7,F}$	0	0	0	0	0	0
$F_{6,F}$	0	0	0	0	0	0	$F_{11,G}$	0	0	0	0	0	0	$F_{7,G}$	0	0	0	0	0	0
$F_{6,G}$	0	0	0	0	0	0	$F_{11,H}$	0	0	0	0	0	0	$F_{7,H}$	0	0	0	0	0	0
$F_{6,H}$	0	0	0	0	0	0	$F_{5,A}$	0	0	0	0	0	0	$F_{12,A}$	0	0	0	0	0	0
							$F_{5,B}$	3.67E-02	3.13E-02	3.14E-02	3.40E-02	3.31E-02	2.41E-01	$F_{12,B}$	0	0	0	0	0	0
							$F_{5,C}$	0	0	0	0	0	0	$F_{12,C}$	0	0	0	0	0	0
							$F_{5,D}$	0	0	0	0	0	0	$F_{12,D}$	0	0	0	0	0	0
							$F_{5,E}$	0	0	0	0	0	0	$F_{12,E}$	0	0	0	0	0	0
							$F_{5,F}$	0	0	0	0	0	0	$F_{12,F}$	0	0	0	0	0	0
							$F_{5,G}$	0	0	0	0	0	0	$F_{12,G}$	0	0	0	0	0	0
							$F_{5,H}$	0	0	0	0	0	0	$F_{12,H}$	0	0	0	0	0	0

C.5 Selection of Manipulated Variables for the Short-horizon control of Separator Level, Stripper Level and Reactor Pressure

Separation Level

The open-loop process models for the separator level by each of the available manipulated variables have been estimated through step tests and they are shown in the table below.

Open-loop Process Model - Separator Level

Manipulation	Deadtime	Integrator Gain					
	all modes	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	10 min	-0.23	-0.1141	0	0.0493	-0.109	0
Product	50 min	-0.0055	0.00066	0.0065	-0.0019	0.00106	-0.0081
Steam	60 min	0.76083	0.81624	0	0.1392	0.09884	0
Condenser CW	10 min	12.054	11.81	0	11.5	10.64	0
Recycle	30 min	0.058	0.141	-6.34	0.0406	0.16	-8.057
Separator Bot	0 min	-10.08	-10.8	-14.46	-8.4	-10.61	-15.74

For the purpose of our analysis, we must evaluate each of the process input under the condition that reactor level is being controlled by the previously selected variables (condenser cooling water at the base case, Modes 2, 4 and 5; recycle flow at Modes 3 and 6). The closed-loop integrator gains can be computed using the procedure described in Section 6.3.2. For the estimation of the deadtime under closed-loop control, consider the following pair of potential assignment:

$$\begin{array}{r c} & \begin{array}{cc} CW_2 & \quad F_{10} \end{array} \\ \begin{array}{r} \text{reactor level} \\ \text{separator level} \end{array} & \begin{pmatrix} \dfrac{-6.198e^{-8s}}{s} & \dfrac{2.26e^{-8s}}{s} \\ \dfrac{12.054e^{-10s}}{s} & \dfrac{-10.08}{s} \end{pmatrix} \end{array}$$

Let A be the process model between reactor level and CW_2, b be the process model between reactor level and F_{10}, c be the process model between separator level and CW_2 and d be the process model between separator level and F_{10}. Then, from Equation [6-27]. the closed-loop model of the separator level for a step change in F_{10} is simply $(d - cA^{-1}b)$, i.e. :

$$\frac{-10.08}{s} - \left(\frac{12.054e^{-10s}}{s} \cdot \frac{s}{-6.18e^{-8s}} \cdot \frac{2.26e^{-8s}}{s} \right)$$

The deadtime of the process model under closed-loop condition can be broken into two components: one from the open-loop model of the process (first term) and another from process interaction (second term). Thus, the effective deadtime of the closed-loop process is simply the smallest deadtime of the two. The deadtime due to interaction, the effective closed-loop deadtime and the closed-loop integrator gain for this output by each of the available inputs have been estimated below:

Separator Level : Deadtime (min) estimation

Manipulation	Base Case, Modes 2, 4, and 5			Modes 3 and 6		
	open-loop	from interaction	effective	open-loop	from interaction	effective
Purge	10 min	8 min	8 min	10 min	120 min	10 min
Product	50 min	40 min	40 min	50 min	600 min	50 min
Steam	60 min	30 min	30 min	60 min	450 min	60 min
Condenser CW	10 min	10 min	10 min	10 min	150 min	10 min
Recycle	30 min	2 min	2 min	30 min	30 min	30 min
Separator Bot	0 min	0 min	0 min	0 min	120 min	0 min

Closed-loop Process Model - Separator Level

Manipulation	Deadtime (min)		Integrator Gain					
	(1,2,4,5)	(3,6)	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	8	10	5.6045	2.5158	0	3.3769	2.3083	0
Product	40	50	-0.0038	-0.0068	-0.0008	-0.0092	0.0129	-0.0029
Steam	30	60	1.4648	1.4148	0	0.4942	0.731	0
Condenser CW	10	10	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	2	30	6.8649	6.3799	*assigned*	5.9773	6.3133	*assigned*
Separator Bot	0	0	-5.6847	-4.945	-7.2832	-2.9246	-4.6857	-6.9056

Using procedure similar to the one for reactor level (see Appendix D.2), the performance indexes of each of the possible pairing can be computed. The gross averages of the performance measures have been estimated to be:

Gross averages of performance measures	$\bar{\bar{V}}_i$
$\bar{\bar{V}}_{deadtime}$	18.88
$\bar{\bar{V}}_{reangeability}$	0.04022
$\bar{\bar{V}}_{integrator}$	0.272

The data for rangeability and integrator gain can be adjusted to the roughly the same order of magnitude as those for deadtime by multiplying the measures by an appropriately chosen normalization factor N_i :

$$N_i = \bar{\bar{V}}_i \,/\, \bar{\bar{V}}_{deadtime} \quad \text{for } i = \text{rangeability, integrator}$$

Using $w_{integrator} = 3$; $w_{deadtime} = 1$; $w_{rangeability} = 0.4$ (the rationale behind the selection of their sizes have been discussed in Section 11.2). The following overall performance indexes have been obtained for all operating modes:

Performance Indexes of Inputs for the control of Separator Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	52.51	95.16	*infinity*	73.63	102.36	*infinity*
Product	54941.25	30722.25	260816.5	22722.31	16215.49	71988.52
Steam	360.29	*infinity*	*infinity*	639.99	503.25	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	220.27	222.58	*assigned*	224.78	222.92	*assigned*
Separator Bot	**49.74**	**55.43**	**35.09**	**84.14**	**57.54**	**35.96**

Clearly, separator bottom flow (F_{10}) is the best choice. Not only does it give a small performance index, it can also be employed throughout the entire operating region.

Stripper Level

Next, we study the stripper level. The open-loop process model has been developed:

Open-loop process Model - Stripper Level

Manipulation	Deadtime all modes	Integrator Gain Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	60 min	-0.2621	-0.125	0	-0.3544	0.00149	0
Product	0 min	-11.12	-11.956	-10.31	-10.89	-11.945	-10.3
Steam	15 min	-0.16259	-0.17102	0	-0.2818	-0.197	0
Condenser CW	20 min	3.62	4.64354	0	0.5627	5.33	0
Recycle	55 min	-0.1566	-0.287	-2.336	-10.03	-0.308	-2.34
Separator Bot	0 min	9.5	20.46	12.38	34	5.57	11.65

The corresponding deadtimes due to interaction, the effective closed-loop deadtime and the closed-loop integrator gain for this output by each of the inputs are shown next:

Stripper Level : Deadtime (min) estimation

Manipulation	Base Case, Modes 2, 4, and 5			Modes 3 and 6		
	open-loop	from interaction	effective	open-loop	from interaction	effective
Purge	60 min	20 min	20 min	60 min	18.3 min	18.3 min
Product	0 min	100 min	0 min	0 min	91.7 min	0 min
Steam	15 min	120 min	15 min	15 min	110 min	15 min
Condenser CW	20 min	20 min	20 min	20 min	18.3 min	18.3 min
Recycle	55 min	60 min	55 min	55 min	55 min	55 min
Separator Bot	0 min	0 min	0 min	0 min	0 min	0 min

Closed-loop process Model - Stripper Level

Manipulation	Deadtime (min)		Integrator Gain					
	(1,2,4 ,5)	(3,6)	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	20	18.3	12.1573	12.4896	0	39.3769	5.4185	0
Product	0	0	-11.1267	-11.9902	-10.3144	-10.9987	-11.9155	-10.3044
Steam	15	15	2.8369	6.5765	0	5.5258	1.4515	0
Condenser CW	20	18.3	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	55	55	14.9539	31.5332	*assigned*	60.2983	14.2778	*assigned*
Separator Bot	0	0	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

The gross averages of performance measures have been estimated to be:

Gross averages of performance measures	$\bar{\bar{V}}_i$
$\bar{\bar{V}}_{deadtime}$	18.15
$\bar{\bar{V}}_{rangeability}$	0.04022
$\bar{\bar{V}}_{integrator}$	0.083

Hence, the data for rangeability and integrator gain can be adjusted to the roughly the same order of magnitude as those for deadtime by multiplying the measures by an appropriately chosen normalization factor N_i :

$$N_i = \bar{\bar{V}}_i / \bar{\bar{V}}_{deadtime} \quad \text{for } i = \text{rangeability, integrator}$$

Using $w_{integrator} = 3$; $w_{deadtime} = 1$; $w_{rangeability} = 0.4$ (the rationale behind the selection of their sizes have been discussed in Section 11.2), the following overall performance indexes for all operating modes have been obtained:

Performance Indexes of Inputs for the control of Stripper Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	81.19	76.82	*infinity*	40.43	145.41	*infinity*
Product	**63.09**	**59.17**	**68.45**	**66.98**	**59.35**	**68.01**
Steam	427.73	*infinity*	*infinity*	314.73	649.37	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	279.56	256.40	*assigned*	246.44	281.65	*assigned*
Separator Bot	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

The product stream (F_{11}) is clearly the best manipulated variable for this output.

Pressure Level

The open-loop process model for reactor pressure level is shown next.

Open-loop process Model - Pressure Level

Manipulation	Deadtime all modes	Integrator Gain Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	5 min	9.3	-1.38	-0.5	1.705	-0.87443	-0.2
Product	40 min	0.0064	-0.02146	-0.0076	-0.02432	0.00559	0.00408
Steam	80 min	2.2808	2.01693	2.15	1.5254	2.15625	2.1
Condenser CW	15 min	-26.34	-32.3567	0	-40.12	-30.54	0
Recycle	5 min	17.1352	18.24	10	19.5	18.7	11.176
Separator Bot	30 min	11.03	20.89	21.31	21.31	22.559	9.189

Again, we have estimated the effective deadtimes and closed-loop integrator gains:

Pressure Level : Deadtime (min) estimation

Manipulation	Base Case, Modes 2, 4, and 5			Modes 3 and 6		
	open-loop	from interaction	effective	open-loop	from interaction	effective
Purge	5 min	6.5 min	5 min	5 min	77 min	5 min
Product	40 min	40 min	40 min	40 min	40 min	40 min
Steam	80 min	0 min	0 min	80 min	0 min	0 min
Condenser CW	15 min	15 min	15 min	15 min	39 min	15 min
Recycle	5 min	0 min	0 min	5 min	5 min	5 min
Separator Bot	30 min	30 min	30 min	30 min	30 min	30 min

Closed-loop process Model - Pressure Level

Manipulation	Deadtime (min)		Integrator Gain					
	(1,2,4,5)	(3,6)	Base Case	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	5	5	-2.042	-6.1267	-0.5	-7.3751	-5.0826	-0.2
Product	40	40	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*
Steam	0	0	1.1102	1.7601	2.15	0.6572	1.2068	2.1
Condenser CW	15	15	*assigned*	*assigned*	0	*assigned*	*assigned*	0
Recycle	0	5	3.9848	7.3821	*assigned*	3.27	8.5063	*assigned*
Separator Bot	30	30	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

Below show the gross averages of performance measures used in our analysis for normalization purposes.

Gross averages of performance measures	$\bar{\bar{V}}_i$
$\bar{\bar{V}}_{deadtime}$	15.28
$\bar{\bar{V}}_{rangeability}$	0.04022
$\bar{\bar{V}}_{integrator}$	1.635

Hence, the data for rangeability and integrator gain can be adjusted to the roughly the same order of magnitude as those for deadtime by multiplying the measures by an appropriately chosen normalization factor N_i :

$$N_i = \bar{\bar{V}}_i / \bar{\bar{V}}_{deadtime} \quad \text{for } i = \text{rangeability, integrator}$$

Using $w_{integrator} = 3$; $w_{deadtime} = 1$; $w_{rangeability} = 0.4$ (the rationale behind the selection of their sizes have been discussed in Section 10.2), we obtain the following overall performance indexes for all operating mode:

Performance Indexes of Inputs for the control of Pressure Level

Manipulations	Base	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Purge	**24.62**	**13.00**	**77.04**	**11.92**	**13.74**	**159.39**
Product	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*
Steam	177.20	*infinity*	*infinity*	194.60	175.18	*infinity*
Condenser CW	*assigned*	*assigned*	*infinity*	*assigned*	*assigned*	*infinity*
Recycle	158.99	155.76	*assigned*	160.53	155.25	*assigned*
Separator Bot	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*	*assigned*

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