DYNAMIC MODELS FOR CONVECTIVE SYSTEMS

by

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ABSTRACT

Recent attempts to apply control theory to chemical processes have shown the need for suitable dynamical models of convective systems. In particular, no models exist for convective systems whose coefficients vary with distance, and many chemical processes which are operated as regulator systems can be approximately represented by this form.

Two models, the modified Galerkin method and the Campbell approximation, are developed, both of which can be used with variable-coefficient systems. The modified Galerkin method gives a model suitable for modal analysis while the Campbell approximation is suitable for most control applications except modal analysis. Modal analysis requires a dynamical model involving eigenfunctions and eigenvalues, and this restriction makes the modified Galerkin method less accurate than the Campbell approximation. The Campbell approximation has gains, zeros, and pure time delays, which depend on distance, and has poles which are independent of distance. The form of the approximation and the numerical values of the parameters can easily be obtained from the system equations.

These two methods give suitable dynamic models for a wide range of systems, and future work can be concentrated on the development of control philosophies for distributed systems.

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CHAPTER I

INTRODUCTION

A. PROBLEM STATEMENT

Recent attempts to apply control theory to chemical processes have shown that one of the main problems is to obtain a suitable model of the system dynamics. Two new simple models of convective systems are developed in this report: the modified Galerkin method and the Campbell approximation. Both of these models are in a form suitable for the application of control design techniques, but the application of such techniques will not be considered. In particular, models are derived which can handle non-linear convective processes for small perturbations about the steady state. Most existing models are only applicable to convective systems whose equations have constant coefficients.

The modified Galerkin method gives a dynamical model which is suitable for modal analysis, and the details are given in Chapter II. It does not give a good approximation to the time delays inherent in convective systems, and to obtain adequate results, some effective diffusion which is much larger than the physical diffusion must be introduced. A similar amount of effective diffusion is introduced by both lumping and the Taylor diffusion model, which are the only other dynamical models known to the author that are suitable for modal analysis. However, this effective diffusion does represent the overall dynamic behavior quite well at low frequencies. It appears that any dynamical model of a convective system suitable for modal analysis must have an effective diffusion; otherwise the high-frequency errors become unacceptable.

The model given by the Campbell approximation has gains, zeros, and pure time delays which depend on distance, and has poles which are independent of distance. This model is suitable for conventional control design techniques, is easy to determine and accurate, and is applicable to both variable and constant-coefficient systems. For all purposes in control design except for modal analysis, the Campbell approximation gives the best dynamical model for convective systems, the best of all the models considered in this report. The details are given in Chapter IV.

Before discussing the determination of the models, the terms convective system, modal analysis, and conventional control design techniques must be defined. The equations which represent a convective process are easily obtained in any chemical system from mass and energy balances. The usual assumption made is that the system is well mixed radially so that a set of partial differential equations in time and in one distance variable are obtained. Thus, a general convective system has the equations

$$-\underline{D}\frac{\partial^2 \underline{y}}{\partial x^2} + \underline{V}\frac{\partial \underline{y}}{\partial x} + \underline{C}\frac{\partial \underline{y}}{\partial t} + \underline{H}\,\underline{y} = 0 \qquad (1.1)$$

where $\underline{y}$ is a vector of the variables of the system, such as temperature or composition.

$\underline{D}$ is a matrix representing axial diffusion.
$\underline{V}$ is a matrix representing axial convection
$\underline{C}$ is a matrix representing capacity.
$\underline{H}$ is a matrix representing the transfer of energy or mass between various elements of $\underline{y}$.
x is the axial distance variable, $0 \leq x \leq 1$.
t is the time variable.

In general, all the matrices are functions of $\underline{y}$, x, t, and, from physical considerations, the matrices $\underline{D}$, $\underline{V}$, $\underline{C}$ are diagonal. Eq. 1.1 will be taken, in this work, as the definition of a general convective system. Chemical processes such as heat exchange, absorption, distillation, and some forms of chemical reaction can be represented by equations of the form of Eq. 1.1.

There are two fundamentally different approaches to control design for convective processes: transfer function analysis, and modal analysis. Both of these methods require simple dynamical models. Transfer function analysis requires a model similar to the forms used in lumped constant systems, while modal analysis requires an eigenvalue and eigenfunction model. Transfer function analysis involves determining the transfer function between each element of $\underline{y}$ at every value of x and for all the disturbances to the system. Then conventional control design techniques [38, 41]* are applied to produce the required system performance. For example, consider the simple case of heat flow in a fluid down an insulated pipe whose walls have negligible heat capacity. A heat balance gives the equation

$$cv\frac{\partial T}{\partial x} + c\frac{\partial T}{\partial t} = 0 \qquad (1.2)$$

where T is the temperature of the fluid.
v is the fluid velocity.
c is the fluid heat capacity.

Let q(t) be a disturbance in temperature at $x = 0$, the input to the system. Then the transfer function of the system is

$$\frac{T(x, s)}{q(s)} = e^{-vsx} \qquad (1.3)$$

where s is the Laplace transform variable with respect to time. If the required performance is to keep the temperature at $x = 1$ at a constant value, conventional control design techniques are used to determine how to vary the input temperature. This form of design has two main drawbacks; the system transfer functions must be evaluated, and by concentrating on the input and output of the system, the distributed nature of the process is ignored. But in systems in which it is impossible to measure or control anywhere except at the input or output of the system, the transfer function approach is perfectly satisfactory.

Modal analysis is an entirely different approach recently developed by Rosenbrock[46] for large interrelated structures and extended by Murray[40] to distributed systems. Modal analysis involves considering the total performance of a distributed system, not just the inputs and outputs. It is a genuine distributed control philosophy which considers the distributed nature of the process. In modal analysis the natural modes, or eigenfunctions, are determined together with their associated eigenvalues, or poles. Then a system of distributed control can

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[*] Superscripts refer to the references given in Appendix J.

be designed to speed up the response of the system. For example, consider the problem of requiring that the temperature in a one-dimensional bar approach a constant value, for instance zero, as quickly as possible, starting from some non-uniform initial distribution. The equation of heat conduction in a bar is

$$\frac{\partial^2 T}{\partial x^2} = \alpha \frac{\partial T}{\partial t} \tag{1.4}$$

where T is the temperature in the bar, and

α is the thermal diffusivity.

Let $T_I(x)$ be the initial temperature distribution of the bar and let $T(0) = T(1) = 0$ be the boundary conditions of Eq. 1.4. Then the solution of Eq. 1.4 is

$$T = \sum_{n=1}^{\infty} a_n \sin n\pi x \, e^{-\frac{n^2\pi^2 t}{\alpha}}$$

$$\text{and} \qquad a_n = \int_0^1 T_I(x) \sin n\pi x \; dx \tag{1.5}$$

The modes of the system are $a_n \sin n\pi x$ with associated poles at $(-\frac{n^2\pi^2}{\alpha})$. Modal analysis suggests a system of control which would produce a heat distribution from a distributed heat source equal to the negative of the first mode $a_1 \sin \pi x$, and thus speed up the rate at which $T(x,t)$ decays to zero by removing the first term of Eq. 1.5. Clearly, modal analysis involves considering the whole distributed system for all values of x. The main problems, in this approach to control design, are determining the eigenvalues and eigenvectors and dealing with the complexity of a distributed control system.

Hence, either the transfer functions or the eigenvalues and eigenvectors must be obtained so that the system dynamics are described in a manner suitable for control design. For convective systems, even in the simplest case of only two streams, Gould[37] has shown that elaborate transcendental transfer functions are obtained which are not amenable to conventional control design techniques. For more complicated convective systems, the transfer functions cannot be evaluated algebraically, and a computer must be used. For modal analysis, although the system appears to have modes, Murray[40] has shown that convective systems with no diffusion have no discrete eigenvalues and eigenvectors. To apply either technique, some simple models are required which approximate the true dynamics and which have a form suitable for conventional control analysis or for modal analysis. The modified Galerkin method and the Campbell approximation are two models which have the required form.

B. CONVECTIVE SYSTEMS

Before considering the problem of obtaining simple models of convective systems, some general properties of convective systems are discussed. The equations of a general convective system are given by Eq. 1.1. These equations are, in general, non-linear but can be linearized about the steady state. This is a reasonable procedure because many process-control systems are operated as regulator systems in which the required objective is to maintain the steady state. In this work only the linearized problem will be considered, and the equations can be written

$$-\underline{D}(x)\,\frac{\partial^2 \underline{y}}{\partial x^2} + \underline{V}(x)\,\frac{\partial \underline{y}}{\partial x} + \underline{C}\,\frac{\partial \underline{y}}{\partial t} + \underline{H}(x)\,\underline{y} = 0 \qquad (1.5)$$

where $\underline{D}$, $\underline{V}$, $\underline{C}$ are diagonal matrices. The non-linear equations are linearized by considering small perturbations from the steady state and ignoring second-order terms in the perturbations. If $\underline{D} = 0$, the system is a pure convective system, and if $\underline{V} = 0$, the system is a diffusive system. In most physical systems in chemical engineering, $\underline{D}$ is very small and is usually neglected. It should be noted that ignoring the diffusion leads to analytical and computational difficulties in the modified Galerkin method which can only be resolved by adding an effective diffusion which, for simple models, is much larger than the physical diffusion. Since the amount of added diffusion does not depend on the physical diffusion but on the computational procedure, most attention will be paid to pure convective systems. The boundary conditions for a pure convective system are

$$y_i(x,t) = q_i(t) \quad \text{at } x = 0 \text{ or } x = 1,\ t>0 \text{ for all } i = 1, \ldots n$$

$$\underline{y}(x,t) = \underline{y}_I(x) \quad \text{for } t < 0 \tag{1.6}$$

If diffusion is included, additional boundary conditions on $\underline{y}(x,t)$ are necessary, and usually the following conditions are used.

$$y_i(x,t) \text{ or } \frac{\partial y_i(x,t)}{\partial x} = 0 \text{ at } x = 0 \text{ or } x = 1, t>0$$
$$\text{for all } i = 1, \ldots n$$

Taking Laplace transforms with respect to time, Eq. 1.5 becomes

$$-\underline{D}(x)\,\underline{y}'' + \underline{V}(x)\,\underline{y}' + s\underline{C}(x)\,\underline{y} + \underline{H}(x)\,\underline{y} = 0 \tag{1.7}$$

where primes mean differentiation with respect to x.
In this work, approximate solutions of Eq. 1.7 will be developed which give models in the frequency domain, but these models can easily be transformed into the time domain. The boundary conditions of Eq. 1.6 are inhomogeneous boundary conditions, and it is frequently easier to solve a problem with homogeneous boundary conditions. Eq. 1.6 and 1.7 can be transformed into a set of equations with homogeneous boundary conditions in the following way.

Let $$\underline{y}(x,t) = \underline{y}_{ss}(x) + \underline{\tilde{y}}(x,t)$$

where $\underline{y}_{ss}(x)$ is the final steady state of $\underline{y}(x,t)$

and $\underline{\tilde{y}}(x,t)$ is the transient portion of $\underline{y}(x,t)$
From Eq. 1.6 and 1.7, since $\underline{y}_{ss}(x)$ satisfies the boundary conditions, the analysis of the system reduces to determining $\underline{y}_{ss}(x)$ and solving the following equation for $\underline{\tilde{y}}(x,t)$:

$$-\underline{D}(x)\underline{\tilde{y}}'' + \underline{V}(x)\underline{\tilde{y}}' + s\underline{C}(x)\underline{\tilde{y}} + \underline{H}(x)\underline{\tilde{y}} = 0 \tag{1.8}$$

with the boundary conditions

$$\tilde{y}_i(x) = 0 \text{ at } x = 0 \text{ or } x = 1 \text{ for all } i = 1, \ldots n$$

$$\underline{\tilde{y}}(x,0) = \underline{y}_I(x) - \underline{y}_{ss}(x) \tag{1.9}$$

The first condition in Eq. 1.9 will be written as

$$\underline{\tilde{y}}(x,t) = 0 \qquad x = 0 \text{ or } 1$$

since it is not significant in the theory which $\tilde{y}_i(x,t)$ are zero at $x = 0$ and which are zero at $x = 1$.

In a non-linear system, $\underline{y}_{ss}(x)$ is already known since the final steady state must be determined in order to linearize the non-linear equations. For the modified Galerkin method Eq. 1.8 is easier to solve than Eq. 1.7.

Associated with every linear system is its adjoint system.[2,14] In the modified Galerkin method a particular property of the adjoint of a convective system will be used. The adjoint to a linear system $L(y)$ is defined as $\mathbb{L}(z)$ where

$$\langle y, \mathbb{L}(z)\rangle - \langle L(y), z\rangle = 0$$

Here $\langle \underline{a}, \underline{b}\rangle$ denotes the inner product of $\underline{a}$ and $\underline{b}$. In particular, if $\underline{a}$ and $\underline{b}$ are functions of x, $\langle \underline{a}, \underline{b}\rangle$ denotes the vector inner product followed by integration over x from 0 to 1.

For a pure convective system

$$\underline{V}\underline{\tilde{y}}' + s\underline{C}\underline{\tilde{y}} + \underline{H}\underline{\tilde{y}} = 0 \tag{1.11}$$

the adjoint is

$$-\left(\underline{V}^T\underline{\tilde{z}}\right)' + s\underline{C}^T\underline{\tilde{z}} + H^T\tilde{z} \tag{1.12}$$

with the boundary conditions

$$\underline{\tilde{y}}(x) = 0 \text{ at } x = 0 \text{ or } 1 \tag{1.13}$$

$$\underline{\tilde{z}}(x) = 0 \text{ at } x = 1 \text{ or } 0 \tag{1.14}$$

By making the substitution $u = 1-x$ in Eq. 1.12, Eq. 1.11 and 1.12 are identical with the same boundary conditions if $\underline{V}$, $\underline{C}$, $\underline{H}$ are constant symmetric matrices. Then

$$\underline{\tilde{y}}(x) = \underline{\tilde{z}}(1-x) \tag{1.15}$$

This relation between the solution of the original system and the solution of the adjoint system will be used in the modified Galerkin method.

C. MODIFIED GALERKIN METHOD

A common approach to solving variable-coefficient equations is to expand the solution in a set of complete orthogonal functions. Galerkin[8, 12] developed a general method and a modification has been developed by the author which makes use of the particular properties of pure convective systems. The model obtained from this method, called the <u>modified Galerkin method</u>, is suitable for modal analysis.

The equations of a pure convective system and its adjoint are given in Eq. 1.11, 1.12, and 1.13. Let $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$ be two sets of complete vector functions with the following properties:

1) $\quad {}_{0}^{1}[\underline{\phi}_n(x)]_i^2\,dx$ and $\int_0^1 [\underline{\psi}_n(x)]_i^2\,dx$ exist for all i and n

2) $\quad \underline{\phi}_n(x) = 0$ for $x = 0$ or 1

$\underline{\psi}_n(x) = 0$ for $x = 1$ or 0

Thus $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$ satisfy the boundary conditions of Eq. 1.13 and 1.14.

3) $$<\underline{\psi}_n(x), \underline{C}\,\underline{\phi}_m(x)> = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

where $\underline{C}$ is the coefficient matrix given in Eq. 1.11. Then the equation of the general convective process

$$\underline{V}\underline{\tilde{y}}' + s\underline{C}\underline{\tilde{y}} + \underline{H}\,\underline{\tilde{y}} = 0 \qquad (1.11)$$

is identical almost everywhere with the set of equations

$$<\underline{\psi}_n(x), \underline{V}\underline{\tilde{y}}' + s\underline{C}\underline{\tilde{y}} + \underline{H}\underline{\tilde{y}}> = 0 \text{ for all } n \qquad (1.16)$$

since the function which is orthogonal to every member of a complete set is identical to the zero function except at a set of points of measure zero

Let
$$\underline{\tilde{y}} = \sum_{n=1}^{\infty} c_n\,\underline{\phi}_n(x) \qquad (1.17)$$

Substitute Eq. 1.17 in Eq. 1.16, and take a finite number of terms, N, as an approximate solution.

Then
$$(\underline{A} + s\underline{I})\underline{c} = 0 \tag{1.18}$$

where
$$A_{nm} = <\underline{\psi}_n(x), \underline{V}\,\underline{\phi}'_m(x) + \underline{H}\,\underline{\phi}_m(x)>$$

$$I_{nm} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

$$\underline{c} = (c_1, \ldots\ldots c_N) \text{ a column vector}$$

Equation 1.18 is a matrix equation which can be solved for its eigenvalues, s_n, and its eigenvectors, $\underline{c}_n$. The eigenvectors have an undetermined constant which is denoted as a_n. From Eq. 1.17, the solution of Eq. 1.11 is

$$\tilde{\underline{y}}(x, s) = \sum_{n=1}^{N} \frac{a_n}{s+s_n} \sum_{m=1}^{N} c_{nm}\underline{\phi}_m(x) \tag{1.19}$$

To complete the solution it is necessary to obtain a_n. The boundary condition which has not yet been used is (Eq. 1.9)

$$\tilde{\underline{y}}(x, 0) = \underline{y}_I(x) - \underline{y}_{ss}(x)$$

Taking the limit of Eq. 1.19 as t→ 0

$$\underline{y}_I(x) - \underline{y}_{ss}(x) = \sum_{n=1}^{N} a_n \sum_{m=1}^{N} c_{nm}\,\underline{\phi}_m(x) \tag{1.20}$$

By expanding the right hand side of Eq. 1.20 in a Fourier series in $\underline{\phi}_m(x)$, the coefficients, a_n, can be determined.

The questions that arise with this method of solution, the modified Galerkin method, are: what set of functions $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$ should be used; and how good is the approximation obtained from Eq. 1.19 and 1.20.

First consider the functions $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$. In Chapter II it is shown that the adjoint system $\tilde{\underline{z}}$ is expanded in the set of functions

$$\underset{\sim}{\tilde{z}} = \sum_{n=1}^{\infty} d_n \underline{\psi}_n(x)$$

and $$(\underline{A}^T + s\underline{I})\,\underline{d} = 0$$

with $$\underline{d} = (d_1, \ldots . d_N), \text{ a column vector}$$

and $\underline{A}$ is given by Eq. 1.18. This means that the modified Galerkin method expands the solution in terms of $\underline{\phi}_n(x)$ and the adjoint solution in terms of $\underline{\psi}_n(x)$. But for pure convective systems with constant symmetric matrix coefficients, it has been shown (Eq. 1.15) that

$$\underline{\tilde{y}}(x) = \underline{\tilde{z}}(1-x)$$

Thus, to imitate this relation it is best to choose

$$\underline{\phi}_n(x) = \underline{\psi}_n(1-x) \tag{1.21}$$

In the original Galerkin method, $\underline{\phi}_n(x) = \underline{\psi}_n(x)$. This can be a very bad choice for a convective system, and it is better to use Eq. 1.21. Many chemical systems, such as heat exchangers, absorbers, and distillation columns, can be considered as small variations from pure convective systems with constant symmetric matrix coefficients. Thus, Eq. 1.21 is a reasonable basis for choosing $\underline{\psi}_n(x)$ given $\underline{\phi}_n(x)$.

$\underline{\phi}_n(x)$ must satisfy the boundary conditions and form a complete set. One such set of functions is

$$[\underline{\phi}_n(x)]_i \begin{cases} \sin\frac{2n-1}{2}\pi x & \text{if } \tilde{y}_i = 0 \text{ at } x = 0 \\ \sin\frac{2n-1}{2}\pi(1-x) & \text{if } \tilde{y}_i = 0 \text{ at } x = 1 \end{cases}$$

However, a method exists for obtaining an approximate solution of constant-coefficient convective systems, called the Taylor diffusion model (Appendix A), which gives a complete set of functions $\underline{\phi}_n(x)$ which satisfy the boundary conditions. A better choice of $\underline{\phi}_n(x)$ is to use the solutions of this approximate system, obtained by averaging the variable coefficients. This is a standard technique in applied mathematics.[22]

The accuracy of the solution is usually investigated by considering how close the eigenvalues of Eq. 1.18 are to the true eigenvalues of the system. Unfortunately Murray[40] has shown that a pure convective system has no discrete eigenvalues, only an essential singularity at infinity. Thus, the only meaningful way of determining the accuracy of the solution is by comparing the frequency responses and time responses for those few cases that can be evaluated exactly.

The two-stream counter-current constant-coefficient convective system has been solved exactly in the frequency domain by Gould.[37] The modified Galerkin method was applied to this case, and the first five terms of Eq. 1.19 were calculated. A schematic diagram is shown in Fig. 1.1, and a typical set of responses is shown in Figs. 1.2 through 1.5. The responses are those of the output of each stream, $y_1(1,t)$ and $y_2(0,t)$ to a disturbance $q(t)$ in the input of y_1, i.e., at $y_1(0,t)$. It is clear that the approximation is adequate for the response of $y_2(0,t)$ and completely inadequate for $y_1(1,t)$. Indeed if more terms were taken, the approximation becomes worse and the high-frequency effects even larger. From the time responses, clearly the main problem is the attempt to approximate the pure time delay. This is known to be a difficult problem.

To improve the accuracy of the method, the high-frequency errors must be reduced. The introduction of some diffusion into the system will attenuate the high frequencies. The amount of diffusion that is required, can be estimated by considering the asymptotic value of the eigenvalues of Eq. 1.18. The following relation which is proved in Chapter II and Appendix D has been found to be satisfactory for determining the additional diffusion, D_i that should be added to each stream

$$D_i = \frac{16}{\pi^2 NM} \sum_{i=1}^{M} |V_i| \qquad (1.22)$$

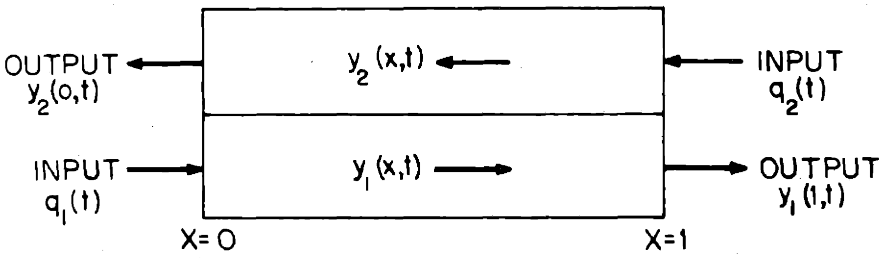


Fig. 1.1 Schematic Diagram of Two-stream Counter-current Convective System

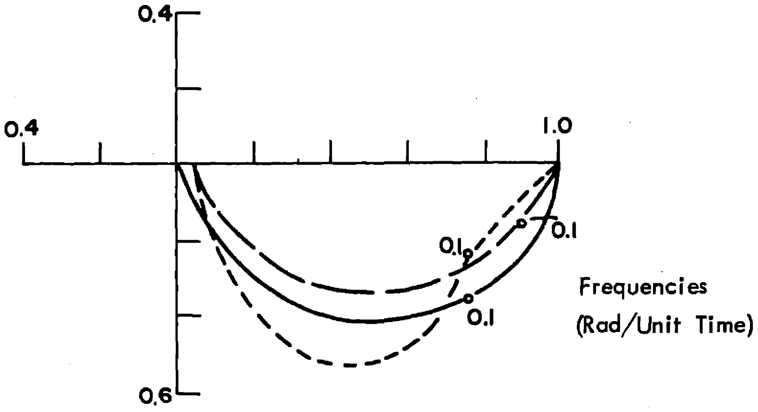


Fig. 1.2 Typical Modified Galerkin Frequency Response $\frac{y_2(0,s)}{q(s)}$

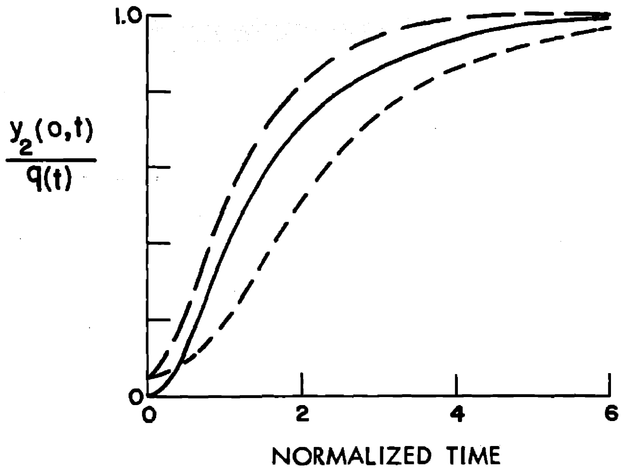


Fig. 1.3 Typical Modified Galerkin Time Response, $y_2(0,t)$

Legend:

——— EXACT TRANSFER FUNCTION
MODIFIED GALERKIN METHOD
- - - - - - a) No Diffusion
— — — b) With Diffusion

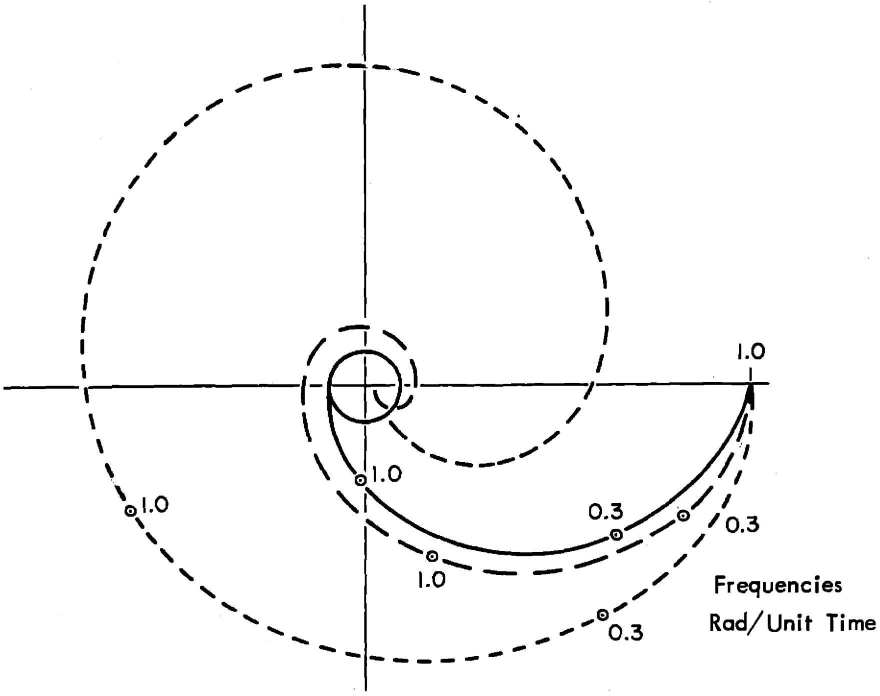


Fig. 1.4 Typical Modified Galerkin Frequency Response $\frac{y_1(1,s)}{q(s)}$

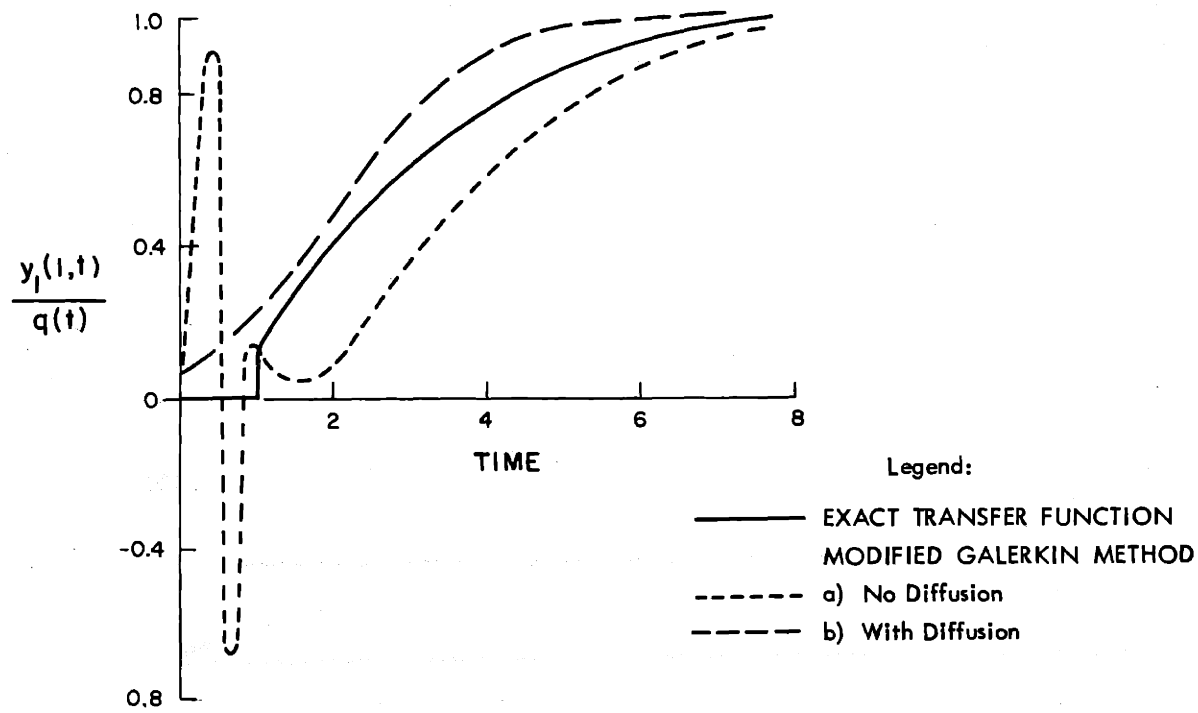


Fig. 1.5 Typical Modified Galerkin Time Response $y_1(1,t)$

where N is the number of terms in the approximation.
M is the number of streams in the system.
V_i is the velocity of the i^{th} stream.

With this additional diffusion, the matrix $\underline{A}$ of Eq. 1.18 becomes

$$A_{nm} = <\underline{\psi}_n(x), \; -\underline{D}\,\underline{\phi}''_m(x) + \underline{V}\,\underline{\phi}'_m(x) + \underline{H}\,\underline{\phi}_m(x)> \tag{1.23}$$

The results, using Eq. 1.22 and 1.23, are shown in Figs. 1.2 through 1.5. The improvement is considerable, but the time delay is not well approximated.

The amount of diffusion implied by Eq. 1.22 is considerably greater than the physical diffusion of convective systems. It is called the <u>effective diffusion</u>. It is of the same order as the effective diffusion introduced by lumping each stream into N lumps. Also the Taylor diffusion model has a similar effective diffusion. These three methods are the only methods which give a dynamical model in the form of a set of eigenvalues and eigenvectors, and, therefore, only these methods are suitable for modal analysis. It appears that any model which is in a form suitable for modal analysis will have an effective diffusion many times greater than the physical diffusion. For counter-current convective systems, the observed physical behavior is quite accurately represented by the effective diffusion because the counterflow action tends to "mix" the transient responses in the axial direction. The main advantage of the modified Galerkin method over lumping is that the dimension of the matrix equations that must be solved is smaller. From the sampling theorem, if N spatial modes are required, at least $2N$ lumps must be used. Thus, for a M-stream system, at least a $(2MN)^{th}$ order matrix equation must be solved, while in the modified Galerkin method only a N^{th} order matrix equation must be solved, However, with powerful digital computers available this advantage may be marginal. The modified Galerkin method is discussed in detail in Chapter II.

It is possible to represent a lumped system as a distributed system with coefficients that are impulses in distance. Thus a mixed distributed system and lumped system can be considered as a single distributed system whose coefficients vary with distance. Such systems can be solved by the modified Galerkin method, and an example of this technique is given in Chapter III.

D. CAMPBELL APPROXIMATION

The modified Galerkin method, considered in the previous section, gives a dynamical model suitable for modal analysis. Such a model is also suitable for conventional control design techniques since the transfer functions between any position in the system and any input can easily be determined. But when conventional control design techniques are used, pure time delays are no inconvenience; whereas modal analysis cannot handle such behavior. Thus, it is reasonable to look for a model involving poles, zeros, gains, and pure time delays, and such a model should be more accurate than the modified Galerkin method since the time delay would be better approximated. Several writers, Campbell,[28] Boyle,[25] and Ziegler and Nichols,[52] have all used dynamical models of this form but the parameters have always been determined experimentally. Further, for complicated systems, the correct form of the model is not obvious.

A new method, called the Campbell approximation, is presented which determines both the form and the numerical values of the parameters directly from the system equations for constant and variable coefficient systems. The method is easy to use and accurate; it has been applied with great success to a complicated non-linear system, an ammonia reactor; and it is apparently the best dynamical model to use for all purposes except for modal analysis.

The Campbell approximation is based on the physical behavior of the system and combines the best features of existing dynamical models for convective systems. To obtain the form of the approximation, a concept is introduced called the transfer path. The transfer paths of a system are defined as the paths by which a disturbance at an input reaches any point in the system for time close to zero. The transfer paths are similar to the paths a wave takes to reach a point where one path is the direct path and other paths are caused by reflections. For time close to zero, the response of a convective system is like the sum of the responses due to each transfer path. This is not true for large time, but it is consistent with the wave-like nature of convective processes. Thus, the transfer paths indicate the form of the desired approximation. Each transfer path has an associated delay caused by convection down a stream, and a pole is introduced each time a boundary is crossed, and this pole is independent of the direction of flow along the transfer path. The simplest system, a two-stream counter-current system, has only one transfer path, while co-current systems and reversed flow systems have two paths. Typical transfer paths for some simple systems are shown in Fig. 1.6.

Four principles are used to determine the parameters of the Campbell approximation:

1) The steady state must be correct.
2) The low frequency is approximated by a simple time lag.
3) The high frequency is given by the integral series method.
4) The system must not respond before the arrival of the disturbance.

To see how to apply these principles, consider the transfer function between $y_i(x,t)$ and a disturbance $q(t)$ at $y_1(0,t)$. Let $L(x,s)$ be the low frequency portion of the transfer function and $H(x,s)$ be the high frequency portion, and let $H(x,s)$ have unity gain at low frequencies.

Then
$$\frac{y_i(x,s)}{q(s)} = L(x,s)\ H(x,s) \tag{1.24}$$

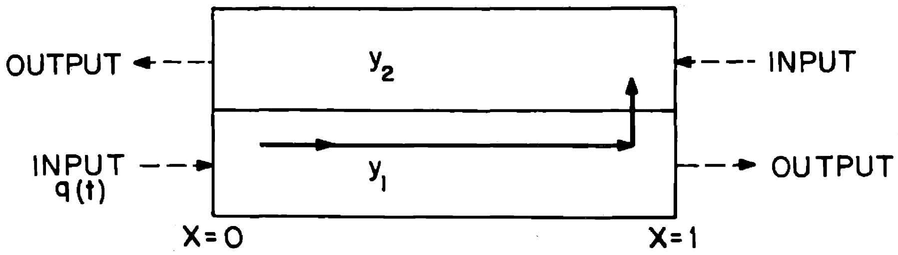
From the first two principles, an approximate form for $L(x,s)$ is

$$L(x,s) = \frac{G(x)}{1+Ts} \tag{1.25}$$

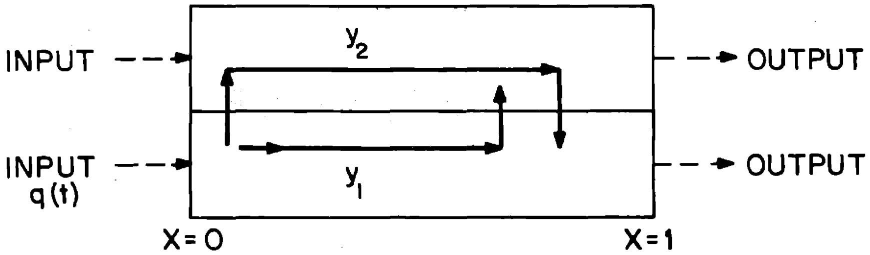
where $G(x)$ is the correct steady state gain.

T is determined by any of three different methods and is the dominant time constant of

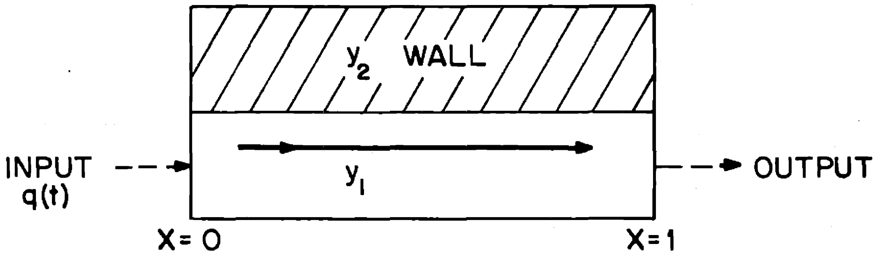
1) The Taylor diffusion model. This is only applicable to constant-coefficient systems (Appendix A).
2) The modified Galerkin method.
3) The system obtained by approximating each stream by one



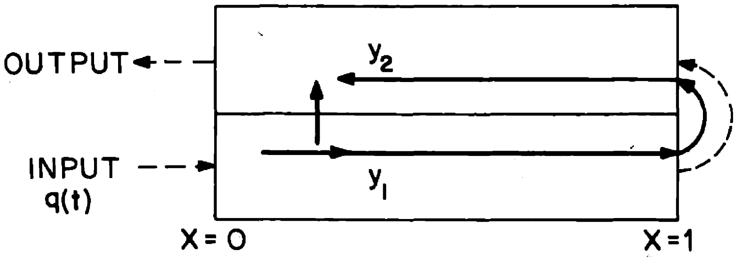
a) Two-stream counter-current system



b) Two-stream co-current system



c) One stream with a wall (Percolation)



d) Two stream reversed flow system

q(t) = The Disturbance

- - → Direction of flow of each stream

——→ Transfer Path

Fig. 1.6 Transfer Paths for Two-stream Systems lump. This is only satisfactory for counter-current systems and is accurate because of the large amount of internal feedback in a counter-current convective system which tends to make the system well-mixed.

The high frequency behavior is obtained from the integral series method (Appendix E) developed by Rinard.[44] The first terms of the series are known to be good high frequency approximations. By averaging the coefficients, the integrals can be evaluated even for variable-coefficient systems. As an example, consider the two-stream counter-current system. This system has only one transfer path (Fig. 1.6) so the form of the approximation is the product of gains, time delays, poles, and zeros. Let $I_1(x, s)$ and $I_2(x, s)$ be the first terms of the integral series of $\frac{y_1(x, s)}{q(s)}$ and $\frac{y_2(x, s)}{q(s)}$ where $q(t)$ is a disturbance at $y_1(0, t)$. Then $I_1(x, s)$ and $I_2(x, s)$ have the form

$$I_1(x, s) = e^{-sx} e^{-ax} \tag{1.26}$$

$$I_2(x, s) = \frac{k e^{-sx} e^{-ax}}{1+T_1 s} \tag{1.27}$$

Then

$$H_1(x, s) = \frac{T}{G_1} e^{-sx} e^{-ax} \tag{1.28}$$

$$H_2(x, s) = \frac{T}{G_2} \cdot \frac{ke^{-sx} e^{-ax}}{1+T_1 s} \tag{1.29}$$

for all s large enough that $|Ts| \gg 1$. This ensures that the high frequency behavior is being studied. Note that the pole in Eq. 1.29 is kept since $|T_1 s|$ is not necessarily larger than unity.

To find the complete approximation, $H_1(x, s)$ and $H_2(x, s)$ must have unity gain at low frequencies. Thus, the Campbell approximation is

$$\frac{y_1(x, s)}{q(s)} = \frac{G_1(x)\ (1+\alpha_1(x)Ts)}{1+Ts} \tag{1.30}$$

$$\frac{y_2(x, s)}{q(s)} = \frac{G_2(x)\ (1+a_2(x)Ts)}{(1+Ts)(1+T_1 s)} \tag{1.31}$$

where
$$a_1(x) = \frac{e^{-ax}}{G_1(x)}$$

$$a_2(x) = \frac{ke^{-ax}}{G_2(x)}$$

Equations 1.30 and 1.31 are in the expected form for one transfer path. If more than one transfer path exists, the results are more complicated. The integral series will give a form consisting of the sum of as many terms as there are transfer paths, but an additional problem arises in how to combine the low and high frequency portions. Some guides have been developed by considering simple cases, and this problem is discussed in Chapter IV.

To test the accuracy of the model, several two-stream counter-current constant-coefficient systems were investigated, and the results were compared with the exact solutions obtained by Gould.[37] A typical frequency response is shown in Fig. 1.7. Clearly the approximation is remarkably accurate.

The Campbell approximation has been applied to an ammonia reactor, which can be represented as four-stream convective system, and the dynamic model was compared with the model obtained by Eymery[31] by direct digital computation. The Campbell approximation gave an excellent dynamical model which indicates how the system response depends on the system parameters. The details of this application are given in Chapter IV.

E. CONCLUSIONS

Two new methods, the modified Galerkin method, and the Campbell approximation, have been developed for obtaining dynamic models of convective systems. Both these methods can be applied to variable-coefficient systems. Therefore, suitable dynamical models of convective systems are available which can be used as a basis for

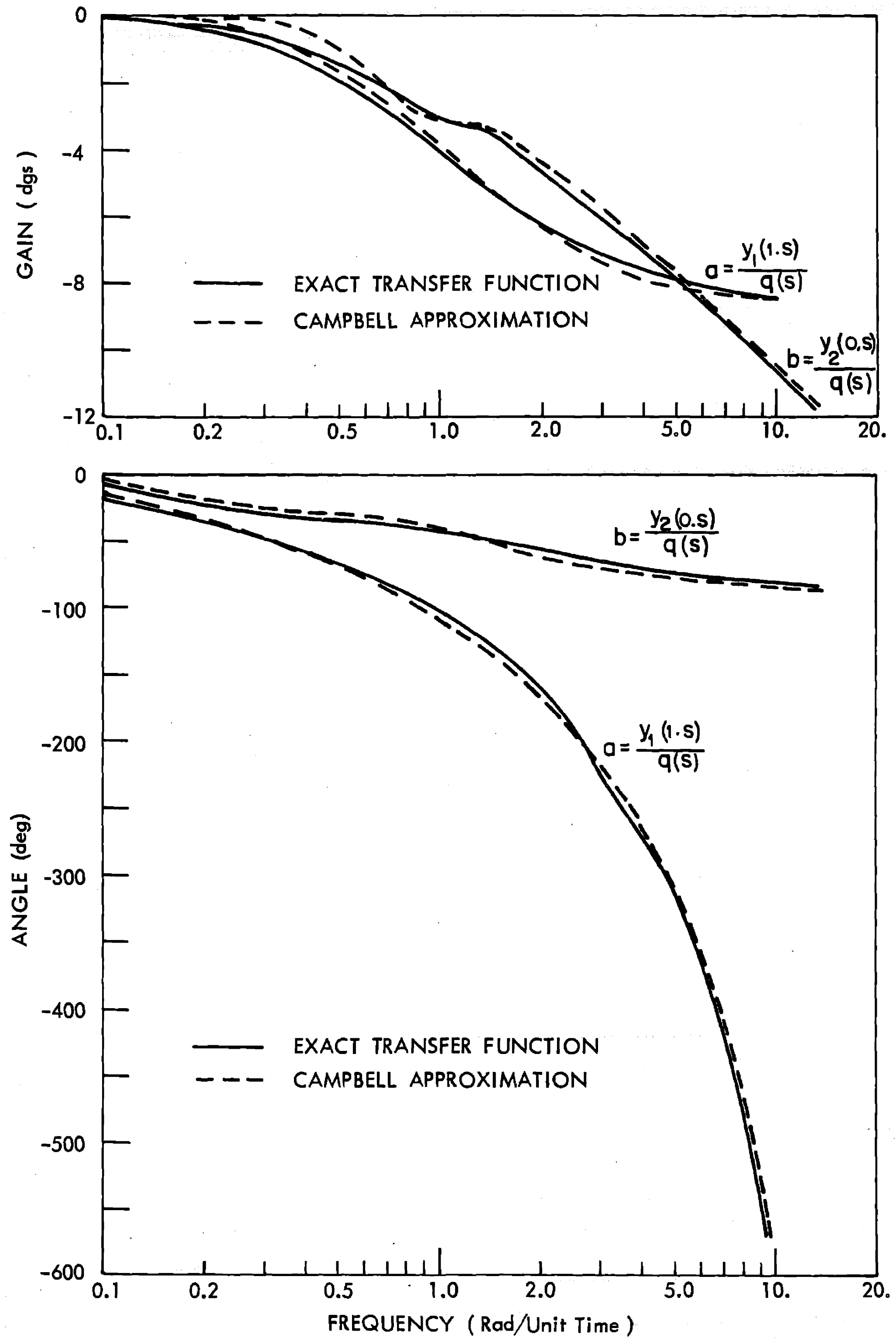


Fig. 1.7 Typical Campbell Approximation Frequency Responses

developing a control philosophy for distributed systems. One such philosophy, modal analysis, has been developed, but it would be interesting to see if a similar philosophy could be developed for systems with a pure time delay. Also the Campbell approximation is a good model for further investigations of the optimal control of chemical processes. Future work can now concentrate on the design of control systems since the problem of adequate dynamic models has essentially been solved. It is the author's opinion that it is dubious whether further work on dynamic models will give any worthwhile results. The primary contribution of this work is the development of suitable dynamic models for convective systems with both constant and variable coefficients.

CHAPTER II

APPROXIMATE SOLUTION OF THE VARIABLE COEFFICIENT CONVECTIVE SYSTEM

A. INTRODUCTION

In this chapter a method of obtaining a convenient model of the dynamics of a convective system with variable coefficients is developed. A general convective system with variable coefficients has the equation

$$-\underline{D}\,\underline{y}'' + \underline{V}\,\underline{y}' + s\underline{C}\,\underline{y} + \underline{H}\,y = 0 \qquad (2.1)$$

where all the coefficient matrices are functions of x and $\underline{D}$, $\underline{V}$, $\underline{C}$ are diagonal matrices.

When $\underline{D}$ is zero the system is a pure convective system and when $\underline{V}$ is zero a pure diffusive system. Since the chemical processes such as heat exchange and distillation have very small diffusion in the x direction, $\underline{D}$ is very small and the systems can be considered as pure convective systems. The method developed in this chapter is applicable to the general convective system (Eq. 2.1) but particular attention is given to pure convective systems.

It has been shown in the previous chapter that two approaches to control system design, conventional control and modal analysis, require simple dynamical models. In particular, modal analysis requires the eigenvalues and eigenfunctions of the system. There are no known methods for solving this problem in general with variable coefficients that are arbitrary. The Taylor diffusion model developed by Gould[36] and Rosenbrock[47] gives a model suitable for modal analysis for pure convective systems with two-streams and constant-coefficients. A general formulation of this method for many streams is given in Appendix A, but several details, especially concerning boundary conditions, have not been solved. The Taylor diffusion model approach could possibly be extended to the variable coefficient problem; however, a completely different approach is considered here. The only other known method which could possibly be applied to variable coefficient systems is the integral series technique.[44] Theoretically, this is possible but in practice the integrals are difficult to evaluate. In

Appendix E a brief summary of the integral series approach is given.

Equations similar to Eq. 2.1 arise in elasticity and quantum mechanics. These problems are usually solved by replacing the differential equations with a matrix problem through the use of a complete set of functions in x. However, the equations that occur in elasticity and quantum mechanics are self-adjoint while the convective equations are not self-adjoint. The exact definitions of a linear system and its adjoint and some general properties are summarized in Appendix C. A physical picture of the difference is that self-adjoint systems are conservative while non-self-adjoint systems are non-conservative. For instance, in both elasticity and quantum mechanics, energy is conserved while in a heat exchanger heat is removed from the system through the output streams. This analogy should not be taken too far but does give some physical feeling to the formal mathematical relations discussed in Appendix C.

The methods used in elasticity were developed from the calculus of variations by Rayleigh[18] and Ritz.[19] Galerkin[8] obtained a similar result from a totally different theoretical point of view and this method is applicable to any linear system, not just a self-adjoint system. A modification of the Galerkin method is developed which is a considerable improvement for convective systems. All three methods are closely related and give identical results for self-adjoint systems. The modification makes use of a special relation between a pure convective system and its adjoint which is proved in Appendix C. This method is called the "Modified Galerkin Method" and is discussed in detail in this chapter. It is shown that there are serious problems with convergence when the modified Galerkin method is applied to pure convective systems but that these problems can be overcome by the addition of some diffusion. The amount of diffusion required depends on the number of terms used in the modified Galerkin method and can be easily determined from a simple inequality.

The modified Galerkin method gives a simple model in terms of eigenfunctions and eigenvalues in exactly the form required by Murray[40] for the application of modal analysis to distributed systems. Thus for the first time a method exists which allows modal analysis to be applied to a wide range of processes. It is now possible to concentrate future work on the control problem if one starts with a dynamical model obtained by the modified Galerkin method. Thus a satisfactory dynamical model is available as a basis for developing a control philosophy for distributed systems. The primary contribution of this work is the demonstration that simple adequate dynamical models can be produced for a wide class of systems.

In this chapter the theory is developed and the results applied to two-stream, counter-current, constant-coefficient, convective systems whose dynamics are well known. Thus it is possible to determine the accuracy of the model. In later chapters the method is applied to more involved processes. Sections B and C outline the Rayleigh-Ritz and Galerkin methods while the modified Galerkin method is given in Section D. The problems of existence and convergence are discussed in Section E and a simple example is considered in Section F to indicate the expected form of the eigenvalues. The complete solution is given in Section G. A summary of the theoretical results is given in Section H. Then the modified Galerkin method is applied to examples taken from typical chemical processes and the numerical details of the examples are given in Section I. In Sections J and K the results with and without added diffusion are discussed including the significance of this added diffusion. Finally in Section L a summary of the modified Galerkin method is given which discusses both its usefulness and the steps involved in applying the method.

In this chapter the inner product $<\underline{a}, \underline{b}>$ denotes the vector inner product followed by integration over x. The notation $\tilde{\underline{y}}(x, t)$ denotes the transient part of the solution $\underline{y}$ and $\underline{y}_{ss}(x)$ is the steady state part of $\underline{y}$. Thus

$$\underline{y}(x, t) = \underline{y}_{ss}(x) + \tilde{\underline{y}}(x, t)$$

B. RAYLEIGH-RITZ METHOD

The Rayleigh-Ritz method is one of the standard methods for solving problems in elasticity involving variable density plates or in quantum mechanics for fields which depend on distance.[2,3,22] This method was first used by Rayleigh[18] to solve problems in acoustics and a rigorous mathematical theory was developed by Ritz.[19] An outline is given below of the method so that it can be compared with different methods in later sections.

The Rayleigh-Ritz method is applicable to self-adjoint systems whose coefficients have certain definite properties. These conditions are equivalent to the conservation of some scalar quantity, usually energy.[22] The method will be applied to a vector equation, although most of the standard works only consider the scalar problem.

Consider the equation

$$-\underline{D}\tilde{\underline{y}}'' + \underline{V}\tilde{\underline{y}}' + \underline{H}\tilde{\underline{y}} + s\underline{C}\tilde{\underline{y}} = 0 \tag{2.2}$$

with $\underline{D}, \underline{V}. \underline{H}, \underline{C}$ and a suitable set of boundary conditions such that the equation is self-adjoint (see Appendix C). This equation is the Euler equation of the following problem in the calculus of variations. Minimize I holding J constant where

$$\begin{aligned} I &= <\tilde{\underline{y}}', \underline{D}\tilde{\underline{y}}'> + <\tilde{\underline{y}}, \underline{V}\tilde{\underline{y}}' + \underline{H}\tilde{\underline{y}}> \\ J &= <\tilde{\underline{y}}, \underline{C}\tilde{\underline{y}}> \end{aligned} \tag{2.3}$$

This problem can be solved approximately by choosing a set of functions $\underline{\phi}_n(x)$ which fulfill the following conditions:

The $\underline{\phi}_n(x)$
1. satisfy the boundary conditions of Eq. 2.2
2. are complete in $0 \leq x \leq 1$
3. $$< \underline{\phi}_m(x), \ \underline{C}\underline{\phi}_n(x) > = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \tag{2.4}$$
4. $\int_0^1 [\underline{\phi}_n(x)]_i^2 \, dx$ exists for all n and for all components l

$[\underline{\phi}_n(x)]_i$ need not be continuous

Let

$$\tilde{\underline{y}} = \sum_{n=1}^{\infty} c_n \underline{\phi}_n(x) \tag{2.5}$$

Substitute for $\tilde{\underline{y}}$ in Eq. 2.3 and minimize with respect to the coefficient c_n.

Then
$$(\underline{A} + s\underline{I})\, \underline{c} = 0 \tag{2.6}$$

where
$$\underline{c} = (c_1, \ldots c_n) \tag{2.7}$$

and $$A_{nm} = \langle \underline{\phi}'_n \, , \, \underline{D}\underline{\phi}'_n \rangle + \langle \underline{\phi}_n, \underline{V}\underline{\phi}'_m + \underline{H}\phi_m \rangle \qquad (2.8)$$

The eigenvalues of $\underline{A}$ are the negative of the eigenvalues of Eq. 2.2 and the eigenvectors of $\underline{A}$, by using Eq. 2.5, give the eigenfunctions of Eq. 2.2.

C. GALERKIN METHOD

An alternative approach was suggested by Galerkin.[8, 12] This method is applicable to any equation and has a quite different theoretical basis. But for systems for which the Rayleigh-Ritz method is applicable, both methods give identical results.

Consider a linear vector equation

$$\underline{L}(\tilde{\underline{y}}) = 0 \qquad (2.9)$$

with a suitable set of boundary conditions and let $\underline{\phi}_n(x)$ be a set of functions complete over $0 \leq x \leq 1$. Since any function which is orthogonal to all members of a complete set must be zero almost everywhere, Eq. 2.9 can be replaced by

$$\langle \underline{\phi}_n(x), \underline{L}(\tilde{\underline{y}}) \rangle = 0 \quad \text{for all } n \qquad (2.10)$$

Let $$\tilde{\underline{y}} = \sum_{n=1}^{\infty} c_n \underline{\phi}_n(x) \qquad (2.11)$$

and $\underline{\phi}_n(x)$ satisfy the boundary conditions of Eq. 2.9. $[\underline{\phi}_n(x)]_i$ need not be continuous and $\int_0^1 [\phi_n(x)]_i^2 \, dx$ must exist for all n and i components. As an approximation to Eq. 2.9 use Eq. 2.11 for $n = 1 \ldots N$. Then the c_n are solutions of the equation

$$\underline{A}\underline{c} = 0 \qquad (2.12)$$

where $$\underline{c} = (c_1, \ldots c_N) \qquad (2.13)$$

and $$A_{nm} = \langle \underline{\phi}_n, \underline{L}(\underline{\phi}_m) \rangle \qquad (2.14)$$

It is obvious that if this result is applied to the self-adjoint Eq. 2.2 then Eqs. 2.6 and 2.12 are identical. However, this method is more general as there are no restrictions on the linear operator $\underline{L}$.

D. MODIFIED GALERKIN METHOD

A modification to Galerkin's method will be developed which offers significant improvement for pure convective processes. In Galerkin's method there is no need to choose the same set of complete functions to be orthogonal to $\underline{L}$ and to expand $\underline{\tilde{y}}$. Let $\underline{\phi}_n(x)$ be a complete set of functions which satisfy the boundary conditions of $\underline{L}$ and let $\underline{\psi}_n(x)$ be another complete set of functions. Then a similar development can be carried out and the only difference is that Eq. 2.14 becomes

$$A_{nm} = < \underline{\psi}_n(x), \ \underline{L}(\underline{\phi}_m(x)) > \tag{2.15}$$

This modification gives greater freedom to the method as there are now two sets of functions to choose. But by considering the adjoint operator $\bar{\underline{L}}$ some guides can be obtained on how to choose $\underline{\phi}_n$ and $\underline{\psi}_n$.

From the definition of a system and its adjoint (Appendix C)

$$< \underline{\tilde{z}}, \ \underline{L}(\underline{\tilde{y}}) > - < \bar{\underline{L}}(\underline{\tilde{z}}), \ \underline{\tilde{y}} > \ = \ 0 \tag{2.16}$$

Let $\underline{\phi}_n(x)$ be complete and satisfy the boundary conditions of $\underline{L}$ and $\int_0^1 [\underline{\phi}_n]_i^2 \, dx$ exist for all n and i. Let $\underline{\psi}_n(x)$ be complete and satisfy the boundary conditions of $\bar{\underline{L}}$ and $\int_0^1 [\psi_n]_i^2 \, dx$ exist for all n and i.

Let
$$\underline{\tilde{y}} = \sum_{n=1}^{\infty} c_n \underline{\phi}_n(x) \quad \text{and} \quad \underline{\tilde{z}} = \sum_{n=1}^{\infty} d_n \underline{\psi}_n(x) \tag{2.17}$$

$$\sum_{m=1}^{\infty} d_m \sum_{n=1}^{\infty} c_n < \underline{\psi}_m, \underline{L}(\underline{\phi}_n)> = \sum_{n=1}^{\infty} c_n \sum_{m=1}^{\infty} d_m < \underline{\phi}_n, \underline{L}(\underline{\psi}_m) > \tag{2.18}$$

The left-hand side of Eq. 2.18 is zero from Eq. 2.15. The right-hand side is zero if

$$\underline{d} = (d_1, \dots d_m \dots)$$

is an eigenvector of $\underline{A}^T$ where $\underline{A}$ is given by Eq. 2.15. Thus $\underline{c}$ is the eigenvector of $\underline{A}$ and $\underline{d}$ is the adjoint eigenvector of $\underline{A}$. This result gives an interpretation of the functions $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$.

$\underline{\phi}_n(x)$ is the set of functions in which the solution $\underline{\tilde{y}}$ is expanded while $\underline{\psi}_n(x)$ is the set of functions in which the solution of the adjoint system $\underline{\tilde{z}}$ is expanded. Clearly the modified Galerkin method reduces to the Galerkin method when $\underline{\phi}_n = \underline{\psi}_n$ and implies that $\underline{\tilde{y}}$ and $\underline{\tilde{z}}$ are expanded in the same set of functions. In the Rayleigh-Ritz case $\underline{\tilde{y}} = \underline{\tilde{z}}$ since the system is self-adjoint and all the methods give identical results. For the pure convective system with constant coefficients it was shown in Appendix C that $\underline{\tilde{y}}(x) = \underline{\tilde{z}}(1 - x)$. If Galerkin's method is used, then a set of $\underline{\phi}_n(x)$ which will approximate well the behavior of $\underline{\tilde{y}}$ in a few terms can be a most indifferent approximation to $\underline{\tilde{z}}$. It is much better to choose a set of the form $\underline{\psi}_n(x) = \underline{\phi}_n(1 - x)$ and thus imitate the relation between $\underline{\tilde{y}}$ and $\underline{\tilde{z}}$.

It is interesting to consider the formal relationship between the modified Galerkin method and the calculus of variations. Consider the problem of minimizing I with J held constant where

$$I = <\underline{\tilde{z}}', \underline{D}\underline{\tilde{y}}'> + <\underline{\tilde{z}}, \underline{V}\underline{\tilde{y}}' + \underline{H}\underline{\tilde{y}}> \tag{2.19}$$

$$J = <\underline{\tilde{z}}, \underline{C}\underline{\tilde{y}}> \tag{2.20}$$

Applying Euler's equations

$$\begin{gathered} -\underline{D}\underline{\tilde{y}}'' + \underline{V}\underline{\tilde{y}}' + \underline{H}\underline{\tilde{y}} + s\underline{C}\underline{\tilde{y}} = 0 \\ -\underline{D}^T\underline{\tilde{z}}'' - (\underline{V}^T\underline{\tilde{z}})' + \underline{H}^T\underline{\tilde{z}} + s\underline{C}^T\underline{\tilde{z}} = 0 \end{gathered} \tag{2.21}$$

which are the equations of the system and its adjoint (Appendix C).

Then if Eq. 2.17 is used results obtained are identical to the modified Galerkin method. The only drawback to this approach is the problem of whether a minimum exists for $I + sJ$. The methods of classical calculus of variations[5] require that a local or weak minimum exist inside the region $0 < x < 1$ and not on the boundary $x = 0$ or $x = 1$. A local or weak minimum exists for a function if the first variation is zero and the second variation is always positive. Consider the variation of $I + sJ$

Let

$$\underline{\tilde{y}} = \underline{\tilde{y}}_{\min} + \epsilon \underline{\eta} \qquad (2.22)$$

$$\underline{\tilde{z}} = \underline{\tilde{z}}_{\min} + \underline{\xi}$$

where $\underline{\tilde{y}}_{\min}, \underline{\tilde{z}}_{\min}$ are the values of $\underline{y}$ and $\underline{z}$ when the first variation is zero

ϵ is a general parameter

$\underline{\eta}, \underline{\xi}$ are general functions satisfying the system boundary conditions

Substitute Eq. 2.22 into $I + sJ$ and consider the variations as ϵ changes. The requirement that the first variation be zero (Euler's equation) gives Eq. 2.21. The second variation gives the equation

$$<\underline{\xi}', \underline{D}\,\underline{\eta}'> + <\underline{\xi}, \underline{V}\underline{\eta}' + \underline{H}\underline{\eta} + s\,\underline{C}\underline{\eta}>$$

Because of the arbitrary nature of $\underline{\eta}, \underline{\xi}$ this equation can be both positive and negative, thus neither weak minima nor weak maxima exist.

For self-adjoint systems (Eq. 2.2) a weak minimum exists provided $\underline{D}, \underline{H}$ are positive definite and $\underline{C}$ is negative definite.[1] Thus for heat conduction in a rod the equations have the form

$$\frac{\partial^2 y}{\partial x^2} = a \frac{\partial y}{\partial t} \qquad a > 0$$

Taking Laplace transforms with respect to time the equations become

$$-y'' + a s y = 0$$

and there exists no weak or local minimum although the equations are self-adjoint. However the one dimensional Laplace equation

$$\frac{\partial^2 y}{\partial x^2} = \alpha \frac{\partial^2 y}{\partial t^2} \qquad \alpha > 0$$

is self-adjoint and has a minimum since taking Laplace transforms with respect to time the equation can be written

$$- y'' + \alpha s^2 y = 0$$

But s is pure imaginary number and putting $s = j\sqrt{\lambda}$ the equation has the required form

$$- y'' - \alpha\lambda = 0$$

E. EXISTENCE AND CONVERGENCE

So far it has been assumed that the eigenvalues exist and nothing has been said about the convergence of the approximate solution as the number of functions used increases. This is an extremely difficult problem in general but some very powerful results have been proved for the Rayleigh-Ritz method. Unfortunately, these results are obtained from the calculus of variations assuming there exists a weak minimum in the interior of the region of the x, namely, $0 < x < 1$ and not on the boundary $x = 0$ or 1. In some special cases results can be obtained even when the minimum is on the boundary. The properties of the Rayleigh-Ritz method are given below. A detailed discussion is given by several standard authors.[1,2,3,7,12]

Since the Rayleigh-Ritz method is applicable only to self-adjoint systems, the eigenvalues are all real and discrete (Appendix C). Then the eigenvalues of the approximation obtained from Eq. 2.6 are least upper bounds to the true eigenvalues and the n^{th} eigenvalue of Eq. 2.6 lies between the n^{th} and $(n+1)^{th}$ true eigenvalue for <u>any</u> complete set of functions $\phi_n(x)$. In practice, the approximation converges very quickly to the correct eigenvalue. Also, the approximate eigenfunctions converge to the true eigenfunctions although not as quickly as the eigenvalues.

For the Galerkin method the situation is much more complicated. Since the method will always produce a finite number of discrete finite eigenvalues, convergence of the eigenvalues can be meaningful only if the system has discrete finite eigenvalues. But it was shown in Appendix C that the eigenvalues could be continuous or at infinity.

In particular, for pure convective systems only an essential singularity at infinity exists and there are no discrete finite eigenvalues. But it was shown in Appendix C that the eigenvalues could be continuous or at infinity. For a system involving diffusion and convection the author suspects, but has not been able to prove, that both discrete finite eigenvalues and an essential singularity at infinity exist. Thus, the only meaningful statement about convergence is to return to the original problem in the time domain and ask whether in the time domain the approximation obtained from the Galerkin method tends to the true solution as the number of functions is increased. For a limited number of scalar cases this has been demonstrated.[13, 17]

Reasonable answers are obtained with the modified Galerkin method depending on the choice of $\underline{\phi}_n$ and $\underline{\psi}_n$. Particularly useful are simple models of the system and their solutions. It is common practice in elasticity to use the solutions of the constant thickness plate as a set of functions to solve variable thickness plate problems. Similar techniques can be used for systems involving diffusion and convection. It is interesting to note the comment of Courant and Hilbert.[2] "In some cases this method (Rayleigh-Ritz) may prove useful for numerical calculations even though convergence is unproved. Its success in any particular case will depend on the proper choice of coordinate functions $\omega_i(\underline{\phi}_n$ and $\underline{\psi}_n)$." To help in estimating the accuracy of the approximations an effort was made to find bounds on the eigenvalues of a system with diffusion and convection assuming the eigenvalues exist. The results obtained were not very helpful and are given in Appendix B.

F. EXPECTED FORM OF THE EIGENVALUES

It is interesting to consider a simple example to show the form of the approximation. Consider the scalar equation

$$\frac{\partial y}{\partial x} + \frac{\partial y}{\partial t} = 0 \qquad (2.23)$$

with the boundary conditions

$$\begin{aligned} y(x,t) &= 0 \quad \text{all } x, \quad 0 < x \leq 1 \quad \text{and} \quad t > 0 \\ y(0,t) &= u_o(t) \quad \text{all } t \end{aligned} \tag{2.24}$$

The solution to Eqs. 2.23 and 2.24 in the time domain is

$$y(x,t) = u_o(t - x) \tag{2.25}$$

and in the frequency domain

$$y(x,s) = e^{-sx} \tag{2.26}$$

The Galerkin method endeavors to approximate e^{-sx} by a set of poles. This is the much-studied problem of approximating a time delay by a rational function of s in the frequency domain. It is known from the theory of waves along a transmission line that one approximation is the set of poles $s = \pm j n \pi$.

The behavior of pure convective systems such as two-pipe counter flow heat exchangers have many wave-like features as is shown particularly well by the integral series solution (Appendix E). Thus the expected form of the Galerkin or modified Galerkin approximation is a pole to represent the large quantity of dissipation in the system and a set of complex poles whole imaginary parts increase much faster than the real parts. A sketch of such a pole configuration is shown in Fig. 2.1

G. COMPLETE SOLUTION

The complete solution of the problem involves more than obtaining the eigenvectors and eigenvalues of $\underline{A}$ from Eqs. 2.6 or 2.12 or 2.15 since the eigenvectors have an undetermined constant. The method of determining this constant is the same for all three methods. Consider

$$\underline{y}(x,t) = \underline{y}_{ss}(x) + \tilde{\underline{y}}(x,t) \tag{2.27}$$

From the boundary conditions

$$\underline{y}(x,t) = \underline{y}_{ss}(x) \quad \text{as} \quad t \to \infty \tag{2.28}$$

$$\underline{y}(x,t) = \underline{y}_I(x) \quad \text{at} \quad t = 0 \tag{2.29}$$

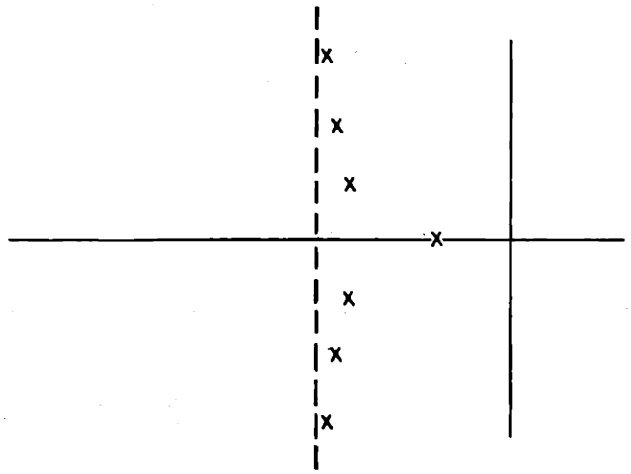


Fig. 2.1 Expected Pole Plot for the Modified Galerkin Method

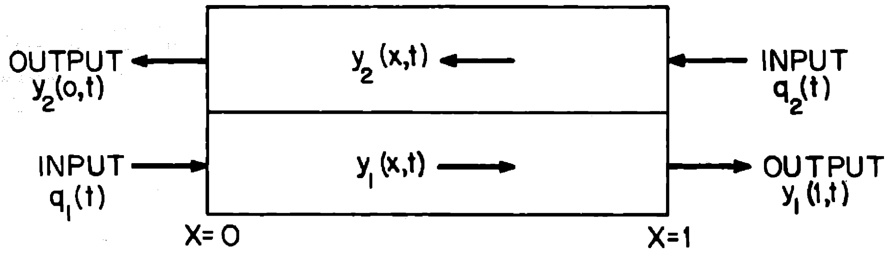


Fig. 2.2 Schematic Diagram of Two-stream Counter-current Convective System

Let $$\underline{y}_D(x) = \underline{y}_I(x) - \underline{y}_{ss}(x) \qquad (2.30)$$

The solution given by Eqs. 2.6 or 2.12 or 2.15 has a set of undetermined coefficients equal to the number of functions $\underline{\phi}_n(x)$. To find these coefficients the known value of $\underline{y}$ at $t = 0$ is used. From Eqs. 2.27, 2.29, and 2.30

$$\tilde{\underline{y}}(x, 0) = \underline{y}_D(x) \qquad (2.31)$$

It is required to express $\underline{y}_D(x)$ as a linear combination of the eigenfunctions. Since the eigenfunctions are themselves linearly independent combinations of a complete set of functions $\phi_n(x)$, they are also complete. To approximate a function by a linear combination of a finite number of terms of a complete orthogonal set is a standard problem in applied mathematics and is often called Fourier expansion.

Let $\gamma_n(x)$ be a complete orthogonal set
and $f(x)$ the function to be approximated

Then let $$c_n = \int_0^1 f(x)\,\gamma_n(x)\,dx \qquad n = 1, \ldots N \qquad (2.32)$$

and $$\bar{f}(x) = \sum_{n=1}^{N} c_n\,\gamma_n(x)$$

and $f(x)$ is approximated by $\bar{f}(x)$. This method of determining the coefficients c_n gives the minimum mean square error between $f(x)$ and $\bar{f}(x)$. Weighting functions can be introduced in Eq. 2.32 to produce weighted mean square error. In this work the minimum mean square error will be used.

It is necessary to approximate each component of $\underline{y}_D(x)$ in its associated functions. Thus to simplify the expressions the following definitions are made.

Let the number of components of $\underline{y}(x)$ be M
the number of functions $\underline{\phi}_n(x)$ be N
$\underline{\xi}_p = (\xi_{p1}, \ldots\ldots \xi_{pN})$ be a column vector
where ξ_{pn} are p^{th} element in n^{th} vector function $\underline{\phi}_n(x)$
$n = 1, \ldots N$
$p = 1, \ldots M$

For example, if $M = 2$ and $N = 3$, then

$$\underline{\Phi}_1 = \begin{pmatrix} \phi_{11} \\ \\ \phi_{12} \end{pmatrix} \quad \underline{\Phi}_2 = \begin{pmatrix} \phi_{21} \\ \\ \phi_{22} \end{pmatrix} \quad \underline{\Phi}_3 = \begin{pmatrix} \phi_{31} \\ \\ \phi_{32} \end{pmatrix}$$

and $\underline{\xi}_1 = \begin{pmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \end{pmatrix} \qquad \underline{\xi}_2 = \begin{pmatrix} \phi_{12} \\ \phi_{22} \\ \phi_{32} \end{pmatrix}$

Let $\underline{k}_p = (k_{p1}, \ldots k_{pN})$ be a set of M constant column vectors.

$\underline{E}$ be a diagonal matrix whole elements are $e^{-s_n t}$
$\underline{C}$ be a matrix whole rows are the eigenvectors.
$\underline{D}$ be a matrix whose rows are the adjoint eigenvectors.

$$\underline{Q}_p = \int_0^1 \underline{\xi}_p(x) \; \underline{\xi}_p^T(x) \, dx \tag{2.33}$$

$$\underline{u}_p^T = \int_0^1 \left[\underline{y}_D(x)\right]_p \underline{\xi}_p^T(x) \, dx \tag{2.34}$$

Then it has been shown (Eqs. 2.6 or 2.12 or 2.15) that

$$\left[\tilde{\underline{y}}(x, t)\right]_p = \underline{k}_p^T \underline{E}\,\underline{C} \, \underline{\xi}_p(x) \qquad p = 1 \ldots M \tag{2.35}$$

and $\underline{k}_p$ are the coefficients to be determined. Putting $t = 0$ in Eq. 2.35 then $\underline{E}$ is the identity matrix and using Eq. 2.31

$$\left[\underline{y}_D(x)\right]_p = \underline{k}_p^T \underline{C} \, \underline{\xi}_p(x) \tag{2.36}$$

Multiply by $\underline{\xi}_p^T(x)$ and integrate over x

$$\underline{u}_p^T = \underline{k}_p^T \underline{C} \, \underline{Q}_p \tag{2.37}$$

Thus the complete solution is

$$[\underline{y}(x,t)]_p = [\underline{y}_{ss}(x,t)]_p + \underline{u}_p^T\, \underline{Q}_p^{-1}\, \underline{C}^{-1}\, \underline{E}\, \underline{C}\, \underline{\xi}_p \qquad (2.38)$$

In computation it is useful to note that $\underline{C}^{-1} = \underline{D}^T$. The second term in Eq. 2.38 can be written as

$$\sum_{n=1}^{N} [\underline{u}_p^T\, \underline{Q}_p^{-1}\, \underline{C}^{-1}]_n\, [\underline{C}\,\underline{\xi}_p(x)]_n\, e^{-s_n t}$$

Then the system poles are s_n and the associated eigenfunctions are

$$[\underline{u}_p^T\, \underline{Q}_p^{-1}\, \underline{C}^{-1}]_n\, [\underline{C}\,\underline{\xi}_p(x)]_n \qquad (2.39)$$

These eigenfunctions give the residues of the poles at each position in the system. The sum of the residues is equal to the error in the Fourier expansion. Put $t = 0$ in Eq. 2.38. Then $\underline{E}$ is the identity matrix and

$$[\underline{y}(x,0)]_p = [\underline{y}_{ss}(x)]_p + \underline{u}_p^T\, \underline{Q}_p^{-1}\, \underline{\xi}_p(x) \qquad (2.40)$$

Hence the accuracy of the solution at $t = 0$ is independent of $\underline{E}$ and $\underline{C}$, i.e., of the eigenvalues and eigenvectors. Thus in the total solution there are two separate sources of error.

1) Error in the eigenvalues and eigenvectors which affects the poles and the residues.

2) Error in the Fourier expansion which affects only the residues.

Sometimes the number of functions needed is determined by the Fourier expansion. To avoid evaluating the residues of poles that have no significant effect on the system dynamics, a modification of Eq. 2.38 is required which permits $\underline{C}$ to be a non-square matrix. The solution can be evaluated if Eq. 2.36 is multiplied by $(\underline{C}\,\underline{\xi}_p)^T$ and integrated. Defining $\underline{u}_p$ as in Eq. 2.37 the solution is

$$[\underline{y}(x,t)]_p = [\underline{y}_{ss}(x)]_p + \underline{u}_p^T\, \underline{C}^T (\underline{C}\, \underline{Q}_p\, \underline{C}^T)^{-1}\, \underline{E}\, \underline{C}\, \underline{\xi}_p$$

(2.41)

since $\underline{C}\,\underline{Q}_p\,\underline{C}^T$ is a square matrix. But this involves finding the inverse of a complex matrix since $\underline{C}\,\underline{Q}_p\,\underline{C}^T$ in general is complex. In Eq. 2.38 this was avoided by using $\underline{C}^{-1} = \underline{D}^T$. However the inverse of $\underline{C}$ can be calculated by noticing that although $\underline{C}$ is a complex matrix each complex row has another row which is its complex conjugate. Let the complex conjugate rows be next to each other. Then

$$\underline{C} = \underline{F}\,\underline{\Gamma} \tag{2.42}$$

There are two cases and the rows of $\underline{\Gamma}$ and $\underline{F}$ will be given for each case.

1) The row of c_{nm} is equivalent to a real eigenvalue

$$F_{nm} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \qquad \text{all } m$$

$$\Gamma_{nm} = c_{nm}$$

2) The rows c_{nm} and $c_{n+1,m}$ are equivalent to a complex conjugate pair of eigenvalues

$$F_{nm} = \begin{cases} 1/\sqrt{2} & n = m \\ j/\sqrt{2} & n = m+1 \\ 0 & \text{elsewhere} \end{cases} \qquad \text{all } m$$

$$F_{n+1,m} = \begin{cases} 1/\sqrt{2} & n = m \\ -j/\sqrt{2} & n = m+1 \\ 0 & \text{elsewhere} \end{cases} \qquad \text{all } m$$

$$\left.\begin{aligned} \Gamma_{nm} &= \sqrt{2}\ \mathrm{Re}\ (c_{nm}) \\ \Gamma_{n+1,m} &= \sqrt{2}\ \mathrm{Im}\ (c_{nm}) \end{aligned}\right\} \qquad \text{all } m$$

Then Eq. 2.41 becomes

$$[\underline{y}(x,t)]_p = [\underline{y}_{ss}(x,t)]_p + \underline{u}_p^T\,\underline{\Gamma}^T\,(\underline{\Gamma}\,\underline{Q}_p\,\underline{\Gamma}^T)^{-1}\,\underline{F}\,\underline{E}\,\underline{C}\,\underline{\xi}_p(x) \tag{2.43}$$

H. SUMMARY OF THEORETICAL RESULTS

Three methods for solving variable coefficient systems were discussed. The Rayleigh-Ritz method is only applicable to self-adjoint systems and cannot be used for convective systems. The Galerkin method is applicable to any system but implies that the system solution and the solution to the adjoint system are expanded in the same set of complete functions. However for pure convective systems this is most unreasonable as there is a simple relationship between a system and its adjoint. The modified Galerkin method makes use of this relation and therefore is the best method for convective systems.

The complete solution is given in Eq. 2.38 and a method of avoiding the need to find the inverse of a complex matrix is developed. The complete solution is also given when some of the eigenvalues are not used. This is useful when it is necessary to use a larger number of functions $\underline{\phi}_n(x)$ to obtain an accurate Fourier expansion than are needed to obtain the dominant poles of the system. Although the form of the solution is more complicated, the matrix algebra can be easily carried out on a computer. An alternative way of obtaining an accurate Fourier expansion is to use a weighted mean square error.

The procedure to carry out the modified Galerkin method can be outlined as follows.

1) Choose sets of functions $\underline{\phi}_n(x)$ and $\underline{\psi}_n(x)$ such that
   a) $\underline{\phi}_n(x) = \underline{\psi}_n(1-x)$
   b) $\underline{\phi}_n(x)$ are complete
   c) $\int_0^1 [\underline{\phi}_n(x)]_i^2 \, dx$ exists for all i
   d) $< \underline{\psi}_n(x), \ \underline{\underline{C}} \, \underline{\phi}_m(x) > \ = \begin{matrix} 0 & n \neq m \\ 1 & n = m \end{matrix}$
2) Evaluate the matrix $\underline{A}$ where

$$A_{nm} = < \underline{\psi}_n(x), \ \underline{\underline{V}} \, \underline{\phi}'_m(x) + \underline{\underline{H}} \, \underline{\phi}_m(x) >$$

3) Evaluate the eigenvalues and eigenvectors of $\underline{A}$
4) Evaluate $\underline{u}_p$ and $\underline{Q}_p$ given by Eqs. 2.33 and 2.34

5) Evaluate the residues given by Eq. 2.39

Frequently it is inconvenient to have to find the combination of $\underline{\phi}_n(x)$ which satisfy 1(d). Since $\underline{\phi}_n$ and $\underline{\psi}_n$ are complete, such a combination can always be found. However, it is simpler in computation to use $\underline{\phi}_n$ and $\underline{\psi}_n$ that satisfy 1(a), (b), (c); then the matrix in 2 becomes $\underline{B}^{-1}\underline{A}$ where

$$\begin{aligned} A_{nm} &= < \underline{\psi}_n(x) , \; \underline{V} \, \underline{\phi}'_m(x) + \underline{\underline{H}} \, \phi_m(x) > \\ B_{nm} &= < \underline{\psi}_n(x) , \; \underline{C} \, \underline{\phi}_m(x) > \end{aligned} \tag{2.44}$$

I. EXAMPLES

To investigate the accuracy of the modified Galerkin method two examples were evaluated. Those examples are two-stream, counter-current, constant-coefficient systems whose solution is known, (Fig. 2.2). When such systems are expressed in normalized, non-dimensional units, the transfer unit is an important parameter which can be used to compare such systems.[37] Just as Reynolds and Prandtl numbers are used to correlate fluid flow experiments under different conditions, so are transfer units used in the dynamics of convective systems.

Consider the single equation

$$cv \frac{\partial y}{\partial x} + c \frac{\partial y}{\partial t} + hy = 0 \qquad 0 \leq x \leq L$$

Let

$$z = \frac{x}{L} \quad \text{and} \quad \tau = {}^{t}/_{T}$$

Then

$$\frac{cv}{L} \frac{\partial y}{\partial z} + \frac{c}{T} \frac{\partial y}{\partial \tau} + hy = 0$$

Let

$$T = \frac{L}{v}$$ then the equations becomes

$$\frac{\partial y}{\partial z} + \frac{\partial y}{\partial \tau} + \frac{hL}{cv} y = 0$$

and

$$N = \frac{hL}{cv}$$ is defined as a transfer unit

If N is large compared with unity, then the system is said to be "long" and a simple lumped approximation is a poor fit to the system dynamics. If N is small compared to unity, a lumped approximation is a good representation of the system dynamics and the system is said to be "short".

The examples were chosen to cover a wide range of transfer units and are based on actual chemical processes. The equations are given in the normalized non-dimensional form

$$\underline{V}y' + s\underline{C}\underline{y} + \underline{H}\underline{y} = 0 \qquad 0\underline{<}x\underline{<}1 \tag{2.45}$$

with boundary conditions

$$\begin{aligned} y_1\,(0,s) &= q(s) \\ y_2\,(1,s) &= 0 \end{aligned} \tag{2.46}$$

and

$$\underline{V} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\underline{C} = \begin{pmatrix} 1 & 0 \\ 0 & \beta \end{pmatrix} \tag{2.47}$$

$$\underline{H} = \begin{pmatrix} +N_1 & -N_1 \\ -N_2 & +N_2 \end{pmatrix}$$

Thus, the time delay down the first stream is one unit of normalized time. In the countercurrent case N_1 is positive while N_2 and β are negative. Sometimes it is desirable to express $\underline{H}$ as a symmetric matrix; then

$$\underline{V} = \begin{pmatrix} \frac{1}{N_1} & 0 \\ 0 & \frac{1}{N_2} \end{pmatrix} \quad \underline{C} = \begin{pmatrix} \frac{1}{N_1} & 0 \\ 0 & \frac{\beta}{N_2} \end{pmatrix} \quad \underline{H} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \tag{2.48}$$

Example A

Water and benzene exchange heat in two concentric pipes in counterflow. The physical data is

Water	Input temperature	150°F
	Flow rate	2000 lbs/hr
Benzene	Input temperature	60°F
	Flow rate	6000 lbs/hr
Pipes	Inside cross-sectional area	0.023 ft^2
	Outside cross-sectional area	0.0206 ft^2
	Surface area per ft. of length	0.6 ft
	Length	280 ft
Heat Transfer Coefficient		48 BTU/hr-ft-°F

This gives a system with

y_1 as water temperature

y_2 as benzene temperature

and $N_1 = 3$, $N_2 = -4$, $\beta = -4$

Example B

Benzene is stripped from a gas by passing through a packed column in counterflow contact with oil. This example is taken from Beusch.[24] The physical data is

Gas	3 per cent benzene by wt at 93.5°F flowing at linear velocity of 13,800 ft/hr
Oil	0.094 per cent benzene by wt at 80°F flowing at linear velocity of 1200 ft/hr
Hold up	0.00484 lb mole/ft
Column	Inside diameter 2.5 ft
	Length 10 ft
	65 per cent available for gas
	3 per cent available for oil
	32 per cent 1 inch Rachig packing rings

Mass transfer coefficient 18.6 lb mole/hr-ft^2 based on the gas phase.

This gives a system where y_1 is the gas mole fraction of benzene divided by the slope of the equilibrium line and y_2 is the liquid mole fraction of benzene. Then

$$N_1 = 8.2, \quad N_2 = -5.6, \quad \beta = -11.5$$

J. RESULTS

The modified Galerkin method was applied to Examples A and B. It was assumed that the boundary conditions were

1) $\underline{y}(x,t) = 0$ for $t<0$, all x

2) $\left.\begin{array}{l} y_1(0,s) = q(s) \\ y_2(1,s) = 0 \end{array}\right\}$ for all t

3) $q(s) = \frac{1}{s}$ i.e., a step disturbance at the input to y_1

From these conditions the steady state was evaluated and is of the form

$$[\underline{y}_{ss}(x)]_1 = a_1 + (1-a_1)e^{px}$$

$$[\underline{y}_{ss}(x)]_2 = a_2e^{p} - a_2e^{px}$$

The transfer function between $\underline{y}(x,s)$ and $q(s)$ can be evaluated by the modified Galerkin method at every position in the system. Two particular responses were evaluated.

$$\frac{y_1(1,s)}{q(s)} \quad \text{and} \quad \frac{y_2(0,s)}{q(s)}$$

These are the responses of the output of each stream to a disturbance at the input of y_1. (Fig. 2.2) The response $\frac{y_1(1,s)}{q(s)}$ is called the long end response since it is the response of y_1 at the end of the system opposite to the disturbance. The response $\frac{y_2(0,s)}{q(s)}$ is called the short end response since it is the response of the output of y_2 at the same end of the system as the disturbance.

These transfer functions have been evaluated algebraically by Gould.[34, 37] This is the most general case in which such an algebraic solution exists. This solution is in the frequency domain and it is impossible to obtain an algebraic solution in the time domain. However, using the integral series approach (Appendis E) the time domain solution can be estimated. The functions $\underline{\phi}_n(x)$ were chosen to be the Taylor diffusion characteristic functions

$$y_1 = e^{px} \sin\omega_n x$$

$$y_2 = e^{px} \sin \omega_n(1-x)$$

This seemed a reasonable choice as the Taylor diffusion characteristic functions are already a reasonable approximation to the system and are complete (Appendix A). This approach is commonly used in elasticity and quantum mechanics. First solve a simpler problem and then use the solution of the simpler problem as a set of $\underline{\phi}_n(x)$ for the more difficult problem. The modified Galerkin method was evaluated with 3, 5, or 7 functions $\underline{\phi}_n(x)$. It was soon clear that an odd number was desirable as the eigenvalues had the expected form of one real and the remainder complex. If an even number is used there are two real eigenvalues, one close to the origin as in the odd case and the other a long way out and of no effect on the system. The results are shown in Figs. 2.3, through 2.11.

It is obvious that the approximation is adequate for the short end response but useless for the long end response. Indeed the more terms that are used the worse the response becomes at high frequency. The long end response is dominated by high frequencies. If the residues of the poles are considered, (Table 2.1) the dominant residue is that of the pole with highest frequency.

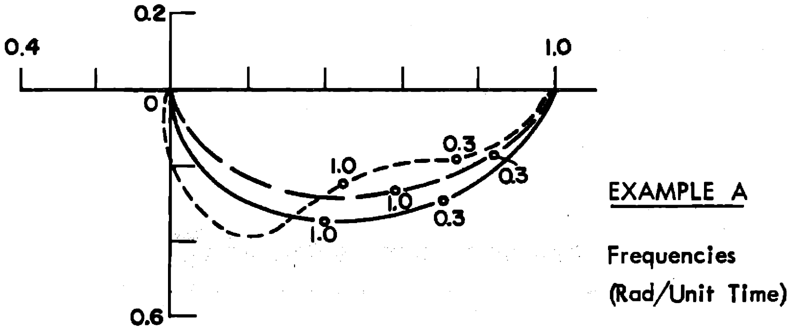


Fig. 2.3 Modified Galerkin Method, Frequency Response $\frac{y_2(0,s)}{q(s)}$ Example A

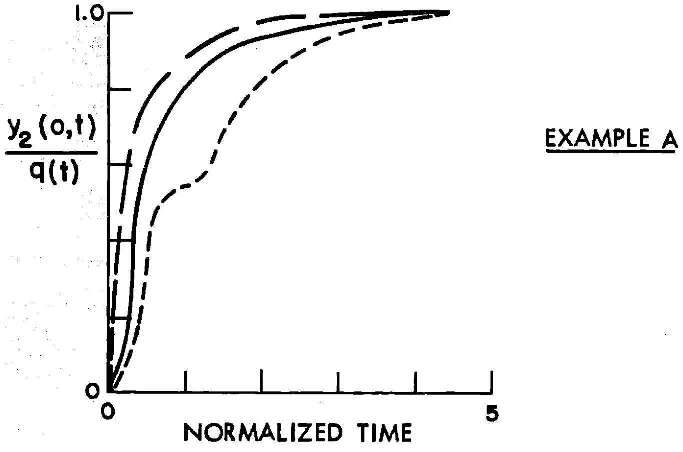


Fig. 2.4 Modified Galerkin Method, Time Response $y_2(0,t)$ Example A

Legend:

——— EXACT TRANSFER FUNCTION

MODIFIED GALERKIN METHOD

- - - - - a) No Diffusion

— — — b) With Diffusion

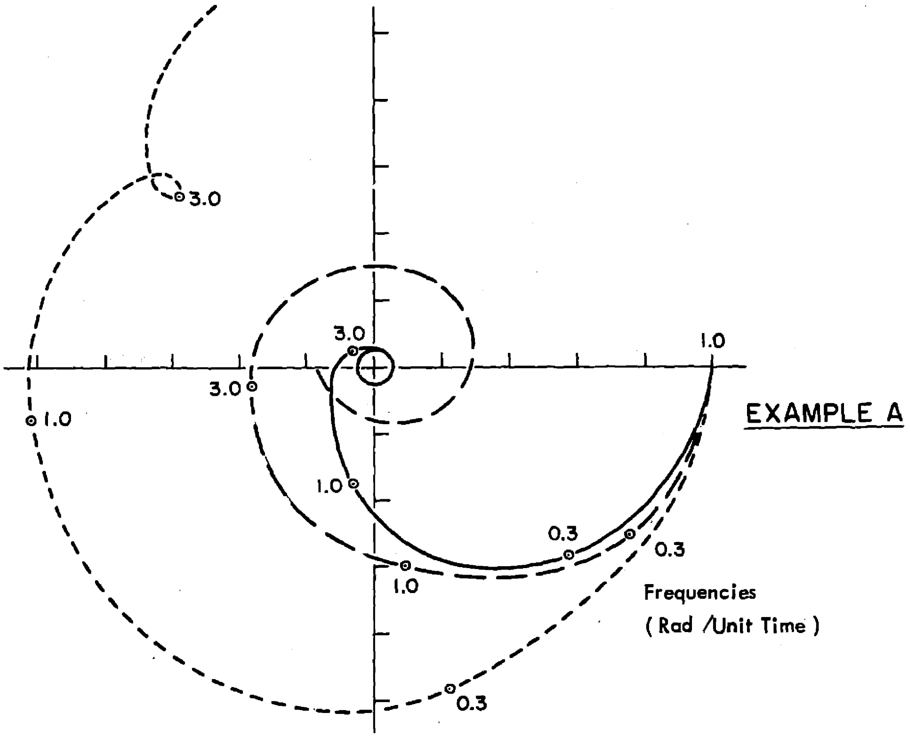


Fig. 2.5 Modified Galerkin Method, Frequency Response $\frac{y_1(1,s)}{q(s)}$ Example A

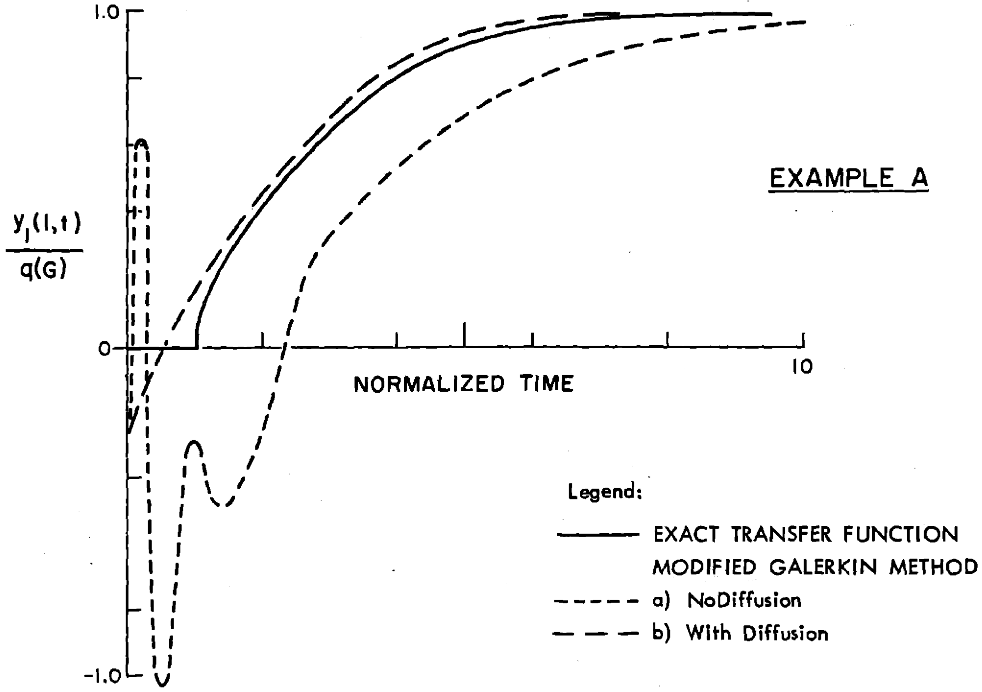


Fig. 2.6 Modified Galerkin Method, Time Response $y_1(1,t)$ Example A

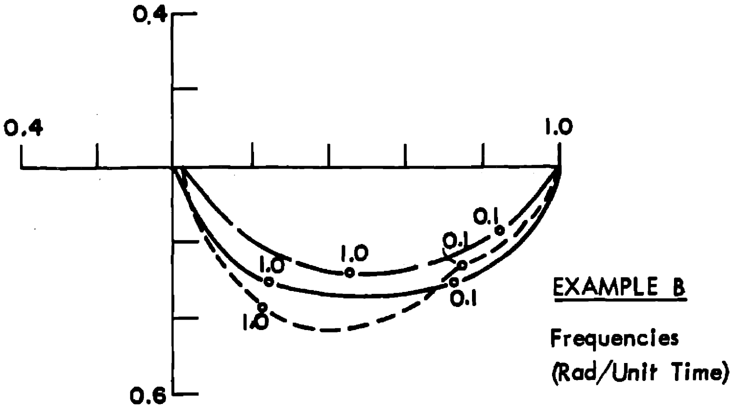


Fig. 2.7 Modified Galerkin Method, Frequency Response $\frac{y_2(0,s)}{q(s)}$ Example B

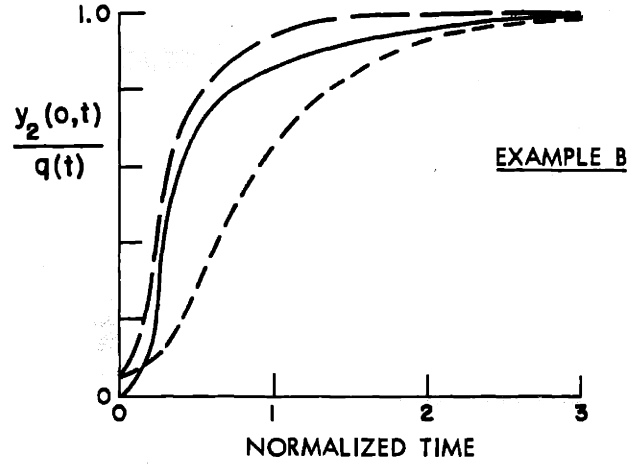


Fig. 2.8 Modified Galerkin Method, Time Response $y_2(0,t)$ Example B

Legend:

——— EXACT TRANSFER FUNCTION

MODIFIED GALERKIN METHOD

- - - - a) No Diffusion

—— —— b) With Diffusion

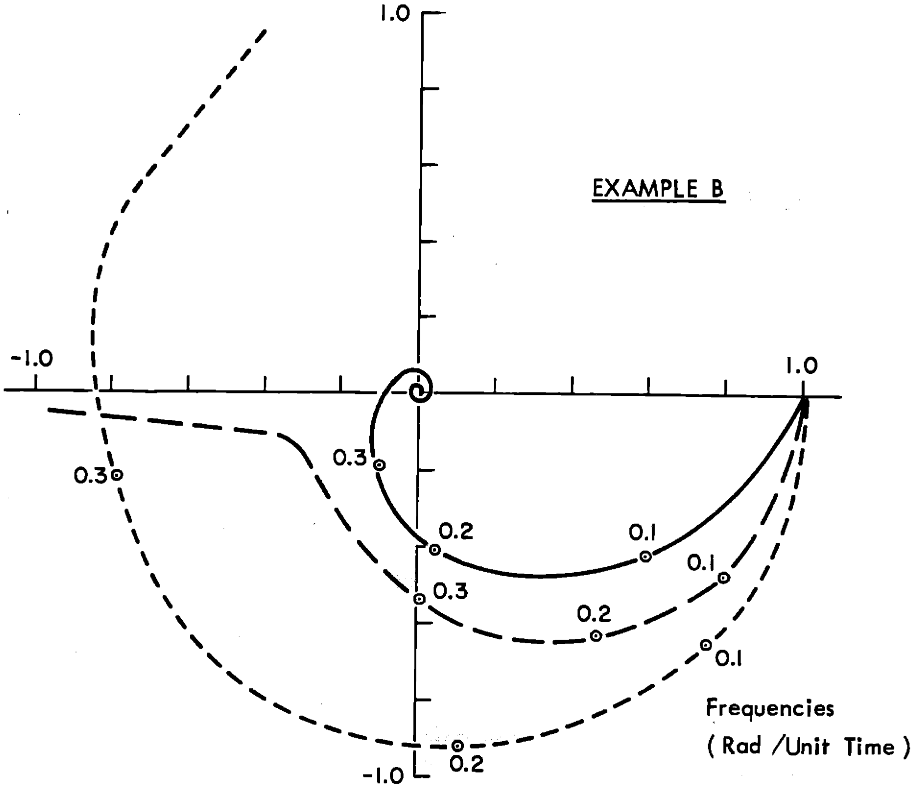


Fig. 2.9 Modified Galerkin Method, Frequency Response $\frac{y_1(1,s)}{q(s)}$ Example B

Legend:

——— EXACT TRANSFER FUNCTION

MODIFIED GALERKIN METHOD

------ a) No Diffusion

— — — — b) With Diffusion

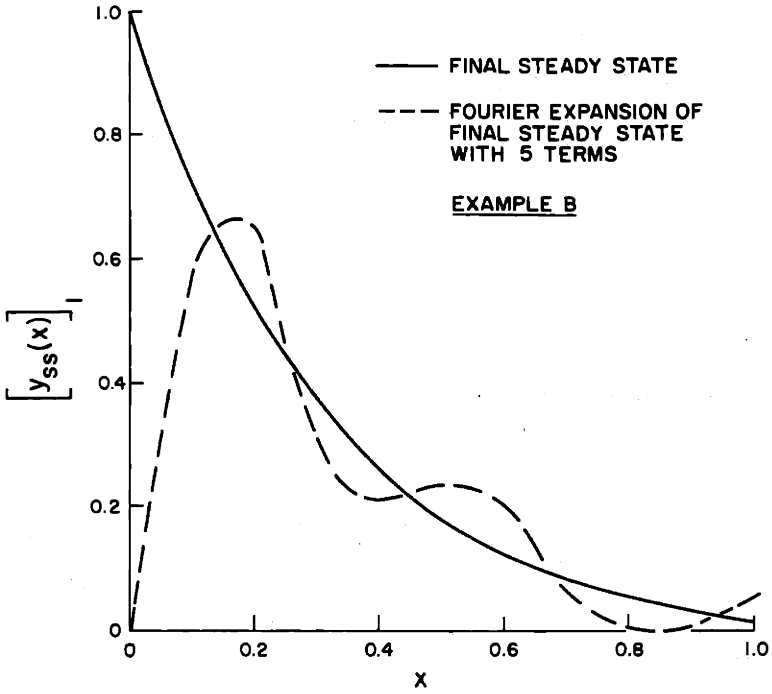


Fig. 2.10 Fourier Expansion of the Steady State, Example B

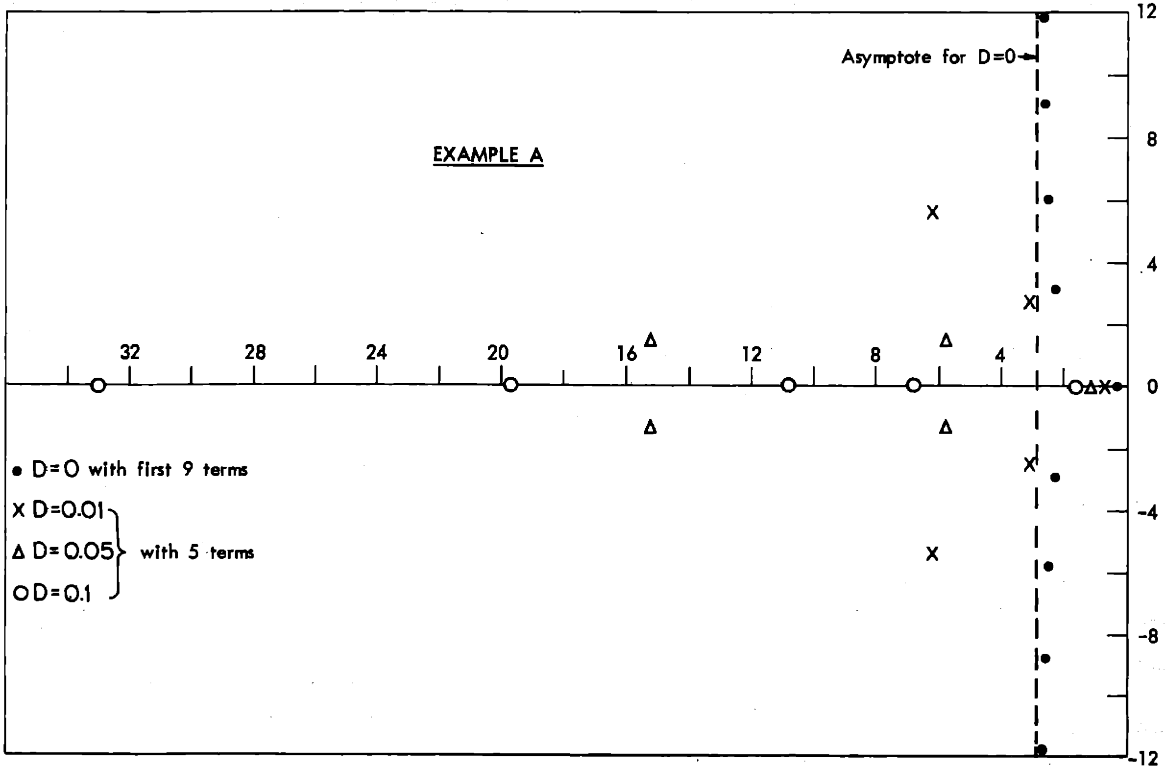


Fig. 2.11 Pole Plot for Example A

Table 2.1

Residues for Example A Long End Response $\frac{y_1(1,s)}{q(s)}$

Pole rad/sec	Residue
0.45	-0.957
2.26 ± j3.03	-0.654 ± j0.385
4.02 ± j5.99	+0.915 ± j1.02

Further, consider the sign of the real part of the residues. The highest frequency pole has a different sign than all the others. To check this result 15 functions were used and still the highest frequency had a different sign to the real part of its residue. Since the sum of the residues is equal to the initial distribution, increasing the number of functions makes the highest frequency more dominant and also tends to make the low frequencies numerically inaccurate. This result is consistent with the fact that the system has no finite discrete eigenvalues, only an essential singularity at infinity. Then, as the number of functions increases to infinity, the system approaches an eigenvalue at infinity with an infinite residue. This is one way of looking at an essential singularity at infinity.

The essential singularity at infinity is similar to a pure time delay. From the time responses it is clear that the time delay is the main source of trouble. The more functions $\underline{\phi}_n$ that are used the larger the oscillations near $t=0$ and the higher their frequency. Clearly, the modified Galerkin model is attempting to approximate a pure time delay with a rational function and this is known to be a difficult problem. However, the response after the time delay is quite adequate. Since the low frequency response is the most important in many applications, it is desirable to modify the method to attenuate the unwanted effects. An obvious way is to add some diffusion to the system. This is considered in the next section.

A second problem is clear from Example B (long response) namely, the gain at $s=\infty$ which is equal to the error in the Fourier expansion of the initial disturbance. In Section G it was shown that this problem is independent of the eigenvalues and eigenvectors. In

Example B the steady state has a very small value at $x = 1$ and the error in the expansion using only 5 functions is very large (Fig. 2.10). One way to avoid this problem is to use more functions. Another possibility is that although the $\underline{\phi}_n(x)$ are complete the initial disturbance is nearly orthogonal to the first few functions. To avoid this it is necessary to change $\underline{\phi}_n(x)$.

A pole plot is shown in Fig. 2.11 for Example A. This entirely agrees with the expectations of Section F and with the asymptotic estimates made in Appendix D.

K. RESULTS WITH DIFFUSION

To attenuate the high frequency effects, some diffusion was added to the system. This reduced the high frequency effects as expected but it also smoothed out the discontinuities. This is entirely to be expected as a system of finite length with diffusion will not propagate discontinuities. The problem is to determine the amount of diffusion necessary to ensure that the high frequency effects are sufficiently attenuated. In Appendix B it is shown that the eigenvalues of a system with diffusion have a bounded imaginary part. In Appendix D the asymptotic values of the eigenvalues obtained from the modified Galerkin method using Taylor characteristic functions (Eq. 2.48) are investigated both with and without diffusion. It is shown that with no diffusion the imaginary parts of the eigenvalues tend to infinity and the real part tends to a finite number. Since the rate of decay of the eigenfunctions is given by the real part of the eigenvalues, this accounts for the importance of the high frequencies. But if the system has some diffusion, however small, the imaginary part of the eigenvalues is bounded and the real part tends to infinity along the negative real axis. The number of functions $\underline{\phi}_n(x)$ that must be used for the real part to be much larger than the imaginary part may be very large if the amount of diffusion is very small, but this result can be used as a method of estimating the diffusion required to attenuate the high frequencies given a fixed number of functions $\underline{\phi}_n(x)$. Let the criteria of a satisfactory system be that the largest eigenvalues have a real part very much larger than the imaginary part. Then if N functions are used, from Appendix D

$$N > > \frac{2}{\pi^2} \frac{\Sigma | V_i |}{\Sigma D_i} \qquad (2.49)$$

where the summation is over the different streams. This assumes that Taylor characteristic functions are used for $\underline{\phi}_n(x)$ and that the Taylor characteristic values ω_i are such that ω_N is close to $(N-1)\pi$ It has been determined experimentally that the inequality of Eq. 2.49 should be satisfied by a factor of at least five. If the highest Taylor characteristic value is more than 30° from $(N-1)\pi$, then a larger factor should be used. When the Taylor characteristic functions are difficult to obtain, it is sometimes convenient to use a complete set based on

$$\sin \frac{2n-1}{2} \pi x \quad \text{and} \quad \sin \frac{2n-1}{2} \pi(1-x)$$

and then a factor of at least eight should be used in Eq. 2.49.

The diffusion is only used to help improve the high frequency performance by modifying the matrix given by the modified Galerkin method. Thus Eq. 2.44 becomes

$$\begin{aligned} A_{nm} &= < \psi_n(x), - \underline{D}\, \phi''_m(x) + \underline{V}\underline{\phi}'_m(x) + \underline{H}\, \underline{\phi}_m(x)> \\ B_{nm} &= < \psi_n(x), \underline{C}\, \phi_m(x) \end{aligned} \qquad (2.50)$$

where $\underline{D}$ is the diagonal matrix containing the added diffusion. No additional boundary conditions are needed and the initial and final steady states which are used to complete the solution (Section G) are unchanged. In Appendix B it is shown that for the eigenvalues to have a bounded imaginary part there must be some diffusion in every stream. However, Eq. 2.49 only gives a value for the sum of the diffusion in all streams. In Appendix C it is shown that the diffusion terms have no effect on the off-diagonal elements of the matrix $\underline{B}^{-1}\underline{A}$ obtained from Eq. 2.50 provided the amount of diffusion in each stream is the same. This relation does not require to be exactly fulfilled as the effect of diffusion on the off-diagonal elements of $\underline{B}^{-1}\underline{A}$ is quite small but it suggests that the amount of diffusion required by Eq. 2.49 be equally divided among all streams.

The results of applying the modified Galerkin method with diffusion to Examples A and B are shown in Figs. 2.3, 2.11. The results show that in the frequency domain the high-frequencies have been heavily attenuated while in the time domain the large oscillations near $t = 0$ have disappeared and the discontinuity has been smoothed over. The addition of diffusion will not solve the problem of the Fourier expansion of the initial disturbance. Only taking more functions $\underline{\phi}_n(x)$, using a weighted mean square error, or using a different set of functions will solve this problem.

The amount of diffusion required by Eq. 2.49 for a small number of functions (between 5 and 9) is several orders larger than the physical diffusion of the system. Thus the additional diffusion is not just the diffusion ignored in assuming a pure convective system. However, it is of the same order as the diffusion implied by both the Taylor diffusion model and by lumping. This will be called the <u>effective diffusion</u> to distinguish it from physical diffusion. In the Taylor diffusion model the entire convective system is replaced by a scalar diffusion equation (Appendix A) and diffusion of this equation is the effective diffusion of the model. In lumping the partial differential equations are replaced by a set of interconnected ordinary differential equations. However, it has been shown [36, 37] that if N lumps are used for a stream with a velocity V, then an effective diffusion D is introduced where

$$D = \frac{V}{2N} \tag{2.51}$$

It is clear that Eqs. 2.49 and 2.51 represent very similar conditions.

It is interesting to note that the only methods which give an approximation to convective system dynamics which are suitable for modal analysis are the Taylor diffusion model, lumping, or the modified Galerkin method. All three methods require an effective diffusion much greater than the physical diffusion. This suggests that an effective diffusion must be introduced to produce an eigenfunction approximation to the system dynamics.

The Taylor diffusion model is only applicable to two-stream constant-coefficient systems. But lumping and the modified Galerkin method can both be used on variable-coefficient systems. The relative advantages of these two methods is largely a matter of personal choice; but the modified Galerkin method does give the eigenfunctions for all values of x and requires the solution of a matrix equation whose order is the same as the number of functions $\underline{\phi}_n(x)$ and is independent of the number of streams. In lumping to obtain a good estimate of the eigenfunctions for all x, at least 10 points will be needed, i.e., 10 lumps in each stream. If the number of streams is M then 10 M-matrix equations must be solved. Thus, lumping requires the solution of a matrix equation of much higher order than that of the modified Galerkin method. This appears to be the main difference between the two approaches.

L. SUMMARY

In this chapter the modified Galerkin method has been developed to obtain a model suitable for modal analysis of a general convective system. It has been shown that to obtain satisfactory results some diffusion must be added. A satisfactory amount of diffusion is

$$\Sigma D_i = \frac{16}{\pi^2} \frac{\Sigma |V_i|}{N}$$

summed over the different streams, where

N is the number of functions $\underline{\phi}_n(x)$ used

V_i is the velocity of each stream

D_i is the required diffusion

This diffusion should be divided equally among all streams so that if there are M streams the diffusion D in each stream is given by

$$D = \frac{16}{MN\pi^2} \sum_{i=1}^{M} |V_i|$$

The steps to be taken in the solution are summarized in Section H and it is necessary to introduce the diffusion into the calculation of the matrix $\underline{A}$.

This method is useful because it gives an eigenvalue and eigenfunction approximation to the dynamics of a general convective system with variable coefficients. Thus it is the basis for modal analysis and for control design following the ideas of Rosenbrock[46] and Murray.[40] The only other possible method for variable-coefficient systems is to use lumping. However, lumping involves matrices of a much larger order, if the eigenfunctions are to be given adequately for all values of x. However, if the main interest is only at one or two positions in the system, typically the outputs, lumping may be a quicker method than the modified Galerkin method. The choice of which method to use in any particular case will depend on personal preferences as well as the control system design philosophy to be pursued, but for many streams the modified Galerkin method does involve lower order matrices and thus less computational problems. However, the recent development by Francis[6] of an accurate and quick computational procedure for solving high-order unsymmetric matrix eigenvalue problems will reduce the problems associated with lumping. Whatever methods are used to obtain an eigenfunction approximation, an effective diffusion several orders larger than the physical diffusion has to be introduced. This is a consequence of the requirement of an eigenfunction model suitable for modal analysis.

The primary contribution of this chapter is the development of a method to obtain an approximation to the dynamics of a convective system with variable coefficients which is suitable for modal analysis.

CHAPTER III

LUMPED CONSTANT SYSTEMS

A. INTRODUCTION

In a large system it is quite common to connect lumped constant or, in chemical engineering terms, stirred tank, systems with distributed systems. To analyze such systems the usual practice is to obtain a lumped approximation to the distributed system and apply the well-developed methods for lumped systems to the resulting model. It will be shown that a lumped system can be considered as a distributed system whose coefficients are impulses in space. Then such a combined lumped and distributed system can be considered as one distributed system with position varying coefficients and solved by the modified Galerkin method. For a large complicated system this will produce a simple approximation with a relatively simple calculation. By using the modified Galerkin method a simple low-order approximation, good at low frequency, can be obtained for any linear plant complex. In Section B the equivalent distributed systems are developed for a single stirred tank and for a plate mass transfer column. As an example an eight-plate absorber was investigated and the results compared with the exact solution of the plate equations. The details are given in Section C.

B. EQUIVALENT DISTRIBUTED SYSTEM

Consider the lumped constant system with equation

$$\dot{y}_o + a y_o = G y_i \qquad (3.1)$$

It will be shown that this is identical to the distributed system

$$\frac{\partial y}{\partial x} + \frac{1}{G} u_o(x - x_n) \frac{\partial y}{\partial t} + \left(\frac{a}{G} - 1\right) u_o(x - x_n)\, y = 0 \qquad 0 \leq x \leq 1 \qquad (3.2)$$

with the boundary condition $y(0) = y_i$ where x_n is any value of x, $0 < x_n < 1$.

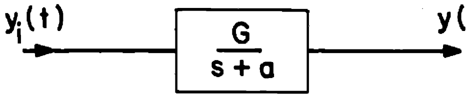


Fig. 3.1 Single Lumped System

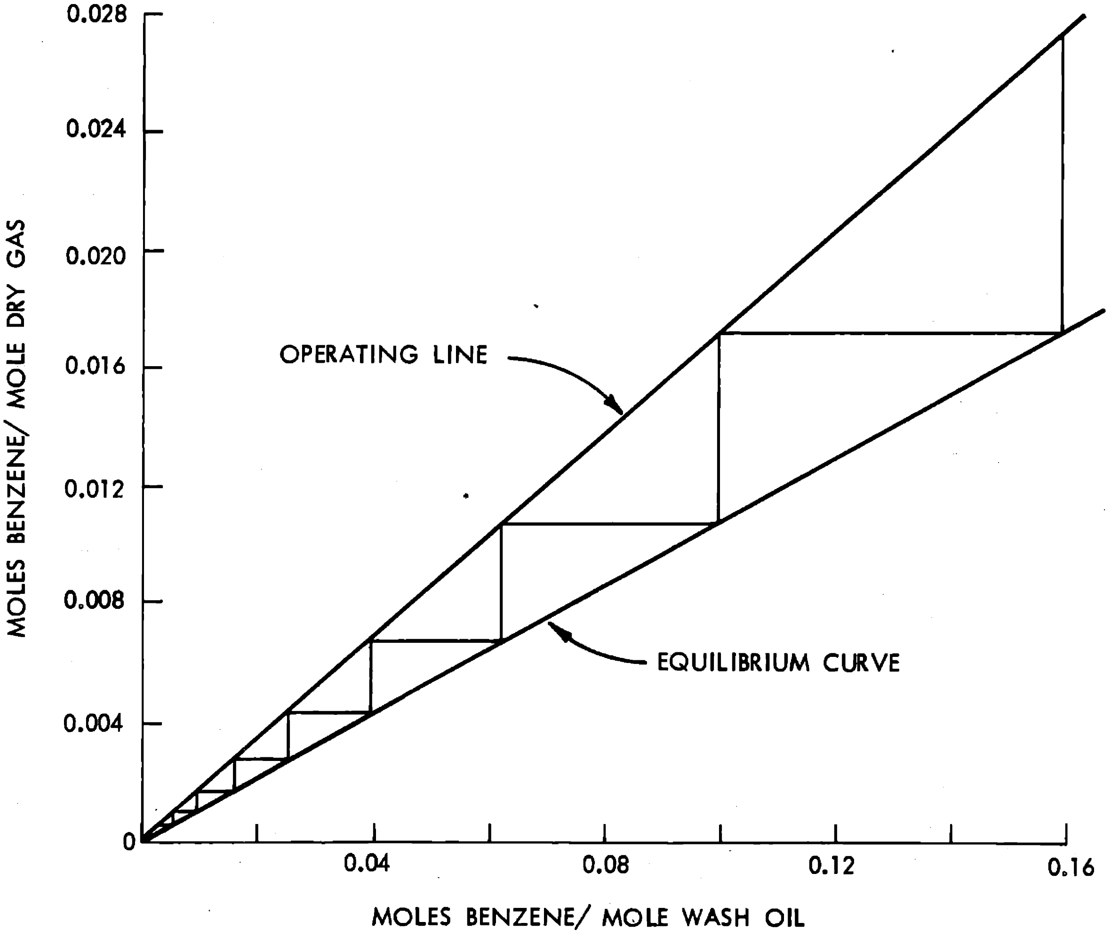


Fig. 3.2 Thiele-McCabe Diagram for Eight-plate Absorber

To prove this, Eq. 3.2 will be integrated over three intervals

1) $0 \leq x \leq x_n^-$

2) $x_n^+ \leq x \leq 1$

3) $x_n^- \leq x \leq x_n^+$

For case (1) we have

$$y(x) = y(0) = y_i \tag{3.3}$$

For case (2) we have

$$y(x) = y(x_n^+) \tag{3.4}$$

For case (3) we have

$$y(x_n^+) - y(x_n^-) + \frac{1}{G}\frac{dy(x_n^+)}{dt} + (\frac{a}{G} - 1)y(x_n) = 0 \tag{3.5}$$

Define $y(x_n) = y(x_n^+)$. This is quite permissible as $y(x_n)$ is clearly undefined at the present. Equation 3.5 gives with Eq. 3.3 and 3.4

$$\frac{dy}{dt} + ay = Gy_i \tag{3.6}$$

Thus the lumped system is considered as a distributed system in which $y(x)$ changes from the input value to the output value as x moves through x_n, and is constant over the intervals,

$$0 \leq x < x_n \text{ and } x_n < x \leq 1$$

It is clear that the value of x_n is arbitrary, and a cascade set of lumped systems can be represented by a series of space impulses along a distributed system. Also the choice of the length of the distributed system is arbitrary and can be chosen in any convenient manner. Usually it is most convenient to let the length of the distributed system be one unit and to arrange the space impulses at equal intervals. In this arrangement the lumped equations of a plate mass transfer column tend to the distributed packed column equations.

For example, consider the equations of a plate mass transfer column.[36] Assuming constant liquid rate and ignoring vapor holdup the equations can be written as (numbering the plates from the top down)

$$H x_r = L\,(x_{r-1} - x_r) + V\,(y_r - y_{r-1})$$
$$y_{r-1} = E\,y^*_{r-1} + (1 - E)\,y_r \qquad (3.7)$$

Where H is the liquid hold up
L is the liquid flow rate
V is the vapor flow rate
E is the efficiency
x_r is the liquid composition leaving the r th plate
y_r is the vapor composition arriving at the r th plate
m is the slope of the equilibrium time

Let $f(x)$ be the vapor/liquid equilibrium curve, then

$$y^*_{r-1} = f(x_r) \qquad (3.8)$$

linearizing

$$y^*_{r-1} = \left.\frac{\partial f}{\partial x}\right|_{ss} x_r = m x_r \qquad (3.9)$$

where m is a function of the plate number. These equations are not quite the usual ones since ordinarily y_r is defined as the vapor leaving the r th plate. For this study it is necessary to define y_r as above since it is desired to express the system as two first order partial differential equations. Such equations can only be obtained from lumped constant equations involving parameters at two positions in space. Physically the definitions used above are equivalent to taking a mass balance about the space between two plates while the usual notation considers a mass balance about a plate.

Equation 3.7 can be represented by the following distributed system, where z is the distance along the column.

$$\underline{V}\frac{\partial \underline{y}}{\partial z} + \underline{C}\frac{\partial \underline{y}}{\partial t} + \underline{H}\underline{y} = 0 \qquad (3.10)$$

where

$$\underline{y} = \begin{pmatrix} x \\ y \end{pmatrix} \quad \underline{V} = \begin{pmatrix} L & 0 \\ 0 & -V \end{pmatrix}$$

$$\underline{C} = \begin{pmatrix} H & 0 \\ 0 & 0 \end{pmatrix} \sum_{r=1}^{n} u_o(z - z_r)$$

$$\underline{H} = \sum_{r=1}^{n} u_o(z - z_r) \begin{pmatrix} EVm(z) & -EV \\ -EVm(z) & EV \end{pmatrix}$$

Note that $m = \left.\frac{\partial f}{\partial x}\right|_{ss}$ is a function of z since $\frac{df}{dx}$ is evaluated at the steady state value of x_r.

These equations demonstrate the essential counter flow nature of the process in the matrix $\underline{V}$. It is easy to show that any process represented by a triple diagonal matrix in its state space is of this form. As the number of plates becomes very large Eq. 3.10 tends to the packed distillation column equations,

$$L\frac{\partial x}{\partial x} + H\frac{\partial x}{\partial t} + k_L(x - x^*) = 0$$

$$-V\frac{\partial y}{\partial z} - k_G(y^* - y) = 0 \qquad (3.11)$$

$$k_G(y - y^*) = k_L(x^* - x)$$

as expected. Thus a complete connection has been made between lumped and distributed systems and the methods proposed to handle position varying distributed systems can also be applied to lumped systems.

If it is necessary to use Eq. 3.7 in the standard notation which involves x_r, x_{r-1}, y_r, y_{r+1}, then a second-order partial differential equation must be used. The second derivative with respect to distance is replaced by $(x_{r+1} + x_{r-1} - 2x_r)$ in the determination of the equivalent lumped model. Such second order partial differential equation can be converted to two first order partial differential equations just as in the case of ordinary differential equations. The main drawback to this form is that it conceals the essential counter-flow nature of the process and is unnecessarily complicated.

Various standard transfer functions and interconnections are shown in Appendix F.

C. ABSORBER

As an example of a lumped system an eight plate absorber is considered. The absorber used is given as an illustration by Treybal.[51] Since Treybal does not give the liquid holdup, the required column size and liquid height on each tray were obtained using the data of Carey.[29] The resulting ratio of liquid holdup to liquid rate is 0.026 hours, a reasonable value. In the absorber, benzene is stripped from a gas by counter flow with a wash oil. Ninety-five per cent removal is required and Henry's Law is assumed. The numerical details are:

Gas	Flow rate	30,000 cu ft/hr
	Av mol. wt	28
	Input benzene	2 per cent by volume
	Density	0.0755 lb/cu ft
Wash Oil	Flow rate	66.7 cu ft/hr
	Av mol. wt	260
	Specific gravity	0.84
	Input benzene	0.005 mole fraction
Column design	Trays	8
	Diameter	5.2 ft
	Tray spacing	20 inches
	Liquid seal	1 inch
	Efficiency	1

Equilibrium data $y = mx$ and $m = 0.12$

where
y is moles benzene/mole dry gas
x is moles benzene/mole wash oil
m the slope of the equilibrium

A Thiele-McCabe diagram is shown in Fig. 3.2.

The system can be represented by Eq. 3.10 where x is replaced by mx so as to make the matrix $\underline{H}$ diagonal.
Then

$$\underline{y} = \begin{pmatrix} mx \\ y \end{pmatrix}$$

$$\underline{V} = \begin{pmatrix} -1.41 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.12}$$

$$\underline{C} = \begin{pmatrix} 0.0372 & 0 \\ 0 & 0 \end{pmatrix} \sum_{r=1}^{8} u_o(z-z_r)$$

$$\underline{H} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \sum_{r=1}^{8} u_o(z-z_r)$$

where

$$z_r = \frac{2r-1}{16} \qquad r = 1 \dots . 8$$

The boundary conditions are

$$x(z,s) = 0 \quad \text{for } z=1$$

$$y(z,s) = q(s) \quad \text{for } z=0$$

To use the modified Galerkin method to solve Eq. 3.10 with the values of Eq. 3.12 it is necessary to introduce some diffusion dependent on the number of terms required. From Eq. 2.49

$$n \gg \frac{2}{\pi^2} \frac{\Sigma |V_{ii}|}{\Sigma D_{ii}} \tag{2.49}$$

Summed over the different streams it was decided to use five functions $\underline{\phi}_n(x)$ and so obtain the first five modes. Hence, for n=5

$$d_1 + d_2 >> 0.1 \tag{3.14}$$

Since the true lumped system has 8 lumps there is an effective diffusion in each stream equal to twice the Peclet number of the stream.[36] The velocities of the streams are 1.41 lb moles/hr on the liquid side and 1.0 lb moles/hr on the gas side. Thus the eight-plate absorber has an effective diffusion

$$d_1 = 0.088 \qquad d_2 = 0.062 \tag{3.15}$$

and

$$d_1 + d_2 = 0.15 \tag{3.16}$$

Clearly, Eq. 3.16 does not adequately satisfy the inequality of Eq. 3.14. It was shown in Chapter II that it is desirable to satisfy Eq. 2.49 by a factor of 8. Then the required diffusion is

$$d_1 = 0.46 \quad \text{and} \quad d_2 = 0.34 \tag{3.17}$$

where it has been divided between d_1 and d_2 in the same proportion as the Eq. 3.15. The functions $\underline{\phi}_n$ used in the modified Galerkin method were

$$\underline{\phi}_n(x) = \begin{pmatrix} \sin \frac{2n-1}{2} \pi x \\ \\ \sin \frac{2n-1}{2} \pi(1-x) \end{pmatrix} \tag{3.18}$$

These were chosen in preference to the Taylor diffusion characteristic functions as they require no additional calculations and the investigations of Chapter II showed that the modified Galerkin method worked satisfactorily with these functions. To apply the Taylor diffusion model it is necessary to replace the 8 plate absorber by an equivalent packed absorber. While this is an entirely reasonable approach for a large number of plates it does not seem that 8 plates is large enough to justify this approximation.

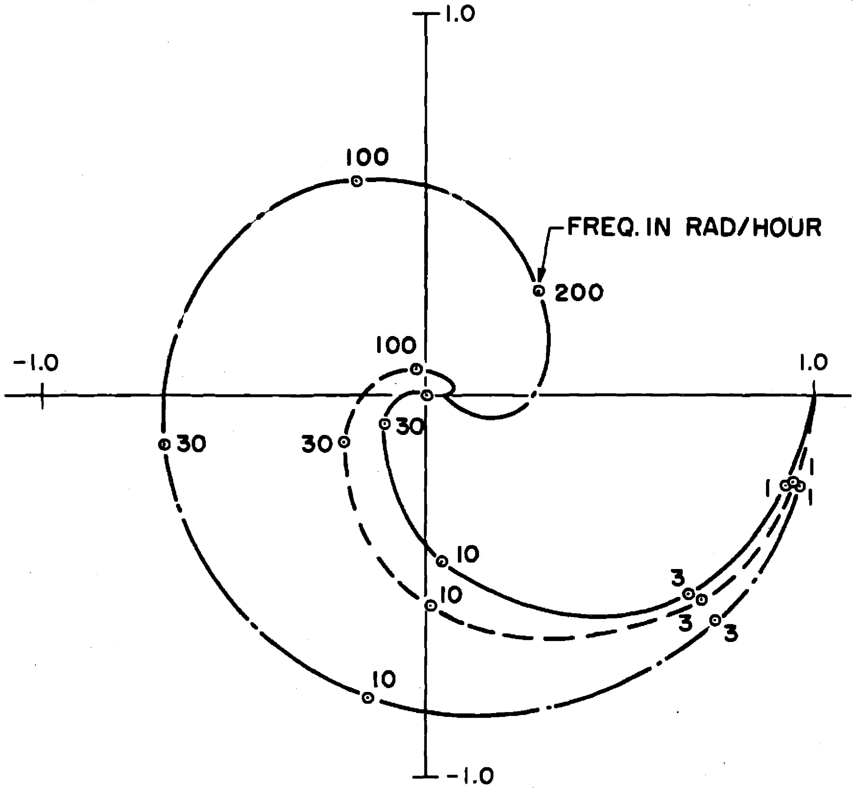


Fig. 3.3 Frequency Response for the Fourth Plate
For a Disturbance in Input Gas Concentration

Legend:

——— EXACT LUMPED RESPONSE

MODIFIED GALERKIN RESPONSE

— — — a) Effective Diffusion of Lumped System

—·— b) Effective Diffusion for 5 terms

In Fig. 3.3 the frequency response of $y(z, s)$ for $z = 1/2$ for a composition disturbance in the gas, $q(s)$, are shown for the exact lumped solution, and for the modified Galerkin method with added diffusion given by both Eq. 3.15 and 3.17. The results are similar to those obtained in Chapter II. More diffusion must be added to obtain a solution using five functions $\underline{\phi}_n(x)$ than is inherent in the eight plate lumped system. In effect the modified Galerkin method is a way of obtaining the first few modes, or eigenfunctions of the lumped system without evaluating the eigenvectors of the lumped system. Whereas this is not difficult for only eight plates it is a considerable undertaking for a hundred plate distillation column.

The most useful application of this approach to lumped systems is to systems consisting of both lumped and distributed elements. Such systems can be considered as a single distributed system and the low frequency behavior of a small plant complex can then be determined by the method described above. The high frequency behavior will not be determined accurately as the modified Galerkin method requires some additional diffusion which alters the high frequency performance. This possible method of investigating plant complexes is dependent on being able to solve variable coefficient convective systems. Thus the modified Galerkin method can handle a large class of nonlinear systems which are operated about the steady state and systems involving both distributed and lumped elements. No methods existed before which could solve these problems. Thus the modified Galerkin method is a powerful method to obtain the dynamics of convective systems such as occur in chemical engineering.

CHAPTER IV

CAMPBELL APPROXIMATION

A. INTRODUCTION

In Chapter II the modified Galerkin method was developed which gave an approximation to the dynamics of a convective system in terms of eigenfunctions and eigenvalues. The form of this approximation is suitable for modal analysis. However, it was necessary to introduce some diffusion to improve the accuracy of the method and it was shown that all the methods that give a form suitable for modal analysis have some effective diffusion which is much larger than the physical diffusion. This effective diffusion must be added because of the difficulties involved in approximating a time delay by a set of poles and their associated residues. But for the application of conventional control theory [38,41] a pure time delay causes no additional difficulty. If conventional control techniques are to be used the transfer functions of the system are required and it is perfectly satisfactory for these transfer functions to contain pure delays. The exact algebraic transfer functions obtained by Gould[37] for the two-stream counter-current constant coefficient system involve a transcendental transfer function which is most inconvenient to use, but a model involving gains, simple poles and zeros, and pure time delays is quite acceptable. This form of the dynamics of chemical systems is not a new idea. Campbell[28] states that any convective system can be satisfactorily modeled in this way, but he did not state how to obtain the numerical values from the system equations. Ziegler and Nichols[52] used two poles and a pure time delay as the process dynamics in their paper on setting the values of a three-term controller. Boyle[25] used a similar form in his investigations of interconnected chemical systems. However, these workers determined the parameters of the transfer functions from the experimental step responses rather than from the system equations.

In this chapter a method is developed to determine from the system equations the required parameters for a model containing only gains, poles, zeros and pure time delays. This model of the system dynamics is called the Campbell approximation. The method can be applied to both constant and variable coefficient systems. No method is available which gives a simple dynamical model in this form. The calculations are easy and can be carried out quite quickly even for variable coefficient systems. Furthermore, the various terms in the model can be directly related to the physical processes. Thus, for a convective system a simple dynamical model can be obtained which does not require elaborate computation. For the application of conventional control design techniques the Campbell approximation is without doubt the quickest and most accurate model to use. One of the main contributions of this work is the development of the Campbell approximation and no methods exist which are both as simple and as accurate.

The Campbell approximation makes use of the best features of the existing methods. At low frequencies the approximation is the same as the Taylor diffusion model or the modified Galerkin method. At high frequencies the approximation approaches the first term of the integral series method. The D.C. gain is always equal to the steady state gain.

The exact form of the Campbell approximation depends on the particular system and on the particular transfer function. The form can be determined from physical considerations and from the mathematical method of obtaining the coefficients. Four principles are used to determine the parameters:

1) The steady state gain is correct $(s = 0)$.
2) The low frequency behavior is represented by a simple first order lag.
3) The high frequency behavior is approximated by the first terms of the integral series.
4) The system does not respond before the arrival of the disturbance. This is called the principle of causality.

Consider a general system with an input disturbance $q(s)$ and consider the transfer function $\frac{y_1(x, s)}{(q(s)}$ where y_i is the i^{th} stream. The transfer function can be divided into two parts, a low frequency portion $L(x, s)$ and a high frequency portion $H(x, s)$. Let $H(x, s)$ have a unit gain at low frequencies, i.e., the steady state gain is included in $L(x,s)$.

$$\frac{y_i(x,s)}{q(s)} = L(x,s)\,H(x,s) \tag{4.1}$$

From the first two principles, the low frequency considerations, $L(x,s)$ has the form

$$L(x,s) = \frac{G(x)}{1+Ts} \tag{4.2}$$

where $G(x)$ is the steady state gain and T is a constant. The pole at $\frac{1}{T}$ is independent of x because the convective system is a system with a large quantity of internal feedback and is analogous to a closed loop control system in which the poles of the system are independent of the particular point in the system being considered.

For high frequencies consider the first term of the integral series $I(x,s)$, then

$$H(x,s) = \frac{Ts}{G(x)}\,I(x,s) \qquad \text{for large } s$$

This result indicates the required form of $H(x,s)$ but is true only for large s, and the exact form of $H(x,s)$ must have unit gain for small s. A typical form for $I(x,s)$ is

$$I(x,s) = \frac{e^{-\gamma x s}\,e^{-bx}}{1+T_\infty s}$$

Then $$H(x,s) = \frac{Tse^{-\gamma x s}\,e^{-bx}}{G(x)\,(1+T_\infty s)} \qquad \text{for large } s$$

Note that large s means that $|Ts| >> 1$ but as T_∞ can be small it is not true that $|T_\infty s| >> 1$. Then the exact form for $H(x,s)$ is

$$H(x,s) = \frac{e^{-\gamma x s}(1+a(x)Ts)}{1+T_\infty s} \tag{4.3}$$

where $$a(x) = \frac{e^{-bx}}{G(x)}$$

Thus the form of the Campbell approximation is

$$\frac{y_i(x,s)}{q(s)} = \frac{e^{-\gamma x s}\,G(x)\,(1+\alpha(x)Ts)}{(1+Ts)\,(1+T_\infty s)} \tag{4.4}$$

Finally, the time delay term $e^{-\gamma x s}$ is checked to see that it satisfies the fourth condition; namely, that the system does not respond before the arrival of the disturbance. This is automatically satisfied for constant-coefficient systems but the delay term has to be adjusted for variable-coefficient systems.

In complicated systems the situation is much more involved. There are essentially two problems, the form of the approximation and the determination of the parameters. Previous work by Campbell,[28] Zeigler and Nichols,[52] and Boyle[25] all assumed a form like Eq. 4.4 which is an obvious choice for simple two-stream constant coefficient systems or any system which is close to such systems. This covers a wide class of problems in heat exchange, distillation and absorption. But the Campbell approximation is applicable to more complicated problems involving reaction, wall effects, and co-current streams. To determine the form of the approximation requires a knowledge of the physical behavior and the concept of a transfer path is most useful.

The transfer path is defined as the way the disturbance is transmitted from the input to any point in the system. It is analogous to the way a wave reaches a point, either directly or by reflection. If a step disturbance occurs at an input, the response at any point in the system can be considered, for time close to zero, as the sum of the responses which have traveled along each transfer path. This concept helps to determine the form of the Campbell approximation and the paths are determined from physical considerations.

In Section B the approximation is developed for a two-stream constant-coefficient, counter-current system and the results compared with the algebraic transfer functions. In Section C the method is extended to variable-coefficient two-stream counter-current systems. In Section D several simple cases are considered so as to help determine the correct form of the approximations for a complicated system. The cases considered are co-current systems, systems with walls, and reversed flow systems. The method of applying the Campbell approximation is summarized in Section E and a procedure for complicated systems is developed. As an application of the model to a complicated process, the dynamics of an ammonia reactor is considered. This reactor has been extensively investigated especially by Eymery[31] who obtained the response of the system to a step disturbance in feed temperature using direct digital simulation. The details of the reactor are given in Section F and the theoretical development of the Campbell model in Section G. The responses obtained from the Campbell approximation are compared in Section H with the responses obtained by Eymery. A summary of the Campbell approximation is given in Section I.

B. CONSTANT-COEFFICIENT COUNTER-CURRENT TWO-STREAM SYSTEMS

To investigate the accuracy of the Campbell approximation it will be applied to a two-stream, constant-coefficient, counter-current system and evaluated numerically for Examples A and B of Chapter II. A schematic of these convective systems is shown in Fig. 4.1. In normalized, non-dimensional form the equations can be written as

$$\begin{aligned} y_1' + sy_1 + N_1(y_1-y_2) &= 0 \\ y_2' + \beta sy_2 + N_2(y_2-y_1) &= 0 \end{aligned} \tag{4.5}$$

Consider a disturbance $q(s)$ at the input of y_1. Then the boundary conditions are

$$\begin{aligned} y_1(0,s) &= q(s) \\ y_2(1,s) &= 0 \end{aligned} \tag{4.6}$$

Following the procedure indicated in the previous section, the low frequency portion of the transfer functions

$$\frac{y_1(x,s)}{q(s)} \quad \text{and} \quad \frac{y_2(x,s)}{q(s)}$$

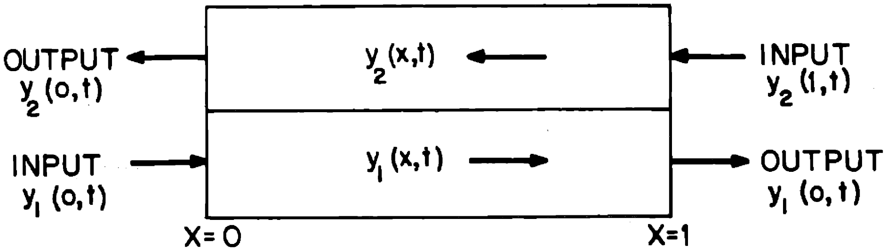


Fig. 4.1 Schematic Diagram of Two-stream, Counter-current Convective System

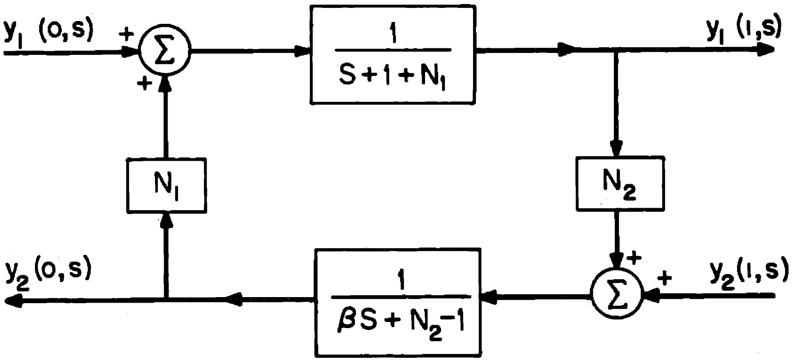


Fig. 4.2 Block Diagram of Single Lumped Model of Two-stream Counter-current Convective System

are given in the form $\frac{G(x)}{1+Ts}$ from Eq. 4.2 where $G(x)$ is the steady state gain of the system.

The value of T can be obtained in three different ways. All the methods give similar results.

1) The dominant time constant of the Taylor diffusion model.
2) The dominant time constant of the modified Galerkin method.
3) The dominant time constant of the system obtained by approximating each stream by one lump.

The Taylor diffusion model is only applicable to constant-coefficient systems and is discussed in Appendix A. The modified Galerkin method can be used with variable-coefficient systems. The details are given in Chapter II. The set of functions $\phi_n(x)$ required for the modified Galerkin method are not critical and the set based on $\sin\frac{2n-1}{2}\pi x$ and $\sin\frac{2n-1}{2}\pi(1-x)$ is quite satisfactory. Best results are obtained if there is no added diffusion to the modified Galerkin method and the first three functions $\phi_n(x)$ will give the dominant pole with sufficient accuracy.

The simplest method is the third method in which each stream is replaced by a single lump. For the two-stream, counter-current, constant-coefficient system a schematic is shown in Fig. 4.1 and the block diagram after lumping in Fig. 4.2. In lumping each stream is replaced by a continuously stirred tank and it is important to notice the direction of flow of each stream. The lumped form of Eq. 4.1 is

$$\begin{aligned} sy_1(1,s) + (N_1+1)y_1(1,s) &= y_1(0,s) + N_1y_2(0,s) \\ \beta sy_2(0,s) + (N_2-1)y_2(0,s) &= y_2(1,s) + N_2y_2(1,s) \end{aligned} \tag{4.7}$$

The poles of a system represented by Eq. 4.7 are

$$s = \frac{1}{2\beta}\left[-(N_2+\beta N_1+\beta-1) \pm \sqrt{(N_2+\beta N_1+\beta-1)^2 + 4\beta(N_1-N_2+1)}\right] \tag{4.8}$$

For a many stream-system Eq. 4.8 can be expressed as a matrix equation. Let the system equations be

$$\underline{V}\underline{y}' + s\underline{C}\underline{y} + \underline{H}\underline{y} = 0 \tag{4.9}$$

Then the dominant time constant T for the Campbell approximation is obtained from the root of the equation, with the smallest magnitude

$$\det (s\underline{C} + |\underline{V}| + \underline{H}) = 0 \tag{4.10}$$

The modulus $|\underline{V}|$ accounts for the direction of flow of the streams.

The reason that the single lumped model gives a reasonable value for the dominant time constant is that counter-current systems are essentially well mixed. If the Campbell approximation is applied to a co-current system, it would be surprising if the lumped model gave the correct dominant time constant of the system. Co-current systems have not been investigated in detail and it would be an interesting case to consider.

To determine the high frequency portion of the transfer function, H(x, s) the first term of the integral series I(x, s) is evaluated and the same procedure followed as in Section A. Let the first term of the integral series I(x, s) be $I_1(x, s)$ for $\frac{y_1(x, s)}{q(s)}$ and $I_2(x, s)$ for $\frac{y_2(x, s)}{q(s)}$

Then
$$I_1(x, s) = e^{-(s+N_1)x} \tag{4.11}$$

$$I_2(x, s) = -e^{-(\beta s+N_2)x} \int_x^1 N_2 e^{[(\beta-1)s + N_2-N_1]x} dx$$

$$= \frac{N_2 e^{-(\beta s+N_2)x}}{(1-\beta)s+(N_1-N_2)} \left[e^{(\beta-1)s + N_2-N_1} - e^{[(\beta-1)s + N_2-N_1]x} \right] \tag{4.12}$$

For a counter-current system N_1 is positive and N_2 and β are negative

Hence
$$e^{(N_2-N_1)} << e^{(N_2-N_1)x} \qquad 0 \le x < 1 \tag{4.13}$$

and

$$I_2(x, s) \simeq \frac{N_2 e^{-(s+N_1)x}}{(1-\beta)s+(N_1-N_2)} \tag{4.14}$$

Thus the complete approximation is given by following Eq. 4.3

$$\frac{y_1(x, s)}{q(s)} = \frac{G_1(x)\ (1 + a_1(x)Ts)\ e^{-sx}}{1+Ts} \tag{4.15}$$

$$\frac{y_2(x, s)}{q(s)} = \frac{G_2(1 + a_2(x)Ts)\ e^{-sx}}{(1+Ts)\ (1+T_\infty s)} \tag{4.16}$$

where G_1 is the steady state gain of $\frac{y_1}{q}$

G_2 is the steady state gain of $\frac{y_2}{q}$

$$a_1 = \frac{e^{-N_1 x}}{G_1} \tag{4.17}$$

$$a_2 = \frac{-N_2 e^{-N_1 x}}{G_2(N_1-N_2)}$$

$$T_\infty = \frac{1-\beta}{N_1-N_2}$$

Equations 4.15 and 4.16 agree with the requirement of causality as the delay in both streams is the same.

To check the accuracy of the approximation the exact algebraic frequency responses were evaluated for the examples considered in Chapter II. Let $H_1(x, s)$ and $H_2(x, s)$ be the analytic response of y_1/q and y_2/q. In Figs. 4.3 through 4.6 the Bode diagrams of

$$\frac{H_1(x, s)\ e^{sx}}{G_1(x)} \quad \text{and} \quad \frac{H_2(x, s)\ e^{sx}\ (1+T_\infty s)}{G_2(x)} \tag{4.16}$$

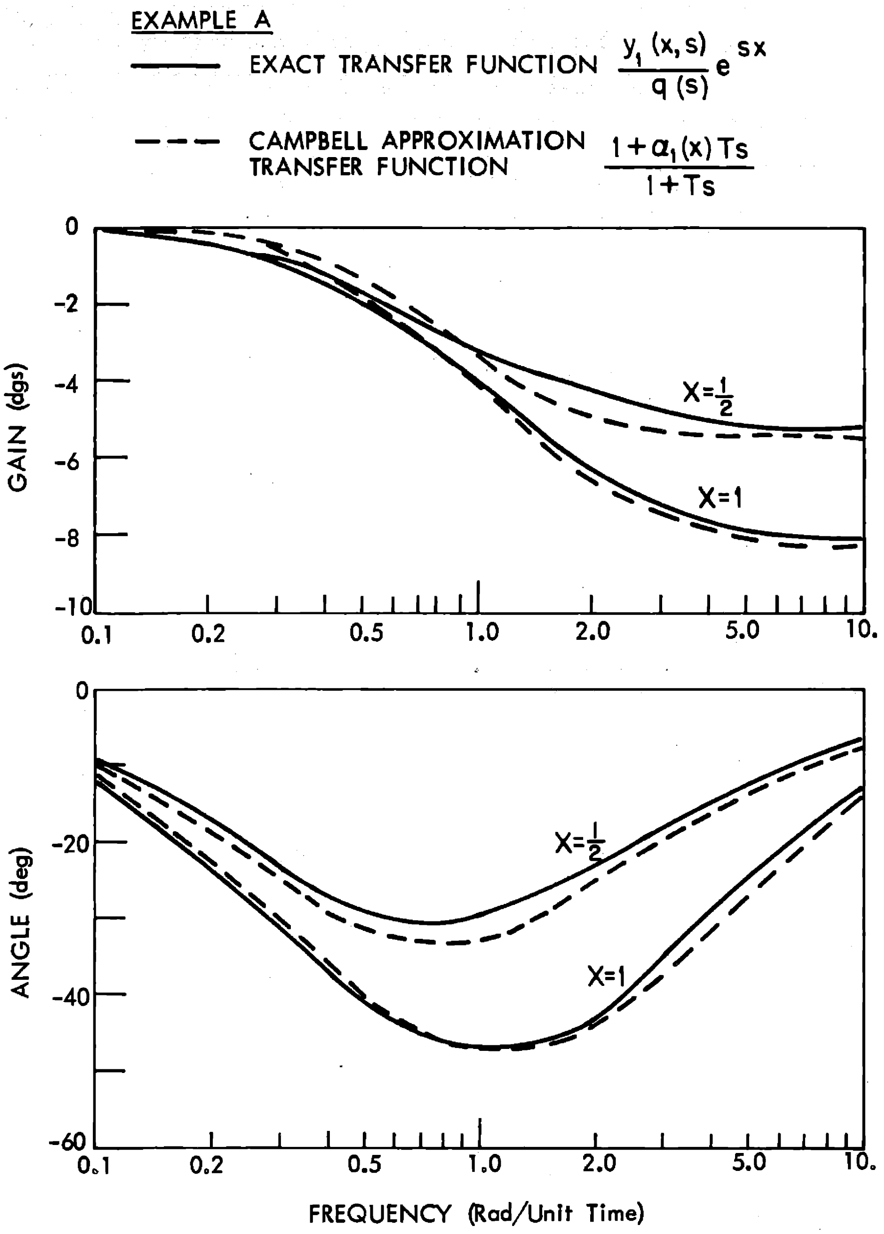


Fig. 4.3 Campbell Approximation, Frequency Response of $\frac{y_1(x,s)}{q(s)}$ Example A

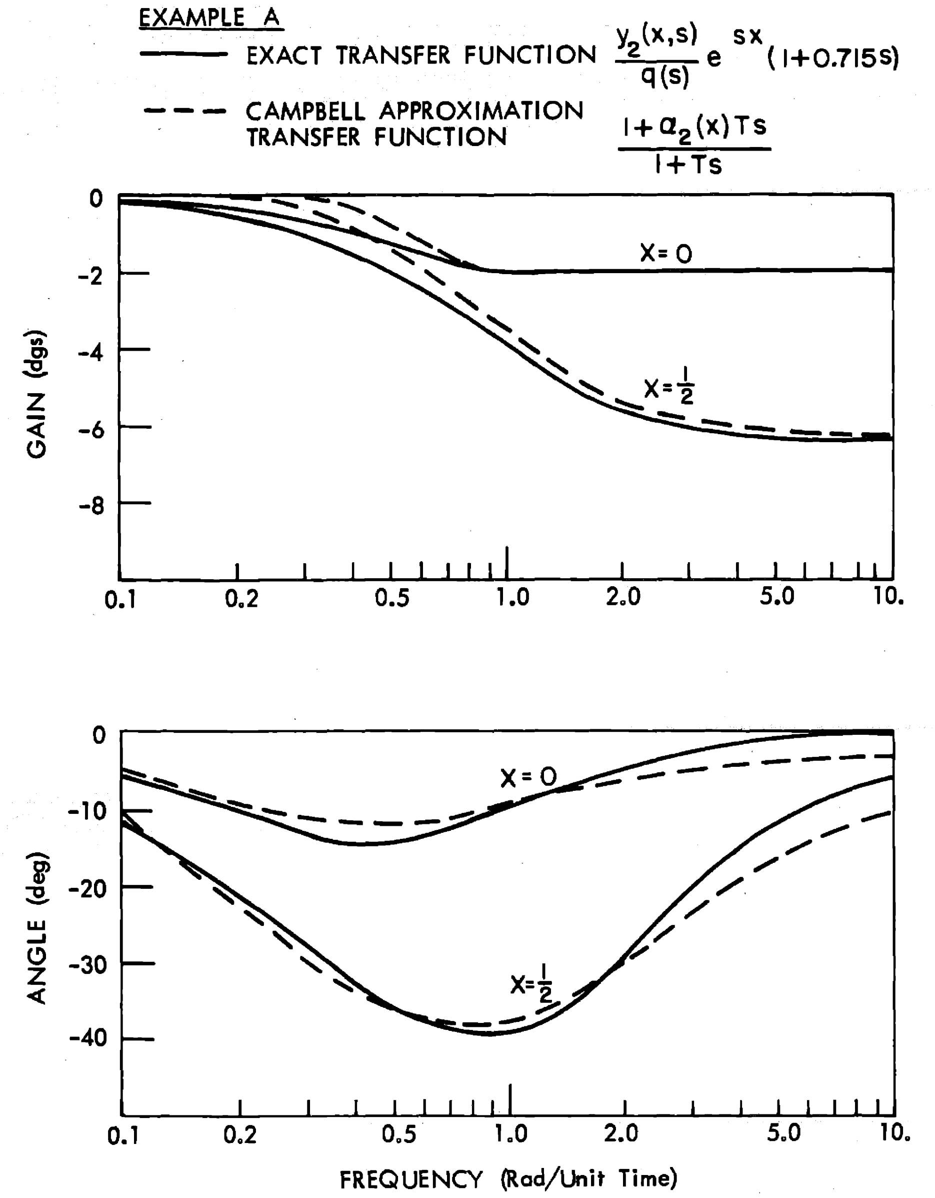


Fig. 4.4 Campbell Approximation, Frequency Response of $\frac{y_2(x,s)}{q(s)}$ Example A

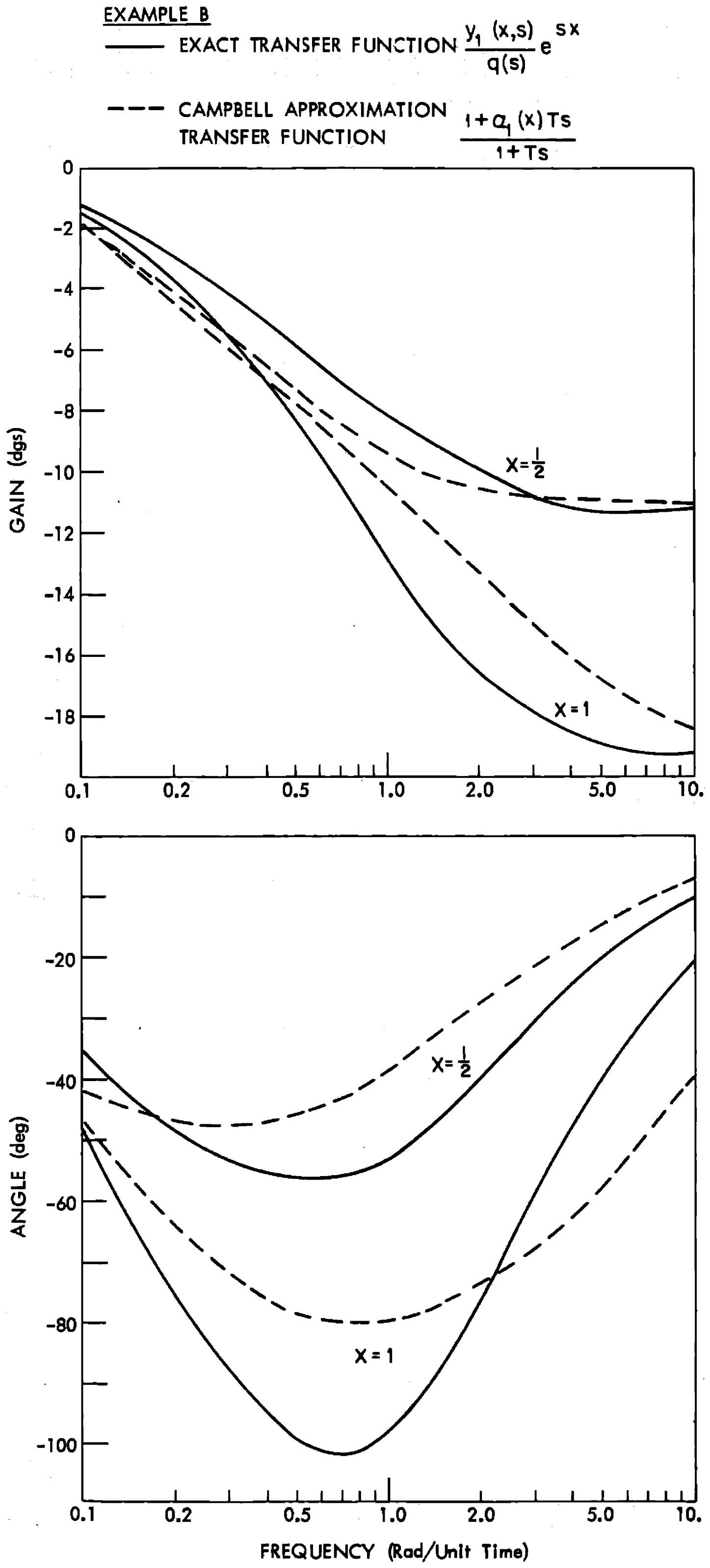


Fig. 4.5 Campbell Approximation, Frequency Response of $\frac{y_2(x,s)}{q(s)}$ Example B

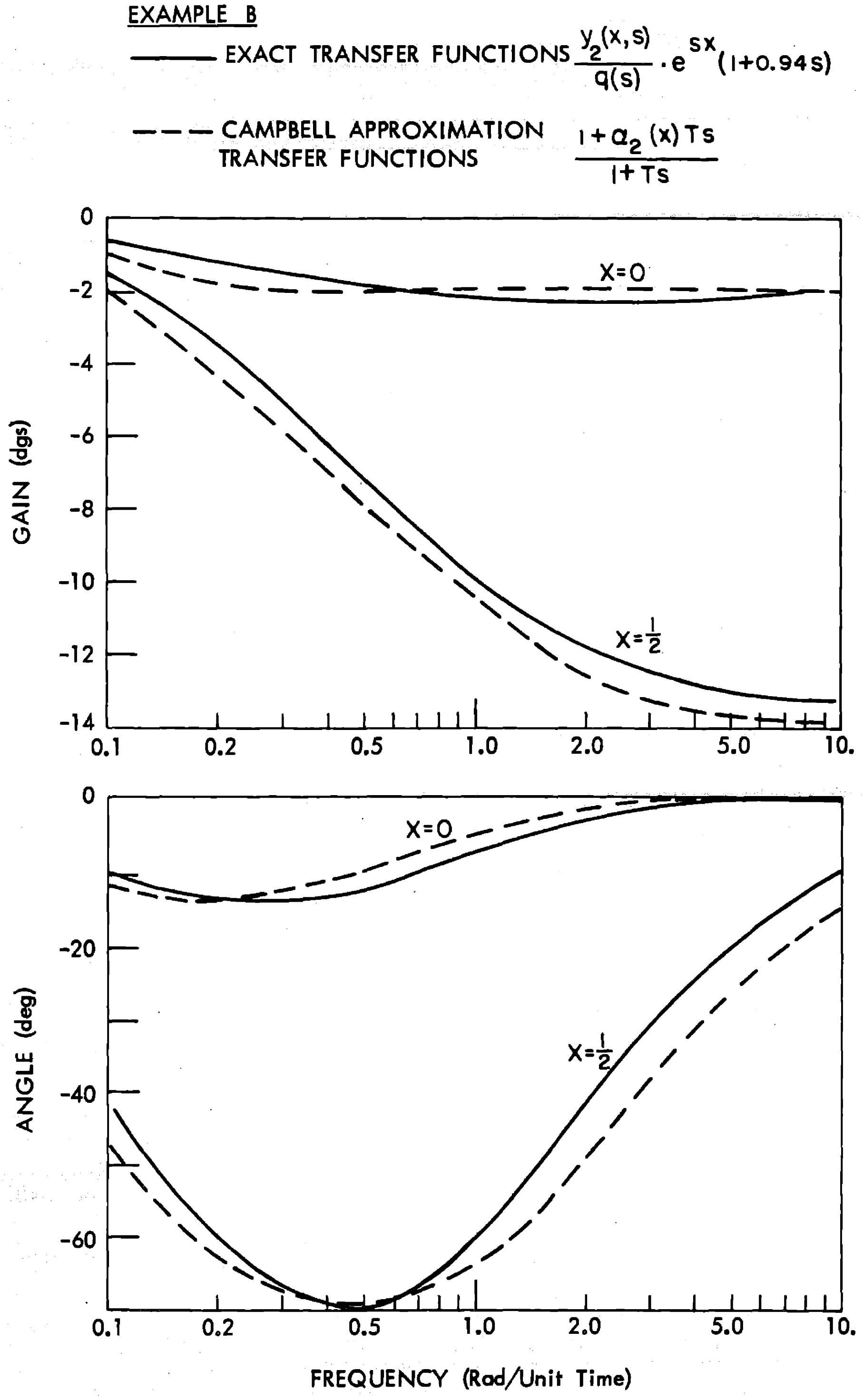


Fig. 4.6 Campbell Approximation, Frequency Response of $\frac{y_2(x,s)}{q(s)}$ Example B

and of $\frac{1+\alpha_1(x)Ts}{1+Ts}$ and $\frac{1+\alpha_2(x)Ts}{1+Ts}$

are plotted. These diagrams clearly show the accuracy of the approximation. The values of T obtained from the modified Galerkin method, Taylor diffusion model, and by lumping are:

Table 4.1

The Dominant Time Constant

Examples	Taylor Diffusion Model	Modified Galerkin Method		Single Lump Model
		Using Taylor Characteristic Functions	Using Sine Functions	
$N_1 = 3$ $N_2 = -4$ $\beta = -4$	2.28	2.25	2.5	2.41
$N_1 = 8.2$ $N_2 = -5.6$ $\beta = -11.5$	11.9	10.6	10.2	8.85

C. VARIABLE-COEFFICIENT TWO-STREAM COUNTER-CURRENT SYSTEM

The Campbell approximation can be applied easily to variable-coefficient systems. The same approach is used as in the previous section.

The gain is equal to the steady state gain. However, the dominant time constant cannot be evaluated by the Taylor diffusion model as this method does not apply to variable coefficient systems. The modified Galerkin method or the lumping technique can be used. In the lumping technique the coefficients must be replaced by their average values. The average of a function f(x) is defined as

$$\bar{f} = \int_0^1 f(x)dx \tag{4.18}$$

Thus, the dominant time constant is obtained from the smallest, in magnitude, root of the equation

$$\det\,(s\underline{\overline{C}} + \underline{\overline{H}} + |\underline{\overline{V}}|\,) = 0 \tag{4.19}$$

when $\underline{C}, \underline{H}, \underline{V}$, are functions of x.

The main problem in the variable-coefficient case is to evaluate the first term of the integral series. To illustrate the procedure consider a two-stream variable-coefficient system with a disturbance $q(s)$ at $y_1(0, s)$. The equations are:

$$v_1(x)y_1' + sc_1(x)y_1 + h(x)\,(y_1 - y_2) = 0 \tag{4.20}$$

$$v_2(x)y_2' + sc_2(x)y_2 + h(x)\,(y_2 - y_1) = 0 \tag{4.21}$$

with boundary conditions

$$\begin{aligned} y_1(0, s) &= q(s) \\ y_2(1, s) &= 0 \end{aligned} \tag{4.22}$$

Hence $$I_1(x, s) = e^{-(\eta_1(x)\,s + \xi_1(x))x} \tag{4.23}$$

where $$\eta_1(x) = \frac{1}{x}\int_0^x \frac{c_1(x)}{v_1(x)}\,dx$$

and $$\xi_1(x) = \frac{1}{x}\int_0^x \frac{h(x)}{v_2(x)}\,dx \tag{4.24}$$

and $$I_2(x, s) = -e^{-(\eta_2(x)s+\xi_2(x))x}\int_x^1 \frac{h(x)}{v_2(x)}\,e^{-[(\eta_1(x)-\eta_2(x))s+\xi_1(x)-\xi_2(x)]x}\,dx \tag{4.25}$$

where $$\eta_2(x) = \frac{-1}{1-x} \int_x^1 \frac{c_2(x)}{v_2(x)}\, dx$$

and $$\xi_2(x) = \frac{-1}{1-x} \int_x^1 \frac{h(x)}{v_2(x)}\, dx \tag{4.26}$$

Equation 4.23 gives the explicit form of $\frac{y_1(x,s)}{q(s)}$ but in Eq. 4.25 the integral must be evaluated. The difficulty of evaluating Eq. 4.25 algebraically is the reason that the integral series is effectively restricted to constant-coefficient systems. Since the integral series approach involves operating on the n^{th} approximation to obtain the $(n+1)^{th}$ approximation it is essential to evaluate the integrals exactly to be able to insure that the method converges (Appendix E). However, in the Campbell approximation, all that is required is an approximate behavior at high frequency. Thus Eq. 4.25 will be integrated by replacing

$$\frac{h(x)}{v_2(x)},\ \eta_1(x),\ \eta_2(x),\ \xi_1(x),\ \xi_2(x)$$

by their average values (Eq. 4.18). Then Eq. 4.25 becomes

$$\frac{y_2(x,s)}{q(s)} = \frac{e^{-(\overline{\eta}_1 s + \overline{\xi}_1)x}}{\overline{\eta_1 - \eta_2}\, s + \overline{\xi_1 - \xi_2}} \left(\frac{\overline{h}}{v_2}\right) \cdot \left[e^{\overline{\eta_1 - \eta_2}\, s - \overline{\xi_1 - \xi_2}} - e^{-\overline{\eta_1 - \eta_2}\, sx}\, e^{-\overline{\xi_1 - \xi_2}\, x} \right] \tag{4.27}$$

But in a counter current system $\overline{\xi}_1$ is positive and $\overline{\xi}_2$ is negative. Therefore

$$e^{-(\overline{\xi_1 - \xi_2})x} \gg e^{-(\overline{\xi_1 - \xi_2})} \quad \text{for } 0 \leq x < 1$$

and the second term of Eq. 4.27 can be neglected. But causality requires that the delay be $e^{-\eta_1(x)xs}$ with an associated attenuation

$e^{-\xi_1(x)xs}$. Hence, Eq. 4.25 can be approximated by

$$\frac{y_2(x,s)}{q(s)} = \frac{e^{-\eta_1(x)sx}\, e^{-\xi_1(x)x}}{\overline{\eta_1-\eta_2}\, s + \overline{\xi_1-\xi_2}} \cdot \left(\frac{\overline{h_2}}{v_2}\right) \tag{4.28}$$

Thus, the approximation is

$$\frac{y_1(x,s)}{q(s)} = \frac{G_1(x)(1+a_1(x)Ts)\, e^{-\gamma(x)s}}{1+Ts} \tag{4.29}$$

$$\frac{y_2(x,s)}{q(s)} = \frac{G_2(x)(1+a_2(x)Ts)\, e^{-\gamma(x)s}}{(1+Ts)\,(1+T_\infty s)} \tag{4.30}$$

where

$$\begin{aligned} \gamma(x) &= \eta_1(x)x \\ a_1(x) &= \frac{e^{-\xi_1(x)x}}{G_1(x)} \\ a_2(x) &= \frac{e^{-\xi_1(x)x}}{G_2(x)(\overline{\xi_1-\xi_2})} \\ T_\infty &= \frac{\overline{\eta_1-\eta_2}}{\overline{\xi_1-\xi_2}} \end{aligned} \tag{4.31}$$

D. THE FORM OF THE CAMPBELL APPROXIMATION

In this section various simple two-stream constant-coefficient systems are investigated to determine the form of their Campbell approximation. These results are useful as a guide to the form of the approximation in a more complicated case. A useful concept is the <u>transfer path</u>. A transfer path is the way a disturbance is transmitted from an input to any point in the system. There can be one or several transfer paths in a system. The transfer paths are similar to the paths a wave travels to reach a point. There is the direct path and there are paths caused by reflections. In convective systems the situation is not as clear cut but a disturbance such as a step change in an input is transmitted to a point in the system in several ways and for times close to $t = 0$ the system response can be considered as the sum of responses caused by different transfer paths. For larger times the responses cannot be separated and the low frequency behavior is like a single time lag, but for high frequencies the system performs like the sum of the responses caused by each of the separate transfer paths. Counter-current systems have only one path which accounts for the simplicity of the results of Section B, but co-current systems have two paths and more involved systems can have several paths. The transfer paths can be determined from physical considerations and are indicated by the first few terms of the integral series method which are used in the Campbell approximation. Thus the mathematical solution is a check that the correct number of transfer paths have been found.

In the examples considered here, the transfer paths are drawn on the schematic diagrams. All cases considered are two-stream constant-coefficient systems.

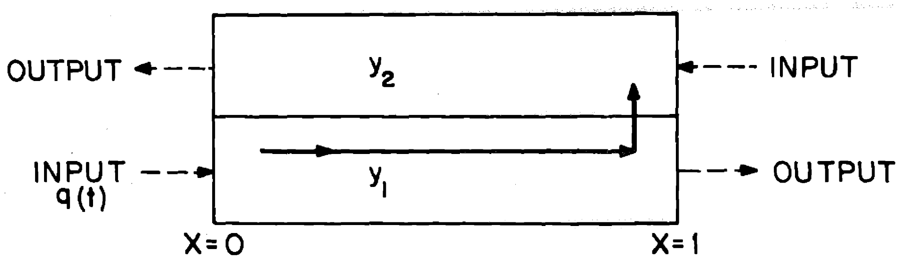
1. Counter-current System

A schematic of the system is shown in Fig. 4.7a. The system has been investigated in Section B and it has been shown that the equations are

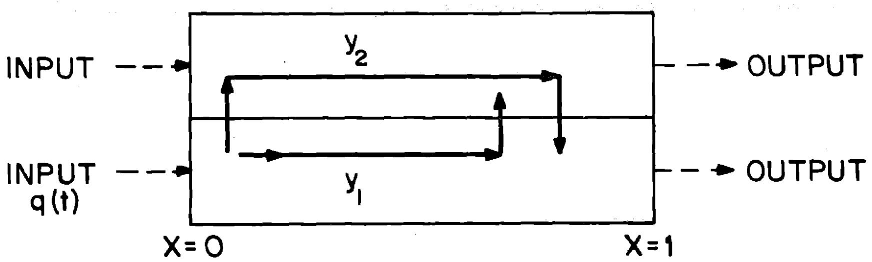
$$\begin{aligned} y_1' + sy_1 + N_1(y_1-y_2) &= 0 \\ y_2' + \beta s y_2 + N_2(y_2-y_1) &= 0 \end{aligned} \tag{4.32}$$

with the boundary conditions

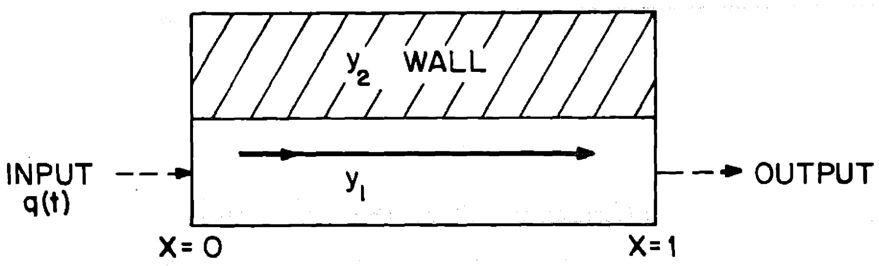
$$\begin{aligned} y_1(0,s) &= q(s) \\ y_2(1,s) &= 0 \end{aligned} \tag{4.33}$$



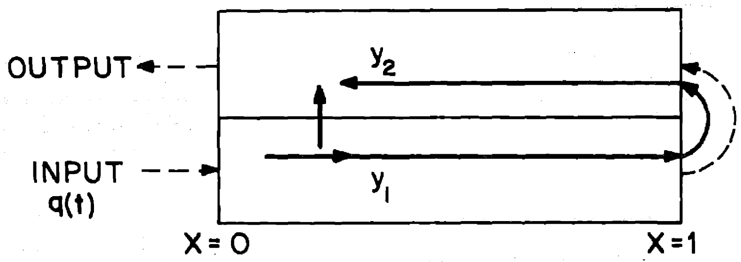
a) Two-stream counter-current system



b) Two-stream co-current system



c) One stream with a wall (Percolation)



d) Two stream reversed flow system

q(t) = The Disturbance

- - → Direction of flow of each stream

——→ Transfer Path

Fig. 4.7 Transfer Paths for Two-stream Systems and N_1 is positive, N_2 and β negative. Then the first term of the integral series is

$$I_1(x,s) = e^{-sx} e^{-N_1 x}$$

$$I_2(x,s) = \frac{-N_2 \; e^{-sx} e^{-N_1 x}}{(1-\beta)s + (N_1 - N_2)} \tag{4.35}$$

Following the same procedure as in Section A, Eqs. 4.34 and 4.35 give the high frequency response while the low frequency response is given by

$$\frac{G(x)}{1+Ts} \tag{4.36}$$

Thus the Campbell approximation has the form

$$\frac{y_1(x,s)}{q(s)} = \frac{G_1(x)\;(1+\alpha_1(x)Ts)\;e^{-sx}}{1+Ts} \tag{4.37}$$

$$\frac{y_2(x,s)}{q(s)} = \frac{G_2(x)\;(1+\alpha_2(x)Ts)\;e^{-sx}}{(1+Ts)\;(1+T_1 s)} \tag{4.38}$$

where G_1 and G_2 are steady state gains

T is the dominant pole

$$\alpha_1(x) = \frac{e^{-N_1 x}}{G_1}$$

$$\alpha_2(x) = \frac{-N_2 \; e^{-N_1 x}}{G_2(N_1 - N_2)}$$

$$T_1 = \frac{1-\beta}{N_1 - N_2}$$

The transfer path in this system is clear. The disturbance is transmitted by convection down the first stream and then through the boundary to the second stream. Since the system is in counter flow any transfer to the second stream at $x = x_1$ $(0 < x_1 < 1)$ cannot affect any point $x > x_1$ except through the first stream. Thus, there is only one transfer path which is indicated in Fig. 4.7a.

2. Co-current System

A schematic is shown in Fig. 4.7b and the system equations are Eq. 4.32 with the boundary conditions

$$\begin{aligned} y_1(0,s) &= q(s) \\ y_2(0,s) &= 0 \end{aligned} \tag{4.39}$$

and N_1, N_2, β are all positive. Using the integral series approach to Eq. 4.32 with the boundary conditions of Eq. 4.39, the first term in the series is

$$I_1(x,s) = e^{-(s+N_1)x} \tag{4.40}$$

$$I_2(x,s) = \frac{N_2}{(\beta-1)s + N_2 - N_1}\left[e^{-(s+N_1)x} - e^{-(\beta s+N_2)x}\right] \tag{4.41}$$

Equation 4.40 gives the form of the Campbell approximation as

$$\frac{y_1(x,s)}{q(s)} = \frac{G_1(x)\,(1+\alpha_1(x)Ts)\,e^{-sx}}{1+Ts} \tag{4.42}$$

where $$\alpha_1(x) = \frac{e^{-N_1 x}}{G_1(x)}$$

Equation 4.41 gives the form of the approximation as the sum of two terms. Sometimes one of the two terms can be neglected depending on the relative magnitude of N_1 and N_2. In general the form of the approximation is

$$\frac{y_2(x,s)}{q(s)} = \frac{G_2(x)\,(1+\alpha_2(x)Ts)}{(1+Ts)\,(1+T_1 s)}\left[e^{-(s+N_1)x} - e^{-(\beta s+N_2)x}\right] \tag{4.43}$$

where
$$a_2(x) = \frac{N_2}{(N_2-N_1)\,G_2(x)}$$

$$T_1 = \frac{\beta-1}{N_2-N_1}$$

The transfer paths for this system are directly down the first stream, and are into the second stream and down the second stream. The relative importance of the two paths is given by the magnitude of the two terms in Eq. 4.41. There are two transfer paths in this case because co-current flow permits the disturbance to be carried down by both streams. Equation 4.43 shows the two terms that occur but if N_2 is much greater than N_1 the second term can be neglected, while if N_1 is much greater than N_2 the first term can be neglected.

To obtain the effect of both transfer paths on y_1 it is necessary to consider the second term in the integral series.

Then

$$I_1(x,s) = e^{-(s+N_1)x}\left[1+\frac{N_1N_2x}{(\beta-1)s+N_2-N_1}+\frac{N_1N_2}{[(\beta-1)s+N_2-N_1]^2}\right] - \frac{N_1N_2\,e^{-(\beta s+N_2)x}}{[(\beta-1)+N_2-N_1]^2} \qquad (4.44)$$

In this expression the first term gives the effect of the direct transfer path through y_1 and the second term the transfer path through y_2.

In the first expression the dominant term is $e^{-(s+N_1)x}$ and the remaining terms can usually be neglected. The second expression has a double pole which is caused by the transfer through the boundary from y_1 to y_2 and back again. From Eq. 4.41 and Eq. 4.44 it is clear that each transfer through a boundary involves a pole and the pole is the same for both directions.

Then a form of the Campbell approximation for y_1 obtained from Eq. 4.44 is

$$\frac{y_1(x,s)}{q(s)} = \frac{G_1(x)}{1+Ts}\left[k_1(1+a_1(x)Ts)e^{-sx} + \frac{k_2(1+a_2(x)Ts)\,e^{-\beta sx}}{(1+T_1 s)^2}\right] \tag{4.45}$$

where
$$T_1 = \frac{\beta-1}{N_2-N_1}$$

$$a_1(x) = \frac{e^{-N_1 x}}{k_1 G_1}$$

$$a_2(x) = -\frac{N_1 N_2\ e^{-N_2 x}}{(N_2-N_1)^2 k_2 G_1}$$

$G_1(x)$ is the steady state gain

T is the low frequency pole

$k_1 + k_2 = 0$

The problem with Eq. 4.45 is that either k_1 or k_2 must be determined. There is no easy way to do this. If $\beta \gg 1$ then the transfer down the direct path arrives first at the point $y_1(x,s)$ and because of the additional double pole in the path through y_2, the dominant effect is caused by the first term in Eq. 4.45. If $\beta \ll 1$ the transfer path through y_2 arrives first at $y_1(x,s)$ and its effect cannot be neglected. A particular case is when $\beta = 0$, i.e., no capacity in the second stream. It is important to remember that in a stream with no capacity any disturbance is instantaneously transmitted through the system. In effect a stream with no capacity is equivalent to a stream with infinite velocity.

Since the second term in Eq. 4.44 is important for the time before the arrival of the effect of the first term and is of less importance later on because of the additional double pole, an alternative form for the Campbell approximation is

$$\frac{y_1(x,s)}{q(s)} = G_1(x)\left[\frac{k_1(1+a_1(x)Ts)\,e^{-sx}}{1+Ts} + \frac{k_2\,e^{-\beta sx}}{(1+T_1 s)^2}\right] \tag{4.46}$$

where

$$T_1 = \frac{\beta-1}{N_2-N_1}$$

$$a_1(x) = \frac{e^{-N_1 x}}{k_1 G_1(x)}$$

$$k_1+k_2 = 1$$

$$k_2 = -\frac{N_1 N_2}{(N_1-N_2)^2 G_1(x)}$$

This is better than Eq. 4.45 as both k_1 and k_2 are determined. It has been found satisfactory for $\beta<<1$, but is not a reasonable form for any other β. If $\beta>>1$ it is satisfactory to ignore the second transfer path and use the result based on the first term of the integral series given by Eq. 4.42.

To summarize, the results for a co-current system are much more complicated because of the two transfer paths. The form of the approximation is given for $\beta>>1$ and $\beta<<1$. However, in the case of β about the same order as unity the exact form is not clear. If $N_1>>N_2$ or $N_2>>N_1$ one of the terms is much smaller and can be neglected and the form of the approximation is clear. If β is close to unity and N_1 close to N_2 it is best to use the complete solution for $\beta=1$, and $N_1 = N_2 = N$, namely

$$\frac{y_1(x,s)}{q(s)} = \left[e^{-sx}\,\frac{1}{2} + \frac{1}{2}\,e^{-2Nx}\right]$$

$$\frac{y_2(x,s)}{q(s)} = \left[e^{-sx}\,\frac{1}{2} - \frac{1}{2}\,e^{-2Nx}\right]$$

Then the Campbell approximation is based on a pure delay with an associated attenuation.

3. One Stream with a Wall

The system consisting of one stream and a wall is the case of a two-stream system with zero velocity in one stream. This is equivalent to $\beta = \infty$ in the co-current system. But it is necessary to solve this problem separately to avoid dividing by infinity. A schematic is shown in Fig. 4.7c.

The equations are

$$\begin{aligned} y_1' + sy_1 + N_1(y_1 - y_2) &= 0 \\ sy_2 + N_2(y_2 - y_1) &= 0 \end{aligned} \qquad (4.47)$$

with the boundary condition $y_1(0, s) = q(s)$. There is only one transfer path down y_1 but there is a secondary effect caused by the wall. The first term of the integral series is

$$I_1(x, s) = e^{-(s+N_1)x}$$

This gives the usual form of the Campbell approximation shown in Eq. 4.37 and 4.42. The second term in the integral series is

$$I_1(x, s) = \frac{e^{-(s+N_1)x}(s+N_2+N_1N_2x)}{(s+N_2)} \qquad (4.48)$$

This shows there is only one transfer path as the integral series is not the addition of two terms with different lags. The wall produces a secondary effect of a pole and a zero shown in Eq. 4.48. If it is necessary to introduce this effect into the Campbell approximation the required form is

$$\frac{Y_1(x, s)}{q(s)} = \frac{G_1(x)\,(1+\alpha_1(x)Ts)\,(1+T_2(x)s)\,e^{-sx}}{(1+Ts)\,(1+T_1 s)} \qquad (4.49)$$

where
$$T_1 = \frac{1}{N_2}$$

$$T_2 = \frac{1}{N_2+N_1N_2x}$$

$$a_1(x) = \frac{e^{-N_1x}}{(1+N_1x)\,G_1(x)}$$

When the wall capacity is of the same order as the stream capacity the wall effect cannot be ignored and the additional terms should be included in Eq. 4.49. If the wall capacity is much smaller than the stream capacity then Eq. 4.48 gives a satisfactory form. If the wall capacity is much larger than the stream capacity then it has been shown by Gould[37] from considering the exact solution that the system is equivalent to a stream with the wall capacity and a wall with zero capacity.

4. Reversed Flow System

Another simple example is a two-stream system in which the output of one stream is the input to the next stream. A schematic diagram is shown in Fig. 4.7d. The equations are

$$y_1' + sy_1 + N_1(y_1-y_2) = 0$$

$$y_2' + \beta sy_2 + N_2(y_2-y_1) = 0$$

with the boundary conditions

$$y_1(0,s) = q(s)$$

$$y_2(1,s) = y_1(1,s)$$

There are two transfer paths in this system. The first is down the first stream and back along the second stream, and the second is through the boundary. For y_1 there is only one transfer path as the effect of y_2 is carried out of the system. This is because the system is in counter-flow. However, for y_2 both transfer paths affect the performance. The first terms in the integral series for y_1 and y_2

are

$$I_1(x, s) = e^{-(s+N_1)x}$$

$$I_2(x, s) = \frac{-N_2 e^{-(s+N_1)x}}{(1-\beta)s+N_2-N_1} + e^{-(\beta s+N_2)(1-x)} e^{-(s+N_1)} \qquad (4.50)$$

Thus the standard form of the Campbell approximation holds for y_1 (Eq. 4.37). For y_2 the same problem exists as in the co-current system. The best form is given by assuming that the main effect is caused by the transfer path down the first stream. Then the form of the Campbell approximation is

$$\frac{y_2(x, s)}{q(s)} = G_2(x) \left[k_1 \frac{(1+\alpha_2(x)Ts)}{1+Ts} e^{-s-\beta(1-x)s} + \frac{k_2 e^{-sx}}{1+T_1 s} \right]$$

where

$$T_1 = \frac{1-\beta}{N_2-N_1}$$

$$\alpha_2(x) = \frac{e^{-N_1-N_2(1-x)}}{k_1 (G_2(x)} \qquad (4.51)$$

$$k_1+k_2 = 1$$

As in the co-current system the problem is to choose k_2. In the co-current case k_2 is made equal to the gain of the appropriate term in Eq. 4.50. Thus,

$$k_2 = \frac{-N_2 e^{-N_1 x}}{(N_2-N_1) G_2(x)} \qquad (4.52)$$

However, it has been found that the value of k_2 given by Eq. 4.52 is usually too small. The main reason for this is that until the arrival of the effect of the first term in Eq. 4.51 the system behaves as if the transfer path through the boundary were the only effect. Thus, the response during this time is as if the first term did not exist. The steady state to which the response is moving is the steady state without the reversed flow at $x = 1$. This steady state can be found by changing the boundary conditions to

$$y_1(0,s) = q(s)$$

$$y_2(1,s) = 0$$

The steady state of y_2 under these conditions

$$y_2(x) = \frac{N_2\left[1-e^{(N_1+N_2)(1-x)}\right]}{N_2-N_1\,e^{N_1+N_2}}$$

and the value of k_2 is

$$k_2 = \frac{N_2\left[1-e^{(N_1+N_2)(1-x)}\right]}{G_2(x)\,N_2-N_1e^{N_1+N_2}} \qquad (4.53)$$

The reason that the value of k_2 given by Eq. 4.53 is different from that of Eq. 4.52 is that the integral series first term does not give a good estimate of the steady state gain except for systems with a number of transfer units much less than unity. It would be desirable to obtain an alternative form of k_2 for the co-current case but there is no way to separate the effects of the two transfer paths. Only for the special case of reversed flow is it possible to obtain the value of k_2 by some means other than the integral series.

E. SUMMARY OF THE CAMPBELL APPROXIMATION

The previous sections have discussed in detail the application of the Campbell approximation to several simple examples and the application to variable-coefficient systems. The concept of a transfer path has been introduced. To apply the method to a complicated system it is desirable to list the steps to be taken. At all stages engineering judgement must be used to check the validity of the approximation but the cases considered in Section D give an indication of what form to expect. The procedure is as follows:

1) Draw a schematic of the system
2) Determine the transfer paths
3) Determine the steady state gain
4) Evaluate the first term of the integral series, making sure that all the transfer paths appear in the expression. If the first term does not include all the transfer paths, evaluate additional terms of the integral series.
5) Determine the simple time lag from any of the follow-methods, if applicable.
    a) Taylor diffusion model
    b) Modified Galerkin method
    c) Single lump approximation
6) Form the Campbell approximation by joining the low frequency and high frequency parts together. In the case of more than one transfer path it is necessary to estimate the gain of each path. The results of Section D give an indication of how this can be done, but there is no firm rule in these cases.
7) Check that the model does not permit the system to respond before the disturbances arrive. Adjust the time delays and associated attenuations accordingly. This has to be done because of the error introduced by averaging in evaluating the integrals in the integral series applied to variable-coefficient systems.

In systems with several transfer paths it is helpful to consider the magnitude of the various terms in the integral series. If one term is clearly dominant,the others can be neglected which simplifies the approximation. This is discussed in the case of the co-current system (D.2). In all cases engineering judgement should be used to determine whether a term is worth including or not.

Useful rules to assist in estimating the form of the approximation from the transfer paths are that each time a boundary is crossed the system has a pole and that pole is the same whichever direction the boundary is crossed, and the form is the sum of a number of terms equal to the number of transfer paths.

F. AMMONIA REACTOR

The performance of an ammonia reactor of the Haber-Bosch form, frequently called the T.V.A. ammonia reactor, has been widely studied by several authors.[26, 31, 39, 43, 48] In particular, Eymery[31] investigated in detail the dynamic behavior of the system. The accuracy of the Campbell approximation for a complicated non-linear system is investigated by applying the technique to the ammonia reactor and comparing the behavior with Eymery's results. The results are most encouraging and suggest that the Campbell approximation is a useful method for complicated systems.

In the T.V.A. ammonia reactor a mixture of hydrogen, nitrogen and inert gases are passed over a catalyst and react to produce ammonia. To heat the gas to the required input temperature the input gas is passed through the catalyst bed in tubes, thus exchanging heat with the reacting gases. A diagram of a typical reactor is shown in Fig. 4.8. The reactor can be considered as a four-variable, convective system whose variables are the ammonia concentration in the catalyst, the catalyst temperature, the reactor wall temperature and the input temperature (Fig. 4.9). Eymery developed, from material and energy balances, four partial differential equations to describe the reactor. These can be written as

$$-d_1 \frac{\partial^2 y_1}{\partial x^2} + v_3 \frac{\partial y_1}{\partial x} + c_1 \frac{\partial y_1}{\partial t} + h_{11} y_1 + h_{13} y_3 + h_{14} y_4 = 0$$

$$v_2 \frac{\partial y_2}{\partial x} + h_{22} y_2 + h_{23} y_3 = 0$$

$$c_3 \frac{\partial y_3}{\partial t} + h_{31} y_1 + h_{32} y_2 + h_{33} y_3 = 0$$

$$v_4 \frac{\partial y_4}{\partial t} + h_{41} y_1 + h_{44} y_4 = 0 \qquad (4.54)$$

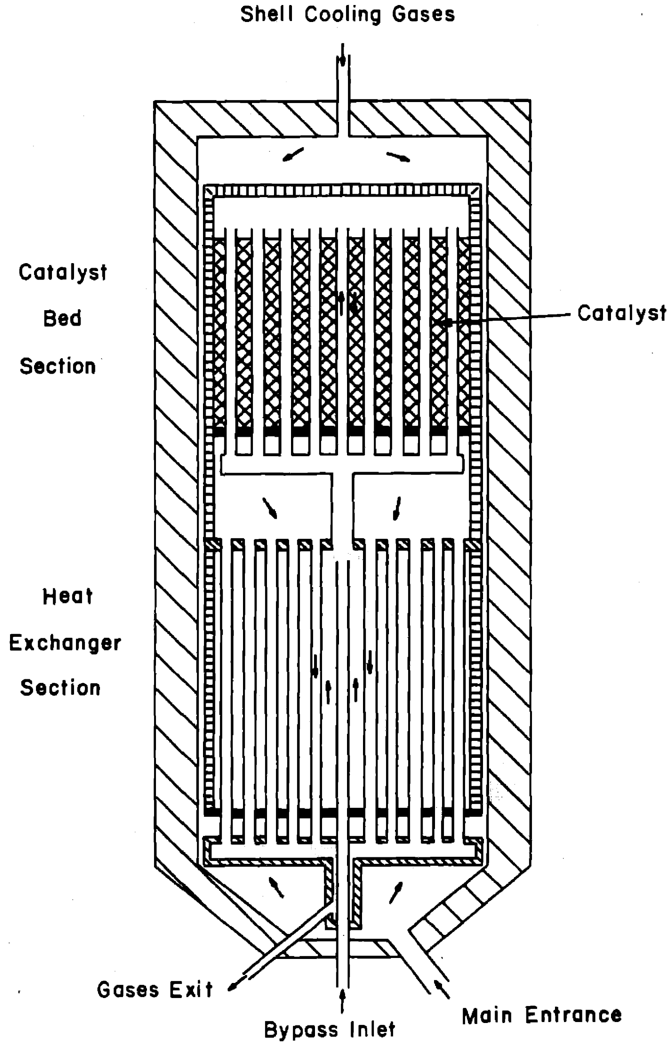
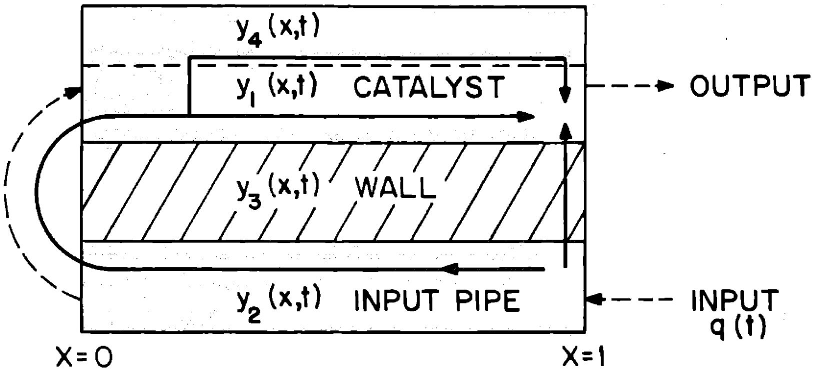


Fig. 4.8 Simplified Diagram of Ammonia Reactor



y_2 IS THE INPUT GAS TEMPERATURE

y_3 IS THE WALL TEMPERATURE

y_1 IS THE CATALYST TEMPERATURE

y_4 IS THE AMMONIA CONCENTRATION IN THE CATALYST

- - -► THE DIRECTION OF FLOW OF THE STREAMS

——► TRANSFER PATHS

Fig. 4.9 Schematic Diagram of Ammonia Reactor where y_1 is catalyst temperature

y_2 is input gas temperature

y_3 is wall temperature

y_4 is ammonia concentration

The notation used here is consistent with the rest of this work and is different from that used by Eymery[31] or Quintero.[43] The central assumptions are

a) The gases are well mixed radially so that a one-dimensional model in distance is obtained.

b) No effective gas hold-up in the catalyst.

c) No effective heat capacity of the input gas.

d) No longitudinal conductivity in the wall or in the gas

e) The reacting gases and the catalyst have the same temperature.

f) The pressure drop in the reactor does not affect the rate of reaction.

g) All radiation effects are neglected.

In general all the coefficients of Eq. 4.32 are functions of y, y_1, y_2, y_3 and y_4. Quintero[43] linearized these equations about the steady state so that the coefficients of Eq. 4.54 are functions of distance only. The numerical details are given in Appendix G. The boundary conditions are

$$\begin{aligned} y_2(1,t) &= q(t), \text{ the disturbance} \\ y_1(0,t) &= y_2(0,t) = y_3(0,t) \qquad (4.55) \\ y_4(0,t) &= 0 \end{aligned}$$

A second boundary condition is required for $y_1(x,t)$ because of diffusion. Eymery suggests that $y_1 + ky_1' = 0$ at $x = 0$ be used but the quantity of diffusion is so small it was decided to neglect it.

Eymery solved the non-linear equations (Eq. 4.54) for a step change in input temperature using the Brian and Stone[49] method of reducing the partial differential equations to a set of difference equations.

To help the convergence he used a variable-length distance grid that is equivalent to replacing x by z where

$$x = 0.2z + 0.8z^2$$

Quintero used the same distance variable as Eymery but since the Campbell approximation relies on the physical nature of the process it is much better to use the original variable x. The only transformation which would be useful for the Campbell approximation is one that made all the coefficients essentially constant. This is because the averaging is exactly correct when the coefficients are constants. All the results are given in terms of the original distance variable x.

Eymery took the Fourier transform of the response of the catalyst temperature to a 5°C step change in temperature of the input gases and the Campbell approximation is compared to the frequency responses obtained under this condition. The size of time increment used in the Brian and Stone solution of the equations was 0.01 units of time, where one unit is the time for a disturbance in catalyst temperature to travel through the reactor. Thus, the frequency responses can be trusted up to 10 rad/unit time with certainty and with some doubt up to 25 rad/unit time and are meaningless for higher frequencies. Similarily there is some doubt as to the form of the time responses at $t = 0$ and when discontinuities occur.

G. APPLICATION OF THE CAMPBELL APPROXIMATION TO THE AMMONIA REACTOR

To apply the Campbell approximation to the ammonia reactor the steps outlined in Section E are followed. The response of the catalyst temperature is investigated for a change in gas input temperature. First, a schematic diagram is drawn with the transfer paths marked (Fig. 4.9). There are three transfer paths in this system for the response of the catalyst temperature, namely

1) The direct path down the input stream and back through the catalyst.
2) The path through the wall.
3) The path down the input stream into the concentration stream and back into the catalyst temperature.

These are combinations of the special cases considered in Section D. The first two are the reversed flow case while the third is caused by the co-current flow of the catalyst temperature and the gas concentration in the reactor. Using the fact that each time a boundary is crossed a pole is introduced; the expected form of the approximation is

$$\frac{y_1(x,s)}{q(s)} = \underbrace{\frac{G_1(x)\, e^{-\gamma(x)s}(1+\alpha(x)Ts)}{1+Ts}}_{\text{Thermal Wave}} + \underbrace{\frac{G_2(x)}{(1+T_1 s)(1+T_2 s)}}_{\text{Wall Effect}} + \underbrace{\frac{G_3(x)}{(1+T_3 s)^2}}_{\text{Concentration Effect}} \qquad (4.56)$$

For convenience the three terms in Eq. 4.56 are called the "thermal wave", the wall effect", and the "concentration effect". The term "thermal wave" is used by Eymery in his discussion of the dynamics of the ammonia reactor.

Next, the first two terms of the integral series are evaluated.

Let

$$\eta_1(x) = \frac{1}{x}\int_0^x \frac{c_1(x)}{v_1(x)}\, dx \qquad (4.57)$$

$$\xi_1(x) = \frac{1}{x}\int_0^x \frac{h_{11}(x)}{v_1(x)}\, dx \qquad (4.58)$$

$$\xi_2(x) = \frac{-1}{1-x}\int_x^1 \frac{h_{22}(x)}{v_2(x)}\, dx \qquad (4.59)$$

$$\xi_4(x) = \frac{1}{x}\int_0^x \frac{h_{44}(x)}{v_4(x)}\, dx \qquad (4.60)$$

Then

$$\frac{y_1(x, s)}{q(s)} = e^{-\xi_2(0) - \xi_1(x)x - \eta_1(x)xs}$$

$$\cdot \left[1 + \left(\overline{\frac{-h_{41}}{v_4}}\right) \left(\overline{\frac{-h_{14}}{v_1}}\right)\left(-x + \frac{1}{\overline{\xi_4-\xi_1} + \bar{\eta}_1 s}\right)\frac{1}{\overline{\xi_4-\xi_1} + \bar{\eta}_1 s}\right]$$

$$+ \frac{e^{-\xi_2(0)-\xi_4(x)x}\left(\overline{\frac{-h_{41}}{v_4}}\right)\left(\overline{\frac{h_{14}}{v_1}}\right)}{(\xi_4-\xi_1 + \eta_1 s)^2} \tag{4.61}$$

$$+ \frac{e^{-\xi_2(0)\,(1-x)}\left(\overline{\frac{h_{13}\,h_{32}}{v_1}}\right)}{(\bar{c}_3 s+\bar{h}_{33})(\overline{\xi_1+\xi_2} + \bar{\eta}_1 s)}$$

Equation 4.61 has the expected form and the term involving

$$-x + \frac{1}{\overline{\xi_4-\xi_1} + \bar{\eta}_1 s}$$

can be neglected. Comparing the result with Eq. 4.56 the time constants are

$$\alpha(x) = e^{-\xi_2(x)-\xi_1(x)x} \tag{4.62}$$

$$\gamma(x) = \eta_1(x) \tag{4.63}$$

$$T_1 = \frac{\bar{c}_3}{\bar{h}_{33}} \tag{4.64}$$

$$T_2 = \frac{\bar{\eta}_1}{\overline{\xi_1+\xi_2}} \tag{4.65}$$

$$T_3 = \frac{\bar{\eta}_1}{\overline{\xi_4-\xi_1}} \tag{4.66}$$

Now consider the steady state behavior. From Eq. 4.56

$$G_{ss}(x) = G_1(x) + G_2(x) + G_3(x) \tag{4.67}$$

Two more equations are required to give $G_1(x)$, $G_2(x)$, and $G_3(x)$. Following the results of the simple cases in Section D and remembering that the wall effect is similar to the reversed flow case and the concentration effect to the co-current case, let $G_3(x)$ be given by the value of the integral series and $G_2(x)$ by the steady state with the modified boundary conditions. Thus, $G_2(x)$ is the steady state gain when the boundary conditions of Eq. 4.55 are replaced by the boundary conditions

$$\begin{aligned} y_2(1,t) &= q(t) \\ y_1(0,t) = y_3(0,t) = y_4(0,t) &= 0 \end{aligned} \tag{4.68}$$

$G_3(x)$ is the gain of the concentration term in the integral series

$$G_3(x) = \frac{e^{-\xi_2(0) - \xi_4(x)x\left(\overline{\frac{-h_{41}}{v_4}}\right)\left(\overline{\frac{-h_{14}}{v_1}}\right)}}{\overline{\xi_4-\xi_1}^{\,2}} \tag{4.69}$$

$G_1(x)$ is obtained from Eq. 4.67 and the known values of $G_2(x)$ and $G_3(x)$.

Finally, the value of T must be computed. If the modified Galerkin method is used the main problem is the choice of suitable functions. Quintero[43] applied the Taylor diffusion technique shown in Appendix A to Eq. 4.54, where the coefficients were replaced with their average values. This gave the diffusion equation,

$$-0.33\,\frac{\partial^2 y_m}{\partial x^2} + 0.41\,\frac{\partial y_m}{\partial x} + \frac{\partial y_m}{\partial t} = 0$$

where y_m is the mean value of $\underline{y}$ used in the Taylor diffusion model, but the correct boundary conditions are not clear since there are too many boundary conditions at $x = 0$. The resulting Taylor characteristic values were markedly different depending on the combination of boundary conditions used. Thus, it was decided not to use the Taylor diffusion characteristic functions but to use the following functions for the modified Galerkin method

$$\underline{\phi}_n(x) = \begin{pmatrix} \sin \frac{2n-1}{\pi}\, x \\ \sin \frac{2n-1}{\pi}\, (1-x) \\ \sin \frac{2n-1}{\pi}\, x \\ \sin \frac{2n-1}{\pi}\, x \end{pmatrix}$$

These functions are complete and satisfy all the requirements of Chapter II, Section H. Then T is the first time constant of the modified Galerkin method.

If lumping each stream into a single lump is used then the coefficients must be averaged first and Eq. 4.19 used, namely

$$\begin{vmatrix} s\bar{c}_1 + \bar{h}_{11} + |\bar{v}_1| & 0 & \bar{h}_{13} & \bar{h}_{14} \\ 0 & \bar{h}_{22} + |\bar{v}_2| & \bar{h}_{23} & 0 \\ \bar{h}_{31} & \bar{h}_{32} & s\bar{c}_3 + \bar{h}_{33} & 0 \\ \bar{h}_{41} & 0 & 0 & \bar{h}_{44} + |\bar{v}_4| \end{vmatrix} = 0 \tag{4.70}$$

The smallest root of Eq. 4.70 will give the appropriate value of T, the dominant time constant.

In all these calculations the diffusion in Eq. 4.32 has been neglected. At low frequency the small diffusion will produce no important effects. However, at high frequency it cannot be neglected. The thermal wave part of Eq. 4.55 is

$$\frac{G_1(x)\, e^{-\gamma(x)s}(1+\alpha(x)Ts)}{1+Ts} \tag{4.71}$$

In the time domain Eq. 4.71 implies that a finite discontinuity of magnitude $\alpha(x)G_1(x)$ occurs after a delay of $\gamma(x)$. The diffusion ensures that this does not occur. To remove the finite discontinuity either the zero at $\frac{1}{\alpha(x)T}$ must be ignored or a second pole introduced

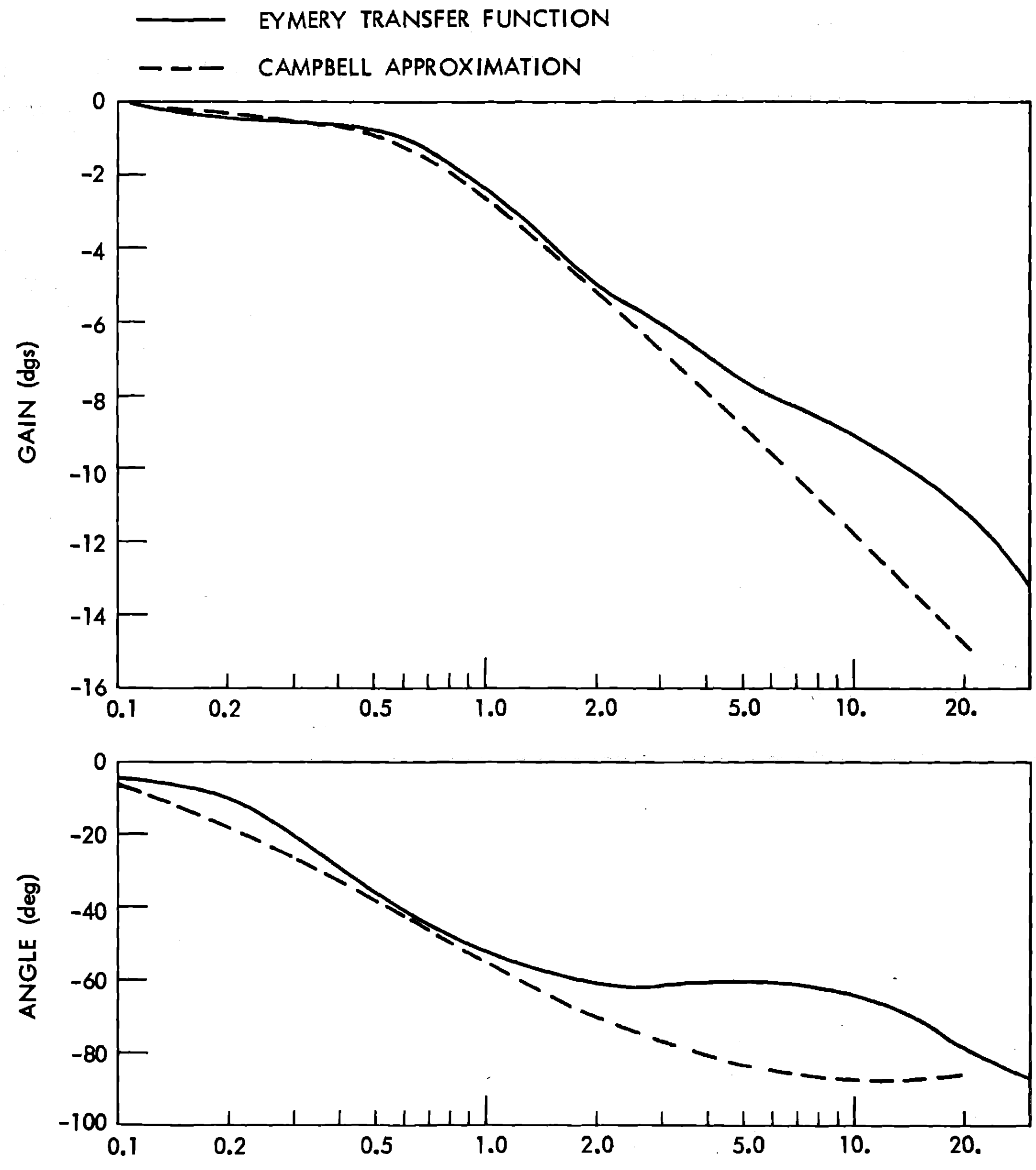


Fig. 4.10 Frequency Response of Ammonia Reactor, x = 0

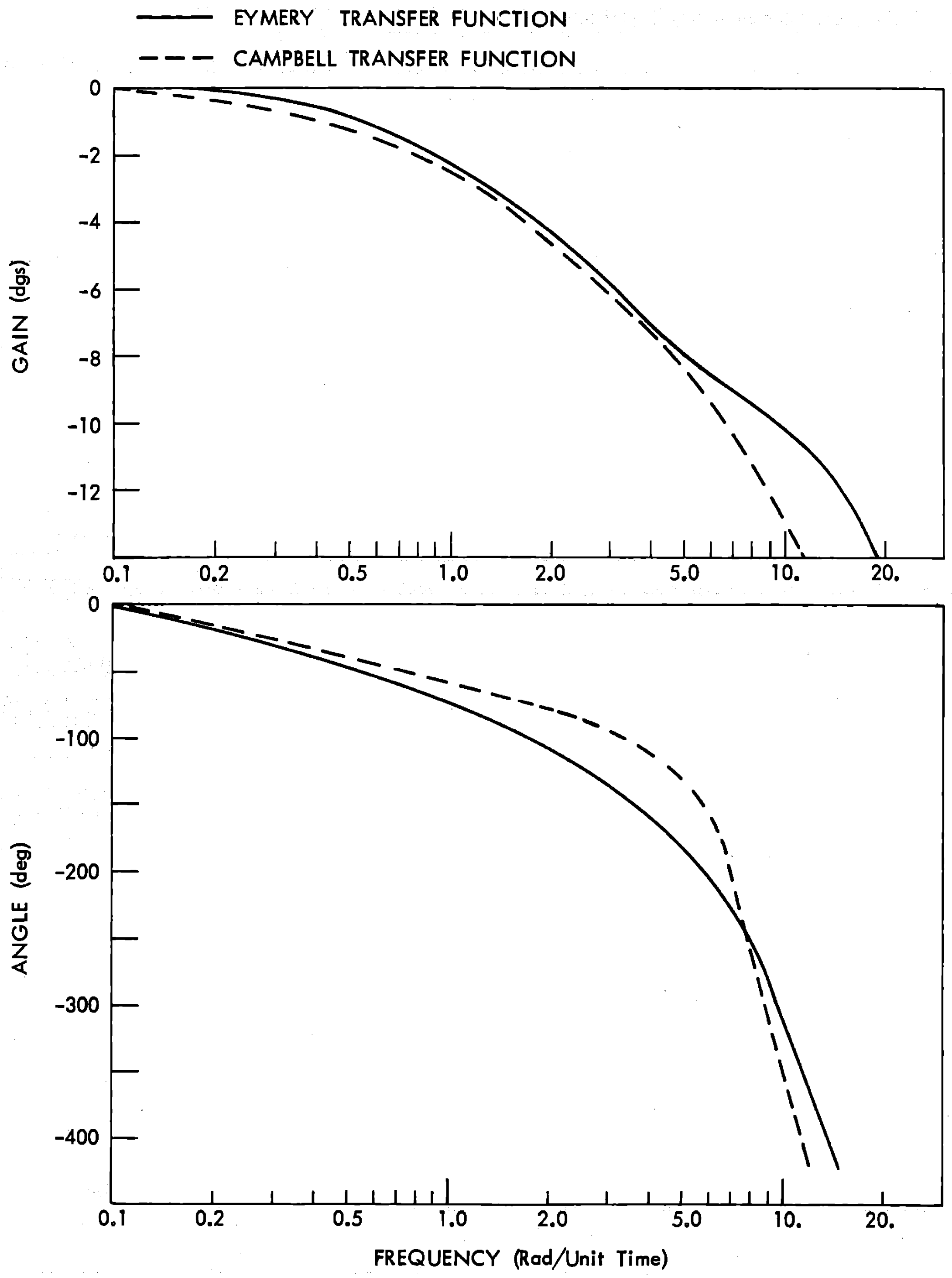


Fig. 4.11 Frequency Response of Ammonia Reactor, x = 0.374

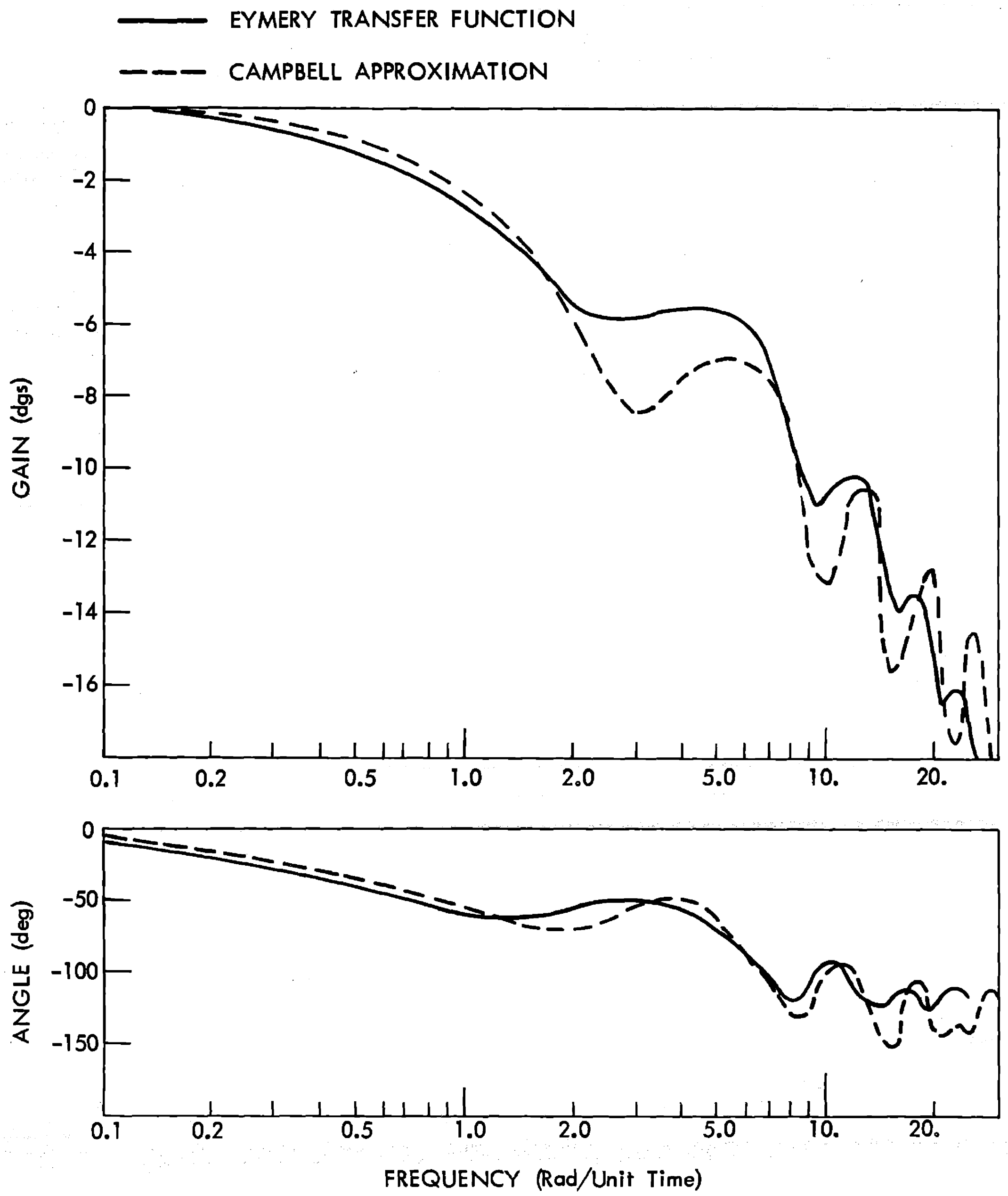


Fig. 4.12 Frequency Response of Ammonia Reactor, x = 1

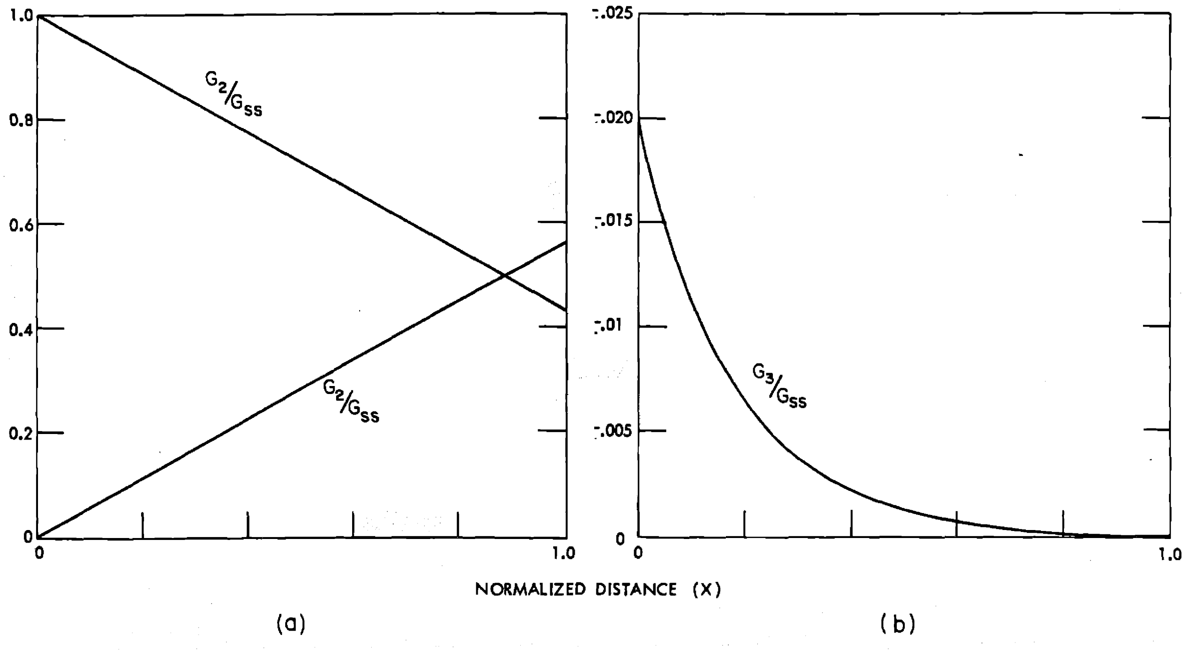


Fig. 4.13 Gains of Campbell Approximation of Ammonia Reactor

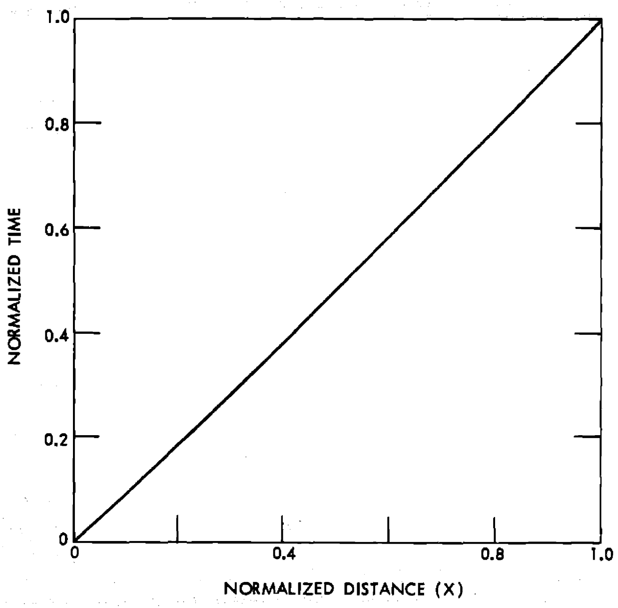


Fig. 4.14 Time Delay in Ammonia Reactor

dependent on the diffusion. Because of the difficulty in estimating another pole and because $\alpha(x)G_1(x)$, the discontinuity is so small it was decided to ignore the zero at $\frac{1}{\alpha(x)T}$. It is essential to do something about the discontinuity as it strongly affects the angle and the magnitude of the response as $s \to \infty$. Thus, the final form of the Campbell approximation is

$$\frac{y_1(x, s)}{q(s)} = \frac{G_1(x)\, e^{-\gamma(x)s}}{1+Ts} + \frac{G_2(x)}{(1+T_1 s)(1+T_2 s)} + \frac{G_3(x)}{(1+T_3 s)^2} \tag{4.72}$$

where T is the first pole of the modified Galerkin method or obtained from lumping.

γ, T_1, T_2, T_3 are given by Eqs. 4.63 to 4.66

$G_1(x)$ and $G_3(x)$ are given by Eqs. 4.67 and 4.69

$G_2(x)$ is the steady state gain with the boundary conditions given by Eq. 4.68.

H. RESULTS

The frequency responses obtained from Eq. 4.72 and by Eymery[31] are shown in Figs. 4.10 to 4.12. The responses have been normalized so that zero frequency gain is unity and the time scale chosen so that the time lag at $x = 1$ is one unit of time. The time lag and normalized gains G_1/G_{ss}, G_2/G_{ss}, G_3/G_{ss}, are plotted against distance in Fig.s. 4.13 and 4.14. The value of the time constants are

$$\begin{aligned} T &= 1.45 \\ T_1 &= 0.056 \\ T_2 &= 0.081 \\ T_3 &= 0.094 \end{aligned} \tag{4.73}$$

Clearly the Campbell approximation gives a very good model of the dynamic performance of the reactor. It will be noticed that $G_3(x)$ is negative and small. It is negative because the rate of reaction expression causes an increase in temperature to decrease the ammonia concentration.

It is small because of the low reactivity of the catalyst. If the catalyst was more active in some region of the reactor the concentration term in Eq. 4.72 will dominate the wall term and a step increase in input temperature will initially decrease the catalyst temperature. This effect was found by Eymery.

Eymery fitted his frequency responses with a simple model on an empirical basis. His results were

$$\begin{aligned} &\text{at} \quad x = 0 \qquad && \frac{y_1(0,s)}{G_{ss}(x)q(s)} = \frac{1}{1+1.25s} \\ &\phantom{\text{at}} \quad x = 0.374 \qquad && \frac{y_1(0.374,s)}{G_{ss}(0.374)q(s)} = \frac{e^{-0.374s}}{1+1.25s} \\ &\phantom{\text{at}} \quad x = 1 \qquad && \frac{y_1(0,s)}{G_{ss}(0)q(s)} = \frac{1}{1+1.25s} \end{aligned} \tag{4.74}$$

These results are similar to those of the Campbell approximation but are inaccurate at $x=1$ because only one pole is used for the wall effect. The low catalyst activity means the concentration effect is negligible. But the time constants are similar. The Campbell approximation gives the frequency response for all x and shows where each term comes from. Thus, the effect of varying various parameters in the reactor can be estimated.

I. SUMMARY

In this Chapter the Campbell approximation is developed for variable-coefficient convective systems. This method gives a simple transfer function between any position in the system and any disturbance. It is easy to evaluate and accurate. The dynamic model given by the Campbell approximation involves only simple constant poles, pure time delays, gains dependent on distance, and zeros dependent on distance. It is an entirely satisfactory model for the application of conventional design techniques.[38, 41] It is a much simpler form than the transcendental transfer functions obtained by Gould[37] for the exact algebraic solution of the two-stream constant-coefficient system.

This model is the only known method of obtaining the system dynamics in this simple form directly from the system equations both for constant and variable coefficient systems. Several people have suggested that this form can be used to approximate the dynamic performance of a large class of chemical systems, but this is the first time a simple procedure has been developed to obtain the necessary parameters from the system equations. The procedure is given in Section E. The model is sufficiently accurate; it can be used as the basis for conventional control design, stability analysis for small perturbations, and the application of optimal control theory to distributed systems. However, the model can not be used for modal analysis[40, 46] as it does not give an eigenfunction expansion of the system dynamics. For modal analysis the modified Galerkin method or lumping are the only methods available for variable-coefficient systems.

The Campbell approximation uses the best features of all the existing methods for representing convective systems. The essential procedure can be outlined as below.

1) Determine the transfer paths of the system.
2) Make the gain at $s = 0$ equal to the steady state gain.
3) Obtain the dominant time constant from either of three methods.
    a) Taylor diffusion model
    b) Modified Galerkin method
    c) System obtained by lumping each stream with one lump.
4) Make the form approach the first term of the integral series model as $s \rightarrow \infty$.

CHAPTER V

APPLICATION OF MODELS

A. INTRODUCTION

In the previous chapters two methods have been developed to obtain a simple model of the dynamical behavior of a general convective system. These methods were investigated so that models would be available for conventional control design[38,41] and for modal analysis.[40,46] Particular attention was paid to variable coefficient systems since there are few methods for handling such systems. Four known techniques exist, most of which apply only to constant coefficient systems. In this chapter different problems which occur in the design of control systems and the investigation of system dynamics are considered and the best model to use is discussed. The choice of the best model inevitably depends on the personal preferences of the engineer but certain general principles can be determined. Also the accuracy of the result and the time available to investigate the problem affect the method used. Certain methods require some digital computations. If such methods are used regularly and the necessary programs developed then the method can be quicker and more accurate than a simpler method. However, if the programs have to be written the additional accuracy may not be worthwhile. In general, if a particular problem occurs repeatedly then special aids such as special slide rules or graphs can be developed. Such aids will not be considered here.

There is a very important distinction between the dynamic response of a system and the dynamic description required for control design. If the only interest is to determine the dynamic response to various disturbances then any mathematical or numerical description is satisfactory. Such a problem arises when it is essential that a system variable does not exceed a certain value during a transient and there is no intention of controlling the system. However, if the objective is to describe the dynamics so that a control system can be designed it is essential to describe the dynamics in a mathematical or graphical form which is suitable for the control theory which is to be applied. Since it is exceedingly difficult to design control systems for non-linear dynamics, it is common to consider small perturbations about the steady state and to attack the linear problem. However, for investigation of dynamics, the non-linear problems can be solved on a digital computer, but the results cannot be used as a basis for control system design.

Computers are a valuable aid in control system design, even for standard techniques. There are three types of computers: digital, analogue, and hybrid. The digital computer will solve a problem in a numerical manner, while an analogue computer solves a problem in real time by using electric circuit analogues. The main advantage of a digital computer is the accuracy of the solution. In analogue computation the speed of computation is most useful, but the accuracy is not so good. A hybrid computer combines these two machines and makes the best use of both. As yet, hybrid computers have not been extensively used, but much work is being done to develop better hybrid computers. Analogue computers have been widely used in dynamic analysis and control investigations. In particular, they are most useful for simulating a non-linear system with a control system designed from linear theory for small perturbations in order to determine whether the non-linearities have any radical effects. The effect of parameter changes can also be easily observed. Digital computers have been used to solve optimal control problems and to determine frequency responses from a set of ordinary differential equations. Three different methods of operating digital computers exist, small computers, batch running on large computers, and time-shared computers. The engineer uses a small computer directly and obtains his answers quickly, but he is limited by the size of the machine. Batch running can give the engineer the advantage of a large machine, but he does not obtain his answers until several hours or even days have passed. In a time-sharing computer, input consoles are placed in convenient locations, and the engineer submits his program directly to the machine, which solves it simultaneously with many other programs. The answers are available immediately, and this system has the power of a large machine and the advantage of a quick return. This enables the engineer to obtain data like frequency responses easily and quickly, even if the equations must be solved numerically.

The usefulness of such methods as the modified Galerkin method and lumping depend on the computers available. Thus, in the following discussion of various problems, different models are suggested depending on the computation facilities available.

Convective systems can be divided into "short" and "long" systems according to the number of transfer units in each stream, (see Chapter II, Section I). When the number of transfer units is much greater than unity, a convective system is said to be long, and when less than unity it is said to be short. The accuracy of the models depends on the number of transfer units, so distinction will be made between long and short systems. Usually heat exchangers have about one transfer unit in each stream while mass transfer devices such as absorbers or distillation columns have more than five transfer units. Counter-current systems that are short convectively behave like a single stirred tank if the disturbance is in a different stream or a pure delay if the disturbance is in the same stream. Long counter-current systems behave more like systems with diffusion and time delay. The Taylor diffusion model is known to be best for long systems, and the modified Galerkin method is also better for long systems. The integral series gives a good approximation easily for short systems. For long systems many terms must be taken, which is arduous. Campbell approximation is satisfactory for both long and short systems. The exact algebraic transfer function applies to both long and short systems. A much used technique is lumping, but many lumps are required to approximate the time delay satisfactorily. The usefulness of lumping depends on the relative significance of the time delay, which depends on the remaining time constants of the system. It is possible for a system to be convectively short and still have a time delay many times larger than any time constant in the control system, but it is also possible for such a system to have a negligible time delay, in which case an adequate dynamical model is a pure gain.

Four different problems are considered: conventional control design (Section B), modal analysis (Section C), dynamic response

(Section D), stability and optimal control theory (Section E). The comments are briefly summarized in Section F. It must be emphasized that the discussion in this chapter is quite subjective and reflects the author's personal preferences and the control philosophy of the chemical process control group at M.I.T. The ultimate choice of a suitable model will depend on the engineer's personal preferences and on the computing equipment available.

B. CONVENTIONAL CONTROL DESIGN

In this section the problem of applying conventional control design techniques to convective systems is considered. To determine which dynamical model is appropriate it is necessary to discuss the objectives and design techniques of conventional control. The objectives of a system are frequently given in terms of only one output. For instance in a heat exchanger the objective could be made to make the output temperature of one stream invariant to disturbances in the inputs to the exchanger. Then the desired dynamic model is concerned only with input-output relationships. The internal dynamic behavior is of no significance. However, this does not mean that the designer should neglect the internal behavior as the best system design may involve measurement and/or control at some internal points. Conventional control design techniques have been concerned mainly with systems in which the input-output relations are given and in which there is no possibility of measurement or control at some internal point.[41] For example, in a motor it is not possible to control the magnetic flux directly but only by adjusting the input voltage to the motor. In chemical systems measurements can frequently be made at an internal point and internal control action is sometimes possible as well.[27] Most applications of conventional control design techniques assume that the input-output relationship of the process is given and no internal effects are considered.

The specifications are usually given in the time domain in terms of overshoot, velocity error, maximum rates of change, or time response to a step. These specifications can be converted into frequency domain requirements and conventional control design techniques applied in the frequency domain. These techniques are mostly graphical and among the most common are the Bode diagram, the Nichols chart and the polar diagram.[41] The required curves in the frequency domain are the transfer functions plotted for $s = j\omega$. In chemical engineering it is common to use the Ziegler-Nichols criteria for setting three term controllers.[52] Harriot[38] gives a good description of conventional control design techniques applied to chemical engineering.

Thus, for conventional control design the transfer functions between each output and the inputs are required. All the different models, the algebraic transfer function, the integral series, the Taylor diffusion model, lumping, the modified Galerkin method, the Campbell approximation will give transfer functions for constant-coefficient systems. Only the last three can be used for variable-coefficient systems. The most convenient form of transfer function for conventional control is in the form of poles and zeros with pure time delays. This is slightly more convenient than a set of poles with their associated residues and much more convenient than a series of poles and time delays. The integral series method (Appendix E) is in the latter form and is the least convenient to use for conventional control except for very short systems. The Taylor diffusion model (Appendix A), lumping and the modified Galerkin method (Chapter II) all give a set of poles and residues while the Campbell approximation (Chapter IV) has poles, zeros and pure time delays. The algebraic transfer functions can be evaluated exactly only for two-stream systems and is an involved transcendental expression.[37] For many stream systems a computer is needed since the roots of a polynomial cannot be found algebraically for a polynominal of higher order than five and not conveniently for more than a quadratic. Thus, a computer is necessary to use the algebraic transfer function with any speed or convenience.

For both constant and variable coefficient systems the Campbell approximation is the most convenient. It has the advantage of also giving the internal behavior of the system as well as the input-output response. Lumping is almost equally convenient if there are only a few transfer functions to be used and only a few lumps in each stream are necessary for an adequate description of the system. However, the smaller the number of lumps the larger the effective diffusion. For a large number of lumps a computer will almost certainly have to be used and the Campbell approximation is definitely quicker.

For constant-coefficient systems the Taylor diffusion model is quite useful but the necessity to expand the initial distribution in a Fourier expansion reduces the usefulness of the approach when only input-output transfer functions are required. The Campbell approximation is still more convenient.

If a time-sharing computer is available and general programs have been written, lumping may be the best approach in general with the algebraic solution which is just as easy for constant-coefficient systems. Insufficient experience has been had with time-shared computers and their associated graphical display systems to show how easy they will make the design of control systems. However, it is clearly desirable to have models which do not depend for their usefulness on such highly sophisticated equipment.

If an analogue computer is to be used for control system design it is most desirable that the model have only poles and zeros and no pure time delays. Thus, lumping is the simplest method but may involve a large number of lumps which means a large number of operational amplifiers. The modified Galerkin method requires a digital computer to solve the matrix equations but the resulting model can easily be simulated on an analogue computer with only a few operational amplifiers. The Taylor diffusion model is similar to the modified Galerkin method but is only applicable to constant-coefficient systems.

To summarize the Campbell approximation is the best for all purposes except for use on an analogue computer when lumping may be better depending on the size of the problem. The integral series is the least convenient. However, among the remaining methods there is little to choose and much will depend on the particular preferences of the designer.

C. MODAL ANALYSIS

Modal analysis has been developed by Rosenbrock[46] and Murray.[40] It is a control philosophy which is concerned with the internal behavior of the system as well as the output behavior. To use modal analysis the dynamical model must be in the form of eigenfunctions and eigenvalues. Thus, only three possible models can be used, lumping, the Taylor diffusion model, and the modified Galerkin method. In lumping the eigenfuctions are replaced by eigenvectors and the space modes are given only at the points where the system has been lumped. Thus for a good description of the modes, from the sampling theorem, at least twice as many lumps are required than modes. Thus for the first five modes at least ten lumps are needed. In Chapter II there is a discussion of the relative merits of the modified Galerkin method and of lumping. The main difference is the order of the matrix equation that has to be solved. The modified Galerkin method seems to be better for more involved systems but with large fast digital computers readily available the advantage may be marginal.

For constant-coefficient systems the Taylor diffusion model is most satisfactory and easier to apply than the modified Galerkin method. However, the boundary value problem for many stream systems (see Appendix A) have not yet been adequately unraveled.

It should be noticed that modal analysis is not suitable for short systems dominated by a pure time delay as none of the dynamical models adequately approximated the delay. All the methods suitable for modal analysis introduce an effective diffusion many times larger than the physical diffusion.

The control design techniques of modal analysis as developed by Rosenbrock[46] and Murray[40] require considerable computation so that the design methods require a reasonably large digital computer, but the calculations can be made quite automatic. The problems of the actual implementation of a control system designed from modal analysis have not been investigated. Indeed now that dynamical models suitable for modal analysis can be found for a wide class of systems there is considerable further work to be undertaken to determine exactly how best to use this design philosophy.[32,33]

D. SYSTEMS DYNAMICS

In the introduction to this chapter the distinction was made between an interest in the system dynamics and a dynamical model suitable for control design. If the engineer is only interested in the dynamic behavior and has no intentions of controlling the system then there is no requirement to express the dynamics in any particular form. However, the dynamical models suitable for any control design are in themselves a description of the dynamic performances. Such models are useful for considering the system providing they are sufficiently accurate. Since all the models considered in this work apply only to linear systems they are accurate for small perturbations from the steady state only. The main possible advantage of the simple models is that the effect of various parameters on the system behavior would be clearer.

For an investigation of the dynamics of a general non-linear convective system, a digital computer solution of the non-linear partial differential equations is frequently used. This is not a simple procedure as the numerical calculations can easily become unstable, but the method of Brian and Stone[49] for replacing the partial differential equations by difference equations has proved most effective. Eymery[31] and Nestor[42] have used it sucessfully on non-linear systems. It is clearly a superior technique to that proposed by Courant, Issacson and Rees.[4] The Brian and Stone method gives the response of the system to any deterministic input. With large computers readily available it is an entirely satisfactory method for determining the system response, but the effect of individual parameters is not obvious and many different cases will have to be computed.

Of the various dynamical models suitable for the design of control systems, only one, the Campbell approximation, offers any advantage over the digital computer solution. The physical picture obtained from the Campbell approximation gives a good idea of the effect of individual parameters. This was clearly shown in Chapter IV in the case of the ammonia reactor. The Campbell approximation can be evaluated as easily as the digital solution and does not require digital computation. The other methods discussed either do not have the accuracy or the physical picture. However, for large disturbances in non-linear systems the digital solution is the only satisfactory method of determining the dynamic behavior.

E. STABILITY AND OPTIMAL CONTROL

The study of any dynamical system must include consideration of stability. The linear dynamical models considered in this work only apply for small perturbations about the steady state. Thus the models cannot be used to study the stability of a non-linear system. However, it is most desirable that the models give the correct high frequency performance so that the gains determined by the control design will not make the system unstable for small perturbations. In particular such models as the Taylor diffusion model, the modified Galerkin method, or lumping never give the correct high frequency behavior because of the large quantity of effective diffusion and the fact that these models use only a finite number of poles to approximate a pure time delay. Thus, from a stability viewpoint the Campbell approximation or the integral series method is much better. However, the really important problems of stability concern the non-linearities and these problems have not been investigated here.

The application of optimal control to convective systems has not been attempted mainly because of the difficulty of handling the partial differential equations. If a design is based on the Weiner-Hopf statistical theory[41] a simple low-order model is required with only poles and zeros and possibly a time lag. The modified Galerkin method or the Taylor diffusion model appear to be the best to use and the Campbell approximation is satisfactory if the additional complication of a time delay is allowed. For optimal design following the methods of Pontryagin a simple model is necessary or the system must be reduced to a set of ordinary differential equations. Thus, the models to use are the Campbell approximation or lumping. For the simplicity of the form and of the number parameters involved, the Campbell approximation may be the most satisfactory. It would be interesting to attempt to apply optimal control theory to a convective system modeled by the Campbell approximation.

F. SUMMARY

Four applications of dynamical models of convective systems have been considered, namely, conventional control design, modal analysis, dynamic response, and stability and optimal control. For all the cases except modal analysis the Campbell approximation is the most convenient to use. In modal analysis there is little to choose between the modified Galerkin method and lumping. If large digital computers are readily available, especially in a time sharing system, and suitable programs are developed, lumping could be the most convenient method to use. However, it is unsatisfactory to be completely dependent on such sophisticated equipment and the Campbell approximation is easy to evaluate and convenient to use in most applications.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

The problem of obtaining dynamic models for linear convective systems has been considered, both for systems whose equations have constant coefficients and for those with coefficients that vary with distance. Many convective systems are operated close to the steady state, and their dynamic behavior is satisfactorily described by the linearized system about the steady state. Such systems have equations whose coefficients are functions of distance. The dynamic behavior of a large class of chemical systems, such as heat exchangers, distillation columns, absorbers, liquid-liquid extractors, and some forms of chemical reactors, can be represented as convective systems with coefficients that vary with distance.

Two new dynamic models, the modified Galerkin method, and the Campbell approximation, have been developed. Both of these methods can be used with variable-coefficient systems. The only existing approach to the dynamic behavior of variable-coefficient systems is by lumping the partial differential equations. The new models have a form suitable for the design of control systems. In particular, the Campbell approximation is suitable for conventional control design techniques, while the modified Galerkin method is suitable for modal analysis. The Campbell approximation is easy to evaluate and is an accurate representation of the system dynamics. The approximation is in a convenient form for all applications, except for modal analysis, and even for a complicated system like an ammonia reactor, the approximation gives an excellent representation of the system dynamics.

For modal analysis, a dynamic model is required in the form of eigenvalues and eigenfunctions. This can be achieved only by the introduction of an effective diffusion many times larger than the physical diffusion, but this effective diffusion does represent the overall low-frequency dynamic behavior quite adequately. The modified Galerkin method gives a model in the form of eigenvalues and eigenfunctions, and the amount of effective diffusion needed can be estimated directly from the system equations and the required number of eigenvalues. The modified Galerkin method has no great advantage over lumping, but the matrix equations are of a smaller order than those produced by lumping.

Suitable dynamic models have been found for convective systems, in particular, for variable-coefficient systems, and this is the primary contribution of this work. No satisfactory methods previously existed to handle these problems. Now models exist on which a control design philosophy for distributed systems can be based. It appears unlikely that further work on dynamic models for convective systems will produce any significant developments. The Campbell approximation can be used for most systems, and when that approximation is not satisfactory, it is best to use lumping with a large computer to handle the computations.

Further work in process control, based on these results, seems promising in several directions, and it is suggested that the following problems be investigated.

a) A control design philosophy for distributed systems using distributed control and measurement. For systems with eigenvalues and eigenfunctions this has already been started by Rosenbrock[46] and Murray[40] although the practicality of the proposed methods has yet to be demonstrated with specific examples. In addition, a philosophy for systems with pure time lags is needed. The Campbell approximation could be used as the dynamic model for such a philosophy.

b) Application of optimal control using either the Campbell approximation or modal decomposition as a description of the system dynamics.

c) The Taylor diffusion model for many-stream systems has too many boundary conditions. Some rules for choosing the boundary conditions are needed. The possibility of applying the Taylor diffusion technique to variable-coefficient systems should be investigated.

d) The best form of the Campbell approximation for co-current systems is not clear. An investigation of the simple two-stream system should indicate the correct result.

e) The dynamics of large inter-related systems involving both distributed and lumped systems can be investigated by replacing the lumped systems by distributed systems with coefficients which are impulses in distance (Chapter III). This seems an excellent method for investigating the dynamics and control of large plant complexes.

To conclude, the problem of suitable dynamic models has been solved, and now attention can be focussed on the development of an effective control philosophy for distributed systems which considers the internal, as well as the external, behavior of the system.

APPENDIX A

TAYLOR DIFFUSION MODEL

A.1 INTRODUCTION

In this appendix the Taylor diffusion model for a general convective system is developed using matrix algebra. The simple two-pipe system has been investigated in detail by Gould.[36,37] The model was first developed by Rosenbrock[47] from the work of Taylor.[50] The purpose of this appendix is to show how to determine the Taylor diffusion model in a general case so as to obtain the functions needed in Chapter IV. The method is applicable only to pure convective systems with constant coefficients. Thus to use this approach to obtain the functions required in Chapter IV, the variable coefficients must be replaced by their average values. In this appendix it is assumed that the coefficient matrices of the pure convective systems are constants.

The solution of the scalar diffusion equation involves the roots of a transcendental equation. A set of tables and curves are given for the first six roots of this equation.

No attempt is made to investigate the accuracy of the model in the general case. Gould has shown that for two-pipe systems the model is an excellent representation for systems with more than two transfer units on each side. It would be most interesting to know how accurate the model is in the general case and in particular how to choose the appropriate boundary conditions.

Standard notation is used. The inner product notation $<\underline{a}, \underline{b}>$ is used to mean $\underline{a}^T\underline{b}$. The vector $\underline{u}$ is defined as a vector whose elements are unity. This gives a convenient notation for the sum of the elements of a vector and the sum of the elements of a matrix. Thus

$$\sum_{i=1}^{n} a_i = \underline{u}^T\underline{a}$$

$$\sum_{i=1}^{n} A_{ij} = \underline{A}^T \underline{u}$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} = <\underline{u}, \underline{A}\,\underline{u}>$$

A.2 GENERAL CONVECTIVE SYSTEM

A general convective system can be represented by the vector equation

$$\underline{V} \frac{\partial \underline{y}}{\partial x} + \underline{C} \frac{\partial \underline{y}}{\partial t} + \underline{H}\,\underline{y} \qquad (A.1)$$

For a large class of processes such as heat exchangers, distillation columns and absorbers, the matrices $\underline{V}, \underline{C}, \underline{H}$ have the following properties.

a) $\underline{V}, \underline{C}$ are diagonal matrices

b) $$\sum_{c=i}^{n} H_{ij} = 0 \quad \text{for all } j = 1 \ldots\ldots u \qquad (A.2)$$

which can be written as $\underline{H}^T \underline{u} = 0$

The second property is a form of conservation, since it implies that the driving force between any two components of $\underline{y}$ is independent of the path taken. Since the sum of the elements of each column of $\underline{H}$ is zero, the rows of $\underline{H}$ are not linearly independent and $\underline{H}$ is a singular matrix with rank $\leq (n-1)$. In this appendix it will be assumed that $\underline{H}$ has rank $= (n-1)$ and a complete set of eigenvectors exist for $\underline{H}$. This implies that there exist one and one only zero eigenvalue of $\underline{H}$. A sufficient, but not necessary, condition on $\underline{H}$ is that the Jordan canonical form be diagonal and have only one zero element.

If the system consists of two or more non-interacting subsystems then $\underline{H}$ will have rank $\leq (n-2)$ and the Jordan canonical form have two or more zero elements. For example

$$\underline{H} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \qquad (A.3)$$

The system consists of four streams but the first two and the last two are separate non-interacting subsystems. Such systems are best treated by two separate Taylor models.

Since $\underline{H}$ is singular $\underline{H}^{-1}$ does not exist. In obtaining the Taylor diffusion model it is necessary to solve simultaneous equations which appear to require the inverse of $\underline{H}$. To avoid this problem it is necessary to diagonalize $\underline{H}$ and the following definitions are made

Let λ_i (i=1 ...n) be the eigenvalues of $\underline{H}$
and $\underline{P}$ be a matrix whose columns are the eigenvectors of $\underline{H}$
Let λ_n be the zero eigenvalue
and the n^{th} column of $\underline{P}$ the corresponding eigenvector

The $\underline{P}$ is a similarity transformation which diagonalizes $\underline{H}$.
Let $\underline{Q}$ be a diagonal matrix such that

$$Q_{ij} \begin{cases} \dfrac{1}{\sqrt{\lambda_i}} & i = j \neq n \\ \mu & i = j = n \\ 0 & i \neq j \end{cases} \qquad (A.4)$$

Where μ is an arbitrary non-zero number.
Let $\underline{D}$ be a diagonal matrix such that

$$D_{ij} \begin{cases} 1 & i = j \neq n \\ 0 & i = j = n \\ 0 & i \neq j \end{cases} \qquad (A.5)$$

Then $\underline{Q}\underline{P}^{-1}\underline{H}\underline{P}\underline{Q} = \underline{D}$ (A.6)

A.3 TAYLOR DIFFUSION MODEL

The central assumption of the Taylor diffusion model is that with respect to axes moving with the mean velocity of the system the time rate of change of $\underline{y}$ can be neglected and the spatial rates of change are approximately equal to the spatial rate of change of a mean of $\underline{y}$.

$$\text{Let } y_m = \frac{<\underline{C}\ \underline{y},\ \underline{u}>}{<\underline{C}\ \underline{u},\ \underline{u}>} = \frac{\sum_i C_{ii} y_i}{\sum_i C_{ii}} \tag{A.7}$$

The system is

$$\underline{V}\frac{\partial \underline{y}}{\partial x} + \underline{C}\frac{\partial \underline{y}}{\partial t} + \underline{H}\,\underline{y} = 0 \tag{A.1}$$

Let the moving axes be given by

$$x' = x - v_m t$$

$$t' = t$$

Then

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x'}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t'} - v_m \frac{\partial}{\partial x'}$$

From Eq. A.1

$$\underline{C}\frac{\partial \underline{y}}{\partial t'} + (\underline{V} - v_m\underline{C})\frac{\partial \underline{y}}{\partial x'} + \underline{H}\ \underline{y} = 0 \tag{A.8}$$

Take the inner product with $\underline{u}$ of Eq. A.8

$$<\underline{u},\ \underline{C}\frac{\partial \underline{y}}{\partial t'}> + <\underline{u},\ (\underline{V} - v_m\underline{C})\frac{\partial \underline{y}}{\partial x'}> + <\underline{u}, \underline{H}\,\underline{y}> = 0 \tag{A.9}$$

From Eq. A.2

$$<\underline{u}, \underline{H}\,\underline{y}> = 0$$

With the Taylor diffusion assumptions replace

$$\frac{\partial y_i}{\partial x'} \text{ by } \frac{\partial y_m}{\partial x'}$$

and set the time derivatives to zero. Then Eq. A.9 is true provided

$$v_m = \frac{<\underline{u}, \underline{V}\,\underline{u}>}{<\underline{u}, \underline{C}\,\underline{u}>} \tag{A.10}$$

and Eq. A.8 becomes

$$(\underline{V} - v_m \underline{C})\, \underline{u} \frac{\partial y_m}{\partial x'} + \underline{H}\underline{y} = 0 \qquad (A.11)$$

From Eqs. A.1 and A.7

$$<\underline{u}, \underline{V} \frac{\partial \underline{y}}{\partial x}> + <\underline{u}, \underline{C}\,\underline{u} \frac{\partial y_m}{\partial t}> = 0 \qquad (A.12)$$

Hence we have developed the following set of equations to describe the system given by Eqs. A.11, A.12, A.7

$$(\underline{V} - v_m \underline{C})\, \underline{u} \frac{\partial y_m}{\partial x} + \underline{H}\underline{y} = 0 \qquad (A.11)$$

$$<u, V \frac{\partial \underline{y}}{\partial x}> + <\underline{u}, \underline{C}\,\underline{u}> \frac{\partial y_m}{\partial t} = 0 \qquad (A.12)$$

$$<\underline{u}, \underline{C}\,\underline{u}>\, y_m - <\underline{u}, \underline{C}\,\underline{y}> = 0 \qquad (A.7)$$

Since $\frac{\partial}{\partial x} = \frac{\partial}{\partial x'}$, the equations are given in the original variables. These equations appear to represent (n+2) equations in (n+1) unknowns, $\underline{y}$ and y_m but Eq. A.11 represents only (n-1) linearly independent equations since the sum of all the equations, or the inner product with u, is zero. The problem is to eliminate $\underline{y}$ from Eq. A.7, A.11 and A.12 and obtain an equation in y_m. This equation is the Taylor diffusion equation of the general convective system. To obtain (n-1) linearily independent equations from Eq. A.11, the variables are transformed to diagonalize $\underline{H}$.

Let

$$\underline{y} = \underline{P}\,\underline{Q}\,\underline{w} \qquad (A.13)$$

Then Eqs. A.7, A.11, A.12 can be written

$$\underline{Q}\,\underline{P}^{-1}(\underline{V} - v_m \underline{C})\, \underline{u} \frac{\partial y_m}{\partial x} + \underline{D}\,\underline{w} = 0 \qquad (A.14)$$

$$<\underline{u}, \underline{C}\,\underline{u}> \frac{\partial y_m}{\partial t} + <\underline{u}, \underline{V}\,\underline{P}\,\underline{Q} \frac{\partial w}{\partial x}> = 0 \qquad (A.15)$$

$$<\underline{u}, \underline{C}\,\underline{u}>\, y_m - <\underline{C}\,\underline{P}\,\underline{Q}\,\underline{w}, \underline{u}> = 0 \qquad (A.16)$$

Consider Eq. A.14 and in particular the n^{th} equation

$$[\underline{Q}\,\underline{P}^{-1}(\underline{V}-v_m\underline{C})\,\underline{u}]_n \frac{\partial y_m}{\partial x} + [\underline{D}\,\underline{w}]_n = 0$$

This equation can be written using the definitions of $\underline{D}$ and $\underline{Q}$ in Eqs. A.4 and A.5 as

$$Q_{nn}[\underline{P}^{1}(\underline{V}-v_m\underline{C})\,\underline{u}]_n = 0$$

Since $Q_{nn} = \mu$ an arbitrary non-zero number therefore

$$[\underline{P}^{-1}(\underline{V}-v_m\underline{C})\,\underline{u}]_n = 0 \qquad \text{(A.17)}$$

To solve Eqs. A.14, A.15, A.16 consider the following analogy

where $\eta_1 \ldots. \eta_n$ corresponds to $w_1 \ldots. w_n$

η_m corresponds to y_m

Then Eq. A.14 has the form of the set of equations

$$\begin{aligned} \eta_1 + a_1\eta_m &= 0 \\ &\vdots \\ \eta_{n-1} + a_{n-1}\eta_m &= 0 \\ a_n &= 0 \end{aligned}$$

Equation A.15 has the form

$$b_1\eta_1 + \ldots + b_{n-1}\eta_{n-1} + b_n\eta_n + c\eta_m = 0$$

Equation A.16 has the form

$$d_1\eta_1 + \ldots + d_{n-1}\eta_{n-1} + d_n\eta_n + e\eta_m = 0$$

These equations can be solved by successive substitution to give a relation connecting η_m.

$$\begin{aligned} &-(d_1a_1 + \ldots + d_na_n)\,b_n\eta_m - d_nc\eta_m \\ &+ (b_1a_1 + \ldots + b_na_n)\,d_n\eta_m + b_ne\eta_m = 0 \end{aligned}$$

Applying this result to Eqs. A.14, A.15, A.16 yields

$$[\langle\frac{\partial}{\partial x}\underline{Q}^T\underline{P}^T\underline{V}^T\underline{u},\ \frac{\partial y_m}{\partial x}\underline{QP}^{-1}(\underline{V}-v_m\underline{C})\underline{u}\rangle - \langle\frac{\partial y_m}{\partial t}\underline{u},\ \underline{Cu}\rangle]$$

$$\cdot\,[\underline{Q}^T\underline{P}^T\underline{C}^T\underline{u}]_n$$

$$= [\langle\underline{u},\underline{C}\,\underline{u}\rangle y_m - \langle\underline{Q}^T\underline{P}^T\underline{C}^T\underline{u},\ \frac{\partial y_m}{\partial x}\underline{QP}^{-1}(\underline{V}-v_m\underline{C})\underline{u}\rangle]$$

$$\cdot\,[\frac{\partial}{\partial x}\underline{Q}^T\underline{P}^T\underline{V}^T\underline{u}]_n$$

This equation can be written as

$$-\alpha_T\frac{\partial^2 y_m}{\partial x^2}+v_T\frac{\partial y_m}{\partial x}+\frac{\partial y_m}{\partial t} = 0 \qquad (A.18)$$

where
$$\alpha_T = \frac{\langle\underline{u},(\underline{V}-v_T\underline{C})\,\underline{P}\underline{Q}^2\underline{P}^{-1}(\underline{V}-v_m\underline{C})\underline{u}\rangle}{\langle\underline{u},\ \underline{C}\,\underline{u}\rangle} \qquad (A.19)$$

or
$$\alpha_T = \frac{\sum_i\sum_j\sum_k(V_{ii}-v_TC_{ii})P_{ij}Q_{jj}^2P_{jk}(V_{kk}-v_mC_{kk})}{\sum_i C_{ii}}$$

and
$$v_T = \frac{[\underline{Q}^T\underline{P}^T\underline{V}^T\underline{u}]_n}{[\underline{Q}^T\underline{P}^T\underline{C}^T\underline{u}]_n} = \frac{\sum_i V_{ii}P_{in}}{\sum_i C_{ii}P_{in}} \qquad (A.20)$$

It will be noticed that the definition of $\underline{Q}$, Eq. A.5 contained an arbitrary number, $\mu = Q_{nn}$. From Eq. A.19 we have that μ is multiplied by a term

$$[\underline{P}^{-1}(\underline{V}-v_m\underline{C})\underline{u}]_n$$

which is identically zero from Eq. A.17. Thus α_T is independent of μ and for the calculation of α_T it is quite permissible and most convenient to put $\mu = 0$ i.e.,

$$\underline{Q}^2 = \begin{pmatrix} \frac{1}{\lambda_1} & & & 0 \\ & \ddots & & \\ 0 & & \frac{1}{\lambda_{n-1}} & \\ & & & 0 \end{pmatrix} \qquad (A.21)$$

To use the Taylor diffusion model the equations relating $\underline{y}$ to y_m are needed. These can be obtained from Eqs. A.14 and A.16

$$\underline{Q}\,\underline{P}^{-1}(\underline{V} - v_m \underline{C})\underline{u}\,\frac{\partial y_m}{\partial x} + \underline{D}\,\underline{w} = 0 \qquad (A.15)$$

$$<\underline{u}, \underline{C}\,\underline{u}>y_m - <\underline{C}\,\underline{P}\,\underline{Q}\,\underline{w}, \underline{u}> = 0 \qquad (A.16)$$

From Eq. A.14 we have

$$<\underline{u}, \underline{C}\,\underline{P}\,\underline{Q}\,\underline{D}\,\underline{w}> + <\underline{u}, \underline{C}\,\underline{P}\,\underline{Q}^2\,\underline{P}^{-1}(\underline{V} - v_m \underline{C})\underline{u}\,\frac{\partial y_m}{\partial x}> = 0$$

Subtracting Eq. A.16

$$<\underline{u}, \underline{C}\,\underline{P}\,\underline{Q}(\underline{I} - \underline{D})\,\underline{w} - \partial> = 0$$

where

$$\partial = <\underline{u}, \underline{C}\,\underline{u}>y_m$$

$$+ <\underline{u}, \underline{C}\,\underline{P}\,\underline{Q}^2\,\underline{P}^{-1}(\underline{V} - v_m \underline{C})\underline{u}>\,\frac{\partial y_m}{\partial x}$$

This equation only has a non-zero value for the n^{th} element of $\underline{Q}^T\,\underline{P}^T\,\underline{C}^T\,\underline{u}$, and is equivalent to

$$[\underline{Q}^T\,\underline{P}^T\,\underline{C}^T\,\underline{u}]_n\,(\underline{I} - \underline{D})\,\underline{w} = \theta\,(\underline{I} - \underline{D})\,\underline{u}$$

Add this equation to Eq. A.14

$$[\underline{Q}^T\,\underline{P}^T\,\underline{C}^T\,\underline{u}]_n\,\underline{w} + \underline{Q}\,\underline{P}^{-1}(\underline{V} - v_m \underline{C})\underline{u}\,[\underline{Q}^T\,\underline{P}^T\,\underline{C}^T\,\underline{u}]_n\,\frac{\partial y_m}{\partial x}$$

$$- \theta\,(\underline{I} - \underline{D})\,\underline{u} = 0$$

But $\underline{y} = \underline{P}\,\underline{Q}\,\underline{w}$

$$y_i = \frac{[<\underline{u}, \underline{C}\,\underline{u}>\underline{P}\,\underline{Q}]_{in}}{[\underline{Q}^T \underline{P}^T \underline{C}^T \underline{u}]_n}\, y_m$$

$$- [\underline{P}\,\underline{Q}^2 \underline{P}^{-1} (\underline{V} - v_m \underline{C})\underline{u}]_i \frac{\partial y_m}{\partial x}$$

$$+ \frac{[<\underline{u}, \underline{C}\,\underline{P}\,\underline{Q}^2 \underline{P}^{-1} (\underline{V} - v_m \underline{C})\underline{u}>\underline{P}\,\underline{Q}]_{in}}{[\underline{Q}^T \underline{P}^T \underline{C}^T \underline{u}]_n} \frac{\partial y_m}{\partial x} \qquad (A.22)$$

Equation A. 22 appears to be a function of $\mu = Q_{nn}$ which is an arbitrary number Eq. A.5. However, Eq. A.22 can be written as below in which $\underline{Q}$ only appears multiplied by $\underline{P}^{-1}(\underline{V} - v_m \underline{C})\underline{u}$. At the end of the previous section it was shown that under these circumstances it is permissible to put $\mu = 0$, or define $\underline{Q}^2$ as in Eq. A.21. Thus Eq. A.22 can be written as

$$y_i = \frac{\sum_j C_{jj}}{\sum_j C_{jj} P_{jn}}\, P_{in}\, y_m$$

$$- \sum_j \sum_k P_{ij}\, Q^2_{jj}\, P^{-1}_{jk}\, (V_{kk} - v_m C_{kk}) \frac{\partial y_m}{\partial x}$$

$$+ \frac{\sum_j \sum_k \sum_l C_{jj}\, P_{jk}\, Q^2_{kk}\, P^{-1}_{kl}\, (V_{ll} - v_m C_{ll})}{\sum_j C_{jj}\, P_{jn}}\, P_{in} \frac{\partial y_m}{\partial x} \qquad (A.23)$$

A.4 SYMMETRIC TRANSFER MATRIX

It is interesting to consider the special case when the matrix $\underline{H}$ is symmetric, particularly as the accuracy of the Taylor diffusion model has been checked only in this case. The general case has not been fully investigated and will not be investigated here.

It is clear from Eq. A.2 that

$$\underline{H}\,\underline{u} = 0 \tag{A.24}$$

Thus the eigenvector corresponding to the zero eigenvalue of $\underline{H}$ is $\underline{u}$ and from Eq. A.4 the n^{th} column of $\underline{P}$ is $\underline{u}$. If these results are used in Eqs. A.19, A.20, A.23

$$v_T = v_m = \frac{<\underline{u},\, \underline{V}\,\underline{u}>}{<\underline{u},\, \underline{C}\,\underline{u}>} \tag{A.25}$$

$$a_T = \frac{<\underline{u},\, (\underline{V} - v_m\underline{C})\, \underline{P}\,\underline{Q}^2\,\underline{P}^{-1}\,(\underline{V} - v_m\,\underline{C})\,\underline{u}>}{<\underline{u},\, \underline{C}\,\underline{u}>}$$

and

$$y_i = y_m + k_i\,\frac{\partial y_m}{\partial x} \qquad i = 1 \cdot\cdot\cdot\cdot\cdot n$$

where

$$k_i = \frac{<\underline{u},\, \underline{C}\,\underline{P}\,\underline{Q}^2\,\underline{P}^{-1}\,(\underline{V} - v_m\,\underline{C})\,\underline{u}>}{<\underline{u},\, \underline{C}\,\underline{u}>} - [\,\underline{P}\,\underline{Q}^2\,\underline{P}^{-1}\,(\underline{V} - v_m\underline{C})\,\underline{u}\,]_i$$

It will be noticed that in the general case Eq. A.18 represents a diffusion equation with a velocity v_T which is not the same as the mean velocity of the system v_m. The physical reasoning for attempting to reduce the vector Eq. A.1 to a single diffusion equation suggests that $v_T = v_m$ and this is true only if $\underline{H}$ is symmetric. However, in a large number of cases $\underline{H}$ is symmetric or can easily be made symmetric. It is thought that the approximations are most reasonable when $\underline{H}$ is symmetric. The two-pipe heat exchanger has a symmetric $\underline{H}$ and this case has been investigated in detail. Any concentric pipe system gives rise to $\underline{H}$ as a triple diagonal matrix, and by a simple change in variables $\underline{H}$ can be made symmetric. In chemical engineering terminology this is equivalent to altering the variables until the equilibrium lines and the operating lines have the same slope.

The results obtained using $\underline{H}$ in an unsymmetric form and in a symmetric form are different as would be expected from the approximations. As an example consider the case of binary absorption in which $\underline{H}$ takes the form

$$\underline{H} = k\begin{pmatrix} 1 & -m \\ -1 & m \end{pmatrix} \text{ and } \underline{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

with

$$\underline{V} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} \text{ and } \underline{C} = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix}$$

Using $\underline{H}$ in this form

$$v_m = \frac{V_1 + V_2}{C_1 + C_2} \text{ and } v_T = \frac{mV_1 + V_2}{mC_1 + C_2}$$

$$a_T = \frac{(V_1 C_2 - V_2 C_1)^2}{k\,(C_1 + C_2)^2\,(mC_1 + C_2)}$$

Now if variables are changed to $\underline{w}$ where $w_1 = y_1$ and $w_2 = my_2$

then
$$\underline{H} = k\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad \underline{V} = \begin{pmatrix} V_1 & 0 \\ 0 & \frac{V_2}{m} \end{pmatrix} \quad \underline{C} = \begin{pmatrix} C_1 & 0 \\ 0 & \frac{C_2}{m} \end{pmatrix}$$

and
$$v_T = v_m = \frac{mV_1 + V_2}{mC_1 + C_2}$$

$$a_T = \frac{m\,(V_1 C_2 - V_2 C_1)^2}{k\,(mC_1 + C_2)^3}$$

A.5 SOLUTION OF DIFFUSION EQUATION

To use the Taylor diffusion model it is necessary to solve Eq. A.18 for a suitable pair of boundary conditions to obtain y_m. Equation A.23 can be used to find the solution to the original problem. In general there are n boundary conditions of the original system

Eq. A.1 and from Eq. A.23 these give n boundary conditions on y_m. But since the diffusion equation is second order, only two boundary conditions on y_m can be satisfied. How to choose these two boundary conditions from the n available is not obvious and considerable further work is required to clarify this point. In this section the equation will be solved for general boundary conditions and the form of the solution of $\underline{y}$ will be obtained.

$$-\alpha_T \frac{\partial^2 y_m}{\partial x^2} + v_T \frac{\partial y_m}{\partial x} + \frac{\partial y_m}{\partial t} = 0 \qquad (A.18)$$

with the boundary conditions

$$\alpha_1 y_m + \alpha_2 \frac{\partial y_m}{\partial x} = 0 \quad \text{at } x = 0$$

$$\beta_1 y_m + \beta_2 \frac{\partial y_m}{\partial x} = 0 \quad \text{at } x = 1 \qquad (A.26)$$

Let

$$p = \frac{v_T}{2\alpha_T} \qquad (A.27)$$

Then solution of Eq. A.18 is

$$y_m = Ae^{px} e^{\lambda_n t} \left[(\alpha_1 + p\alpha_2) \sin \omega_n x - \omega_n \alpha_2 \cos \omega_n x\right] \qquad (A.28)$$

where

$$\lambda_n = \alpha_T (\omega_n^2 - p^2) \ ; \ \text{A is a constant} \qquad (A.29)$$

and ω_n is a root of the equation

$$(\alpha_2 \beta_1 - \alpha_1 \beta_2) \ \omega \cot \omega = (\alpha_1 + \alpha_2 p)(\beta_1 + \beta_2 p) + \alpha_2 \beta_2 \omega^2 \qquad (A.30)$$

To solve the transcendental Eq. A.30 the solution of

$$\omega \cot \omega = A\omega^2 - B \qquad (A.31)$$

is considered in the next section.

To obtain the solution of the original problem Eq. A.23 can be written as

$$y_i = \gamma_i y_m + \delta_i \frac{\partial y_m}{\partial x} \qquad i = 1 \ldots n \tag{A.32}$$

Hence from Eq. A.28 and A.30 after considerable algebra

$$y_i = C e^{px} e^{\lambda_n t} [\omega_n \beta_2 (\alpha_2 \gamma_i - \alpha_1 \delta_i) \sin \omega_n (1 - x)$$

$$+ (\beta_2 \gamma_i - \beta_1 \delta_i) (\alpha_2 \omega_n \cos \omega_n - (\alpha_1 + \alpha_2 p) \sin \omega_n) \sin \omega_n x] \tag{A.33}$$

For a two-pipe system with original boundary conditions

$y_1 = 0$ at $x = 0$ and $y_2 = 0$ at $x = 1$

the solutions are

$$y_1 = C_1 e^{px} e^{\lambda_n t} \sin \omega_n x$$

$$y_2 = C_2 e^{px} e^{\lambda_n t} \sin \omega_n (1-x) \tag{A.34}$$

It will be noticed that Eq. A.34 satisfies exactly the boundary conditions of the original problem. In a higher order system this will not be true.

If the solutions of the Taylor diffusion model are used as a base set of functions as in Chapter IV, it is essential to ensure that the functions satisfy the boundary conditions of the problem and that the functions are a complete set. To satisfy the boundary conditions it will be necessary to modify the results of Eq. A.33 and to use the two-pipe solutions Eq. A.34 as a guide. The functions so chosen will be members of a complete set in nearly all cases. The solutions for y_m given in Eq. A.28 are complete as they are the solutions of a self-adjoint Sturm-Liouville equation.

Let $(y_m)_r$ be the r^{th} solution of y_m given in Eq. A.28. Then $(y_m')_r$ can be expanded in terms of $(y_m)_r$ since y_m are complete

$$(y'_m)_r = \sum_p b_{rp}(y_m)_p$$

Then y_i, $i = 1 \ldots n$, given by Eq. A.33 are complete provided $\frac{\delta i}{\gamma i}$ are not eigenvalues of the matrix b_{rp}.

A.5 SOLUTION OF THE TRANSCENDENTAL EQUATION

To facilitate the solution of Eq. A.31, a set of tables and graphs have been prepared to give the first six roots of

$$\omega \cot \omega = A\omega^2 - B \tag{A.31}$$

for A and B positive. (Figures A.1 to A.6 and Tables A.1 to A.6) The positive values were chosen since these appear to occur in all the simple cases. Certain general properties of the roots of Eq. A.31 are given below which help to determine intermediate values from the tables and to extrapolate to higher roots if required.

a) ω_n lies between $n\pi$ and $(n-1)\pi$

b) For fixed A and B, ω_n tends to $(n-1)\pi$ as n tends to infinity.

c) For fixed A and n, ω_n tends to $n\pi$ as B tends to infinity.

d) For fixed B and n, ω_n tends to $(n-1)\pi$ as A tends to infinity.

e) When A = 0, the roots are given by the equation

$$\omega \cot \omega = a = 0 \qquad a = B$$

whose solution is given by Carslaw and Jaeger.[30]

f) When B = 0, the roots are given by the equation

$$\omega \tan \omega = a \qquad a = 1/A$$

whose solution is given by Carslaw and Jaeger.[30]

g) $\omega_n = \frac{(2n-1)\pi}{2}$ whenever $B = \frac{A^2\pi^2}{4}(2n-1)^2$

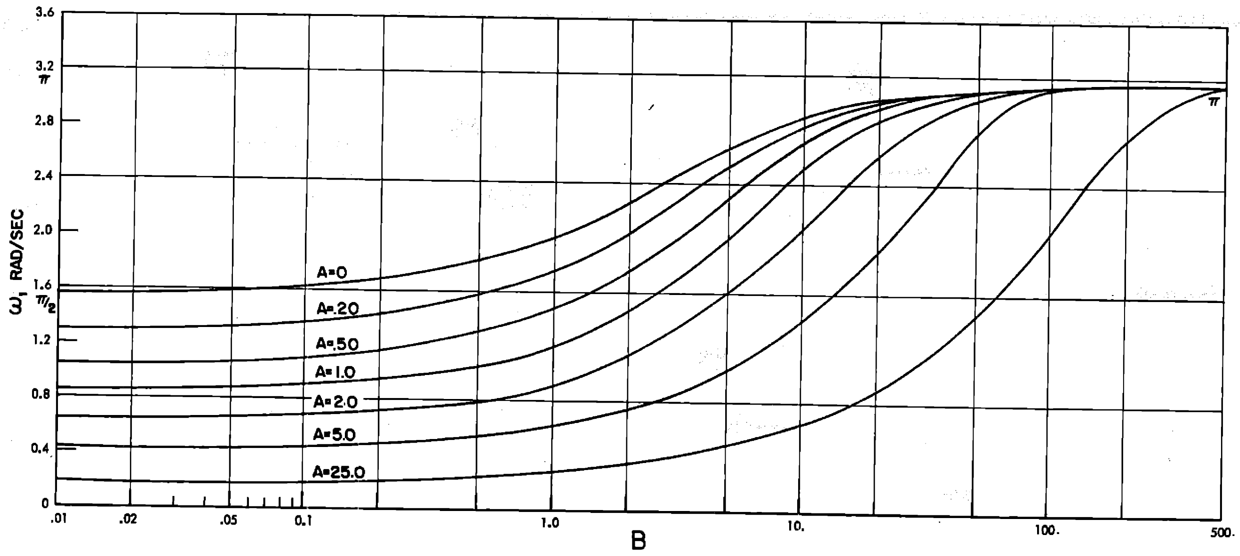


Fig. A.1 Solution of $\omega \cot \omega = A\omega^2 - B$ 1st root

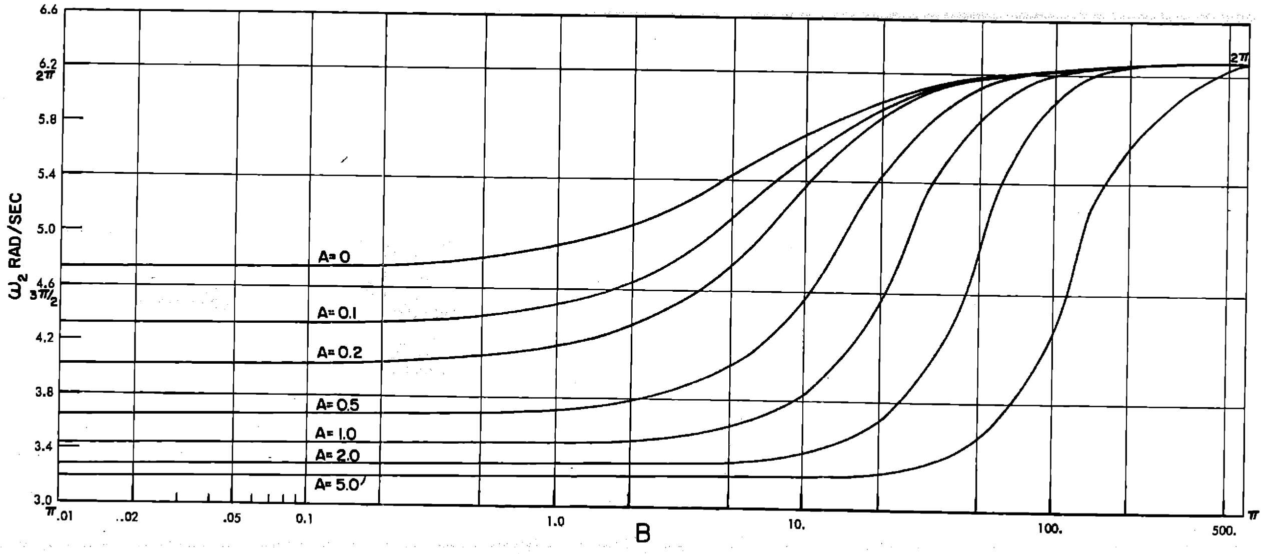


Fig. A.2 Solution of $\omega \cot \omega = A\omega^2 - B$ 2nd root

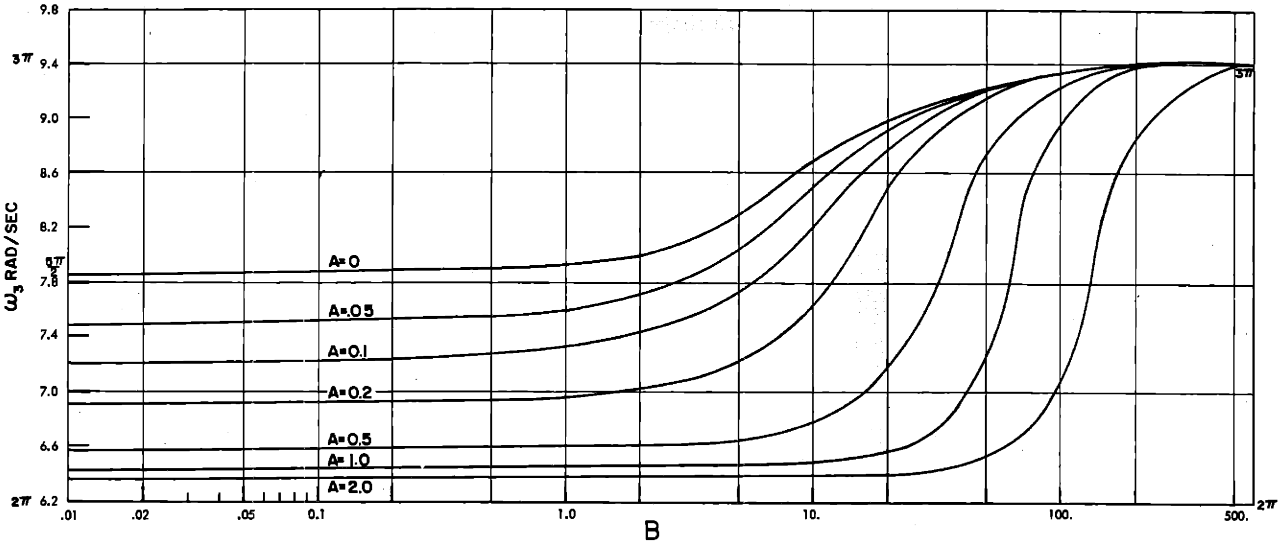


Fig. A.3 Solution of $\omega \cot \omega = A\omega^2 - B$ 3rd root

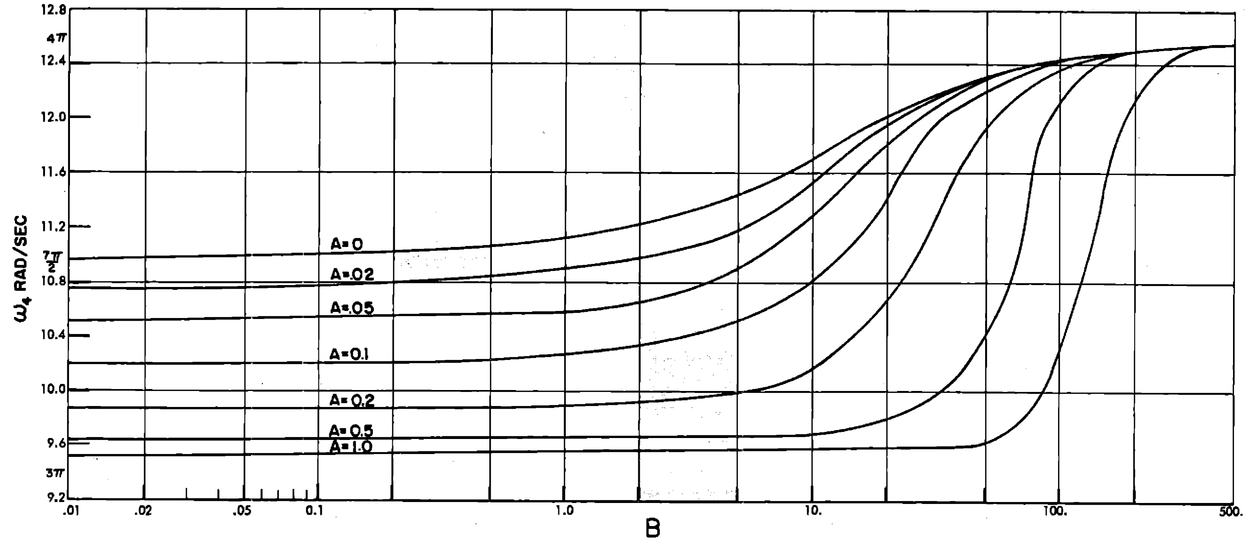


Fig. A.4 Solution of $\omega \cot \omega = A\omega^2 - B$ 4th root

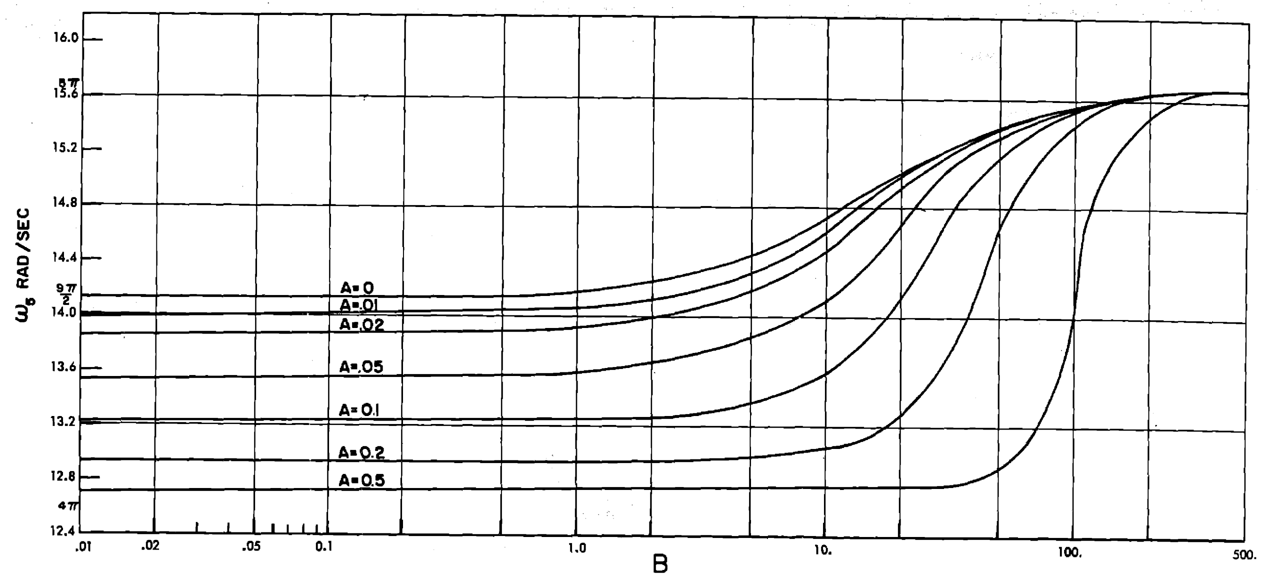


Fig. A.5 Solution of $\omega \cot \omega = A\omega^2 - B$ 5th root

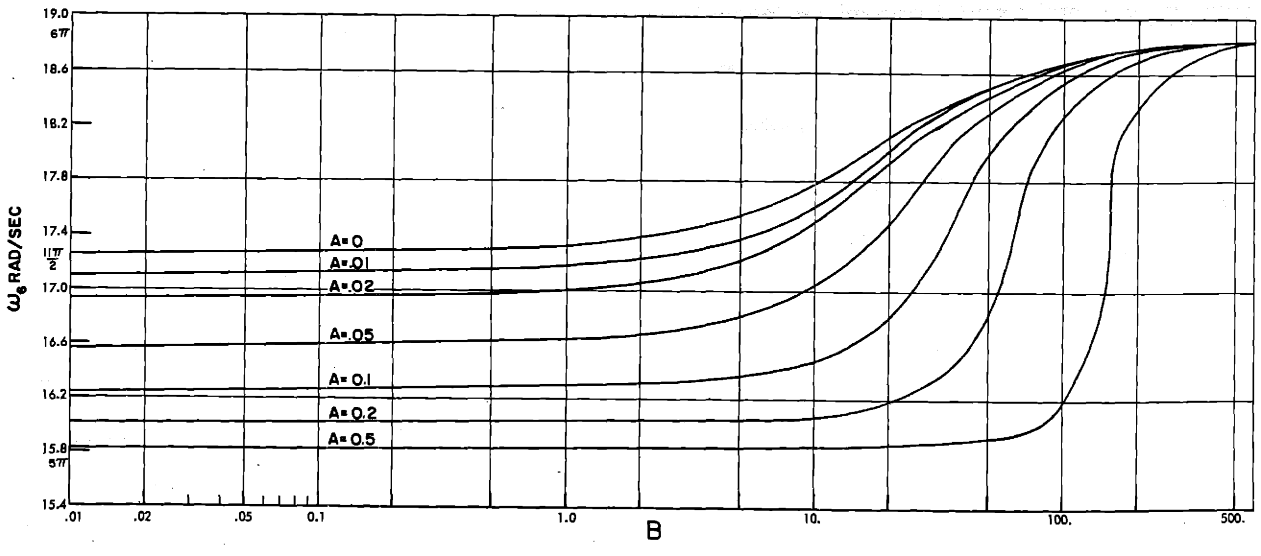


Fig. A.6 Solution of $\omega \cot \omega = A\omega^2 - B$ 6th root

Table A-1

Solution of $\omega \cot \omega = A\omega^2 - B$ 1st root

B	A= 0.	A= .20	A= .50	A= 1.00	A= 2.00	A= 5.00	A=25.00
0.	1.5708	1.3138	1.0769	.8603	.6533	.4328	.1987
.1	1.6320	1.3720	1.1274	.9017	.6850	.4539	.2084
.2	1.6887	1.4267	1.1753	.9411	.7153	.4741	.2176
.5	1.8366	1.5738	1.3065	1.0499	.7992	.5300	.2433
1.0	2.0288	1.7758	1.4936	1.2078	.9218	.6119	.2810
2.0	2.2889	2.0735	1.7898	1.4672	1.1262	.7491	.3441
5.0	2.6537	2.5409	2.3396	2.0122	1.5791	1.0579	.4866
10.0	2.8628	2.8183	2.7309	2.5294	2.0959	1.4286	.6588
20.0	2.9930	2.9795	2.9548	2.8970	2.6893	1.9595	.9101
50.0	3.0801	3.0777	3.0738	3.0662	3.0451	2.8484	1.4173
100.0	3.1105	3.1099	3.1089	3.1072	3.1032	3.0829	1.9911
200.0	3.1260	3.1258	3.1256	3.1252	3.1243	3.1210	2.7766
500.0	3.1353	3.1353	3.1353	3.1352	3.1351	3.1346	3.1290

Table A-2

Solution of $\omega \cot \omega = A\omega^2 - B$ 2nd root

B	A= 0.	A= .10	A= .20	A= .50	A= 1.00	A= 2.00	A= 5.00
0.	4.7124	4.3058	4.0336	3.6436	3.4256	3.2923	3.2039
.1	4.7335	4.3239	4.0470	3.6493	3.4278	3.2930	3.2041
.3	4.7751	4.3604	4.0745	3.6611	3.4321	3.2943	3.2043
1.0	4.9132	4.4899	4.1753	3.7051	3.4482	3.2991	3.2051
2.0	5.0870	4.6731	4.3287	3.7762	3.4739	3.3065	3.2064
5.0	5.4544	5.1420	4.7957	4.0457	3.5728	3.3328	3.2105
10.0	5.7606	5.5990	5.3774	4.5933	3.8292	3.3959	3.2185
20.0	5.9921	5.9373	5.8631	5.4619	4.5532	3.6466	3.2409
40.0	6.1311	6.1161	6.0981	6.0152	5.6630	4.5209	3.3475
70.0	6.1949	6.1899	6.1843	6.1629	6.0993	5.6105	3.8582
100.0	6.2211	6.2186	6.2159	6.2065	6.1834	6.0590	4.4943
150.0	6.2416	6.2405	6.2393	6.2355	6.2272	6.1986	5.3963
500.0	6.2706	6.2705	6.2704	6.2701	6.2696	6.2683	6.2614

Table A-3

Solution of $\omega \cot \omega = A\omega^2 - B$ 3rd root

B	A= 0.	A= .05	A= .10	A= .20	A= .50	A= 1.00	A= 2.00
0.	7.8540	7.4954	7.2281	6.9096	6.5783	6.4373	6.3616
.1	7.8667	7.5066	7.2367	6.9143	6.5796	6.4377	6.3617
1.0	7.9787	7.6099	7.3172	6.9587	6.5911	6.4410	6.3626
2.0	8.0962	7.7271	7.4134	7.0132	6.6050	6.4448	6.3636
5.0	8.3913	8.0671	7.7287	7.2112	6.6536	6.4574	6.3667
10.0	8.7083	8.4986	8.2281	7.6387	6.7665	6.4829	6.3724
20.0	9.0018	8.9170	8.8018	8.4493	7.1777	6.5606	6.3865
40.0	9.1987	9.1738	9.1435	9.0581	8.3811	6.9673	6.4325
60.0	9.2715	9.2601	9.2469	9.2138	8.9937	7.7821	6.5349
80.0	9.3089	9.3025	9.2952	9.2781	9.1864	8.5424	6.7904
100.0	9.3317	9.3276	9.3230	9.3126	9.2639	8.9875	7.2469
150.0	9.3624	9.3606	9.3586	9.3543	9.3372	9.2805	8.4810
500.0	9.4060	9.4058	9.4056	9.4052	9.4041	9.4019	9.3932

Table A-4

Solution of $\omega \cot \omega = A\omega^2 - B$ 4th root

B	A= 0.	A= .02	A= .05	A= .10	A= .20	A= .50	A= 1.00
0.	10.9956	10.7832	10.5117	10.2003	9.8927	9.6296	9.5293
.1	11.0047	10.7919	10.5189	10.2049	9.8947	9.6300	9.5294
1.0	11.0855	10.8708	10.5854	10.2479	9.9132	9.6339	9.5305
3.0	11.2560	11.0462	10.7432	10.3548	9.9589	9.6430	9.5328
10.0	11.7027	11.5605	11.3047	10.8362	10.1836	9.6816	9.5420
20.0	12.0250	11.9573	11.8283	11.5235	10.7231	9.7641	9.5579
40.0	12.2688	12.2467	12.2075	12.1198	11.7965	10.1481	9.6065
60.0	12.3632	12.3528	12.3351	12.2989	12.1841	10.9750	9.7018
80.0	12.4124	12.4065	12.3966	12.3773	12.3230	11.7478	9.9194
100.0	12.4426	12.4387	12.4324	12.4205	12.3895	12.1351	10.3687
150.0	12.4833	12.4816	12.4788	12.4739	12.4620	12.3984	11.7690
200.0	12.5039	12.5029	12.5014	12.4987	12.4925	12.4648	12.3167
500.0	12.5413	12.5411	12.5409	12.5405	12.5396	12.5366	12.5298

Table A-5

Solution of $\omega \cot \omega = A\omega^2 - B$ 5th root

B	A= 0.	A= .01	A= .02	A= .05	A= .10	A= .20	A= .50
0.	14.1372	13.9981	13.8666	13.5420	13.2142	12.9352	12.7223
.1	14.1442	14.0050	13.8732	13.5469	13.2169	12.9362	12.7225
1.0	14.2074	14.0677	13.9332	13.5923	13.2416	12.9453	12.7242
3.0	14.3433	14.2062	14.0691	13.7010	13.3021	12.9669	12.7281
10.0	14.7335	14.6301	14.5164	14.1376	13.5809	13.0626	12.7435
20.0	15.0625	15.0061	14.9420	14.6965	14.1380	13.2819	12.7710
40.0	15.3417	15.3215	15.2992	15.2164	14.9994	14.1386	12.8591
60.0	15.4558	15.4460	15.4354	15.3984	15.3113	14.9371	13.0458
80.0	15.5164	15.5107	15.5046	15.4841	15.4397	15.2780	13.4668
100.0	15.5537	15.5499	15.5460	15.5331	15.5066	15.4219	14.1397
150.0	15.6043	15.6026	15.6009	15.5953	15.5846	15.5560	15.2777
200.0	15.6300	15.6290	15.6280	15.6250	15.6192	15.6052	15.5155
500.0	15.6766	15.6764	15.6763	15.6758	15.6750	15.6732	15.6665

Table A-6

Solution of $\omega \cot \omega = A\omega^2 - B$ 6th root

B	A= 0.	A= .01	A= .02	A= .05	A= .10	A= .20	A= .50
0.	17.2787	17.1093	16.9519	16.5864	16.2593	16.0106	15.8336
.1	17.2845	17.1149	16.9571	16.5899	16.2610	16.0112	15.8337
1.0	17.3364	17.1658	17.0046	16.6220	16.2762	16.0162	15.8346
3.0	17.4490	17.2796	17.1133	16.6987	16.3126	16.0279	15.8366
10.0	17.7908	17.6506	17.4968	17.0211	16.4736	16.0760	15.8443
20.0	18.1136	18.0274	17.9268	17.5365	16.8207	16.1721	15.8569
40.0	18.4180	18.3843	18.3456	18.1898	17.7290	16.5498	15.8902
60.0	18.5497	18.5329	18.5143	18.4443	18.2499	17.2907	15.9414
80.0	18.6209	18.6110	18.6003	18.5620	18.4670	17.9841	16.0275
100.0	18.6650	18.6586	18.6517	18.6279	18.5733	18.3389	16.1888
150.0	18.7254	18.7224	18.7194	18.7093	18.6885	18.6226	17.2996
200.0	18.7560	18.7544	18.7527	18.7472	18.7364	18.7066	18.3296
500.0	18.8119	18.8116	18.8114	18.8106	18.8091	18.8058	18.7915

APPENDIX B

BOUNDS ON THE EIGENVALUES OF SYSTEMS WITH CONVECTION AND DIFFUSION

B.1. INTRODUCTION

In this appendix some bounds on the eigenvalues of systems with convection and diffusion are developed. It is assumed that such eigenvalues exist and are discrete. It is shown that no useful bounds are obtained for a pure convective system. Bounds are obtained for the real part, the imaginary part, and the ratio of the imaginary part to the real part of the eigenvalues. The significance of the results is that it is shown that the imaginary part of the eigenvalues is bounded however small the quantity of diffusion and thus the eigenvalues tend to infinity along the negative real axis. The actual numerical bounds are much larger than the actual limits but the proof of the existence of a bound is useful.

B.2. EIGENVALUE BOUNDS

Consider the system represented by

$$-\underline{D}y'' + \underline{V}\,\underline{y}' + \underline{H}\underline{y} + \lambda\underline{C}\underline{y} = 0 \qquad \text{(B.1)}$$

with the boundary conditions

$$\begin{aligned} \underline{y} + \underline{A}\underline{y}' &= 0 \quad \text{at } x = 0 \\ \underline{y} + \underline{B}\underline{y}' &= 0 \quad \text{at } x = 1 \end{aligned} \qquad \text{(B.2)}$$

where $\underline{D}$ is a diagonal matrix independent of x,

$\underline{V}, \underline{C}$ are diagonal matrices which are functions of x,

$\underline{H}$ is an unsymmetric matrix that is a function of x,

$\underline{A}, \underline{B}$ are diagonal matrices independent of x.

Multiply Eq. B.1 by $e^{-\underline{D}^{-1}\underline{V}x}$ and the system can be written as

$$-(\underline{P}\,\underline{y}')' + \underline{Q}\underline{y} + \lambda\underline{R}\,\underline{y} = 0 \qquad \text{(B.3)}$$

with the boundary conditions of Eq. B.2.

Consider the following integral, where $\underline{y}_n$, $\underline{y}_m$ are solutions of Eq. B.3

$$I_{mn} = \int_0^1 \underline{y}_m^T [-(\underline{P}\underline{y}'_n)' + \underline{Q}\underline{y}_n + \lambda_n \underline{R}\underline{y}_n] \, dx = 0 \qquad (B.4)$$

Integrating by parts

$$I_{mn} = \int_0^1 \underline{y}'^T_m \underline{P}\underline{y}'_n + \underline{y}_m^T \underline{Q}\underline{y}_n + \lambda_n \underline{y}_m^T \underline{R}\underline{y}_n] dx \qquad (B.5)$$

Since $\underline{y}_m$ and $\underline{y}_n$ satisfy the boundary conditions.

Since $\underline{P}$, $\underline{Q}$, $\underline{R}$ are real, if $\underline{y}_n$, λ_n is a solution of Eq. B.3 then $\underline{y}_n^*$, λ_n^* is another solution. Let $\underline{y}_m = \underline{y}_n^*$. Hence, from $I_{mn} + I_{nm}$ and $I_{mn} - I_{nm}$ the following equations are obtained

$$2j \, \mathrm{Im}(\lambda_n) \int_0^1 \underline{y}_n^{*T} \underline{R}\underline{y}_n \, dx = -\int_0^1 \underline{y}_n^{*T} (\underline{Q} - \underline{Q}^T) \underline{y}_n \, dx \qquad (B.6)$$

$$2 \, \mathrm{Re}(\lambda_n) \int_0^1 \underline{y}_n^{*T} \underline{R}\underline{y}_n \, dx = \int_0^1 2 \underline{y}_n^{*'T} \underline{P}\underline{y}'_n + \underline{y}_n^{*T} (\underline{Q} + \underline{Q}^T) \underline{y}_n \, dx$$

(B.7)

Let $\underline{Q}_1 = \frac{1}{2}(\underline{Q} + \underline{Q}^T)$ be the symmetric part of $\underline{Q}$

$\underline{Q}_2 = \frac{1}{2}(\underline{Q} - \underline{Q}^T)$ be the skew-symmetric part of $\underline{Q}$

$\underline{y}_n = \underline{\xi}_n + j\underline{\eta}_n$ (B.8)

$$\tan\theta = \frac{\mathrm{Im}(\lambda n)}{\mathrm{Re}(\lambda n)}$$

Then

$$\operatorname{Im}(\lambda_n) = \frac{-2\int_0^1 \underline{\xi}_n^T \, \underline{Q}_2 \, \underline{\eta}_n \, dx}{\int_0^1 \left(\underline{\xi}_n^T \, \underline{R} \, \underline{\xi}_n + \underline{\eta}_n^T \, \underline{R} \, \underline{\eta}_n \, dx \right)} \tag{B.9}$$

$$\operatorname{Re}(\lambda_n) = \frac{\int_0^1 \left(\underline{y}_n^{*'T} \, \underline{P} \underline{y}_n' + \underline{y}_n^{*T} \, \underline{Q}_1 \, \underline{y}_n \right) dx}{\int_0^1 \underline{y}_n^{*T} \, \underline{R} \, \underline{y}_n \, dx} \tag{B.10}$$

$$\tan\theta = \frac{j\int_0^1 \underline{y}_n^{*T} \, \underline{Q}_2 \, \underline{y}_n \, dx}{\int_0^1 \underline{y}_n^{*'T} \, \underline{P} \, \underline{y}_n' + \underline{y}_n^{*T} \, \underline{Q}_1 \, \underline{y}_n \, dx} \tag{B.11}$$

To determine the maximum value of $|\operatorname{Im}(\lambda_n)|$ from Eq. B.9 the following lemma is required.

Lemma

$$|\underline{x}^T \underline{A} \, \underline{u}| \leq \frac{1}{2} [\underline{x}^T \underline{B} \, \underline{x} + \underline{u}^T \underline{B} \underline{u}] \sqrt{\lambda_{\max}(\underline{F}\underline{F}^T)}$$

where $\underline{B}$ is a positive definite diagonal matrix and $\underline{F} = \underline{B}^{-1/2} \underline{A} \, \underline{B}^{-1/2}$.

Proof

Consider the maximum value of $\underline{x}^T \underline{A} \underline{u}$ subject to the constraint. $\underline{x}^T \underline{B} \underline{x} + \underline{u}^T \underline{B} \underline{u} = k$ is a constant.

Let $$f = \underline{x}^T \underline{A} \underline{u} - \mu [\underline{x}^T \underline{B} \, \underline{x} + \underline{u}^T \underline{B} \underline{u}]$$

At an extremum $\frac{\partial f}{\partial \underline{x}}, \frac{\partial f}{\partial \underline{u}}$ are zero

$$\underline{A} \underline{u} = 2\mu \, \underline{B} \underline{x}$$

$$\underline{A}^T \underline{x} = 2\mu \, \underline{B} \underline{u}$$

Hence $\quad \underline{x}^T \underline{Au} = \mu k \quad$ and $\quad \underline{B}^{-1/2}\,\underline{AB}^{-1}\;\;\underline{AB}^{-1/2}\underline{x} = 4\mu^2\underline{x}$

Thus $$\mu = \frac{1}{2}\sqrt{\lambda(\underline{F}\,\underline{F}^T)}$$

Note that $\underline{FF}^T$ is a symmetric matrix so that all the eigenvalues are real. Thus the lemma is proved, namely

$$|\underline{x}^T\underline{Au}| \le \frac{1}{2}[\underline{x}^T\underline{B}\underline{x} + \underline{u}^T\,\underline{B}\underline{u}]\sqrt{\lambda_{max}(\underline{F}\,\underline{F}^T)}$$

Using the lemma it is clear that

$$|\mathrm{Im}\,(\lambda_n)| \le \sqrt{\lambda_{max}(F\,F^T)}$$
$$\max\ 0 \le x \le 1$$

where $$\underline{F} = \underline{R}^{-1/2}\underline{Q}_2\,\underline{R}^{-1/2}$$

But $\underline{Q}_2$ is a skew-symmetric matrix and $\underline{R}^{-1/2}\underline{Q}_2\,\underline{R}^{-1/2}$ is also skew-symmetric.

$$|\mathrm{Im}\,(\lambda_n)| \le [\,j\,\lambda_{max}(\underline{F})\,] \qquad \text{(B. 12)}$$
$$\max\ 0 \le x \le 1$$

To solve Eq. B. 10 and B. 11, replace $\underline{y}_n$ (a set of discrete functions) by $\underline{u}$ (a continuous function). Then

$$\mathrm{Re}(\lambda_n) \le \left.\frac{\int_0^1 (\underline{u}^{*'T}\underline{P}u' + \underline{u}^{*T}\underline{Q}_1\underline{u})\,dx}{\int_0^1 \underline{u}^{*T}\underline{R}\,\underline{u}\;\;dx}\right|_{\max} \qquad \text{(B. 13)}$$

$$\tan\theta \le \left.\frac{\int_0^1 \underline{u}^{*T}\underline{Q}_2\,\underline{u}\;\;dx}{\int_0^1 (\underline{u}^{*'T}\underline{Pu}' + \underline{u}^{*T}\underline{Q}_1\underline{u})\,dx}\right|_{\max} \qquad \text{(B. 14)}$$

Eqs. B. 13 and B. 14 can be solved by the classical calculus of variations. Euler's equations give

$$\mathrm{Re}\,(\lambda_n) < \mu_{1\ \max} \qquad \text{(B. 15)}$$

$$|\tan\,\theta| < |\mu_{2\,\max}| \tag{B.16}$$

where $\mu_{1\,\max}$ is the largest eigenvalue, or the smallest in magnitude since the eigenvalues are all negative.

$$-(\underline{P}\,\underline{u}')' + \underline{Q}_1\,\underline{u} + \mu\,\underline{R}\,\underline{u} = 0 \tag{B.17}$$

and $\mu_{2\,\max}$ is the smallest eigenvalue of the equation

$$-(\underline{P}\,\underline{u}')' + \underline{Q}_1\,\underline{u} + j\,\mu\,\underline{Q}_2\,\underline{u} = 0 \tag{B.18}$$

The boundary conditions for Eqs. B.17 and B.18 are the original boundary conditions of the system given by Eq. B.2. Also both equations are self-adjoint and have all real eigenvalues since all the matrices are hermitian. In Eq. B.18 if $\underline{u}$, μ is a solution then $\underline{u}^*$ and $-\mu$ is also a solution. This result is to be expected as the eigenvalues of the original system occur in complex pairs.

Eqs. B.15 and B.16 have inequality signs since equality would occur only if the solution $\underline{u}$ of Eqs. B.17 and B.18 also satisfied the original system, Eq. B.3. This cannot occur except in very degenerate cases.

Eqs. B.17 and B.18 can be solved by Galerkin's method. In Eq. B.17 the $\underline{u}$ are real and a real set of functions can be used. However, in Eq. B.18 the $\underline{u}$ are complex and a complex set of $\underline{\phi}_n$ must be used, together with the conjugate set $\underline{\phi}_n^*$. This will ensure approximation to the largest in magnitude of the values of μ_2 with both plus and minus signs.

B.3. EXAMPLE

Consider the bound on $\mathrm{Im}(\lambda_n)$ for Example A considered in Chapter II. The equations are

$$-\,d_1\,\frac{\partial^2 y_1}{\partial x^2} + \frac{\partial y_1}{\partial x} + \frac{\partial y_1}{\partial t} + N_1(y_1 - y_2) = 0$$

$$-\,d_2\,\frac{\partial^2 y_2}{\partial x^2} + \frac{\partial y_2}{\partial x} + \beta\,\frac{\partial y_2}{\partial t} + N_2\,(y_2 - y_1) = 0$$

Then the matrices $\underline{P}$, $\underline{Q}$ and $\underline{R}$ are

$$\underline{P} = \begin{pmatrix} -d_1 e^{-x/d_1} & 0 \\ 0 & -d_2 e^{-x/d_2} \end{pmatrix} \quad \underline{R} = \begin{pmatrix} e^{-x/d_1} & 0 \\ 0 & \beta e^{-x/d_2} \end{pmatrix}$$

$$\underline{Q} = \begin{pmatrix} N_1 e^{-x/d_1} & -N_1 e^{-x/d_1} \\ -N_2 e^{-x/d_2} & N_2 e^{-x/d_2} \end{pmatrix}$$

Then $\underline{Q}_2$ (the skew-symmetric part of $\underline{Q}$) is

$$\underline{Q}_2 = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix} \text{where} \quad q = \frac{1}{2}\left[N_2 e^{-x/d_2} - N_1 e^{-x/d_1} \right]$$

From Eq. B.12

$$\underline{F} = \begin{pmatrix} 0 & f \\ -f & 0 \end{pmatrix}$$

where
$$f = \frac{1}{2\beta^{1/2}} \left[N_2 e^{-x/d_2} - N_1 e^{-x/d_1} \right] e^{\left(\frac{1}{d_1} + \frac{1}{d_2}\right)\frac{x}{2}}$$

and
$$|\operatorname{Im}(\lambda_n)| \leq [\,|f|\,]_{\max} \quad 0 \leq x \leq 1$$

For example A of Chapter II where $N_1 = 3$, $N_2 = -4$, $\beta = -4$ with the added diffusion of $d_1 = 0.0033$ and $d_2 = -0.0025$ then $|\operatorname{Im}(\lambda_n)| \leq e^{350}$. In the actual example the maximum imaginary part of the eigenvalues of 6.

B.4. SIGNIFICANCE OF THE RESULTS

The importance of the results of this appendix are not the numerical value of the bounds as the example showed that the bound is far removed from the least bound. But it has been shown that a bound exists for the imaginary part of the eigenvalues when there is some diffusion however small in each stream of the system. It is well known property of a second-order <u>scalar</u> differential equation that it can be put in self-adjoint form providing the boundary conditions are given by

Eq. B.2. Such a scalar equation is a one-stream system with diffusion and convection, and has real negative eigenvalues. However, the vector equation given by Eq. B.1 cannot, in general, be put in self-adjust form (see Appendix C) and the eigenvalues can be complex. In this appendix it has been shown that such complex eigenvalues have a bounded imaginary part and thus tend to infinity parallel to the negative real axis.

When there is no diffusion present the methods used here do not apply, but if the limiting case is considered as the diffusion tends to zero, it is clear that the bound on the imaginary part goes to infinity and θ tends to $\pi/2$. This is consistent with the results of Appendix D where the asymptotic values of the eigenvalues obtained by the modified Galerkin method are considered.

APPENDIX C

PROPERTIES OF A LINEAR SYSTEM AND ITS ADJOINT

C.1 INTRODUCTION

In Chapter II various results from the theory of linear systems are used, especially those concerned with eigenvalues and eigenvectors. In this appendix a summary is made of the properties of a linear system and its adjoint. Since all the results except those in Section C.5 are standard results, no proofs are given. Details of the proofs are available in the standard mathematical texts.[1, 7, 9, 11, 14] The particular linear system considered in this work is the general convective system whose equations are

$$-\underline{D}\underline{y}'' + \underline{V}\underline{y}' + \lambda\underline{C}\underline{y} + \underline{H}\underline{y} = 0 \qquad \text{(C.1a)}$$

where $\underline{D}, \underline{V}, \underline{C}$ are diagonal matrices which are functions of x and $\underline{H}$ is a general matrix which is a function of x.

If $\underline{D}$ is zero then the system is a pure convective system, and if $\underline{V}$ is zero the system is a pure diffusive system. The results of linear system theory for convective systems are stated.

In Section C.2 the adjoint system is defined and in Section C.3 the properties of the eigenvalues and eigenvectors are given. To illustrate the points made in the previous sections a simple example is considered in Section C.4. Finally a relation between the solution of a system and the solution of its adjoint for pure convective systems with constant coefficients is obtained in Section C.5. This relation is useful in Chapter II since the Galerkin[8] method involves solving simultaneously the system and its adjoint any information concerning a system and its adjoint is useful. This result is particularily helpful as such processes as heat exchange and distillation are very close to being pure convective systems with constant coefficients.

In this appendix it is assumed that the range of x is $0 \leq x \leq 1$. The inner product $\langle a, b \rangle$ denotes integration over x and if a, b are vectors, the vector inner product followed by integration over x.

C.2 ADJOINT OPERATOR

Consider a scalar system represented by the equation

$$L(y) = \lambda y \tag{C.1}$$

where L is any real linear operator with its set of boundary conditions. Then there exists an associated operator called the adjoint operator $\overline{L}$ such that

$$\overline{L}(z) = \lambda z \tag{C.2}$$

and

$$<y, \overline{L}(z)> - <L(y), z> = k \tag{C.3}$$

where k is not a function of y and z, the solutions of Eqs. C.1 and C.2.

Ince[11] defines adjoint systems as such that k is constant, but modern practice is to define the adjoint system with the set of boundary conditions which makes k zero. Thus to conform to current practice to construct an adjoint system one chooses the operator $\overline{L}$ to satisfy Eq. C.3 and then chooses a set of boundary conditions for z such that with the given boundary conditions for y, k is zero.

These definitions can be extended to the case where $\underline{y}, \underline{z}$ are vectors and $\underline{L}, \underline{\overline{L}}$ are matrix operators.

A system is said to be self-adjoint if $L = \overline{L}$ and the boundary conditions are identical. The classical Sturm-Liouville[20,16] equation is a scalar second-order self-adjoint system, namely

$$(py')' + qy + \lambda ry = 0 \tag{C.4}$$

with boundary conditions

$$\alpha_1 y + \beta_1 y' = 0 \quad \text{at } x = 0$$

$$\alpha_2 y + \beta_2 y' = 0 \quad \text{at } x = 1$$

It is easy to show[22] that any second-order scalar differential equation can be put in self-adjoint form by any of three transformations, multiplying by a function, changing the dependent variable or changing the independent variable.

For vector systems there are no such simple results. Consider the set of equations

$$(\underline{A}\underline{y}')' + \underline{B}\underline{y}' + \underline{C}\underline{y} + \lambda\underline{D}\underline{y} = 0 \qquad \text{(C.5)}$$

with a suitable set of boundary conditions where $\underline{A}$, $\underline{B}$, $\underline{C}$, $\underline{D}$ are real matrices. The adjoint equations are

$$(\underline{A}^T\underline{z}')' - (\underline{B}^T\underline{z})' + \underline{C}^T\underline{z} + \lambda\underline{D}^T\underline{z} = 0 \qquad \text{(C.6)}$$

For Eq. C.5 to be self-adjoint,

$$\begin{aligned} &\underline{A},\ \underline{C},\ \underline{D} \text{ must be symmetric} \\ &\underline{B} \text{ must be skew-symmetric} \end{aligned} \qquad \text{(C.7)}$$

and the set of boundary conditions must be the same for both the system and its adjoint. In particular consider the convective system given by Eq. C.1a. The matrix $\underline{V}$ must be skew-symmetric and $\underline{D}$, $\underline{C}$, $\underline{H}$ must be symmetric. But $\underline{V}$ is always diagonal in a convective system so a convective system can never be self-adjoint. However a pure diffusive system can be self-adjoint provided $\underline{H}$ is symmetric. Clearly it is not possible in general to reduce the vector Eq. C.5 to self-adjoint form as in the case of the second-order scalar equation. When the coefficient matrices are complex, the conditions of Eq. C.7 become hermitian and skew-hermitian.[1]

C.3 EIGENVALUES AND EIGENFUNCTIONS

To show the difference between self-adjoint and non-self-adjoint systems, particularly their eigenvalues and eigenfunctions, some properties are listed below.

For non-self-adjoint systems

a) The eigenvalues may or may not exist and can be finite or infinite.

b) If the eigenvalues exist then they are identical for a system and its adjoint.

c) The eigenvalues can be real or complex, discrete or essential singularities or branch points.

d) There is not necessarily a separate eigenfunction for each eigenvalue nor can separate eigenfunctions be constructed for multiple eigenvalues.

e) If $\underline{y}_n$ and $\underline{z}_n$ are eigenfunctions of a system and its adjoint corresponding to an eigenvalue λ_n, then

$$<\underline{y}_n, \underline{z}_m> = \begin{cases} 1 & n=m \\ 0 & n \neq m \end{cases}$$

f) The eigenfunctions do not necessarily span the function space.

For a self-adjoint system

a) The eigenvalues exist and are all real, discrete and usually negative.

b) The eigenfunctions are distinct, orthogonal and span the function space.

c) To each eigenvalue there exists a distinct eigenfunction and for a multiple eigenvalue of order r, r distinct orthogonal eigenfunctions can be constructed.

C.4 EXAMPLE: SINGLE-PIPE HEAT EXCHANGER

To illustrate some of the points in the preceeding sections and to obtain some physical representation of the adjoint system, consider a single-pipe heat exchanger whose walls are kept at a constant temperature, taken to be zero for convenience. In non-dimensional time and distance the equation of such a system is

$$T' + NT + \lambda T = 0 \qquad (C.8)$$

with boundary condition

$$T(0,t) = 0$$

To obtain the adjoint system consider the equation

$$-R' + NR + \lambda R = 0 \qquad (C.9)$$

where R is the adjoint variable.

Then from Eq. C.3

$$\int_0^1 [T(-R' + NR + \lambda R) - R(T' + NT + \lambda T)\, dx$$

$$= [-TR']_0^1 = -T(1)R(1) + T(0)R(0)$$

From the boundary condition on T the second term is zero. To make the expression zero the required boundary condition on R is

$$R(1,t) = 0$$

Thus it is clear that the adjoint system is an identical system flowing in the opposite direction with an input at $x = 1$ identical to the input at $x = 0$ of the original system. Considering the two systems together (Fig. C.1) it is clear that there is no net heat transferred in the x direction across any section. However, heat is transferred to the walls by both systems and thus heat leaves the system. The addition therefore of the adjoint system produces a system with no net flow along the x direction.

Finally consider the solution of Eq. C.8

$$T = \Sigma a_n e^{-(N + \lambda)x}$$

The boundary condition $T(0,t) = 0$ is used to determine the values of λ. Unfortunately this gives only that $\lambda = \infty$. Thus there are no discrete eigenvalues but only an essential singularity at infinity. This is typical behavior for a non-self-adjoint system and makes approximations difficult. Eq. C.8 can easily be solved in the time domain and the solution is

$$T = e^{-Nx} u_{-1}(t - x)$$

It is the time delay which causes difficulty. In the general case of a system with pure convection more complicated essential singularities at infinity exist but the basic problem is caused by the time delay.

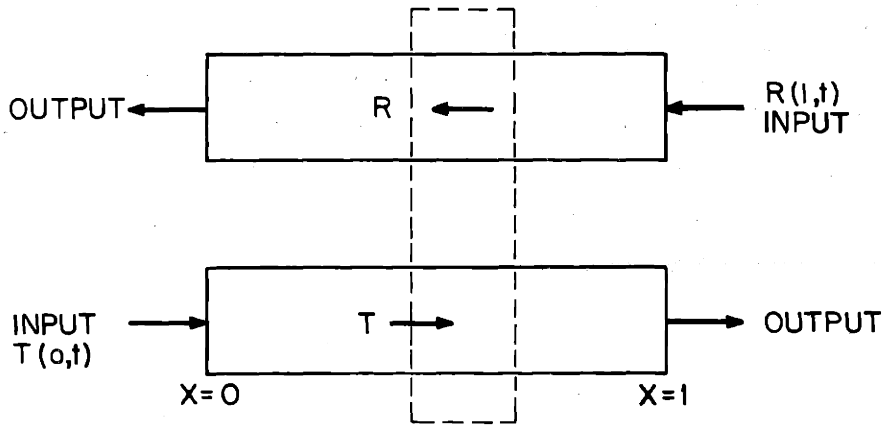


Fig. C.1 A Representation of a System and its Adjoint

C.5 PURE CONVECTIVE SYSTEM

The pure convective system has one particular property which is used in Chapter II, namely, the relation between the solution of the system and of the adjoint system. The equations of a pure convective system and its adjoint are

$$\underline{V}\,\underline{y}' + \lambda\underline{C}\,\underline{y} + \underline{H}\,\underline{y} = 0 \tag{C.10}$$

$$-(\underline{V}^T\underline{z})' + \lambda\underline{C}^T\underline{z} + \underline{H}\,\underline{z} = 0 \tag{C.11}$$

where $\underline{V}$, $\underline{C}$, $\underline{H}$ are functions of x

Let the boundary conditions of Eq. C.10 be $\underline{y} = 0$ at $x = 0$ or 1. This notation denotes that each element of $\underline{y}$, is zero at $x = 0$ or $x = 1$. It is not significant in the theory which elements of $\underline{y}$ are zero at $x = 0$ and which at $x = 1$. Usually the elements of $\underline{y}$ are zero at $x = 0$ when the corresponding element of $\underline{V}$ is positive and zero at $x = 1$ when the corresponding elements of $\underline{V}$ are negative. The boundary conditions of $\underline{z}$ are that if

$$y_i = 0 \text{ at } x = 0 \text{ then } z_i = 0 \text{ at } x = 1$$

and if

$$y_i = 0 \text{ at } x = 1 \text{ then } z_i = 0 \text{ at } x = 0$$

Thus the boundary conditions of Eq. C.10 and C.11 can be written

$$\underline{y} = 0 \quad x = 0 \text{ or } 1 \tag{C.12}$$

$$\underline{z} = 0 \quad x = 1 \text{ or } 0 \tag{C.13}$$

In Eq. C.11 and C.12 let $u = 1 - x$

$$(\underline{V}^T(1-u)\underline{z})' + \lambda\underline{C}^T(1-u)\,\underline{z} + \underline{H}^T(1-u)\,\underline{z} = 0 \tag{C.14}$$

and boundary condition

$$\underline{z} = 0 \quad u = 0 \text{ or } 1 \tag{C.15}$$

Equations C.12 and C.15 are identical and Eqs. C.10 and C.14 will be identical if the coefficient matrices satisfy the following conditions

$$\underline{V}(x) \text{ is symmetric and constant} \tag{C.16}$$

$$\underline{C}(x) = \underline{C}^T(1 - x)$$
$$\underline{H}(x) = \underline{H}^T(1 - x) \qquad (C.17)$$

This is true if $\underline{C}$ and $\underline{H}$ are symmetric and have elements which are symmetric with respect to x about $x = 1/2$. A special case occurs when $\underline{C}$ and $\underline{H}$ are symmetric constant matrices.
Then

$$\underline{y}(x) = \underline{z}(1 - x) \qquad (C.18)$$

In general there is no simple relation like Eq. C.18 relating $\underline{y}$ and $\underline{z}$ but in a large class of systems such as heat exchangers and distillation columns the coefficient matrices do not differ markedly from a constant as x changes and Eq. C.18 can be useful in selecting the functions required in the Galerkin method discussed in Chapter II.

APPENDIX D

ASYMPTOTIC EIGENVALUES OF CERTAIN MATRICES

D.1. INTRODUCTION

In Chapter II the modified Galerkin method was applied to a two pipe constant coefficient system with the Taylor diffusion characteristic functions used as a set of base functions. In this appendix the asymptotic value of the eigenvalues will be considered as the number of functions used is increased. In particular if no diffusion is added it is shown that the real part of the eigenvalues tends to a finite value while the imaginary part tends to infinity, but with diffusion added the imaginary part tends to zero and the real part tends to minus infinity. This is true however small a quantity of diffusion is added; however, a very large number of terms may be necessary. Thus it is possible to estimate the amount of diffusion necessary to ensure that the largest eigenvalues are real.

D.2. DETERMINATION OF MATRICES

Consider the two pipe constant coefficient system

$$\underline{V}\tilde{\underline{y}} + \lambda \underline{C}\tilde{\underline{y}} + \underline{H}\tilde{\underline{y}} = 0 \tag{D.1}$$

where

$$\underline{V} = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix} \quad \underline{C} = \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix}$$

$$\underline{H} = h\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \tag{D.2}$$

with boundary conditions

$$\tilde{y}_1(x, s) = 0 \qquad x = 0$$

$$\tilde{y}_2(x, s) = 0 \qquad x = 1$$

The Taylor diffusion characteristic functions given in Appendix A are

$$\underline{\Phi}_n = \begin{pmatrix} e^{px} & \sin \omega_n x \\ \\ e^{px} & \sin \omega_n (1 - x) \end{pmatrix} \tag{D.3}$$

Using these functions and applying the modified Galerkin method given in Chapter II, the eigenvalues of Eq. D.1 are the negative of the eigenvalues of the matrix $\underline{B}^{-1}\underline{A}$ where

$$\underline{A} = [\, p(v_1 + v_2) + 2h \,]\, \underline{\Delta} + (v_1 - v_2)\underline{\Gamma} - 2h\underline{\textcircled{H}} \tag{D.4}$$

$$\underline{B} = (c_1 + c_2)\underline{\Delta} \tag{D.5}$$

and

$$\Delta_{nm} = \begin{cases} \dfrac{\omega_m \sin \omega_n - \omega_n \sin \omega_m}{\omega_m^2 - \omega_n^2} & n \neq m \\ \\ \dfrac{1}{2}\, \dfrac{\sin \omega_n}{\omega_n} - \cos \omega_n & n = m \end{cases} \tag{D.6}$$

$$\Gamma_{nm} = \begin{cases} \dfrac{\omega_n \omega_m (\cos \omega_n - \cos \omega_m)}{\omega_m^2 - \omega_n^2} & n \neq m \\ \\ \dfrac{1}{2} \sin \omega_n & n = m \end{cases} \tag{D.7}$$

$$\textcircled{H}_{nm} = \begin{cases} \dfrac{1}{2}\left[\dfrac{\sin(\omega_m - \omega_n)}{\omega_m - \omega_n} - \dfrac{\sin(\omega_m + \omega_n)}{\omega_m + \omega_n}\right] & m \neq n \\ \\ \dfrac{1}{2}\left[\, 1 - \dfrac{\sin 2\omega_n}{2\omega_n} \,\right] & n = m \end{cases} \tag{D.8}$$

D.3. PURE CONVECTIVE SYSTEM

It is shown in Appendix A that as the number of Tayler diffusion characteristic functions increases the characteristic values tend to $(n - 1)\pi$. Consider the elements of $\underline{B}^{-1}\underline{A}$ for large n by letting

$$\omega_n = (n - 1)\pi$$

in Eqs. D.6, D.7 and D.8. Then

$$\Delta_{nm} = \begin{cases} 1/2(-1)^n & n = m \\ 0 & n \neq m \end{cases} \qquad \text{(D.9)}$$

$$\Gamma_{nm} = \begin{cases} \dfrac{-2(n-1)(m-1)(-1)^n}{\pi[(m-1)^2 - (n-1)^2]} & \text{n, m are not both even or both odd} \\ 0 & \text{elsewhere} \end{cases} \qquad \text{(D.10)}$$

$$\textcircled{H}_{nm} = \begin{cases} 1/2 & n \neq m \\ 0 & n = m \end{cases} \qquad \text{(D.11)}$$

and

$$(B^{-1}A)_{nm} = \begin{cases} \dfrac{(v_1 + v_2)p + 4h}{c_1 + c_2} & m = n \quad \text{even} \\ \dfrac{(v_1 + v_2)p}{c_1 + c_2} & m = n \quad \text{odd} \\ \dfrac{4(v_1 - v_2)(n-1)(m-1)}{(c_1 + c_2)[(n-1)^2 - (m-1)^2]} & \text{m, n are not both even or both odd} \\ 0 & \text{elsewhere} \end{cases}$$

From Eq. D.2 it is clear that as $n, m \to \infty$ the diagonal elements remain of the same order but the upper and lower diagonal elements increase proportionally with n. Further if the diagonal elements are removed from $\underline{B}^{-1}\underline{A}$ the remaining matrix is skew symmetric. Since the eigenvalues of a skew-symmetric matrix are pure imaginary the asymptotic value of the eigenvalues of $\underline{B}^{-1}\underline{A}$ lie on a curve approaching infinity in the direction of the imaginary axis. Thus the real part of the eigenvalues of $\underline{B}^{-1}\underline{A}$ tends to a finite limit.

Unfortunately the author has been unable to derive an expression giving this limit. The number of eigenvalues required to reach the limit is dependent on the number of characteristic values which must be used so that the highest value is close to $(n - 1)\pi$.

D.4. SYSTEM WITH CONVECTION AND DIFFUSION

In Chapter II it was shown that the addition of some diffusion improved the convergence of the Galerkin method. Consider the value of $\underline{B}^{1}\underline{A}$ under the same conditions as in the previous section with the addition of some diffusion. Eq. D. 12 becomes

$$(B^{-1}A)_{nm} = \begin{cases} \dfrac{(n^2\pi^2 - p^2)(d_1 + d_2) + (\sigma_1 + \sigma_2)p + 4h}{c_1 + c_2} & m = n \quad \text{even} \\[2ex] \dfrac{(n^2\pi^2 - p^2)(d_1 + d_2) + (v_1 + v_2)p}{c_1 + c_2} & m = n \quad \text{odd} \\[2ex] \dfrac{4(v_1 - v_2)(n - 1)(m - 1)}{(c_1 + c_2)[(n - 1)^2 - (m - 1)^2} & \begin{array}{l} m, n \text{ are not} \\ \text{both even or} \\ \text{both odd} \end{array} \\[2ex] 0 & \text{elsewhere} \end{cases}$$

where the term $-\underline{D}\tilde{y}''$ is added to Eq. C. 1 and

$$\underline{D} = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}$$

From Eq. D. 13 it is clear that as $n \rightarrow \infty$ the dominant terms are on the leading diagonal. Thus

$$\text{Eigenvalues of } (\underline{B}^{-1}\underline{A}) \rightarrow \frac{(n^2\pi^2 - p^2)(d_1 + d_2)}{c_1 + c_2} \tag{D. 14}$$

To estimate when the eigenvalues will behave as given by Eq. D. 14, compare the upper and lower diagonal elements with the leading diagonal elements. The leading diagonal element will be dominant if

$$n >> \frac{2(v_1 - v_2)}{\pi^2(d_1 + d_2)} \tag{D.15}$$

This assumes that n is large enough that

a) ω_n is close to $(n - 1)\pi$ (D.16)

b) $n >> b/\pi$ (D.17)

c) $\frac{n^2}{n - 1} \underline{\Omega}\ n$ (D.18)

For small values of n Eq. D.16 can be the limiting case but it depends on the numerical parameters of the system.

APPENDIX E

INTEGRAL SERIES

One method of obtaining the solution of a general convective system is to convert the equations from a set of differential equations into a set of integral equations. Then the integral equations can be solved by an iterative technique which is a special case of the Neumann series.[2] This method was investigated by Rinard[44] and he showed it to be useful for linear constant-coefficient systems. However, for variable coefficient systems the integrals can not be easily evaluated. The integral series solution is good at high frequencies; however, several terms may be required to obtain an accurate value of the steady state gain. Even though only three or four terms may be required, the labor involved in determining the third and higher order terms is enormous. In the Campbell approximation the first term in the integral series is used to give the form of the transfer function as $s \rightarrow \infty$. An outline is given here of the integral series solution for a two-stream constant coefficient counter-current system.

The equations are in normalized non-dimensional form (Chapter II) after taking Laplace transforms with respect to time.

$$\begin{aligned} y_1' + s\,y_1 + N_1(y_1 - y_2) &= 0 \\ y_2' + \beta s y_2 + N_2(y_2 - y_1) &= 0 \end{aligned} \qquad (E.1)$$

with boundary conditions

$$\begin{aligned} y_1(0, s) &= q_1(s) \\ y_2(1, s) &= q_2(s) \end{aligned} \qquad (E.2)$$

Eq. E.1 can be written as

$$y_1 = e^{-a_1 x} \int_0^x N_1\, y_2\, e^{a_1 x}\, dx + e^{-a_1 x}\, q_1(s) \qquad (E.3)$$

$$y_2 = e^{a_2(1-x)} \int_x^1 -N_2 e^{-a_2(1-x)} y_1 \, dx + e^{a_2(1-x)} q_2(s) \tag{E.4}$$

where
$$a_1 = s + N_1$$
$$a_2 = \beta s + N_2$$

Substitute for y_2 from Eq. E.4 into Eq. E.3, then

$$y_1(x,s) = F(x,s) + I[y_1(x,s)] \tag{E.5}$$

where
$$F(x,s) = e^{-a_1 x} q_1(s) + \frac{N_1}{a_1 - a_2} e^{a_2} q_2(s) \left[e^{-a_2 x} - e^{-a_1 x} \right]$$

and I is the integral operator.

$$I = -N_1 N_2 e^{-a_1 x} \int_0^x e^{(a_1 - a_2)\xi} \, d\xi \int_0^1 e^{a_2 \eta} \, d\eta$$

To solve Eq. E.5 assume $y_1(x,s) = F(x,s)$ as a first approximation. Then the second approximation is

$$y_1(x,s) = F(x,s) + I[F(x,s)]$$

This procedure can be continued and will generate a series of terms that when truncated can be used as an approximate solution. The n^{th} approximation

$$y_1(x,s) = F(x,s) + \sum_{i=1}^{n-1} I^i [F(x,s)] \tag{E.6}$$

where I^i means applying the operator I i-times. The general result for the third order approximation is given by Gould.[37]

For constant coefficient systems, a_1 and a_2 are independent of x although functions of s; thus there is no problem in evaluating the integral operator as many times as is necessary. However, in the variable coefficient system similar equations can be developed but a_1 and a_2 will be functions of x and s. Thus the integrals cannot be easily evaluated.

As an example consider Example B of Chapter II. The equations are given by Eqs. E. 1 and E. 2 where

$$N_1 = 8.22 \qquad N_2 = -5.6 \qquad \beta = -11.5$$

In particular consider the response of $y_2(x, t)$ at $x = 0$ to be a disturbance $q_1(t)$ in $y_1(x, t)$ at $x = 0$. The the first approximation is

$$\frac{y_2(0, s)}{q_1(s)} = \frac{3.40}{1 + 0.897s}\left[1 - e^{-13.83 - 12.5s}\right] \tag{E.7}$$

$$= \frac{3.40}{1 + 0.897s}$$

since the second term can be neglected. The second approximation is

$$\frac{y_2(0, s)}{q_1(s)} = \frac{3.40}{1 + 0.897s}\left[1 + \frac{0.241}{(1 + 0.897s)^2}\right] \tag{E.8}$$

The third approximation is

$$\frac{y_2(0, s)}{q_1(s)} = \frac{3.40}{1 + 0.897s}\left[1 + \frac{0.241}{\gamma^2}\left(1 - \frac{0.482}{\gamma}\left(1 + \frac{0.072}{\gamma}\right)\right)\right]$$

where

$$\gamma = 1 + 0.897s$$

It is clear from the example that the approximation becomes progressively more involved for each term. This is worse if the simplification of Eq. E.7 cannot be carried out. Equation E.7 shows the wave-like behavior of the system in the sum of the two terms. One is the direct transfer through the boundary and the other is delayed by the time the disturbance takes to travel down y_1 and back along y_2. The steady state gain is correctly given by the third approximation but the error in the steady state gain for the earlier approximation is considerable as is shown below. The correct value is 3.80.

1st approx.	3.40	error	- 10.5 percent
2nd approx.	4.22	error	+ 11.5 percent
3rd approx.	3.78	error	- 0.5 percent

APPENDIX F

STANDARD TRANSFER FUNCTIONS AND INTERCONNECTIONS CONSIDERED AS DISTRIBUTED SYSTEMS

In this appendix various standard lumped transfer functions and interconnections are expressed in terms of a standard distributed system whose coefficients are space distributed impulses. The proofs follow exactly the same pattern as those given in Chapter III and are not given here.

The standard distributed system is

$$\underline{A}\frac{\partial \underline{y}}{\partial x} + \underline{B}\ \frac{\partial \underline{y}}{\partial t} + \underline{C}\underline{y} = 0 \qquad 0 \leq x \leq 1 \qquad \text{(F.1)}$$

The following are general properties of $\underline{A}, \underline{B}, \underline{C}$ when Eq. F.1 can be reduced to a lumped system.

a) $\underline{A}$ and $\underline{B}$ are diagonal matrices.

b) $\underline{A}$ is not a space distributed impulse function.
$\underline{B}$ and $\underline{C}$ are space distributed impulse functions.

c) The sign of the element of $\underline{A}$ indicates the direction of flow along the path. In particular feedforward is positive and feedback is negative. The matrix $\underline{C}$ determines whether positive or negative feedforward or feedback is used.

d) It is generally desirable to normalize the equations so that the elements of A are ± 1.

e) The boundary conditions are that the components of $\underline{y}$ are zero at $x = 0$ or $x = 1$, according to the direction of flow, i.e., the sign of the corresponding element of $\underline{A}$.

f) If a path has no memory the corresponding element of $\underline{B}$ is zero.

g) There is a non-zero element of $\underline{C}$ for each addition to a flow path and a zero element for a tap of a flow path.

It is assumed that the lumps or interconnections occur at $x = X$, i.e., the impulses are placed at $x = X$. In Chapter III it is shown that X can be anywhere in the interval $0 \leq x \leq 1$.

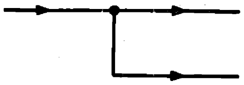
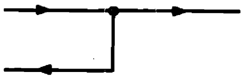
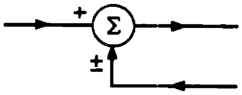
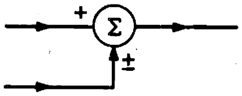
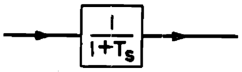
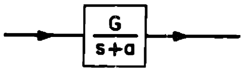
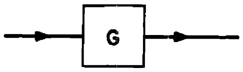
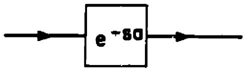
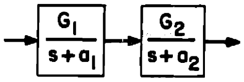
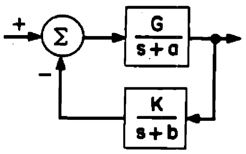
	SYSTEM	A	B	C
1.		$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\underline{0}$	$\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} u_0(x-X)$
2.		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\underline{0}$	$\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} u_0(x-X)$
3.		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\underline{0}$	$\begin{pmatrix} 0 & \mp 1 \\ 0 & 0 \end{pmatrix} u_0(x-X)$
4.		$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\underline{0}$	$\begin{pmatrix} 0 & \pm 1 \\ 0 & 0 \end{pmatrix} u_0(x-X)$
5.		1	$Tu_0(x-X)$	0
6.		1	$\frac{1}{G}u_0(x-X)$	$\left(\frac{a}{G}-1\right)u_0(x-X)$
7.		1	0	$\left(\frac{1}{G}-1\right)u_0(x-X)$
8.		1	a	0
9.		1	$\frac{1}{G_1}u_0(x-X_1)+\frac{1}{G_2}u_0(x-X_2)$	$\left(\frac{a_1}{G_1}-1\right)u_0(x-X_1)+\left(\frac{a_2}{G_2}-1\right)u_0(x-X_2)$
10.		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{G}u_0(x-X_2) & 0 \\ 0 & \frac{1}{K}u_0(x-X_2) \end{pmatrix}$ $0<X_1<X_2<X_3<1$	$\begin{pmatrix} \left(\frac{a}{G}-1\right)u_0(x-X_2) & u_0(x-X_1) \\ -u_0(x-X_3) & \left(\frac{b}{K}-1\right)u_0(x-X_2) \end{pmatrix}$
11.	FOR A PLATE DISTILLATION COLUMN SEE CHAPTER III			
	SYSTEM	A	B	C

Fig. F.1 Standard Transfer Functions Expressed as Distributed Systems

APPENDIX G

NUMERICAL VALUES OF AMMONIA REACTOR PARAMETERS

The numerical values used in the study of the ammonia reactor were taken from Eymery[31] and Quintero.[43] The non-linear partial differential equations are

$$-D\frac{\partial^2 y_1}{\partial x^2} + s\left[\left(1 - h\frac{y_4 - y_4^*}{1 + y_4}\right)\right]\frac{\partial y_1}{\partial x} + \frac{\partial y_1}{\partial t}$$

$$+ (y_1 + y_2) - [e + h(y_1 - 0.3725)]\,sr = 0$$

$$\frac{\partial y_2}{\partial x} - \beta(y_2 - y_3) = 0$$

$$g\frac{\partial y_3}{\partial t} + y_3(1 + d) - y_1 - dy_2 = 0 \qquad \text{(G.1)}$$

$$\frac{\partial y_4}{\partial t} - r\frac{(1 + y_4)^2}{1 + y_4^*} = 0$$

where

y_1	is the normalized catalyst temperature
y_2	is the normalized input gas temperature
y_3	is the normalized wall temperature
y_4	is the ammonia concentration
y_4^*	is the ammonia concentration of the feed

The coefficients in Eq. G.1 are

$D = 0.0002$

$d = 1.455$

$e = 1.878$

$g = 0.3209$

$h = 0.4444$

$s = 0.4382$

$\beta = 3.320$

The coefficient r is the rate of reaction and is a function of temperature and composition

$$r = 3.28.10^{11} \exp\left(\frac{-25.37}{y_1}\right)$$

$$\cdot \left[L^2 \; 0.1952 \; \frac{(0.8584 - y_4)^{2.5}}{y_4} - \frac{0.355}{(0.8584 - y_4)^{1.5}} \right]$$

where $L = 1271 \; y_1^{-2.49} \exp\left[2.2 - 0.23\, y_1 + 0.27\, y_1^2 + \frac{5.97}{y_1} \right]$

Quintero linearized Eq. G.1 about the steady state solution. The equations become

$$-\underline{D} \frac{\partial^2 \underline{y}}{\partial x^2} + \underline{V} \frac{\partial \underline{y}}{\partial x} + \underline{C} \frac{\partial \underline{y}}{\partial t} + \underline{H}\, \underline{y} = 0 \qquad \text{(G.2)}$$

where $$\underline{D} = \begin{pmatrix} d_1 & & & 0 \\ & 0 & & \\ & & 0 & \\ 0 & & & 0 \end{pmatrix}$$

$$\underline{V} = \begin{pmatrix} v_1 & & & 0 \\ & v_2 & & \\ & & 0 & \\ 0 & & & v_4 \end{pmatrix}$$

$$\underline{C} = \begin{pmatrix} c_1 & & & 0 \\ & 0 & & \\ & & c_3 & \\ 0 & & & 0 \end{pmatrix}$$

$$\underline{H} = \begin{pmatrix} h_{11} & 0 & h_{13} & h_{14} \\ 0 & h_{22} & h_{23} & 0 \\ h_{31} & h_{32} & h_{33} & 0 \\ h_{41} & 0 & 0 & h_{44} \end{pmatrix}$$

$$\underline{y} = (y_1, y_2, y_3, y_4)$$

The numerical values of the parameters are

$d = 0.0002$

$v_2 = 0.4365$

$c_1 = 1.0$

$c_2 = 0.3209$

$h_{13} = -1.0$

$h_{22} = 1.455$

$h_{23} = -1.455$

$h_{31} = -1.0$

$h_{32} = -1.455$

$h_{33} = 2.455$

Curves of v_1, v_4, h_{11}, h_{14}, h_{41}, h_{44} are shown in Fig. G.1. and of the initial and final steady states in Fig. G.2 and G.3. Tables of the values of these coefficients and of the initial and final steady states at every 0.01 units of distance are given in Tables G.1 to G.6. It should be noted that these results are given in terms of the true distance variable x. Both Eymery and Quintero use a modified distance variable

$$x = 0.2z + 0.8z^2 \tag{G.3}$$

This was used by Eymery to improve the convergence of the Brian and Stone difference equation.[49] In this work which depends on physical aspects of the process it is important to use the true distance variable. The only reason for using a transformation such as Eq. G.3 is if it reduces the variation of the coefficients with distance.

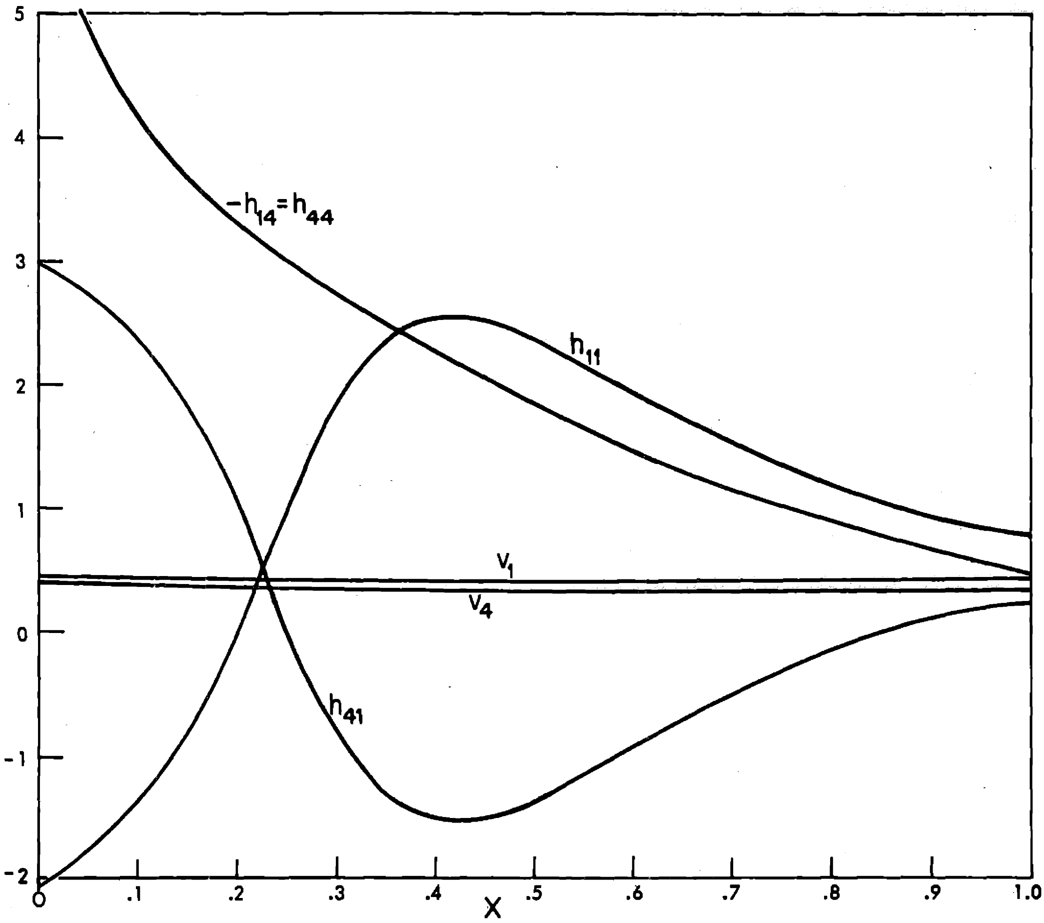


Fig. G.1 Variable Coefficients of Linear Model of Ammonia Reactor

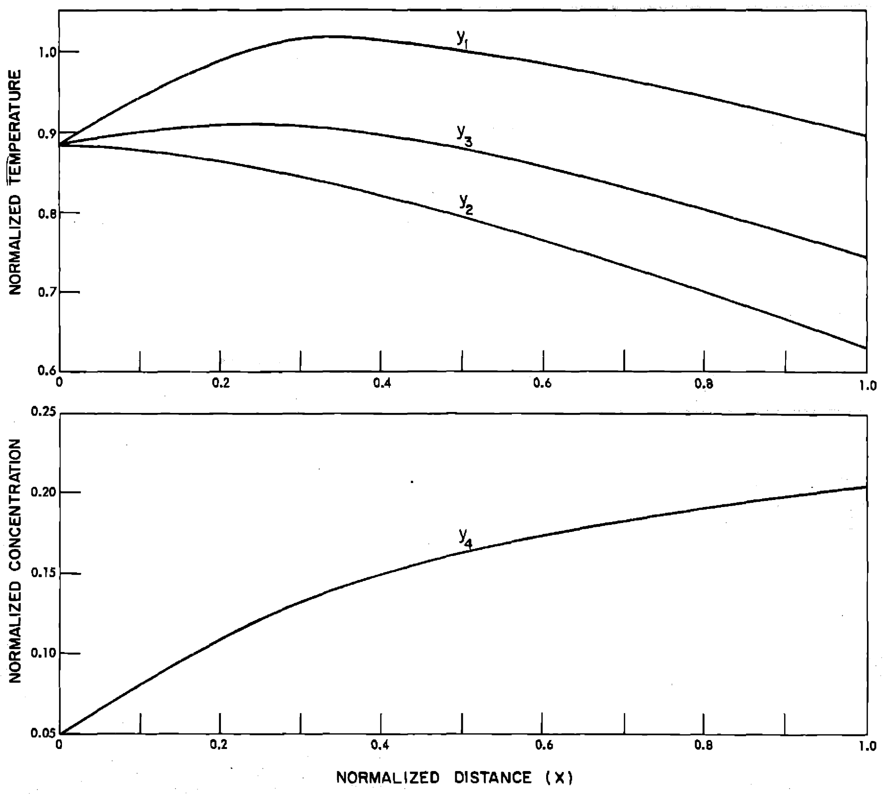


Fig. G.2 Initial Steady State of Ammonia Reactor

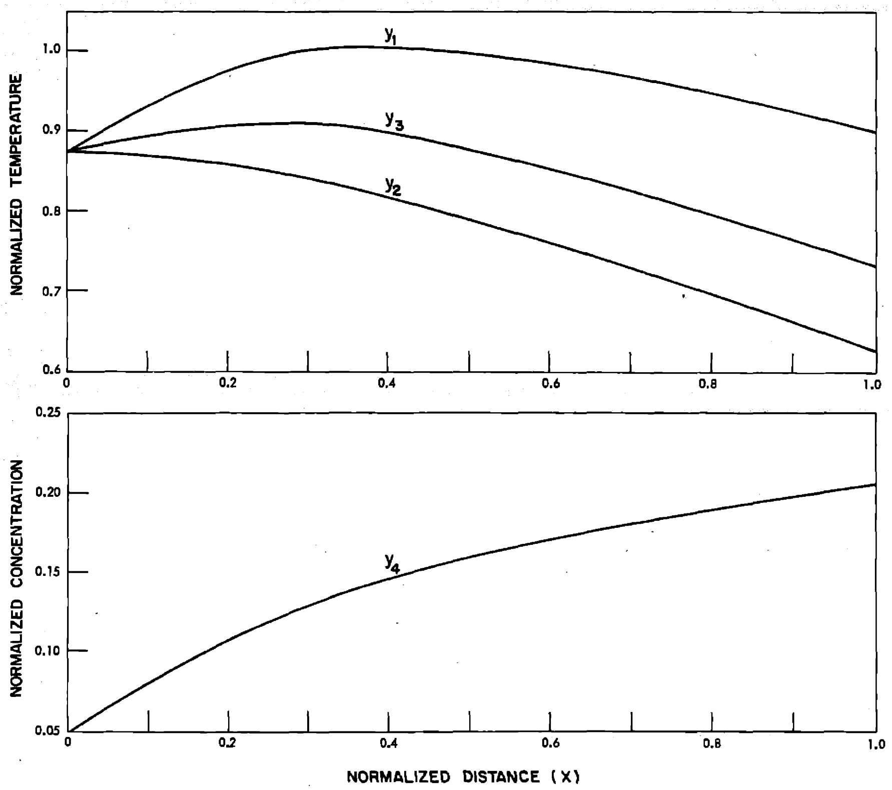


Fig. G.3 Final Steady State of Ammonia Reactor

Table G-1

Variable Coefficients of Linear Model of Ammonia Reactor X=0 to X=0.5

X	V1	V3	H11	H14	H41	H44
.	.4542	.4173	-2.1178	-6.4087	3.1178	6.4087
.01	.4487	.4168	-2.0508	-6.0690	3.0508	6.0690
.02	.4447	.4137	-1.9861	-5.7685	2.9861	5.7685
.03	.4423	.4109	-1.9235	-5.5055	2.9235	5.5055
.04	.4400	.4076	-1.8608	-5.2705	2.8608	5.2705
.05	.4395	.4057	-1.7989	-5.0664	2.7989	5.0664
.06	.4377	.4025	-1.7325	-4.8761	2.7325	4.8761
.07	.4369	.4001	-1.6646	-4.7084	2.6646	4.7084
.08	.4359	.3976	-1.5915	-4.5542	2.5915	4.5542
.09	.4362	.3962	-1.5176	-4.4206	2.5176	4.4206
.10	.4354	.3938	-1.4336	-4.2915	2.4336	4.2915
.11	.4339	.3907	-1.3370	-4.1668	2.3370	4.1668
.12	.4339	.3890	-1.2405	-4.0601	2.2405	4.0601
.13	.4323	.3857	-1.1224	-3.9502	2.1224	3.9502
.14	.4322	.3839	-1.0058	-3.8567	2.0058	3.8567
.15	.4316	.3818	-.8737	-3.7661	1.8737	3.7661
.16	.4307	.3792	-.7269	-3.6778	1.7269	3.6778
.17	.4303	.3774	-.5744	-3.5980	1.5744	3.5980
.18	.4297	.3752	-.4066	-3.5201	1.4066	3.5201
.19	.4287	.3728	-.2244	-3.4438	1.2244	3.4438
.20	.4284	.3710	-.0435	-3.3748	1.0435	3.3748
.21	.4279	.3691	.1502	-3.3072	.8498	3.3072
.22	.4272	.3671	.3533	-3.2406	.6467	3.2406
.23	.4271	.3658	.5459	-3.1803	.4541	3.1803
.24	.4269	.3643	.7425	-3.1207	.2575	3.1207
.25	.4265	.3627	.9406	-3.0616	.0594	3.0616
.26	.4259	.3611	1.1375	-3.0029	-.1375	3.0029
.27	.4252	.3594	1.3301	-2.9446	-.3301	2.9446
.28	.4252	.3583	1.4988	-2.8917	-.4988	2.8917
.29	.4250	.3572	1.6592	-2.8390	-.6592	2.8390
.30	.4240	.3554	1.8244	-2.7810	-.8244	2.7810
.31	.4244	.3549	1.9479	-2.7335	-.9479	2.7335
.32	.4239	.3537	2.0732	-2.6807	-1.0732	2.6807
.33	.4234	.3525	2.1845	-2.6279	-1.1845	2.6279
.34	.4235	.3518	2.2716	-2.5802	-1.2716	2.5802
.35	.4228	.3505	2.3549	-2.5272	-1.3549	2.5272
.36	.4227	.3498	2.4170	-2.4793	-1.4170	2.4793
.37	.4226	.3491	2.4676	-2.4314	-1.4676	2.4314
.38	.4223	.3483	2.5072	-2.3833	-1.5072	2.3833
.39	.4221	.3475	2.5363	-2.3353	-1.5363	2.3353
.40	.4217	.3467	2.5554	-2.2871	-1.5554	2.2871
.41	.4219	.3463	2.5650	-2.2443	-1.5650	2.2443
.42	.4215	.3454	2.5672	-2.1962	-1.5672	2.1962
.43	.4216	.3450	2.5613	-2.1534	-1.5613	2.1534
.44	.4210	.3441	2.5484	-2.1053	-1.5484	2.1053
.45	.4210	.3436	2.5315	-2.0627	-1.5315	2.0627
.46	.4209	.3431	2.5100	-2.0201	-1.5100	2.0201
.47	.4208	.3425	2.4845	-1.9776	-1.4845	1.9776
.48	.4207	.3420	2.4547	-1.9352	-1.4547	1.9352
.49	.4205	.3414	2.4211	-1.8930	-1.4211	1.8930
.50	.4203	.3407	2.3847	-1.8509	-1.3847	1.8509

Table G-2

Variable Coefficients of Linear Model of Ammonia Reactor X=0.5 to X=1.0

X	V1	V3	H11	H14	H41	H44
.50	.4203	.3407	2.3847	-1.8509	-1.3847	1.8509
.51	.4200	.3401	2.3458	-1.8090	-1.3458	1.8090
.52	.4202	.3399	2.3100	-1.7725	-1.3100	1.7725
.53	.4199	.3392	2.2665	-1.7310	-1.2665	1.7310
.54	.4195	.3384	2.2212	-1.6898	-1.2212	1.6898
.55	.4196	.3375	2.1805	-1.6539	-1.1340	1.6161
.56	.4197	.3370	2.1389	-1.6181	-1.0900	1.5793
.57	.4192	.3380	2.0899	-1.5777	-1.1780	1.6499
.58	.4192	.3366	2.0463	-1.5425	-1.0463	1.5425
.59	.4192	.3362	2.0023	-1.5075	-1.0023	1.5075
.60	.4191	.3358	1.9577	-1.4727	-.9577	1.4727
.61	.4186	.3349	1.9063	-1.4334	-.9063	1.4334
.62	.4185	.3344	1.8611	-1.3993	-.8611	1.3993
.63	.4183	.3339	1.8159	-1.3653	-.8159	1.3653
.64	.4182	.3334	1.7706	-1.3318	-.7706	1.3318
.65	.4180	.3328	1.7254	-1.2985	-.7254	1.2985
.66	.4182	.3327	1.6868	-1.2702	-.6868	1.2702
.67	.4180	.3321	1.6420	-1.2375	-.6420	1.2375
.68	.4178	.3315	1.5976	-1.2052	-.5976	1.2052
.69	.4175	.3309	1.5535	-1.1731	-.5535	1.1731
.70	.4177	.3307	1.5162	-1.1459	-.5162	1.1459
.71	.4173	.3301	1.4732	-1.1145	-.4732	1.1145
.72	.4175	.3298	1.4367	-1.0878	-.4367	1.0878
.73	.4171	.3291	1.3950	-1.0571	-.3950	1.0571
.74	.4172	.3289	1.3599	-1.0310	-.3599	1.0310
.75	.4168	.3282	1.3195	-1.0009	-.3195	1.0009
.76	.4169	.3279	1.2859	-.9754	-.2859	.9754
.77	.4165	.3272	1.2474	-.9460	-.2474	.9460
.78	.4165	.3268	1.2150	-.9211	-.2150	.9211
.79	.4165	.3265	1.1838	-.8966	-.1838	.8966
.80	.4164	.3261	1.1532	-.8722	-.1532	.8722
.81	.4164	.3258	1.1235	-.8482	-.1235	.8482
.82	.4159	.3250	1.0902	-.8206	-.0902	.8206
.83	.4158	.3246	1.0624	-.7972	-.0624	.7972
.84	.4158	.3242	1.0359	-.7741	-.0359	.7741
.85	.4157	.3238	1.0103	-.7514	-.0103	.7514
.86	.4155	.3234	.9855	-.7289	.0145	.7289
.87	.4154	.3230	.9622	-.7068	.0378	.7068
.88	.4153	.3226	.9396	-.6849	.0604	.6849
.89	.4152	.3221	.9185	-.6634	.0815	.6634
.90	.4150	.3217	.8984	-.6422	.1016	.6422
.91	.4152	.3216	.8824	-.6248	.1176	.6248
.92	.4150	.3212	.8645	-.6042	.1355	.6042
.93	.4148	.3207	.8473	-.5839	.1527	.5839
.94	.4147	.3203	.8321	-.5640	.1679	.5640
.95	.4148	.3202	.8198	-.5476	.1802	.5476
.96	.4146	.3197	.8065	-.5283	.1935	.5283
.97	.4144	.3192	.7943	-.5094	.2057	.5094
.98	.4145	.3191	.7850	-.4938	.2150	.4938
.99	.4143	.3187	.7751	-.4755	.2249	.4755
.00	.4140	.3182	.7658	-.4574	.2342	.4574

Table G-3

Initial Steady State of Ammonia Reactor X=0 to X=0.5

X	Y1	Y2	Y3	Y4
0.	.8833	.8827	.8841	.0500
.01	.8811	.8753	.8776	.0529
.02	.8869	.8752	.8799	.0559
.03	.8926	.8750	.8821	.0589
.04	.8983	.8747	.8843	.0619
.05	.9038	.8743	.8863	.0648
.06	.9094	.8739	.8883	.0679
.07	.9148	.8733	.8902	.0710
.08	.9202	.8727	.8921	.0740
.09	.9252	.8721	.8937	.0769
.10	.9303	.8713	.8954	.0800
.11	.9356	.8705	.8970	.0832
.12	.9404	.8696	.8984	.0861
.13	.9456	.8685	.8999	.0894
.14	.9502	.8675	.9012	.0923
.15	.9548	.8663	.9024	.0953
.16	.9594	.8651	.9035	.0984
.17	.9636	.8638	.9045	.1013
.18	.9678	.8624	.9053	.1043
.19	.9720	.8609	.9061	.1074
.20	.9757	.8594	.9068	.1102
.21	.9793	.8578	.9073	.1130
.22	.9828	.8561	.9077	.1158
.23	.9859	.8544	.9080	.1184
.24	.9888	.8526	.9081	.1209
.25	.9916	.8507	.9081	.1235
.26	.9941	.8488	.9080	.1260
.27	.9965	.8467	.9077	.1284
.28	.9985	.8447	.9074	.1306
.29	1.0002	.8427	.9069	.1327
.30	1.0019	.8403	.9062	.1350
.31	1.0031	.8383	.9055	.1368
.32	1.0043	.8360	.9046	.1387
.33	1.0052	.8337	.9035	.1406
.34	1.0059	.8314	.9025	.1423
.35	1.0064	.8289	.9012	.1440
.36	1.0067	.8265	.8999	.1456
.37	1.0069	.8241	.8986	.1471
.38	1.0069	.8216	.8971	.1485
.39	1.0067	.8190	.8955	.1499
.40	1.0065	.8164	.8938	.1513
.41	1.0061	.8140	.8923	.1525
.42	1.0056	.8113	.8904	.1538
.43	1.0050	.8088	.8887	.1549
.44	1.0042	.8059	.8867	.1562
.45	1.0034	.8033	.8848	.1573
.46	1.0026	.8007	.8829	.1584
.47	1.0016	.7979	.8809	.1594
.48	1.0006	.7952	.8789	.1605
.49	.9995	.7924	.8767	.1615
.50	.9983	.7895	.8746	.1626

Table G-4

Initial Steady State of Ammonia Reactor X=0.5 to X=1.0

X	Y1	Y2	Y3	Y4
.50	.9983	.7895	.8746	.1626
.51	.9971	.7866	.8723	.1636
.52	.9959	.7840	.8703	.1645
.53	.9945	.7810	.8680	.1655
.54	.9931	.7779	.8656	.1665
.55	.9918	.7752	.8634	.1674
.56	.9905	.7724	.8612	.1683
.57	.9888	.7692	.8587	.1693
.58	.9874	.7663	.8564	.1702
.59	.9859	.7634	.8540	.1711
.60	.9843	.7605	.8517	.1720
.61	.9825	.7571	.8489	.1730
.62	.9809	.7540	.8464	.1739
.63	.9792	.7510	.8439	.1748
.64	.9774	.7478	.8414	.1757
.65	.9757	.7447	.8388	.1766
.66	.9741	.7419	.8365	.1774
.67	.9722	.7387	.8338	.1783
.68	.9703	.7354	.8311	.1792
.69	.9683	.7321	.8283	.1801
.70	.9666	.7292	.8259	.1809
.71	.9646	.7258	.8230	.1818
.72	.9628	.7228	.8206	.1826
.73	.9606	.7193	.8176	.1835
.74	.9587	.7163	.8150	.1842
.75	.9565	.7127	.8120	.1852
.76	.9545	.7096	.8094	.1859
.77	.9522	.7059	.8062	.1868
.78	.9501	.7028	.8035	.1876
.79	.9480	.6995	.8008	.1884
.80	.9459	.6963	.7980	.1892
.81	.9437	.6930	.7951	.1899
.82	.9411	.6891	.7918	.1908
.83	.9389	.6858	.7889	.1916
.84	.9365	.6824	.7859	.1923
.85	.9342	.6790	.7829	.1931
.86	.9318	.6755	.7799	.1938
.87	.9293	.6720	.7768	.1946
.88	.9268	.6685	.7737	.1953
.89	.9242	.6650	.7706	.1960
.90	.9216	.6614	.7674	.1967
.91	.9194	.6583	.7647	.1973
.92	.9167	.6547	.7614	.1980
.93	.9139	.6510	.7581	.1987
.94	.9111	.6473	.7547	.1994
.95	.9087	.6442	.7519	.2000
.96	.9058	.6404	.7485	.2007
.97	.9028	.6366	.7450	.2013
.98	.9003	.6334	.7421	.2019
.99	.8972	.6295	.7385	.2025
1.00	.8941	.6256	.7350	.2031

Table G-5

Final Steady State of Ammonia Reactor X=0 to X=0.5

X	Y1	Y2	Y3	Y4
0.	.8758	.8753	.8765	.0507
.01	.8890	.8827	.8853	.0532
.02	.8953	.8826	.8878	.0564
.03	.9015	.8824	.8902	.0596
.04	.9077	.8821	.8925	.0629
.05	.9136	.8817	.8947	.0661
.06	.9197	.8812	.8969	.0694
.07	.9255	.8806	.8989	.0727
.08	.9313	.8800	.9009	.0760
.09	.9367	.8793	.9026	.0791
.10	.9422	.8785	.9044	.0824
.11	.9478	.8775	.9062	.0858
.12	.9529	.8766	.9077	.0889
.13	.9584	.8754	.9092	.0924
.14	.9632	.8743	.9105	.0955
.15	.9680	.8731	.9118	.0987
.16	.9728	.8717	.9129	.1019
.17	.9772	.8703	.9139	.1050
.18	.9815	.8688	.9147	.1081
.19	.9857	.8672	.9155	.1112
.20	.9894	.8656	.9160	.1140
.21	.9929	.8639	.9165	.1169
.22	.9963	.8621	.9167	.1197
.23	.9991	.8603	.9169	.1222
.24	1.0018	.8585	.9169	.1247
.25	1.0043	.8565	.9167	.1271
.26	1.0065	.8544	.9164	.1295
.27	1.0085	.8523	.9159	.1318
.28	1.0100	.8502	.9153	.1338
.29	1.0114	.8481	.9146	.1357
.30	1.0126	.8457	.9137	.1378
.31	1.0134	.8436	.9128	.1394
.32	1.0141	.8412	.9116	.1412
.33	1.0145	.8388	.9104	.1428
.34	1.0148	.8365	.9091	.1443
.35	1.0149	.8339	.9076	.1458
.36	1.0148	.8315	.9062	.1472
.37	1.0146	.8291	.9046	.1485
.38	1.0142	.8265	.9030	.1497
.39	1.0137	.8239	.9012	.1510
.40	1.0131	.8213	.8994	.1522
.41	1.0125	.8189	.8977	.1532
.42	1.0116	.8161	.8958	.1544
.43	1.0108	.8136	.8939	.1554
.44	1.0098	.8107	.8918	.1565
.45	1.0088	.8081	.8899	.1575
.46	1.0078	.8054	.8878	.1585
.47	1.0066	.8027	.8858	.1594
.48	1.0055	.8000	.8837	.1604
.49	1.0042	.7971	.8815	.1614
.50	1.0029	.7943	.8793	.1623

Table G-6

Final Steady State of Ammonia Reactor X=0.5 to X= 1.0

X	Y1	Y2	Y3	Y4
.50	1.0029	.7943	.8793	.1623
.51	1.0015	.7914	.8770	.1633
.52	1.0003	.7888	.8749	.1641
.53	.9988	.7858	.8726	.1651
.54	.9973	.7827	.8701	.1661
.55	.9959	.7800	.8679	.1669
.56	.9945	.7772	.8657	.1678
.57	.9929	.7740	.8632	.1687
.58	.9913	.7712	.8609	.1696
.59	.9898	.7683	.8585	.1704
.60	.9882	.7654	.8561	.1713
.61	.9864	.7620	.8534	.1723
.62	.9847	.7589	.8509	.1732
.63	.9830	.7559	.8484	.1740
.64	.9812	.7528	.8458	.1749
.65	.9794	.7496	.8432	.1758
.66	.9779	.7469	.8410	.1766
.67	.9760	.7437	.8383	.1774
.68	.9741	.7404	.8356	.1783
.69	.9721	.7371	.8328	.1792
.70	.9704	.7342	.8304	.1800
.71	.9684	.7308	.8276	.1809
.72	.9666	.7279	.8251	.1817
.73	.9645	.7244	.8222	.1826
.74	.9626	.7214	.8196	.1834
.75	.9604	.7178	.8166	.1843
.76	.9584	.7147	.8140	.1850
.77	.9561	.7111	.8109	.1859
.78	.9541	.7079	.8082	.1867
.79	.9520	.7047	.8054	.1875
.80	.9499	.7015	.8027	.1883
.81	.9477	.6982	.7999	.1890
.82	.9452	.6944	.7965	.1899
.83	.9429	.6910	.7936	.1907
.84	.9407	.6877	.7907	.1915
.85	.9383	.6842	.7877	.1922
.86	.9359	.6808	.7847	.1930
.87	.9335	.6773	.7817	.1937
.88	.9311	.6738	.7786	.1945
.89	.9285	.6703	.7755	.1952
.90	.9260	.6667	.7723	.1960
.91	.9238	.6637	.7696	.1966
.92	.9211	.6600	.7664	.1973
.93	.9184	.6564	.7631	.1980
.94	.9156	.6527	.7598	.1987
.95	.9133	.6496	.7570	.1993
.96	.9104	.6458	.7536	.2000
.97	.9075	.6420	.7501	.2006
.98	.9050	.6388	.7472	.2012
.99	.9020	.6349	.7437	.2019
1.00	.8989	.6310	.7402	.2025

APPENDIX H

PROGRAMS

H. 1. INTRODUCTION

All the calculations were evaluated by programs written in Fortran II and carried out on the I. B. M. 7094 at the Computation Center, Massachusetts Institute of Technology. Most of the programs are of no general interest but the eigenvalue program used in the modified Galerkin calculations is given. However recent developments in eigenvalue calculations suggest that better methods now exist.[6] The program used to evaluate the roots of the transcendental equation in Appendix A is given since it could be used to extend the tables.

H. 2. EIGENVALUE AND EIGENVECTOR PROGRAMS

The calculations required for the modified Galerkin method consists of four stages

a) Calculation of the matrix
b) Solution of eigenvalues and eigenvectors
c) Fourier expansion of the initial distribution
d) Final solution

Items a) and c) require integration of variable coefficients multiplied by known functions and are easy to carry out. Item d) requires considerable but straightforward matrix multiplication to evaluate Eq. 2.38. For b) Lanczos'[15] method was used. However, recently Francis[6] has developed a superior method called the Q-R transform which can accurately obtain the eigenvalues of high order unsymmetric matrices. Van Ness[10] has written a program in Fortran IV for this method which is available in the I. B. M. Share catalogue. He has used it successfully on a 51 x 51 matrix.[24] The subroutines TRIPLE, UNVAL, UNVEC are listed which give the eigenvalues, the eigenvectors and the adjoint eigenvectors for a real unsymmetric matrix $\underline{A}$.

A	is the matrix
N	is the order of matrix
REAL	is the real part of the eigenvalues
XIMAG	is the imaginary part of the eigenvalues
VECR	is the real part of eigenvectors
VECI	is the imaginary part of the eigenvectors
ADVECR	is the real part of the adjoint eigenvector
ADVECI	is the imaginary part of the adjoint eigenvectors
U, V	are initial guess at quadratic root (usually taken as 1.0 and 0.5)

H. 3. TRANSCENDENTAL EQUATION

In Appendix A the first six roots of the equation

$$\omega \cot \omega = A\omega^2 - B$$

were given. These were evaluated by the program listed here

NA	is number of values of A, Max 7
NB	is number of values of B, Max 100
NR	is the root required

$$\text{NCASE} = \begin{cases} 1 & \text{if not the last case} \\ 2 & \text{if the last case} \end{cases}$$

Data cards are required to give the values of A and B. The format is 7F 10.0.

The calculation is carried out in three steps. Let the required root be the n^{th} root which lies between $n\pi$ and $(n-1)\pi$.

a) For $A = 0$ evaluate ω for each B; call this Ω

b) Evaluate B for ω_m where

$$\omega_m = \left(\frac{n\pi - \Omega}{10}\right) m \qquad m = 0, 1, \ldots 10$$

c) Iterate by linear interpolation between values of ω_m closest to the required value of B. This procedure, a combined iterative and search method, gives good convergence even when the curves have sharp corners.

```
  TODF  TO SOLVE THE EQUATION COTW=AW-B/W
      DIMENSION A(7),W(7),BB(100),UU(12),BU(12)
   80 READ 40,NA,NB,NR,NCASE
      READ 41,(A(I),I=1,NA)
      READ 41,(BB(I),I=1,NB)
      XNR=NR
      PRINT 113
      PRINT 110
      PRINT 111,NR
      PRINT 112,A(1),A(2),A(3),A(4),A(5),A(6),A(7)
      TE=XNR*3.14159
C     CALCULATE VALUES FOR B=0.0
      DO 10 I=1,NA
      W(I)=TE
      IF(A(I))13,15,13
   15 W(I)=TE-0.5*3.14159
      GO TO 10
   13 U=ATANF(1.0/(A(I)*W(I)))+(XNR-1.0)*3.14159
      IF(ABSF(W(I)-U)-1.0E-6)10,10,12
   12 W(I)=U
      GO TO 13
   10 CONTINUE
      B=0.0
      PRINT 103,B,(W(I),I=1,NA)
      DO 30 J=1,NB
      B=BB(J)
      DO 20 I=1,NA
      K=1
   42 XK=K
      UU(K)=W(I)+(TE-W(I))*(XK-1.0)/10.0
   47 C=COTF(UU(K))
      BU(K)=(A(I)*UU(K)-C)*UU(K)
      IF(BU(K)-B)90,45,91
   45 W(I)=UU(K)
      GO TO 20
   91 WP=UU(K-1)
      WQ=UU(K)
      BP=BU(K-1)
      BQ=BU(K)
      GO TO 60
   90 IF(K-10)43,46,44
   43 K=K+1
      GO TO 42
   44 PRINT 114
      CALL EXIT
   46 UU(11)=TE-0.001
      K=11
      XK=11.0
      GO TO 47
   60 WR=(WP*BQ-WQ*BP+B*(WQ-WP))/(BQ-BP)
      IF(ABSF(1.0-WR/WP)-1.0E-5)70,70,71
   71 IF(ABSF(1.0-WR/WQ)-1.0E-5)70,70,72
   72 C=COTF(WR)
      BR=(A(I)*WR-C)*WR
      IF(BR-B)61,70,63
   61 WP=WR
      BP=BR
      GO TO 60
   63 WQ=WR
      BQ=BR
      GO TO 60
   70 W(I)=WR
   20 CONTINUE
      PRINT 103,B,(W(I),I=1,NA)
   30 CONTINUE
      GO TO (80,81),NCASE
   81 CALL EXIT
   40 FORMAT (4I10)
   41 FORMAT (7F10.0)
  103 FORMAT (F13.1,F19.4,6F16.4)
  110 FORMAT(25X38H ROOTS OF THE EQUATION   COT(W)=AW-B/W//)
  111 FORMAT(33X17H FOR ROOT NUMBER I2//)
  112 FORMAT (10X2H B10X3H A=F5.2,8X3H A=F5.2,8X3H A=F5.2,8X3H A=F5.2,8X
     13H A=F5.2,8X3H A=F5.2,8X3H A=F5.2//)
  113 FORMAT (1H1)
  114 FORMAT (11H ERROR IN K)
      END(1,1,0,0,0,0,1,1,0,1,0,0,0,0,0)

JOB TIME =     .08 MIN.
```

```
      SUBROUTINE TRIPLE(N,A,B,ALPHA,BETA,Y,YTR)
CTRIPLE  TO FORM THE TRIPLE DIAGONAL FORM OF UNSYMMETRIC MATRIX
      DIMENSION A(10,10),Y(10,10),YTR(10,10),
     1B(10),C(10),CTR(10),ANORM(10),ALPHA(10),BETA(11)
C    TO OBTAIN THE TRIPLE DIAGONAL FORM OF A UNSYMMETRIC MATRIX
      DO 56 I=1,N
      DO 56 J=1,N
      Y(I,J)=0.0
   56 YTR(I,J)=0.0
      DO 57 J=1,N
      C(J)=0.0
      CTR(J)=0.0
      ANORM(J)=0.0
      ALPHA(J)=0.0
      BETA(J)=0.0
      Y(1,J)=B(J)
   57 YTR(1,J)=B(J)
      BETA(1)=0.0
      ALNUM=0.0
C      FIRST ITERATION
      DO 59 J=1,N
      DO 58 K=1,N
      C(J)=C(J)+A(J,K)*Y(K,1)
   58 CTR(J)=CTR(J)+A(K,J)*YTR(K,1)
      ANORM(1)=ANORM(1)+Y(J,1)*YTR(J,1)
   59 ALNUM=ALNUM+C(J)*YTR(J,1)
      IF(ANORM(1))40,61,40
   40 ALPHA(1)=ALNUM/ANORM(1)
      DO 41 J=1,N
      Y(J,2)=C(J)-ALPHA(1)*Y(J,1)
   41 YTR(J,2)=CTR(J)-ALPHA(1)*YTR(J,1)
      E=0.0
      ETR=0.0
      DO 42 K=1,N
      E=E+Y(K,2)*YTR(K,1)
   42 ETR=ETR+YTR(K,2)*Y(K,1)
      DO 43 K=1,N
      Y(K,2)=Y(K,2)-E*Y(K,1)/ANORM(1)
   43 YTR(K,2)=YTR(K,2)-ETR*YTR(K,1)/ANORM(1)
C     SUBSEQUENT ITERATIONS
      DO 55 I=2,N
      ALNUM=0.0
      BTNUM=0.0
      DO 51 J=1,N
      C(J)=0.0
      CTR(J)=0.0
      DO 50 K=1,N
      C(J)=C(J)+A(J,K)*Y(K,I)
   50 CTR(J)=CTR(J)+A(K,J)*YTR(K,I)
      ANORM(I)=ANORM(I)+Y(J,I)*YTR(J,I)
      ALNUM=ALNUM+C(J)*YTR(J,I)
   51 BTNUM=BTNUM+C(J)*YTR(J,I-1)
      IF(ANORM(I))60,61,60
   60 ALPHA(I)=ALNUM/ANORM(I)
      BETA(I)=BTNUM/ANORM(I-1)
      IF(N-I)72,73,74
   74 DO 52 J=1,N
      Y(J,I+1)=C(J)-ALPHA(I)*Y(J,I)-BETA(I)*Y(J,I-1)
   52 YTR(J,I+1)=CTR(J)-ALPHA(I)*YTR(J,I)-BETA(I)*YTR(J,I-1)
      DO 70 J=1,I
      CTR(J)=0.0
      C(J)=0.0
      DO 70 K=1,N
       C(J)=C(J)+Y(K,I+1)*YTR(K,J)
   70  CTR(J)=CTR(J)+YTR(K,I+1)*Y(K,J)
       DO 71 K=1,N
       DO 71 J=1,I
       Y(K,I+1)=Y(K,I+1)-C(J)*Y(K,J)/ANORM(J)
   71  YTR(K,I+1)=YTR(K,I+1)-CTR(J)*YTR(K,J)/ANORM(J)
   55  CONTINUE
   73  RETURN
   61  PRINT 100
       CALL EXIT
   72  PRINT 101
       CALL EXIT
  100  FORMAT (25H INCORRECT INITIAL VECTOR)
  101  FORMAT (16H ERROR IN TRIPLE)
       END
```

```
      SUBROUTINE UNVAL(N,U,V,ALPHA,BETA,REAL,XIMAG)
CUNVAL  TO EVALUATE THE EIGENVALUES OF A TRIPLE DIAGONAL MATRIX
      DIMENSION ALPHA(10),BETA(11),P(11),Q(13),T(11),REAL(10),XIMAG(10)
C       FORM POLYNOMIAL FROM TRIPLE DIAGONAL MATRIX
      IF(N-2*(N/2))99,73,71
   73 M=N
      GO TO 74
   71 M=N-1
   74 NA=N
   72 DO 60 K=1,N
      P(K)=0.0
   60 Q(K)=0.0
      P(1)=-ALPHA(1)
      P(2)=1.0
      Q(1)=1.0
      DO 62 I=2,M,2
      Q(1)=-ALPHA(I)*P(1)-BETA(I)*Q(1)
      DO 61 K=2,N
   61 Q(K)=P(K-1)-ALPHA(I)*P(K)-BETA(I)*Q(K)
      IF(N-I)99,64,63
   64 DO 65 K=1,N
   65 P(K)=Q(K)
      GO TO 66
   63 P(1)=-ALPHA(I+1)*Q(1)-BETA(I+1)*P(1)
      DO 62 K=2,N
   62 P(K)=Q(K-1)-ALPHA(I+1)*Q(K)-BETA(I+1)*P(K)
   66 P(N+1)=1.0
C       OBTAIN COMPLEX ROOTS OF REAL POLYNOMIAL, BAIRSTOWS METHOD
      L1=N+1
      L3=N+3
      NCT=0
      NR=0
      SUM=P(N)
      TEST =P(1)
      PRINT 251,TEST,SUM
C       ITERATION USING QUADRATIC FACTOR
   87 Q(1)=0.0
      Q(2)=0.0
      NCT=NCT+1
      IF(NCT-300)110,110,111
  111 PRINT 112
      GO TO 86
  110 DO 80 K=3,L3
      L4=N+4-K
   80 Q(K)=P(L4)+U*Q(K-1)+V*Q(K-2)
      T(1)=0.0
      T(2)=0.0
      DO 81 K=3,L1
   81 T(K)=Q(K)+U*T(K-1)+V*T(K-2)
      XPL=U*T(N+1)+V*T(N)
      DPL=T(N+1)**2-XPL*T(N)
      IF(ABSF(DPL)-1.0E-8)99,99,82
   82 UINC=(T(N)*Q(N+3)-T(N+1)*Q(N+2))/DPL
      VINC=(XPL*Q(N+2)-T(N+1)*Q(N+3))/DPL
      U=U+UINC
```

```
      V=V+VINC
      IF(ABSF(U)-1.0E+0)121,120,120
  121 IF(ABSF(UINC)-1.0E-8)122,122,87
  120 IF(ABSF(UINC/U)-1.0E-8)122,122,87
  122 IF(ABSF(V)-1.0E+0)84,123,123
   84 IF(ABSF(VINC)-1.0E-8)86,86,87
  123 IF(ABSF(VINC/V)-1.0E-8)86,86,87
C       OBTAIN ROOTS OF QUADRATIC FACTORS
   86 DSCRM=(0.25*U*U)+V
      IF(DSCRM)88,89,90
   89 RT1R=U*0.5
      RT2R=RT1R
      GO TO 91
   90 RT1R=(U*0.5)+SQRTF(DSCRM)
      RT2R=U-RT1R
   91 RT1I=0.0
      RT2I=0.0
      GO TO 93
   88 RT1R=U*0.5
      RT2R=RT1R
      RT1I=SQRTF(-DSCRM)
      RT2I=-RT1I
   93 NR=NR+1
      REAL(NR)=RT1R
      XIMAG(NR)=RT1I
      NR=NR+1
      REAL(NR)=RT2R
      XIMAG(NR)=RT2I
C       DETERMINE WHETHER ALL ROOTS HAVE BEEN OBTAINED
      IF(N-4)94,95,96
   96 N=N-2
      L1=N+1
      L3=N+3
      DO 98 K=1,L1
      L4=N+4-K
   98 P(K)=Q(L4)
      NCT=0
      GO TO 87
   95 U=-Q(4)
      V=-Q(5)
      N=2
      GO TO 86
   94 IF(N-3)130,97,99
   99 PRINT 101
      GO TO 100
   97 NR=NR+1
      REAL(NR)=-Q(4)
      XIMAG(NR)=Q(1)
  130 N=NA
      RETURN
  100 CALL EXIT
   92 FORMAT(2E20.8)
  101 FORMAT(17H INCORRECT ANSWER)
  112 FORMAT (24H EXCEEDED 300 ITERATIONS//)
  251 FORMAT (36H PRODUCT AND SUM OF EIGENVALUES ARE 2E20.8//)
```

```
      SUBROUTINE UNVEC(N,ALPHA,BETA,Y,YTR,REAL,XIMAG,VECR,VECI,
     1ADVECR,ADVECI)
CUNVEC  TO OBTAIN THE EIGENVECTORS
      DIMENSION Y(10,10),YTR(10,10),P(10,10),Q(10,10),
     1VECR(10,10),VECI(10,10),ADVECR(10,10),ADVECI(10,10),
     2ALPHA(10),BETA(11),REAL(10),XIMAG(10),TR(10),TI(10),
     3ATR(10),ATI(10)
      BETA(N+1)=0.0
      DO 20 I=1,N
      P(I,N)=1.0
      Q(I,N)=0.0
      P(I,N-1)=REAL(I)-ALPHA(N)
      Q(I,N-1)=XIMAG(I)
      DO 20 J=3,N
      K=N-J+1
      P(I,K)=P(I,K+1)*(+REAL(I)-ALPHA(K+1))-BETA(K+2)*P(I,K+2)-XIMAG(I)*
     1Q(I,K+1)
   20 Q(I,K)=Q(I,K+1)*(+REAL(I)-ALPHA(K+1))+P(I,K+1)*XIMAG(I)-BETA(K+2)
     1*Q(I,K+2)
      DO 25 I=1,N
      DO 25 J=1,N
      VECR(I,J)=0.0
      VECI(I,J)=0.0
      ADVECR(I,J)=0.0
      ADVECI(I,J)=0.0
      DO 25 K=1,N
      VECR(I,J)=VECR(I,J)+P(I,K)*Y(J,K)
      VECI(I,J)=VECI(I,J)+Q(I,K)*Y(J,K)
      ADVECR(I,J)=ADVECR(I,J)+P(I,K)*YTR(J,K)
   25 ADVECI(I,J)=ADVECI(I,J)+Q(I,K)*YTR(J,K)
      DO 26 I=1,N
      ZR=0.0
      ZI=0.0
      DO 27 J=1,N
      ZR=ZR+VECR(I,J)*ADVECR(I,J)-VECI(I,J)*ADVECI(I,J)
   27 ZI=ZI+VECR(I,J)*ADVECI(I,J)+VECI(I,J)*ADVECR(I,J)
      IF(ABSF(ZI)-0.0001)204,204,201
  204 IF(ZR)200,205,206
  205 PRINT 250
      CALL EXIT
  200 WR=0.0
      WI=SQRTF(-ZR)
      GO TO 203
  206 WR=SQRTF(ZR)
      WI=0.0
      GO TO 203
  201 WR=SQRTF(0.5*(ZR+SQRTF(ZR*ZR+ZI*ZI)))
      WI=ZI/(2.0*WR)
  203 WN=WR*WR+WI*WI
      DO 26 J=1,N
      TR(J)=(VECR(I,J)*WR+VECI(I,J)*WI)/WN
      TI(J)=(VECI(I,J)*WR-VECR(I,J)*WI)/WN
      ATR(J)=(ADVECR(I,J)*WR+ADVECI(I,J)*WI)/WN
      ATI(J)=(ADVECI(I,J)*WR-ADVECR(I,J)*WI)/WN
      VECR(I,J)=TR(J)
      VECI(I,J)=TI(J)
      ADVECR(I,J)=ATR(J)
   26 ADVECI(I,J)=ATI(J)
  250 FORMAT (24H ZERO LENGTH EIGENVECTOR//)
      RETURN
      END
```

APPENDIX I

NOMENCLATURE

General

z	Scalar
z	Complex conjugate of z
z'	Derivative of z with respect to x
$\overline{z}$	Average value of $z(x)$
$\underline{z}$	Column vector
$\underline{z}^T$	Row vector
z_n	Element of $\underline{z}$
$\underline{Z}$	Matrix
$\underline{Z}^{-1}$	Inverse of $\underline{Z}$
$\underline{Z}^T$	Transpose of $\underline{Z}$
Z_{nm}	Element of $\underline{Z}$
$\langle a, b\rangle$	Inner product of a, and b, followed by integration over x
$\frac{\partial z}{\partial x}$	Partial derivative of z, holding t constant
$\frac{\partial z}{\partial t}$	Partial derivative of z, holding x constant
$\tilde{z}$	Transient part of z
z_{ss}	Steady state part of z

Roman Letters

$\underline{A}$	Matrix of modified Galerkin method
$\underline{A}$	Eq. F.1
a_1, a_2	Appendix E
a_n	Undetermined coefficient of eigenvectors
$\underline{B}$	Matrix of modified Galerkin method
$\underline{B}$	Eq. F.1
$\underline{C}$	Generalized capacity matrix
$\underline{C}$	Matrix of eigenvectors in rows

c_i	i^{th} element of $\underline{C}$
$\underline{D}$	Generalized diffusion matrix
$\underline{D}$	Matrix of adjoint eigenvectors in rows
$\underline{D}$	Eq. A.5
d_i	i^{th} element of $\underline{D}$
$\underline{E}$	Eq. 2.38
E	Mass transfer efficiency
$\underline{F}$	Eq. 2.42
F(x, s)	Eq. E.6
f(x)	Vapor/liquid equilibrium curve
G	Gain
$\underline{H}$	Generalized transfer matrix
h_{ij}	Element of H
H	Liquid hold-up
H(x, s)	High-frequency portion of transfer function
Im(z)	Imaginary part of z
I(x, s)	Integral series solution
k_L, k_G	Mass transfer coefficients
k_i	Gain
L(y)	Linear operator
L(z)	Adjoint linear operator
L(x, s)	Low-frequency portion of transfer function
L	Liquid flow rate
M	Number of streams
m	Slope of the equilibrium line
N_i	Number of transfer units in the i^{th} stream
N	Number of terms in modified Galerkin method

$\underline{P}$	Eqs. A.6 and B.3
p	Half the Pecelet number
$\underline{Q}_p$	Eq. 2.33
$\underline{Q}$	Eqs. A.4 and B.3
q	Disturbance
$\mathrm{Re}(z)$	Real part of z
$\underline{R}$	Eq. B.3
R	Eq. C.9
s	Laplace transform variable with respect to time
t	Time in normalized units
T	Dominant time constant
T_i	Time constants of Campbell approximation
u	$(1, \ldots . 1)$ in Appendix A
$u_o(x-X)$	Unit impulse at $x=X$
$\underline{u}_p$	Eq. 2.34
$\underline{V}$	Generalized velocity matrix
v_i	i^{th} element of $\underline{V}$
v_m	Mean velocity of system
V_T	Taylor diffusion velocity
w	Eq. A.13
x	Normalized distance $0 \leq x < 1$
x	Liquid composition
$\underline{y}$	Vector of system variables
y_i	i^{th} element of $\underline{y}$
y_i, y_o	Eq. 3.1
y	Vapor composition
ym	Mean value of $\underline{y}$

$\underline{z}$	Adjoint variable to $\underline{y}$
z	Normalized distance

Greek Letters

α_1, α_2	Coefficients of boundary conditions
$\alpha_i(x)$	Ratio of zero to pole in Campbell approximation
α_T	Taylor diffusivity
β	Velocity ratio of two-stream system
β_1, β_2	Coefficients of boundary conditions
$\underline{\phi}_n(x)$	Complete set of functions
$\underline{\psi}_n(x)$	Complete set of functions
λ	Eigenvalue
$\underline{\xi}_p$	Eq. 2.33
$\underline{\xi}_n$	Real part of $\underline{y}_n$
ξ_i	Attenuation in i^{th} stream
η_i	Delay in i^{th} stream
$\underline{\eta}_n$	Imaginary part of $\underline{y}_n$
$\underline{\eta}$	Variation of $\underline{\tilde{y}}$
$\underline{\zeta}$	Variation of $\underline{\tilde{z}}$
ω_n	Taylor characteristic values
θ	Eq. A.22
	Appendix D
Δ	Appendix D
$\underline{\Gamma}$	Appendix D and Eq. 2.42

APPENDIX J

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BIOGRAPHICAL NOTE

Matthew Richard Gordon-Clark was born in London on 24 September, 1933. He was educated at Cheltenham College (1942-51), being awarded an exhibition in 1947, and at Trinity Hall, Cambridge University (1952-55) where he read mathematics obtaining a B. A. in 1955 and M. A. in 1959. He returned to Cambridge University in 1959 to take a Post-Graduate course in Control Engineering, and in 1961 he entered the Massachusetts Institute of Technology and obtained a S. M. in Electrical Engineering in 1962.

From 1955-59 he worked for the Bristol Aeroplane Company of Filton, England, on the control and guidance of guided weapons, especially the Bloodhound ground-to-air missile. In 1960 he joined the Transcoil Division of Daystrom, Inc. of Worcester, Pa. and worked on the design and development of tachometers and synchros.

While at the Massachusetts Institute of Technology he was a teaching assistant in 1963-64 and an instructor in electrical engineering in 1964-65. He taught courses in linear circuit theory (6.01 and 6.02), in electromechanical components (6.42), and in feedback control laboratory (6.213).

He published a paper based on his masters thesis, entitled "A Novel Approach to the Control of Dynamically Unfavorable Processes" in the I.E.E.E. Transactions on Automatic Control, Vol. AC-9, 1964.

In 1962 he married Katherine Yates Massela of Philadelphia.