Multi-Variable Optimization of Pressurized Oxy-Coal Combustion

by

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Abstract

Simultaneous multi-variable gradient-based optimization with multi-start is performed on a 300 MWe wet-recycling pressurized oxy-coal combustion process with carbon capture and sequestration. The model accounts for realistic component behavior such as heat losses, steam leaks, pressure drops, cycle irreversibilities, and other technological and economical considerations. The optimization study involves 16 variables, three of which are integer valued, and 10 constraints with the objective of maximizing thermal efficiency. The solution procedure follows active inequality constraints which are identified by thermodynamic-based analysis to facilitate convergence. Results of the multi-variable optimization are compared to a pressure sensitivity analysis similar to those performed in literature; the basecase of both assessments performed here is a favorable solution found in literature. Significant cycle performance improvements are obtained compared to this literature design at a much lower operating pressure and with moderate changes in the other operating variables. The effect of the variables on the cycle performance and on the constraints are analyzed and explained to obtain increased understanding of the actual behavior of the system. This study reflects the importance of simultaneous multi-variable optimization in revealing the system characteristics and uncovering the favorable solutions with higher efficiency than the atmospheric operation or those obtained by single variable sensitivity analysis.

Thesis Supervisor: Alexander Mitsos
Title: Rockwell International Assistant Professor
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Chapter 1

Introduction

One of the major products of fossil fuel combustion is carbon dioxide, which is widely considered to be a greenhouse gas and a major contributor to global warming [8]. Given the potential implications of the fast rise of CO$_2$ levels in the atmosphere [8, 15], policies and regulations against anthropogenic CO$_2$ emissions are expected to be implemented in the near future [1].

Electrical power generation relies heavily on the combustion of fossil fuels and demand for electricity is only expected to increase. Due to the abundance of reserves and relatively cheap price, coal is the fuel of choice for electricity production [18]. Thus, coal combustion with Carbon Capture and Sequestration (CCS), where Oxy-Coal Combustion (OCC) combustion is one of the promising options, is considered as a solution to these emissions [2]. In OCC with CCS oxygen is separated from air before being used as an oxidizer. Combustion occurs in the presence of large amounts of recycled flue gas to dilute the mixture and control the combustion temperature. Due to the absence of nitrogen in the oxidizer stream, the combustion products are predominantly CO$_2$ and H$_2$O, and the CO$_2$ is separated relatively easily by removing the H$_2$O via condensation. After purification treatment, the CO$_2$ gas is compressed for sequestration [16].

The high concentration of water vapor in the flue gas, which carries a significant amount of latent energy, and the compression requirement for the CO$_2$ sequestration motivates pressurized oxy-combustion, i.e., oxycombustion at an elevated pressure.
Different flowsheets have been suggested to utilize the benefits of this technology. One flowsheet is given in a case study of an OCC process operating at 80 bar with dry recycling, recycling after condensing the H$_2$O, [7]. A ThermoEnergy Integrated Power System (TIPS) cycle operating pressure of 80 bar is presented in a feasibility study, [22]. Another flowsheet based on wet recycling, recycling before condensing the H$_2$O, is proposed in [9] and further investigated by [13, 14]. In [14], a sensitivity analysis of the combustor pressure indicates that 10 bar is the favorable operating pressure. Technological issues of pressurized oxy-coal combustion are investigated in [10]. These flowsheet configurations share the same main principles. Flue gas from combustion contains a large amount of water vapor due to the combustion of hydrogen atoms and more significantly due to the water introduced with the coal slurry mixture. A recovery heat exchanger (RHE) is used to condense the water in the flue gas and heat the working fluid of the Rankine cycle and as a result eliminating the need for low pressure feedwater heaters and low pressure bleed extractions. The RHE is also referred to as Acid Condenser in some contexts because it must be able to withstand the presence of acids since sulfur and nitrogen oxides are byproducts of coal combustion. As operating pressure increases, the saturation temperature of the water in the flue gas increases, resulting in a larger amount of H$_2$O condensation occurring at a higher average temperature. Thus a larger amount and higher quality of thermal energy transfer at the RHE is achieved, which includes both "latent and sensible heat". Moreover, the flue gas to be purified and sequestrated is already pressurized reducing the power required by the CO$_2$ Sequestration Unit (CSU). However, pressurized operation implies a need to compress O$_2$. Due to the smaller heat capacity ratio of CO$_2$, oxygen compression is more expensive than CO$_2$ compression for identical molar flowrate of both molecules. Also the O$_2$ flowrate is larger than that of CO$_2$ due to the oxidation of the H atoms forming H$_2$O and any excess oxygen used. Moreover, with increasing pressure, cycle pressure losses in the Heat Recovery Steam Generator (HRSG) increase. The capital cost of the pressurized system is higher than the capital cost of normal a OCC process which in turn is higher than the capital cost of a coal power cycle without CCS. Other new technologies like selective oxygen
transport separation membranes and reactive membranes, the latter typically considered for natural gas, are investigated [11], however, they are still in a premature state with many design, manufacturing, technical, and economical challenges.

A comprehensive analysis and optimization of pressurized oxy-coal combustion has not been addressed in literature yet, especially not one which considers high-fidelity modeling of components and irreversibilities. Herein, multi-variable optimization for a 300 MWe pressurized oxy-coal combustion plant is performed on a wet recycling OCC for CCS to accurately assess the concept's advantages and tradeoffs. The effect of each optimization variable on the different cycle sections and on the efficiency is then analyzed and presented. The importance of simultaneous variable optimization is demonstrated by the complex state variable interactions and the improvement in cycle efficiency. Section ?? describes the cycle’s flowsheet with an emphasis on the detailed unit operation models used to represent an actual power plant. Section 2 deals with the pressure loss calculations required for an accurate assessment of pressurized OCC. Section 3 provides a thorough description of the optimization formulation including the objective function, variables, and constraints. A description of the numerical scheme allowing for optimization based partially on following active constraints is also given. Results are shown in Section 4, where the influence of the critical variables on the different sections of the cycle and on the cycle performance are analyzed. Motivated by the system response and the results observed, Section 5 describes and analyzes the effect of water addition to the temperature controlling/recirculation sections of the flowsheet.
Chapter 2

Flue Gas Pressure Drop

Combustion in pure oxygen can in principle reach extremely high temperatures, however, due to material properties, the temperature of the flue gas entering the HRSG is limited to 800°C [19]. The temperature of the combustion process also has an upper bound set by material properties and a lower bound set by the ash melting point. Ash present in the coal is deposited on the walls of the combustor where it melts and flows to the combustor outlet. For an accurate assessment of the cycle performance the behavior of the different cycle sections is taken into consideration. Pressure drops due to friction, bends, and obstructions are significant, mainly in the HRSG and in the recirculation pipes. Fans are employed to compensate for the pressure drop. The flue gas pressure drop and thus the fans’ compression requirements are functions of the operating pressure; therefore, it is important to accurately evaluate these pressure losses during optimization to find the optimum operating conditions.

2.1 Recirculation Pipes Pressure Drop

Flue gas is recycled into the combustion chamber by the primary recirculation pipe, and into the Temperature Controller by the secondary recirculation pipe. The associated pressure drop in each pipe, \( \Delta P_{\text{pipe}} \), is estimated by the following equations [17, 20]:

\[
\Delta P_{\text{pipe}} = \rho f \frac{L_p V^2}{d^2}
\]
where \( V \) is the bulk gas velocity in the pipe, \( d \) is the pipe diameter, \( L_p \) is the pipe equivalent length, \( \rho \) is the gas density, and \( f \) is the friction factor calculated by

\[
f_{pipe} = \left\{ -2.0 \log \left[ \frac{(2\epsilon/d)}{7.4} - \frac{5.02}{Re_d} \log \left( \frac{(2\epsilon/d)}{7.4} + \frac{13}{Re_d} \right) \right] \right\}^{-2}
\]

where \( \epsilon \) is the pipe roughness, \( Re_d = \frac{\rho V_d}{\mu} \) is the Reynolds number based on the pipe diameter, \( \rho \) is the flue gas density, and \( \mu \) is the dynamic viscosity of the gas.

The pipe diameter, \( d \), and the gas velocity, \( V \), are related by \( \dot{m} = \rho V \frac{\pi d^2}{4} \), where \( \dot{m} \) is the recirculated gas mass flowrate through each of the two pipes. The flowrates are specified by the amount of dilution required to control each temperature limit but also depend on the pipe properties and dimensions. Section 4.5 discusses how pressure drop and its compensation affect dilution requirements. For practical considerations the pipes diameters and the gas velocities in the pipes have to fall within fixed ranges [19]. The acceptable ranges are shown in Table 2.2. The equivalent length was obtained by considering a 63.5 mbar pressure drop in each pipe at the base-case operating pressure of 10 bar [19].

Table 2.1: Recirculation pipe diameters and gas velocity ranges [19]

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The larger the pipe diameter, the smaller the gas flow velocity, and the smaller the pressure drop. Thus, a larger pipe is always favored in terms of efficiency but not necessarily from an economical point of view as the capital, installation, and maintenance costs would increase. However, very large flow velocities can cause structural failure and acoustic resonance. Herein, at each iteration within the optimization study, the largest allowable diameter, for each of the two pipes, is chosen such that the gas velocity remains within the velocity range. In the case the flowrate is too high, the upper bound on the diameter is chosen and the velocity range is violated.


2.2 HRSG Pressure Drop

The HRSG transfers thermal energy from the hot flue gas to the working fluid of the Rankine cycle. As the flue gas passes through the HRSG and through the tube bundles that form the heat exchanger's surface area, it is subjected to a pressure drop. An HRSG with a larger cross section and larger heat exchange area causes lower pressure losses for the same thermal energy transfer because the flue gas passage is less restricted. However, the high capital and maintenance costs of the HRSG are determined by its surface area, and it is economically favorable to allow significant pressure losses for the sake of having a smaller and less expensive HRSG. The HRSG model relies on industrial considerations and data to obtain a small size and cost while maintaining a high heat transfer coefficient, [19].

A high entrance velocity is required to limit the exchanger’s size and surface area. A typical value is \( V_0 = 15.5 \text{ m/s} \) with a 0.527 bar pressure drop at the 10 bar base-case operation [19]. A simple procedure based on similarity analysis is proposed for the estimation of the pressure drop; the geometric design and arrangement of the heat exchanger is identical to the base-case design where the entrance velocity \( V_0 \) is fixed to the typical suggested value.

The flue gas pressure drop in the HRSG is expressed as
\[
\Delta P_{HRSG} = f N \rho \frac{V_{\text{max}}^2}{2}
\]
where \( V_{\text{max}} = V_0 \frac{S_T}{S_T-D} \) is the maximum velocity between the tubes [17]. \( N \) is the number of tube bundles/rows along the longitudinal direction, and the constant parameters \( D \) and \( S_T \) are the tube diameter and the transverse pitch of the fixed design heat exchanger, respectively. So for a required constant \( V_0 \), \( V_{\text{max}} \) is also a constant. The friction factor, \( f \), is a function of Reynold’s number. All operating conditions considered herein result in high Reynold’s numbers and thus an approximately constant friction factor. Therefore,
\[
\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{N_a \rho_a}{N_b \rho_b}
\]
The subscripts \( a \) and \( b \) stand for actual and base-case, respectively. \( N \) is directly
and linearly proportional to $L$, the length of the heat exchanger, by a factor of $1/S_L$, where $S_L$ is the longitudinal pitch and is also constant for a fixed design.

The heat exchanger surface area is given by $A_s = \pi D \times W \times \frac{H}{S_T} \times \frac{L}{S_L}$, where $H$ is the exchanger’s height and $H/S_T$ represents the number of tubes in the transverse direction. $W$ is the exchanger’s width which is also the length of the tubes through which water/steam pass. Therefore $A_s = \text{constant} \times A_c L$ where $A_c = x^2$ is the HRSG cross sectional area when a square cross section of side $x$ is assumed ($H = W = x$). $A_c$ is calculated from the mass flow rate $\dot{m}$: $A_c = \frac{\dot{m} x}{\rho_0 v_0} = x^2$. Therefore

$$\frac{L_a}{L_b} = \frac{A_{s,a} x_b^2}{A_{s,b} x_a^2} \tag{2.2}$$

The total heat transfer, $\dot{Q}$, is related to the heat exchanger’s surface area, $A_s$, by: $\dot{Q} = U A_s F \Delta T_{lm}$, where $U$ is the effective heat transfer coefficient, $\Delta T_{lm}$ is the log mean temperature difference for the particular chosen design and $F$ is its respective correction factor. $\Delta T_{lm}$ and $F$ are solely a function of the entry and exit temperatures, and since a fixed design is considered, their functional expression is identical for any operating condition. The hot gas entry temperature and the cold streams exit temperatures of both the main and the reheat streams are fixed parameters, and only small variations in the temperature at the extremes of the heat exchanger are seen during optimization (the exit flue gas temperature is around 300°C and the feedwater entry temperature is around 290°C as discussed later in Section 4.3). Keeping in mind that a fixed internal temperature approach is specified for the heat exchanger, as explained in Section 3.5 and discussed in Section 4.3, the $\Delta T_{lm}$ and $F$ can be considered invariant. So

$$\frac{A_{s,a}}{A_{s,b}} = \frac{\dot{Q}_a U_b}{\dot{Q}_b U_a} \tag{2.3}$$

The Reynolds number based on the hydraulic diameter $D_h$ is given by $\text{Re}_{D_h} = \frac{\rho \dot{V}_Q D_h}{\mu}$. For the square cross sectional area considered, $D_h = \left(\frac{\dot{m}}{\rho_0 v_0}\right)^{1/2}$ which means $\text{Re}_{D_h} = \frac{\rho^{1/2} \dot{m}^{1/2} v_0^{1/2}}{\mu}$. The mass flowrate $\dot{m}$ increases with increasing pressure as will be ex-
plained later in Section 4.5. \( V_0 \) is constant, \( \mu \) is a weak function of the operating pressure, and \( \rho \) increases with increasing pressure, so \( Re_{D_h} \) slightly increases with increasing operating pressure primarily due to the density change.

The Nusselt number is proportional to the Reynolds number raised to a power lower than unity, and thus less sensitive to changes in operation. The functional form relating the two numbers cannot be obtained without a detailed representation of the HRSG in particular since both convection and radiation can play a role. Two approaches that in principle lead to two different pressure drop correlations but in practice have relatively similar results, are investigated.

In the first approach, the Nusselt number, \( Nu = \frac{UxD_a}{K} \) where \( K \) is the thermal conductivity of the flue gas at each operating condition, is assumed constant. Under this approximation, dividing the Nusselt number by that of the base-case number and rearranging gives:

\[
\frac{U_a}{U_b} = \frac{Nu_a K_a D_{h,b}}{Nu_b K_b D_{h,a}} = \frac{K_a x_b}{K_b x_a} \tag{2.4}
\]

which with (2.7), (2.8), and (2.9) gives:

\[
\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{\dot{Q}_a K_b \dot{m}_b^{1/2} \rho_a^{1/2} \rho_b}{\dot{Q}_b K_a \dot{m}_a^{1/2} \rho_b^{1/2} \rho_a} = \frac{\dot{Q}_a K_b \dot{m}_b^{3/2}}{\dot{Q}_b K_a \dot{m}_a^{3/2}} \tag{2.5}
\]

The second approach is to consider the heat transfer coefficient \( U \), the combined convective and radiative heat transfer, equal to the base-case. So for a constant \( U \) we get from equation (2.9): \( A_a = \frac{A_b}{A_b} \). Substituting and rearranging we finally get:

\[
\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{Q_a \rho_a^2 \dot{m}_b}{Q_b \rho_b^2 \dot{m}_a} \tag{2.6}
\]

Both approximations lead to comparable pressure drops in the range of expected optimum, so only the second approach, defined by equation (2.12), is incorporated in
this study. Combustion in pure oxygen can in principle reach extremely high temperatures, however, due to material properties, the temperature of the flue gas entering the HRSG is limited to 800°C. The temperature of the combustion process also has an upper bound set by material properties and a lower bound set by the ash melting point, [5]. Ash present in the coal is deposited on the walls of the combustor where it melts and flows to the combustor outlet. For an accurate assessment of the cycle performance the behavior of the different cycle sections is taken into consideration. Pressure drops due to friction, bends, and obstructions are significant, mainly in the HRSG and in the recirculation pipes. Fans are employed to compensate for the pressure drop. The flue gas pressure drop and thus the fans' compression requirements are functions of the operating pressure; therefore, it is important to accurately evaluate these pressure losses during optimization to find the optimum operating conditions.

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where $\epsilon$ is the pipe roughness, $\text{Re}_d = \frac{\rho V d}{\mu}$ is the Reynolds number based on the pipe diameter, $\rho$ is the flue gas density, and $\mu$ is the dynamic viscosity of the gas.

The pipe diameter, $d$, and the gas velocity, $V$, are related by $\dot{m} = \rho V \pi d^2 / 4$, where $\dot{m}$ is the recirculated gas mass flowrate through each of the two pipes. The flowrates are specified by the amount of dilution required to control each temperature limit but also
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$$\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{N_a \rho_a}{N_b \rho_b}$$

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The total heat transfer, $\dot{Q}$, is related to the heat exchanger’s surface area, $A_s$, by:
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where \( U \) is the effective heat transfer coefficient, \( \Delta T_{lm} \) is the log mean temperature difference for the particular chosen design and \( F \) is its respective correction factor. \( \Delta T_{lm} \) and \( F \) are solely a function of the entry and exit temperatures, and since a fixed design is considered, their functional expression is identical for any operating condition. The hot gas entry temperature and the cold streams exit temperatures of both the main and the reheat streams are fixed parameters, and only small variations in the temperature at the extremes of the heat exchanger are seen during optimization. As discussed in Section 5.3 the flue gas temperature is around 300°C and the feedwater entry temperature is around 290°C; note that this is significantly higher than the acid dew point, see also Figure 4-5 and reference [10] for the pressure dependence of the acid dew point. Keeping in mind that a fixed internal temperature approach is specified for the heat exchanger, as explained in Section 3.5 and discussed in Section 4.3, the \( \Delta T_{lm} \) and \( F \) can be considered invariant. So

\[ \frac{A_{s,a}}{A_{s,b}} = \frac{\dot{Q}_a U_b}{\dot{Q}_b U_a} \quad (2.9) \]

The Reynolds number based on the hydraulic diameter \( D_h \) is given by \( Re_{D_h} = \frac{\rho V_0 D_h}{\mu} \). For the square cross sectional area considered, \( D_h = (\frac{m}{V_0})^{1/2} \) which means \( Re_{D_h} = \frac{\rho^{1/2} \dot{m}^{1/2} V_0^{1/2}}{\mu} \). The mass flowrate \( \dot{m} \) increases with increasing pressure as will be explained later in Section 4.5. \( V_0 \) is constant, \( \mu \) is a weak function of the operating pressure, and \( \rho \) increases with increasing pressure, so \( Re_{D_h} \) slightly increases with increasing operating pressure primarily due to the density change.

The Nusselt number is proportional to the Reynolds number raised to a power lower than unity, and thus less sensitive to changes in operation. The functional form relating the two numbers cannot be obtained without a detailed representation of the HRSG in particular since both convection and radiation can play a role. Two approaches that in principle lead to two different pressure drop correlations but in practice have relatively similar results, are investigated.

In the first approach, the Nusselt number, \( Nu = \frac{U \times D_h}{K} \) where \( K \) is the thermal conductivity of the flue gas at each operating condition, is assumed constant. Under
this approximation, dividing the Nusselt number by that of the base-case number and rearranging gives:

\[
\frac{U_a}{U_b} = \frac{N u_a K_a D_{h,b}}{N u_b K_b D_{h,a}} = \frac{K_a x_b}{K_b x_a}
\]  

(2.10)

which with (2.7), (2.8), and (2.9) gives:

\[
\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{\dot{Q}_a K_b \dot{m}_b^{1/2} \rho_a \rho_b}{\dot{Q}_b K_a \dot{m}_a^{1/2} \rho_a \rho_b} = \frac{\dot{Q}_a K_b \dot{m}_b^{1/2} \rho_a^{3/2}}{\dot{Q}_b K_a \dot{m}_a^{1/2} \rho_b^{3/2}}
\]

(2.11)

The second approach is to consider the heat transfer coefficient \( U \), the combined convective and radiative heat transfer, equal to the base-case. So for a constant \( U \) we get from equation (2.9): \( \frac{\dot{A}_a}{\dot{A}_b} = \frac{\dot{Q}_a}{\dot{Q}_b} \). Substituting and rearranging we finally get:

\[
\frac{\Delta P_{HRSG,a}}{\Delta P_{HRSG,b}} = \frac{Q_a \rho_a^2 \rho_b \dot{m}_b}{Q_b \rho_b^2 \rho_a \dot{m}_a}
\]

(2.12)

Both approximations lead to comparable pressure drops in the range of expected optimum, so only the second approach, defined by equation (2.12), is incorporated in this study.
Chapter 3

Optimization

To capture the true behavior of the system and the potential advantages of OCC, simultaneous optimization of all variables is required. Varying a single variable over-constrains the optimization problem and masks the potential advantages. Moreover, a single variable manipulation may result in simulation errors and violations, as well as violation of the optimization constraints. Thus, only a small range for the variable is possible when a single or small number of variables are optimized for. In contrast, because of the variables' influence on the many constraints and flowsheet sections, the constraints can be met in a multi-variable optimization while utilizing larger variable ranges, which in turn uncover potential improvements.

3.1 Objective Function

The aim is to have a nearly zero emissions (in particular CO₂), yet efficient and profitable, power plant. For the problem at hand, two objective functions, very similar in concept, can be formulated. The first is maximizing the power output for a fixed fuel input. This is equivalent to maximizing the first-law-efficiency holding the denominator, input chemical energy, constant. The alternative objective function is the profit. Maximizing the profit implies having the maximum difference between the total revenue and the total cost. This is similar to minimizing the levelized cost of electricity assuming a given electricity price. To maximize profit, the model needs to
account for the different components' material, size, cost, etc. It also needs to account for the operation and maintenance cost as well as the opportunity cost or the interest rate on capital. Such an economic optimization provides valuable information, for example the operation strategies, input and output price sensitivity, demand and supply sensitivity, etc. However, profit maximization should be considered after the engineering/performance optimization. Moreover, it depends strongly on parameters that vary such as the market input prices, output prices, interest rates, wages, etc. Therefore, herein the technological objective of maximal power will be used while taking into consideration economical concerns such as reasonable HRSG size and recirculation pipe diameters, as explained in Section 2.

Whether capital, operation and maintenance costs are considered or not, the exact representation of the objective function depends on the CO2-emission regulations. If in the regulations CO2 production is subjected to a fixed upper bound then the objective is to maximize efficiency subject to a CO2 production constraint. In contrast, if in the regulations power plants are fined for the amount of CO2-emission then the emission is no longer a constraint, but rather added as a penalty to the objective function. The penalty weight relative to the objective function would be proportional to the emission-fine relative to the electricity price.

In this study the efficiency is considered as the objective, i.e., maximizing the net-power output for a fixed fuel input, with CO2 capture and purity taken as a constraint. The net-power is equal to the gross power produced by the Rankine cycle minus the power demands of the pumps, the recirculation fans, the ASU, and the CSU. The ASU power requirement is the total power needed to produce the the oxidizer stream to compress the stream to the required operating pressure.

### 3.2 Optimization Variables and Constraints

The model consists of 10 constraints and 13 optimization variables, not counting the three integer variables described in Section 3.3. As discussed in Section 3.5 some constraints and variables were coupled in design specifications to accelerate
convergence and avoid suboptimal solutions. Figure 3-1 shows the optimization in purple circles marked by (o) and optimization constraints in green circles marked by (x).

### 3.2.1 Optimization Variables

Table 3.1 shows the 13 optimization variables, as they appear in Figure 3-1, their ranges, and their default base-case values. The default values are the results of the parametric study performed by [13] where 10 bar was found to be the favorable operating combustor pressure. $P_{\text{Comb}}$, the Oxygen delivery pressure, specifies the combustion operating pressure and the flue gas pressure which affects not only the flue gas condensation properties and the recovered thermal energy but also the pressure...
drops in the HRSG and the recirculation pipes and the compression load distribution between the ASU and the CSU. The feedwater can absorb almost all the Combustor’s thermal leaks/duty, \( Q_{\text{Comb}} \), although decreasing this duty is associated with an increase in the cost of insulation and refractory material around the combustor. M_BLD1,2,&3 and P_BLD1,2,&3, are the three bleeds’ mass flowrates and extraction pressures responsible for the regeneration process, respectively. The thermal energy transferred to the feedwater at the low temperature section changes with variables 1 and 2, so the bleeds’ variables need to change to achieve proper regeneration. The optimization of the regeneration changes the feedwater temperature at the inlet of the HRSG, so the feedwater flowrate through the HRSG, M_FW_Main, has to change accordingly. The turbines’ performance is considered to be unaffected by the change in the steam flowrate. Q_FWH1&2 are the amounts of thermal energy transferred from the bleed to the feedwater in the two closed feedwater heaters, which have to change as the conditions and properties of the bleeds and feedwater change. The deaerator pressure, P_Deaerator, is also an important part of the regeneration section. The temperature of the flue gas at the exit of the RHE, T_FG_RHE, specifies the amount of thermal energy transferred to the feedwater and has an effect on the compression requirements of the CSU. Both the flue gas pressure and feedwater flowrate also have an influence on the amount of thermal energy that can be recovered in the RHE. In principal a cooler can be used to decrease the flue gas temperature down to atmospheric after it exits the RHE. The cooler reduces the compression requirements and is mostly utilized at low operating pressures where the flue gas temperature at the RHE exit is high. However, for a proper fair economical comparison between operating pressures and to maintain a fixed capital cost no cooler was introduced.

### 3.2.2 Optimization Constraints

The 10 optimization constraints are stated in Table 3.2 as they appear in Figure 3-1. All heat exchangers have a minimum internal temperature approach (MITA) constraint between the hot and cold streams (MITA_HRSG, MITA_FWH1, MITA_FWH2, MITA_RHE). As typically done in systems-level analysis, the MITA is used instead
Table 3.1: Optimization Variables

<table>
<thead>
<tr>
<th>Number</th>
<th>Variable</th>
<th>Range</th>
<th>Base-case default value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>P_Comb</td>
<td>[1.283 - 30] bar</td>
<td>10 bar</td>
</tr>
<tr>
<td>2</td>
<td>Q_Comb</td>
<td>[1 - 30] MW</td>
<td>16 MW</td>
</tr>
<tr>
<td>3</td>
<td>M_FW_Main</td>
<td>[240-340] kg/s</td>
<td>269 kg/s</td>
</tr>
<tr>
<td>4</td>
<td>P_BLD1</td>
<td>[250 - 30] bar</td>
<td>55.96 bar</td>
</tr>
<tr>
<td>5</td>
<td>M_BLD1</td>
<td>[0 - 60] kg/s</td>
<td>34.04 kg/s</td>
</tr>
<tr>
<td>6</td>
<td>P_BLD2</td>
<td>[120 - 10] bar</td>
<td>18.76 bar</td>
</tr>
<tr>
<td>7</td>
<td>M_BLD2</td>
<td>[0 - 30] kg/s</td>
<td>7.962 kg/s</td>
</tr>
<tr>
<td>8</td>
<td>P_BLD3</td>
<td>[30 - 4.5] bar</td>
<td>10.5 bar</td>
</tr>
<tr>
<td>9</td>
<td>M_BLD3</td>
<td>[0 - 30] kg/s</td>
<td>3.815 kg/s</td>
</tr>
<tr>
<td>10</td>
<td>QFWH1</td>
<td>[0 - 200] MW</td>
<td>75.8 MW</td>
</tr>
<tr>
<td>11</td>
<td>QFWH2</td>
<td>[0 - 200] MW</td>
<td>21.2 MW</td>
</tr>
<tr>
<td>12</td>
<td>P_Deaerator</td>
<td>[0.1 - 30] bar&lt;sup&gt;a&lt;/sup&gt;</td>
<td>10 bar</td>
</tr>
<tr>
<td>13</td>
<td>T_FG_RHE</td>
<td>[30 - 150] °C</td>
<td>36.9°C</td>
</tr>
<tr>
<td>14</td>
<td>BLD1_Pos integer variable</td>
<td>Stages: 1-4</td>
<td>Stage: 3</td>
</tr>
<tr>
<td>15</td>
<td>BLD2_Pos integer variable</td>
<td>Stages: 3-6</td>
<td>Stage: 5</td>
</tr>
<tr>
<td>16</td>
<td>BLD3_Pos integer variable</td>
<td>Stages: 5-7</td>
<td>Stage: 6</td>
</tr>
</tbody>
</table>

<sup>a</sup> The Deaerator operating pressure should be above atmospheric, but here the lower bound was intentionally taken sub-atmospheric to examine if it would lead to any advantage in performance.

of the respective heat exchanger area specification. The allowed values of the MITA are identical for all runs and equal to those specified in the base-case and the pressure only parametric study. The Deaerator is responsible for the separation of the gases dissolved in the feedwater, which is achieved by allowing the mixture of the feedwater and bleeds to reach saturation in the Deaerator tank situated at an elevated height while having a pressure higher than atmospheric. q_Deaerator, ensures that the feedwater in the deaerator tank reaches saturation, which automatically guarantees that the feedwater at the exit of the deaerator is all liquid. Besides the physical reasons for implementing this constraint, simulation results in major errors otherwise. T_Cool-Gas, T_FW-HRSG-in, and T_Com-Gas-in guard against undesired acid condensation. The temperature of the Cool-Gas has to be at least 20°C above the acid condensation temperature. Also, the temperature of FW-HR-in has to be at least 5°C above the acid condensation temperature to prevent film condensation in the HRSG. The tem-
perature of Com-Gas-in also has to be 20°C above the acid condensation temperature especially that dilution and temperature drop occurs after mixing with a relatively cool oxygen stream for low operating pressures. Finally, CO2_cap and CO2_pure force the CSU to capture 94% of the total amount of CO2 with a purity of 96.5%.

Table 3.2: Optimization Constraints

<table>
<thead>
<tr>
<th>Number</th>
<th>Constraint</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>MITA_HRSG</td>
<td>120°C superheat and reheat sections; 3.7°C economizer section^a</td>
</tr>
<tr>
<td>2</td>
<td>MITA_FWH1</td>
<td>2.1°C</td>
</tr>
<tr>
<td>3</td>
<td>MITA_FWH2</td>
<td>2.1°C</td>
</tr>
<tr>
<td>4</td>
<td>MITA_RHE</td>
<td>7.5°C</td>
</tr>
<tr>
<td>5</td>
<td>Q_Deaerator</td>
<td>Saturated Liquid</td>
</tr>
<tr>
<td>6</td>
<td>T_Cool-Gas</td>
<td>20°C above acid condensation temperature</td>
</tr>
<tr>
<td>7</td>
<td>T_FW-HRSG-in</td>
<td>5°C above acid condensation temperature</td>
</tr>
<tr>
<td>8</td>
<td>T_Com-Gas-in</td>
<td>20°C above acid condensation temperature</td>
</tr>
<tr>
<td>9</td>
<td>CO2_Cap</td>
<td>94% of total CO2 produced</td>
</tr>
<tr>
<td>10</td>
<td>CO2_Pur</td>
<td>96.5% purity</td>
</tr>
</tbody>
</table>

^a The temperature of the flue gas is initially high as it enters the HRSG, 800°C; it is guaranteed that the temperature difference between the flue gas and the water/stream of the Rankine cycle, which reach a maximum of 610°C, is large in the superheat section; the temperature approach in the economizer is limiting due to the flue gas temperature drop.

3.3 Integer Variables

The characteristics and properties of the Rankine cycle sections and blocks are based on current best practices in coal fired power plants. Recall that the modeled blocks represent realistic plant components and specifications. The most interesting and challenging aspect in this realistic modeling is the steam expansion line. The expansion line is formed of different turbine stages with different efficiencies (isentropic
and mechanical efficiencies) as well as steam leaks. Modeling the expansion line requires taking into account for each stage separately. Each stage is represented by different turbine block(s) with the respective stage specifications. Incorporating the bleeds, which are the extractions that proceed to the feedwater heaters and deaerator for purpose of regeneration, as variables while having a realistic expansion line presents a major challenge due to the separate turbine stages. The bleed extraction pressure is an optimization variable, but the range of this variable is bounded by the pressure range of the particular stage the bleed is extracted from. Going beyond the stage’s pressure boundaries requires changing the bleed extraction position. In order to avoid having a different flowsheet for each of the possible combinations of bleed extractions (three bleeds in the current design and 12 different turbine expansion stages), each bleed going to its respective feedwater heater is allowed to be a combination of multiple streams extracted from the different turbine stages. Note that the multiple sub-bleeds are just a modeling trick. Figure 3-2 shows how three streams (sub-bleeds) extracted from the high pressure stages combine into a single bleed stream. Among these, a single sub-bleed should be active for each feedwater heater and the other sub-bleeds should have a zero flowrate. In Figure 3-2, Bleed 1 is considered to be extracted from the high pressure stages and thus has three possible extraction positions, but blindly choosing the bleed extractions would require incorporating all 12 stages of the steam expansion line.

Having multiple sub-bleeds in reality would result in unnecessary irreversibilities. In particular, the mixing of the sub-bleeds results in the throttling of the higher pressure sub-bleeds to the pressure of the lowest one. This creates considerable losses and destroys exergy that could have otherwise been used in the turbine, without adding any advantages to the heat regeneration process. In Appendix A it is analytically proven that each bleed should be drawn from only one stage for maximum efficiency. A numerical example is also provided in the same appendix.

Optimizing for efficiency as the objective function with all sub-bleeds as optimization variables should return only one nonzero sub-bleed. However, Aspen’s built in optimizer typically terminates with a suboptimal solution with more than one ac-
ative sub-bleed. This is likely a result of nonconvexity, small gradients, or simulation failures for zero flowrates of sub-bleeds. To avoid these numerical difficulties, one sub-bleed per bleed is activated at a time. The choice of the bleed extraction stage, or choice of active sub-bleed, is an integer variable. However, integer variables are not supported by the optimizer, so optimization is performed by explicitly accounting for the possible bleed extraction positions. There are a total of 12 turbine stages along the expansion line, and three regenerative bleeds. In addition, there is the possibility of no bleed. Thus, the total number of integer realizations is $13 \times 13 \times 13 = 2197$. However, it is not required to account for all these possibilities since most are obviously suboptimal. Herein, $4 \times 4 \times 3 = 48$ possibilities are chosen, which reflects that the first bleed should belong to the high pressure turbine stages as it requires having a high saturation temperature, and the second bleed should come from lower pressure stages to gradually increase the feedwater temperature in the feedwater heaters, and so on. In addition to the 48 different integer combinations, whenever a run results in a bleed pressure at the bounds of the allowed stage pressure range, the consecutive stage is tested with initial conditions being the converged results of the preceding bounded run.
3.3.1 Parameters Considered Constant

Ensuring a realistic representation of the components in the Rankine cycle section necessitates excluding some variables from the optimization process. The temperature and pressure of the feedwater exiting the HRSG, and more importantly, the reheat extraction pressure and the reheat delivery temperature are not incorporated as optimization variables. Typically, the main feedwater stream specifications on temperature and pressure are limited by technological constraints and metallurgical properties. As mentioned before, for a realistic assessment of the pressurized OCC process, the turbine stages that define the steam expansion line have fixed efficiency values over fixed pressure ranges. The efficiency of each stage is a strong function of the steam conditions. Here, the efficiencies of the stages are known as fixed values for the given main stream and reheat stream pressures and temperatures. The functional form of the stages' efficiency in terms of the steam pressure and temperature is not known. Changing the feedwater pressure or its temperature at the exit of the HRSG changes the conditions of the steam entering the different turbine stages, which in turn causes the stages' efficiency to change. Also, manipulating the reheat extraction pressure from the expansion line or the reheat delivery temperature at the exit of the HRSG would effect all downstream turbine stages and sections of the adjacent upstream stages, leading to an unknown value for the stages' efficiency. Therefore, the four mentioned parameters are kept fixed for the purpose of this study.

The oxidizer stream purity is a fixed parameter in this study. Varying the oxygen purity changes the ASU power demand and capital cost but also requires a different oxidizer stream flowrate to match the combustor's equivalence ratio specifications, which in turn affects the performance of the cycle downstream. The oxygen purity affects efficiency and capital cost significantly and thus would be interesting to optimize for, but would require a more elaborate model for each of the ASU and CSU which is beyond the scope of this work.
3.4 Multi-Start

Multi-Start refers to executing a large number of optimization runs with different initial guesses for the optimization variables distributed over their allowable range. The optimization problem is non-convex, meaning that there are multiple suboptimal local optima. The optimizer may converge to any of the local optima depending on the initial guesses of the variables. As a result, the solution furnished by local solvers depends on the initial guess used. The multi-start procedure generates multiple local optimal solutions. If a sufficient number of optimization runs are performed, the probability of finding a global optimum is acceptable. Figure 3-3 shows favorable results of the multi-start procedure. The plot represents 42 different optimization runs belonging to a single combination of the bleeds' extraction position. The combination of bleeds' extraction positions in this plot is the one which resulted in the highest maximum objective function value of its multi-start runs. The runs are plotted by descending order of the obtained objective function value, efficiency based on the Lower Heating Value (LHV) of coal. It is evident that there are several suboptimal local optima. Since multiple initial guesses converged very closely to 34.46% efficiency, it suggests that the global optimum has been found. However, no optimality guarantees can be given. Other extraction positions, combinations of integer variables, also experience a similar structure signifying the high non-convexity of the problem and the importance of (heuristic or deterministic) global optimization technique.

3.5 Active Constraint Optimization

In some cases it can be shown that at optimal conditions an inequality constraint is active. In that case and assuming that a variable affects the constraints significantly, the pair of constraint and variable, can be combined in a design specification. The variable can then be explicitly manipulated at the simulation level to obtain the desired constraint value. The advantages of this manipulation include reducing constraint violations in the optimization, simulation violations and fatal errors, and the
Figure 3-3: Favorable solutions of the multi-start optimization runs for the optimum value of integer variables plotted in decreasing order of the objective function.

optimization problem size. Some constraints enforce practical or economical operating limits which are a subset of physical operation limits e.g., heat exchangers have a positive MITA which is strictly greater than zero, where temperature cross over between the hot and cold streams occur. For variable values that result in a violation of such constraints, typically a simulation failure also occurs. Since the optimizer has no explicit information about the constraints, it invariably selects such variable values during the optimization iterations. Adding suitable design specifications avoids these violations in the first place. The design specifications are constructed using physical insight, e.g., decrease the heat duty in the heat exchanger to avoid cross over. Avoiding such failures is particularly important in AspenPlus since they result in termination. Another advantage of explicitly activating the constraint is avoiding some suboptimal solution points. Note however, that activating the constraint may be suboptimal during the iterations of the optimizer but is optimal at the final converged result. Explicitly accounting for each sub-bleed could be viewed as an active constraint optimization, so one option is to activate all sub-bleeds and add a constraint for each bleed. The constraint would then require that the sum of all the multiplications of two sub-bleeds' flowrates to be identically zero. Such a constraint, which
would be required for each bleed, is highly nonlinear and very difficult to satisfy, so explicit enumeration guarantees the required single sub-bleed per bleed constraint in a much simpler and direct approach. Activating design specifications also has some disadvantages such as more expensive function evaluations for the optimizers and potential convergence complications or increase number of total iterations. The proposed procedure contradicts some recommendations in the literature. For instance, in the recent excellent treatment of of chemical plant optimization it is recommended to do optimization and design specifications simultaneously, [6]. However, for the problem at hand the design specifications helped optimization significantly.

In order to reduce the complexity of the optimization problem, four variables and an equal number of constraints are eliminated and replaced by design specifications at the simulation level. The four pairs (constraint/variable) are:

1. MITA.RHE/T.FG.RHE. It is favorable to reach the constraint lower limit for any operating condition (i.e., for any value of the other optimization variables). The smaller the temperature approach in the RHE the lower the exit temperature of the condensing flue gas, which means more latent and sensible energy is transferred to the working fluid. Moreover, the compression requirement of the CSU is lowered due to a lower flue gas inlet temperature.

2. MITA.HRSG/M.FW.Main. Increasing the feedwater main flowrate in the HRSG increases the power output of the cycle while decreasing the temperature approach between the hot and cold streams. Therefore, the HRSG MITA is maintained at its lower limit in its respective design specification by varying the feedwater flowrate. The optimization of the bleeds’ variables and the regeneration process changes the temperature of the feedwater entering the HRSG (FW-HR-in), as discussed in Section 4.3, so the feed water main flowrate is adjusted accordingly by this design specification for optimum performance.

3. MITA.FWH(1 & 2)/ Q.FWH(1 & 2). For any bleed extraction conditions, increasing the duty transferred from the hot bleed to the colder feedwater decreases the MITA while providing more heat regeneration and causing a larger increase
in the feedwater temperature. In other words, a bleed with a certain flowrate and extraction pressure gives the same regeneration effect as that of a lower energy cost bleed (lower flowrate and/or lower extraction pressure) if the latter has a smaller MITA in the feedwater heater. Therefore, for a fixed extraction stream it is always favorable for the cycle to have the feedwater MITA equal to the lower bound of the constraint. For a more formal discussion see [21], where a new criterion for optimum operation is established.

Alternatively using the smallest MITA allowed can be viewed as a minimization of entropy generation within the heat exchanger. However, due to coupling between units, minimal entropy generation in a given component does not necessarily imply optimal performance.
Chapter 4

Results and Analysis

Pressurized OCC provides advantages over atmospheric OCC with CCS [7, 13], but in order to utilize its benefits and target its limitations with future advancements it is vital to know the influencing parameters and the behavior of the different sections of the cycle. Multi-variable optimization of the cycle, like the one performed here, not only results in favorable operating conditions and improvement in efficiency, but it also provides valuable insight into the aspects affecting the cycle and the reasons behind that improvement. The constant heat transfer coefficient approach, described by Equation (2.12), is used to account for the pressure drop in the HRSG.

4.1 General Results

Performing multi-variable optimization with multi-start runs results in favorable solutions that cannot be achieved by a single variable parametric analysis. To understand the system's behavior and response to the pressurization process, the cycle is monitored at its optimum operating conditions over a range of combustor pressures. Essentially a parametric NLP, [3], is approximated by discretization. First multistart optimization is performed for all variables including pressure. Then, the optimal solution among all runs is taken as an initial guess for the optimization with all variables except for pressure, which is incrementally varied. The initial guesses of each new pressure run are the converged results of the preceding one. Table 4.1
reports the values of optimization and some dependent simulation variables for the optimum solution found. Figure 4-1 shows the results of the plants efficiency versus pressure at optimum operating conditions based on the LHV. A maximum efficiency of 34.48%LHV (33.14%HHV) is achieved at an operating pressure in the range of 3.75 to 6.25 bar, an improvement of 0.82% based on LHV (0.79% HHV) over the 10 bar basecase design. Thus the multi-variable optimization results in both higher efficiency and lower capital cost due to the significantly lower operating pressure. The case studies of pressurized OCC presented in some literature operating at very high pressures, 80 bar for [7, 22], do not account for irreversibilities and losses. In particular, they don’t account for the penalty of increasing pressure drop with increasing operating pressure that accompanies a realistic behavior without an increase in capital cost. The initial oxygen stream is thus directly compressed to the high pressure required for the sequestration of the CO₂ rich flue gas. In multi-variable optimization, it is worth noting that the efficiency is relatively insensitive to pressure around the optimum. This behavior has favorable implications. First, it suggests that in the optimum range the system is insensitive to fluctuations and accidental or unavoidable variations in the operating conditions like part load operations and changes in coal batches or types. Second, it means that it is possible to take practical, design, economical, and technological considerations into account without sacrificing performance, e.g., pipes and combustor pressure limits, components size and capital cost, etc. Third, it signifies that approximations and inaccuracies in the equations used or in the modeling procedure do not significantly alter the favorable solutions or mask the optimum performance. Finally, it shows that it might be possible for part load operation not to have a big difference in the optimal operating conditions. It is worth noting that the high pressure FWH is a a HARP, Heater Above the Re-heat Point. This is thermodynamically favorable especially in supercritical cycles as expected. However, recall that the reheat pressure was not included in optimization and it’s current extraction is not considered to be at its optimum.

Figure 4-1 also plots the efficiency of the basecase pressure sensitivity analysis versus the operating pressure, similar to that performed in [13]. For consistency with
the optimization considered herein, the sensitivity is repeated with i) more accurate physical property methods for the acid and water condensation in the flue gas, ii) more accurate pressure drop calculations in the HRSG and the recirculation pipes, and iii) design specifications resulting in constraint satisfaction and improved performance. Both cascading and non-cascading bleed designs are investigated for the single variable sensitivity analysis with the latter resulting in a minor but definite improvement at every operating pressure, on the order of $10^{-4}$. The multi-variable optimum operating conditions of 3.75-6.25 bar achieves a 0.58% (0.55%) points higher efficiency than the 4.75 bar favored operation of the pressure only sensitivity study based on the LHV (HHV). The improvement is even bigger, 3.18%(3.05%), when compared to atmospheric operation. To understand these responses and the reasons behind them it is required to break down the cycle and analyze the different sections.
Pressurized OCC requires an ASU that delivers the oxygen oxidizer stream at elevated pressures, a CSU that compresses the carbon dioxide stream for purification and sequestration, and blowers or fans that compensate for the pressure drops of the recycled flue gas. These units require power from the Rankine cycle so it is important to understand their behavior.

With increasing operating pressure the gas compression power requirements shift from the CSU to the ASU, as seen in Figure 4-2, however, they do not change in equal amounts. Initially the combined power requirement decreases as the CSU power falls rapidly for three main reasons: First, with increasing operating pressure, the pressure ratio across the first CSU compressor required to raise the flue gas pressure to the pressure of the first purification stage decreases. Second, as explained later in
Section 4.4, the temperature of the flue gas exiting the Acid Condenser decreases, rapidly at first, thus flue gas requires less compression work. Third, also mentioned in Section 4.4, the amount of condensed water vapor increases, also rapidly at first, with increasing operating pressure, thus decreasing the flowrate at the stream entering the first CO$_2$ sequestration compressor. Moreover, the intercooling to 63°C of the two stage oxygen compressor leads to a relatively slow rise in the power required by the ASU compression. However, as the operating pressure further increases, the ASU power increase becomes more significant than the CSU power decrease. The CSU is formed of multistage intercooled compression processes between stages of fixed operating conditions, both in temperature and pressure, over a relatively large pressure range. The change in the flue gas pressure only affects the first compression process, and this effect becomes less significant at larger operating pressures. Moreover, a higher operation pressure is associated with a higher pressure drop of the stream entering the CSU, equal to that of the HRSG pressure drop which increases with increasing operation pressure as later seen in Figure 4-3-a, reducing the savings in the CSU compression power. Also, the temperature of the flue gas at the exit of the RHE levels off at 36.9°C starting from a pressure of 3.5 bar as explained in Section 4.4, which leads to additional reductions in the CSU power savings. On the other hand, the increase in pressure ratio across the oxygen compressor that accompanies higher operating pressure causes a significant increase in the consumed power leading to an overall increase in the combined ASU and CSU power for operating pressures above around 4.25 bar.

To compensate for the flue gas pressure losses, as discussed in Chapter 2, and maintain the proper gas recycling, a fan is installed at the end of each of the two recirculation pipes. Within the ranges evaluated here, the fans’ pressure ratio and thus the power required are slightly lower when they are installed at the duct’s end than when installed at the duct’s inlet mainly due to the density effect on the pressure drop of the recirculation pipes. Figure 4-3-a shows the value of the three pressure drops – the HRSG, the primary recirculation pipe, and the secondary recirculation pipe – versus the operating pressure at optimum cycle conditions. The HRSG pressure loss
increases with increasing operating pressure and that is expected from the limited heat exchanger surface area required, and obvious from equation (2.12). The primary recirculation pipe causes a relatively high pressure drop at atmospheric operating condition due to the very high velocity of flue gas resulting from the low gas density and the upper bound on the diameter. As pressure increases so does the density, therefore, the velocity and thus the pressure drop in the primary recirculation pipe decrease. However, with higher operating pressures, the pressure drop starts to increase due to the lower bound on velocity which forces a smaller diameter. This also applies to the secondary recirculation pipe and explains the rise in its pressure drop. The fans’ compression power is plotted in Figure 4-3-b, where the initial decrease in power requirement is due to the fast decrease of pressure losses in the primary recirculation pipe.

Figure 4-3: Flue gas pressure drops(a), and Fans power requirement(b) versus operating pressure at optimum conditions
Finally, Figure 4-4 shows the total gas compression power and the interesting initial drop in the total compression power requirements. This graph suggests that even without adjusting the power cycle to incorporate all the advantages of the pressurized process, e.g., flue gas recovery in the RHE, the pressurized OCC process is favorable over the atmospheric process at an operating pressure of around 3.5 bar where gas compression is minimal. Note that removing the RHE would require a new optimization study to determine the optimum operating conditions in such a cycle configuration. At an operating pressure in the range of 3.75-6.25 bar, where the optimum performance is achieved, the total compression power is still lower than that required for an atmospheric OCC for CCS.

Note that the fans' power requirements also depend on the amount of flue gas recycled which is a complex function of the temperature of the Cool-Gas exiting the HRSG and the amount of compression power (ASU and fans) put into the flue gas. Both aspects are dependent on several optimization and state variables and will be discussed in detail later in Sections 4.3 & 4.5.

As a final remark, it is seen in Figure 4-3-a that at low operating pressures the pressure drop associated with the primary recycled flue gas is significantly higher than that of the secondary recycling and the HRSG pressure drop. As the primary recycling pressure drop initially decreases with increasing operating pressure (while the value of the two other pressure drops increase), the fan compression power decreases signifying that indeed the primary recycling pressure drop dominates the fan power requirements. Recalling that the combustion temperature is not necessarily limited at 1550°C and can go higher if the combustor can withstand such conditions, the primary recycling flowrate can be decreased and thus decreasing the pressure drop and power requirement associated with it. This would require a larger secondary flowrate to maintain the Hot-Gas temperature at 800°C adding to its power demand, but overall causes a decrease in the fans compression power, particularly at low operating pressures. The efficiency of the cycle and the optimum solution may be affected when adding the combustion temperature as a variable. Although since there are a lot of practical, design, and technological constraints that tightly bound the combus-
Figure 4-4: Total gas compression power requirement versus operating pressure at optimum conditions
tion temperature, the performance is not expected to change much. This point was mentioned for sake of completion and not modeled in the current work.

4.3 Temperature of Cooled Flue Gas

The cold side of the HRSG – hot stream exit and cold stream inlet – is subjected to temperature constraints guarding against acid condensation which should only occur in the Acid Condenser/RHE. The temperature of the flue gas exiting the HRSG (Cool-Gas) should be at least 20°C above the acid condensation temperature, and the temperature of the feedwater entering the HRSG (FW-HRSG-in) should be at least 5°C above the acid condensation temperature. Optimization results in a counterintuitive high value for the Cool-Gas temperature. It would seem that a lower temperature for the Cool-Gas is favorable since more thermal energy would be transferred to the high temperature section of the Rankine cycle instead of the lower temperature at the Acid Condenser level. For the majority of the multi-start runs, including all the runs resulting in the highly favorable solutions, as well as the runs of the pressure parametric optimization (solid curve of Figure 4-1), Cool-Gas has a temperature of around 300°C or higher, which is significantly above the acid condensation temperature and the resulting minimum allowed temperatures (180-270°C), see also [10] for the pressure dependence of the acid dew point. The same is observed with the temperature of FW-HRSG-in. Figure 4-5 plots the acid condensation temperature versus operating pressure on primary x-axis and flue gas pressure on secondary x-axis. The flue gas pressure in the RHE is lower than the combustor operating pressure by the amount of the HRSG pressure drop which is also a function of the operating pressure. Acid condensation temperature increases with increasing operating pressure but remains low relative to the optimum temperature of the Cool-Gas and the FW-HRSG-in which are also depicted on the same figure and seem independent to the operating pressure. The high temperature of the Cool-Gas ensures that the temperature of Comb-Gas-in satisfies the inequality constraint associated to it. The difference between the temperature of the Cool-Gas and FW-HRSG-in seems to be a constant as will be explained
Figure 4-5: Acid condensation temperature and water dew point in flue gas, and temperature of constrained streams versus operating pressure (on bottom) and flue gas pressure (on top)

in the following. With a higher Cool-Gas temperature more thermal energy is carried away by the stream entering the RHE, FG-RHE-in, where this energy is transferred to the low temperature section of the Rankine Cycle. Note that the mass flowrate of the FG-RHE-in stream is constant at any operating condition and equal to the total mass entering the cycle, 120.4kg/s (oxidizer stream, slurry mixture minus the separated slag and ash, and atomizer stream), but the recycled flue gas mass flowrate is dependent on the Cool-Gas temperature. A larger temperature of Cool-Gas requires more internal recirculation in order to dilute the combustion mixture and control the temperature of the flue gas entering the HRSG (Hot-Gas). More recycling also results in a larger pressure drop and an increase in the recirculation fan power requirement to compensate for this larger loss of the now larger flowrate.
Although a hotter Cool-Gas transfers more thermal energy to the low temperature section of the Rankine cycle and leads to larger fan power requirements, optimization results in a high value of that stream's temperature for any operating pressure. The apparent contradiction is resolved after inspecting the temperature of FW-HRSG-in, the flowrate of the FW-HRSG-in or through the turbine expansion stages, and the flowrate of the flue gas through the HRSG. Due to the optimization of the Rankine cycle and the heat regeneration process, the temperature of FW-HRSG-in can reach higher values, above 290°C instead of the 260°C of the basecase. Recall that the temperature of the supercritical feedwater at the exit of the HRSG is fixed at 600°C, so the temperature rise of the feedwater in the HRSG is now smaller. This translates in the ability to circulate a larger amount of feedwater through the HRSG and through the turbine expansion stages producing a larger power output for the same thermal input as shown by the fact that the feedwater flowrate increases from 269.0kg/s in the basecase to 295.3kg/s in the optimized run. Note that the reheat stream is also entering the HRSG but its inlet temperature and temperature rise are invariant as explained in Section 3.3.1.

Second law arguments can also explain the reasons behind this preferred behavior. The optimized regeneration allows for a larger FW-HRSG-in temperature and thus a smaller feedwater temperature rise across the HRSG. This results in a smaller temperature drop of the hot stream in the HRSG and thus a higher Cool-Gas temperature. With a hotter Cool-Gas, flue gas recirculation requirements increase in order to control the critical temperatures and the flue gas flowrate in the HRSG increases from 1040kg/s in the basecase to 1111kg/s in the optimized run. Now whether we look at the HRSG flue gas or the HRSG feedwater, and referring to the second-law, we find that each stream has a larger flowrate with a larger average temperature. This signifies that the thermal energy transfer to the Rankine cycle occurs at a higher effective temperature reducing the irreversibility in that section. The irreversibility reduction in the HRSG due to the increase in the average temperature of the high temperature section (i.e., due to the increase in the Cool-Gas temperature) is larger than the additional irreversibility caused by transferring a small portion of the thermal energy.
from the HRSG to the RHE by the hotter FG-RHE-in stream.

The optimization process gives the insight that a larger Cool-Gas temperature is more favorable independent of the operating pressure, but the stream temperature chosen requires further explanation. With larger temperature of the Cool-Gas and larger recirculation flowrates, the pressure drop across the recirculation pipes increase which means that the fans require more power to recover the larger pressure drop for the larger amount of recycled flue gas. Moreover, the regeneration process might also be a limiting factor. Therefore, including an additional high pressure FWH to provide larger regeneration could result in a higher temperature of FW-HRSG-in and thus a higher temperature of Cool-Gas. In other words, there are competing aspects with higher Cool-Gas temperature: on one hand there is an increase in power production due to a larger feedwater flow rate and higher effective temperature for the high temperature section, and on the other hand there are the additional irriversibility created at the RHE, higher fan compression power requirements, and probably a lower regeneration efficiency with the current assembly. The limiting factor could be determined by adding a third high pressure feedwater heater and re-optimizing for the new flowsheet but this is beyond the scope of this work. The complex interactions would not have been understood without a complete simultaneous multi-variable optimization process.

It is interesting to consider the Cool-Gas temperature in the base-case without optimization. In that case increasing the temperature of the Cool-Gas requires decreasing the main feedwater flowrate. However, this results in a completely different behavior. The flowrate through the turbines decreases and so does the power output and cycle efficiency. The contradicting results show the importance of simultaneous multi-variable optimization. Clearly a sensitivity assessment of this section results in an incorrect interpretation of the behavior.
4.4 Flue Gas Recovery Heat Exchanger

Water vapor is a major component in the flue gas, with a molar fraction close to 0.5, and holds significant amount of thermal energy which can be recovered at the level of the RHE. Recall that a large amount of H$_2$O is introduced to the combustion process, coal water slurry, atomizer stream, and more is produced by combustion. Figure 4-6 plots the total thermal energy recovered and the amount of condensed water in the RHE versus the operating pressure at optimum conditions. Both curves are monotonically increasing as a function of pressure but almost constant at pressures above approximately 3.5 bar, which validates with [22] where it is reported that 97% of recovery in the RHE is obtained at a relatively low pressure of 3.5 bar although their case study with no pressure losses is performed at 80 bar. The small fluctuations in the recovered thermal energy beyond 3.5 bar are due to the fluctuations in the temperature of Cool-Gas, however, they are a small percentage of the actual recovery and doesn’t mask the characteristic behavior of the system. Figure 4-5 also plots the water vapor condensation temperature in the flue gas versus the Combustor operating pressure on the primary x-axis and the flue gas pressure on the secondary x-axis. As the operating pressure increases so does the condensation temperature allowing earlier condensation of water vapor in the flue gas.

Water vapor in the flue gas holds a significant amount of latent energy which is transferred during condensation at temperatures lower than the water vapor dew point. As explained in Sections 4.3 & 4.5, the flue gas entering the RHE/Acid Condenser holds almost equal amounts of thermal energy at any operating pressure. The overall behavior is seen clearly in Figure 4-7 which plots the flue gas and feedwater temperature profiles within the RHE for different operating pressures at optimum operating conditions. This plot covers the region of the RHE where acid condensation in flue gas starts all the way to the RHE’s cold end, and can be used as a reference for the following discussion. A low pressure flue gas has a low water dew point, thus the thermal energy available in that low pressure gas as it condenses is more than sufficient to increase the feedwater temperature from the latter’s inlet of 29.5°C to
Figure 4-6: Thermal energy recovered and water condensed in RHE versus operating pressure at optimum conditions
the flue gas dew point (minus the MITA specification), and as a result encountering
the pinch at that very same point. The excess thermal energy in the flue gas is car-
ried away as the latter leaves the heat exchanger with a relatively high temperature
and high water vapor molar fraction. With a larger operating pressure, the water
dew point increases, so the thermal energy, both latent and sensible, required by the
condensing flue gas to raise the feedwater temperature up to the flue gas dew point
increases. This causes the flue gas to exit with a lower temperature and a smaller
vapor molar fraction. The advantages further propagate to the CSU since a lower
flue gas temperature and a lower water content in the flue gas (lower flowrate of flue
gas), reduces the compression requirements of the CSU’s first stage compressor.

At a pressure of approximately 3.5 bar the flue gas at the exit of the RHE en-
counters the pinch at the cold end of the RHE too. Beyond that operating pressure
the temperature of flue gas as it exits the RHE is constant at 36.6°C. Beyond an
operating pressure of around 3.5 bar the pinch is no longer encountered at the dew
point of the flue gas; this is because the amount of latent and sensible thermal energy
available in the condensing section of the gas, as it cools from the dew point temper-
ature to the now constant exit temperature of 29.5°C, is not sufficient to raise the
feedwater temperature up to that level. This is seen in the temperature profiles of
the high pressure flue gas in Figure 4-7 where the flue gas temperature at the point of
condensation, start of the nonlinear region, is higher than the feedwater temperature
at the same section. The non-condensing section of the flue gas, which increases de-
creasing lower operating pressure, transfers only sensible thermal energy and does not
add any advantages over the higher operating pressure regimes since the condensing
section of the latter involves both sensible and latent thermal energy. Finally, we can
see that although the amount of thermal energy carried by the gas as it enters the
RHE is more or less constant, the operating pressure dictates the amount that can
be recovered. One could also say that the availability of the high pressure flue gas is
larger since latent heat is transfered at a higher temperature increasing the average
or effective temperature of energy transfer into the Rankine cycle. This is analogous
to saying that the feedwater temperature as it exits the RHE is higher. The section
of the flue gas temperature profile above the water vapor dew point is almost linear and parallel at any operating pressure because the amount of acids present in the flue gas is small with regards to their influence on the enthalpy of the stream or the temperature profile.

Increasing the pressure of the flue gas results in a smaller slope of the feedwater temperature profile due to the increase in the feedwater flowrate through the RHE as a result of the increased thermal recovery. When the pinch is reached at the outlet of the RHE, at a pressure of 3.5 bar, water condensation and thus recovery from the RHE is constant. Note that the flowrate as a function of pressure increases beyond 3.5 bar due to the behavior of the HRSG and the recirculating sections described next in Section 4.5.

The advantage of increasing the main feedwater flowrate is not limited to the increase in the expansion line flowrate and increase in turbines power output. With increasing feedwater flowrate within the RHE, the pinch point restriction is alleviated and the amount of thermal energy required to raise the feedwater temperature from its inlet temperature to the water dew point temperature of the flue gas increases. This means that a given low pressure flue gas can transfer more thermal energy to the feedwater if the latter has a larger flowrate. Thus, the operating pressure at which thermal recovery levels off and reaches its maximum value decreases. Therefore, the maximum recovery coexists within a region of lower compression power requirements.

As a final note, notice that although for large operating pressure the flue gas temperature at the outlet of the RHE does not change as it encounters the pinch and the duty recovered does not increase in any significant amount, the temperature difference between the flue gas and the feed water is at every point larger with increasing pressure signifying smaller area requirement and a less costly RHE. Taking economic optimization into consideration, this effect could play a role in favoring a slightly higher pressure than the one leading to optimal performance in order to reduce the capital, operation, and maintenance costs of the RHE.
Figure 4-7: Temperature profile of the streams in the RHE versus the heat duty transferred for different operating pressures. Only a section of the RHE is shown ranging from the point where acids start to condense till the cold end.
4.5 HRSG Analysis

The behavior of the Cool-Gas temperature, Section 4.3, motivated taking a closer look at the HRSG and the thermal energy transfer process. Figure 4-8 plots the thermal energy transferred from the flue gas to the feedwater in the HRSG as a function of pressure at optimum conditions and shows an interesting behavior. Surprisingly, the thermal energy transfer has a pronounced minimum at around 3 bar. At any operating pressure, the FG-RHE-in (which has exactly the same intensive properties as those of the Cool-Gas) going from the HRSG to the RHE has constant flowrate, the same species concentration, and almost the same temperature (see Section 4.3). Moreover, the effect of pressure on the FG-RHE-in enthalpy is negligible especially compared to the large variations in the HRSG thermal energy transfer. Thus, the dependence of transferred energy as a function of pressure requires explanation.

Figure 4-9 shows a control volume around a section of the flue gas cycle. An energy balance explains the reason for the variation of the HRSG thermal energy transfer. The enthalpy flow into the control volume by the low pressure $O_2$ stream and the coal water slurry stream are constant for any operating condition. The enthalpy flow out of the control volume by the slag stream is also fixed due to the fixed combustion temperature and coal specifications. The enthalpy outflow by the FG-RHE-in is almost invariant as discussed above and seen in Section 4.3 and Figure 4-5. Also, as will be discussed in Section 4.6.1, the combustor duty ($\dot{Q}_{\text{Comb}}$) is always set to the lower bound by the optimizer and thus is independent of the operating pressure. Therefore, at steady state, the variation in the fan and the Oxygen compressor's work requirement accompanying the change in the operation pressure results in a change in the thermal energy transfer across the HRSG. Neglecting the small variations in the temperature of the FG-RHE-in or the effect of the gas pressure on its enthalpy, the change in the HRSG thermal energy transfer would be equal to the change in the sum of the fan work requirement and the oxygen enthalpy rise. The oxygen enthalpy rise is equal to the oxygen compressor work minus the thermal energy rejected by the compressor's intercooling.
Figure 4-8: Thermal energy transfer in the HRSG versus operating pressure at optimum operating conditions
Figure 4-9: Control volume explaining the variation in the HRSG transferred thermal energy
Figure 4-10: Compression Enthalpy Rise (CER), i.e., the sum of the fans compression power and enthalpy increase of the oxygen oxidizer stream, versus operating pressure at optimum conditions.
Figure 4-10 plots the fan compression power and the enthalpy rise of the oxygen stream (oxidizer stream) as it crosses the oxygen compressor of the ASU versus the operating pressure at optimum conditions. Their sum is also plotted on the same figure and is referred to as Compression Enthalpy Rise (CER) in the rest of the text. The enthalpy change of the oxygen stream is more relevant than the work of the oxygen compressor due to the thermal rejection in the intercooler. In Figure 4-10 the fans’ compression requirement initially decrease, as explained in Section 4.2, which decreases the CER despite the increase in the $O_2$ enthalpy rise. This explains the initial decrease in the thermal energy transfer into the HRSG and then its increase beyond an operating pressure of 3.0 bar. Now subtracting the CER from the HRSG thermal energy transferred we obtain the curve in Figure 4-11 which is almost flat reflecting the validity of the above analysis and accuracy of the approximations made. Actually, $Q_{HRSG}$ minus CER shown in Figure 4-11 is around 83.5% of the total LHV of the fuel (80.2% of its HHV). The rest is leaving with the exiting flue gas and combustor duty ($\dot{Q}_{\text{Comb}}$). This shows that the fuel thermal energy available at the low temperature section is almost constant and that the RHE is recovering different portions of that energy depending on the operating condition. This also stresses on the importance of multi-variable optimization in enhancing the recovery process of that fixed amount of energy. Note that with the increase of operating pressure the pressure drop in HRSG and recirculation pipes increase, thus requiring more power from the recirculating fans. Therefore, at higher operating pressures the recirculating stream carries more enthalpy. Similarly is the case for the oxygen stream. As a result, more dilution is required to maintain the $800^\circ$C temperature at the inlet of the HRSG. Which explains the reason behind the increase in the flowrate of the flue gas through the HRSG as mentioned in Section 2.4.

The CER contributes in transferring additional thermal energy to the Rankine cycle thus producing some additional power output which is referred to as Work of Compression Enthalpy Rise (WCER) in this document. To accurately assess the gas compression requirements previously presented in Section 4.2 and in particular Figure 4-4, it is important to see how much WCER these expensive compression
Figure 4-11: Effect of CER, caused by the gas compression processes, on the thermal energy transferred in the HRSG at optimum operating conditions.
processes provide. As explained above and seen in Figure 4-11, the variations in the HRSG’s thermal power transfer is almost identical to the CER; therefore, the CER is considered to be primarily transferred at the high temperature section of the cycle. Consequently, WCER is related to CER by the efficiency of that section only and not the efficiency of the total Rankine cycle. To obtain an estimate of the efficiency of the high temperature section, the operating conditions of each of the optimized pressure runs (previously presented in Figure 4-1) are evaluated while having a common thermal energy input to the low temperature section of the power cycle, meaning that each optimized pressure run is re-executed with a fixed Combustor duty ($Q_{\text{Comb}}$, set to the lower bound which is the value chosen by the optimizer in the first place) and more significantly, a common and fixed RHE flue gas recovery set to a value of zero. For the zero-recovery runs the Rankine net power output is due to the single thermal energy source, the HRSG. Therefore, the efficiency of the zero-recovery cycle at each operating pressure is representative to the efficiency of the HRSG in the optimized runs at the same operating pressure, i.e.,

$$\eta_{\text{HRSG}}(p) = \frac{\dot{W}_{\text{NET-Rankine}}(P)}{\dot{Q}_{\text{HRSG}}(P)} = \frac{\dot{W}_{\text{NET-Rankine}}(P)}{\dot{W}_{\text{Coal}}(P)} = \frac{\dot{W}_{\text{Coal}}(P)}{\dot{Q}_{\text{HRSG}}(P)}$$

The obtained efficiency is then multiplied by the CER to get a rough estimate of the resultant WCER.

The WCER is a small compensation for the power required to compress the gas. Figure 4-12 shows the gas compression breakdown similar to that seen in Figure 4-4 with one additional curve labeled the effective compression power, being the total compression power minus the WCER. The effective compression requirement is flat compared to the total actual compression power. An even flatter curve is expected for optimal integration of the thermal energy of the intercooling stages of both the ASU and CSU.

Figure 4-13 plots two curves: the first is the net Rankine cycle power output and
Figure 4-12: Total and effective gas compression power required versus operating pressure at optimum conditions.
the second is the net Rankine power output minus the WCER versus the operating pressure at optimum conditions. The second curve, labeled effective net Rankine power, roughly represents the effect of the RHE on the cycle as a function of pressure at optimum conditions without the contribution of the CER. With increasing pressure the recovered thermal energy at the RHE increases, therefore increasing the Rankine cycle net power output, however, at pressures higher than around 3.5 bar the net power levels-off. This agrees with the results of Section 4.4 and Figures 4-6 and 4-7 where flue gas thermal recovery levels-off at a pressure of 3.5 bar.

The figures and analysis presented here are more representative of the cycle behavior than those seen in Sections 4.1 & 4.2, where both the actual gas compression power requirements and the actual Rankine cycle net power output increase indefinitely. Splitting the power demands and contributions into effective power consumption and
effective power production gives a better idea of the behavior. Understanding this behavior is possible after the observed results of the optimum cycle performance for each operating pressure which is possible with multi-variable optimization. These complex interactions most likely would not have been understood with a simple parametric study.

4.6 Behavior of Other Optimization Variables

The effects of the remaining optimization variables are described next.

4.6.1 Combustor Duty

The Combustor duty, $Q_{\text{Comb}}$, represents heat transfer from the combustion temperature of 1550°C to the low temperature section of the Rankine cycle (140-160°C). This transfer results in large irreversibilities. A smaller heat duty results in a larger enthalpy for the flue gas and thus more heat exchange in the HRSG, which is transferred to the Rankine cycle working fluid at the high temperature section with less irreversibilities. However, the decrease in the value of this variable requires a larger flow of recycled flue gas in order to control the key temperatures, which results in larger fans compression requirements to compensate for the larger pressure drop of the now larger flowrate. Optimization results in low values close to the lower bound of 1MW. This suggests that the decrease in the irreversibilities associated with the heat transfer process dominate over the increase in the irreversibilities associated with the pressure drop; It is worth mentioning that with lower duty transfer the system becomes less sensitive to further decrease in this variable’s value due to the further increase in pressure drop.

In contrast to the multi-variable optimization, a sensitivity analysis seemingly favors high heat duty. Figure 4-14 plots the efficiency of the optimum operation, 5.75bar $\in [3.75-6.25]$ bar, and the efficiency of the basecase operation versus the combustor duty, $Q_{\text{Comb}}$. For the optimum operation, increasing the duty results in an efficiency decrease in accordance to the optimization results. In contrast, for the base-case op-
Figure 4-14: Effective Rankine cycle net power output (Rankine Cycle net power minus WCER, caused by the CER) versus operating pressure at optimum conditions

Operating condition decreasing the duty results in a decrease in the cycle efficiency. This reflects the complex dependence of the objective function on the optimization variables. This observation highlights the importance of multi-variable optimization in unveiling the true system behavior and potential while a single variable optimization would clearly result in a suboptimal solution and false interpretations of the cycle responses. The sensitivity analysis plot of the optimum operation efficiency versus combustor duty in Figure 4-14 should not be used to calculate the exact contribution of this variable to the cycle because the sensitivity analysis performed here has all other variables fixed. The sensitivity analysis should be used for qualitative purposes only.

Adding insulation and refractory material to the combustor in order to limit this transferred duty is possible but not without an increase in capital cost, so it might be worth taking into account additional economic considerations regarding the combustor duty.
4.6.2 Deaerator Pressure

At the optimum solution, the Deaerator pressure, $P_{\text{Deaerator}}$, takes on a value larger than that of the base-case, 13-14 bar as opposed to 10 bar. The Deaerator’s optimum pressure also slight increases with increasing operating pressure. As the operating pressure increases, water in the Deaerator can reach saturation at higher pressures due to the increase in the thermal energy recovery at the RHE, which results in a reduction of irreversibilities from bleed mixing in the Deaerator. Moreover, the power requirement decreases due to the shift of the required load and pressure ratio from the high pressure pump to the low pressure pump. The high pressure pump has a larger flow rate and larger feed inlet temperature (larger specific volume despite its small effect).

4.6.3 Regenerative Bleeds

All bleeds have higher flowrates and extraction pressures than those of the base-case as can be seen in Table 4.1. As discussed in Section 4.3, the optimal regeneration increases the temperature of the feedwater entering the HRSG to its optimal value. Since this temperature was found insensitive to the operating pressure, it is likely that the bleeds’ specifications are insensitive too. In fact the bleeds’ extraction pressure normalized by the deaerator pressure are insensitive to operating pressure. The same holds for the bleeds’ flowrate normalized by the flowrate of feedwater and for the duty across each of the closed feedwater heaters normalized by the total duty across both feedwater heaters. A reasonable explanation is that the optimum regeneration in a cycle requires a specific and fixed contribution from each feedwater heater. Recall the well-known approximate rule of equal enthalpy rise across feedwater heaters [4, 12]. Recall however, that herein reheat and nonidealities are considered and thus the approximate rule is not expected to be a good approximation especially regarding the equal fractional distribution of duty among the feedwater heater. But in essence
the optimal distribution of the regeneration section is a constant and insensitive to the combustor operating pressure. Note that the results of regeneration are analyzed in the normalized form because the flowrate through the system is increasing with increasing operating pressure and the absolute results scale accordingly.
Table 4.1: Key results of the base-case, the pressure only parametric study, and optimization runs

<table>
<thead>
<tr>
<th>Variable</th>
<th>base-case</th>
<th>Pressure-only-variation</th>
<th>Optimization</th>
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<tbody>
<tr>
<td>P_Comb</td>
<td>10bar</td>
<td>4.75bar</td>
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<tr>
<td>Objective Function (LHV)</td>
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<td>34.48%</td>
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<tr>
<td>Q_Comb</td>
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<td>1MW</td>
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<tr>
<td>M_FW_Main</td>
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<td>75.6MW</td>
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</tr>
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<td>262.9°C</td>
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<td>235.0kg/s</td>
<td>235.0kg/s</td>
<td>234.1kg/s</td>
</tr>
<tr>
<td>ΔP_HRSG</td>
<td>0.527bar</td>
<td>0.118bar</td>
<td>0.164bar</td>
</tr>
<tr>
<td>ΔP_pipe primary</td>
<td>0.0649bar</td>
<td>0.068bar</td>
<td>0.066bar</td>
</tr>
<tr>
<td>ΔP_pipe secondary</td>
<td>0.0650bar</td>
<td>0.022bar</td>
<td>0.0253bar</td>
</tr>
<tr>
<td>Prim. recircul.</td>
<td>266.5kg/s</td>
<td>264.6kg/s</td>
<td>278.0kg/s</td>
</tr>
<tr>
<td>pipe flowrate</td>
<td>652.5kg/s</td>
<td>646.5kg/s</td>
<td>712.5kg/s</td>
</tr>
</tbody>
</table>

For the base-case and pressure only variation FWH2 has cascading bleeds
Chapter 5

Water Addition

The temperature control processes necessitate a large amount of flue gas recycling which results in high compression power for the fans. Adding water to the Combustor and the Temperature Controller dilutes the mixtures and reduces the amount of recycled flue gas and the gas pressure drop, which reduces the fans compression requirements. Moreover, given the right operating pressure almost all the water is condensed, so the thermal energy used for evaporating and superheating the added water would still be transferred to the power cycle. Thus, the addition of water to the Combustor and the Temperature Controller is a way to satisfy the temperature limits while lowering the fans’ compression power and having the same net amount of thermal energy transferred to the Rankine cycle. On the other hand, a large portion of the energy absorbed by the added water is transferred at the level of the RHE during water condensation. Water addition reduces the quality of the thermal energy transferred which contributes in reducing the efficiency of the cycle.

Optimization runs are performed with the addition of these two variables; however, their values are set to the lower bound, zero flowrate, by the optimizer. Moreover, when given the chance to further reduce the water addition by manipulating the water content in the coal slurry, the optimizer selected a flowrate lower than the necessary design value of 35.38% by weight of the slurry mixture. Performing an optimization run from the previously found optimum, 5.75 bar, while having slurry water input as a variable results in an operating pressure of 5.73 bar and a slurry water flowrate
of 8.3 kg/s (from 16.5 kg/s) with an efficiency of 34.75% (from 34.48%) based on LHV. Complete assessment and optimum performance requires a new multi-start run which is not performed here due to the impracticality of such operating conditions. The optimum pressure of the single optimization run belongs to the range of optimum operating pressure found in this study; this has favorable implications suggesting that the optimum operation range is insensitive towards changes in coal specifications and coal water content. Although the water content in coal or the resulting amount of water vapor in the flue gas is unlikely to vary by the amount seen here (16.5 kg/s compared to 8.3 kg/s) for a given change in coal type, other factors may affect the process and a proper assessment requires a separate optimization study. In conclusion, the water necessary for technical reasons (coal slurry) is more than the optimal water addition from a thermodynamic limit. The promising finding is that the two give significant but not drastically different performance or operation points.
Chapter 6

Conclusion

Pressurized OCC has an advantage over regular coal combustion with CCS due to the ability to recover a large amount of thermal energy from the high moisture content of the flue gas. Previous literature studies dealing with pressurized OCC showed improvements in performance over the atmospheric operation. Such studies however utilized a single variable sensitivity analysis which does not allow capturing all the complex cycle interactions or the true response of the system with the changes in variables’ values.

In this work, a simultaneous multi-variable optimization was performed for a high fidelity model of a pressurized OCC with CCS. Multi-start runs were also performed to increase the chances of finding a global optimum and its results reflected the presence of several local optima. The optimum solution was found within a range of operating pressure, 3.75-6.25 bar, reflecting a favorable system behavior towards operation fluctuations and/or modeling approximations. Both flue gas pressure losses and thermal energy recovery from the high moisture pressurized flue gas play major roles in dictating the optimum operating conditions. This optimum range was dictated by the concurrence of the minimum compression power and the maximum thermal recovery. This favorable matching was possible due to the simultaneous variables optimization. Moreover, optimizing the regeneration process in the power cycle contributed in enhancing the cycle performance at any operating pressure. Regeneration exhibits an interesting behavior where by it is insensitive to the operating pressure and is al-
most constant for the given parameters of the Rankine cycle, a behavior discussed in literature for simple and ideal cycles.
Appendix A

Sub-bleed Mixing Is Always Non-Optimal

In a cycle with realistic expansion line, sub-bleed mixing is a modeling trick proposed herein to eliminate the need for multiple flowsheets each with a different combination of bleeds' extraction positions. If a perfect global is used, this trick eliminates the need for integer variables or explicit enumeration and facilitates the optimization problem and time requirements for finding the optimum solution. We now argue that a single sub-bleed per is necessary for optimality.

For a given constant but arbitrary regeneration heat duty, $Q_{\text{regen}}$, in a FWH

Suppose that for a given bleed two sub-bleeds are active, namely sub-bleed1 and sub-bleed2 (high and low pressure respectively).

$h_T(P_x)$ is the specific enthalpy of the stream extracted from the steam expansion line at a pressure $P_x$.

$h_{B,o}^l$ is the specific enthalpy of the bleed stream exiting the feedwater heater where it is considered to be in the subcooled region and so the superscript $l$ (liquid) is added.

Consider the work that could have been produced in the turbine from the two sub-bleeds.

$$\dot{W}_{\text{lost}} = \dot{m}_{b,1}(h_T(P_1) - h_{T,o}) + \dot{m}_{b,2}(h_T(P_2) - h_{T,o})$$
Take its derivative with respect to the high pressure $P_1$, for the constant conditions of sub-bleed $2$

$$\frac{d\dot{W}_{\text{lost}}}{dP_1} = \frac{d\dot{m}_{b,1}(h_T(P_1) - h_{T,o}) + \dot{m}_{b,1}}{dP_1} \left|_{P=P_1} \right. \frac{dh_T}{dP_1} \quad (A.1)$$

If $\frac{d\dot{m}_{b,1}}{dP_1} \geq 0$, then $\frac{d\dot{W}_{\text{lost}}}{dP_1} > 0$ as claimed above, so $P_{b,1}$ should decrease to decrease losses. We can now consider when $\frac{d\dot{m}_{b,1}}{dP_1} \leq 0$. The required heating of the feedwater in the FWH is given by:

$$\dot{Q}_{\text{regen}} = \dot{m}_{b,2}(h_T(P_2) - h_{B,o}^l) + \dot{m}_{b,1}(h_T(P_1) - h_{B,o}^l)$$

where $h_{B,o}^l$ is the enthalpy at the outlet of the FWH, calculated at the pressure of the lower pressure sub-bleed. Differentiate both sides with respect to $P_1$:

$$0 = \frac{d\dot{m}_{b,1}}{dP_1}(h_T(P_1) - h_{B,o}^l) + \dot{m}_{b,1} \left|_{P=P_1} \right. \frac{dh_T}{dP_1}$$

and therefore

$$\frac{d\dot{m}_{b,1}}{dP_1}(h_T(P_1) - h_{B,o}^l) = -\dot{m}_{b,1} \left|_{P=P_1} \right. \frac{dh_T}{dP_1} \quad (A.2)$$

The turbine outlet enthalpy can be safely assumed to be greater than the FWH outlet enthalpy because the former is at least within the saturation region closer to the superheat side, while the latter is subcooled liquid, [21] explains this in more details. i.e.,

$$h_{T,o} > h_{B,o}^l$$

and therefore

$$-h_{T,o} < -h_{B,o}^l$$

or

$$h_T(P_1) - h_{T,o} < h_T(P_1) - h_{B,o}^l$$

Since $\frac{d\dot{m}_{b,1}}{dP_1} < 0$ we obtain:

$$\frac{d\dot{m}_{b,1}}{dP_1}(h_T(P_1) - h_{T,o}) > \frac{d\dot{m}_{b,1}}{dP_1}(h_T(P_1) - h_{B,o}^l)$$
and therefore by (A.2)

\[ \frac{d\dot{m}_{b,1}}{dP_1} (h_T(P_1) - h_{T,e}) > -\dot{m}_{b,1} \frac{dh_T}{dP_1} \bigg|_{P=P_1} \]

The last inequality together with (A.1) implies

\[ \frac{dW_{\text{lost}}}{dP_1} > 0 \]

Therefore, the power loss decreases with decreasing sub-bleed1 extraction pressure with the latter having a lower bound equal to the extraction pressure of sub-bleed2. This signifies suboptimal operation for any sub-bleed mixing, and concludes the proof by contraposition. Note that this argument does not imply that low extraction pressures are optimal, but rather that two sub-bleeds giving the required regeneration are suboptimal.

Figure A-1 plots the power output versus the flowrates of two active sub-bleeds from the intermediate pressure stage where sub-bleed1 and sub-bleed2 are the higher and lower pressure sub-bleeds respectively. It can be seen that for a range of flowrates of sub-bleed2 adding flow from sub-bleed1 increases the power output, and that having one active sub-bleed does not result in a larger power output at any operating condition. A larger thermal regeneration (larger \( Q_{\text{regen}} \)) is sometimes preferred over a smaller one even if the former includes irreversible sub-bleed mixing. In other words, if the flowrate of sub-bleed2 is below the optimal flowrate for it's specified extraction pressure, then a nonzero flowrate from sub-bleed1 increases the power output. However, the optimum solution is one with a single bleed at a specific extraction pressure and flowrate, i.e., when the regeneration is attained without irreversible mixing of sub-bleeds.
Figure A-1: Net work output for a combination of sub-bleeds flowrates from the intermediate turbine stages
Bibliography


