

Modeling of Integrated Environmental Control Systems for Coal-Fired Power Plants

Quarterly Progress Report

To

Pittsburgh Energy Technology Center
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From

Center for Energy and Environmental Studies
Carnegie Mellon University
Pittsburgh, Pennsylvania 15213

Prepared by

E.S. Rubin, Principal Investigator

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Nomenclature

English Letter Symbols

| | |
|--|---|
| A_{device} | = area of device (ft^2) |
| C_{category} | = capital charges associated with startup (\$) |
| C_{idx} | = chemical engineering cost index |
| C_o | = molar gas concentration of SO_2 in the fluegas entering the adsorber ($\text{lbmole}/\text{ft}^3$) |
| CF | = capacity factor of power plant (fraction) |
| $\text{DCC}_{\text{device}}$ | = capital cost for device (M\$) |
| $e^{\#}$ | = notation for specifying power of 10. |
| $E_{\text{specie, device, inlet or outlet}}$ | = energy flow rate of specie for the inlet or outlet of the specified device (lbmole/hr) |
| $\text{EC}_{\text{device}}$ | = electricity consumption of the specified device (kW) |
| f_{makeup} | = attrition rate of sorbent (fraction) |
| $f_{\text{specie, wet air}}$ | = amount of specie in ambient moist air (fraction) |
| $f_{\text{Pspecie, device}}$ | = quantity of specie produced in device (fraction) |
| F_{oil} | = constant used to estimate amount of sulfur from oil (fraction) |
| FOC | = fixed operating cost (\$/yr) |
| $G_{\text{device, inlet or outlet}}$ | = gas flow rate for the inlet or outlet of the specified device (ft^3/min) |
| $\hat{h}_{\text{specie, temperature}}$ | = molar enthalpy of species at specified temperature (Btu/lbmole) |
| H | = fluidized bed height in adsorber (ft) |
| $\text{HHV}_{\text{specie}}$ | = higher heating value of specie (Btu/lb) |
| HR | = heat rate of power plant ($\text{kW}\cdot\text{Hr}/\text{MBtu}$) |
| i | = inflation rate (fraction) |
| K_a | = apparent rate constant ($\text{atm}^{-1} \text{sec}^{-1}$) |
| $\text{LMTD}_{\text{device}}$ | = log mean temperature difference of device ($^{\circ}\text{F}$) |
| m_{specie} | = mass flow of species (lbs/hr or tons/hr) |
| $M_{\text{specie, device, inlet or outlet}}$ | = molar flow rate of specie for the inlet or outlet of the specified device (lbmole/hr) |
| MW_g | = gross electrical capacity of power plant (MW) |
| N_t | = initial loading of the active Na on sorbent (lbmole/lb) |
| NOP | = number of operating adsorbers |
| NRD | = number of spare adsorbers |
| $\text{OC}_{\text{catagorie}}$ | = annual operating cost (\$/yr) |
| Q_{device} | = heat load across heat exchanger device (Btu/hr) |
| p | = interest rate (fraction) |
| $P_{\text{device, inlet or outlet}}$ | = pressure of the specified device at inlet or outlet (" water or atm) |
| $\text{RT}_{\text{device}}$ | = residence time of sorbent in device (hours) |
| $T_{\text{specie, device, inlet or outlet}}$ | = temperature of specie for the specified device at inlet or outlet ($^{\circ}\text{F}$) |
| TCC | = total capital cost (\$) |
| TPC | = total plant cost (\$) |
| TPI | = total plant investment (\$) |
| TDC | = total direct cost (\$) |
| TVC | = total operating and maintenance cost, sum of FOC and VOC (\$/yr) |

| | |
|------------------------------|--|
| U_{device} | = universal heat transfer coefficient for device (Btu/hr-ft ² °F) |
| UC_{specie} | = unit cost of specie (\$/unit) |
| U_{specie} | = utilization constant for species in regenerator (fraction) |
| V | = superficial velocity of flue gas through adsorber (ft/sec) |
| VOC | = variable operating cost (\$/yr) |
| W_{Na} | = weight fraction of sodium to sorbent (fraction) |
| X | = mean value of the fractional conversion of the sorbent in the entire adsorber (fraction) |
| $Y_{\text{inlet or outlet}}$ | = molar fraction of SO ₂ in the flue gas (fraction) |

Greek Letter Symbols

| | |
|-------------------------------|--|
| δ_{NO_x} | = fraction of NO _x returned to boiler which is destroyed (fraction) |
| ΔH_{device} | = heat of reaction in device (Btu/hr) |
| $\eta_{\text{specie,device}}$ | = efficiency of device (fraction) |
| λ | = molar stoichiometry of SO ₂ to active sorbent |
| ρ_{sorb} | = bulk density of sorbent (lbs/ft ³) |

Subscripts

| | |
|-------|---|
| 1 | = specifies the first part or half of a device |
| guess | = used to indicate the guess of a value in the interpolating algorithms |
| i | = stands for inlet |
| j,k | = used in sums to specify equipment or species. |
| o | = stands for outlet |
| std | = emission standard for either SO _x or NO _x |

Species:

| | |
|--------|--|
| acid | = sulfuric acid |
| air | = air |
| ash | = ash |
| c | = combustion air for gas burner not including air needed to maintain maximum temperature |
| CD | = carbon dioxide |
| CM | = carbon monoxide |
| CS | = carbon oxide sulfide, COS |
| ex | = excess air for the gas burner needed to maintain temperature |
| H | = hydrogen, H ₂ |
| HS | = hydrogen sulfide, H ₂ S |
| M | = methane, CH ₄ |
| makeup | = makeup sorbent |
| N | = nitrogen, N ₂ |
| NO | = nitrogen oxide, NO |
| ND | = nitrogen dioxide, NO ₂ |
| O | = oxygen, O ₂ |
| st | = steam |
| sorb | = sorbent |
| S | = sulfur, S ₂ |

SC = sulfur compounds, includes COS, H₂S, S₂, SO₂, and SO₃
 SD = sulfur dioxide, SO₂
 SOX = sulfur dioxide and sulfur trioxide
 ST = sulfur trioxide, SO₃
 W = water, H₂O

Equipment:

aph = air preheater
 AD = adsorber
 AH = air heater for sorbent heater
 AP = acid plant
 b = boiler in acid plant
 B = boiler of power plant
 BF = dilution air blower and filter
 CS = catalytic converter contact section
 D = drying tower
 ES = effluent strippers
 GB = gas burner
 GC = gas humidification and cooling tower
 HP = heat recovery preheater
 IC = inlet compressor
 MC = main compressor
 PA = product acid
 R = regenerator
 R&S = regenerator and steam treatment vessel
 s = superheater
 SC = sorbent cooler
 SH = sorbent heater
 SS = strong acid handling system
 STV = steam treatment vessel
 T = interpass and final towers and associated equipment
 WA = weak acid system

Categories for capital and operating cost:

acid = acid plant
 admin = support and administration labor
 credit = income from sale of sulfuric acid
 eng = engineering and home office fees
 gf = general facilities
 inv = inventory capital
 maint-labor = maintenance labor
 maint-matl = maintenance material
 makeup = makeup catalyst due to attrition loss
 marketing = marketing and shipping charges for selling sulfuric acid
 misc = royalty and land charges
 oper = operating labor
 proc = process contingency
 proj = project contingency
 startup = startup charges for one month
 work = working capital

1. Introduction

This is the third quarterly report of DOE Contract No. DE-AC22-87PC79864, entitled "Modeling of Integrated Environmental Control Systems for Coal-Fired Power Plants." This report summarizes accomplishments during the period April 1, 1988 to June 30, 1988. Our efforts during the last quarter focused on, (1) completion of a sulfuric acid plant model (used in conjunction with by-product recovery processes for SO_2/NO_x removal) and, (2) an update the NOXSO process model. Other accomplishments involved revision and expansion of the enthalpy data algorithms used for process energy balances. The sections below present the details of these developments. References are included at the end of each section.

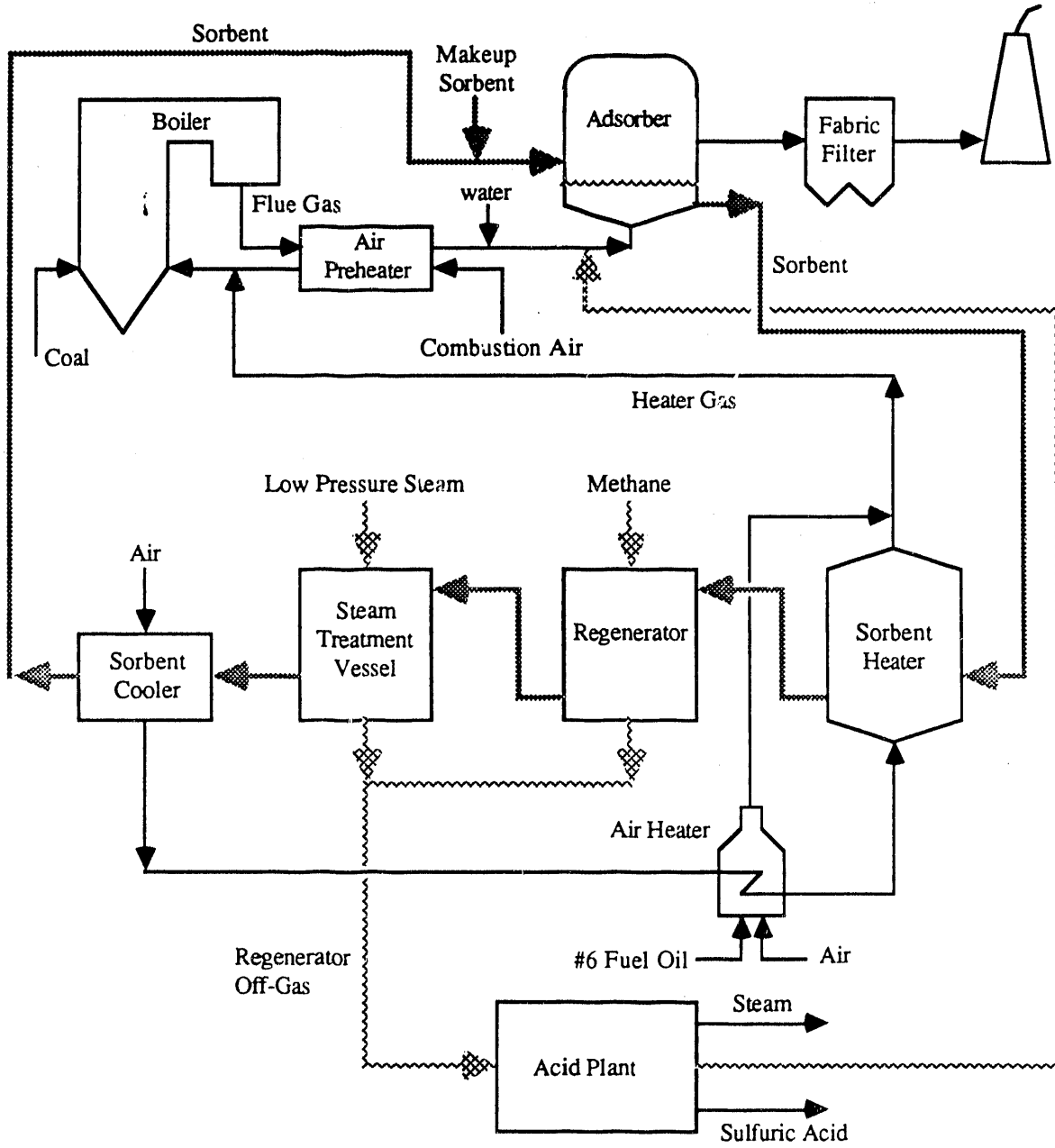
2. NOXSO Process Model

The NOXSO process model incorporated in our integrated modeling framework was originally developed by Barrett [1]. The present NOXSO model is based on designs by NOXSO Corp. [2,3,4,5], and Stearns-Rogers [6]. The design of the process has changed over time to incorporate potential improvements. The current process design for this model is based on a study for EPRI [6], with one modification suggested by NOXSO Corp [7], i.e., using methane as the reducing gas instead of synthesis gas produced from a Texaco Coal Gasification System.

The NOXSO process is intended to remove over 90 percent of the SO_x and NO_x from the flue gas of a coal-fired power plant. The pollutants are adsorbed onto a sodium coated alumina sorbent in a fluidized bed reactor. The sorbent is regenerated producing various sulfur compounds and NO_x . The NO_x and some of the SO_x are returned to the boiler, while the rest of the sulfur compounds are sent either to a sulfuric acid or Claus plant. The NO_x returned to the boiler is expected to partially decompose into nitrogen leading to a steady-state NO_x concentration.

A proposed process diagram is shown in Figure 2-1. There are four major mass flows in the NOXSO process: (1) the sorbent recirculation stream; (2) the regenerator off-gas sent to the acid plant; (3) the sorbent heater gas stream containing NO_x and SO_x returned to the boiler; and, (4) the combustion/flue gas stream. This process diagram differs from the one used for the initial model developed by Barrett [1] in the following ways:

Figure 2-1: NOXSO Process Diagram



- oil is used instead of coal in the sorbent heater
- the cyclone in front of the adsorber has been removed
- methane is used for the reducing gas
- the adsorber by-pass option has been removed.

Figure 2-1 is best examined by examining each major mass flow separately. The first mass flow to examine is the sorbent stream. The sorbent entering the adsorber contains some residual sulfur compounds. The sorbent removes NO_x and SO_x from the flue gas while raising the temperature of the flue gas. Then it enters the sorbent heater, where it releases all the NO_x and about 8 to 10 percent of the SO_x in the sorbent. The sorbent then enters the regenerator where methane (or some other reducing gas) is used to remove additional SO_x in the sorbent. After the regenerator, the sorbent enters the steam treatment vessel where steam is used to removed most of the remaining sulfur compounds. Finally, the sorbent is cooled and makeup sorbent is added before it is returned to the adsorber.

The second major mass stream is the off gas from the regenerator. This gas stream is critical to the cost and performance of the acid plant, since its composition can drastically affect the cost of the sulfur recovery system. Its composition depends upon the type and quantity of reducing gas used and the design of the regenerator and steam treatment vessels. In the latest communications with NOXSO Corp. they have suggested that these two vessels be replaced with a single vessel.

The third major stream is the air stream used to heat and cool the sorbent and to return the NO_x (and some SO_x) to the boiler. Recent tests have indicated that approximately 65% of the NO_x returned to the boiler is decomposed [8]. This air stream also contains a significant amount of oxygen, so it is used to reduce the amount of combustion air entering the air preheater. This gas stream enters the sorbent cooler where it is heated by cooling the sorbent to approximately 210 °F. Then it enters the sorbent heater where it picks up the NO_x and some SO_x . After leaving the sorbent heater it mixes with combustion air and enters the boiler.

The last mass flow is the combustion/flue gas stream. The inlet air passes through the air preheater and picks up the gas stream exiting the sorbent heater. This gas stream contains NO_x and SO_x , as well as the products of combustion from the air heater, plus air used to heat and cool the sorbent. The inlet gas entering the air preheater is reduced in proportion to the amount of

oxygen entering in this stream. The SO_x comes from the sorbent heater and the combustion of #6 fuel oil. This combined gas stream enters the boiler where some of the NO_x decomposes. After the boiler it passes through the air preheater, where it picks up additional air leaking across air preheater. After the air preheater, the flue gas is cooled by adding water. It then enters the adsorber, where most of the NO_x and SO_x are removed by the sorbent. The cleaned flue gas picks up the attrition particles of the sorbent and enters the fabric filter. Here, particulate matter is removed before the gas is vented to the atmosphere.

The adsorption and regeneration chemistry of NO_x and SO_x are explained in detailed in many of the reports cited earlier, so only a brief summary will be given here. SO_x is adsorbed onto both the sodium and alumina substrate and is dependent upon a number of parameters:

- Sorbent flow rate
- Available sodium on sorbent
- Oxygen content of flue gas
- NO_x concentration
- Steam concentration
- Degree of dehydration on the sorbent surface
- Temperature of sorbent

The adsorption of NO_x is dependant upon the temperatures and flow rates of sorbent, SO_x , steam, oxygen, and the type of reducing gas used. It has been found that increasing the temperature decreases NO_x removal, while using methane for regeneration of SO_2 improves the NO_x removal efficiency.

The regeneration of SO_x is a multi-step process. The first step is to heat the sorbent to approximately 1000°F, where approximately 8 - 10% of the sulfur compounds and all the NO_x are released. The next step is to treat the sorbent with a reducing gas, which releases COS, H_2S , S_2 , and SO_2 , which are sent to the acid plant. Finally the sorbent is treated with steam to convert as many of the sulfites to H_2S as possible. NO_x is regenerated by heating the sorbent to 1000°F.

2.1 Performance Model

The primary purpose of the process performance model is to characterizes the major flow rates defined in the previous section and to predict the NO_x and SO_x removal efficiencies in the adsorber. The NOXSO process recycles some of the NO_x and SO_2 removed by the adsorber,

which requires the adsorber to have a removal efficiency higher than the efficiency required by the emission standards. The recycled SO_2 comes from the sorbent heater and the acid plant, while another source of SO_2 is the air heater. The NO_x and SO_2 removal efficiencies are also linked. In the previous model, an equation was developed relating the NO_x and SO_2 removal efficiencies based on the adsorber temperature. For all the NOXSO designs proposed, the adsorber temperature has remained approximately the same, 250°F. At this temperature the NO_x and SO_2 removal efficiencies are the same. Therefore, our current model assumes a bed temperature of 250°F with equal removal efficiencies for SO_2 and NO_x .

The following procedure is then used to determine the sorbent flow rate:

- The required SO_2 removal efficiency in the adsorber needed to meet the emission standard is determined which includes the effects of recycled SO_2 , and SO_2 from the air heater.
- The required NO_x removal efficiency in the adsorber needed to meet the emission standard is determined which includes the effects of recycled NO_x and the NO_x 'destroyed' in the boiler.
- The higher of these removal efficiencies is used to determine the NO_x and SO_2 removed by the adsorber and the sorbent flow rate.

Figure 2-2 shows a simplified diagram of the flow of sulfur compounds through the NOXSO process. It should be noted that the steam treatment vessel and the regenerator have been lumped together, and that the sulfur dioxide from the air heater isn't shown. The sulfur dioxide from the air heater is dependant upon the sorbent flow rate, which depends upon the sulfur removal efficiency in the adsorber. Since this is an iterative problem, the approach taken was to first determine the removal efficiency in the adsorber without the addition of sulfur dioxide from the air heater. Then, the removal efficiency in the adsorber is increased by a small amount to account for the sulfur dioxide from the air heater. The following efficiencies are either known or assumed:

- SO_x emission standard and removal efficiency, η_{std}
- fraction of sulfur retained in bottom ash, η_{ash}
- fraction of sulfur compounds not released in the sorbent heater, η_{SH}
- fraction of sulfur compounds regenerated in the regenerator, η_{R}
- fraction of sulfur compounds regenerated in the steam treatment vessel, η_{STV}
- fraction of sulfur compounds converted to sulfuric acid in acid plant, η_{AP}

Figure 2-2: Simplified Diagram of Mass Flows for Sulfur Compounds

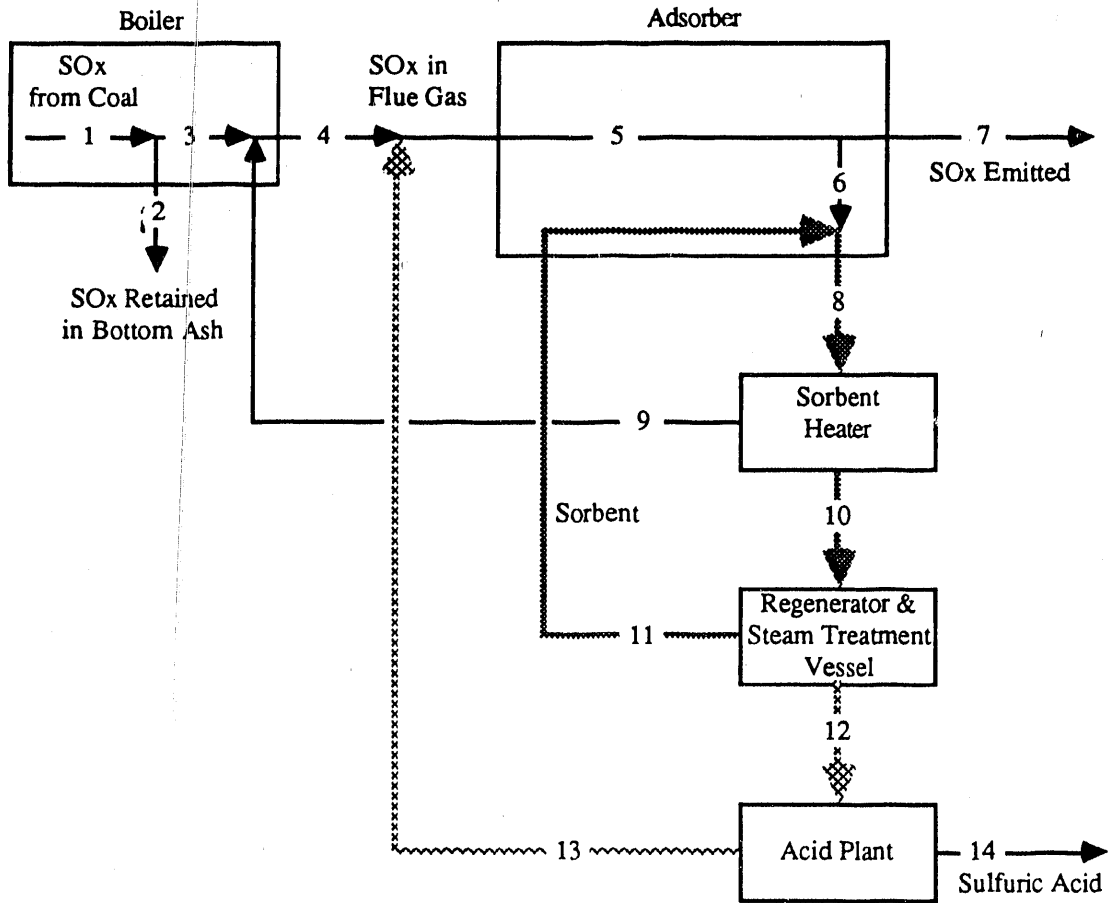
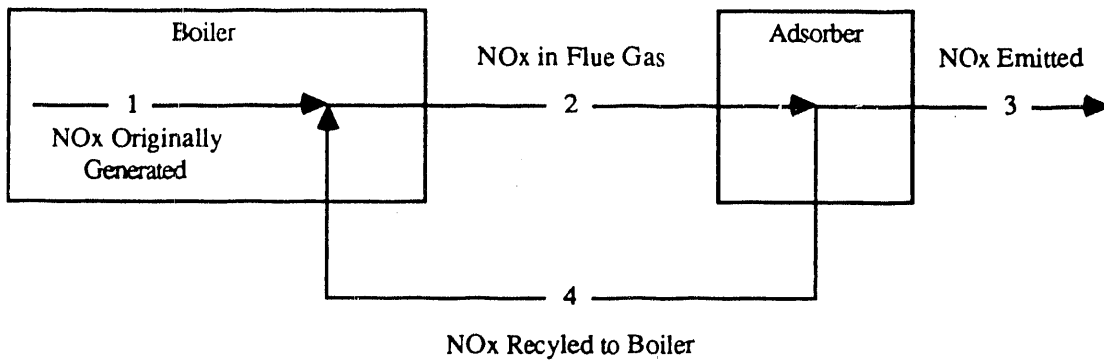


Figure 2-3: Simplified Diagram of Mass Flows for NO_x



The objective is to derive the actual SO₂ removal efficiency in the adsorber knowing the SO_x in the flue gas from the coal, the removal efficiency required by the emission standard, and the efficiencies of the sorbent heater, regenerator, and the acid plant. It is assumed that none of the SO₂ returned to the boiler from the sorbent heater is retained in the bottom ash. These conservation of mass equations (Equations 2.1) are needed to determine the apparent and actual SO_x removal efficiencies in the adsorber:

$$\begin{aligned}
 M_6 &= M_8 - M_{11} & M_{12} &= \frac{M_{14}}{\eta_{AP}} \\
 M_8 &= \frac{M_{10}}{\eta_{SH}} & M_{14} &= \eta_{std} M_3 \\
 M_{11} &= M_{10}(1 - \eta_{R\&S}) & M_5 &= M_6 + M_7 \\
 M_{10} &= \frac{M_{12}}{\eta_{R\&S}} & M_7 &= M_3(1 - \eta_{std}) \\
 \text{where } \eta_{R\&S} &= \eta_R + (1 - \eta_R)\eta_{STV}
 \end{aligned} \tag{2.1}$$

The apparent removal efficiency is defined as the SO_x removed by the adsorber, M₆, divided by the SO_x from the coal, M₃. Substituting for M₆ and simplifying yields Equation 2.2, which determines the apparent removal efficiency based on known values:

$$\begin{aligned}
 \eta_{app} &= \frac{M_6}{M_3} = \frac{M_8 - M_{11}}{M_3} = \frac{\frac{M_{10}}{\eta_{SH}} - M_{10}(1 - \eta_{R\&S})}{M_3} = \frac{M_{10}(\eta_{R\&S} - 1 + \frac{1}{\eta_{SH}})}{M_3} \\
 \eta_{app} &= \frac{M_{12}(\eta_{R\&S} - 1 + \frac{1}{\eta_{SH}})}{M_3 \eta_{R\&S}} = \frac{M_{14}(\eta_{R\&S} - 1 + \frac{1}{\eta_{SH}})}{M_3 \eta_{R\&S} \eta_{AP}} = \frac{M_3 \eta_{std}(\eta_{R\&S} - 1 + \frac{1}{\eta_{SH}})}{M_3 \eta_{R\&S} \eta_{SH}} \\
 \eta_{app} &= \frac{\eta_{std}(\eta_{R\&S} - 1 + \frac{1}{\eta_{SH}})}{\eta_{R\&S} \eta_{AP}}
 \end{aligned} \tag{2.2}$$

The actual SO₂ removal efficiency in the adsorber is defined as the SO_x removed, M₆, divided by the SO_x entering the adsorber, M₅. Substituting $\eta_{app} M_3$ for M₆ and simplifying, yields the actual removal efficiency. This value is multiplied by a constant to account for the sulfur from the oil burned in the air heater.

$$\eta_{SOX} = \frac{M_6}{M_5} = \frac{\eta_{app} M_3}{M_6 + M_7} = \frac{\eta_{app} M_3}{\eta_{app} M_3 + (1 - \eta_{std}) M_3} = \frac{\eta_{app} (1 + F_{oil})}{\eta_{app} + 1 - \eta_{std}} \tag{2.3}$$

The next step is to determine the NO_x removal efficiency required by the emission standard (including the effects of recycling NO_x to the boiler). Figure 2-3 shows a simplified NO_x flow diagram. The following parameters are known: the NO_x produced originally, M_1 ; the emission constraint, M_3 ; and the fraction of NO_x "destroyed" in the boiler. The actual NO_x removal efficiency is defined as the NO_x removed, M_4 , divided by the NO_x entering the adsorber, M_2 . Substituting for M_4 and M_2 and simplifying yields:

$$\eta_{\text{NOX}} = \frac{M_4}{M_2} = \frac{M_4}{M_1 + (1 - \delta_{\text{NOX}})M_4} = \frac{\frac{\eta_{\text{NOX}}M_3}{1 - \eta_{\text{NOX}}}}{M_1 + \frac{(1 - \delta_{\text{NOX}})\eta_{\text{NOX}}M_3}{1 - \eta_{\text{NOX}}}} = \frac{M_1 - M_3}{M_1 - (1 - \delta_{\text{NOX}})M_3} \quad (2.4)$$

where,

$$M_2 = M_1 + (1 - \delta_{\text{NOX}})M_4 \quad M_4 = \frac{\eta_{\text{NOX}}M_3}{(1 - \eta_{\text{NOX}})}$$

Since the removal efficiencies for NO_x and SO_x are equal, the SO_x removal efficiency for the adsorber equals the larger of the two values. NOXSO has reported that the actual NO_x removal efficiency is based on the concentration of SO_x [8]. However, a steady state relationship between η_{NOX} and the concentration of SO_x could not be determined from the available data.

$$\text{if } \eta_{\text{SOX}} > \eta_{\text{NOX}} \text{ then} \quad (2.5)$$

$$\eta_{\text{SOX,A}} = \eta_{\text{SOX}}$$

else

$$\eta_{\text{SOX,A}} = \eta_{\text{NOX}}$$

$$\eta_{\text{NOX,A}} = \eta_{\text{SOX,A}} \quad (2.6)$$

With NO_x removal efficiency determined, the amount of NO_x removed by the adsorber and the NO_x entering the adsorber can be determined with the following equations:

$$M_2 = M_1 + (1 - \delta_{\text{NOX}})M_4 = M_1 + (1 - \delta_{\text{NOX}})\eta_{\text{NOX,A}}M_2 = \frac{M_1}{1 - (1 - \delta_{\text{NOX}})\eta_{\text{NOX,A}}} \quad (2.7)$$

$$M_4 = \eta_{\text{NOX,A}}M_2 \quad (2.8)$$

With the actual SO_x removal efficiency in the adsorber known, it is possible to determine the SO_x removed by the adsorber and the SO_x remaining in the flue gas. The derivation of Equations 2.9 and 2.10 are quite involved and are not presented here. Equations 2.11 and 2.12 are easily derived from Figure 2-2.

$$C = (1 - \eta_{\text{SOX,A}}) \left(\frac{1 - \eta_{\text{SH}}}{h_{\text{SH}} \eta_{\text{R\&S}}} + 1 \right) \quad (2.9)$$

$$M_7 = \frac{CM_3}{C + \eta_{\text{SOX,A}} \eta_{\text{AP}}} \quad (2.10)$$

$$M_6 = \frac{\eta_{\text{SOX,A}} M_7}{1 - \eta_{\text{SOX,A}}} \quad (2.11)$$

$$M_8 = \frac{M_6}{1 - (1 - \eta_{\text{R\&S}}) \eta_{\text{SH}}} \quad (2.12)$$

The sorbent flow rate is determined by an algorithm developed by NOXSO [8]. The numerator in Equation 2.13 is the SO_x removed by the adsorber, M₆. λ is the ratio of available sodium to sulfur removed and is assumed to be unity [7]. The parameter X can be determined by existing algorithms [8].

$$m_{\text{sorb}} = \frac{A_A VC_o(y_i - y_o)}{\lambda N_t X} = \frac{M_6}{\lambda N_t X} \quad (2.13)$$

$$X = \frac{\ln\left(\frac{y_o}{y_i}\right)V}{k_a PH} + 1 = \frac{\ln(1 - \eta_{\text{SOX,A}})V}{k_a PH} + 1 \quad (2.14)$$

H, K_a, P, and λ are input parameters. K_a is currently set to 3.7 according to Ref. 8, while P is assumed to be 1 atmosphere. N_t is the loading of active sorbent material to the weight of sorbent. This can be determined by the following equation:

$$N_t = \frac{w_{\text{Na}}}{23 \eta_{\text{R\&S}}} \quad (2.15)$$

Once the sorbent flow rate is known, the makeup sorbent rate and the energy required to pump the sorbent can be determined. The makeup sorbent rate is assumed to be a fraction of the sorbent rate, and is an input parameter. Energy to pump the sorbent is assumed to be proportional to the energy estimated in the EPRI report [6]:

$$m_{\text{makeup}} = f_{\text{makeup}} m_{\text{sorb}} \quad (2.16)$$

$$EC_{\text{sorb}} = 1795 \text{ kW} / 1.3486e^6 \text{ lb/hr} * m_{\text{sorb}} = 1.32e^{-3} m_{\text{sorb}} \quad (2.17)^1$$

The energy required to raise the sorbent temperature to 1110°F from the exit temperature of the adsorber is simply the difference in enthalpy times the sorbent flow rate. This determines the

¹ e# is used to signify "x 10#."

amount of air needed by the sorbent heater. It is assumed that the air temperature drops from 1280°F to 610°F in the sorbent heater.

$$E_{\text{sorb,SH}} = (\hat{h}_{\text{sorb}}(1110) - \hat{h}_{\text{sorb}}(250)) m_{\text{sorb}} \quad (2.18)$$

$$M_{\text{air,SH}} = \frac{E_{\text{sorb,SH}}}{\hat{h}_{\text{air}}(1,280) - \hat{h}_{\text{air}}(610)} \quad (2.19)$$

Once the flow rate of the air is determined, the amount of energy needed to heat the air to 1280°F is equal to the energy flow rate of air at 1280°F minus the heat given up in the sorbent cooler minus the energy flow rate of air at 100°F, which is the temperature of the air after the compressor. The sorbent flow rate at the sorbent cooler is approximately 7% less than when it left the adsorber; it is also assumed to drop from 970°F to 210°F.

The energy required to heat the air determines the oil requirement for the air heater. The efficiency of the air heater is an input parameter. The electricity consumption of the compressor is determined by the flow rate of air and the pressure increase, which is assumed to be 84" of water.

$$E_{\text{air,AH}} = \left[(\hat{h}_{\text{air}}(1280) - \hat{h}_{\text{air}}(100)) \right] M_{\text{air,SH}} - 0.93 \left[(\hat{h}_{\text{sorb}}(970) - \hat{h}_{\text{sorb}}(210)) \right] m_{\text{sorb}} \quad (2.20)$$

$$EC_{\text{air,SH}} = \left(\frac{1,545 M_{\text{air,SH}}}{0.75 * 60 * 44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2*84}}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460) \quad (2.21)$$

Once the energy requirement to heat the air is known, this determines the oil requirement for the air heater. The efficiency of the air heater is an input parameter, and 18% excess air is assumed. With the oil consumption known, the amount of combustion air for the air heater can be determined. The oil is assumed to be a heavy fuel oil, with a higher heating value of 18,400 Btu/lb and the following composition: 87.87% carbon, 10.33% hydrogen, 1.16% sulfur, 0.14% nitrogen, and 0.50% oxygen [9]. The actual composition is not extremely critical; however, all the components are in place in case another fuel, such as coal, is used.

$$m_{\text{oil}} = \frac{E_{\text{air,SH}}}{\text{HHV}_{\text{oil}} \eta_{\text{AH}}} \quad (2.22)$$

$$m_{\text{air,AH}} = \frac{\left(\frac{0.8787}{12} + \frac{0.1033}{4} + \frac{0.0116}{32} - \frac{0.005}{32} \right) 1.18 m_{\text{oil}}}{f_{\text{O, wet air}}} \quad (2.23)$$

The amount of steam and methane used in the regenerator and steam treatment vessels can be calculated once the sulfur flow rate exiting the sorbent heater is found. The methane requirement for the regenerator is assumed to be proportional to the sulfur dioxide entering the regenerator. According to NOXSO, approximately 3690 SCFM of methane are needed for 575 lb-moles per hour of sulfur dioxide [10]. Also 3.34 moles of steam are needed for each mole of sulfur dioxide entering the steam treatment vessel. The constant converting SCFM to lb-moles/hr is 0.1585 assuming at standard temperature of 58°F.

$$M_{SC,R,i} = M_{SC,A,o} \eta_{SH} \quad (2.24)$$

$$M_{M,R,i} = 3690 / 575 * 0.1585 M_{SC,R,i} \quad (2.25)$$

$$M_{W,STV,i} = 3.34 (1 - \eta_{STV}) M_{SC,R,i} \quad (2.26)$$

The utilization of methane and steam and the fractions of SO_2 , H_2S , and S_2 produced in the regenerator are input parameters. It is assumed that there is sufficient oxygen to convert all the carbon in the methane to CO_2 ; that no COS is formed; and that all only H_2S and steam are produced in the steam treatment vessels. The moisture content of the regenerator gas is assumed to be the steam not utilized in the steam treatment vessel plus the hydrogen released when methane is converted to carbon dioxide minus the hydrogen used to form hydrogen sulfide. This gas is sent to either a sulfuric acid plant or an elemental sulfur (Claus) plant.

$$M_{M,R,o} = (1 - \eta_R) M_{M,R,i} \quad (2.27)$$

$$M_{SD,R,o} = f_{PSD,R} \eta_R M_{SD,R,i} \quad (2.28)$$

$$M_{HS,R,o} = (f_{PHS,R} \eta_R + (1 - \eta_R) \eta_{STV}) M_{SD,R,i} \quad (2.29)$$

$$M_{S,R,o} = (1 - f_{PSD,R} - f_{PHS,R}) \eta_R M_{SD,R,i} / 2 \quad (2.30)$$

$$M_{M,R,o} = (1 - U_{tM}) M_{M,R,i} \quad (2.31)$$

$$M_{CD,R,o} = U_{tM} M_{M,R,i} \quad (2.32)$$

$$M_{W,R,o} = (1 - U_{tW}) M_{W,STV,i} + 2M_{CD,R,o} - f_{PHS,R} \eta_R M_{SD,R,i} \quad (2.33)$$

The next step is to determine the composition of the gas returned to the boiler. This gas stream consist of three other streams. The first is the air used to heat and cool the sorbent, $M_{air,SH}$. The second is the NO_x and SO_x picked up by this stream in the sorbent heater. Finally, there is the flue gas from the air heater. The off gas from the acid plant is returned to the flue gas upstream of

the adsorber; however, since it is a small stream, and to simplify the calculations, it is treated as SO₂ returned to the boiler. It is assumed that only SO₂ is returned to the boiler from the sorbent heater, acid plant, and air heater. The composition of NO_x returned to the boiler is assumed to be in the same proportions as that generated in the boiler. The temperature of this gas stream is estimated to be 620°F [6].

$$M_{N,B,i} = f_{N,wet\ air} M_{air,SH} + 0.0014 / 28 M_{oil} \quad (2.34)$$

$$M_{O,B,i} = f_{O,wet\ air} (M_{air,SH} + 0.18 / 1.18 M_{air,AH}) \quad (2.35)$$

$$M_{W,B,i} = f_{W,wet\ air} (M_{air,SH} + M_{air,AH}) + 0.1033 / 2 M_{oil} \quad (2.36)$$

$$M_{CD,B,i} = 0.8787 / 12 M_{oil} \quad (2.37)$$

$$M_{SD,B,i} = [(1 - \eta_{SH}) + (1 - \eta_{AP})\eta_{SH}\eta_{R\&S}] M_{SD,A,o} + 0.0116 / 32 M_{oil} \quad (2.38)$$

$$M_{NO,B,i} = f_{PNO,B} M_{NOX,A,o} \quad (2.39)$$

$$M_{ND,B,i} = (1 - f_{PNO,B}) M_{NOX,A,o} \quad (2.40)$$

Now the inlet combustion air and the composition of the flue gas exiting the boiler can be determined. The oxygen being returned to the boiler reduces the combustion air entering the air preheater. Since the nitrogen and moisture are based on the oxygen content, the only variable which needs to be modified is the oxygen required. See the analytical documentation for the IEC model [1]. Once these parameters are known, the composition of the flue gas exiting the boiler can be determined:

$$M_{O,AP,i} = M_{O,required} - M_{O,B,i} \quad (2.41)$$

$$M_{CD,B,o} = M_{C,coal} + M_{CD,B,i} \quad (2.42)$$

$$M_{W,B,o} = M_{W,coal} + M_{W,AP,i} + 0.5 M_{H,coal} + M_{W,B,i} \quad (2.43)$$

$$M_{SD,B,o} = f_{PSD,B} \eta_{ash} M_{S,coal} + M_{SD,B,i} \quad (2.44)$$

$$M_{ST,B,o} = (1 - f_{PSD,B}) \eta_{ash} M_{S,coal} \quad (2.45)$$

$$M_{ND,orig} = \frac{NO_{x,ef} m_{coal}}{46 + \frac{30 f_{PNO,B}}{1 - f_{PNO,B}}} \quad (2.46)$$

$$M_{NO,orig} = \frac{f_{PNO,B} M_{ND,orig}}{1 - f_{PNO,B}} \quad (2.47)$$

$$M_{ND,B,o} = M_{ND,orig} + (1 - \delta_{NOX})M_{ND,B,i} \quad (2.48)$$

$$M_{NO,B,o} = M_{NO,orig} + (1 - \delta_{NOX})M_{NO,B,i} \quad (2.49)$$

$$M_{N,B,o} = 0.5M_{N,coal} + M_{N,AP,i} - 0.5(M_{NO,orig} + M_{ND,orig}) + M_{N,B,i} + 0.5M_{NOX,A,o} \quad (2.50)$$

$$M_{O,B,o} = M_{O,AP,i} + 0.5M_{O,coal} - M_{C,coal} - 0.25M_{H,coal} - f_{PSD,B}\eta_{ash}M_{S,coal} - 1.5M_{ST,B,o} \\ - 0.5M_{NO,orig} - M_{ND,orig} + M_{O,B,i} + \delta_{NOX}(M_{ND,B,i} + 0.5M_{NO,B,i}) \quad (2.51)$$

With the flue gas flow rate and combustion air determined, the air preheater model can be used to determine the flue gas temperature leaving the air preheater, $T_{fg,AP,o}$, and the temperature of the combustion exiting the air preheater, $T_{air,AP,o}$. Now the amount of water added to cool the flue gas to 210°F and the volumetric flow rate into the adsorber can be determined. The water needed to cool the flue gas is the energy loss of the flue gas between the exit temperature of the air preheater and 210°F divided by 20,204 (the energy needed to raise a mole of water from 60°F to 212°F saturated steam). Now the gas flow rate into and exiting the adsorber can be determined:

$$M_{W,fg,added} = \frac{\sum_{i=1}^8 (\hat{h}_i(T_{fg,AP,o}) - \hat{h}_i(210))M_{i,fg}}{20,204} \quad (2.52)$$

$$G_{A,i} = \frac{\left(\sum_{i=1}^8 M_{i,fg} + M_{W,fg,added} \right) 1,545 * (210 + 460)}{14.687 * 144 * 60} \quad (2.53)$$

$$G_{A,o} = G_{A,i} \frac{250 + 460}{210 + 460} \quad (2.54)$$

With the volumetric flow rate determined, the number of operating train and the size of each adsorber can be determined. Each adsorber in EPRI report handled 450,000 acfm [6]. The algorithm to determine the number of redundant trains is retained from Ref.[1]. The electricity consumption is required to overcome the pressure drop, in the adsorber (22" water) and to power the blower for the air heater. This blower is assumed to have a 4" water pressure drop.

$$NOP = \text{round} \left(\frac{G_{A,i}}{450,000} \right) \quad (2.55)$$

$$NRD = 1 + \text{if} \left(\frac{NOP}{4} - 1 \right) > 1 \text{ then } \text{round} \left(\frac{NOP}{4} - 0.5 \right) - 1 \text{ else } 0 \quad (2.56)$$

$$A_A = \frac{G_{A,i}}{60 \text{ NOP V}} \quad (2.57)$$

$$EC_{FG} = 1.38e^{-4} * 22 G_{A,o} \quad (2.58)$$

$$EC_{AH} = \frac{1,545 (80 + 460) M_{AH}}{14.687 * 144 * 60} * 4 * 1.38e^{-4} \quad (2.59)$$

The NOXSO process consumes low pressure steam in the steam treatment vessel, while the acid plant may produce steam. Therefore, the net steam consumption or credit is the difference between the steam consumed by NOXSO and that generated by the acid plant. The temperature of the steam from the acid plant is set to 665°F, the temperature of the steam required for the NOXSO process. Then, 15,940 Btu is the energy required to raise a mole of saturated water at 226°F to saturated steam at 338°F minus the value from the enthalpy algorithms at 338°F. The boiler is assumed to be 88% efficient. Therefore, the total power consumption of the NOXSO and acid plant is the sum of the requirements for the pressure drop in the flue gas, transport of the sorbent, compressor for the sorbent cooler, blower for the air heater, the acid plant, and (if required) the steam consumption:

$$EC_{\text{steam}} = (M_{W,STV} - M_{\text{steam,AP}}) \frac{\hat{h}_W(665^\circ\text{F}) + 15,940}{0.88 * \text{HR}} \quad (2.60)$$

$$EC_{\text{total}} = EC_{fg} + EC_{\text{air,SC}} + EC_{AH} + EC_{\text{sorb}} + EC_{AP} + \text{if } EC_{\text{steam}} > 0 \quad (2.61)$$

The energy is added to the power plant from the steam generated by the acid plant and the air recycled to the boiler. The electrical equivalent for the steam is straight forward. The energy credit for the air recycled to the boiler is more complicated, since it also reduces the amount of inlet combustion air and changes the performance of the air preheater. The energy credit for the recycled air is the energy flow rate of the recycled air plus inlet combustion air at the new air preheater exit temperature minus the energy flow rate of the original combustion air at 515°F. The original combustion air is defined as the air required for the coal consumed.

$$EC_{\text{recycled}} = (M_{\text{recycled}} \hat{h}(620) + M_{\text{comb,air}} \hat{h}(T_{AP,o}) - M_{\text{comb,air}} \hat{h}(515)) / \text{HR} \quad (2.62)$$

$$\text{if } EC_{\text{steam}} < 0 \text{ then } EC_{\text{r_steam}} = -EC_{\text{steam}} \text{ else } 0 \quad (2.63)$$

$$EC_{\text{r_total}} = EC_{\text{recycled}} + EC_{\text{steam}} \quad (2.64)$$

2.2 Economic Model

The current economics model for the NOXSO process is based primarily on the recent case study by EPRI [6]. The major difference is that methane is used for the regeneration step rather than a synthesis gas produced on-site.

The capital costs are scaled to five key parameters: flue gas flow rate, sorbent flow rate, makeup flow rate, area of the adsorbers, and oil consumption. The values of these parameters for the EPRI base case plant (1000MW, 4% S coal) are: $3.6e^6$ acfm, $1.36e^6$ lb/hr, 880 lb/hr, 2542 ft², and 7200 lb/hr. The area of the adsorber, 2545 ft², is estimated from the gas flow rate into the adsorber, the number of operating trains, and the gas velocity through the adsorber. The capital cost for a larger air preheater, if that option is chosen, is also included as a part of the capital cost for the NOXSO process.

2.2.1 Capital Costs

The EPRI report lists plant components by section with delivered equipment costs itemized. The report also gives the total cost of each plant area. The cost of the components can be summed and divided into the total cost to determine a multiplier for each area. The total equipment cost, total process capital, and the appropriate multiplier are given in Table 2-1. Note that the design plant size is two 500 MW units. The regeneration system, area 40, contains a Texaco Coal Gasification System for producing regeneration gas. This item has been removed from the total listed in area 40 of Table 2-1. It was assumed to have a multiplier of one, since it is a delivered system. The sulfuric acid plant, particulate removal, and waste disposal areas are not listed since they have been explicitly modeled elsewhere in the IEC model.

The capital cost coefficients for each of the major parameters are estimated by adding all the component costs associated with each parameter, then divide through by the base value of the parameter (from the EPRI report) raised to the 0.7 power. The makeup rate of sorbent and oil consumption are used to scale the reagent feed system. Since the Texaco Coal Gasification System is not used, liquid oxygen storage is not needed. Miscellaneous process equipment is included in the coefficient for oil. Therefore the total capital cost for area 10 is:

$$DCC_{10} = \frac{1,651,777}{880^{0.7}} m_{\text{makeup}}^{0.7} + \frac{965,006}{7200^{0.7}} m_{\text{oil}}^{0.7} = 14,350 m_{\text{makeup}}^{0.7} + 1.925 m_{\text{oil}}^{0.7} \quad (2.65)$$

Table 2-1: Area Cost Multipliers for NOXSO Process

| <u>Area</u> | <u>Description</u> | <u>Equipment Costs</u> | <u>Total Cost</u> | <u>Multiplier</u> |
|-------------|--------------------------------|------------------------|-------------------|-------------------|
| 10 | Reagent Feed System | 12.76 | 5.57 | 2.29 |
| 20 | SO ₂ Removal System | 7.52 | 2.52 | 2.99 |
| 30 | Flue Gas Handling System | 27.00 | 13.65 | 1.98 |
| 40 | Sorbent Regeneration System | 15.66 | 9.99 | 1.57 ^a |
| 70 | General Support Equipment | 0.30 | 0.17 | 1.77 |

^a Does not include the Texaco Coal Gasification System.

The capital cost for the flue gas equipment is broken into two components. The first component is area 30, with a slight modification to the capital cost for the I.D. fans. Since the adsorber does not cause the entire pressure drop across the I.D. fans, it is only charged for its portion of the pressure drop, 22" water. Since the I.D. fans is sized for 30" of water, the NOXSO process is charged for 73% of the I.D. fans and dampers. The capital cost for the ductwork associated with the mu! lones and ESP are not included. The second component is the adsorber, which is in the SO₂ removal system in the EPRI report. However, its cost is related to the flue gas flow rate, so it is included with the flue gas handling system. Thus:

$$DCC_{30} = \frac{20,599,176}{3,600,000^{0.7}} G_{A,i}^{0.7} + \frac{5,292,001}{10 * 2,542^{0.7}} (NOP + NRD) A_A^{0.7}$$

$$DCC_{30} = 530G_{A,i}^{0.7} + 2,188 (NOP + NRD) A_A^{0.7} \quad (2.66)$$

The capital cost associated with the sorbent flow rate includes part of area 20 and most of area 40. The Texaco Coal Gasification System, regenerative gas burner, and the acid plant compressor are not included. The regenerative gas burner and acid plant compressor are part of the acid plant model. The equipment from area 20 is the regenerated sorbent transfer hopper and the pneumatic conveying system. The capital cost associated with general support equipment is taken as a fraction of the previous capital cost areas. The results are:

$$DCC_{40} = \frac{15,132,844}{1,358,600^{0.7}} m_{sorb}^{0.7} = 770m_{sorb}^{0.7} \quad (2.67)$$

$$DCC_{70} = \frac{296,121}{43,640,804}(DCC_{10} + DCC_{30} + DCC_{40})$$

$$DCC_{70} = 0.007(DCC_{10} + DCC_{30} + DCC_{40}) \quad (2.68)$$

The total direct capital cost is the sum of Equations 2.65 through 2.68, plus the cost of a larger air preheater (if needed). The indirect capital charges include general facilities, engineering fees, project and project contingencies. These are assumed to be 10%, 12.5%, 21.2%, and 13.4% respectively, of the total direct capital cost. The total plant cost is the sum of the following items, plus the total capital cost of the acid plant.

$$DCC_{total} = DCC_{10} + DCC_{30} + DCC_{40} + DCC_{70} + DCC_{APH} \quad (2.69)$$

$$DCC_{gf} = 0.10DCC_{total} \quad (2.70)$$

$$DCC_{eng} = 0.125DCC_{total} \quad (2.71)$$

$$DCC_{proj} = 0.212DCC_{total} \quad (2.72)$$

$$DCC_{proc} = 0.134DCC_{total} \quad (2.73)$$

$$TPC = DCC_{total} + DCC_{gf} + DCC_{eng} + DCC_{proj} + DCC_{proc} + TCC_{acid} \quad (2.74)$$

The cost of interest during construction is a function of the interest and inflation rates, and is taken as a fraction of the total plant cost. The project is assumed to take three years to complete, with an equal amount of money spent each year. All funds are expended in the middle of each year. The interest rate is a function of the debt/equity ratio and is calculated according to EPRI guidelines [11]. The startup charges are estimated to be one month of the fixed and variable operating costs plus 2% of the total plant inventory cost. The royalty charges are assumed to be 0.5% of the total direct capital cost. The land costs are scaled to the size of the gross size of the plant. In sum:

$$TPI = \left(\left(\frac{1+i}{1+p} \right)^{0.5} + \left(\frac{1+i}{1+p} \right)^{1.5} + \left(\frac{1+i}{1+p} \right)^{2.5} \right) \frac{TPC}{3} \quad (2.75)$$

$$C_{startup} = (FOC + VOC) / 12 + 0.02TPI \quad (2.76)$$

$$C_{misc} = 0.005DCC_{total} + 4.97e^{-5}MW_g \quad (2.77)$$

Working capital is estimated as 60 days of consumption at full capacity for the makeup sorbent, methane, and oil. The sorbent cost is \$2.5 / lb; the cost of oil is expressed in \$ per Btu, while 0.378 converts lb-moles/hr to MSCF.

$$C_{\text{work}} = (2.5m_{\text{makeup}} + 0.378UC_M M_{M,R,i} + UC_{\text{oil}} \text{HHV}_{\text{oil}} m_{\text{oil}}) 24 * 60 \quad (2.78)$$

The inventory capital cost of the sorbent is estimated from the mass of sorbent in the process equipment. The settled bed height is estimated to be one-half of the expanded bed height. The amount of sorbent in the adsorber is estimated from the area of the adsorber, settled bed height, and density. The amount of sorbent in the rest of the system is estimated from the residence times of equipment and the mass flow rate of sorbent. The total capital cost is the sum of the total plant inventory, startup charges, working capital, inventory cost, land and royalty fees:

$$C_{\text{inv}} = \left(\frac{H}{2} A_A \rho_{\text{sorb}} + \frac{m_{\text{sorb}}}{\text{NOP}} (RT_R + RT_{\text{SH}} + RT_{\text{SC}}) \right) (\text{NOP} + \text{NRD}) * 2.5 \quad (2.79)$$

$$\text{TCC} = \text{TPI} + C_{\text{startup}} + C_{\text{work}} + C_{\text{inv}} + C_{\text{misc}} \quad (2.80)$$

2.2.2 Operating and Maintenance Costs

Annual operating charges consist of fixed and variables charges. The fixed charges consist of the operating, maintenance, administrative labor, and the maintenance materials. It is estimated that 5.2 workers per hour at \$19.70/hr are needed for operating labor. Maintenance labor and materials and administration labor charges are estimated using the EPRI guidelines [11]. Maintenance cost is 4.8% of the total plant cost excluding the total capital cost for the acid plant. Labor accounts for 40%, while materials account for 60% of the total maintenance cost. Administrative and support labor is estimated to be 30% of the operating and maintenance labor. The variable charges include the costs for makeup sorbent, methane, oil, and miscellaneous charges. The result is:

$$\text{OC}_{\text{oper}} = 5.2 * 19.7 * 8766 \quad (2.81)$$

$$\text{OC}_{\text{maint-labor}} = 0.40 * 0.048 (\text{TPC} - \text{TCC}_{\text{acid}}) \quad (2.82)$$

$$\text{OC}_{\text{maint-matl}} = 0.60 * 0.048 (\text{TPC} - \text{TCC}_{\text{acid}}) \quad (2.83)$$

$$\text{OC}_{\text{admin}} = 0.30(\text{OC}_{\text{oper}} + \text{OC}_{\text{maint-labor}}) \quad (2.84)$$

$$\text{FOC} = \text{OC}_{\text{oper}} + \text{OC}_{\text{maint-labor}} + \text{OC}_{\text{maint-matl}} + \text{OC}_{\text{admin}} \quad (2.85)$$

$$\text{OC}_{\text{sorb}} = 2.5 * 8,766 \text{ CF } m_{\text{makeup}} \quad (2.86)$$

$$\text{OC}_M = 0.378 * 8,766 \text{ CF } UC_M M_{M,R,i} \quad (2.87)$$

$$\text{OC}_{\text{oil}} = 8,766 \text{ CF } \text{HHV}_{\text{oil}} UC_{\text{oil}} m_{\text{oil}} \quad (2.88)$$

$$\text{OC}_{\text{misc}} = 0.019 \text{DCC}_{\text{total}} \quad (2.89)$$

$$VOC = OC_{\text{sorb}} + OC_M + OC_{\text{oil}} + OC_{\text{misc}} \quad (2.90)$$

The NOXSO process typically produces an energy credit. In the IEC model, energy credits are accounted for by increasing the output of the power plant while keeping coal consumption the same. The capital and operating costs, including the additional energy cost, of the increased size are charged to the basic power plant while the NOXSO process is given a credit for the energy it supplies to the power plant. This is equivalent to assuming that the NOXSO process decreases the amount of coal burned in the boiler. Since the energy credit and the cost of the NOXSO are dependent upon the coal consumption, it becomes an iterative problem.

$$TCC_{BP, \text{incre}} = \frac{ECr_{\text{total}}}{MWg * 1000} TCC_{BP} \quad (2.91)$$

$$TVC_{BP, \text{incre}} = \frac{ECr_{\text{total}}}{MWg * 1000} TVC_{BP} \quad (2.92)$$

$$OCr_{\text{coal}} = 8766 \text{ CF } UC_{\text{coal}} \frac{ECr_{\text{total}} \text{ HR}}{2000 \text{ HHV}_{\text{coal}}} \quad (2.93)$$

The total capital and operating cost of the power plant are increased by $TCC_{BP, \text{incr}} + TVC_{BP, \text{incr}}$. The total variable cost of the NOXSO process is the sum of the fixed and variable operating costs minus the credits for coal and the sale of sulfuric acid. Utility consumption is charged separately. The result is:

$$TVC = FOC + VOC - OCr_{\text{coal}} - OC_{\text{credit, acid}} \quad (2.94)$$

$$\text{Util} = 8766 \text{ CF } UC_{\text{elec}} EC_{\text{total}} \quad (2.95)$$

2.3 References

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3. Sulfuric Acid Plant

This section of the report describes an update version of a sulfuric acid plant model developed by Frey [1]. The sulfuric acid plant performance and economic models were developed based on an interpass absorption (2/1) contact acid plant design by Monsanto for SMC [2,3]. Subsequent information from Monsanto [4,5], and studies [6] also were used for this model.

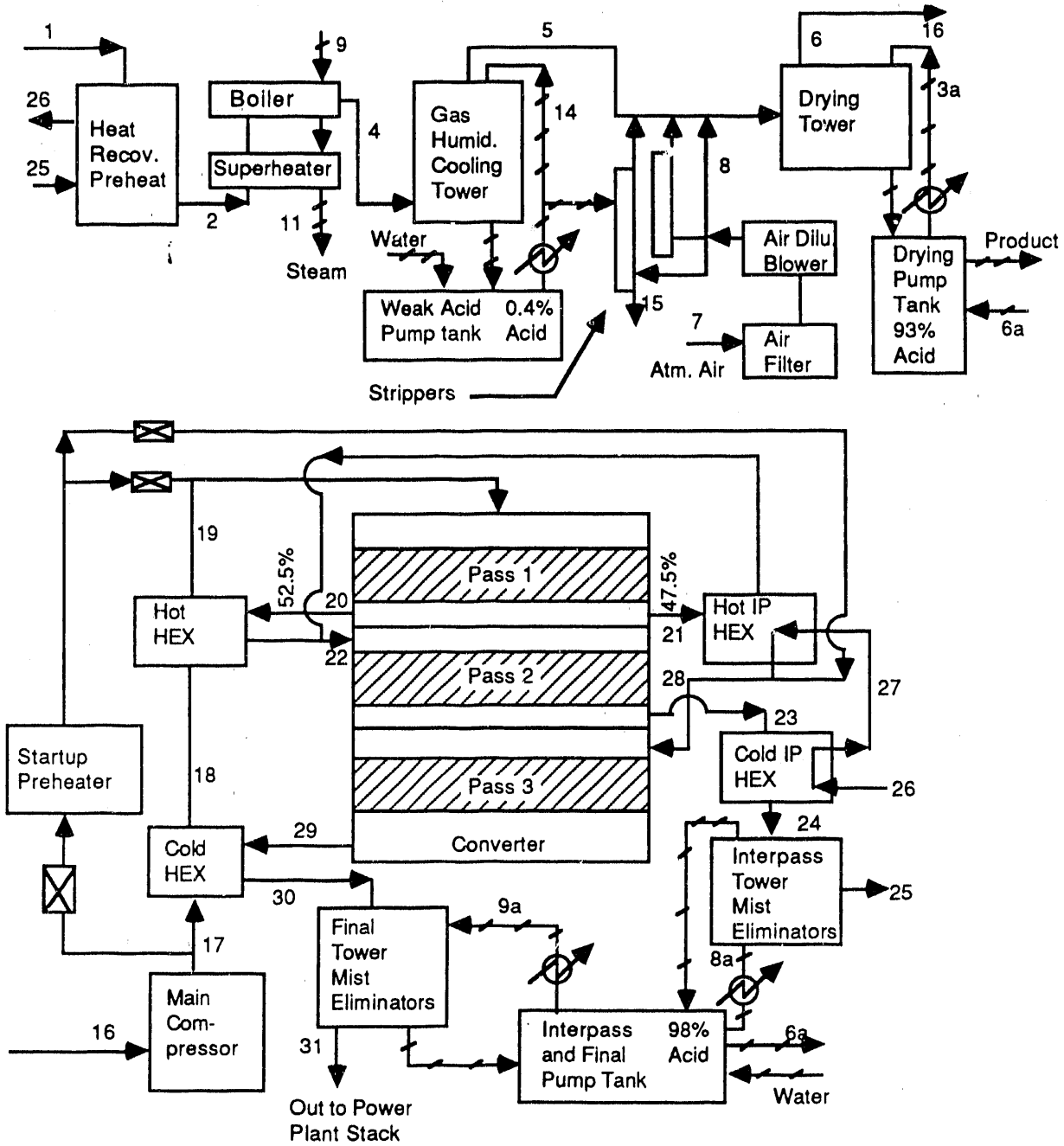
The Monsanto design has a conversion efficiency of 99.5% and is based on a regenerator off-gas composition specified by SMC, which consisted of CH_4 , CO_2 , H_2O , and SO_2 . The current design, shown in Figure 3-1, was modified to accommodate off-gases with different compositions, temperatures, and pressures. Presently it can handle these additional gases: CO , COS , H_2 , H_2S , N_2 , O_2 , and SO_2 . The only major changes are an additional inlet gas compressor and gas burner. The inlet gas compressor is only used if the inlet off gas is below 97" of water, while the gas burner is used to burn combustible compounds in the inlet gas. The inlet gas compressor and gas burner are shown in Figure 3-2.

To understand this model, it is important to understand the characteristics of contact acid plants, overall strategy, assumptions, and algorithms used for this model, and how it interacts with the rest of the IEC model. Contact acid plants have high initial capital cost and low operating cost, excluding utilities; therefore, it is more important to estimate the capital cost than the operating cost. The most expensive and critical component is the converter.

Another important point is that acid plants can either be net energy producers or consumers depending upon the composition of the inlet gas. So the amount of energy consumed and produced have to be accurately estimated. Acid plants are very reliable and maintenance requirements are small.

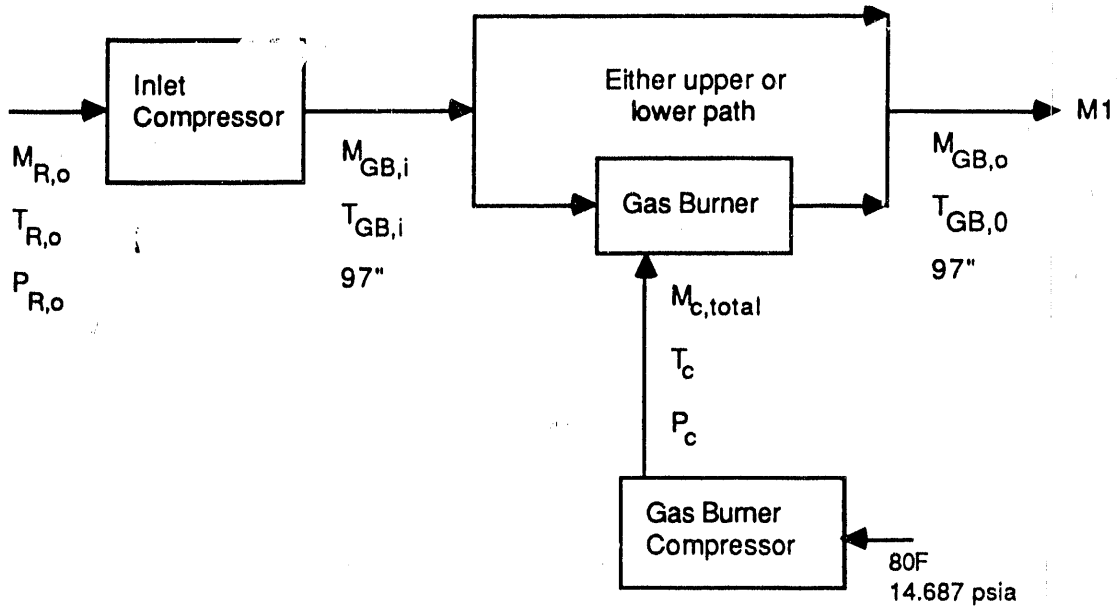
Generally an acid plant only has to be shut down once a year for a week, to maintain the catalyst in the converter. The attrition rate per year is approximately 2% for the entire converter, if the gas does not contain any dust, arsenic, chlorine, and flourine. Dust clogs the catalyst, while the other chemicals react with the catalyst and reduce its reactivity. The actual attrition rate per bed varies. The first stage or bed has the highest rate; the second stage has the second highest, and the last stage has the lowest.

Figure 3-1: Schematic Diagram of Sulfuric Acid Plant

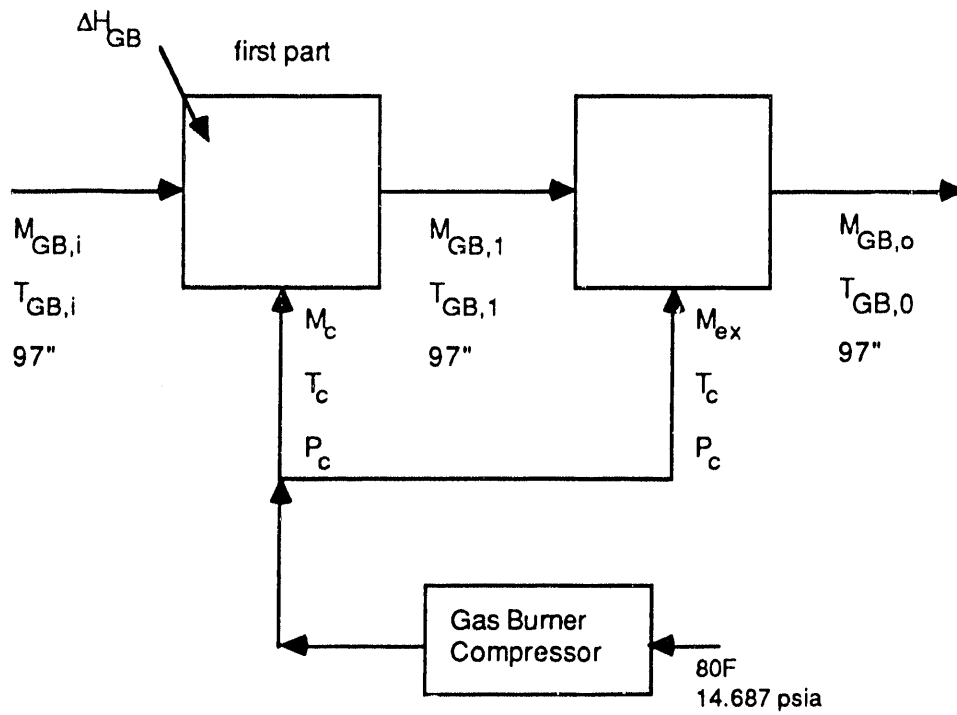


| | | | | | | | | | | | | | | | |
|---------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| Stream | 1 | 2 | 4 | 5 | 6 | 7 | 8 | 9 | 11 | 14 | 16 | 17 | 18 | 19 | 20 |
| Temp. F | 824 | 609 | 506 | 169 | 120 | 85 | 115 | 226 | 450 | 163 | 120 | 171 | 603 | 779 | 1158 |
| * Water | 97 | | | 67 | 51 | 0 | 67 | 100 | 100 | | 51 | 167 | | 155 | |
| Stream | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 3a | 6a | 8a | 9a |
| Temp. F | 1158 | 828 | 918 | 570 | 180 | 256 | 667 | 850 | 877 | 380 | 180 | 120 | 180 | 180 | 180 |
| * Water | | | | 97 | | | | 37 | | | 1 | | | | |

Figure 3-2: Schematic Diagrams of Inlet Compressor and Gas Burner



Break down of Gas Burner



Before proceeding with a detailed description of the acid plant chemical processes, an overview is given below. It is assumed the reader will refer to Figures 3-1 and 3-2 for information to understand where the output of one piece of equipment is the input to another.

The principal steps of the process are:

- Oxidizing combustible gases other than SO_2 , if economical
- Gas purification, cooling, and drying
- Conversion of SO_2 to SO_3
- Conversion of SO_3 to sulfuric acid

A contact sulfuric acid plant is based upon the chemical reaction of SO_3 and H_2O forming sulfuric acid. This reaction takes place in the final and interpass towers. The SO_3 in the gas actually reacts with the water in the 98.5% sulfuric acid that is circulated through these towers. A strong acid is used to help prevent acid mist from forming.

Acid mist is formed if the SO_3 is brought in contact with free water vapor. This acid mist can cause corrosion problems downstream unless it is removed. Some mist is always created, so mist eliminators are used downstream of the towers, although these are relatively expensive and have a significant pressure drop. To prevent moisture from entering the converter, drying towers are used upstream; however, moisture is also formed from any hydrogen compounds entering the converter, since they burn in the first stage.

The SO_3 is generated in the converter by oxidizing SO_2 in the presence of a catalyst. The oxidation of SO_2 is highly temperature dependent. The rate of reaction increases with increasing temperature; however, the conversion efficiency decreases with increasing temperature. Therefore a three pass converter design is used to achieve a 99.5% conversion efficiency. The first stage oxidizes 70% of the SO_2 operating at a temperature of 1158°F; the second stage converts an additional 25% at 918°F; the final stage converts all but the last 0.5% of the SO_2 at 877°F. The catalyst has a maximum operating temperature of 1158°F, which is maintained by adding dilution air upstream of the converter. Since the oxidation of SO_2 is exothermic, the maximum concentration of SO_2 in the gas stream to the converter is approximately 11% if the gas stream does not contain any combustible gases. Any combustible gases in the inlet gas react with oxygen

in the first stage and cause additional heat to be released in the first stage of the converter, so additional dilution air is required to ensure that the catalyst does not get too hot. This significantly increases the capital and operating costs. The amount of dilution air is determined by an energy balance on the first stage of the converter.

The gas must be cooled for the second and third stages. This is accomplished by five heat exchanges which either cool or heat the gas after it leaves the first stage. After the second stage, the gas passes through the interpass tower and mist eliminator which cools the gas and converts the SO_3 into sulfuric acid. The gas has to be heated for the third stage, so it passes through the heat recovery preheater and two heat exchangers.

The gas stream, 6, into the converter (see Figure 1) must be dry and have a maximum SO_2 concentration of approximately 11%. The gas is prepared by a series of heat exchangers and drying towers, upstream of the converter. The inlet gas stream, 1, is cooled from 824°F to 609°F by the heat recovery preheater, while the gas stream, 25, from the interpass tower is heated from 180°F to 256°F . If the heat recovery preheater cools the inlet gas below 506°F , the boiler or superheater are not used. This usually occurs when there are a lot combustible gases entering the converter. The combustible gases increase the dilution air requirement, which increases the size of stream 25 relative to stream 1.

A gas burner can be used to burn any combustible gases before it enters the converter, and is usually placed upstream of the heat recovery preheater. These burners are fired by natural gas; however, it is assumed that the natural gas is just used to ignite and maintain combustion, and does not add any significant energy to the gas stream. Therefore the energy and molar balances ignore any effects of the natural gas. These burners generally have a maximum temperature of 2000°F , so additional air over stoichiometric may be needed to maintain this temperature. Using a gas burner increases the temperature and flow rate of the gases into the heat recovery preheater, superheater, boiler, and gas humidification and cooling tower. The overall effect is to increase the cost of the superheater, boiler, gas humidification and cooling tower, weak acid, and effluent stripper components. However, the dilution air, inlet and exit converter flow rates are lower and additional energy is recovered by the superheater and boiler. This reduces the cost for the heat recovery preheater, dilution blower, drying tower and converter. These trade-offs make it difficult to

determine *a priori* whether it is more profitable to use the gas burner, so the user must specify its use.

The boiler and superheater are primarily used to generate high quality steam, which can be used elsewhere in the power plant or to generate electricity. The gas humidification and cooling tower drops the temperature to 169°F, while reducing the moisture content by 30%. This is accomplished by circulating a weak acid through the gas.

Finally the dilution air is added to the inlet gas stream and this combined stream is sent to the drying tower, which removes the remaining moisture by circulating a 93% acid through the gas. The dilution air is determined by an energy balance on the first stage of the converter.

3.1 Performance Model for Acid Plant

The sulfuric acid plant model developed is meant to respond to a number of the factors that affect sulfuric acid plant cost. These include the volume flow rate, moisture content, temperature, pressure, combustible gases, and SO₂ content of the inlet gas stream. To achieve this, mass and energy balances are performed upon key components to determine critical mass and heat loads. These mass and heat loads are used to estimate the capital cost and operating cost.

To perform energy balances, enthalpy data over a large temperature range (77 - 3000°F) are needed for the 11 chemicals listed in the Introduction. These data are obtained by integrating the polynomial correlations for specific heat with respect to temperature obtain from Barin and Knacke [7] and Barin, Knacke and Kubaschewski [8]. These polynomial equations are functions in this model, and are explained in more detail in Appendix A. When a temperature of a gas flow needs to be estimated, an initial estimate is made, which is used to interpolate or extrapolate to the final estimated temperature. This procedure reduces the error to less than 5% and is also a non iterative technique. Some of the assumptions for this model are that the inlet gas is free of dust, arsenic, chlorine, and fluorine; that the inlet pressure entering the heat recovery preheater is 95 - 97" of water; and that the temperatures exiting the gas humidification and cooling tower and the drying tower are 169°F and 120°F respectively. The temperatures in the converter and exiting the heat exchangers surrounding it are the same as those estimated in the Monsanto design for SMC [2]. The pressure drops for all the equipment remains the same. The gases are assumed to be ideal, and

all energy transfers are assumed to be adiabatic. The atmosphere is assumed to have a pressure of 14.687 psi, a temperature of 80°F, contain 21% oxygen, 79% nitrogen on a dry basis, and 0.018 lbs moisture per pound of dry air. These values appear as constants in this report; however, they are actually variables in the model.

The first step is to calculate the characteristics of the inlet gas before and after the inlet compressor. The inlet compressor is used if the pressure exiting the regenerator is less than 95" of water. The gas flow rates are based on the ideal gas law, while the energy consumed by the compressor is depended upon the pressure difference. If the pressure difference is greater than 50" of water, a compressor is used with an efficiency of 75% [9]; otherwise, a blower is used with an efficiency of 85% [10]. The main difference between a blower and a compressor is that a blowers pressure drop is low enough to assume incompressible flow. The temperature, inlet and exit gas flow rate and energy consumed by the inlet compressor are shown below.

$$T_{IC,o} = (T_{R,o} + 460) \left(\frac{14.687 + 3.612e^{-2*97}}{14.687 + 3.612e^{-2}P_{R,o}} \right)^{\frac{1.4-1}{1.4}} - 460 \quad (3.1)$$

$$G_{IC,i} = \frac{1545 M_{R,o} (T_{R,o} + 460)}{60*144 (14.687 + 3.612e^{-2} P_{R,o})} \quad (3.2)$$

$$G_{IC,o} = \frac{1545 M_{R,o} (T_{IC,o} + 460)}{60*144(14.687 + 3.612e^{-2}*97)} \quad (3.3)$$

if $P_{R,o} < 47$ then

$$EC_{IC} = \left(\frac{1545M_{R,o}}{0.75*60*44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2*97}}{14.687 + 3.612e^{-2}P_{R,o}} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (T_{R,o} + 460) \quad (3.4)$$

$$\text{else } EC_{IC} = 1.38e^{-4}G_{IC,i}(97 - P_{R,o})$$

The next step is to determine if the gas burner is used and it affects on the gas flow rate. The model assumes that the pressure drop across the gas burner is negligible. The gas burner is assumed to be fired by natural gas; however, it is also assumed that only enough natural gas is used to maintain and ignite the combustible gases in the inlet stream. Therefore, the energy and mass balances ignore the effects of it. The gas burner has a maximum operating temperature of

2000°F, and completely oxidize all the combustible gases. To prevent the gas burner from operating above 2000°F, additional air is added above the stoichiometric requirement to oxidize the combustible gases. To solve for the additional air requirement, the gas burner is assumed to be divided into two parts, shown in Figure 3-2. The first part burns the gases with 5% excess air. If the total energy flow rate into the first part of the gas burner is greater than the energy flow rate of the exhaust gases at 2000°F, then additional air is added. If it isn't, then the exit temperature of the gas burner is estimated by interpolating between the inlet temperature and 2000°F. The oxygen needed for combustion is,

$$M_{O,c,1} = 2M_{M,R,o} + 0.5M_{H,R,o} + 0.5M_{CM,R,o} + 1.5M_{CS,R,o} + 1.5M_{HS,R,o} + 2M_{S,R,o} \quad (3.5)$$

The additional air needed for 5% excess air is,

$$\text{if } 1.05M_{O,c,1} > M_{O,R,o} \text{ then} \quad (3.6)$$

$$M_{O,c} = 1.05M_{O,c,1} - M_{O,R,o}$$

$$\text{else } M_{O,c} = 0$$

$$M_{N,c} = 3.76M_{O,c} \quad (3.7)$$

$$M_{W,c} = 1.611 * 0.018 (M_{O,c} + M_{N,c}) \quad (3.8)$$

The combustion air has to be raised to 97° of water; therefore its temperature into the gas burner is,

$$T_c = (80 + 460) \left(\frac{14.687 + 3.612e^{-2*97}}{14.687} \right)^{\frac{1.4-1}{1.4}} - 460 \quad (3.9)$$

The next step is to determine the exhaust gases exiting the first part of the gas burner and the energy produced. It is assumed that all the methane, hydrogen, carbon monoxide, hydrogen sulfide, sulfur and COS are oxidized.

$$M_{j,GB,1} = 0$$

$$M_{SD,GB,1} = M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o} \quad (3.10)$$

$$M_{W,GB,1} = M_{W,R,o} + M_{W,c} + 2M_{M,R,o} + M_{H,R,o} + M_{HS,R,o} \quad (3.11)$$

$$M_{CD,GB,1} = M_{CD,R,o} + M_{M,R,o} + M_{CM,R,o} + M_{CS,R,o} \quad (3.12)$$

$$M_{N,GB,1} = M_{N,R,o} + M_{W,c} \quad (3.13)$$

if $M_{O,R,o} > 1.05M_{O,c,l}$ then (3.14)

$$M_{O,GB,1} = M_{O,R,o} - M_{O,c,l}$$

else $M_{O,GB,1} = 0.05M_{O,c,l}$

where $j = CM, CS, H, HS, M, S$

$$\Delta H_{GB} = 345,200M_M + 104,000M_H + 121,700M_{CM} + 255,400M_S + \quad (3.15)$$

$$222,900M_{HS} + 236,000M_{CS}$$

Now an energy balance is performed upon the first part of the gas burner to see if more air is needed to cool the gas burner. Two estimates are made for the exit temperature: one is made at the maximum allowable temperature of 2000°F, the other is made at the inlet temperature. If the total energy entering the gas burner is greater than the energy flow rate of the exhaust gases at 2000°F, then additional air is needed to cool the gas. If the temperature is less than 2000°F, then no additional air is added, and the exit temperature is estimated by a linear interpolation between the inlet temperature and 2000°F. Finally, the total molar and volumetric flow rates of the combustion air are calculated, along with the energy consumed by the gas burner combustion air compressor.

$$E_{GB,i} = \sum_{k=1}^{11} \hat{h}_k(T_{GB,i})M_{GB,i} \quad (3.16)$$

$$E_c = \hat{h}_O(T_c)M_{O,c} + \hat{h}_N(T_c)M_{N,c} + \hat{h}_{W,c}(T_c)M_{w,c} \quad (3.17)$$

$$E_{GB,total} = E_{BG,i} + E_c + \Delta H_{GB} \quad (3.18)$$

$$E_{GB,max} = \sum_{j=1}^5 \hat{h}_j(2000)M_{j,1} \quad (3.19)$$

$$E_{GB,min} = \sum_{j=1}^5 \hat{h}_j(T_{GB,i})M_{j,1} \quad (3.20)$$

where $k = CD, CM, CS, H, HS, M, N, O, S, SD, W$

and $j = CD, N, O, SD, W$

if $E_{GB,total} > E_{GB,max}$ then (3.21)

$$M_{O,ex} = \frac{E_{GB,total} - E_{GB,max}}{15,180 - \hat{h}_O(T_c) + 3.76(14,440 - \hat{h}_N(T_c)) + 1.611*0.018*(17,920 - \hat{h}_W(T_c))}$$

$$T_{GB,o} = 2000$$

$$\text{else } M_{O,ex} = 0$$

$$T_{GB,o} = \frac{2000 - T_{GB,i}}{E_{GB,max} - E_{GB,min}} (E_{GB,total} - E_{GB,min}) + T_{GB,i}$$

$$M_{N,ex} = 3.76M_{O,ex} \quad (3.22)$$

$$M_{W,ex} = 1.611*0.018*4.76M_{O,ex} \quad (3.23)$$

$$M_{c,total} = M_{O,c} + M_{N,c} + M_{W,c} + M_{O,ex} + M_{N,ex} + M_{W,ex} \quad (3.24)$$

$$G_{c,total} = \frac{1545M_{c,total} (80 + 460)}{60*14.687*144} \quad (3.25)$$

$$EC_{GBC} = \left(\frac{1545M_{c,total}}{0.75*60*44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687+3.612e^{-2}*97}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460) \quad (3.26)$$

The next step is to determine the composition and temperature of the gas steam entering the heat recovery preheater. It should be noted that the composition of the gas stream between the gas burner and the first stage of the converter is the same, except for the moisture content. This allows the use of the same variable names for the composition of the gas stream between the gas burner and converter, which saves space and increases execution speed. The composition of the gas stream entering the heat recovery preheater depends on whether the gas burner is used. If it isn't used, the composition and temperature are the same as those exiting the regenerator.

If a gas burner is not used then,

$$M_{k,HP,i} = M_{k,R,o} \quad (3.27)$$

$$T_{HP,i} = T_{R,o} \quad (3.28)$$

else

$$M_{j,HP,i} = 0 \quad (3.29)$$

$$M_{SD,HP,i} = M_{SD,GB,1} \quad (3.30)$$

$$M_{CD,HP,i} = M_{CD,GB,1} \quad (3.31)$$

$$M_{W,HP,i} = M_{W,GB,1} + M_{W,ex} \quad (3.32)$$

$$M_{N,HP,i} = M_{N,GB,1} + M_{N,ex} \quad (3.33)$$

$$M_{O,HP,i} = M_{O,GB,1} + M_{O,ex} \quad (3.34)$$

$$T_{HP,i} = T_{GB,o} \quad (3.35)$$

$$M_{HP,i} = \sum_{k=1}^{11} M_{k,HP,i} \quad (3.36)$$

$$G_{HP,i} = \frac{1545 M_{HP,i} (T_{HP,i} + 460)}{60 \cdot 144 \cdot (14.687 + 3.612e^{-2} \cdot 97)}$$

where $k = CD, CM, CS, H, HS, M, N, O, S, SD, W$

and $j = CM, CS, H, HS, M, S$

So far the algorithms has followed the gas stream into the acid plant, and it would seem logical to model the heat recovery preheater next. However, the heat load on the preheater is determined by the gas flow exiting the second stage of the converter, M25, which hasn't been determined, and this gas flow is depended upon the gas flow entering the converter. This cyclic problem is eliminated by the assumptions made at the beginning of this section and noting that the composition of the gas entering the converter can be predicted by the composition exiting the gas burner. Another important assumption is dividing the first stage of the converter into two parts. The first part burns the combustible gases and converts 70% of the SO_2 to SO_3 ; the second part adds dilution air to lower the temperature to 1158°F. This is the same procedure used for the gas burner. Some other important points are:

- The combustible gases entering the converter are the same as those exiting the gas burner; therefore, the energy released in the first stage of the converter can be determined.
- The oxygen requirement for complete conversion of SO_2 to SO_3 and the oxidation of the other combustible gases can be calculated.
- The gas entering the first stage of the converter is assumed to be 997°F, and free of moisture, since the drying tower removes all moisture.

The oxygen consumed in the first stage is calculated, along with the oxygen needed for oxidization all the combustible gases and converting all the SO₂ to SO₃ is calculated below. This ensures that enough oxygen is available to convert the SO₂ to SO₃. Once these values are known the composition of the gas exiting the converter, not including additional dilution air needed to maintain 1158°F, can be determined:

$$M_{O,CS,1} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.35M_{SD,PH,i} + 1.85M_{CS,PH,i} + 1.85M_{HS,PH,i} + 2.7M_{S,PH,i} \quad (3.37)$$

$$M_{O,CS,all} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.5M_{SD,PH,i} + 2M_{CS,PH,i} + 2M_{HS,PH,i} + 3M_{S,PH,i} \quad (3.38)$$

$$\text{if } M_{O,CS,all} > M_{O,PH,i} \text{ then } M_{O,CS,c} = M_{O,CS,all} - M_{O,PH,i} \quad (3.39)$$

else $M_{O,CS,c} = 0$

$$M_{N,CS,c} = 3.76M_{O,CS,c} \quad (3.40)$$

$$M_{W,CS,c} = 1.611 * 0.018 (M_{O,CS,c} + M_{O,CS,c}) \quad (3.41)$$

$$\text{if } M_{O,CS,all} > M_{O,PH,i} \text{ then } M_{O,CS,1,o} = M_{O,CS,all} - M_{O,CS,1} \quad (3.42)$$

else $M_{O,CS,1,o} = M_{O,PH,i} - M_{O,CS,1}$

$$M_{N,CS,1,o} = M_{N,PH,i} + M_{N,CS,c} \quad (3.43)$$

$$M_{CD,CS,1,o} = M_{CD,PH,i} + M_{M,PH,i} + M_{CM,PH,i} + M_{CS,PH,i} \quad (3.44)$$

$$M_{W,CS,1,o} = M_{H,PH,i} + 2M_{M,PH,i} + M_{HS,PH,i} \quad (3.45)$$

$$M_{ST,CS,1,o} = 0.7(M_{SD,PH,i} + 2M_{S,PH,i} + M_{HS,PH,i} + M_{CS,PH,i}) \quad (3.46)$$

$$M_{SD,CS,1,o} = 0.3(M_{SD,PH,i} + 2M_{S,PH,i} + M_{HS,PH,i} + M_{CS,PH,i}) \quad (3.47)$$

$$\Delta H_{CS,1} = 42,570 * 0.7M_{SD,PH,i} + 345,200M_{M,PH,i} + 104,000M_{H,PH,i} + 121,700M_{CM,PH,i} + 315,000M_{S,PH,i} + 261,500M_{HS,PH,i} + 265,800M_{CS,PH,i} \quad (3.48)$$

With this information an energy balance can be performed on the second part of the first stage to determine the additional amount of dry air needed to cool the catalyst to 1158°F. Then the total molar flow rate of moist dilution air can be calculated. The energy flow rate into the second part of the first stage is the energy flow of all the species entering the heat recovery preheater at 779°F, except for the moisture, plus the energy flow from the combustion air at 779°F, plus the energy

released in the first part. The energy flow out of the second part of the first stage is the sum of the product gases at 1158°F. The constants in Equation 3.49 are the enthalpies of oxygen and nitrogen at 779°F. The constant 2864.2 in Equation 3.51 is the enthalpy difference for dry air between 1158°F and 779°F.

$$E_{CS,1} = \sum_{k=1}^{10} \hat{h}_k(779)M_{k,PH,i} + 5,235.7M_{O,CS,c} + 5,028.4M_{N,CS,c} + \Delta H_{CS,1} \quad (3.49)$$

$$E_{CS,1,max} = \sum_{j=1}^6 \hat{h}_j(1158)M_{j,CS,1,o} \quad (3.50)$$

$$M_{air,CS,ex} = \frac{E_{CS,1} - E_{CS,1,max}}{2,864.2} \quad (3.51)$$

$$M_{BF} = (1 + 1.611*0.018)M_{air,CS,ex} + M_{O,CS,c} + M_{N,CS,c} + M_{W,CS,c} \quad (3.52)$$

where $k = CD, CM, CS, H, HS, M, N, O, S, SD$

and $j = CD, N, O, SD, ST, W$

Now the molar flow rates for the gas streams entering and exiting the drying tower and gas streams, 23 & 25 can be determined. The gas stream entering the drying tower is the same as the gas stream entering the heat recovery preheater minus the moisture removed in the gas humidification and cooling tower plus the moist dilution air. This includes all the moisture added with the dilution air, since the dilution air compressor is upstream of the drying tower. The gas streams, 23 & 25, are a bit more complicated to figure out. Stream 23 is after the second stage of the converter, which converts an additional 83% of the SO_2 exiting the first stage to SO_3 , which consumes oxygen. Therefore gas stream 23 is the sum of $M_{k,CS,1,o}$, the air added for temperature control, $M_{air,CS,ex}$, minus the oxygen consumed in the second stage. After the second stage it passes through the interpass tower, which removes all the moisture and converts all the SO_3 to sulfuric acid. Note that the variables $M_{N,CS,1,o}$, $M_{O,CS,1,o}$, and $M_{CD,CS,1,o}$ do not include the dry air needed to cool the catalyst to 1158°F.

$$M_{D,i} = M_{PH,i} + M_{BF} - 0.3M_{W,PH,i} \quad (3.53)$$

$$M_{D,o} = M_{D,i} - 0.7M_{W,PH,i} - 1.611*0.018M_{air,CS,ex} - M_{W,CS,c} \quad (3.54)$$

$$M_{23} = \sum_{k=1}^6 M_{k,CS,1,o} + M_{air,CS,ex} - 0.5*0.83M_{SD,CS,1,o} \quad (3.55)$$

$$M_{CD,25} = M_{CD,CS,1,o} \quad (3.56)$$

$$M_{N,25} = M_{N,CS,1,o} + 0.79M_{air,CS,ex} \quad (3.57)$$

$$M_{O,25} = M_{O,CS,1,o} + 0.21M_{air,CS,ex} - 0.5*0.83*M_{SD,CS,1,o} \quad (3.58)$$

$$M_{SD,25} = 0.17M_{SD,CS,1,o} \quad (3.59)$$

$$M_{25} = \sum_{j=1}^4 M_{j,25} \quad (3.60)$$

where $k = CD, N, O, SD, ST, W$

and $j = CD, N, O, SD$

With this information, it is possible to model the heat recovery preheater, superheater, and boiler. Schematic diagrams for the heat recovery preheater, boiler, and superheater are shown in Figure 3-3. The factor which will most directly affect the cost of heat exchangers are the required heat transfer surface area. This is calculated based on knowledge of the heat transfer load, the heat transfer coefficient U , and the log mean temperature difference (LMTD) for the heat exchanger. The heat transfer coefficients for the heat recovery preheater, superheater, and boiler are 4.5, 6, and 15 respectively, which are taken from the Monsanto design.

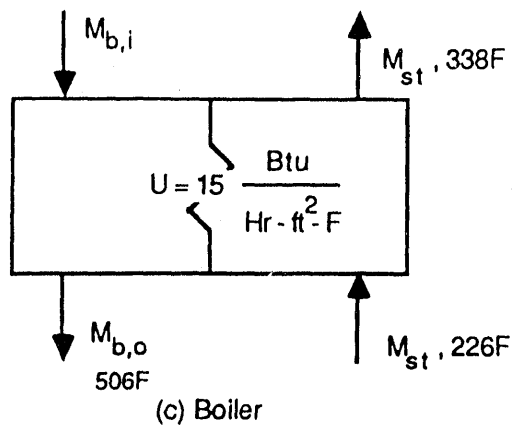
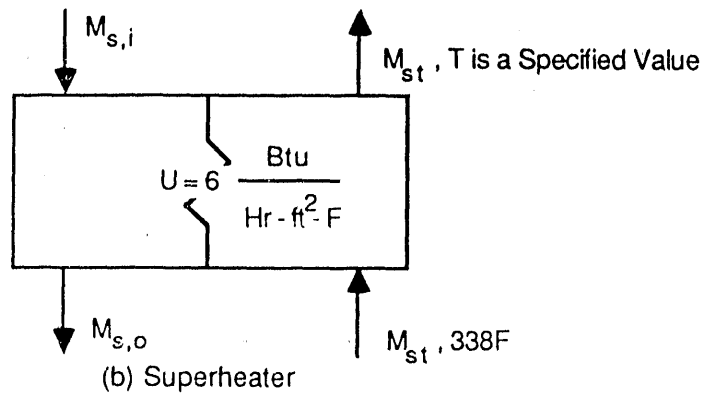
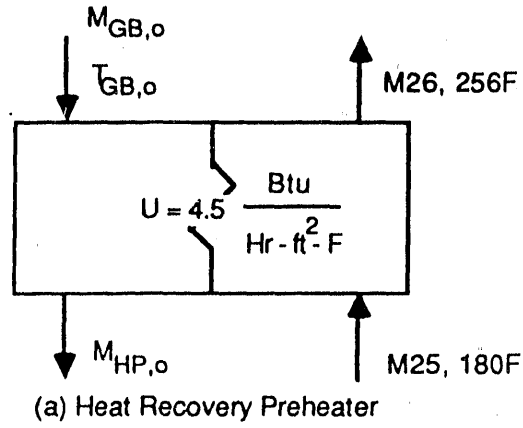
The heat load in the heat recovery preheater is energy needed to raise the gas stream, 25, from 180°F to 256°F. The exit temperature of the heat recovery preheater is estimated by making a guess of the exit temperature based on the ratio of the heat load to the energy entering heat recovery preheater. This algorithm is used instead of a constant since it provides a reasonable estimate of the exit temperature. This temperature estimate is used to estimate the energy flow rate exiting the heat recovery preheater. The energy estimate is used to calculate the exit temperature. The exit temperature is used to calculate the log mean temperature difference, which is used to determine the area of the heat recovery preheater.

$$Q_{HP} = \sum_{j=1}^4 (\hat{h}_j(256) - \hat{h}_j(180))M_{j,25} \quad (3.61)$$

$$E_{HP,i} = \sum_{k=1}^{11} \hat{h}_k(T_{HP,i})M_k \quad (3.62)$$

$$T_{guess} = T_{HP,i} \left(1 - \frac{Q_{HP}}{E_{HP,i}} \right) \quad (3.63)$$

Figure 3-3: Inlet Gas Cooling Heat Exchangers



$$E_{\text{guess}} = \sum_{k=1}^{11} \hat{h}_k(T_{\text{guess}})M_k \quad (3.64)$$

where $j = \text{CD, N, O, SD}$

and $k = \text{CD, CM, CS, H, HS, M, N, O, S, SD, W}$

$$T_{\text{HP,o}} = -Q_{\text{HP}} \frac{T_{\text{HP,i}} - T_{\text{guess}}}{E_{\text{HP,i}} - E_{\text{guess}}} + T_{\text{HP,i}} \quad (3.65)$$

$$\text{LMTD}_{\text{HP}} = \frac{(T_{\text{HP,i}} - 256) - (T_{\text{HP,o}} - 180)}{\ln \left(\frac{T_{\text{HP,i}} - 256}{T_{\text{HP,o}} - 180} \right)} \quad (3.66)$$

$$A_{\text{HP}} = \frac{Q_{\text{HP}}}{4.5 \text{LMTD}_{\text{HP}}} \quad (3.67)$$

The calculations for the boiler and superheater are similar, except that first the amount of water that can be heated to steam must be determined, and then the calculations for the LMTD and heat transfer areas of the boiler and superheater can be made. In order to parallel the design work performed by Monsanto, the off-gas temperature leaving the boiler is specified as 506°F, unless the exit temperature of the heat recovery preheater is less. If this occurs, the superheater and boiler are not used, no steam is generated, and the temperature of the gas entering the gas humidification and cooling tower is the exit temperature of the heat recovery preheater.²

The water mass flow rate required for conversion to steam is calculated by determining how much energy is available in the hot regenerator off-gas to heat water from 226°F to superheated steam at a specified temperature and 100 psia. The constant 17,929 is the energy needed to raise a mole of saturated water at 226 to 338°F, while 2134.8 is the enthalpy of saturated steam at 338°F. The temperature of the superheated steam is a user specified value, since this steam can be used by some FGD processes, which require steam at different temperatures.

$$E_{\text{HP,o}} = E_{\text{HP,i}} - Q_{\text{HP}} \quad (3.68)$$

² Instead of testing the exit temperature of the heat recovery preheater to see if it is greater than 506, the energy flow of the gas stream exiting the heat recovery preheater is compared against the energy flow of the gas stream at 506. This method is used since the exit temperature is just an interpolated estimate, while the energy flow exiting the preheater can be determined more accurately by subtracting the heat load from the energy entering the preheater.

$$E_{506} = \sum_{k=1}^{11} \hat{h}_k (506) M_k \quad (3.69)$$

if $E_{HP,o} > E_{506}$ then

$$E_{GC,i} = E_{506} \quad (3.70)$$

$$T_{GC,i} = 506 \quad (3.71)$$

else

$$E_{GC,i} = E_{HP,o}$$

$$T_{GC,i} = T_{HP,o}$$

$$M_{st} = \frac{E_{HP,o} - E_{GC,i}}{\hat{h}_W(T_{\text{specified}}) - 2134.8 + 17,929} \quad (3.72)$$

Now the boiler and superheater energy loads can be determined, and after an energy balance calculation, the boiler inlet temperature can be determined. The inlet temperature of the boiler can be estimated in a similar manner to the exit temperature of the heat recovery preheater. From this, the LMTD for both the superheater and the boiler can be calculated. Finally, the required heat transfer areas for both heat exchangers are calculated from knowledge of the heat transfer coefficient, heat load, and LMTD.

$$Q_b = 17,929 M_{st} \quad (3.73)$$

$$Q_s = (\hat{h}_W(T_{\text{specified}}) - 2134.8) M_{st} \quad (3.74)$$

$$T_{\text{guess}} = T_{HP,i} \left(1 - \frac{Q_{HP}}{E_{HP,i}} \right) \quad (3.75)$$

$$E_{\text{guess}} = \sum_{k=1}^{11} \hat{h}_k (T_{\text{guess}}) M_k \quad (3.76)$$

$$T_{bi,i} = -Q_s \frac{T_{HP,o} - T_{\text{guess}}}{E_{HP,o} - E_{\text{guess}}} + T_{HP,o} \quad (3.77)$$

The log mean temperature differences for the boiler and superheater are based on the inlet and outlet temperatures of the two heat exchangers. The required heat transfer surface area for each is calculated based on the heat load, the log mean temperature difference, and the universal heat transfer coefficient. The values for the heat transfer coefficients are adopted from the Monsanto estimate.

$$\text{LMTD}_s = \frac{(T_{\text{HP,o}} - T_{\text{specified}}) - (T_{\text{b,i}} - 338)}{\ln \left(\frac{T_{\text{HP,o}} - T_{\text{specified}}}{T_{\text{b,i}} - 338} \right)} \quad (3.78)$$

$$\text{LMTD}_b = \frac{(T_{\text{b,i}} - 338) - (506 - 226)}{\ln \left(\frac{T_{\text{b,i}} - 338}{506 - 226} \right)} \quad (3.79)$$

$$A_s = \frac{Q_s}{6\text{LMTD}_s} \quad (3.80)$$

$$A_b = \frac{Q_b}{15\text{LMTD}_b} \quad (3.81)$$

The off-gas enters the cooling and humidification tower at a temperature of 506°F and leaves at 169°F. It is assumed that about 30 percent of the water vapor is removed based on the Monsanto design. Cooling is effected by the circulation of a weak acid stream through the cooling tower. The mass flow of this stream is calculated by an energy balance. The constant 324.6 is amount of energy needed to raise the temperature of the weak acid from 163°F to 181°F. The constants 840.6 and 17,813 are the enthalpy and heat of vaporization at 181°F.

$$E_{\text{GC,o}} = \sum_{k=1}^{11} \hat{h}_k(169)M_k - 0.3\hat{h}_w(169)M_{\text{W,HP,i}} \quad (3.82)$$

$$M_{\text{WA}} = \frac{E_{\text{GC,i}} - E_{\text{GC,o}} + 0.3(\hat{h}_w(T_{\text{GC,i}}) - 840.6 + 17,813)M_{\text{W,HP,i}}}{324.6} \quad (3.83)$$

The electricity usage for the main and dilution compressors, as well as, the pumps used for the strong, weak, and product acid pumps can be determined. The pressure drops across the main and dilution compressors are 116" and 67" of water respectively.

$$\text{EC}_{\text{BF}} = \left(\frac{1545M_{\text{BF}}}{0.75 \cdot 60 \cdot 44240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} \cdot 67}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460) \quad (3.84)$$

$$\text{EC}_{\text{MC}} = \left(\frac{1545M_{\text{D,o}}}{0.75 \cdot 60 \cdot 44240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} \cdot 167}{14.687 + 3.612e^{-2} \cdot 51} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (120 + 460) \quad (3.85)$$

The total acid produced can be determined along with the energy consumption of the pumps. The pressure drops for the strong, weak, and product acid pumps are 80 feet of water, 120 psi,

and 80 psi respectively. The efficiency for the strong and weak acid pumps are 80%, while the product pump is much smaller and has an efficiency of 70%. The specific gravity for sulfuric acid greater than 95% is 1.83, while the specific gravity for weak acid is assumed to be 1. The specific gravity for the product acid at 93% concentration, is estimated to be 1.77, which equals $1.83 \cdot 0.93 + 1 \cdot 0.07$. The energy needed for the weak acid pump is based on the molar flow rate of weak acid. The strong acid system which supplies acid to the drying, interpass, and final towers has three pumps. Therefore the energy usage is based on scaling the total flow rate for these pumps on the sulfuric acid produced. In the Monsanto design, 3501 gallons per minute of strong acid is pumped against a head of 80 feet of water for 17.3 tons per hour of acid produced.

$$m_{\text{acid}} = \frac{0.995 (M_{\text{SD,R,o}} + M_{\text{CS,R,o}} + M_{\text{HS,R,o}} + 2M_{\text{S,R,o}}) * 98 \text{ lbm/lbmole}}{2000 \text{ tons/lbm}} \quad (3.86)$$

$$EC_{\text{WA}} = \frac{120 \frac{\text{lbf}}{\text{in}^2} * 18 \frac{\text{lbm}}{\text{lbmole}} * 144 \frac{\text{in}^2}{\text{ft}^2} M_{\text{WA}}}{44,240 \frac{\text{ft-lbf/min}}{\text{kW}} * 7.4805 \frac{\text{gal}}{\text{ft}^3} * 60 \frac{\text{min}}{\text{hr}} * 8.33 \frac{\text{lbm}}{\text{gal}} * 0.80}$$

which simplifies to

$$EC_{\text{WA}} = \frac{120 \frac{\text{lbf}}{\text{in}^2} M_{\text{WA}}}{63,813 \frac{\text{lbmole/hr} * \text{lbf/in}^2}{\text{kW}} * 0.80} \quad (3.87)$$

$$EC_{\text{SS}} = \frac{\left(\frac{3501 \frac{\text{gal}}{\text{min}}}{17.3 \frac{\text{tons}}{\text{hr}}} \right) 80 \text{ ft} * 61.2 \frac{\text{lbm}}{\text{ft}^3} * 32.174 \frac{\text{ft}}{\text{sec}^2} * 1.83 m_{\text{acid}}}{7.4805 \frac{\text{gal}}{\text{ft}^3} * 32.174 \frac{\text{lbm-ft}}{\text{lbf-sec}^2} * 44,240 \frac{\text{ft-lbf/min}}{\text{kW}} * 0.80}$$

which simplifies to

$$EC_{\text{SS}} = \frac{202.4 \frac{\text{gal/min}}{\text{tons/hr}} * 80 \text{ ft} m_{\text{acid}}}{2955 \frac{\text{gal/min} * \text{ft}}{\text{kW}} * 0.80} \quad (3.88)$$

$$EC_{\text{PA}} = \frac{2000 \frac{\text{lbm}}{\text{ton}} * 144 \frac{\text{in}^2}{\text{ft}^2} * 80 \frac{\text{lbf}}{\text{in}^2} m_{\text{acid}}}{60 \frac{\text{min}}{\text{hr}} * 8.33 \frac{\text{lbm}}{\text{gal}} * 7.4805 \frac{\text{gal}}{\text{ft}^3} * 44,240 \frac{\text{ft-lbf/min}}{\text{kW}} * 1.77 * 0.70} \quad (3.89)$$

which simplifies to

$$EC_{PA} = \frac{80 \frac{\text{lb}}{\text{in}^2} m_{\text{acid}}}{1017 \frac{\text{tons/hr lb/in}^2}{\text{kW}} * 0.70} \quad (3.90)$$

The total energy consumed is the sum of the inlet, gas burner, dilution air, and main compressor plus the weak, strong, and product acid pumps. The equivalent electric power of the steam produced is calculated by assuming an 88% efficient boiler and the heat rate specified by the main power plant.

$$EC_{\text{total}} = EC_{IC} + EC_{GB} + EC_{BF} + EC_{MC} + EC_{WA} + EC_{SS} + EC_{PA} \quad (3.91)$$

$$EC_{\text{st}} = \frac{E_{\text{PH},o} - E_{\text{GC},i}}{0.88\text{HR}} \quad (3.92)$$

3.2 Economic Model

The cost estimate for the sulfuric acid plant is based on physical parameters that affect the cost of the equipment in the plant. An experimental scaling factor of 0.6 is assumed and all the capital cost are in mid-83 dollars, except for the inlet compressor and gas burner which are mid-82 dollars. All costs may later be adjusted to a current basis using appropriate cost-escalators included in the IEC model.

3.2.1 Capital Cost

The cost of the inlet compressor depends on the pressure drop and the inlet gas flow rate. The cost is split by pressure drop since the capital cost of blowers and compressors increase with increasing pressure. The cost estimates came from the NOXSO chapter in the EPRI Economic Evaluation of FGD System [6]. For both estimates, it is assumed that there are two operating and one spare. The algorithm is:

$$\text{if } P_{R,o} < 47" \text{ of water} \quad (3.93)$$

$$DCC_{IC} = \$1.04e^6 \left(\frac{G_{R,o}}{35,000 \text{ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314}$$

else if $47 \leq P_{R,o} < 95$

$$DCC_{IC} = \$5.64e^6 \left(\frac{G_{R,o}}{1.80e^6 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314}$$

The capital gas of the gas burner is also taken from reference [6]. It is assumed that there are two operating and one spare, and that the cost includes the cost of the combustion air compressor.

$$DCC_{GB} = \$7.07e^5 \left(\frac{G_{IC,o}}{68,000 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314} \quad (3.94)$$

The heat recovery preheater cost is scaled to the Monsanto cost estimate of \$29,000 for a heat exchanger with an area of 1100 square feet. The cost of the boiler is based on an estimated cost of \$53,000 for a heat exchanger with 350 square feet of heat exchange area. The cost of the superheater is scaled from the estimate of \$80,000 for a heat exchanger with an area of 50 square feet.

$$DCC_{HP} = \$29,000 \left(\frac{A_{HP}}{1,100 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.95)$$

$$DCC_b = \$53,000 \left(\frac{A_b}{350 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.96)$$

$$DCC_s = \$80,000 \left(\frac{A_s}{50 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.97)$$

The gas humidification and cooling tower cost estimate is based on the Monsanto estimate of \$367,000 for a gas stream of 1063 lbmole/hr. The cost of the tower is scaled to the off-gas flow $M_{GC,i}$ entering the sulfuric acid plant.

$$DCC_{GC} = \$367,000 \left(\frac{M_{GC}}{1,063 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.98)$$

The weak acid system is associated with the gas humidification and cooling tower. The cost of this system is proportional to the flow rate of weak acid, M_{WA} , required to achieve the necessary cooling in the tower.

$$DCC_{WA} = \$39,000 \left(\frac{M_{WA}}{19,250 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.99)$$

The drying tower is sized to accommodate the inlet gas stream consisting of the regenerator

off-gas and dilution air, $M_{D,i}$. Monsanto estimated a cost of \$636,000 for a tower that handles 5325 lbmole/hr of gas.

$$DCC_D = \$636,000 \left(\frac{M_{D,i}}{5,325 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.100)$$

The blower and filter are required to pump and clean the dilution air mass flow, M_{BF} , and are sized accordingly. Monsanto estimated the cost of these components based on a dilution air inlet flow of 4407 lbmole/hr.

$$DCC_{BF} = \$518,000 \left(\frac{M_{BF}}{4,407 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.101)$$

The contact section of the sulfuric acid plant includes the inter-pass heat exchangers and the catalytic converter. The total cost of this part of the system was estimated by Monsanto to be \$2,681,000. The cost of this part of the plant is scaled to the gas flow exiting the drying tower.

$$DCC_{CS} = \$2,681,000 \left(\frac{M_{D,o}}{4,854 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.102)$$

The cost for the interpass and final towers and their associated equipment was estimated to be \$988,000. This cost is scaled to the gas stream M_{23} .

$$DCC_T = \$988,000 \left(\frac{M_{23}}{4,685 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.103)$$

The strong acid system is proportional in size to the amount of sulfur in the off-gas stream. The cost of the effluent stripper is assumed to be proportional to the off-gas flow rate.

$$DCC_{SA} = \$739,000 \left(\frac{M_{SD,HP,i} + M_{CS,HP,i} + M_{HS,HP,i} + 2M_{S,HP,i}}{354 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.104)$$

$$DCC_{ES} = \$70,000 \left(\frac{M_{GC,i}}{1,063 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.105)$$

The total direct cost of the sulfuric acid plant is the sum of the individual equipment direct capital costs. The indirect capital cost, not including AFUDC, is estimated to be 27.5%, 41.9%, and 8.1% of the total direct cost for the labor and general field cost, home office cost, and contingency respectively.

$$DCC_{total} = \sum_{k=1}^{13} DCC_k \quad (3.106)$$

$$TCC_{\text{acid}} = (1 + 0.275 + 0.419 + 0.081)DCC_{\text{total}} = 1.776DCC_{\text{total}} \quad (3.107)$$

3.2.2 Operating and Maintenance Costs

The non-utility operating costs of an acid plant consist of the operating, maintenance, and administration labor, plus maintenance material, catalyst makeup, marketing, and shipping cost. The labor costs and makeup requirements are estimated from letters with Monsanto [4,5]. The maintenance personnel are assumed to only work 1/3 of the total number of hours in a year; whereas, it is assumed that 2 operators are always working around the clock. Acid plants of this size require 2 operators per shift, with 2 full time maintenance people. The administration and support labor cost is estimated to be 30% of the operating and maintenance labor cost.

$$OC_{\text{oper}} = 2 \text{ persons} * 19.70 \text{ \$/hr} * 8766 \text{ hrs/yr} * C_{\text{idx}}/325.3 \quad (3.108)$$

$$OC_{\text{maint-labor}} = 2 \text{ persons} * 19.70 \text{ \$/hr} * 8766 \text{ hrs/yr} / 3 * C_{\text{idx}}/325.3 \quad (3.109)$$

$$OC_{\text{admin}} = 0.30 * (OC_{\text{oper}} + OC_{\text{maint-labor}}) \quad (3.110)$$

The maintenance material costs is estimated as a fraction of the direct capital cost. The fraction is 0.9%. The makeup of the catalyst is approximately 2% per year and the converter requires approximately \$35.2 per lbmole/hr of gas flow (1985\$) [5]. The marketing and shipping cost are estimated to be 10% of the sulfuric acid credit [11]. Sulfuric acid is assumed to sell for \$50/ton (1985\$). [11].

$$OC_{\text{maint-matl}} = 0.009 * DCC_{\text{total}} \quad (3.111)$$

$$OC_{\text{makeup}} = 0.02 * 35.2 \text{ \$/lbmole/hr} * M_c * C_{\text{idx}}/325.3 \quad (3.112)$$

$$OC_{\text{credit}} = 50 \text{ \$/ton} * CF * 8766 * m_{\text{acid}} * C_{\text{idx}}/325.3 \quad (3.113)$$

$$OC_{\text{marketing}} = 0.1 * OC_{\text{credit}} \quad (3.114)$$

$$OC_{\text{total}} = OC_{\text{oper}} + OC_{\text{maint-labor}} + OC_{\text{admin}} + OC_{\text{maint-mater}} + OC_{\text{makeup}} \\ + OC_{\text{marketing}} - OC_{\text{credit}} \quad (3.115)$$

3.3 Numerical Example

This section contains a numerical example of the sulfuric acid plant model presented in the previous sections. The input parameters and their values necessary to run the model are given in Table 1. The model will be illustrated by using a gas stream with a large quantity of combustible gases, which requires the use of the gas burner. The gas stream is not from any particular report or FGD process. The composition consist of all the species with which this model has been designed for except for nitrogen and oxygen.³ The pressure exiting the regenerator in the FGD process is 28" of water; therefore, the inlet compressor is required to raise the pressure to 97" of water.

Since the pressure of the regenerator off-gas is less than 97" of water, the inlet compressor is needed. Equations 3.1, 3.2, 3.3, and 3.4 are used to calculate the temperature exiting the inlet compressor, gas flow rate in actual cubic feet per minute, and electricity consumption of the compressor.

$$T_{IC,o} = (T_{R,o} + 460) \left(\frac{14.687 + 3.612e^{-2} * 97}{14.687 + 3.612e^{-2} P_{R,o}} \right)^{\frac{1.4-1}{1.4}} - 460 \quad (3.1)$$

$$T_{IC,i} = (550 + 460) \left(\frac{14.687 + 3.612d^{-2} * 97}{14.687 + 3.612e^{-2} * 28} \right)^{\frac{1.4-1}{1.4}} - 460$$

$$T_{IC,i} = 958.5^{\circ}F$$

$$G_{IC,i} = \frac{1545 M_{R,o} (T_{R,o} + 460)}{60 * 144 (14.687 + 3.612e^{-2} P_{R,o})} \quad (3.2)$$

$$G_{IC,i} = \frac{1545 * 1,568 * (550 + 460)}{60 * 144 (14.687 + 3.612e^{-2} * 28)}$$

$$G_{IC,i} = 24,290 \text{ acfm}$$

$$G_{IC,o} = \frac{1545 M_{R,o} (T_{IC,o} + 460)}{60 * 144 (14.687 + 3.612e^{-2} * 97)} \quad (3.3)$$

³ There are two reasons for not including oxygen and nitrogen in the gas stream for the numerical example. Since there are products of incomplete oxidation in this particular gas stream, it is not likely to contain oxygen. Nitrogen could have been added to the gas; however, any nitrogen available would probably have been added with air to completely oxidize the gas in the regenerator.

Table 1: Input Parameters for Sulfuric Acid Plant Numerical Example

| Input Parameter | Sample Value | Input Parameter | Sample Value |
|------------------------|---------------|-----------------|-----------------|
| $T_{R,o}$ | 900°F | $M_{M,R,o}$ | 10 lbmole/hr |
| $P_{R,o}$ | 28" of water | $M_{N,R,o}$ | 0 lbmole/hr |
| $T_{\text{specified}}$ | 550°F | $M_{O,R,o}$ | 0 lbmole/hr |
| $M_{CD,R,o}$ | 500 lbmole/hr | $M_{S,R,o}$ | 41 lbmole/hr |
| $M_{CO,R,o}$ | 50 lbmole/hr | $M_{SD,R,o}$ | 200 lbmole/hr |
| $M_{COS,R,o}$ | 17 lbmole/hr | $M_{W,R,o}$ | 500 lbmole/hr |
| $M_{H,R,o}$ | 100 lbmole/hr | $M_{R,o}$ | 1,568 lbmole/hr |
| $M_{HS,R,o}$ | 150 lbmole/hr | | |

$$G_{IC,o} = \frac{1,545 \cdot 1,568 \cdot (958.54 + 460)}{60 \cdot 144 \cdot (14.687 + 3.612e^{-2} \cdot 97)}$$

$$G_{IC,o} = 21,865 \text{ acfm}$$

if $P_{R,o} < 47$ then

$$EC_{IC} = \left(\frac{1545 M_{R,o}}{0.75 \cdot 60 \cdot 44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} \cdot 97}{14.687 + 3.612e^{-2} P_{R,o}} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (T_{R,o} + 460) \quad (3.4)$$

$$\text{else } EC_{IC} = 1.38e^{-4} G_{IC,i} (97 - P_{R,o})$$

Since 28" is less than 97"

$$EC_{IC} = \left(\frac{1,545 \cdot 1,568}{0.75 \cdot 60 \cdot 44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} \cdot 97}{14.687 + 3.612e^{-2} \cdot 28} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (T_{R,o} + 460)$$

$$EC_{IC} = 249.3 \text{ kW}$$

The gas burner is used since the inlet gas contains a lot of combustible gases. The algorithm of the gas burner divides it into two parts, see Figure 3-3. The first part determines the amount of energy released by burning the combustible gases. This is used to determine the total energy flow exiting the first part of the gas burner, and the composition of the outlet gas. The air needed for combustion and its temperature are calculated first.

$$M_{O,c,1} = 2M_{M,R,o} + 0.5M_{H,R,o} + 0.5M_{CM,R,o} + 1.5M_{CS,R,o} + 1.5M_{HS,R,o} + 2M_{S,R,o} \quad (3.5)$$

$$M_{O,c,1} = 2*10 + 0.5*100 + 0.5*50 + 1.5*17 + 1.5*150 + 2*41 = 427.5 \text{ lbmole/hr}$$

since $1.05*427.5 > 0$ (3.6)

$$M_{O,c} = 1.05*427.5 - 0 = 448.9 \text{ lbmole/hr}$$

$$M_{N,c} = 3.76M_{O,c} = 3.76*448.88 = 1,688 \text{ lbmole/hr} \quad (3.7)$$

$$M_{W,c} = 1.611*0.018(448.88 + 1,687.77) = 61.96 \text{ lbmole/hr} \quad (3.8)$$

$$T_c = (80 + 460) \left(\frac{14.687 + 3.612e^{-2*97}}{14.687} \right)^{\frac{1.4-1}{1.4}} - 460 \quad (3.9)$$

$$T_c = 114.1^\circ\text{F}$$

Now the exhaust gas from the first part and the energy released are calculated.

$$M_{CO,GB,1} = M_{COS,GB,1} = M_{H,GB,1} = M_{HS,GB,1} = M_{M,GB,1} = M_{S,GB,1} = 0$$

$$M_{SD,GB,1} = M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o} \quad (3.10)$$

$$M_{SD,GB,1} = 200 + 17 + 150 + 2*41 = 449 \text{ lbmole/hr}$$

$$M_{W,GB,1} = M_{W,R,o} + M_{W,c} + 2M_{M,R,o} + M_{H,R,o} + M_{HS,R,o} \quad (3.11)$$

$$M_{W,GB,1} = 500 + 61.96 + 2*10 + 100 + 150 = 832.0 \text{ lbmole/hr}$$

$$M_{CD,GB,1} = M_{CD,R,o} + M_{M,R,o} + M_{CM,R,o} + M_{CS,R,o} \quad (3.12)$$

$$M_{CD,GB,1} = 500 + 10 + 50 + 17 = 577 \text{ lbmole/hr}$$

$$M_{N,GB,1} = M_{N,R,o} + M_{W,c} \quad (3.13)$$

$$M_{N,GB,1} = 0 + 1,688 = 1,688 \text{ lbmole/hr}$$

since $0 > 1.05*427.5$ is false (3.14)

$$M_{O,GB,1} = 0.05M_{O,c,1} = 0.05*417.5 = 21.38$$

$$\Delta H_{GB} = 345,200M_M + 104,000M_H + 121,700M_{CM} + 255,400M_S + 222,900M_{HS} + 236,000M_{CS} \quad (3.15)$$

$$\Delta H_{GB} = 345,200*10 + 104,000*100 + 121,700*50 + 255,400*41 + 222,900*150 + 236,000*17$$

$$\Delta H_{GB} = 67.86e^6 \text{ Btu/hr}$$

The total energy exiting the first part of the gas burner is calculated next, along with the energy flow rates of the exhaust gases at two estimated temperatures 2000°F and 958.54°F. Then the energy flow exiting the first part is compared to the energy flow rate of the exhaust gas, if it is

greater than additional air is needed to cool the gas burner. Then the total volumetric flow rate of the combustion gas is calculated along with the electricity consumed by the compressor for the combustion air.

$$E_{GB,i} = \sum_{k=1}^{11} \hat{h}_k(T_{GB,i})M_{GB,i} = \sum_{k=1}^{11} \hat{h}_k(958.54)M_{GB,i} \quad (3.16)$$

$$E_{GB,i} = 9,567*500 + 6,414*50 + 10.34e^3*17 + 6,166*100 + 7,950*150 + \\ 10,33e^3*10 + 6,359*0 + 7.426*41 + 9,833*200 + 7,576*500$$

$$E_{GB,i} = 13.25e^6 \text{ Btu/hr}$$

$$E_c = \hat{h}_O(T_c)M_{O,c} + \hat{h}_N(T_c)M_{N,c} + \hat{h}_{W,c}(T_c)M_{W,c} \quad (3.17)$$

$$E_c = 261.3*448.9 + 258.6*1,688 + 298.2*61.96 = 572.2e^3 \text{ Btu/hr}$$

$$E_{GB,total} = E_{BG,i} + E_c + \Delta H_{GB} \quad (3.18)$$

$$E_{GB,total} = 13.25e^6 + 572.2e^3 + 67.86e^6 = 81.68e^6$$

$$E_{GB,max} = \sum_{j=1}^5 \hat{h}_j(2000)M_{j,1} \quad (3.19)$$

$$E_{GB,max} = 22.78e^3*577 + 14.44e^3*1,688 + 15.18e^3*21.38 + 23.36e^3*449 + \\ 17.92e^3*832.0$$

$$E_{GB,max} = 63.24e^6 \text{ Btu/hr}$$

$$E_{GB,min} = \sum_{j=1}^5 \hat{h}_j(T_{GB,i})M_{j,1} \quad (3.20)$$

$$E_{GB,min} = 9,569*577 + 6,359*1,688 + 6,640*21.38 + 9,833*449 + \\ 7,576*832.0$$

$$E_{GB,min} = 27.11e^6 \text{ Btu/hr}$$

$$\text{if } E_{GB,total} > E_{GB,max} \text{ then} \quad (3.21)$$

$$M_{O,ex} = \frac{E_{GB,total} - E_{GB,max}}{15,180 - \hat{h}_O(T_c) + 3.76(14,440 - \hat{h}_N(T_c)) + 1.611*0.018*(17,920 - \hat{h}_W(T_c))}$$

$$T_{GB,o} = 2000$$

else $M_{O,ex} = 0$

$$T_{GB,o} = \frac{2000 - T_{GB,i}}{E_{GB,max} - E_{GB,min}} (E_{GB,total} - E_{GB,min}) + T_{GB,i}$$

since $81.68e^6 > 63.24e^6$

$$M_{O,ex} = \frac{81.68e^6 - 63.24e^6}{(15,180 - 261.3) + 3.76(14,440 - 258.6) + 1.611*0.018*4.76(17,920 - 298.2)}$$

$$M_{O,ex} = 260.9 \text{ lbmole/hr}$$

$$T_{GB,o} = 2000^\circ\text{F}$$

$$M_{N,ex} = 3.76M_{O,ex} = 3.76*260.9 = 981.1 \text{ lbmole/hr} \quad (3.22)$$

$$M_{W,ex} = 1.611*0.018*4.76M_{O,ex} = 1.611*0.018*4.76*260.9 = 36.02 \text{ lbmole/hr} \quad (3.23)$$

$$M_{c,total} = M_{O,c} + M_{N,c} + M_{W,c} + M_{O,ex} + M_{N,ex} + M_{W,ex} \quad (3.24)$$

$$M_{c,total} = 448.9 + 1,688 + 61.96 + 260.9 + 981.1 + 36.02 = 3,477 \text{ lbmole/hr}$$

$$G_{c,total} = \frac{1,545M_{c,total}(80 + 460)}{60*14.687*144} = \frac{1,545*3,477*(80 + 460)}{60*14.687*144} = 22,860 \text{ acfm} \quad (3.25)$$

$$EC_{GB} = \left(\frac{1545M_{c,total}}{0.75*60*44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2}*97}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460) \quad (3.26)$$

$$EC_{GB} = \left(\frac{1,545*3,477}{0.75*60*44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2}*97}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460)$$

$$EC_{GB} = 321.8 \text{ kW}$$

Since the gas burner is used, the actual exhaust gas and volumetric gas flow rate needs to be calculated. It is important to note that the molar flow rate has tripled, while the volumetric flow rate has increased almost five times. Since the gas burner is located upstream of the superheater and boiler, the energy released in the gas burner can be partially recovered by the superheater and boiler.

$$M_{CO,HP,i} = M_{COS,HP,i} = M_{H,HP,i} = M_{HS,HP,i} = M_{M,HP,i} = M_{S,HP,i} = 0 \text{ lbmole/hr}$$

$$M_{SD,HP,i} = M_{SD,GB,1} = 449 \text{ lbmole/hr} \quad (3.29)$$

$$M_{CD,HP,i} = M_{CD,GB,1} = 577 \text{ lbmole/hr} \quad (3.30)$$

$$M_{N,HP,i} = M_{N,GB,1} + M_{N,ex} = 1,688 + 981.1 = 2669 \text{ lbmole/hr} \quad (3.31)$$

$$M_{O,HP,i} = M_{O,GB,1} + M_{O,ex} = 21.38 + 260.9 = 282.3 \text{ lbmole/hr} \quad (3.32)$$

$$M_{W,HP,i} = M_{W,GB,1} + M_{W,ex} = 832.0 + 36.02 = 868.0 \text{ lbmole/hr} \quad (3.33)$$

$$T_{HP,i} = T_{GB,o} = 2000^\circ\text{F} \quad (3.34)$$

$$M_{HP,i} = \sum_{k=1}^{11} M_{k,HP,i} = 577 + 2,669 + 282.3 + \dots + 449 + 868.0 = 4,845 \text{ lbmole/hr} \quad (3.35)$$

$$G_{HP,i} = \frac{1,545 M_{HP,i} (T_{HP,i} + 460)}{60 \cdot 144 \cdot (14.687 + 3.612e^{-2} \cdot 97)} = \frac{1,545 \cdot 4,845 \cdot (2,000 + 460)}{60 \cdot 144 \cdot (14.687 + 3.612e^{-2} \cdot 97)} \quad (3.36)$$

$$G_{HP,i} = 117.2e^3 \text{ acfm}$$

The next step is to calculate the oxygen needed for the converter and the energy released in the first stage of the converter. The first stage of the catalytic converter is divided into two parts to solve for the amount of dilution air. The first part burns any combustibles and converts above 70% of the SO_2 to SO_3 .

$$M_{O,CS,1} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.35M_{SD,PH,i} + 1.85M_{CS,PH,i} + 1.85M_{HS,PH,i} + 2.7M_{S,PH,i} \text{ lbmole/hr} \quad (3.37)$$

$$M_{O,CS,1} = 2 \cdot 0 + 0.5 \cdot 0 + 0.5 \cdot 0 + 0.35 \cdot 449 + 1.85 \cdot 0 + 1.85 \cdot 0 + 2.7 \cdot 0 = 157.2$$

$$M_{O,CS,all} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.5M_{SD,PH,i} + 2M_{CS,PH,i} + 2M_{HS,PH,i} + 3M_{S,PH,i} \quad (3.38)$$

$$M_{O,CS,all} = 20 + 0.5 \cdot 0 + 0.5 \cdot 0 + 0.5 \cdot 449 + 2 \cdot 0 + 2 \cdot 0 + 3 \cdot 0 = 224.5 \text{ lbmole/hr}$$

$$\text{if } M_{O,CS,all} > M_{O,PH,i} \text{ then } M_{O,CS,c} = M_{O,CS,all} - M_{O,PH,i} \quad (3.39)$$

$$\text{else } M_{O,CS,c} = 0$$

since 224.5 is not greater than 282.3 then

$$M_{O,CS,c} = 0 \text{ lbmole/hr}$$

$$M_{N,CS,c} = 3.76M_{O,CS,c} = 3.76 \cdot 0 = 0 \text{ lbmole/hr} \quad (3.40)$$

$$M_{W,CS,c} = 1.611 \cdot 0.018(M_{O,CS,c} + M_{O,CS,c}) = 1.611 \cdot 0.018(0 + 0) = 0 \text{ lbmole/hr} \quad (3.41)$$

$$\text{if } M_{O,CS,all} > M_{O,PH,i} \text{ then } M_{O,CS,1,o} = M_{O,CS,all} - M_{O,CS,1} \quad (3.42)$$

$$\text{else } M_{O,CS,1,o} = M_{O,PH,i} - M_{O,CS,1}$$

since 224.5 is not greater than 282.3 then

$$M_{O,CS,1,o} = M_{O,PH,i} - M_{O,CS,1} = 282.3 - 157.2 = 125.2 \text{ lbmole/hr}$$

$$M_{N,CS,1,o} = M_{N,PH,i} + M_{N,CS,c} = 2,669 + 0 = 2,669 \text{ lbmole/hr} \quad (3.43)$$

$$M_{CD,CS,1,o} = M_{CD,PH,i} + M_{M,PH,i} + M_{CM,PH,i} + M_{CS,PH,i} \quad (3.44)$$

$$M_{CD,CS,1,o} = 577 + 0 + 0 + 0 + 0 = 577 \text{ lbmole/hr}$$

$$M_{W,CS,1,o} = M_{H,PH,i} + 2M_{M,PH,i} + M_{HS,PH,i} = 0 + 0 + 2*0 = 0 \text{ lbmole/hr} \quad (3.45)$$

$$M_{ST,CS,1,o} = 0.7(M_{SD,PH,i} + 2M_{S,PH,i} + M_{HS,PH,i} + M_{CS,PH,i}) \quad (3.46)$$

$$M_{ST,CS,1,o} = 0.7(449 + 0 + 0 + 0 + 0) = 314.3$$

$$M_{SD,CS,1,o} = 0.3(M_{SD,PH,i} + 2M_{S,PH,i} + M_{HS,PH,i} + M_{CS,PH,i}) \quad (3.47)$$

$$M_{SD,CS,1,o} = 0.3(449 + 0 + 0 + 0 + 0) = 134.7$$

$$\Delta H_{CS,1} = 42,570*0.7M_{SD,PH,i} + 345,200M_{M,PH,i} + 104,000M_{H,PH,i} + \quad (3.48)$$

$$121,700M_{CM,PH,i} + 315,000M_{S,PH,i} + 261,500M_{HS,PH,i} + 265,800M_{CS,PH,i}$$

$$\Delta H_{CS,1} = 42,570*0.7*449 + 345,200*0 + 104,000*0 + 121,700*0 + 315,000*0$$

$$+ 261,500*0 + 265,800*0 = 13.38e^6$$

An energy balance can be made to determine the amount of air needed for cooling the first stage of the converter. Once this value is known, the total amount of moist dilution air can be determined; along with the molar flow rates exiting the drying tower (M6), second stage (M23), and entering the heat recovery preheater (M25).

$$E_{CS,1} = \sum_{k=1}^{10} \hat{h}_j (779) M_{k,PH,i} + 5,235.7 M_{O,CS,c} + 5,028.4 M_{N,CS,c} + \Delta H_{CS,1} \quad (3.49)$$

$$E_{CS,1} = 7,456*577 + 5,068*0 + 8,082*0 + 4,888*0 + 6,202*0 + 7,779*0 +$$

$$5,028*2,669 + 5,236*282.3 + 5,869*0 + 7,680*449 + 5,236*0 + 5,028*0 +$$

$$13.38e^6$$

$$E_{CS,1} = 36.03e^6 \text{ Btu/hr}$$

$$E_{CS,1,max} = \sum_{j=1}^6 \hat{h}_j (1158) M_{j,CS,1,o} \quad (3.50)$$

$$E_{CS,max} = 11,980*577 + 7,859*2,669 + 8,226*125.2 + 12,290*134.7 + 16,970*314.3$$

$$+ 9,439*0$$

$$E_{CS,max} = 35.91e^6 \text{ Btu/hr}$$

where $k = CD, CM, CS, H, HS, M, N, O, S, SD$

and $j = CD, N, O, SD, ST, W$

$$M_{air,CS,ex} = \frac{E_{CS,1} - E_{CS,1,max}}{2,864.2} = \frac{36.03e^6 - 35.91e^6}{2,864.2} = 42.53 \text{ lbmole/hr} \quad (3.51)$$

$$M_{BF} = (1 + 1.611*0.018)M_{air,CS,ex} + M_{O,CS,c} + M_{N,CS,c} + M_{W,CS,c} \quad (3.52)$$

$$M_{BF} = (1 + 1.611*0.018)42.53 + 0 + 0 + 0 = 43.76 \text{ lbmole/hr}$$

$$M_{D,i} = M_{PH,i} + M_{BF} - 0.3M_{W,PH,i} = 4845 + 43.76 - 0.3*868.0 = 4,629 \text{ lbmole/hr} \quad (3.53)$$

$$M_{D,o} = M_{D,i} - 0.7M_{W,PH,i} - 1.611*0.018M_{air,CS,ex} - M_{W,CS,c} \quad (3.54)$$

$$M_{D,o} = 4,629 - 0.7*868.0 - 1.611*0.018*43.76 - 0 = 4,020 \text{ lbmole/hr}$$

$$M_{23} = \sum_{k=1}^6 M_{k,CS,1,o} + M_{air,CS,ex} - 0.5*0.83M_{SD,CS,1,o} \quad (3.55)$$

$$M_{23} = 577 + 2,669 + 125.2 + 134.7 + 314.3 + 0 + 42.53 - 0.5*0.83*134.7$$

$$M_{23} = 3,807 \text{ lbmole/hr}$$

$$M_{CD,25} = M_{CD,CS,1,o} = 577 \text{ lbmole/hr} \quad (3.56)$$

$$M_{N,25} = M_{N,CS,1,o} + 0.79M_{air,CS,ex} = 2,669 + 0.79*42.53 = 2,702 \text{ lbmole/hr} \quad (3.57)$$

$$M_{O,25} = M_{O,CS,1,o} + 0.21M_{air,CS,ex} - 0.5*0.83*M_{SD,CS,1,o} \quad (3.58)$$

$$M_{O,25} = 125.2 + 0.21*42.53 - 0.5*0.83*134.7$$

$$M_{O,25} = 78.19 \text{ lbmole/hr}$$

$$M_{SD,25} = 0.17M_{SD,CS,1,o} = 0.17*134.7 = 22.90 \text{ lbmole/hr} \quad (3.59)$$

$$M_{25} = \sum_{j=1}^4 M_{j,25} = 577 + 270 + 78.18 + 22.90 = 3,381 \text{ lbmole/hr} \quad (3.60)$$

where $k = CD, N, O, SD, ST, W$

and $j = CD, N, O, SD$

The heat load on the heat recovery preheater can be determined now. The initial guess for the exit temperature is estimated by the ratio of the heat load to the inlet energy flow rate. This algorithm is used because it makes a very good initial guess for a wide range of inlet temperatures, compositions, and heat loads. Note that in Equations 3.62 and 3.64, the molar flow rates of the combustible gases are zero, and weren't shown in the calculation.

$$Q_{HP} = \sum_{j=1}^4 (\hat{h}_j(256) - \hat{h}_j(180))M_{j,25} \quad (3.61)$$

$$Q_{HP} = (1,715 - 961.0)*577 + (1,256 - 720.3)*2,702 + (1,285 - 732.3)*78.19 + (1,802 - 1,017)*22.29$$

$$Q_{HP} = 1.943e^6 \text{ Btu/hr}$$

$$E_{HP,i} = \sum_{k=1}^{11} \hat{h}_k(T_{HP,i})M_k = \sum_{k=1}^{11} \hat{h}_k(2000)M_k \quad (3.62)$$

$$E_{HP,i} = 22.78e^3 * 577 + 14.44e^3 * 2,669 + 15.18e^3 * 282.3 + 23.36e^3 * 449 + 17.92e^3 * 868.0$$

$$E_{HP,i} = 82.01e^6 \text{ Btu/hr}$$

$$T_{\text{guess}} = T_{HP,i} \left(1 - \frac{Q_{HP}}{E_{HP,i}} \right) = 2,000 \left(1 - \frac{1.943e^6}{82.01e^6} \right) = 1,953^\circ\text{F} \quad (3.63)$$

$$E_{\text{guess}} = \sum_{k=1}^{11} \hat{h}_k(T_{\text{guess}})M_k = \sum_{k=1}^{11} \hat{h}_k(1,953)M_k \quad (3.64)$$

$$E_{\text{guess}} = 22.15e^3 * 577 + 14.06e^3 * 2,669 + 14.78e^3 * 282.3 + 22.70e^3 * 449 + 17.42e^3 * 868.0$$

$$E_{\text{guess}} = 79.79e^6 \text{ Btu/hr}$$

where $j = \text{CD, N, O, SD}$

and $k = \text{CD, CM, CS, H, HS, M, N, O, S, SD, W}$

$$T_{HP,o} = -Q_{HP} \frac{T_{HP,i} - T_{\text{guess}}}{E_{HP,i} - E_{\text{guess}}} + T_{HP,i} = -1.943e^6 \frac{2,000 - 1,953}{82.01e^6 - 79.79e^6} + 2,000 = 1,959^\circ\text{F} \quad (3.65)$$

$$\text{LMTD}_{HP} = \frac{(T_{HP,i} - 256) - (T_{HP,o} - 180)}{\ln \left(\frac{T_{HP,i} - 256}{T_{HP,o} - 180} \right)} = \frac{(2,000 - 256) - (1,959 - 180)}{\ln \left(\frac{1,959 - 256}{2,000 - 180} \right)} = 1,761^\circ\text{F} \quad (3.66)$$

$$A_{HP} = \frac{Q_{HP}}{4.5 \text{LMTD}_{HP}} = \frac{1.943e^6}{4.5 * 1,761} = 245.1 \text{ ft}^2 \quad (3.67)$$

The amount of steam generated; along with, the heat and area of the boiler and superheater are determined in a similar manner to the heat recovery preheater. The energy flow rate exiting the heat recovery preheater is compared to the energy flow at 506°F to determine if any steam can be generated.

$$E_{HP,o} = E_{HP,i} - Q_{HP} = 82.01e^6 - 1.943e^6 = 80.07 \text{ Btu/hr} \quad (3.68)$$

$$E_{506} = \sum_{k=1}^{11} \hat{h}_k(506)M_k \quad (3.69)$$

$$E_{506} = 4,366*577 + 3,040*2,669 + 3,143*282.3 + 4,527*449 + 3,556*868.0$$

$$E_{506} = 16.64e^6 \text{ Btu/hr}$$

and $k = \text{CD,CM,CS,H,HS,M,N,O,S,SD,W}$

if $E_{\text{HP,o}} > E_{506}$ then

$$E_{\text{GC,i}} = E_{506} \quad (3.70)$$

$$T_{\text{GC,i}} = 506 \quad (3.71)$$

else

$$E_{\text{GC,i}} = E_{\text{HP,o}}$$

$$T_{\text{GC,i}} = T_{\text{HP,o}}$$

since $80.07e^6$ is greater than $16.64e^6$

$$E_{\text{GC,i}} = 16.64e^6 \text{ Btu/hr}$$

$$T_{\text{GC,i}} = 506^\circ\text{F}$$

$$M_{\text{st}} = \frac{E_{\text{HP,o}} - E_{\text{GC,i}}}{\hat{h}_W(T_{\text{specified}}) - 2,134.8 + 17,929} = \frac{80.07e^6 - 16.64e^6}{3,934 - 2,134.8 + 17,929} \quad (3.72)$$

$$M_{\text{st}} = 3215 \text{ lbmole/hr}$$

Now the boiler and superheater heat loads, as well as, the log mean temperature differences, and areas can be determined. It should be noted that the model is not smart enough to determine whether the exit temperature of the heat recovery preheater is lower than the specified temperature of the steam. If this occurs a warning will be generated by Demos, when the model tries to evaluate the log mean temperature difference for the superheater. At this point the user should check the exit temperature of the heat recovery preheater and set the temperature of the steam accordingly.

$$Q_b = 17,929M_{\text{st}} = 17,929*3,215 = 57.65e^6 \text{ Btu/hr} \quad (3.73)$$

$$Q_s = (\hat{h}_W(T_{\text{specified}}) - 2134.8)M_{\text{st}} = (3,934 - 2,134.8)*3,215 = 5,786e^6 \text{ Btu/hr} \quad (3.74)$$

$$T_{\text{guess}} = T_{\text{HP,o}} \left(1 - \frac{Q_s}{E_{\text{HP,o}}} \right) = 1,959 \left(1 - \frac{5.786e^6}{80.07e^6} \right) = 1,817^\circ\text{F} \quad (3.75)$$

$$E_{\text{guess}} = \sum_{k=1}^{11} \hat{h}_k(T_{\text{guess}})M_k = \sum_{k=1}^{11} \hat{h}_k(1,817)M_k \quad (3.76)$$

$$E_{\text{guess}} = 20.35e^3 * 577 + 12.98e^3 * 2,669 + 13.63e^3 * 282.3 + 20.86e^3 * 449 + 15.99e^3 * 868.0$$

$$E_{\text{guess}} = 73.49e^6 \text{ Btu/hr}$$

$$T_{b,i} = -Q_s \frac{T_{\text{HP},o} - T_{\text{guess}}}{E_{\text{HP},o} - E_{\text{guess}}} + T_{\text{HP},o} = -5.786e^6 \frac{1,959 - 1,817}{80.07e^6 - 73.49e^6} + 1,959 = 1,834^\circ\text{F} \quad (3.77)$$

$$LMTD_s = \frac{(T_{\text{HP},o} - T_{\text{specified}}) - (T_{b,i} - 338)}{\ln\left(\frac{T_{\text{HP},o} - 338}{T_{b,i} - 338}\right)} = \frac{(1,959 - 550) - (1,834 - 338)}{\ln\left(\frac{1,959 - 550}{1,834 - 338}\right)} = 1,452^\circ\text{F} \quad (3.78)$$

$$LMTD_b = \frac{(T_{b,i} - 338) - (506 - 226)}{\ln\left(\frac{T_{b,i} - 338}{506 - 226}\right)} = \frac{(1,834 - 338) - (506 - 226)}{\ln\left(\frac{1,834 - 338}{506 - 226}\right)} = 725.8^\circ\text{F} \quad (3.79)$$

$$A_s = \frac{Q_s}{6LMTD_s} = \frac{5.786e^6}{6 * 1,452} = 664 \text{ ft}^2 \quad (3.80)$$

$$A_b = \frac{Q_b}{15LMTD_b} = \frac{57.65e^6}{15 * 725.8} = 5,295 \text{ ft}^2 \quad (3.81)$$

The weak acid needed for the gas humidification and cooling tower, as well as, the electricity consumption of the compressors and pumps can be calculated now.

$$E_{\text{GC},o} = \sum_{k=1}^{11} \hat{h}_k (169) M_k - 0.3 \hat{h}_w (169) M_{\text{W,HP},i} \quad (3.82)$$

$$E_{\text{GC},o} = 854.7 * 577 + 643.1 * 2,669 + 653.2 * 282.3 + 905.2 * 449 + 742.9 * 868.0 - 0.3 * 742.9 * 868.0$$

$$E_{\text{GC},o} = 3.252e^6 \text{ Btu/hr}$$

$$M_{\text{WA}} = \frac{E_{\text{GC},i} - E_{\text{GC},o} + 0.3(\hat{h}_w(T_{\text{GC},i}) - 840.6 + 17,813)M_{\text{W,HP},i}}{324.6} \quad (3.83)$$

$$M_{\text{WA}} = \frac{16.64e^6 - 3.252e^6 + 0.3(3,556 - 840.6 + 17,813)868.0}{324.6}$$

$$M_{\text{WA}} = 57,710 \text{ lbmole/hr}$$

$$EC_{\text{BF}} = \left(\frac{1545 M_{\text{BF}}}{0.75 * 60 * 44240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} * 67}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460) \quad (3.84)$$

$$EC_{\text{BF}} = \left(\frac{1,545 * 43.76}{0.75 * 60 * 44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2} * 67}{14.687} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (80 + 460)$$

$$EC_{BF} = 2.862 \text{ kW}$$

$$EC_{MC} = \left(\frac{1545M_{D,o}}{0.75*60*44240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2*167}}{14.687 + 3.612e^{-2*51}} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (120 + 460) \quad (3.85)$$

$$EC_{MC} = \left(\frac{1,545*4,020}{0.75*60*44,240} \right) \left(\frac{1.4}{1.4-1} \right) \left[\left(\frac{14.687 + 3.612e^{-2*167}}{14.687 + 3.612e^{-2*51}} \right)^{\frac{1.4-1}{1.4}} - 1 \right] (120 + 460)$$

$$EC_{MC} = 422.7 \text{ kW}$$

$$m_{acid} = 0.995(M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o}) \frac{98 \text{ lbm/lbmole}}{2000 \text{ tons/lbm}} \quad (3.86)$$

$$m_{acid} = 0.995(200 + 17 + 50 + 41) * \frac{98}{2000} = 21.89 \text{ tons/hr}$$

$$EC_{WA} = \frac{120 \frac{\text{lb}}{\text{in}^2} M_{WA}}{63,813 \frac{\text{lbmole/hr} * \text{lb}/\text{in}^2}{\text{kW}} * 0.80} \quad (3.87)$$

$$EC_{WA} = \frac{120 * 57,710}{63,813 * 0.8} = 135.7 \text{ kW}$$

$$EC_{SS} = \frac{202.4 \frac{\text{gal,om}}{\text{tons/hr}} * 80 \text{ ft } m_{acid}}{2955 \frac{\text{gal/min*ft}}{\text{kW}} * 0.80} \quad (3.88)$$

$$EC_{SS} = \frac{202.4 * 21.89 * 80}{2,955 * 0.8} = 149.9 \text{ kW}$$

$$EC_{PA} = \frac{80 \frac{\text{lb}}{\text{in}^2} m_{acid}}{1017 \frac{\text{tons/hr lb}/\text{in}^2}{\text{kW}} * 0.70} \quad (3.89)$$

$$EC_{PA} = \frac{21.89 * 80}{1,017 * 0.7} = 2.46$$

$$EC_{total} = EC_{IC} + EC_{GB} + EC_{BF} + EC_{MC} + EC_{WA} + EC_{SS} + EC_{PA} \quad (3.90)$$

$$EC_{total} = 249.3 + 321.8 + 2.862 + 422.7 + 135.7 + 149.9 + 2.46 = 1,285 \text{ kW}$$

$$EC_{st} = \frac{E_{PH,o} - E_{GC,i}}{0.88HR} \quad (3.91)$$

$$EC_{st} = \frac{E_{PH,o} - E_{GC,i}}{0.88HR} = \frac{80.07e^6 - 16.64e^6}{0.88*9500} = 7,587 \text{ kW}$$

The direct capital cost of the power plant is calculated next.

if $P_{R,o} > 47$ then

(3.92)

$$DCC_{IC} = \$1.04e^6 \left(\frac{G_{R,o}}{35,000 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314}$$

else if $47 \leq P_{R,o} < 95$

$$DCC_{IC} = \$5.64e^6 \left(\frac{G_{R,o}}{1.80e^6 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314}$$

since $P_{R,o} > 47$

$$DCC_{IC} = \$1.04e^6 \left(\frac{G_{R,o}}{35,000 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314} = \$1.04e^6 \left(\frac{24,290}{35,000} \right)^{0.6} \frac{316.9}{314} = \$843.0e^3$$

$$DCC_{GB} = \$7.07e^5 \left(\frac{G_{IC,o}}{68,000 \text{ ft}^3/\text{min}} \right)^{0.6} \frac{C_{idx}}{314} = \$7.07e^5 \left(\frac{21,870}{68,000} \right)^{0.6} \frac{316.9}{314} = \$361.2e^3 \quad (3.93)$$

$$DCC_{HP} = \$29,000 \left(\frac{A_{HP}}{1,100 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} = \$29,000 \left(\frac{245.1}{1,100} \right)^{0.6} \frac{316.9}{316.9} = \$11.78e^3 \quad (3.94)$$

$$DCC_b = \$53,000 \left(\frac{A_b}{350 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} = \$53,000 \left(\frac{5,295}{350} \right)^{0.6} \frac{316.9}{316.9} = \$270.5e^6 \quad (3.95)$$

$$DCC_s = \$80,000 \left(\frac{A_s}{50 \text{ ft}^2} \right)^{0.6} \frac{C_{idx}}{316.9} = \$80,000 \left(\frac{664.0}{50} \right)^{0.6} \frac{316.9}{316.9} = \$377.6e^3 \quad (3.96)$$

$$DCC_{GC} = \$367,000 \left(\frac{M_{GC}}{1,063 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$367,000 \left(\frac{4,845}{1,063} \right)^{0.6} \frac{316.9}{316.9} \quad (3.97)$$

$$DCC_{GC} = \$911.9e^3$$

$$DCC_{WA} = \$39,000 \left(\frac{M_{WA}}{19,250 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$39,000 \left(\frac{57,710}{19,250} \right)^{0.6} \frac{316.9}{316.9} \quad (3.98)$$

$$DCC_{WA} = \$75.36e^3$$

$$DCC_D = \$636,000 \left(\frac{M_{D,i}}{5,325 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$636,000 \left(\frac{4,629}{5,325} \right)^{0.6} \frac{316.9}{316.9} \quad (3.99)$$

$$DCC_D = \$586.7e^3$$

$$DCC_{BF} = \$518,000 \left(\frac{M_{BF}}{4407 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$518,000 \left(\frac{43.76}{4407} \right)^{0.6} \frac{316.9}{316.9} \quad (3.100)$$

$$DCC_{BF} = \$32.55e^3$$

$$DCC_{CS} = \$2,681,000 \left(\frac{M_{D,o}}{4854 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$2,681,000 \left(\frac{4020}{4854} \right)^{0.6} \frac{316.9}{316.9} \quad (3.101)$$

$$DCC_{CS} = \$2.394e^6$$

$$DCC_T = \$988,000 \left(\frac{M_{23}}{4685 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$988,000 \left(\frac{3807}{4685} \right)^{0.6} \frac{316.9}{316.9} \quad (3.102)$$

$$DCC_T = \$872.3e^3$$

$$DCC_{SA} = \$739,000 \left(\frac{M_{SD,HP,i} + M_{CS,HP,i} + M_{HS,HP,i} + 2M_{S,HP,i}}{354 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} \quad (3.103)$$

$$DCC_{SA} = \$739,000 \left(\frac{449 + 0 + 0 + 0}{354} \right)^{0.6} \frac{316.9}{316.9} = \$852.3e^3$$

$$DCC_{ES} = \$70,000 \left(\frac{M_{GC,i}}{1,063 \text{ lbmole/hr}} \right)^{0.6} \frac{C_{idx}}{316.9} = \$70,000 \left(\frac{4,845}{1,063} \right)^{0.6} \frac{316.9}{316.9} \quad (3.104)$$

$$DCC_{ES} = \$173.9e^3$$

$$DCC_{total} = \sum_{k=1}^{13} DCC_k = \$843.0e^3 + \$361.2e^3 + \$11.78e^3 + \$270.5e^3 + \$377.6e^3 + (3.105)$$

$$\$911.9e^3 + \$75.36e^3 + \$584.7e^3 + \$32.55e^3 + \$2,394e^3 + \$872.3e^3 +$$

$$\$852.3e^3 + \$173.9e^3$$

$$DCC_{total} = \$7.761e^6$$

$$TCC_{acid} = (1 + 0.275 + 0.419 + 0.081)DCC_{total} = 1.776DCC_{total} \quad (3.106)$$

$$TCC_{acid} = 1.776 * \$7.761e^3 = \$13.784e^3$$

Now the operating cost are calculated.

$$OC_{oper} = 2 \text{ persons} * 19.70 \text{ \$/hr} * 8766 \text{ hrs/yr} * C_{idx}/325.3 \quad (3.107)$$

$$OC_{oper} = 2 * 19.70 * 8766 * 316.9 / 325.3 = \$336.5e^3/\text{yr}$$

$$OC_{maint-labor} = 2 \text{ persons} * 19.70 \text{ \$/hr} * 8766 \text{ hrs/yr} / 3 * C_{idx}/325.3 \quad (3.108)$$

$$OC_{maint-labor} = 2 * 19.70 * 8766 / 3 * 316.9 / 325.3 = \$112.3e^3/\text{yr}$$

$$OC_{admin} = 0.30(OC_{oper} + OC_{maint-labor}) \quad (3.109)$$

$$OC_{\text{admin}} = 0.30(336.5e^3 + 112.3e^e) = \$134.6e^3/\text{yr}$$

$$OC_{\text{maint-mater}} = 0.009DCC_{\text{total}} = 0.009 * 7.761e^6 = 69.85e^3/\text{yr} \quad (3.110)$$

$$OC_{\text{makeup}} = 0.02 * 35.2 \text{ 85\$/lbmole/hr} * M_6 * C_{\text{idx}}/325.3 \quad (3.111)$$

$$OC_{\text{makeup}} = 0.02 * 35.2 * 4,020 * 316.9 / 325.3 = \$2,757/\text{yr}$$

$$OC_{\text{credit}} = 50 \text{ 85\$/ton} * CF * 8766 * m_{\text{acid}} * C_{\text{idx}}/325 \quad (3.12)$$

$$OC_{\text{credit}} = 50 * .65 * 8766 * 21.89 * 316.9 / 325.3 = \$6,076e^3/\text{yr}$$

$$OC_{\text{marketing}} = 0.1 * OC_{\text{credit}} = 0.1 * 6,076e^3 = \$607.6e^3/\text{yr} \quad (3.113)$$

$$OC_{\text{total}} = OC_{\text{oper}} + OC_{\text{maint-labor}} + OC_{\text{admin}} + OC_{\text{main-mater}} + OC_{\text{makeup}} + OC_{\text{marketing}} - OC_{\text{credit}} \quad (3.114)$$

$$OC_{\text{total}} = \$336.5e^3 + \$112.2e^3 + \$134.6e^3 + \$69.85e^3 + \$2,757 + \$607.6e^3 - \$6,076e^3$$

$$OC_{\text{total}} = 1,264e^3 - \$6,076e^3 = -\$4,812e^3$$

3.4 References

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A. Appendix. Thermodynamic Data

This appendix documents the thermodynamic data used in the IEC model. This data includes the heats of reaction for chemical processes occurring in the copper oxide, NOXSO, and sulfuric acid plant systems. All the data is from Barin and Knacke [7], or Barin, Knacke, and Kubaschewski [8], except for the enthalpy data for the alumina substrate. This data is from the SMC report [12]. All the enthalpies are set to zero at 77°F, and are assumed to be at a constant pressure. The heats of reaction and formation are calculated at this temperature. All data are shown to four significant digits; however, at least six significant digits were used to calculate the heats of reaction.⁴ Table A.1 shows the heats of formation for 18 species, while Table A.2 shows the heats of reaction for 21 chemical reactions.

The enthalpy data for all the compounds is obtained by integrating polynomial correlations for the specific heat at constant pressure between 77°F and the specified temperature. The correlations are in cal/(g-mole °K), except for the alumina substrate, so they have to be converted to Btu/(lbmole °R). The polynomial correlations are shown below. The values of the constants for all the species are shown in Table A.3.

$$C_p = A + Be^{-3}T + \frac{Ce^5}{T^2} + De^{-6}T^2 \quad (\text{A.1})$$

The correlation for the alumina substrate in J/(g-mole °K) is

$$C_p = Ae^2 + Be^{-3}T + \frac{Ce^2}{\sqrt{T}} + \frac{De^6}{T^2} \quad (\text{A.2})$$

Integrating with respect to temperature and choosing 298.15°K as a reference temperature gives for Equation A.1 gives,

$$\hat{h} = \int_{298.15}^{T_k} \left(A + Be^{-3}T + \frac{Ce^5}{T^2} + De^{-6}T^2 \right) dT \quad (\text{A.3})$$

$$\hat{h} = \left(AT + \frac{Be^{-3}T^2}{2} - \frac{Ce^5}{T} + \frac{De^{-6}T^3}{3} \right) dT \quad (\text{A.4})$$

⁴ All the original data are in metric units and had to be converted to english units.

Next evaluate Equation A.4 and substitute H_{298} for the constant terms. Converting from cal/g-mole to Btu/lbmole by multiplying by 1.8 gives,

$$\hat{h} = 1.8AT_K + \frac{1.8Be^{-3}T_K^2}{2} - \frac{1.8Ce^5}{T_K} + \frac{1.8De^{-6}T_K^3}{3} - 1.8H_{298} \quad (A.5)$$

However the input temperature is still in degrees Kelvin, and it is desirable to the temperature in degrees Fahrenheit. Substituting $T_K = (T_F + 459.67)/1.8$ gives,

$$\hat{h} = \frac{1.8A(T_F + 459.67)}{1.8} + \frac{1.8Be^{-3}(T_F + 459.67)^2}{2*1.8} - \frac{1.8^2Ce^5}{T_F + 459.67} \quad (A.6)$$

$$+ \frac{1.8De^{-6}(T_F + 459.67)^3}{3*1.8^3} - 1.8H_{298}$$

simplifying yields,

$$\hat{h} = A(T_F + 459.67) + \frac{Be^{-3}(T_F + 459.67)^2}{3.6} - \frac{3.24Ce^{-5}}{T_F + 459.67} + \frac{De^{-6}(T_F + 459.67)^3}{9.72} \quad (A.7)$$

$$- 1.8H_{298}$$

Equation A.7 is used as a function for all the species except for the alumina substrate, since its units are Btu/lb and the correlation for the specific heat has a different form. The final form of the enthalpy equation for the alumina substrate is.

$$\hat{h} = 0.23901(Ae^2(T_F + 459.67) + \frac{Be^3(T_F + 459.67)}{3.6} + Ce^2\sqrt{7.2(T_F + 459.67)} \quad (A.8)$$

$$- \frac{3.24De^6}{T_F + 459.67} - 1.8H_{298}) / 102$$

The constant 0.23901 converts J to calories, while 102 is the molecular weight.

Table A.1: Standard Heat of Formation

| Species | H _o (77°F) Btu/lbmoie |
|-------------------|-------------------------------------|
| CH ₄ | -32,180 |
| CO | -47,560 |
| CO ₂ | -169,300 |
| COS | -61,020 |
| Cu | 0 |
| CuO | -67,050 |
| CuSO ₄ | -331,300 |
| H ₂ | 0 |
| H ₂ O | -104,000 |
| H ₂ S | -8820 |
| N ₂ | 0 |
| NH ₃ | -19,760 |
| NO | 38,840 |
| NO ₂ | 14,240 |
| O ₂ | 0 |
| S ₂ | 55,350 |
| SO ₂ | -127,700 |
| SO ₃ | -170,300 |

Table A.2: Heats of Reactions

| Reaction | ΔH (77°F) Btu/lbmole |
|--|---------------------------------|
| $\text{CH}_4 + \text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O}$ | -345,200 |
| $\text{CO} + 0.5\text{O}_2 = \text{CO}_2$ | -121,700 |
| $\text{COS} + 1.5\text{O}_2 = \text{CO}_2 + \text{SO}_2$ | -236,000 |
| $\text{COS} + 1.85\text{O}_2 = \text{CO}_2 + 0.3\text{SO}_2 + 0.7\text{SO}_3$ | -265,800 |
| $\text{Cu} + 0.5\text{O}_2 = \text{CuO}$ | -67,050 |
| $\text{CuO} + 0.25\text{CH}_4 = \text{Cu} + 0.25\text{CO}_2 + 0.5\text{H}_2\text{O}$ | -19,240 |
| $\text{CuO} + \text{CO} = \text{Cu} + \text{CO}_2$ | -54,680 |
| $\text{CuO} + \text{H}_2 = \text{Cu} + \text{H}_2\text{O}$ | -36,980 |
| $\text{CuO} + \text{SO}_2 + 0.5\text{O}_2 = \text{CuSO}_4$ | -136,500 |
| $\text{CuO} + \text{SO}_3 = \text{CuSO}_4$ | -93,940 |
| $\text{CuSO}_4 + 0.5\text{CH}_4 = \text{Cu} + \text{SO}_2 + 0.5\text{CO}_2 + \text{H}_2\text{O}$ | 30,980 |
| $\text{CuSO}_4 + 2\text{CO} = \text{Cu} + \text{SO}_2 + 2\text{CO}_2$ | -39,910 |
| $\text{CuSO}_4 + 2\text{H}_2 = \text{Cu} + \text{SO}_2 + 2\text{H}_2\text{O}$ | -4500 |
| $\text{H}_2 + 0.5\text{O}_2 = \text{H}_2\text{O}$ | -104,000 |
| $\text{H}_2\text{S} + 1.5\text{O}_2 = \text{H}_2\text{O} + \text{SO}_2$ | -222,900 |
| $\text{H}_2\text{S} + 1.85\text{O}_2 = \text{H}_2\text{O} + 0.3\text{SO}_2 + 0.7\text{SO}_3$ | -261,500 |
| $\text{NO} + \text{NH}_3 + 0.25\text{O}_2 = \text{N}_2 + 1.5\text{H}_2\text{O}$ | -175,100 |
| $\text{NO}_2 + 2\text{NH}_3 + 0.5\text{O}_2 = 1.5\text{N}_2 + 3\text{H}_2\text{O}$ | -286,800 |
| $\text{S}_2 + 2\text{O}_2 = 2\text{SO}_2$ | -255,400 |
| $\text{S}_2 + 2.7\text{O}_2 = 0.3*2*\text{SO}_2 + 0.7*2*\text{SO}_3$ | -315,000 |
| $\text{SO}_2 + 0.5\text{O}_2 = \text{SO}_3$ | -42,570 |

Table A.3: Constants for the Specific Heat Correlations

| Species | A | B | C | D | H ₂₉₈ cal/g-mole | Temperature Range °K |
|---|--------|--------|---------|---------|--------------------------------|-------------------------|
| CH ₄ | 2.975 | 18.329 | 0.346 | -4.303 | 1,547.6 | 298 - 2000 |
| CO | 6.790 | 0.980 | -0.110 | - | 2,104.9 | 298 - 2500 |
| CO ₂ | 10.550 | 2.160 | -2.040 | - | 3,925.7 | 298 - 2500 |
| COS | 11.330 | 2.180 | -1.830 | - | 4,088.7 | 298 - 1800 |
| Cu (s) | 5.940 | 0.905 | -0.332 | - | 1,922.6 | 298 - 1357 |
| CuO (s) | 10.476 | 4.007 | -1.406 | - | 3,773.1 | 298 - 1359 |
| CuSO ₄ (s) | 17.545 | 36.532 | -2.942 | -17.110 | 7,690.4 | 298 - 1078 |
| H ₂ | 6.520 | 0.780 | 0.120 | - | 1,938.4 | 298 - 3000 |
| H ₂ O | 7.170 | 2.560 | 0.080 | - | 2,224.7 | 298 - 2500 |
| H ₂ S | 7.020 | 3.680 | - | - | 2,256.6 | 298 - 1800 |
| N ₂ | 6.660 | 1.020 | - | - | 2,031.0 | 298 - 2500 |
| NH ₃ | 6.165 | 7.558 | 0.084 | - | 2,145.9 | 298 - 800 |
| | 12.601 | 2.500 | -15.231 | - | 7,590.5 ⁵ | 800 - 2000 |
| NO | 6.616 | 1.778 | -0.036 | -0.342 | 2,060.6 | 298 - 3000 |
| NO ₂ | 8.529 | 5.475 | -1.124 | -1.514 | 3,149.9 | 298 - 1500 |
| | 12.848 | 0.305 | - | - | 5,440.5 ⁶ | 1,500 - 3000 |
| O ₂ | 7.160 | 1.000 | -0.400 | - | 2,313.4 | 298 - 3000 |
| S ₂ | 8.720 | 0.160 | -0.900 | - | 2,908.8 | 298 - 2000 |
| SO ₂ | 10.380 | 2.540 | -1.420 | - | 3,684.0 | 298 - 1800 |
| SO ₃ | 13.658 | 6.536 | -3.086 | -1.847 | 4,972.4 | 298 - 2000 |
| Al ₂ O ₃ (s) ⁷ | 1.534 | 1.968 | -9.006 | -2.031 | 20,804 | 298 - 1800 |

Note all species are assumed to be gaseous, except where noted.

⁵ Value of enthalpy at 800°K.

⁶ Value of enthalpy at 1,500°K.

⁷ Units of correlations J/(g-mole °K)

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