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

Final Report

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1 INTRODUCTION

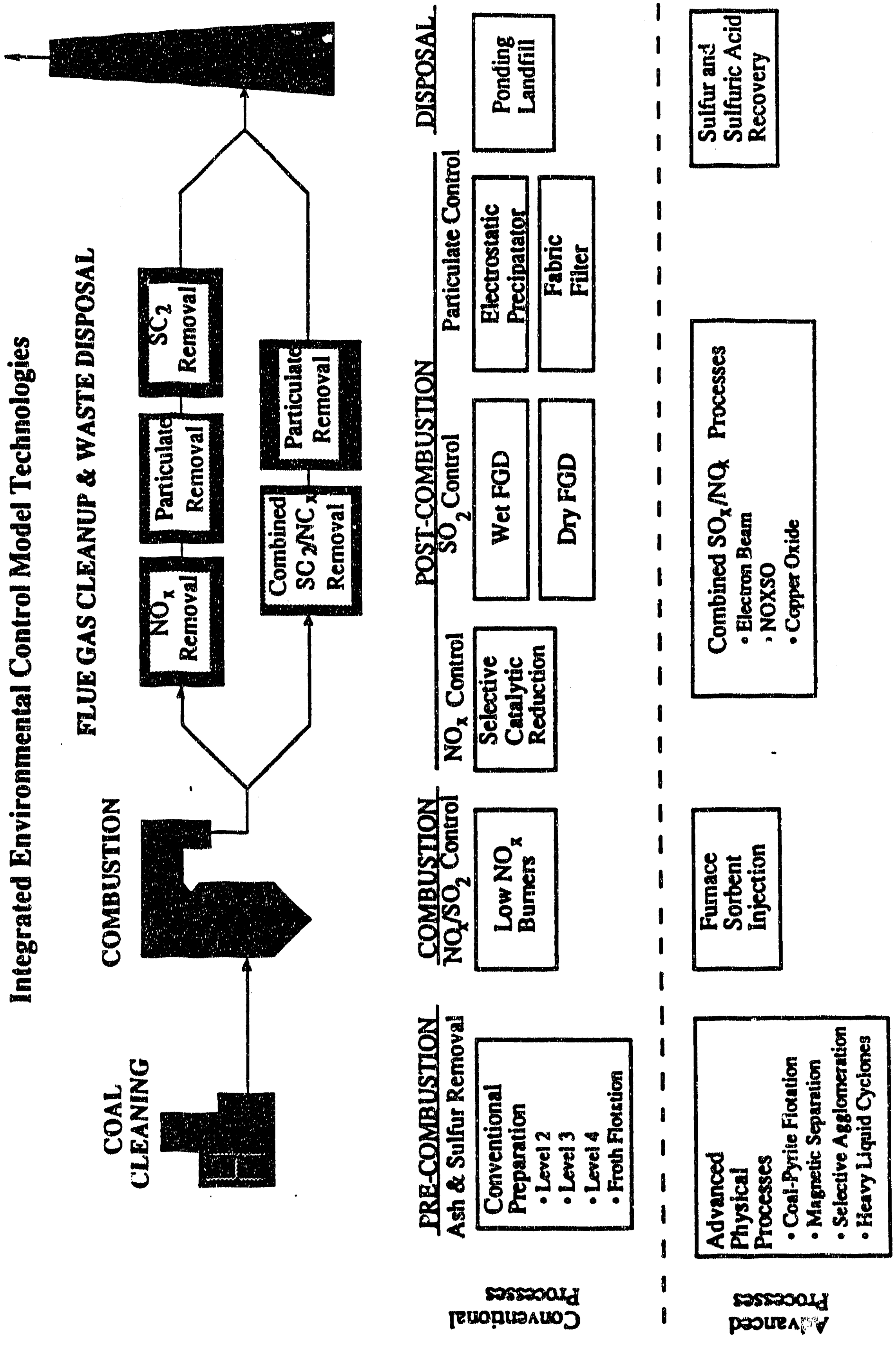
This report summarizes the analytical improvements and model updates to the Integrated Environmental Control Model (IECM) originally developed for the U.S. Department of Energy's Pittsburgh Energy Technology Center (DOE/PETC) under Contract No. DE-FG22-83PC60271. The result of that initial effort was documented in a final report detailing the background and analytical basis for the IECM computer model (1). The current report, conducted under Contract No. DE-AC22-87PC79864, builds upon that initial effort.

An overview of the current IECM structure appears in Figure 1-1. Briefly, the IECM was designed to permit the systematic evaluation of environmental control options for pulverized coal-fired (PC) power plants. Of special interest was the ability to compare the performance and cost of advanced pollution control systems to "conventional" technologies for the control of particulate, SO_2 and NO_x. Of importance also was the ability to consider pre-combustion, combustion and post-combustion control methods employed alone or in combination to meet tough air pollution emission standards. Finally, the ability to conduct probabilistic analyses is a unique capability of the IECM. Key results are characterized as distribution functions rather than as single deterministic values.

In this report we document the analytical basis for several model enhancements and also document updates to various process technology models described in Reference (1). Chapter 2 begins with a summary of refinements to the base power plant model representing conventional technology. Chapters 3 through 7 describe several improvements for advanced post-combustion control methods, including new models of byproduct recovery systems. Finally, Chapters 8 to 10 present several new models for pre-combustion control methods employing advanced coal beneficiation techniques. Illustrative examples of model applications are contained within the various chapters. An additional Case study illustrating the use of the IECM for probabilistic analyses and process evaluations appears in the Appendix.

A companion document to this report is the IECM Technical Manual (2) that gives detailed documentation of the IECM computer code and model default values. Other background information is contained in Reference (1), upon which this report builds.

Figure 1-1: Schematic of Control Model Technologies



2 ENHANCEMENTS TO BASELINE PLANT MODEL

The "baseline" power plant in the IECM is a plant consisting of a conventional PC boiler with low NO_x burners plus a selective catalytic reduction (SCR) system for NO_x control, either a wet or dry flue gas desulfurization (FGD) system for SO_2 removal and (depending on the choice of FGD system) either a cold-side electrostatic precipitator (ESP) or fabric filter for particulate control. Physical coal cleaning with post-combustion controls also is part of the baseline system.

Enhancements to the original model were made to improve the characterization of plant stream quantities and composition, update certain process performance algorithms and expand the capabilities of the economic analysis modules. The sections below detail these enhancements. The format employed throughout this report begins with a detailed nomenclature list to support the equations used in each chapter.

2.1 Nomenclature

English Symbols

a	Advalorem tax rate (fraction)
A_n	Annuity factor per year (fraction)
$A_{overhead}$	Overhead ash (fraction)
AC	Annual cost (M$/yr)
AFUDC	Accumulated funds used during construction (M$)
B	Rate of return for bonds in current dollars (fraction)
B_l	Booklife (years)
B_r	Rate of return for bonds in constant dollars (fraction)
Byp	Bypass (fraction)
C	Weighted cost of capital or return on investment (fraction)
C_{ash}	Carbon in collected ash (mass fraction)
C_{CO}	Carbon in fuel oxidized to carbon monoxide (fraction)
C_f	Capacity factor (fraction)
C_{idx}	Chemical Engineering Plant cost index for current year
$C_{idx,\#}$	Chemical Engineering Plant cost index for year #
c_k	Chemical cost for k^{th} level coal cleaning plant (78$/dry ton of cleaned coal)
$C_{Unburned}$	Unburned carbon (lb carbon/lb fuel)
$CC_{L,n}$	Levelized carrying charge per year (fraction)
CC_n	Carry charges per year (fraction)
$CC_{pv,n}$	Cumulative present value of carrying charges per year (fraction)
Cp	Heat capacity of fluid (Btu/°R)
Cp'	Specific heat (Btu/lb-mole °R)
$Cp_{\#,avg}$	Average heat capacity of flue gas at point # (Btu/°R)
CS	Rate of return for common stock in current dollars (fraction)
CS_r	Rate of return for common stock in constant dollars (fraction)
d	Temporary variable used in heat exchanger analysis (dimensionless)
D_b	Book depreciation per year including investment tax credit (fraction)
D_f	Fraction of capital cost financed by bonds
$D_{s,n}$	Depreciation schedule per year for tax purposes (fraction)
DC	Direct capital cost (M$)
DCC	Cost coefficient for cleaning equipment (78$/dry ton of raw coal)
dis	Nominal discount rate (fraction)

E	Weighted rate of return for preferred and common stock (fraction)
e_{boiler}	Excess air for boiler (fraction of stoichiometric air)
E_{cost}	Cost of electricity (mills/kWhr)
E_d	Energy needed for thermal drier (Btu/lb of dry coal)
E_{wetfgd}	Energy needed to reheat flue gas (Btu/hr)
e_f	Apparent escalation rate of variable and fuel costs (fraction)
e_i	Inflation rate (fraction)
e_k	Electricity cost for k^{th} level coal cleaning plant (78$/dry ton of cleaned coal)
e_{leak}	Leakage air across the air preheater (fraction of stoichiometric air)
e_r	Real escalation rate of variable and fuel costs (fraction)
EF_{NO_2}	Emission factor for NO_x (lb equivalent of NO_2 per ton fuel)
ES	Emission standard (lb/million Btu into furnace)
f_k	Mass fraction of component k in fuel (fraction)
fs_i	Weight fraction of coal in stream i(fraction)
FCF	Fixed charge factor (fraction)
$h_j(T)$	Enthalpy of component j in flue gas at temperature, T (Btu/lb•mole)
Hhv	Higher heating value of fuel (Btu/lb)
Hhv_{natgas}	Higher heating value of natural gas (Btu/ft^3)
HR	Heat rate of power plant (Btu/kWhr)
HR_{cycle}	Gross cycle heat rate, includes the boiler efficiency (Btu/kWhr)
HR_{steam}	Steam cycle heat rate (Btu/kWhr)
HW_{idx}	Handy - Whitman electric utility cost index for current year
$HW_{idx,\#}$	Handy - Whitman electric utility cost index for year #
ICF	Indirect charge factor (fraction)
itc	Investment tax credit (fraction)
k	Temporary variable used in levelization factor (fraction)
L_i	Losses from category i (fraction)
LE	Latent heat of vaporization loss (Btu/lb fuel)
LHV	Lower heating value of coal (Btu/lb)
m'	Total moisture content of coal (fraction)
mi'	Inherent moisture content of coal (fraction)
ms'	Surface moisture content of coal (fraction)
$m_{\#,j}$	Pound moles of component j in gas at point # (lb•mole/lb fuel)
$\dot{m}_{\#,j}$	Molar flow rate of component j at point # (lb•mole/hr)
$\dot{M}_{\#,j}$	Mass flow rate of component j at point # (tons/hr)
MW_g	Gross electrical output of power plant (MW)
N	Years of construction (integer)
N_{NO}	Fraction of NO_x that is NO
NTU	Number of transfer units (dimensionless)
O_{comb}	Stoichiometric oxygen needed for combustion (lb•mole/lb fuel)
Ox	Oxidation of calcium sulfite to calcium sulfate (fraction)
P_{atm}	Atmospheric pressure (psia)
P_{fuel}	Price of fuel ($/ton)
P_g	Guage pressure (inches of water)
PS	Rate of return for preferred stock in current dollars (fraction)
PS_f	Fraction of capital cost financed by preferred stock
PS_r	Rate of return for preferred stock in constant dollars (fraction)
PV_n	Present value factor per year
Q	Heat transfer (Btu/hr)
R_{H_2O}	Moisture content of reagent (fraction)
R_{purity}	Purity of reagent (fraction)

RB_n	Remaining balance per year (fraction)
RD_n	Return on debt per year (fraction)
RE_n	Return on equity per year (fraction)
S_{ret}	Sulfur retained in bottom ash and fly ash streams (fraction)
S_{SO_2}	Sulfur in fuel oxidized to sulfur dioxide (fraction)
SE_i	Sensible heat losses from category i (Btu/lb fuel)
t	Overall tax rate (fraction)
$t_{d,n}$	Deferred income tax per year (fraction)
t_f	Federal tax rate (fraction)
$t_{p,n}$	Taxes paid per year (fraction)
t_s	State tax rate (fraction)
$T_\#$	Temperature at point # (°R)
TDC	Direct capital cost (M$)
TCC	Total capital cost (M$/yr)
TCC_n	Total capital charges in a given year (current M$/yr)
TCE	Total cash expended (M$)
TPI	Total plant investment (M$)
TRR	Levelized total revenue requirement (M$/yr)
TRR_n	Total revenue requirement in a given year (current M$/yr)
TVC	Total variable cost without utilities (M$/yr)
TVC_n	Total variable cost in a given year (current M$/yr)
UA_{aph}	Overall heat transfer coefficient times the surface area for the air preheater (Btu/°R)
v_j	Volume fraction of component k (fraction)
VCLF	Levelization factor (fraction)
w_k	Water cost for kth level coal cleaning plant (78$/dry ton of cleaned coal)
W	Water content (fraction)
$\dot{W}_{evp}$	Evaporated water in scrubber (lb-mole/hr)
w'	Weight of water evaporated in thermal drier per pound of dry coal processed (fraction)
w'_e	Weight of water evaporated in thermal drier (tons/hr)
x_i	Electricity or steam consumption (fraction)
Y	Mass yield (fraction)
Y_i	Mass yield of the stream i in coal cleaning plant (fraction)
Y_{od}	Ratio of coal mass exiting wash streams to coal mass exiting plant (fraction)

Greek Symbols

δ_i	Equals 0 if wash stream i is not thermally dried and 1 if it is thermally dried.
Δh	Enthalpy difference (Btu/lb-mole)
ΔT	Temperature difference (°F)
ε	Heat exchanger effectiveness (fraction)
η	Efficiency (fraction)
σ	Molar stoichiometry (fraction)
ω	Specific humidity of air (mass of moisture per mass of dry air)

Subcategories for Losses

C	Losses from unburned and incomplete combustion of carbon
Gas	Sensible heat losses for dry flue gas
H_2O	Latent and sensible heat losses for moisture
R	Radiation losses
Unacc	Unaccounted losses

Subcategories for Combustion Air and Flue Gas Components

CO	Carbon monoxide

CO_2	Carbon dioxide
H_2O	Moisture
N_2	Nitrogen
NO	Nitrogen oxide
NO_2	Nitrogen dioxide
O_2	Oxygen
SO_2	Sulfur dioxide
SO_3	Sulfur trioxide

Subcategories for Fuel Components

Ash	Ash
C	Carbon
H	Hydrogen (monatomic)
H_2O	Moisture
N	Nitrogen (monatomic)
O	Oxygen (monatomic)

Subcategories for Natural Gas Components

CH_4	Methane
C_2H_6	Ethane
CO_2	Carbon dioxide
N_2	Nitrogen
O_2	Oxygen

Subcategories for Solid Stream Components

Ash	Ash
CaO	Lime
$CaCO_3$	Limestone
$CaSO_3\cdot.5H_2O$	Hydrated calcium sulfite
$CaSO_4$	Calcium Sulfate
$CaSO_4\cdot2H_2O$	Hydrated calcium sulfate
H_2O	Water or Moisture
Misc	Miscellaneous

Subcategories for Stream Location

apho	Exiting air preheater on combustion air side
botash	Bottom ash stream
econo	Exiting the economizer
fdfan	Exiting forced draft fan
fg1	Located at point 1 in flue gas stream (see Figure 2-1)
fg2	Located at point 2 in flue gas stream (see Figure 2-1)
fg3	Located at point 3 in flue gas stream (see Figure 2-1)
fgaphi	Entering air preheater on flue gas side
fgapho	Exiting air preheater on flue gas side
fuel	Fuel stream
furn	In furnace after combustion
leak	Leakage across air preheater
stack	Entering stack
unc	"Uncorrected" flue gas temperature

Subcategories for Utility Consumption

c	Cooling system
f	Fans
misc	Miscellaneous
p	Pulverizers
sp	Steam pumps

Subcategories for Economic Variables

fuel	Fuel charges
non	Non fuel charges
util	Utility charges, i.e. steam and electricity consumption (M$/yr)
w/o cc	Without coal cleaning
w/o util	Without utility charges

Subcategories for FGD Variables

evp	Evaporated
max	Maximum
min	Minimum
reag	Reagent
rem	Removed
rh	Reheater
S	Sulfur or sulfur compound
sd	Spray dryer
sat	Saturation
sludge	Sludge exiting bottom of scrubber
SO_2	Sulfur dioxide
std	Based on emission standard
TSP	Total suspended particulates in flue gas

General Subcategories

aph	Air preheater
bp	Base power plant
c	Coal exiting the washing equipment
credit	Credit
d	Thermal drier
delta	Change between current and original
exit	Exiting device
ff	Fabric filter
in	Entering device
natgas	Natural gas
new	Current or modified
o	Final product of coal cleaning plant
orig	Original or without pollution control equipment
oil	Fuel oil
op	Overall power plant (including pollution control equipment)
out	Exiting device
p	Cleaning equipment in coal cleaning plant
pce	Pollution control equipment
ref	Refuse stream in coal cleaning plant
ROM	Run-of-mine coal
t	Overall coal cleaning plant
total	Sum or total

2.2 Stream Properties and Composition

This section describes how the IECM calculates the quantity and quality of solid and gaseous streams in fossil-fuel fired power plants. A schematic of the solid and gaseous streams for the base power plant is shown in Figure 2-1. These basic streams are always present in the model. As the plant is configured with pollution control equipment, additional streams are created and the equations defining the streams in Figure 2-1 may be modified.

The phrases in quotation marks in Figure 2-1 are the stream labels. They are used as variable subscripts in this documentation to show the variable location in the power plant. For example, the variable T_{fgaphi} refers the temperature of the flue gas at the air preheater inlet. The subscripts "fg1", "fg2" and "fg3" refer to locations downstream from the air preheater. Pollution control equipment is placed between these locations. For example, an ESP is placed between "fgapho" and "fg1". The variables at "fgapho" and "fg1" are respectively the inlet and outlet variables for the ESP. The equations for some variables at "fg1" are redefined to reflect the changes caused by the ESP. The following section describes in more detail the stream variables and their equations.

2.2.1 Fuel and Other Solid Streams

This section describes the fuel and other solid streams in the base power plant. The IECM tracks the following chemical compounds in most solid streams (tons per hour): final ash, lime, limestone, hydrated calcium sulfite, calcium sulfate, hydrated calcium sulfate, moisture and miscellaneous[1]. The total mass flow of any stream is the sum of these chemical compounds. For the fuel stream, the total mass flow rate is determined instead of the mass flow rates of the chemical components.

Oil or natural gas is added to coal in the IECM as boiler fuels. The model requires the following property variables for coal and oil:

Hhv	Higher heating value of the fuel (Btu/lb)
f_{Ash}	Ash content (mass fraction)
f_C	Carbon content (mass fraction)
f_H	Hydrogen content (mass fraction)
f_{H_2O}	Moisture content (mass fraction)
f_N	Nitrogen content (mass fraction)
f_O	Oxygen content (mass fraction)
f_S	Sulfur content (mass fraction)

For coal and oil these variables define the ultimate analysis of the fuel. Natural gas analysis usually reports methane, ethane, carbon dioxide, nitrogen and oxygen content on a percent volume basis and the higher heating value in Btu per standard cubic foot. The standard temperature and pressure are 80°F and 30 inches of mercury respectively. Therefore the input parameters for natural gas are:

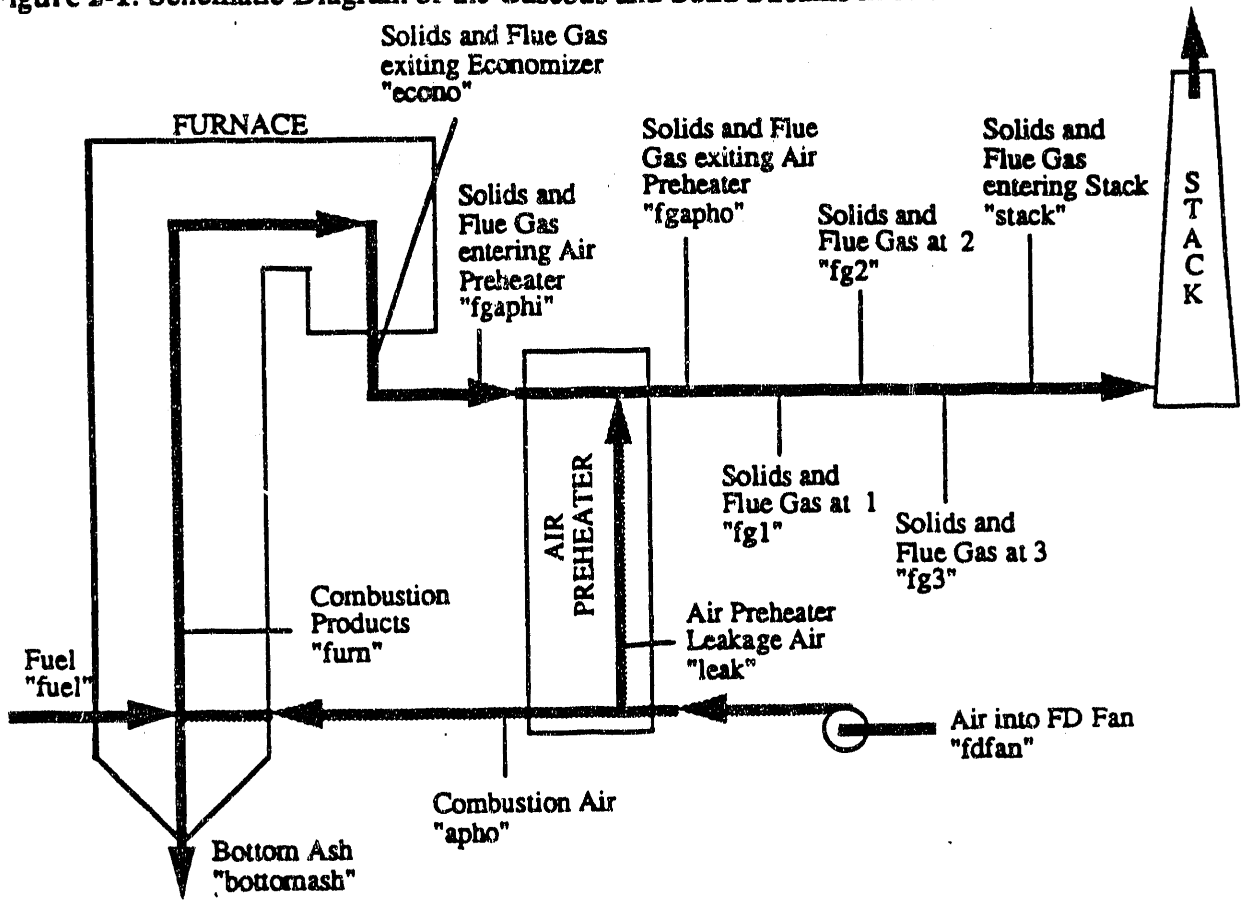
Hhv_{natgas}	Higher heating value of the natural gas (Btu/ft^3)
v_{CH_4}	Methane content (volume fraction)
$v_{C_2H_6}$	Ethane content (volume fraction)

---

[1] The exceptions are the fuel stream and some solid streams used by pollution control equipment. For example a wet scrubber has a lime or limestone slurry, which only contains the reagent plus miscellaneous material.

v_{CO_2}	Carbon dioxide content (volume fraction)
v_{N_2}	Nitrogen content (volume fraction)
v_{O_2}	Oxygen content (volume fraction)

Figure 2-1: Schematic Diagram of the Gaseous and Solid Streams in IECM



Since the analysis of natural gas is not in elemental units, it has to be converted to the mass fraction of carbon, hydrogen, nitrogen, oxygen and sulfur. In addition, the higher value has to be converted to Btu per pound. Natural gas is assumed to behave as an ideal mixture, so volume fractions are equivalent to molar fractions. Therefore, the average molecular weight and density are estimated by[2]

$$\widehat{M}_{natgas} = 16.04 v_{CH_4} + 30.07 v_{C_2H_6} + 44.01 v_{CO_2} + 28.01 v_{N_2} + 32.00 v_{O_2}$$

$$\rho_{natgas} = 0.04246 v_{CH_4} + 0.08029 v_{C_2H_6} + 0.1170 v_{CO_2} + 0.07439 v_{N_2} + 0.08461 v_{O_2}$$

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[2] The values for the densities are from "Combustion: Fossil Power Systems" (3)

The higher heating value on a mass basis can be determined by dividing the higher heating value on a volume basis by the density.

$$\mathrm{Hhv} = \frac{\mathrm{Hhv}_{\mathrm{natgas}}}{\rho_{\mathrm{natgas}}}$$

The mass fractions of carbon, hydrogen, nitrogen and oxygen are found by determining the mass of the individual components (i.e. carbon, hydrogen, etc.) and dividing by the average molecular weight. Since the natural gas is assumed to be free of ash, sulfur and moisture, these values are set to zero.

$$f_C = \frac{12.01 v_{CH_4} + 24.02 v_{C_2H_4} + 12.01 v_{CO_2}}{\widehat{M}_{\mathrm{natgas}}}$$

$$f_H = \frac{4.04 v_{CH_4} + 6.06 v_{C_2H_4}}{\widehat{M}_{\mathrm{natgas}}}$$

$$f_N = \frac{28.01 v_{N_2}}{\widehat{M}_{\mathrm{natgas}}}$$

$$f_O = \frac{32.00 v_{O_2} + 32.00 v_{CO_2}}{\widehat{M}_{\mathrm{natgas}}}$$

$$f_{Ash} = f_S = f_{H_2O} = 0$$

With the fuel characteristics it is possible to calculate the mass flow rates and composition of the gaseous and solid streams in the power plant. The mass flow rate of fuel must be calculated first.

The base power plant is sized to produce a specified amount of electricity, MW_g, which is the amount of electricity that the generators produce. The amount of fuel needed to produce the gross electric capacity, MW_g, depends upon the gross cycle heat rate, boiler efficiency and higher heating value of the fuel. It is determined by

$$\dot{M}_{\mathrm{fuel}} = \frac{MW_g\,HR_{\mathrm{cycle}}}{2\,\mathrm{Hhv}}$$

where

$$HR_{\mathrm{cycle}} = \frac{HR_{\mathrm{steam}}}{\eta_{\mathrm{boiler}}}$$

The gross electrical capacity, steam cycle heat rate and the higher heating value of the fuel are input parameters. The boiler efficiency is calculated and described in more detail in Section 2.3.

With the mass flow rate of fuel determined, it is now possible to determine the mass flow rates of the other solids streams in the power (e.g. the bottom ash or flyash). The solids produced by combustion are from three sources: ash in the fuel, sulfur retained in the ash and any unburned carbon. The mass from sulfur in the ash and the unburned carbon is accounted for in the variable $\dot{M}_{furn,misc}$. The base power plant does not inject lime or limestone slurries into the flue gas stream. Therefore, mass flow rates of lime, limestone, calcium sulfate, hydrated calcium sulfate calcium sulfite and moisture are zero.

$$\dot{M}_{furn,ash} = f_{Ash}\dot{M}_{fuel} \; ; \; \dot{M}_{furn,Misc} = (f_S S_{ret} + f_C C_{Unburned})\, \dot{M}_{fuel}$$

$$\dot{M}_{furn,k} = 0 \quad \text{for } k = CaO,\ CaCO_3,\ CaSO_3{\bullet}0.5H_2O,\ CaSO_4,\ CaSO_4{\bullet}2H_2O,\ H_2O$$

The unburned carbon is a solid entrained in the bottom ash and flyash streams. Utilities measure the fraction of carbon in their collected ash streams. This value is called the percent carbon in refuse and is used in the following formula to determine the amount of unburned carbon per pound of fuel.

$$C_{Unburned} = f_{ash}\,\frac{C_{ash}}{1 - C_{ash}} \tag{2.1}$$

The solids produced by combustion can either exit the furnace with the flue gas or drop out the bottom of the furnace. The fraction that exists with the flue gas is the overhead ash fraction and is a function of the furnace design and coal rank. The bottom ash flow rate is determined by

$$\dot{M}_{botash,k} = \dot{M}_{furn,k}\,(1 - A_{overhead}) \quad \text{for all } k$$

The solids exiting the economizer is equal to the overhead ash fraction times the solids produced by combustion.

$$\dot{M}_{econo,k} = \dot{M}_{furn,k}\, A_{overhead} \quad \text{for all } k$$

For the base power plant, no pollution control equipment can change the mass flow rates of solids in the flue gas. The mass flow rates of solids at each location are the mass flow rate of solids at the previous location. When pollution control equipment is added the definitions of these variables change depending upon the specific choice of equipment.

$$\dot{M}_{stack,k} = \dot{M}_{fg3,k} = \dot{M}_{fg2,k} = \dot{M}_{fg1,k} = \dot{M}_{fgapho,k} = \dot{M}_{fgaphi,k} = \dot{M}_{econo,k} \quad \text{for all } k$$

2.2.2 Air and Flue Gas Streams

This section describes the gaseous streams in the base power plant. The IECM tracks the following chemical compounds in all gaseous streams (lb•mole/lb fuel and lb•mole/hour): diatomic nitrogen, diatomic oxygen, moisture, carbon dioxide, carbon monoxide, sulfur dioxide, sulfur trioxide, nitrogen oxide and nitrogen dioxide. At every location in Figure 2-1, the IECM determines the gaseous stream flow rate in lb•mole/lb fuel and lb•mole/hour. The gaseous stream variables with units of lb•mole/lb fuel describe the gas stream created by the base power plant. They do not change as pollution control equipment is added. These variables are needed by different algorithms in the IECM for comparison with the base power plant[3]. The gaseous stream variables with units of lb•mole/hour describe the gas stream for the current power plant configuration.

The gas streams are assumed to act as ideal mixtures and obey the ideal gas law. Therefore, the total value of a stream property can be determined by summing the values of the property of the individual components. Since the gases obey the ideal gas law, the enthalpy is a function of temperature only. The enthalpy functions are described in more detail in Section 2.2.3. The total volumetric flow rate and enthalpy of a gaseous stream are determined by

$$\dot{V} = \frac{1545\,T}{144 * 60\,(P_{atm} + 0.036127P_g)} \sum_{j=1}^{9} \dot{m}_j$$

$$h(T) = \sum_{j=1}^{9} h_j(T)\,.$$

The IECM assumes that dry air consist of 79% nitrogen and 21% oxygen. The specific humidity is an input parameter. The volumetric fraction of nitrogen, oxygen and moisture can be determined from

$$v_{N_2} = \frac{0.79}{1 + \frac{0.79*28.01 + 0.21*32.00}{18.02}\,\omega} = \frac{0.79}{1 + 1.601\omega}$$

$$v_{H_2O} = \frac{1.601\omega}{1 + 1.601\omega}\ ; \quad v_{O_2} = \frac{0.21}{1 + 1.601\omega}$$

The amount of oxygen needed for stoichiometric combustion of the fuel is the sum of the oxygen needed to convert of carbon to carbon dioxide, hydrogen to water and sulfur to sulfur

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[3] The boiler efficiency algorithm uses the gaseous stream variables in units of lb•mole/lb fuel to prevent a cyclic dependency between the boiler efficiency and the mass flow rate of fuel.

dioxide minus any oxygen in the fuel. To minimize incomplete combustion losses, the combustion air entering the furnace is more than the stoichiometric air requirement. This additional air is called excess air and is an input parameter.

$$O_{comb} = \frac{f_C}{12.01} + \frac{f_H}{1.01} + \frac{f_S}{32.06} - \frac{f_O}{16.00}$$

$$m_{apho,N_2} = \frac{v_{N_2}(1 + e_{boiler})O_{comb}}{v_{O_2}} \; ; \; m_{apho,H_2O} = \frac{v_{H_2O}(1 + e_{boiler})O_{comb}}{v_{O_2}}$$

$$m_{apho,O_2} = (1 + e_{boiler})O_{comb} \; ; \; m_{apho,j} = 0 \text{ for } j = CO_2, CO, SO_2, SO_3, NO, NO_2$$

$$\dot{m}_{apho,j} = 2000\,\dot{M}_{fuel}\, m_{apho,j}$$

The leakage air across the air preheater is based upon the stoichiometric air requirement and is an input parameter. The air entering the forced draft fans is the sum of the leakage air and the air entering the furnace.

$$m_{leak,N_2} = \frac{v_{N_2}(1 + e_{leak})O_{comb}}{v_{O_2}} \; ; \; m_{leak,H_2O} = \frac{v_{H_2O}(1 + e_{leak})O_{comb}}{v_{O_2}}$$

$$m_{leak,O_2} = (1 + e_{leak})O_{comb} \; ; \; m_{leak,j} = 0$$

$$\text{for } j = CO_2, CO, NO, NO_2, SO_2, SO_3$$

$$\dot{m}_{leak,j} = 2000\,\dot{M}_{fuel}\, m_{leak,j}$$

$$m_{fdfan,j} = m_{apho,j} + m_{leak,j} \; ; \; \dot{m}_{fdfan,j} = \dot{m}_{apho,j} + \dot{m}_{leak,j}$$

The products of combustion are determined by specifying extent of combustion for carbon, sulfur and nitrogen and an emission factor for NO_2. The carbon in the fuel can oxides to carbon monoxide or carbon dioxide or it can remain unburned. The amount of unburned carbon, $C_{Unburned}$, is determined with Equation (2.1). The amount of carbon monoxide is determined by the input parameter C_{CO}, the fraction of carbon that oxidizes to carbon monoxide. The sulfur in the fuel can oxidize to either sulfur dioxide or sulfur trioxide. It also can be captured in the ash.

The amount sulfur retained in the ash is determined by the input parameter, S_{ret}. The amount of sulfur dioxide is determined by the input parameter S_{SO_2}. The nitrogen in the fuel can remain unchanged or oxidize to nitrogen oxide or nitrogen dioxide. The amount of NO_x formed is controlled by the NO_2 emission factor. The units of the NO_2 emission factor for coal, oil and natural gas are pounds NO_2 per ton, pounds NO_2 per thousand gallons and pounds NO_2 per million cubic feet respectively. The NO_2 emission factor for oil is converted to pounds NO_2 per ton if the density of oil is 7.8 pounds per gallon (4). The fraction of NO_x that is nitrogen oxide is determined by the input parameter N_{NO}.

$$EF_{NO_2} = \frac{2000\ EF_{oil}}{7.8 * 1000} = 0.2564EF_{oil}\ ;\ EF_{NO_2} = \frac{2000\ EF_{natgas}}{1,000,000\rho_{natgas}} = \frac{2x10^{-3}\ EF_{natgas}}{\rho_{natgas}}$$

With these parameters, it is possible to find the combustion products from a molar balance of the air and the fuel entering the furnace.

$$m_{furn,N_2} = m_{apho,N_2} + \frac{f_N}{2 * 14.01} - \frac{EF_{NO_2}}{2 * 46.01 * 2000}$$

$$m_{furn,O_2} = m_{apho,O_2} + \frac{f_O}{2 * 16.00} - \frac{f_C\,(1 - C_{Unburned} - 0.5C_{CO})}{12.01} - \frac{f_H}{4 * 1.01} - \frac{f_s\,(1 - S_{ret})(1.5 - 0.5S_{SO_2})}{32.06} - \frac{EF_{NO_2}\,(1 - 0.5N_{NO})}{46.01 * 2000}$$

$$m_{furn,H_2O} = m_{apho,H_2O} + \frac{f_H}{2 * 1.01} + \frac{H_{H_2O}}{18.02}$$

$$m_{furn,CO_2} = m_{apho,CO_2} + \frac{f_C\,(1 - C_{Unburned} - C_{CO})}{12.01}\ ;\ m_{furn,CO} = m_{apho,CO} + \frac{f_C\,C_{CO}}{12.01}$$

$$m_{furn,SO_2} = m_{apho,SO_2} + \frac{f_S\,S_{SO_2}\,(1 - S_{ret})}{32.06}\ ;\ m_{furn,SO_3} = m_{apho,SO_3} + \frac{f_S\,(1 - S_{SO_2})(1 - S_{ret})}{32.06}$$

$$m_{furn,NO} = m_{apho,NO} + \frac{EF_{NO_2}\,N_{NO}}{46.01 * 2000}\ ;\ m_{furn,NO_2} = m_{apho,NO_2} + \frac{EF_{NO_2}\,(1 - N_{NO})}{46.01 * 2000}$$

$$\dot{m}_{furn,j} = 2000\ \dot{M}_{fuel}\ m_{furn,j}$$

The flue gas flow rate remains the same until it exits the air preheater in the base power plant. At the air preheater, the leakage air is added to the flue gas. Pollution control equipment do not alter the flue gas flow rates after the air preheater in the base power plant. The molar flow rates of the gases at each location are defined to be the molar flow rate of the gases at the previous location. When pollution control equipment is added, the definitions of these variables will change depending upon the specific pollution control equipment added.

$$m_{fgaphi,j} = m_{econo,j} = m_{furn,j} \;\; ; \;\; m_{fgaphi,j} = m_{econo,j} = m_{furn,j}$$

$$m_{fgapho,j} = m_{fgaphi,j} + m_{leak,j} \;\; ; \;\; \dot{m}_{fgapho,j} = \dot{m}_{fgaphi,j} + \dot{m}_{leak,j}$$

$$m_{stack,j} = m_{fg3,j} = m_{fg2,j} = m_{fg1,j} = m_{fgapho,j}$$

$$\dot{m}_{stack,j} = \dot{m}_{fg3,j} = \dot{m}_{fg2,j} = \dot{m}_{fg1,j} = \dot{m}_{fgapho,j}$$

2.2.3 Thermodynamic Data

This section documents the thermodynamic data used in the IECM. This data includes the heats of reaction for chemical processes occurring in the copper oxide, NOXSO and sulfuric acid plant systems. All the data except the enthalpy for the alumina substrate is from Barin and Knacke (5) or Barin, Knacke and Kubaschewski (6). This data is from the SMC report (7). 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. Although most data are shown to four significant digits, at least six significant digits were used to calculate the heats of reaction.[4] Table 2-1 shows the heats of formation for 18 species. Table 2-2 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 ^{O}K), except the alumina substrate, and must be converted to Btu/(lb•mole ^{O}R). The polynomial correlations are shown below. The values of the constants for all the species are shown in Table 2-3.

$$Cp = A + Be^{-3}T + \frac{Ce^{5}}{T^{2}} + De^{-6}T^{2} \tag{2.2}$$

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

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[4] All the original data are in metric units and had to be converted to English units.

$$Cp_{Al_2O_3} = Ae^2 + Be^{-3}T + \frac{Ce^2}{\sqrt{T}} + \frac{De^6}{T^2}$$

Integrating Equation (2.2) with respect to temperature and choosing 298.15°K as a reference temperature gives

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

$$h(T_K) = AT_K + \frac{Be^{-3}T_K^2}{2} - \frac{Ce^5}{T_K} + \frac{De^{-6}T_K^3}{3} - \tag{2.3}$$

$$\left(A\ 298.15 + \frac{Be^{-3}298.15^2}{2} - \frac{Ce^5}{298.15} + \frac{De^{-6}298.15^3}{3} \right)$$

Next, evaluate Equation (2.3) and substitute H_{298} for the sum of the terms evaluate at 298.15°K. Converting this from cal/g-mole to Btu/lb•mole by multiplying by 1.8 gives

$$h(T_K) = 1.8AT_K + \frac{1.8Be^{-3}T_K^2}{2} - \frac{1.8Ce^5}{T_K} + \frac{1.8De^{-6}T_K^3}{3} - 1.8H_{298.15}$$

Yet the input temperature is still in degrees Kelvin and it is desirable to the temperature in degrees Rankine. Substituting $T_K = T_R/1.8$ gives

$$h(T_R) = \frac{1.8AT_R}{1.8} + \frac{1.8Be^{-3}T_R^2}{2*1.8^2} - \frac{1.8^2Ce^5}{T_R} + \frac{1.8De^{-6}T_R^3}{3*1.8^3} - 1.8H_{298.15}$$

Simplifying $h(T_R)$ yields

$$h(T_R) = AT_R + \frac{Be^{-3}T_R^2}{3.6} - \frac{3.24Ce^5}{T_R} + \frac{De^{-6}T_R^3}{9.72} - 1.8H_{298.15} \tag{2.4}$$

Equation (2.4) is used as a function for all the species except 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

$$h_{Al_2O_3}(T_R) = 0.23901\left(Ae^2T_R + \frac{Be^3T_R}{3.6} + Ce^2\sqrt{7.2T_R} - \frac{3.24De^6}{T_R} - 1.8H_{298.15} \right) / 102$$

The constant 0.23901 converts joules to calories. 102 is the molecular weight.

Table 2-1: Standard Heat of Formation

Species	H_o (77°F) Btu/lb•mole
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_2O	-104,000
H_2S	-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 2-2: Heats of Reactions

Reaction	ΔH (77°F) Btu/lb•mole
$CH_4 + O_2 = CO_2 + 2H_2O$	-345,200
$CO + 0.5O_2 = CO_2$	-121,700
$COS + 1.5O_2 = CO_2 + SO_2$	-236,000
$COS + 1.85O_2 = CO_2 + 0.3SO_2 + 0.7SO_3$	-265,800
$Cu + 0.5O_2 = CuO$	-67,050
$CuO + 0.25CH_4 = Cu + 0.25CO_2 + 0.5H_2O$	-19,240
$CuO + CO = Cu + CO_2$	-54,680
$CuO + H_2 = Cu + H_2O$	-36,980
$CuO + SO_2 + 0.5O_2 = CuSO_4$	-136,500
$CuO + SO_3 = CuSO_4$	-93,940
$CuSO_4 + 0.5CH_4 = Cu + SO_2 + 0.5CO_2 + H_2O$	30,980
$CuSO_4 + 2CO = Cu + SO_2 + 2CO_2$	-39,910
$CuSO_4 + 2H_2 = Cu + SO_2 + 2H_2O$	-4500
$H_2 + 0.5O_2 = H_2O$	-104,000
$H_2S + 1.5O_2 = H_2O + SO_2$	-222,900
$H_2S + 1.85O_2 = H_2O + 0.3SO_2 + 0.7SO_3$	-261,500
$NO + NH_3 + 0.25O_2 = N_2 + 1.5H_2O$	-175,100
$NO_2 + 2NH_3 + 0.5O_2 = 1.5N_2 + 3H_2O$	-286,800
$S_2 + 2O_2 = 2SO_2$	-255,400
$S_2 + 2.7O_2 = 0.3*2*SO_2 + 0.7*2*SO_3$	-315,000
$SO_2 + 0.5O_2 = SO_3$	-42,570

Table 2-3: Constants for the Specific Heat Correlations

Species	A	B	C	D	$H_{298.15}$ 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_2O	7.170	2.560	0.080	-	2,224.7	298 - 2500
H_2S	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_2O_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.

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[5] Value of enthalpy at 800°K.

[6] Value of enthalpy at 1,500°K.

[7] Units of correlations J/(g-mole °K)

2.3 Boiler Efficiency

This section describes the algorithm used to calculate the boiler efficiency. The boiler efficiency is determined for a power plant without any pollution control equipment. This fixes the amount of fuel entering the furnace. Any changes in the energy efficiency of the boiler caused by pollution control equipment is considered by the energy credit algorithm. The air preheater is described in more detail in the next section. Yet, it is necessary to understand that the air preheater is divided into an ideal heat exchanger (i.e., no leakage) followed by a section where air leaks into the flue gas (see Figure 2-2). The uncorrected air preheater temperature, $T_{unc,orig}$, is the flue gas temperature after the heat exchanger.

The boiler efficiency in the IECM is based on the algorithm in "Steam/ Its Generation and Use", by Babcock and Wilcox (8) and "Combustion, Fossil Power Systems", by Combustion Engineering, Inc (9). The boiler efficiency is the energy absorbed by the steam cycle divided by the energy in the fuel. The energy that is not absorbed by the steam cycle is lost to the environment. These losses can be categorized into five areas:

- sensible heat loss of the dry flue gas
- sensible and latent heat loss from water vapor
- unburned carbon and carbon monoxide
- radiation loss
- unaccounted losses

Therefore, the boiler efficiency is

$$\eta_{boiler} = 1 - L_{Gas} - L_{H_2O} - L_C - L_R - L_{Unacc}$$

The sensible heat loss of the dry flue gas is the energy that could be used if the dry flue gas were cooled to the inlet air temperature of the air preheater, $T_{fdfan,orig}$. The inlet fuel temperature is assumed to be the same as the combustion air. This energy loss in Btu per pound of fuel can be defined as

$$SE_{Gas} = \sum_{j=1}^{8} m_{fgaphi,j,orig}(h_j(T_{unc,orig}) - h_j(T_{fdfan,orig}))$$

where j equals all the flue gas components except H_2O

This energy loss can be expressed as a fraction of the fuel's energy content by dividing it by the higher heating value.

$$L_{Gas} = \frac{SE_{Gas}}{Hhv}$$

The heat loss due to water vapor in the flue gas can be split into the latent heat of vaporization and the sensible heat loss. The latent heat loss is the energy that could be used if the water vapor in the flue gas was condensed. Every pound of water vapor that is condensed releases 1,040 Btu of energy. The water vapor in the flue gas is produced by the vaporization of moisture in the fuel and the combustion of hydrogen in the fuel. The latent heat loss can be calculated as follows:

$$LE = \left(f_{H_2O} + \frac{18.02 f_H}{2*1.01}\right)1{,}040$$

The sensible heat loss due to water vapor is the energy that could be used if the water vapor could be cooled to the inlet air temperature, $T_{fdfan,orig}$. This energy loss can be calculated as follows:

$$SE_{H_2O} = m_{fgaphi,H_2O,orig}\left(h_{H_2O}(T_{unc,orig}) - h_{H_2O}(T_{fdfan,orig})\right)$$

The total loss from moisture expressed as a fraction is the sum of the latent heat and sensible heat losses divided by the higher heating value of the fuel.

$$L_{H_2O} = \frac{(LE + SE_{H_2O})}{Hhv}$$

Since the fuel's higher heating value is based on the complete oxidation of carbon to carbon dioxide, the boiler efficiency has to account for energy loss from unburned carbon and carbon monoxide. Pure carbon has a higher heating value of 14,100 Btu/lb. The energy lost per pound of unburned carbon is 14,100 Btu. For every pound of carbon converted to carbon monoxide, 9755 Btu of energy are lost. The total energy loss due to unburned carbon and carbon monoxide is

$$L_C = (12.01*9{,}755 m_{fgaphi,co} + 14{,}100 C_{Unburned}) / Hhv$$

The loss from radiation exchange with the surroundings is estimated based on Figure 27 in reference (8) and Figure 6-5 in reference (9). Modern utility boilers usually have four water cooled walls and range in output from 800 to 6,000 million Btu per hour. Therefore, this curve was fitted to the following equation between 800 and 6,000 million Btu per hour:

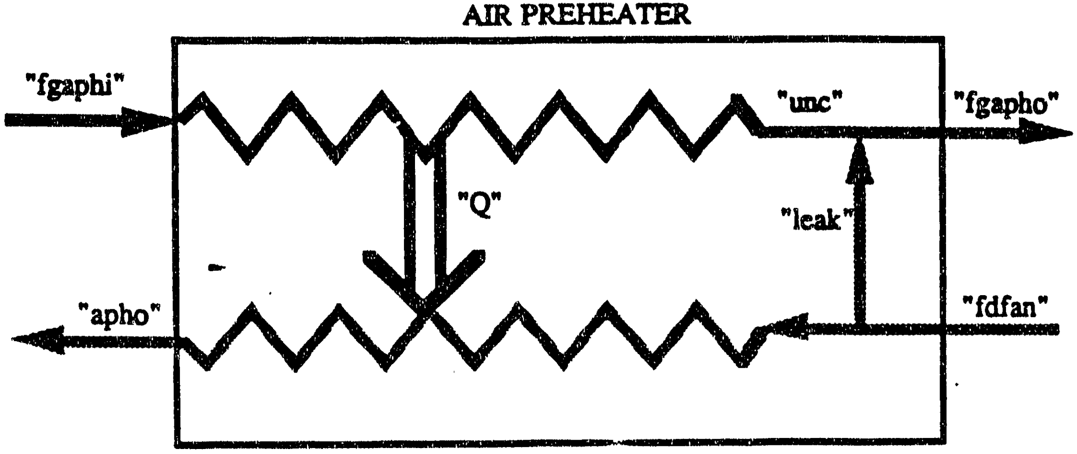
$$L_R = 0.0015 + \frac{6000}{MW_g HR_{steam}}$$

There are other minor losses that are not determined in this algorithm. An example of one of these losses is the sensible heat loss from the ash exiting the boiler. Theses losses and other miscellaneous tolerance errors are entered as an input parameter in L_{Unacc}.

2.4 Air Preheater

This section describes the performance and economic algorithms for the air preheater. Figure 2-2 shows a schematic the air preheater. The purpose of the air preheater is to heat the combustion air entering the boiler by cooling the flue gas exiting the boiler. Typically, there is a significant amount of leakage between the inlet boiler air and the outlet flue gas. The model assumes that the mixing due to the leakage air occurs independently of the heat transfer across the heat exchanger. This allows separate consideration of the effect of the leakage air and the characteristics of the heat exchanger. The heat exchanger is assumed to be a counterflow type.

Figure 2-2: Schematic Diagram of Air Preheater



The air preheater algorithms must calculate the performance of the air preheater for a power plant with and without pollution control equipment so that the effects of adding pollution control equipment can be determined. When the term "original" or "design" is used to describe a parameter, it signifies that the parameter is determined for a power plant without pollution control equipment. The term "modified" or "actual" signifies that the parameter is determined for a power plant with pollution control equipment. The purpose of the air preheater model is to calculate

- the design "uncorrected" air preheater temperature for the boiler efficiency algorithm
- the original amount of heat transferred by the air preheater
- the original size of the air preheater
- the actual "uncorrected" air preheater temperature
- the actual amount of heat transferred by the air preheater
- the difference in the amount of energy captured by the air preheater due to the addition of pollution control equipment
- the new size of the air preheater if requested
- the additional capital cost for a larger air preheater if requested

The "uncorrected" flue gas temperature, $T_{unc,orig}$, can be determined from an energy balance of the streams "leak", "fgaphi" and "fgapho" shown in Figure 2-2. This energy balance is shown below, where the temperature of the flue gas exiting the air preheater, $T_{fgapho,orig}$, and the leakage air temperature, $T_{leak,orig}$, are known.

$$\sum_{j=1}^{9}\left(m_{leak,j,orig}h_j(T_{leak,orig}) + m_{fgaphi,j,orig}h_j(T_{unc,orig})\right) = \sum_{j=1}^{9} m_{fgapho,j,orig}h_j(T_{fgapho,orig})$$

Stream "fgapho" is equal to the sum of streams "leak" and "fgaphi". Therefore, the energy balance can be rearranged as follows

$$\sum_{j=1}^{9} m_{fgaphi,j,orig}\left(h_j(T_{unc,orig}) - h_j(T_{fgapho,orig})\right) = \sum_{j=1}^{9} m_{leak,j,orig}\left(h_j(T_{fgapho,orig}) - h_j(T_{leak,orig})\right)$$

The temperature difference between $T_{fgapho,orig}$ and $T_{unc,orig}$ is usually less than 40°F, so the left hand side of this equation can be estimated by the average heat capacity times the temperature difference between $T_{unc,orig}$ and $T_{fgapho,orig}$. The average heat capacity is estimated between $T_{fgapho,orig}$ and $T_{fgapho,orig}$ + 40°F. Therefore, $T_{unc,orig}$ is determined by

$$T_{unc,orig} = \frac{\sum_{j=1}^{9} m_{leak,j,orig}\left(h_j(T_{fgapho,orig}) - h_j(T_{leak,orig})\right)}{Cp_{fgaphi,avg,orig}} + T_{fgapho,orig}$$

where

$$Cp_{unc,avg,orig} = \frac{\sum_{j=1}^{9} m_{fgaphi,j,orig}\left(h_j(T_{fgapho,orig}+40) - h_j(T_{fgapho,orig})\right)}{40}$$

The amount of energy transferred from the flue gas to the combustion air for a power plant without pollution control equipment is

$$Q_{aph,orig} = 2000\dot{M}_{fuel}\sum_{j=1}^{9} m_{fgaphi,j,orig}\left(h_j(T_{fgaphi,orig}) - h_j(T_{unc,orig})\right)$$

The temperature of the combustion air exiting the air preheater is typically less than 535°F. It can be estimated by

$$T_{apho,orig} = \frac{Q_{aph,orig}}{2000\dot{M}_{fuel}Cp_{apho,avg,orig}} + T_{fdfan,orig}$$

where

$$Cp_{apho,avg,orig} = \frac{\sum_{j=1}^{9} m_{apho,j,orig}\left(h_j(985) - h_j(T_{fdfan,orig})\right)}{985 - T_{fdfan,orig}}$$

The size of the air preheater is estimated by the quantity UA, where U is the overall heat transfer coefficient and A is the surface area. For a given heat exchanger, the heat transfer can be estimated by the equation below, where the subscripts "i" and "o" represent "in" and "out" and "h" and "c" represent "hot" and "cold" respectively (10).

$$Q = \frac{UA\left[(T_{h,i} - T_{c,o}) - (T_{h,o} - T_{c,i})\right]}{\ln\left\{\frac{T_{h,i} - T_{c,o}}{T_{h,o} - T_{c,i}}\right\}}$$

Solving the above equation for UA for the original air preheater. Substituting the appropriate subscripts yields

$$UA_{aph,orig} = \frac{Q_{aph,orig}}{(T_{fgaphi,orig} - T_{apho,orig}) - (T_{unc,orig} - T_{fdfan,orig})} \ln\left(\frac{T_{fgaphi,orig} - T_{apho,orig}}{T_{unc,orig} - T_{fdfan,orig}}\right) \quad (2.65)$$

Certain pollution control equipment, such as the copper oxide and NOXSO processes, significantly change the composition and temperature of the flue gas entering the air preheater. These changes may increase or decrease the amount of energy captured by the air preheater or change the exit temperature of the flue gas exiting the air preheater. Two cases can be considered. The first (or base) case is using the original air preheater without modifications. The alternative is to resize the air preheater so that additional energy can be captured by the air preheater.

For the base case, the original air preheater is used so its size is fixed and the overall heat transfer coefficient is assumed to be constant. Therefore, the known values are

- flue gas flow rate, m_{fgaphi} and inlet temperature, T_{fgaphi}
- combustion air flow rate, m_{apho} and inlet temperature, $T_{fdfan,orig}$
- leakage air flow rate, $m_{leak,orig}$ and inlet temperature, $T_{leak,orig}$
- the product of the overall heat transfer coefficient and surface area, UA

It should be noted that m_{apho}, m_{fgaphi} and T_{fgaphi} are known, but their values may be different from their value for the original power plant without pollution control equipment.

The output parameters are the energy transferred across the air preheater, Q_{aph}, the flue gas exit temperature, T_{fgapho}, the "uncorrected" flue gas temperature, T_{unc} and the combustion air exit temperature, T_{apho}. To simplify the algorithms the average heat capacity of the flue gas entering the air preheater and the combustion air exiting the air preheater is determined.

$$Cp_{apho,avg} = \frac{\sum_{j=1}^{9} m_{apho,j}\left(h_j(T_{fgaphi}-100) - h_j(T_{fdfan,orig})\right)}{T_{fgaphi}-100 - T_{fdfan,orig}}$$

$$Cp_{fgaphi,avg} = \frac{\sum_{j=1}^{9} m_{fgaphi,j}\left(h_j(T_{fgaphi}) - h_j(T_{fgapho,input})\right)}{T_{fgaphi} - T_{fgapho,input}}$$

The variable $T_{fgapho,input}$ is the new flue gas exit temperature when the air preheater is resized. It is used for the base case as a matter of convenience to determine the average heat capacity of the flue gas. Once the average heat capacities are calculated, the "uncorrected" flue gas temperature, T_{fgapho}, is determined using the *effectiveness-NTU* method. The effectiveness, ε, is the ratio of the actual heat transfer rate for the heat exchanger to the maximum heat transfer rate.

$$\varepsilon = \frac{Q}{Q_{max}} = \frac{Cp_h(T_{h,i} - T_{h,o})}{Cp_{min}(T_{h,i} - T_{c,i})} \quad (2.5)$$

The subscript "min" indicates the stream with the lower heat capacity, while the subscript "max" indicates the stream with the higher heat capacity. For a counterflow heat exchanger with both fluids unmixed, the effectiveness can approximated with the following relation.

$$\varepsilon = \frac{1 - \exp\left[-NTU\left(1 - \frac{Cp_{min}}{Cp_{max}}\right)\right]}{1 - \frac{Cp_{min}}{Cp_{max}}\exp\left[-NTU\left(1 - \frac{Cp_{min}}{Cp_{max}}\right)\right]} \tag{2.6}$$

In fossil fuel fired power plants, the hot fluid stream (flue gas) is significantly larger than the cold fluid stream. Therefore, the hot fluid stream has a greater heat capacity rate than the cold fluid. Equations (2.5) and (2.6) can be solved for $T_{h,o}$ by substituting C_c for C_{min} and C_h for C_{max} and eliminating ε.

$$T_{h,o} = T_{h,i} - (T_{h,i} - T_{c,i}) \frac{1 - \exp\left[-NTU\left(1 - \frac{Cp_{min}}{Cp_{max}}\right)\right]}{\frac{Cp_h}{Cp_c} - \exp\left[-NTU\left(1 - \frac{Cp_{min}}{Cp_{max}}\right)\right]} \tag{2.7}$$

The number of transfer units (NTU) is a dimensionless parameter in heat exchanger analysis and is

$$NTU = \frac{UA}{Cp_{min}}$$

Since UA is known, the term in the exponential of Equation (2.7) can be replaced by

$$d = -NTU\left(1 - \frac{Cp_c}{Cp_h}\right) = \frac{-UA}{Cp_c}\left(1 - \frac{Cp_c}{Cp_h}\right) = UA\left(Cp_h^{-1} - Cp_c^{-1}\right)$$

Therefore, Equation (2.7) can be written as

$$T_{h,o} = T_{h,i} - (T_{h,i} - T_{c,i}) \frac{1 - e^d}{\frac{Cp_h}{Cp_c} - e^d}$$

Substituting the appropriate subscripts for the air preheater into the above equations yields

$$T_{unc} = T_{fgaphi} - (T_{fgaphi} - T_{fdfan}) \frac{1 - e^d}{\frac{Cp_{fgaphi,avg}}{Cp_{apho,avg}} - e^d}$$

$$d = UA_{aph,orig}(Cp_{fgaphi,avg}^{-1} - Cp_{apho,avg}^{-1})$$

Once the "uncorrected" flue gas temperature is determined the flue gas and combustion temperatures exiting the air preheater and the heat transfer across the air preheater can be determined.

$$Cp_{leak,avg} = \frac{\sum_{j=1}^{9} m_{leak,j}(h_j(T_{unc}) - h_j(T_{leak,orig}))}{T_{unc} - T_{leak,orig}}$$

$$T_{fgapho} = \frac{Cp_{leak,avg}T_{leak,orig} + Cp_{fgaphi,avg}T_{unc}}{Cp_{leak,avg} + Cp_{fgaphi,avg}}$$

$$Q_{aph} = Cp_{fgaphi,avg}(T_{fgaphi} - T_{unc})$$

$$T_{apho} = \frac{Q_{aph}}{Cp_{apho,avg}} + T_{fdfan,orig}$$

For the resize case, the air preheater is resize so that the flue gas has an exit temperature of $T_{fgapho,input}$. Therefore, the known values are

- flue gas flow rate, m_{fgaphi} and inlet temperature, T_{fgaphi}
- combustion air flow rate, m_{fgapho} and inlet temperature, $T_{fdfan,orig}$
- leakage air flow rate, $m_{leak,orig}$ and inlet temperature, $T_{leak,orig}$
- the flue gas exit temperature, $T_{fgapho,input}$

The output parameters are the energy transferred across the air preheater, Qaph, the "uncorrected" flue gas temperature, T_{fgapho} and the combustion air exit temperature, T_{fgapho} and the air preheater size, UA. Since $T_{fgapho,input}$ is specified, the "uncorrected" flue gas temperature is

$$T_{unc} = \frac{\sum_{j=1}^{9} m_{leak,j,orig}(h_j(T_{fgapho,input}) - h_j(T_{fgapho,input}))}{Cp_{fgaphi,avg}} + T_{fgapho,input}$$

With the "uncorrected" flue gas temperature, the flue gas and combustion temperatures exiting the air preheater and the heat transfer across the air preheater can be determined. The flue gas exit temperature, T_{fgapho}, should be very close to $T_{fgapho,input}$.

$$T_{fgapho} = \frac{Cp_{leak,avg}T_{leak,orig} + Cp_{fgaphi,avg}T_{unc}}{Cp_{leak,avg} + Cp_{fgaphi,avg}}$$

$$Q_{aph} = Cp_{fgaphi,avg}(T_{fgaphi} - T_{unc})$$

$$T_{apho} = \frac{Q_{aph}}{Cp_{apho,avg}} + T_{fdfan,orig}$$

Once all the exit temperatures are determined, the new air preheater size, UA_{aph}, can be determined with

$$UA_{aph} = \frac{Q_{aph}}{(T_{fgaphi} - T_{apho}) - (T_{unc} - T_{fdfan,orig})} \ln\left(\frac{T_{fgaphi} - T_{apho}}{T_{unc} - T_{fdfan,orig}}\right)$$

Once the new size is determined, the additional capital cost in millions of current dollars can be estimated by

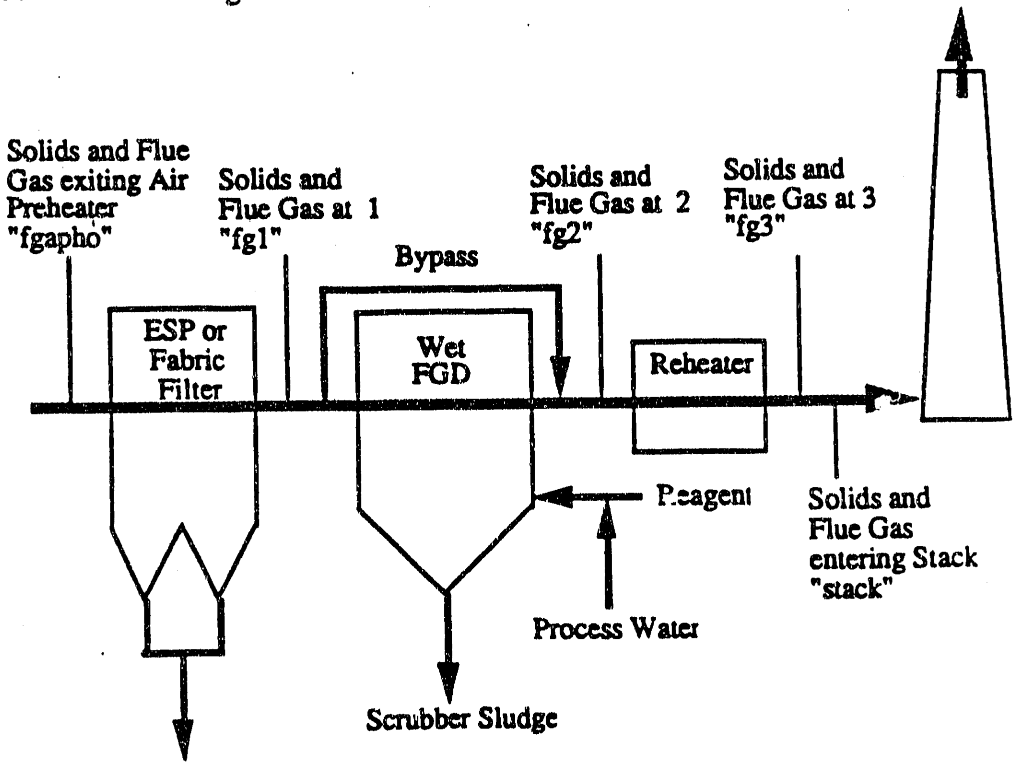
$$Cap_{aph} = 2.6x10^{3}(UA_{aph}^{0.6} - UA_{aph,orig}^{0.6})\frac{C_{idx}}{C_{idx,1984}}$$

For either the base case or the resize case, the difference in the energy transfer across the air preheater can be determined by

$$Q_{aph,delta} = Q_{aph} - Q_{aph,orig}$$

This difference in the energy transfer is an energy credit and how it affects the economics of the power plant is discussed in Section 2.7.

Figure 2-3: Schematic Diagram of the Wet FGD Model



2.5 Wet FGD Performance

This section describes the improvements to the wet flue gas desulfurization (FGD) model since the original model development (1). The quantities that were modified are the reagent composition, water evaporation in the scrubber, flue gas composition exiting scrubber, energy needed for reheat, characterization of the scrubber waste and the capital cost when using lime as a reagent. A schematic diagram of the wet scrubber is shown in Figure 2-3. The diagram shows a configuration with bypass and a reheater. These options are mutually exclusive, since it is not likely that a scrubber would be built with both. So, if there is a bypass, the reheater is not used. Conversely, if there is no bypass, the reheater is used to raise the flue gas temperature to a specified value.

2.5.1 Reagent and SO_2 Efficiency

The SO_2 removal efficiency is a key parameter governing the performance of the FGD system. The removal efficiency can either be specified or it can be calculated to meet a desired SO_2 emission standard. The SO_2 removal efficiency, η_{SO_2}, based on the emission standard is calculated by

$$\eta_{SO_2,std} = 1 - \frac{2000\, ES_{SO_2}\, \dot{M}_{fuel}\, Hhv_{fuel}}{64.06 * 1{,}000{,}000\, (\dot{m}_{in,SO_2} + \dot{m}_{in,SO_3})}$$

$$\eta_{SO_2,std} = 1 - \frac{ES_{SO_2}\, \dot{M}_{fuel}\, Hhv_{fuel}}{64.06 * 500\, (\dot{m}_{in,SO_2} + \dot{m}_{in,SO_3})} \qquad (2.8)$$

The wet FGD system has an option to allow bypassing of some flue gas around the scrubber. This option may lower the cost of the wet FGD system if the efficiency calculated by Equation (2.8) is not very high. When the bypass option is chosen the scrubber operates at its maximum removal efficiency, $\eta_{SO_2,max}$, provided the amount of bypass is greater than the minimum bypass specified by the user, Byp_{min}. Since the bypass does not affect the total amount of sulfur removed, the moles of sulfur removed by the scrubber are determined from the Equation (2.8).

$$\text{if} \left(1 - \frac{\eta_{SO_2,std}}{\eta_{SO_2,max}}\right) \geq Byp_{min} \text{ then}$$

$$Byp = 1 - \frac{\eta_{SO_2,std}}{\eta_{SO_2,max}}; \quad \eta_{SO_2} = \eta_{SO_2,max}$$

$$\text{else } Byp = 0.0\ ; \ \eta_{SO_2} = \eta_{SO_2,std}$$

$$\dot{m}_{rem,S} = \eta_{SO_2,std}\, (\dot{m}_{in,SO_2} + \dot{m}_{in,SO_3})$$

The reagent for the wet scrubber can be either lime or limestone. The reagent purity, R_{purity} and moisture content, W_{reag}, must be specified. Any remaining material is considered inert. The molar stoichiometry, σ, (moles of calcium required per mole of sulfur removed) must be specified. The default values for the molar stoichiometry are 1.15 and 1.05 for limestone and lime, respectively. With the molar stoichiometry, the mass flow rate of reagent is calculated by

$$\dot{M}_{reag} = \frac{100.09\ \dot{m}_{rem,S}\ \sigma}{2000\ R_{purity}} \text{ for } CaCO_3\ ;\ \dot{M}_{reag} = \frac{56.08\ \dot{m}_{rem,S}\ \sigma}{2000\ R_{purity}} \text{ for } CaO$$

2.5.2 Water Balance

Makeup water to the FGD system is required principally to offset evaporative losses in the scrubber. The mass of water evaporated in the FGD system is determined by an energy balance assuming adiabatic conditions and neglecting the solid mass flow rates in the scrubber. With these assumptions, the sensible energy released by the flue gas entering the scrubber has to equal the energy needed to evaporate the water evaporated and raise it to the exit temperature. The equation for the energy balance is shown by Equation (2.9) for a scrubber without bypass[8]. The function, $Cp'_{in,avg}$ is the average specific heat of the flue gas between the inlet temperature and the T_{exit}. The function, Δh, is the energy needed to raise the makeup water to saturated steam at T_{exit}.

$$Cp'_{in,avg}(T_{in}, T_{exit})\ (T_{in} - T_{exit}) \sum_{j=1}^{9} \dot{m}_{in,j} = \dot{W}_{evp}\ \Delta h(T_{exit}) \tag{2.9}$$

$$T_{in} = T_{fg1} + \Delta T_{idfan}$$

The temperature T_{in} is higher than T_{in}, since the induce draft fan raises the inlet temperature by ΔT_{idfan}. The induced draft fan is assumed to be located between the scrubber and the particulate collector. The flue gas is assumed to behave as an ideal mixture, so the molar fraction of water in the flue gas is equal to the parcel pressure of water divided by the total pressure of the flue gas. Since the flue gas is saturated when it exits the scrubber, the amount of water evaporated is constrained by the saturation pressure of the water in the flue gas at the exit temperature. Since the change in the flue gas' total molar flow rate caused by the chemical equations is very small, the water evaporation constraint is show in Equation (2.10).

$$\frac{P_{sat}(T_{exit})}{P_{atm} + P_{g,exit}} = \frac{\dot{W}_{evp} + \dot{m}_{in,H_2O}}{\dot{W}_{evp} + \sum_{i=1}^{9} \dot{m}_{in,j}} \tag{2.10}$$

Equations (2.9) and (2.10) represent two non-linear equations in two unknowns, T_{exit} and $\dot{W}_{evp}$. These two equations can be turned into a quadratic equation of $\dot{W}_{evp}$, provided the P_{sat} and Δh are linear functions of the exit temperature and $Cp'_{in,avg}$ is constant. Figure 2-4 shows the typical variation in the average specific heat between 300°F and the exit temperature. The flue

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[8] Bypassing flue gas around the scrubber does not change the exit temperature, but it does change the amount of water evaporated. For these reasons, the bypass variable is excluded from the derivation of the flue gas exit temperature. Once the exit temperature is determined, the amount of evaporated water can be determined for the scrubber with bypass.

gas for Figure 2-4 is from an Illinois #6 coal and the average specific heat is determined using the enthalpy functions presented in Section 2.2. The initial estimate of the average specific heat, $Cp'_{in,avg}$, is determined by guessing the exit temperature.

$$Cp'_{in,avg}(T_{in}, T_{guess}) = \frac{\sum_{j=1}^{9} \dot{m}_{in,j}\left(h_j(T_{in}) - h_j(T_{guess})\right)}{(T_{in} - T_{guess}) \sum_{j=1}^{9} \dot{m}_{in,j}}$$

Figure 2-4: Flue Gas Specific Heat versus Exit Temperature

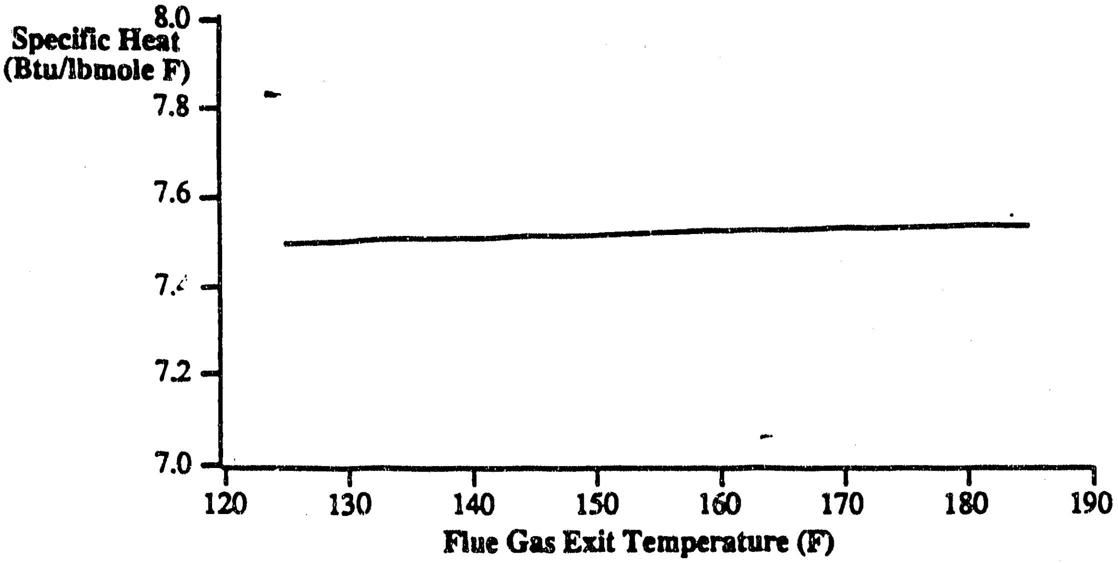
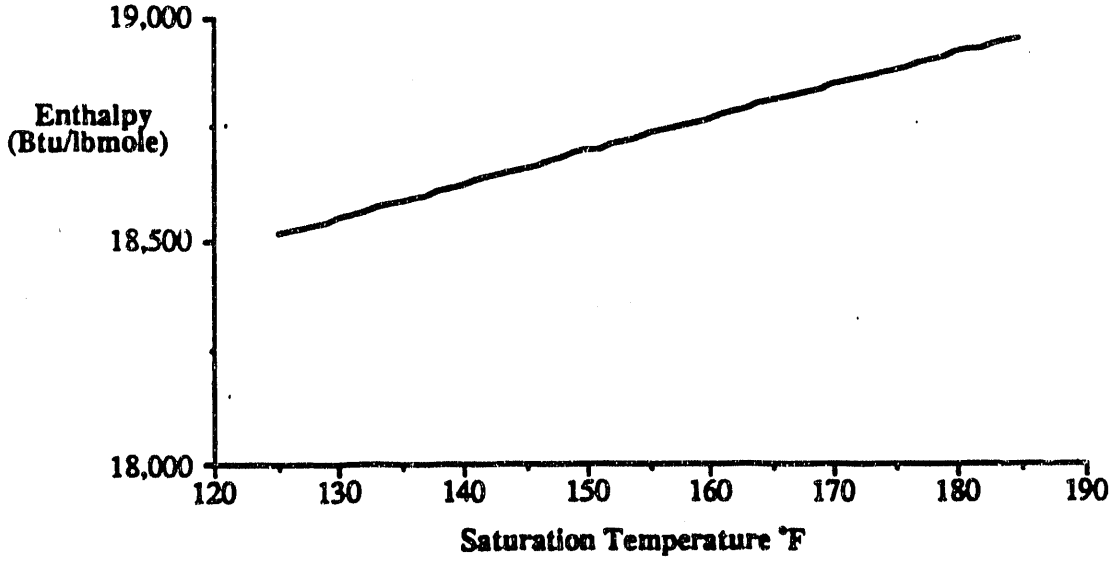


Figure 2-5: Enthalpy Difference between Saturated Steam and Saturated Water at 120°F



The linear equation, (2.11), for energy absorbed by the evaporating water was determined from a linear regression of the enthalpy of saturated steam minus the enthalpy of saturated water at 120°F, between 125°F and 185°F (10). Figure 2-5 shows the enthalpy at 120°F, between 125°F and 185°F (10). Figure 2-5 shows the enthalpy difference between saturated steam versus saturated water at 120°F. It was found that the amount of water evaporated is not sensitive to the inlet water temperature, so the inlet water temperature is assumed to be 120°F. The correlation coefficient for the linear regression was greater than 99%.

$$\Delta h(T) = 7.3660\ T_F + 17{,}593.7 \qquad (2.11)$$

The saturation pressure of water versus temperature is shown in Figure 2-6 (11). Because of the curvature of the data and the sensitivity of Equation (2.10) to the saturation pressure, this data was fitted to a piecewise line between 125 and 185°F, (2.12). The correlation coefficient was greater than 99% for each segment.

$$P_{sat}(T_F) = A_{sat}\ T_F + B_{sat} \qquad (2.12)$$

where

$A_{sat} = 59.5475\times10^{-3}$, $B_{sat} = -5.5087$ for $125 \leq T_F \leq 135$,

$A_{sat} = 74.4615\times10^{-3}$, $B_{sat} = -7.5238$ for $135 < T_F \leq 145$

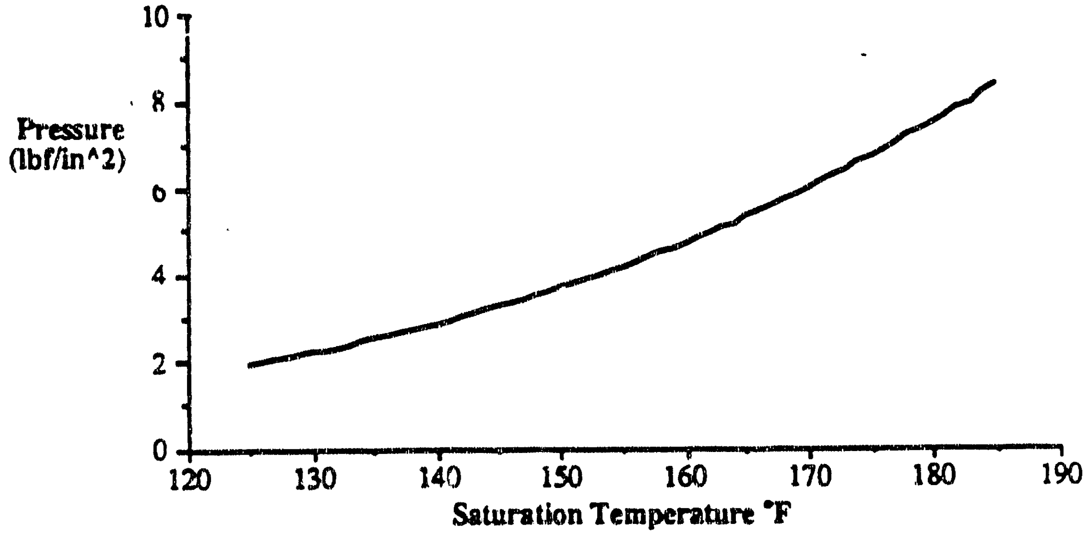
$A_{sat} = 92.2619\times10^{-3}$, $B_{sat} = -10.1068$ for $145 < T_F \leq 155$

$A_{sat} = 113.333\times10^{-3}$, $B_{sat} = -13.3749$ for $155 < T_F \leq 165$

$A_{sat} = = 138.0782\times10^{-3}$, $B_{sat} = -17.4604$ for $165 < T_F \leq 175$

$A_{sat} = = 166.8782\times10^{-3}$, $B_{sat} = -22.5032$ for $175 < T_F \leq 185$

Figure 2-6: Saturation Pressure of Water versus Temperature



Substituting Equations (2.11) and (2.12) into Equations (2.9) and (2.10) and solving for evaporated water yields Equation (2.13). Once the evaporated water is known, the exit temperature can be found by substituting P_{sat} from Equation (2.12) into Equation (2.10) and solving for the exit temperature, (2.14).

$$\dot{W}_{evp} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \tag{2.13}$$

where

$$a = 7.366\,(-B_{sat} + 1) + 17{,}593.7A_{sat}$$

$$b = \left(Cp'_{in,avg}(T_{in}, T_{guess})\,(-A_{sat}T_{in} - B_{sat} + 1) - 7.366B_{sat} + 17{,}593.7A_{sat}\right)\sum_{j=1}^{9} \dot{m}_{in,j}$$

$$+ 7.366\dot{m}_{in,H_2O}$$

$$c = \left(\dot{m}_{fg1,H_2O} + (-A_{sat}T_{in} - B_{sat})\sum_{j=1}^{9} \dot{m}_{fg1,j}\right) Cp'_{fg1,avg}(T_{in}, T_{guess}) \sum_{j=1}^{9} \dot{m}_{fg1,j}$$

$$T_{exit} = \frac{\dot{W}_{evp} + \dot{m}_{in,H_2O}}{A_{sat}\left(\dot{W}_{evp} + \sum_{j=1}^{9} \dot{m}_{in,j}\right)} - \frac{B_{sat}}{A_{sat}} \tag{2.14}$$

Since a single linear equation for the saturation pressure does not represent the data, the solution of the quadratic equation for the evaporated water depends on the slope and intercept of Equation (2.12), that are functions of the exit temperature. To eliminate this cyclic dependency, the procedure shown below is used. It has been found that the temperature converges to within a degree and the evaporated water to within one percent on step five.

1. Determine $\dot{W}_{evp,1}$ from (2.13) assuming an exit temperature of 155°F
2. Determine $T_{exit,1}$ from (2.14) with $\dot{W}_{evp,1}$
3. Determine $\dot{W}_{evp,2}$ with $T_{exit,1}$
4. Determine T_{exit} with $\dot{W}_{evp,1}$
5. Determine $\dot{W}_{evp}$ from (2.13) times (1 - Byp) with T_{exit}

Figure 2-7: Evaporated Water versus Temperature

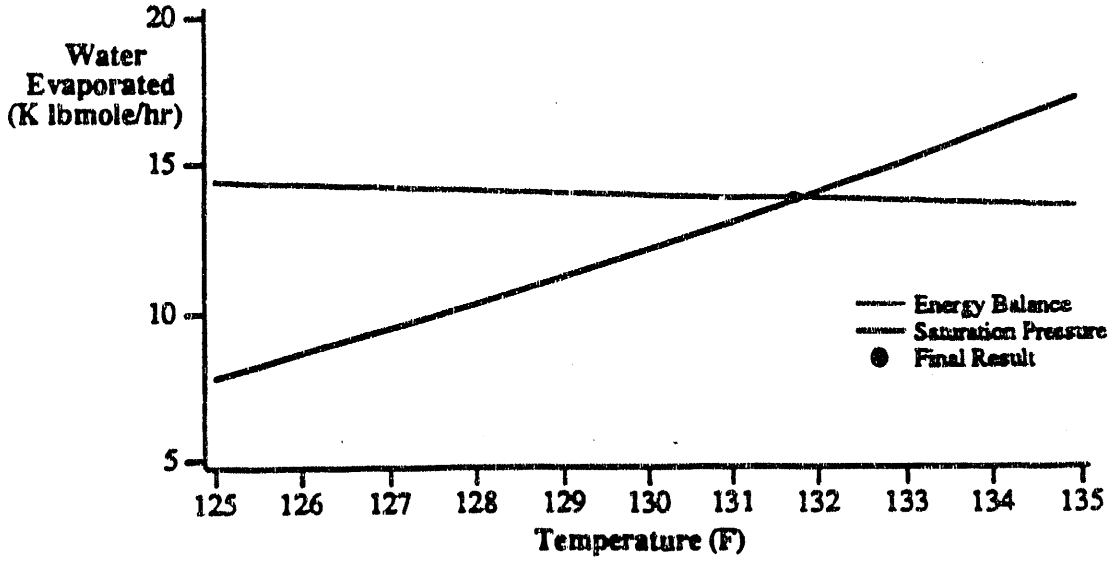


Figure 2-7 shows evaporated water based on Equations (2.9), (2.10) and the iterative procedure shown above for an Illinois #6 coal, an inlet temperature of 314°F and gauge pressure of 4" of water. The graph indicates that the iterative solution is very accurate.

2.5.3 Flue Gas Composition and Reheat

The composition of the flue gas changes in the scrubber. The two most significant changes are the reduction in the sulfur dioxide content and the increase in the moisture content. The sulfur dioxide and sulfur trioxide are removed from the flue gas by a complex set of chemical reactions. These chemical reactions have been greatly simplified in the IECM and are shown below.

$$\begin{aligned}
&0.5H_20 + SO_2 + CaCO_3 \dashrightarrow CaSO_3{\bullet}0.5H_20 + CO_2 \qquad (2.15)\\
&2H_20 + 0.5O_2 + SO_2 + CaCO_3 \dashrightarrow CaSO_4{\bullet}2H_20 + CO_2\\
&0.5H_20 + SO_3 + CaCO_3 \dashrightarrow CaSO_3{\bullet}0.5H_20 + CO_2 + 0.5O_2\\
&2H_20 + SO_3 + CaCO_3 \dashrightarrow CaSO_4{\bullet}2H_20 + CO_2\\
&0.5H_20 + SO_2 + CaO \dashrightarrow CaSO_3{\bullet}0.5H_20\\
&2H_20 + 0.5O_2 + SO_2 + CaO \dashrightarrow CaSO_4{\bullet}2H_20\\
&0.5H_20 + SO_3 + CaO \dashrightarrow CaSO_3{\bullet}0.5H_20 + 0.5O_2\\
&2H_20 + SO_3 + CaO \dashrightarrow CaSO_4{\bullet}2H_20
\end{aligned}$$

Using these chemical reactions the composition of the flue gas exiting the scrubber can be determined from a molar balance and is shown below. It is assumed that the oxygen needed to oxidize the calcium sulfite to calcium sulfate is taken from the flue gas. In practice this oxygen may be supplied by blowing air through the sludge outside the scrubber vessel. It is assumed that the water needed to hydrate the scrubber sludge comes directly from the makeup slurry and does not reduce the moisture content of the flue gas. The symbol Ox represents the fraction of calcium sulfite oxidized to calcium sulfate.

$$\dot{m}_{exit,j} = (1 - Byp)\,\dot{m}_{in,j} \quad \text{for } j = N_2,\ CO,\ NO,\ NO_2$$

$$\dot{m}_{exit,O_2} = (1 - Byp)\,\dot{m}_{in,O_2} + (0.5(1 - Ox)\,\dot{m}_{in,SO_3} - 0.5\,Ox\,\dot{m}_{in,SO_2})\,\eta_{SO_2,std}$$

$$\dot{m}_{exit,H_2O} = (1 - Byp)\,\dot{m}_{in,H_2O} + \dot{W}_{evp}$$

$$\dot{m}_{exit,CO_2} = (1 - Byp)\,\dot{m}_{in,CO_2} + \{\dot{m}_{rem,S} \text{ if regent} = CaCO_3\}$$

$$\dot{m}_{exit,SO_2} = (1 - Byp)\,\dot{m}_{in,SO_2} - \dot{m}_{in,SO_2}\,\eta_{SO_2,std}$$

$$\dot{m}_{exit,SO_3} = (1 - Byp)\,\dot{m}_{in,SO_3} - \dot{m}_{in,SO_3}\,\eta_{SO_2,std}$$

The flue gas exiting the scrubber contains water droplets that the demister has not removed. These droplets evaporate either in the reheater or after the flue gas is remixed with the bypassed flue gas. These droplets are assumed to be a fraction, W_{demis}, of the evaporated water:

$$\dot{m}_{stack,j} = \dot{m}_{exit,j} + Byp\ \dot{m}_{in,j} \text{ for all j except } H_2O$$

$$\dot{m}_{stack,H_2O} = \dot{m}_{exit,H_2O} + Byp\ \dot{m}_{in,H_2O} + W_{demis}\ \dot{W}_{evp}$$

The flue gas exiting the scrubber is either remixed with the bypass flue gas or it passes through a reheater. Therefore, the flue gas temperature entering the stack is either the average temperature of the bypass flue gas and the flue gas exiting the scrubber or the exit temperature of the reheater. The exit temperature of the reheater is an input parameter, $T_{stack,input}$. The energy needed to raise the flue gas temperature to T_{stack} is the sum of the sensible energy of the flue gas and the energy needed to evaporate the water droplets and raise their temperature to T_{stack}.

If no bypass then

$$T_{stack} = T_{stack,input}$$

$$E_{wetfgd} = W_{demis}\ \dot{W}_{evp}\ (7.366T_{stack} + 17593.7) + \sum_{j=1}^{9} \dot{m}_{in,j}\ (h_j(T_{stack}) - h_j(T_{exit}))$$

else

$$T_{stack} = Byp\ T_{in} + (1 - Byp)\ T_{exit}$$

$$E_{wetfgd} = 0$$

2.5.4 Waste Stream Composition

A major environmental flow stream emanating from a wet FGD system is the stream of wet solids. Two model options affect the mass flow rate of wet solids. The user specifies either a forced oxidation FGD system producing a gypsum waste or a natural oxidation FGD system that produces a wet sludge. The basic chemistry for these two options is shown in Equation (2.15). The difference in the composition and mass flow rates of FGD waste depends on the extent of oxidation of calcium sulfite to sulfate, Ox and the extent of dewatering of the final product, W_{sludge}. Other constituents of the FGD solids stream include unreacted reagent (that depends on the molar stoichiometry), inert materials introduced with the reagent (as dictated by the level of reagent purity) and flyash that has been removed by the scrubber (that depends on the particulate removal efficiency, η_{TSP}). The mass flow rates of the component are shown below.

$$\dot{M}_{sludge,j} = (1 - Byp)\ \eta_{TSP}\ \dot{M}_{in,j} \text{ for } j = \text{Ash, } CaSO_4$$

$$\dot{M}_{sludge,CaO} = (1 - Byp)\,\eta_{TSP}\,\dot{M}_{in,CaO} + \left\{\frac{56.08\,(\sigma - 1)\,\dot{m}_{rem,S}}{2000} \text{ if reagent} = \mathrm{CaO}\right\}$$

$$\dot{M}_{sludge,CaCO_3} = (1 - Byp)\,\eta_{TSP}\,\dot{M}_{in,CaCO_3} + \left\{\frac{100.09\,(\sigma - 1)\,\dot{m}_{rem,S}}{2000} \text{ if reagent} = \mathrm{CaCO_3}\right\}$$

$$\dot{M}_{sludge,CaSO_3\cdot 0.5H_2O} = (1 - Byp)\,\eta_{TSP}\,\dot{M}_{in,CaSO_3\cdot 0.5H_2O} + \frac{129.14\,(1 - Ox)\,\dot{m}_{rem,S}}{2000}$$

$$\dot{M}_{sludge,CaSO_4\cdot 2H_2O} = (1 - Byp)\,\eta_{TSP}\,\dot{M}_{in,CaSO_4\cdot 2H_2O} + \frac{172.17\,Ox\,\dot{m}_{rem,S}}{2000}$$

$$\dot{M}_{sludge,Misc} = (1 - Byp)\,\eta_{TSP}\,\dot{M}_{in,Misc} + (1 - R_{purity} - W_{reag})\,\dot{M}_{reag}$$

$$\dot{M}_{sludge,H_2O} = \left(\frac{1}{W_{sludge}} - 1\right)\sum_{j=1}^{8} \dot{M}_{sludge,j} \text{ for all j except } H_2O$$

2.5.5 Economics Algorithm

The economic algorithm for the wet scrubber has remained unchanged except two items. The first is that the single indirect charge factor originally employed for capital cost estimates has been split into its component categories following the nomenclature used by the Tennessee Valley Authority (TVA), author of the basic FGD cost model. The second change is in the direct capital cost for reagent handling. If lime is used as the reagent, the direct capital cost of reagent handling is the same as the algorithm used for a spray dryer (1). If limestone is used, the algorithm remains unchanged. The direct capital cost of reagent handling is shown below.

If Reagent = $CaCO_3$

$$DC_{reag} = \left(\text{If } \dot{M}_{reag} < 18 \text{ Then } 0.1323\,\dot{M}_{reag} + 2.859 \text{ else } 0.07288\,\dot{M}_{reag} + 5.393\right)\frac{C_{idx}}{C_{idx,1981}}$$

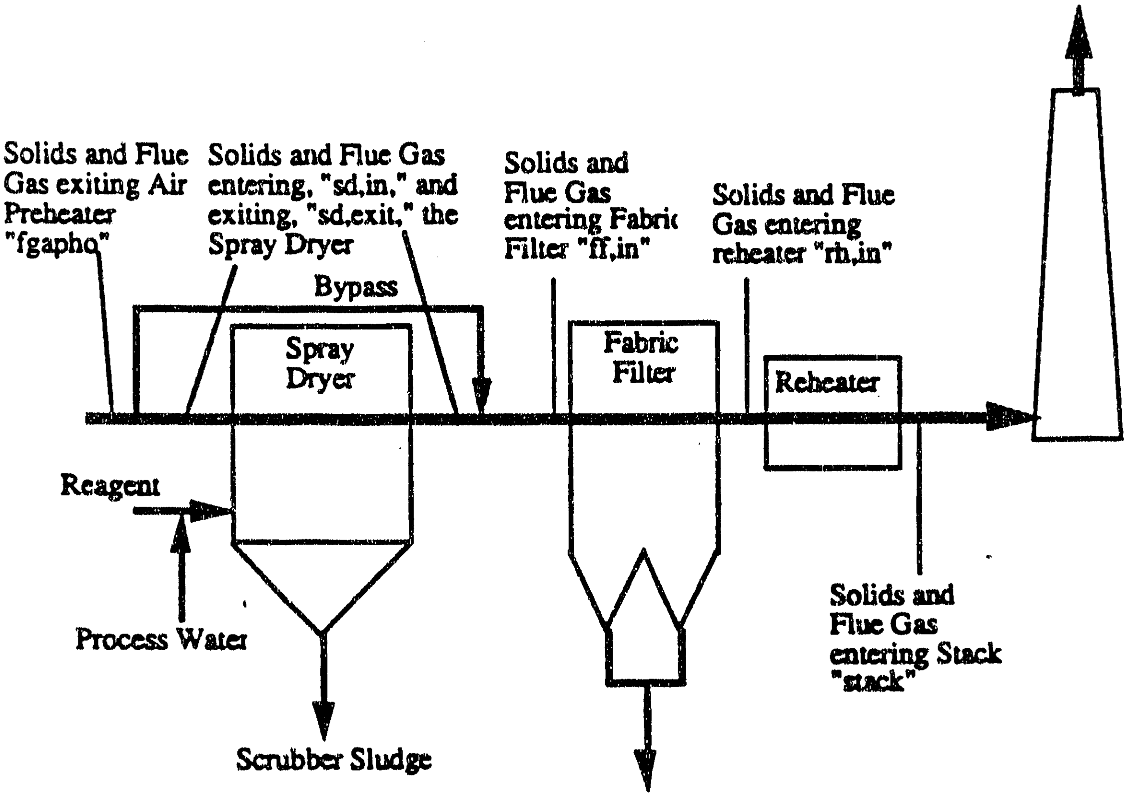
else

$$DC_{reag} = \left(\text{If } \dot{M}_{reag} < 2 \text{ Then } 0.2997\,\dot{M}_{reag} + 1.546 \text{ else } 0.1986\,\dot{M}_{reag} + 2.042\right)\frac{C_{idx}}{C_{idx,1981}}$$

2.6 Spray Dryer Performance

This section describes improvements to the lime spray dryer performance model relative to the previous report (1). The areas that were modified are the reagent composition, water evaporation in the spray dryer, flue gas composition exiting spray dryer, energy needed for reheat and characterization of the scrubber waste. A schematic diagram of the spray dryer is shown in Figure 2-8. The diagram shows a configuration with bypass and a reheater. These options are mutually exclusive, since it is not likely that a spray dryer would be built with both. If there is a bypass, the reheater is not used. Conversely, if there is no bypass, the reheater is used to raise the flue gas temperature to a specified value.

Figure 2-8: Schematic Diagram of the Spray Dryer FGD Model



2.6.1 Reagent and SO_2 Efficiency

The SO_2 removal efficiency is a key parameter governing the performance of the spray dryer system. The removal efficiency can either be specified or it can be calculated to meet a desired SO_2 emission standard. The SO_2 removal efficiency, η_{SO_2}, based on the emission standard is the same as Equation (2.8) shown in Section 2.5.

The spray dryer system has an option to allow bypassing of some flue gas around the scrubber. This option may lower the cost of the spray dryer system if the efficiency calculated by Equation (2.16) is not very high. When the bypass option is chosen the amount of bypass is based on either the spray dryer operating at its maximum efficiency, $\eta_{SO_2,max}$, or the flue gas temperature entering the stack. No bypass will be used if the amount of bypass is less than the minimum bypass specified by the user, Byp_{min}. If the user wants the bypass to be based on the maximum efficiency of the spray dryer then Equation (2.16) is used.

$$\text{if}\left(1 - \frac{\eta_{SO_2,std}}{\eta_{SO_2,max}}\right) \geq Byp_{min} \text{ then} \tag{2.16}$$

$$Byp = 1 - \frac{\eta_{SO_2,std}}{\eta_{SO_2,max}}; \quad \eta_{SO_2} = \eta_{SO_2,max}$$

else

$$Byp = 0.0; \quad \eta_{SO_2} = \eta_{SO_2,std}$$

The user may desire to have the bypass based on a desired stack temperature, $T_{stack,input}$. With this option, a bypass is only allowed if the bypass is greater than the minimum, Byp_{min}, and less than the amount determined by Equation (2.16). The induced draft fan is after the fabric filter, (that is after the gases remix) and raises the temperature of the flue gas by a user specified amount, T_{idfan}. The flue gas exiting the spray dryer and the flue gas bypassed around the spray dryer are assumed to have the same specific heat; therefore, Equation (2.17) is used if the user wants the bypass to be based on the $T_{stack,input}$. The inlet temperature, T_{in}, equals the temperature exiting the air preheater, T_{fgapho}, while the exit temperature, T_{exit}, is determined in the next section.

$$\text{if } Byp_{min} \leq \frac{T_{stack,input} - T_{idfan} - T_{sd,exit}}{T_{fgapho} - T_{sd,exit}} \leq \left(1 - \frac{\eta_{SO_2,std}}{\eta_{SO_2,max}}\right) \text{then} \tag{2.17}$$

$$Byp = \frac{T_{stack,input} - T_{idfan} - T_{sd,exit}}{T_{fgapho} - T_{sd,exit}}; \quad \eta_{SO_2} = \frac{\eta_{SO_2,std}}{1 - Byp}$$

else

$$Byp = 0.0; \quad \eta_{SO_2} = \eta_{SO_2,std}$$

The flue gas that is not bypassed and the moles of sulfur removed by the scrubber are determined by

$$\dot{m}_{sd,in,j} = (1 - Byp)\, \dot{m}_{fgapho,j}$$

$$\dot{m}_{rem,S} = \eta_{SO_2} (\dot{m}_{sd,in,SO_2} + \dot{m}_{sd,in,SO_3})$$

The reagent for the spray dryer is lime. The reagent purity, R_{purity} and moisture content, W_{reag}, must be specified. Any remaining material is considered inert. The molar stoichiometry, σ, (moles of calcium required per mole of sulfur into the system) is a function of the SO_2 removal efficiency and the approach to saturation temperature (1). With the molar stoichiometry, the mass flow rate of reagent can be determined.

$$\sigma_{sd} = \exp(3.322\, \eta_{SO_2} + 0.025\, \Delta T_{sat} - 2.900) \tag{2.18}$$

$$\dot{M}_{reag} = \frac{56.08\,(\dot{m}_{sd,in,SO_2} + \dot{m}_{sd,in,SO_3})\,\sigma_{sd}}{2000\, R_{purity}} \tag{2.19}$$

2.6.2 Water Balance

Makeup water to the spray dryer system is required principally to offset evaporative losses in the scrubber. The mass of water evaporated in the spray dryer system is determined by an energy balance assuming adiabatic conditions and neglecting the solid mass flow rates in the system. With these assumptions, the sensible energy released by the flue gas entering the scrubber has to equal the energy needed to evaporate the water evaporated and raise it to the exit temperature. This is identical with the wet scrubber, except that the flue gas exiting the spray dryer is not saturated. The user specifies an approach to saturation temperature, ΔT_{sat}, which is a measure of how close the flue gas is to being saturated. The procedure for the spray dryer is identical with the algorithm shown in Section 2.5, except steps 4 and 5[9]. Once the saturation temperature, T_{sat}, of the flue gas is determined, the approach to saturation temperature is added to find the exit temperature. The evaporated water is determined with Equation (2.20), shown below, as follows:

1. Determine $\dot{W}_{evp,1}$ from (2.13) assuming an exit temperature of 155°F
2. Determine $T_{sat,1}$ from (2.14) with $\dot{W}_{evp,1}$
3. Determine $\dot{W}_{evp,2}$ with $T_{exit,1}$
4. Determine T_{sat} with $\dot{W}_{evp,1}$, then $T_{exit} = T_{sat} + \Delta T_{sat}$.
5. Determine $\dot{W}_{evp}$ from (2.20)[10]

$$\dot{W}_{evp} = \frac{(1 - Byp) \sum_{j=1}^{9} \dot{m}_{sd,in,j}\,(h_j(T_{fg,apho}) - h_j(T_{sd,exit}))}{7.366\, T_{sd,exit} + 17{,}593.7} \tag{2.20}$$

2.6.3 Flue Gas Composition and Reheat

The composition of the flue gas changes in the spray dryer. The two most significant changes are the reduction in the sulfur dioxide content and the increase in the moisture content. The sulfur dioxide and sulfur trioxide are removed from the flue gas by a complex set of chemical reactions. These chemical reactions have been greatly simplified in the IECM and are shown below:

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[9] An additional assumption is needed for the spray dryer which is that the enthalpy of the water in the flue gas is approximately equal to the enthalpy of saturated steam at the same temperature.

[10] Bypassing flue gas around the scrubber does not change the exit temperature, but it does change the amount of water evaporated. For these reasons, the bypass variable is excluded from the derivation of the flue gas exit temperature. Once the exit temperature is determined, the amount of evaporated water can be determined for the spray dryer with bypass.

$$SO_2 + CaO + 0.5H_20 \dashrightarrow CaSO_3 \cdot 0.5H_20 \qquad (2.21)$$
$$SO_2 + CaO + 2H_20 + 0.5O_2 \dashrightarrow CaSO_4 \cdot 2H_20$$
$$SO_3 + CaO + 0.5H_20 \dashrightarrow CaSO_3 \cdot 0.5H_20 + 0.5O_2$$
$$SO_3 + CaO + 2H_20 \dashrightarrow CaSO_4 \cdot 2H_20$$

Using these chemical reactions the composition of the flue gas exiting the scrubber can be determined from a molar balance and is shown below. It is assumed that the oxygen needed to oxidize the calcium sulfite to calcium sulfate is taken from the flue gas. In practice this oxygen may be supplied by blowing air through the sludge outside the scrubber vessel. It is assumed that the water needed to hydrate the scrubber sludge comes directly from the makeup slurry and does not reduce the moisture content of the flue gas. The symbol Ox represents the fraction of calcium sulfite oxidized to calcium sulfate.

$$\dot{m}_{sd,exit,j} = \dot{m}_{sd,in,j} \quad \text{for } j = N_2, CO_2, CO, NO, NO_2$$

$$\dot{m}_{sd,exit,O_2} = \dot{m}_{sd,in,O_2} + (0.5(1 - Ox)\, \dot{m}_{sd,in,SO_3} - 0.5\, Ox\, \dot{m}_{sd,in,SO_2})\, \eta_{SO_2}$$

$$\dot{m}_{sd,exit,H_2O} = \dot{m}_{sd,in,H_2O} + \dot{W}_{evp}$$

$$\dot{m}_{sd,exit,SO_2} = \dot{m}_{sd,in,SO_2} - \dot{m}_{sd,in,SO_2}\, \eta_{SO_2}$$

$$\dot{m}_{sd,exit,SO_3} = \dot{m}_{sd,in,SO_3} - \dot{m}_{sd,in,SO_3}\, \eta_{SO_2}$$

After the spray dryer there are two options depending if a bypass is used. The first is that the flue gas is remixed with the bypassed flue gas before going into the fabric filter. After the fabric filter the flue gas temperature is raised by the induced draft fan before entering the stack. The second is that the flue gas passes through the fabric filter and induced draft fan before going into the reheater. After exiting the reheater the flue gas enters the stack. For either case, the flue gas composition and temperature do not change in the fabric filter. The equations governing the flue gas temperature and composition for the bypass case are shown below.

$$\dot{m}_{ff,in,j} = \dot{m}_{sd,exit,j} + Byp\, \dot{m}_{fgapho,j} \qquad (2.22)$$

$$T_{ff,in} = Byp\, T_{fgapho} + (1 - Byp)\, T_{sd,exit} \qquad (2.23)$$

$$\dot{m}_{stack,in,j} = \dot{m}_{ff,in,j} \qquad (2.24)$$

$$T_{stack} = T_{ff,in} + \Delta T_{idfan} \qquad (2.25)$$

$$E_{dryfgd} = 0 \qquad (2.26)$$

The equations governing the flue gas temperature and composition for the reheater case are shown below. The exit temperature of the reheater is an input parameter, $T_{stack,input}$. The energy needed to raise the flue gas temperature to T_{stack} is the sensible energy of the flue gas.

$$\dot{m}_{stack,in,j} = \dot{m}_{ff,in,j}\dot{m}_{stack,j} = \dot{m}_{rh,in,j} = \dot{m}_{ff,in,j} = \dot{m}_{sd,exit,j} \tag{2.27}$$

$$T_{ff,in} = T_{sd,exit} \tag{2.28}$$

$$T_{rh,in} = T_{ff,in} + \Delta T_{idfan} \tag{2.29}$$

$$T_{stack} = T_{stack,input} \tag{2.30}$$

$$E_{dryfgd} = \sum_{j=1}^{9} \dot{m}_{rh,in,j}\left(h_j(T_{stack}) - h_j(T_{rh,in})\right) \tag{2.31}$$

2.6.4 Waste Stream Composition

A major environmental flow stream emanating from a spray dryer system is the stream of dry waste solids. The basic chemistry for the creation of these solids is shown in Equation (2.21). The difference in the composition and mass flow rates of spray dryer waste depends on the extent of oxidation of calcium sulfite to sulfate, Ox. Other constituents of the spray dryer solids stream include unreacted reagent (that depends on the molar stoichiometry), inert materials introduced with the reagent (as dictated by the level of reagent purity) and flyash. The total mass flow rate of the solids created in the spray dryer and the flyash entering the spray dryer is shown below.

$$\dot{M}_{sd,total,j} = \dot{M}_{sd,in,j} \text{ for } j = \text{Ash, } CaCO_3\text{, } CaSO_4$$

$$\dot{M}_{sd,total,CaO} = \dot{M}_{sd,in,CaO} + \left\{\frac{56.08\left[\sigma\left(\dot{m}_{sd,in,SO_2} + \dot{m}_{sd,in,SO_3}\right) - \dot{m}_{rem,S}\right]}{2000}\right\}$$

$$\dot{M}_{sd,total,CaSO_3\cdot 0.5H_2O} = \dot{M}_{sd,in,CaSO_3\cdot 0.5H_2O} + \frac{129.14\,(1 - Ox)\,\dot{m}_{rem,S}}{2000}$$

$$\dot{M}_{sd,total,CaSO_4\cdot 2H_2O} = \dot{M}_{sd,in,CaSO_4\cdot 2H_2O} + \frac{172.17\,Ox\,\dot{m}_{rem,S}}{2000}$$

$$\dot{M}_{sd,total,Misc} = \dot{M}_{sd,in,Misc} + (1 - R_{purity} - W_{reag})\,\dot{M}_{reag}$$

The total solids in the spray dryer either exit with the flue gas or drop out the bottom of the spray dryer. The removal efficiency, η_{TSP}, of the solids is an input parameter, that specifies what fraction of the total solids exit out the bottom. The solids that exit with the flue gas remix with the flyash bypassed around the spray dryer (if present) before entering the fabric filter. After the fabric filter removes most of the solids, the solids from the spray dryer and fabric filter are remixed before being disposed.

$$\dot{M}_{sd,bottom,j} = \eta_{TSP}\,\dot{M}_{sd,total,j}$$

$$\dot{M}_{sd,exit,j} = (1 - \eta_{TSP})\,\dot{M}_{sd,total,j}$$

$$\dot{M}_{ff,in,j} = Byp\,\dot{M}_{fgapho,j} + \dot{M}_{sd,exit,j}$$

2.6.5 Economics Algorithm

The economic algorithm for the spray dryer has remained unchanged except one item. The single indirect charge factor for capital cost has been split into different categories of indirect charges following the nomenclature of the TVA.

2.7 Power Plant Economics

This section describes the economics of the base (original) power plant. Subsequent sections then describe how the pollution control equipment affects the economics of the base plant. The following section will describe how the economics changes when pollution control equipment is added. For purposes of cost estimate and internal consistency, the IECM effectively considers the power plant and pollution control equipment to be separate entities. The base power plant essentially consumes fuel and produces electricity and flue gas, while the pollution control equipment consumes some electricity and removes the pollutants from the flue gas.

2.7.1 Base Plant Costs

The base power plant uses electricity and steam for running pulverizers, steam cycle pumps, flue gas fans, cooling system and miscellaneous other equipment. These components represent internal utility (auxiliary power) consumption that reduces the amount of electricity that the power plant can sell to customers (including the pollution control equipment). The auxiliary power consumption reduces the electricity available for sale and increases the heat rate.

$$MW_{bp} = MW_g(1 - x_p - x_{sp} - x_f - x_c - x_{misc})$$

$$HR_{bp} = \frac{HR_{cycle}}{1 - x_p - x_{sp} - x_f - x_c - x_{misc}}$$

The capital and operating cost of a power plant is based on the algorithms presented in Molberg (11). The direct and total capital costs are estimated as follows:

$$TDC_{bp} = 600\left(\frac{MW_{bp}}{1{,}000{,}000}\right)^{0.85} \frac{HW_{idx}}{HW_{idx,1988}}$$

$$TCC_{bp} = TDC_{bp}\,(1 + ICF)$$

The operating cost is divided into two categories: fuel cost and non-fuel cost. The non-fuel expenses include labor, maintenance, overhead, taxes, etc... The fuel cost depends on the fuel consumption and cost of fuel, while the non-fuel cost is proportional to the size of the power plant.

$$AC_{fuel} = 8766x10^{-6}\, C_f m_{fuel} P_{fuel}$$

$$AC_{non} = 8766x10^{-6}\, C_f\, 4.35\, MW_{bp} \frac{C_{idx}}{C_{idx,1988}}$$

$$AC_{bp} = AC_{fuel} + AC_{non}$$

The total revenue requirement excluding any income from "selling" electricity to the pollution control equipment can be calculated by annualizing the total capital cost and levelizing the total operating and maintenance costs. The model does not explicitly charge the power plant for its own utility consumption. The main reason is that any charge to the power plant is collected by the power plant, so the net effect is zero. The price of electricity, E_{cost}, charged to the pollution control equipment can be set to any value by the model user (as is typically done in most economic analyses). However, the default is to use the marginal electricity cost based on the total revenue requirement of the base plant without utilities:

$$TRR_{w/o\ util,bp} = TCC_{bp} FCF + AC_{bp} VCLF \tag{2.32}$$

$$E_{cost} = \frac{TRR_{w/o\ util,bp} x10^6}{8766 C_f MW_{bp}} \tag{2.33}$$

where 8766 is the average number of hours in a year (including leap years).

2.7.2 Pollution Control Equipment Energy Penalties

This section gives a brief overview of the economics of pollution control equipment and describes in detail how the pollution control equipment affects the economics of the base power plant. This section assumes that the pollution control equipment is a consumer of energy. The next section describes the effects when pollution control equipment *contributes* energy (e.g. from exothermic chemical reactions). How the capital and operating costs of specific pollution control equipment are determined is described in other chapters and is not covered in this section. Once the total capital and operating costs are determined for a specific pollution control equipment the total revenue requirement can be calculated.

$$TRR_{w/o\ util,pce,j} = TCC_{pce,j}FCF + AC_{pce,j}VCLF$$

However, this does not reflect the cost of electricity and steam consumption charged to the pollution control equipment by the power plant. The utility cost is the equivalent electricity consumption times the cost of electricity. Given the utility cost, the total revenue requirement can be determined. This total revenue requirement can be expressed in mills per kilowatt hour by divided it by the net electric capacity of the power plant.

$$AC_{util,pce,j} = 8766C_f\, MW_{bp}\, x_{pce,j}\, E_{cost}$$

$$TRR_{pce,j} = TRR_{w/o\ util,pce,j} + AC_{util,pce,j}$$

$$E_{pce,j} = \frac{TRR_{pce,j} x 10^6}{8766C_f MW_{net}}$$

The electricity consumption of the pollution control equipment reduces the amount of electricity available for sale to external customers. Therefore, the net electric capacity is the gross capacity minus the internal consumption, including all pollution control equipment:

$$MW_{net} = MW_g\left(1 - x_p - x_{sp} - x_f - x_c - x_{misc} - \sum_{j=1}^{n} x_{pce,j}\right)$$

Since the pollution control equipment "pays" the base power plant for electricity consumption, these charges are income for the base power plant. The pollution control equipment utility costs appear as negative charges (i.e. income) in the base power plant utility cost. This procedure is a bookkeeping operation to change pollution control equipment for utility use:

$$AC_{util,bp} = -\sum_{j=1}^{n} AC_{util,pce,j}$$

The total revenue requirement including utility cost for the power plant can be calculated as the sum of the total revenue requirement without utilities plus the utility cost for the base power plant. The total revenue requirement can be divided by the net capacity to determine the cost of electricity including utility costs of the base power plant, E_{bp}. This cost of electricity, E_{bp}, will equal the price of electricity charged to the pollution control equipment, E_{cost}, if the price charged to the pollution control equipment is equal to the value determined by Equation (2.33).

$$TRR_{bp} = TRR_{w/o\,util,bp} + AC_{util,bp} \tag{2.34}$$

$$E_{bp} = \frac{TRR_{bp} x 10^6}{8766 C_f MW_{net}} \tag{2.35}$$

2.7.3 Pollution Control Equipment Energy Credits

This section describes the changes in economics when pollution control equipment contributes energy that can be converted to electricity (as is true of an exothermic process that increases the potential heat input to the boiler). There are a variety of ways to treat this case. For the IECM, the pollution control equipment is assumed to sell the energy back to the power plant, that converts the additional energy into electricity for sale. Therefore, the revenue generated from the sale of energy to the power plant shows up as a credit in the operating costs for the pollution control equipment and a debit in the fuel cost of the power plant.

The power plant is considered to have two choices for treating this energy. Either it can reduce the amount of purchased fuel while the gross amount of electricity remains constant or it can "build" additional equipment to convert this energy into additional electricity (i.e., increase the gross plant size). The first choice requires an iterative solution since the energy generated by the pollution control equipment is a function of the fuel consumption of the power plant.[11] Because of the complexities of the IECM, it is not possible to solve this iterative problem explicitly.

Instead, the IECM assumes the power plant builds additional equipment to convert the additional energy into electricity. Since the IECM models new power plants, the additional equipment is "built" simultaneously with the base power plant, yet is accounted separately in the economics. This approach allows a simpler solution. Or, the user simply can neglect the change in size since it is generally small and does not change the economics substantially. The additional equipment has capital and non-fuel operating costs, that are charged to the base power plant.

The equivalent electric capacity of this energy is needed to determine the charges and debits for energy generated by pollution control equipment. If the additional energy is in the form of heat captured by the air preheater, it is treated the same as the energy from coal. The additional

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[11] The energy generated by the pollution control equipment is based on the fuel flow rate into the power plant and the characteristics of the specific pollution control equipment. So reducing the fuel flow rate into the power plant, changes the energy generated by the pollution control equipment, which changes the fuel flow rate. To accurately solve this problem requires an interactive solution, since it is not possible to *a priori* determine the appropriate fuel flow rate and energy from the pollution control equipment to produce a specific amount of electricity.

energy is divided by the original heat rate. If the additional energy is in the form of steam, it is treated the same as energy in the steam cycle, so the additional energy is divided by the original heat rate times the boiler efficiency. With the equivalent electric capacity, the electric capacity of the power plant with and without pollution control equipment also can be determined.

$$MW_{credit} = \frac{Q_{aph,delta}}{HR_{orig}} + \frac{Q_{steam}}{\eta_{boiler} HR_{orig}}$$

$$MW_{bp,new} = MW_g(1 - x_p - x_{sp} - x_f - x_c - x_{misc}) + MW_{credit}$$

$$MW_{net} = MW_g\left(1 - x_p - x_{sp} - x_f - x_c - x_{misc} - \sum_{j=1}^{n} x_{pce,j}\right) + MW_{credit}$$

Multiplying the electric capacity by the heat rate and dividing by the higher heating value of the fuel gives the equivalent fuel consumption. The equivalent fuel consumption is multiplied by the cost of fuel to determine the revenue from the sale of the energy to the power plant. This revenue is credited to the operating cost of the pollution control equipment that generated the energy.

$$m_{fuel,credit} = \frac{MW_{credit} HR_{bp}}{2Hhv}$$

$$AC_{fuel,credit} = 8766x10^{-6} C_f m_{fuel,credit} P_{fuel}$$

$$AC_{pce,j} = AC_{w/o\ credit,pce,j} + AC_{fuel,credit}$$

Several base plant economic variables must be modified to account for the energy credit. The direct capital cost for the additional equipment is estimated to be proportional to the direct capital cost of the original power plant. Therefore, the direct capital cost is determined by

$$TDC_{bp} = 600\left(1 + \frac{MW_{credit}}{MW_{bp}}\right)\left(\frac{MW_{bp}}{1,000,000}\right)^{0.85} \frac{HW_{idx}}{HW_{idx,1988}}$$

The non-fuel operating and maintenance costs are estimated to be proportional to the non-fuel operating and maintenance cost of the original power plant. The total operating cost for the base plant is

$$AC_{non} = 8766x10^{-6}\, C_f\, 4.35\, (MW_{bp} + MW_{credit}) \frac{C_{idx}}{C_{idx,1988}}$$

$$AC_{bp} = AC_{fuel} + AC_{non} + AC_{fuel,credit}$$

The equations for the total revenue requirement, (2.34) and (2.32) and the cost of electricity of the base power plant, (2.35), do not change, but the equation for the default price of electricity charged to pollution control equipment, (2.33), does change:

$$E_{cost} = \frac{TRR_{w/o\ util,bp} x10^6}{8766 C_f MW_{bp,new}}$$

2.7.4 Total Pollution Control Cost

The total capital, operating, utility and revenue requirements for pollution control excluding coal cleaning can be determined by summing the values the pollution control equipment:

$$TCC_{total,pce} = \sum_{j=1}^{n} TCC_{pce,j} \ ; \ AC_{total,pce} = \sum_{j=1}^{n} AC_{pce,j}$$

$$TRR_{w/o\ util,total,pce} = \sum_{j=1}^{n} TRR_{w/o\ util,pce,j} \ ; \ AC_{util,total,pce} = \sum_{j=1}^{n} AC_{util,pce,j}$$

$$TRR_{total,pce} = \sum_{j=1}^{n} TRR_{pce,j} \ ; \ E_{total,pce} = \sum_{j=1}^{n} E_{pce,j}$$

The total capital, operating, utility and revenue requirements of the power plant are the sum of the base power plant and the total pollution control equipment.

$$TCC_{total} = TCC_{bp} + TCC_{total,pce}$$

$$AC_{total} = AC_{bp} + AC_{total,pce}$$

$$TRR_{w/o\ util,total} = TCC_{w/o\ util,bp} + TCC_{w/o\ util,total,pce}$$

$$AC_{util,total} = AC_{util,bp} + AC_{util,total,pce}$$

$$TRR_{total} = TCC_{bp} + TCC_{total,pce}$$

$$EC_{total} = EC_{bp} + EC_{total,pce}$$

The total cost for pollution control including coal cleaning has to be determined by examining two identical power plant. One power plant uses cleaned coal, while the other does not. The total pollution control costs are calculated by subtracting the base plant costs for the plant that is not using cleaned coal from the total plant costs for the plant that is using cleaned coal. This procedure is necessary since the coal cleaning plant is assumed to be separate from the power plant. The capital and operating costs of the coal cleaning plant are added to the cost of raw coal, so delivered cost of coal to the power plant increases.

$$TCC_{total,pce} = TCC_{total} - TCC_{bp,w/o\ cc}$$

$$AC_{total,pce} = AC_{total} - AC_{bp,w/o\ cc}$$

$$TRR_{w/o\ util,total,pce} = TCC_{w/o\ util,total} - TCC_{w/o\ util,bp,w/o\ cc}$$

$$AC_{util,total,pce} = AC_{util,total} - AC_{util,bp,w/o\ cc}$$

$$TRR_{total,pce} = TCC_{total} - TCC_{bp,w/o\ cc}$$

$$EC_{total,pce} = EC_{total} - EC_{bp,w/o\ cc}$$

2.8 Key Financial Parameters

2.8.1 Fixed Charge Factor

The fixed charge factor is used to convert the future carrying charges of the plant investment into a uniform series of payments over the plant life. It is calculated based on the revenue requirement methodology presented in the EPRI Technical Assessment Guide (12, 13).

Revenue requirements consist of two main components, carrying charges (fixed charges) and expenses (operating costs). Carrying charges are related to the capital investment and are incurred despite how the plant is used. They consist of return on investment, book depreciation, income taxes, local property taxes and insurance. Expenses are related to the operation and maintenance of the plant and generally used within one year and generally consist of fuel, operating and maintenance costs.

Book depreciation is the annual charge to repay the original investment. A straight line method is used in the IECM and it is assumed that the salvage value is equal to the cost of retiring the plant. The current tax laws allow for an investment tax credit. This credit is an immediate reduction in the income taxes for the year that the plant goes into services. The investment tax credit is normalized as opposed to "flow through" (these terms are explained later). Therefore, the book depreciation calculation is

$$D_b = \frac{1 - itc}{B_l}$$

Money to cover the total capital investment comes from the sale of bonds (known as debt financing) and the sale of common and preferred stock (equity financing). The ratio of debt financing to equity financing is generally around 50%. The return on debt and equity is the money a utility must pay to its investors for using their money. The weighted average of the return on debt and equity is often called the "return on investment", "cost of money" or the "weighted cost of capital". This return is based on the undepreciated investment or the remaining balance on the initial investment, that will be defined later in Equation (2.42). The annual rate of return on debt and equity is related to the inflation rate. The IECM assumes that the real rate of return or the return in the absence of inflation remains constant. Therefore, the rates of return are input parameters expressed in constant dollars and the nominal or current rates of returns are calculated with Equations (2.36), (2.37), (2.38). The weighted cost equity is shown in Equation (2.39), while the weighted cost of capital is shown in Equation (2.40).

$$B = (1 + e_i)(1 + B_r) - 1 \qquad (2.36)$$

$$CS = (1 + e_i)(1 + CS_r) - 1 \qquad (2.37)$$

$$PS = (1 + e_i)(1 + PS_r) - 1 \qquad (2.38)$$

$$E = \frac{PS\,PS_f + CS(1 - PS_f - D_f)}{1 - D_f} \qquad (2.39)$$

$$C = B\,D_f + E\,(1 - D_f) \qquad (2.40)$$

Income taxes are based on company profit within a given year. The profit is equal to the total revenue minus all the deductible expenditures. Income taxes consist of state and federal taxes, with state taxes being deductible for federal tax purposes. Therefore, the effective total tax rate is.

$$t = t_s + (1 - t_s)\,t_f$$

Table 2-4: Federal Tax Depreciation Schedule

Year	Depreciation %	Year	Depreciation%
1	7.5	16	4.4
2	6.9	17	4.4
3	6.4	18	4.4
4	5.9	19	4.4
5	5.5	20	4.4
6	5.1	21	0
7	4.7	22	0
8	4.5	23	0
9	4.5	24	0
10	4.5	25	0
11	4.5	26	0
12	4.5	26	0
13	4.5	28	0
14	4.5	29	0
15	4.5	30	0

Federal tax laws also allow for an accelerated cost recovery or depreciation. This accelerated depreciation schedule, $D_{s,n}$ used for tax purposes is a 200% declining balance method over 15 years and is shown below. It allows for a shorter recovery time and a greater deduction in the early years that the straight line depreciation schedule.

Deferred income tax is the difference between income tax actually paid and the income tax that would have been paid if a straight line tax recovery schedule had been used, Equation (2.41). There are two methods of handling deferred taxes: "flow through" and "normalization". The flow through method pass the tax deferrals immediately to the rate payers or to the stockholders. The normalized method, which the IECM uses, accumulates the deferred taxes in a reserve account to pay for new investment items. The utility collects revenue as if a straight line recovery schedule was used. The utility then has use of the funds until the tax obligation has to be paid in the later years of the booklife. The deferred income taxes and the investment tax credit are called tax preferences.

$$t_{d,n} = (D_{s,n} - 1/B_l)\, t \text{ for } n = 1, B_l \tag{2.41}$$

As mentioned earlier, the return on investment was based on the remaining balance. The remaining balance per year is the initial investment minus the book depreciation, deferred income tax per year and investment tax credit in the first year, Equation (2.42). The returns on debt and equity per year are shown in Equation (2.43) and (2.44). The taxes paid per year are shown in Equation (2.45). The year by year carrying charges is just the sum of the book depreciation, deferred taxes, return on debt, return on equity, income taxes paid and the advalorem tax, Equation (2.46).

$$RB_n = RB_{n-1} - D_b - t_{d,n-1} \tag{2.42}$$

$$RD_n = RB_n D_f B \tag{2.43}$$

$$RE_n = RB_n (1 - D_f) E \tag{2.44}$$

$$t_{p,n} = \frac{t}{1 - t} (D_b - D_{s,n} + t_{d,n} + RE_n) \tag{2.45}$$

$$CC_n = D_b + t_{d,n} + RD_n + RE_n + t_{p,n} + a \text{ for } n = 1, B_l \tag{2.46}$$

$$RB_1 = 1 - itc$$

The discount rate used for present value calculations is related to the weighted cost of capital. The most common method used in the utility industry is a "before tax discount rate" that is equal to the weighted cost of capital. Some industries use an "after tax discount rate" that is equal to the weighted cost of capital less the tax rate times the return on debt. The IECM uses a "before tax discount rate", Equation (2.47). The present value factor of a future expense in a given year is given by Equation (2.48). It is assumed for present value calculations that all expenses are paid at the end of year. The annuity factor shown in Equation (2.49), calculates the present value of a uniform series of payments in the future, while the reciprocal of the annuity factor calculates an equivalent uniform annual amount for a single payment.

$$dis = C \tag{2.47}$$

$$PV_n = (1 + dis)^n \tag{2.48}$$

$$A_n = \frac{1 - PV_n}{dis} \tag{2.49}$$

The present value of future carrying charges is the sum of carrying charges times the present value factor, Equation (2.50). The levelized carrying charge converts the actual carrying charges that vary from year to year into a uniform payment for the tax life of the plant. The levelized carrying charge per year is just the cumulative present value of the carrying charge divided by the annuity, Equation (2.51). The levelized carrying charge for the last year of the book life is the fixed charge factor, Equation (2.52).

$$CC_{pv,n} = \sum_{m=1}^{n} CC_m \, PV_m \tag{2.50}$$

$$CC_{l,n} = \frac{CC_{pv,n}}{A_n} \tag{2.51}$$

$$FCF = CC_{l,B_l} \tag{2.52}$$

2.8.2 Levelization Factor

The levelization algorithm is used to convert a series of future payments that have a uniform escalation rate into a uniform series of payments over the same period. The IECM assumes that the real escalation rate for expenses is constant, so the apparent escalation rate is calculated from Equation (2.53). The levelization factor is calculated with Equation (2.54). The total revenue requirement is calculated in Equation (2.55).

$$e_f = (1 + e_r)(1 + e_i) - 1 \tag{2.53}$$

$$L_n = \frac{k(1 - k^n)}{A_{B_l}(1 - k)}$$

$$\text{where } k = \frac{1 + e_f}{1 + dis} \tag{2.54}$$

$$TRR = TCC \; FCF + TVC \; L_{B_l} \tag{2.55}$$

2.8.3 Year-by-Year Revenue Requirement Analysis

A year-by-year revenue requirement analysis is also available in the IECM. This method has the advantage of showing the revenue requirement in current dollars over the entire tax life. The total revenue requirement in a future year is the sum of the carrying charges and the operating expenses.

$$TCC_n = TCC \; CC$$

$$TVC_n = TVC \, (1 + e_f)^n$$

$$TRR_n = TCC_n + TVC_n$$

2.8.4 Accumulated Funds Used During Construction

The accumulated funds used during construction, AFUDC, or interest during construction is determined from the total plant cost, TPC. It is assumed that the equipment begins service at the beginning of January and that the construction takes place during the preceding years. Also the IECM determines the total plant cost in the same year dollars that the equipment begins services. The actual cashed expended for construction is assumed to be spent uniformly at the middle of each year during construction. Therefore, the total cash expended, TCE, in mixed year dollars, is found by de-escalating the total plant cost back in time.

$$TCE = \frac{TPC}{N} \sum_{j=1}^{N} \frac{1}{(1+i)^{j-0.5}}$$

After the money is spent, interest charges are accumulated as part of the AFUDC at a discount rate, dis. The discount rate is determined from Equation (2.47). Therefore, the total plant investment, TPI, is

$$TPI = \frac{TPC}{N} \sum_{j=i}^{N} \frac{(1+dis)^{j-0.5}}{(1+i)^{j-0.5}} = \frac{TPC}{N} \sum_{j=1}^{N} \left(\frac{1+dis}{1+i}\right)^{j-0.5}$$

The AFUDC is the difference between the total plant investment and the total cash expended.

$$AFUDC = TPI - TCE$$

2.9 Conventional Coal Cleaning

2.9.1 Introduction

This section describes the changes to the conventional coal cleaning model. A detailed description of the conventional coal cleaning model is contained in Reference (1). Figures 2-9 - 2-11 show the schematic diagrams for coal cleaning plants of levels 2, 3 and 4. The subscript "i" in this section refers to the coarse, medium or fine streams of the coal cleaning plant.

2.9.2 Level 4 Plant Cost

After reviewing the economics for a level four plant, several cost coefficients were modified to more accurately represent level four plants that use hydrocyclones. These changes are minor and do not change the cost of cleaning a given coal significantly. The new cost coefficients were modified for the direct capital cost, chemicals, electricity and water are:

$DCC_4 = 45{,}700$

$c_4 = 0.065$

$e_4 = 0.158$

$w_4 = 0.0041$

2.9.3 Moisture Content of Cleaned Coal

Another improvement to the coal cleaning model is that it now more accurately calculates the moisture content of the cleaned and refuse coal. Previously the model did not explicitly calculate the moisture content of the cleaned or refuse coal and it did not adjust the final quality of the coal to account for the thermal drier. These assumptions made the model less sensitive to the effects of the different moisture content associated with different size wash streams.

The revised model assumes that the total moisture content of the raw coal is composed of two components: the inherent moisture and the surface moisture. The inherent moisture is assumed to remained constant even if the coal is washed or thermally dried. The surface moisture of the coal changes if it is washed or thermally dried. The model requires that the surface moisture associated with each wash stream be entered as an input parameter. The value should be typical of the surface moisture associated with the wash size stream after it has been through mechanical dewatering. In other words, as the wash stream size decreases the surface moisture should increase. For example, 28x0 mesh coal would have a surface moisture of approximately 20%, while 1.375"x0.25" would have a value of approximately 4%.

The total moisture content of each wash stream is equal to the inherent moisture content of the raw coal plus the surface moisture of either the wash stream (if the stream was washed) or the raw coal Equation.

If $Y_i < 1$ then

$$m'_i = mi'_{ROM} + ms'_i$$

else

$$m'_i = mi'_{ROM} + ms'_{ROM}$$

To calculate the average properties of the coal entering the thermal drier, the fraction of coal to be thermally dried needs to be determined. Equation (2.56) calculates the weight fraction of the coal exiting the washing equipment, while Equation (2.57) calculates the fraction of coal to be thermally dried. The input parameter, δ_i, is used to determine which streams should be thermally dried. It is set to 1 if the stream is to be thermally dried; otherwise, it is 0. This allows any combination of wash streams to be sent to the thermal drier.

$$fs_{c,i} = \frac{fs_{ROM,i} Y_i}{Y_p} \tag{2.56}$$

$$fs_d = \sum_{i=1}^{3} fs_{c,i} \delta_i \tag{2.57}$$

The surface moisture associated with a wash stream, ms'_i, is an input parameter. Equations (2.58) and (2.59) show the equations for the average moisture content and higher heating value of the coal entering the thermal drier.

$$m'_{in} = \frac{\sum_{i=1}^{3} \frac{m'_i fs_{c,i} \delta_i}{(1 - m'_i)}}{\sum_{i=1}^{3} \frac{fs_{c,i} \delta_i}{(1 - m'_i)}} \tag{2.58}$$

$$HHV_d = \frac{\sum_{i=1}^{3} HHV_i fs_{c,i} \delta_i}{fs_d} \tag{2.59}$$

The moisture content of the refuse streams is equal to the inherent moisture content of the raw coal plus surface moisture associated with the washed streams. Therefore, the average moisture content of the refuse coal is estimated with the equation below.

$$m'_{ref} = \frac{\sum_{i=1}^{3} \frac{(mi'_{ROM} + ms'_i)(1 - Y_i) fs_{ROM,i}}{(1 - mi'_{ROM} - ms'_i)}}{\sum_{i=1}^{3} \frac{(1 - Y_i) fs_{ROM,i}}{(1 - mi'_{ROM} - ms'_i)}}$$

With the moisture content and higher heating value of the coal entering the thermal drier determined, it is possible to calculate the performance of the thermal drier. Since the model explicitly calculates the moisture content of the coal entering the thermal drier, m'_{in}, it is possible for that coal to be drier than the specified moisture content of the coal exiting the thermal drier, m'_{out}. Thus, the thermal drier is used only if the coal entering the drier has a moisture content above a certain level. If the thermal drier is not used the thermal drier yield is set to 100 percent and the fraction of coal dried and water evaporated are set to zero. If it is used the fraction of coal dried is calculated with Equation (2.57) and the other parameters are calculated as follows.

```
$m'_{out} = mi'_{ROM} + ms'_{out}$
If $m'_{in} < m'_{out}$ then
    $w' = 0.0$
    $E_d = 0.0$
    $LHV = 0.0$
    $Y_d = 1.0$
    $Yo_d = 1.0$                                        (2.60)
    $w'_e = 0.0$
    $fs_d = 0.0$
    $\delta_i = 0$
else
```

$$w' = \frac{m'_{in} - m'_{out}}{(1 - m'_{in})(1 - m'_{out})}$$

$$E_d = \frac{1020\ m'}{\eta_d}$$

$$LHV = 0.96\ HHV_d - \frac{1020\ m'_{out}}{(1 - m'_{out})}$$

$$Y_d = 1 - \frac{E_d}{LHV}$$

$$Yo_d = (1 - fs_d) + fs_d\ Y_d \qquad (2.61)$$

$$w'_e = \frac{w'\ m_o\ fs_d}{Yo_d}$$

The ratio of the coal exiting the washing equipment to the coal leaving the plant is defined by Equation (2.60) or (2.61). This parameter is needed to calculate the amount of coal leaving the wash streams based on the out capacity of the plant.

The thermal drier does not change the quality of the coals. It does change the weight fraction of coal in each stream. Therefore, the mass yield and weight fraction of each stream must be adjusted to account for the losses of water and coal in thermal drier. At this point it is more appropriate to describe the drier yield by individual stream though the streams to be dried are combined before entering the thermal drier and the yield is the same across both streams.

If $\delta_i = 1$ then

$$Y_{d,i} = Y_d$$

else

$$Y_{d,i} = 1$$

With the thermal drier yield described as above, the weight fraction and mass yield of each stream can be calculated as follows:

$$fs_{o,i} = \frac{fs_{c,i}\ \delta_i}{Yo_d}$$

$$Y_{t,i} = Y_i\ Y_{d,i}$$

Figure 2-9: Schematic Diagram of a Level 2 Conventional Coal Cleaning Plant

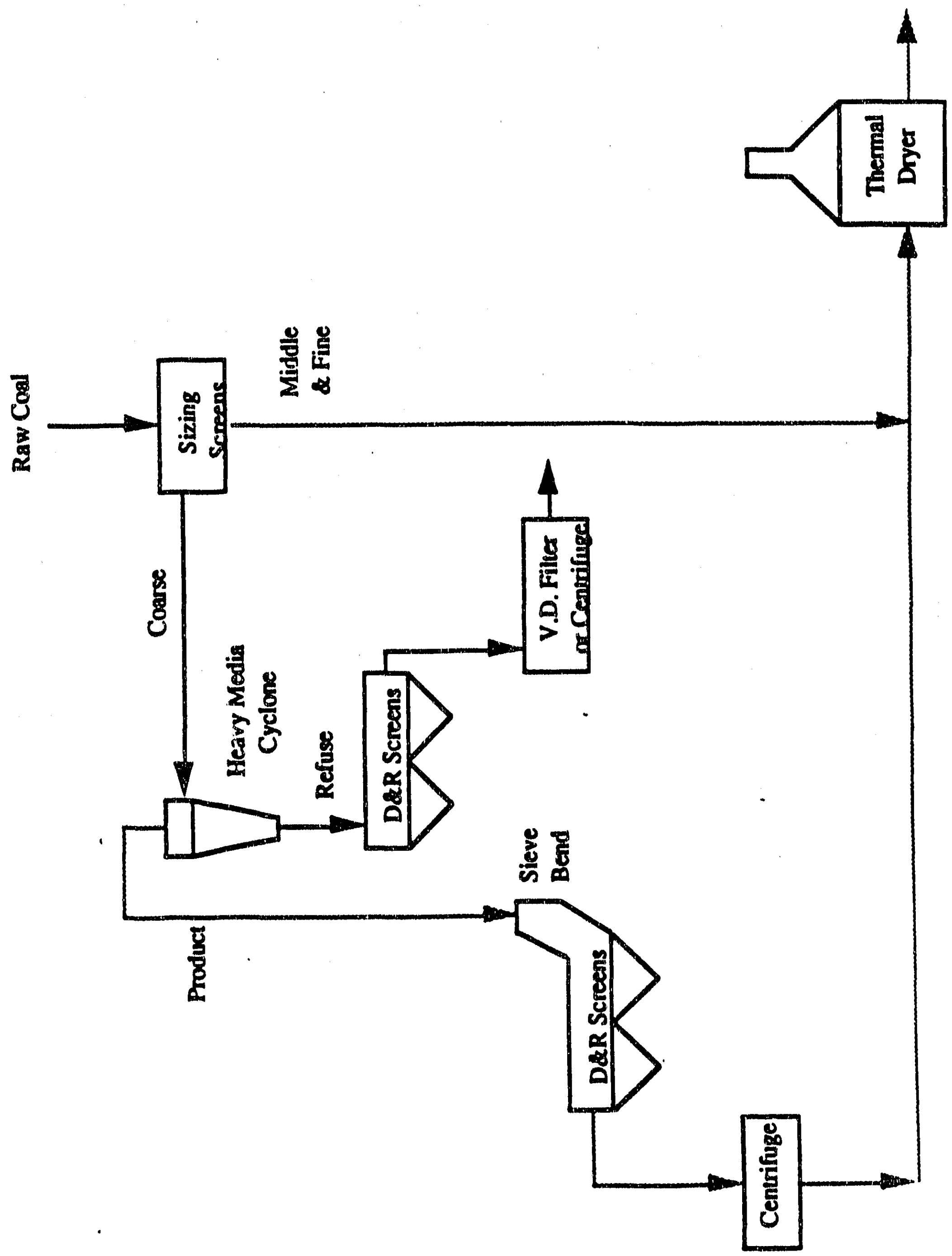


Figure 2-10: Schematic Diagram of a Level 3 Conventional Coal Cleaning Plant

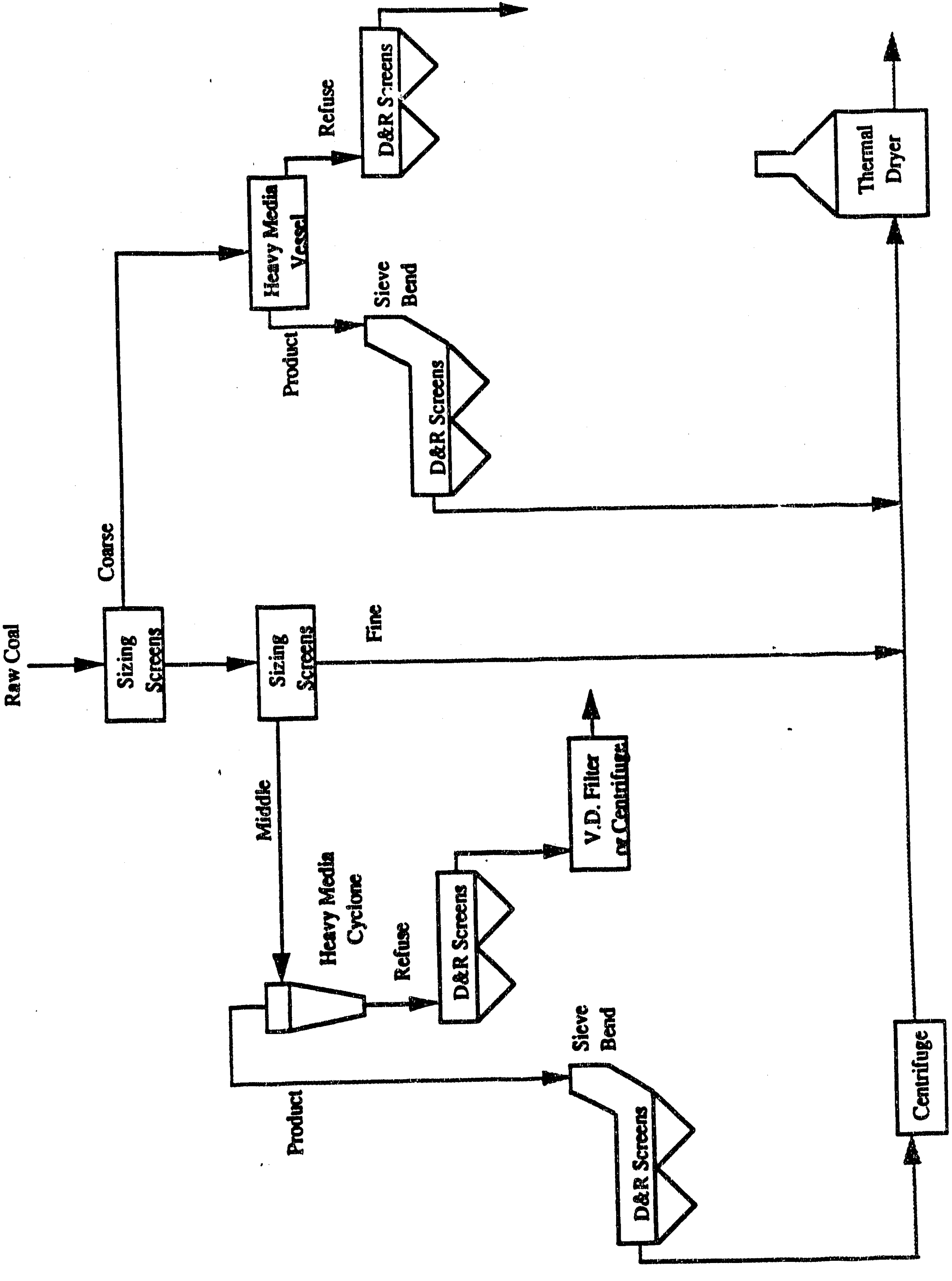
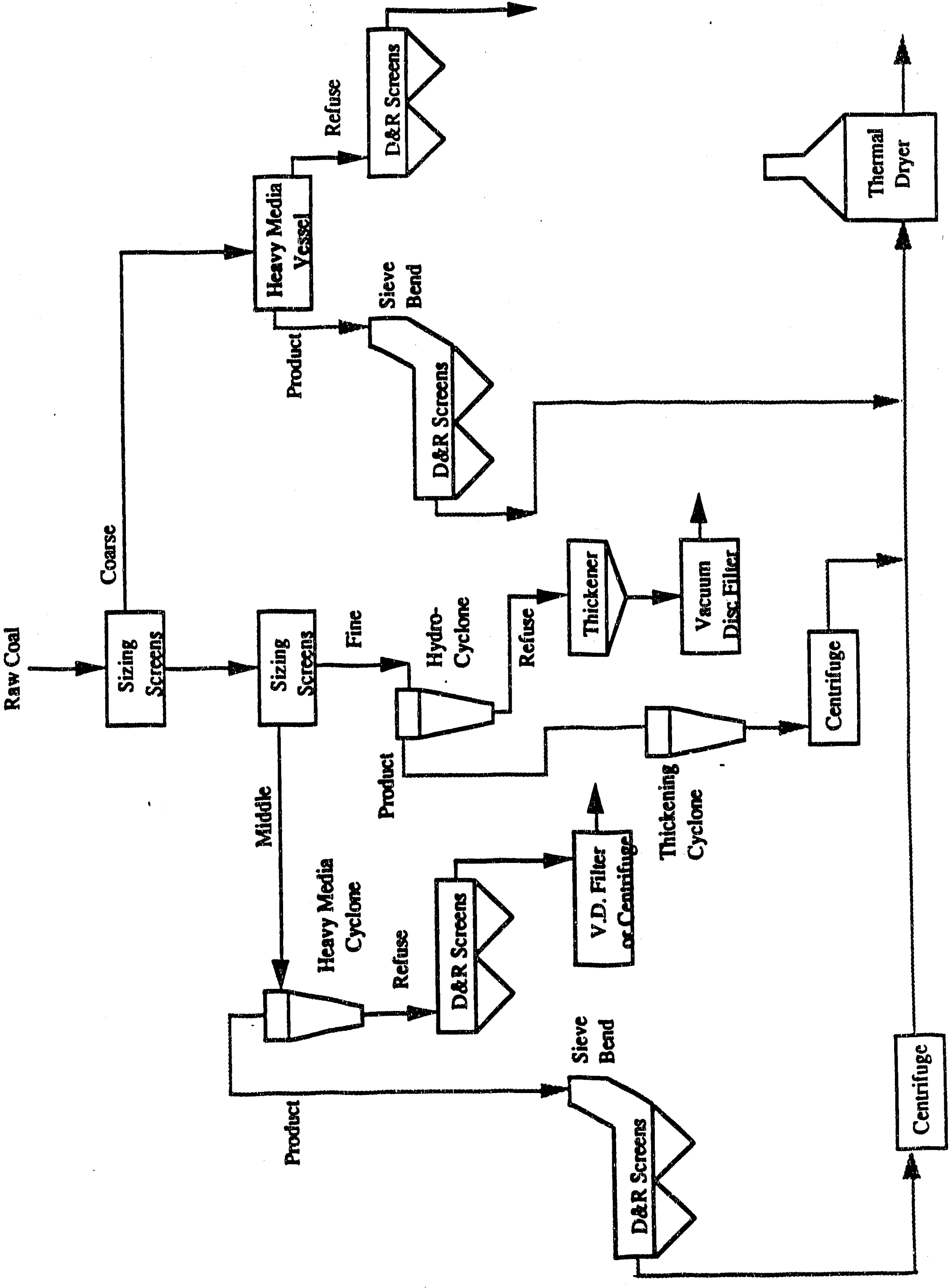


Figure 2-11: Schematic Diagram of a Level 4 Conventional Coal Cleaning Plant



With the new weight fraction data it is possible to calculate the quality of the coal leaving the coal cleaning plant. The moisture content of the final product depends on whether any stream was thermally dried. From this, the higher heating value, ash and sulfur content on a wet basis can be calculated with the equations shown below.

If $\delta_i = 1$ then

$$m'_{o,i} = m'_{out}$$

else

$$m'_{o,i} = m'_{in,i}$$

$$m'_o = \frac{\sum_{i=1}^{3} \frac{m'_{o,i} fs_{o,i}}{1 - m'_{o,i}}}{\sum_{i=1}^{3} \frac{fs_{o,i}}{1 - m'_{o,i}}}$$

$$HHV_o = (1 - m'_{o,i}) \sum_{i=1}^{3} HHV_{o,i} fs_{o,i}$$

$$A_o = (1 - m'_{o,i}) \sum_{i=1}^{3} A_{o,i} fs_{o,i}$$

$$S_o = (1 - m'_{o,i}) \sum_{i=1}^{3} S_{o,i} fs_{o,i}$$

The quality of the final product after the thermal drier may differ slightly from the target quality specified because the optimization algorithm is based on dry coal properties. The difference should not be very large since the thermal drier usually has a mass yield well above 98%. Also note, that if all the streams are picked to be thermally dried, the model will only attempt to dry to coal if the moisture content exceeds a specified value.

3 COPPER OXIDE PROCESS MODEL

3.1 Nomenclature

a	Slope of linear approximation of enthalpy function (Btu/lb•mole °R)
A	reactor cross-sectional area, m^2
b	Intercept of linear approximation of enthalpy function (Btu/lb•mole °R)
C_o	initial CuO content, kg CuO/kg Al_2O_3
Cp_{avg}	Heat capacity (Btu/°R)
D	fluidized bed (expanded) density, kg Al_2O_3/m^3
E	activation energy, KJ/gmole
F	sorbent feed rate, kg Al_2O_3/hr
Ff	frequency factor, 1/hr
G	molar volume of gas at reaction temperature, m^3/kgmole
h_i	Enthalpy of i (Btu/lb•mole °R)
k	reaction rate constant, 1/hr
M	molecular weight of CuO, kg/kgmole
m_j	mass flow rate of j, lb/hr
M_j	Molar flow rate of j, lb•mole/hr
MW_j	molecular weight of j, lb/lb•mole
p	fractional partial pressure of SO_2 at absorber outlet
p_o	fractional partial pressure of SO_2 at absorber inlet
Q_{reac}	Total energy released or absorbed by reaction (Btu/hr)
Q_{total}	Total energy entering device including Q_{reac} (Btu/hr)
r	Molar ratio of sulfur dioxide entering absorber to available copper
R	universal gas constant, 0.008314 KJ/(gmole-K)
R_c	ratio of the molecular weights of Cu and CuO
T	absolute reaction temperature, K
V_o	inlet flue gas volumetric flow rate, m^3/hr
x_{Cu}	weight fraction of available copper in sorbent (kg Cu/kg fresh sorbent)
Z	expanded bed depth, m.
η_r	regeneration efficiency, fraction

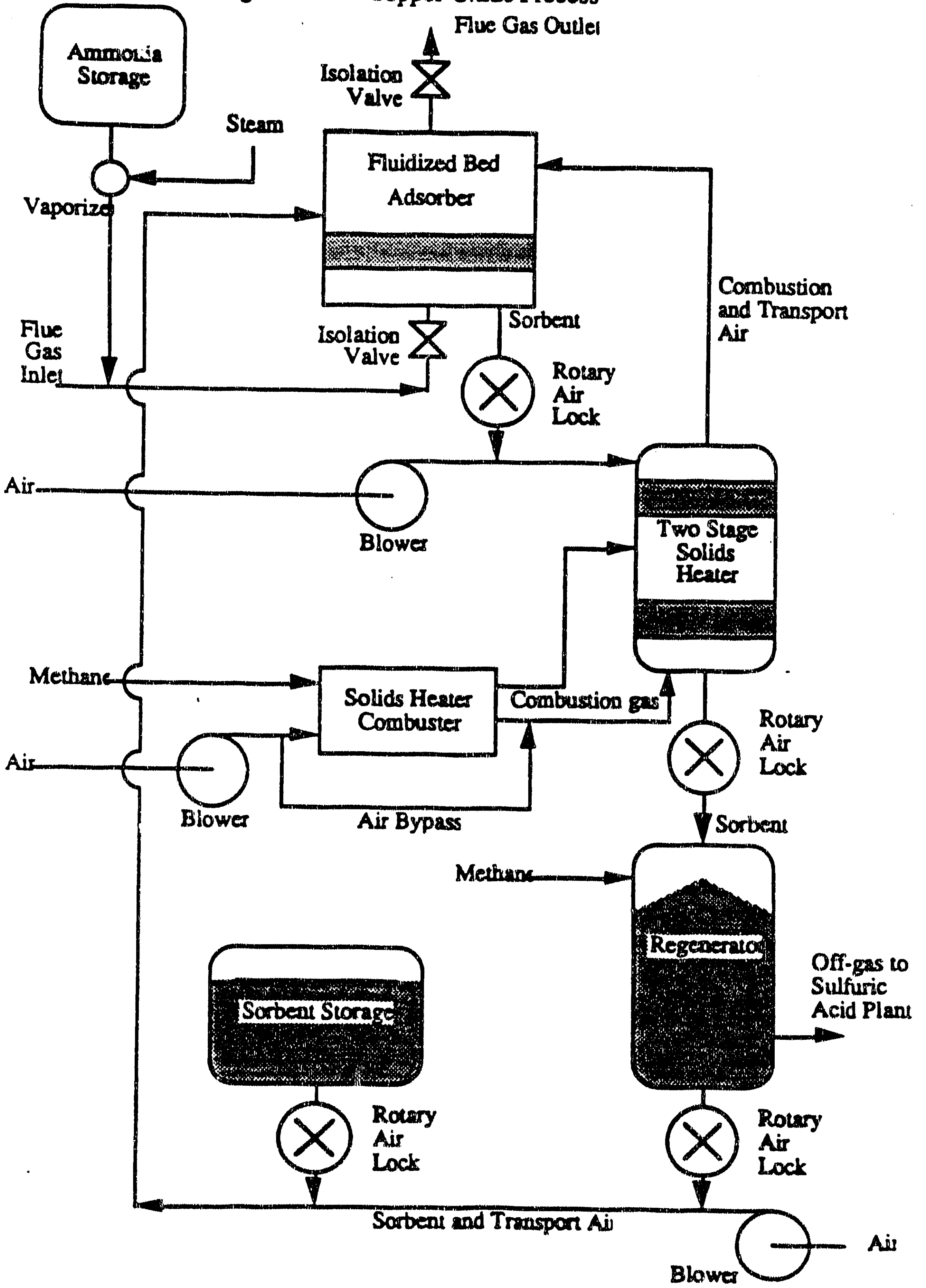
Subcategories

Al_2O_3	Alumina substrate
Cu	Copper
CuO	Copper Oxide
$CuSO_4$	Copper sulfate
s	Sorbent
SO_2	Sulfur dioxide

3.2 Introduction

This chapter describes improvements to the copper oxide process model relative to the original formulation (1). The areas that were modified are the sulfation reaction algorithm in the absorber, the enthalpy functions used to calculate the temperatures of various streams, and the energy captured by the air preheater. The sulfation reaction algorithm is described below in Section 3.3. The new enthalpy functions and the heats of reactions are described in Section 2.2, while the changes in the copper oxide model caused by the new enthalpy functions are described in Section 3.4. The algorithms that determined the energy captured by the air preheater are described in Section 2.4. A schematic diagram of the copper oxide process is shown in Figure 3-1.

Figure 3-1: Schematic Diagram of the Copper Oxide Process



3.3 Sulfation Reaction Algorithm

The revised model for the copper oxide process determines the copper-to-sulfur ratio using a sulfation reaction algorithm developed by PETC (14) instead of an equation based on the regression analysis of experimental data. The new algorithm accounts for available copper oxide initially resident in the fluidized bed, the molar ratio of sulfur oxides to inlet available copper and incomplete regeneration of the sorbent. The derivation is given below.

The sorbent flow rate is a key parameter that affects the mass and energy balances, sizing and cost of most components of the copper oxide process. The sorbent entering the fluidized bed absorber includes regenerated copper oxide and unregenerated copper sulfate. The required flow rate of copper oxide, also referred to as available copper, is determined based on the copper-to-sulfur (Cu/S) molar ratio required to meet the emission control requirement and the amount of sulfur oxides in the flue gas. This rate is given by.

$$m_{CuO} = \frac{MW_{CuO}}{r} M_{SO_2} \qquad (3.1)$$

The amount of unregenerated copper sulfate entering the absorber is given by

$$m_{CuSO_4} = \left[MW_{CuSO_4} \left(\frac{\eta_s}{\eta_r} \right) (1 - \eta_r) \right] M_{SO_2}$$

The total sorbent mass flow rate, including copper oxide, copper sulfate and the alumina substrate, is given by

$$m_s = \left(\frac{MW_{CuO}}{X_{Cu}} \right) (M_{CuO} + M_{CuSO_4} (1 + 1.260 X_{Cu}))$$

The available Cu/S molar ratio, 1/r, required to achieve a specified SO_2 reduction requirement is estimated based on a first-order sulfation reaction kinetics model developed by PETC (14). The fractional partial pressure of SO_2 exiting the absorber can be estimated by

$$p = \frac{\left(1 - \frac{p_o V_o M}{G F C_o} \right) p_o}{\exp\left[\frac{k D A G Z C_o}{M V_o} \left(1 - \frac{p_o V_o M}{G F C_o} \right) \right] - \frac{p_o V_o M}{G F C_o}} \qquad (3.2)$$

The terms on the right-hand side of the model may be redefined as follows

$$r = \frac{p_o V_o M}{G F C_o} = \frac{\text{Inlet } SO_2\text{, kgmole/hr}}{\text{Inlet CuO, kgmole/hr}} \qquad (3.3)$$

$$B = k \left(\frac{k D A G Z C_o}{M V_o} \right) = k \left(\frac{\text{kgmole CuO in fluidized bed}}{\text{kgmole/hr flue gas flow rate}} \right) \qquad (3.4)$$

Equation (3.3) is the inverse of the available copper-to-sulfur molar ratio. Equation (3.4) is the ratio of the copper oxide resident in the bed to the incoming flue gas molar flowrate, multiplied by the reaction rate constant. Equation (3.2) may be rewritten in terms of Equations (3.3) and (3.4) and the SO_2 removal efficiency as follows

$$\eta_{SO_2} = \frac{p_o - p}{p_o} = \frac{\exp[B(1-r)] - 1}{\exp[B(1-r)] - r} \tag{3.5}$$

This is a convenient formulation if we wish to calculate the removal efficiency when regeneration efficiency is 100 percent and B and r are known. However, more typically, we desire to calculate the value of r required to meet a specified removal efficiency, for arbitrary regeneration efficiencies.

The PETC algorithm accounts for two main effects: (1) the amount of available copper oxide initially resident in the fluidized bed per unit molar gas flow, B, and (2) the molar ratio of sulfur oxides to inlet available copper, r. However, the PETC algorithm neglects the regeneration efficiency of the sorbent. When regeneration of the sorbent is complete, the available copper content, C_o, will be the same as the sorbent copper loading. However, in the more likely case where regeneration is incomplete, the available copper will be less than the sorbent copper loading. Since incomplete regeneration reduces the amount of available copper entering the absorber compared to fresh sorbent, by that reducing the sulfur absorption efficiency, the PETC model was modified explicitly to include the effect of regeneration efficiency on the Cu/S ratio requirement. Thus, an expression for C_o was developed that includes regeneration efficiency as a parameter.

The mass flow of the alumina substrate is given by the difference between the total sorbent mass flow rate and the mass flow rates of copper oxide and copper sulfate in the sorbent.

$$m_{Al_2O_3} = \left\{ \frac{MW_{Cu}}{x_{Cu}} \left[\frac{1}{r} + \left(\frac{\eta_{SO_2}}{\eta_r} \right) (1 - \eta_r)(1 + 1.260\, x_{Cu}) \right] \right.$$

$$\left. - \frac{MW_{CuO}}{r} - M_{CuSO_4} \left(\frac{\eta_{SO_2}}{\eta_r} \right) (1 - \eta_r) \right\} M_{SO_2} \tag{3.6}$$

The mass ratio of the available copper (copper oxide) to the alumina oxide substrate, C_o, is then given by the ratio of Equations (3.1) and (3.6). After expanding and then collecting terms and approximating the ratio of the molecular weights of copper sulfate to copper oxide to be 2, rather than 2.006, the following expression results.

$$C_o = \frac{x_{Cu}}{(R_c - x_{Cu}) \left[1 + r \left(\frac{\eta_{SO_2}}{\eta_r} \right) (1 - \eta_r) \right]} \tag{3.7}$$

In the limit where the regeneration efficiency is 100 percent, Equation (3.7) reduces to

$$C_o = \frac{x_{Cu}}{(R_c - x_{Cu})}$$

However, when regeneration is less than complete, the weight ratio of actual copper oxide to alumina substrate is shown to depend on the sulfur-to-available-copper molar ratio, r, the sulfur dioxide removal efficiency and the weight percent copper in fresh sorbent.

Substituting Equation (3.7) into (3.4) and then substituting the resulting equation into (3.5) we obtain the following expression.

$$\eta_s = \frac{\exp\left\{\alpha\left[\dfrac{1-r}{1+r\left(\dfrac{\eta_{SO_2}}{\eta_r}\right)(1-\eta_r)}\right]\right\} - 1}{\exp\left\{\alpha\left[\dfrac{1-r}{1+r\left(\dfrac{\eta_{SO_2}}{\eta_r}\right)(1-\eta_r)}\right]\right\} - r} \qquad (3.8)$$

where

$$\alpha = \frac{k\,D\,A\,G\,Z}{M\,V_o}\left(\frac{x_{Cu}}{R_c - x_{Cu}}\right) \qquad (3.9)$$

In most applications, we wish to solve Equation (3.8) for r as a function of η_s. However, an interactive numerical technique is required to obtain the solution. Newton's method is very effective and convergences within four iterations.

The rate constant used in Equation (3.9) is estimated as follows

$$k = Ff\,\exp\left(-\frac{E}{R\,T}\right)$$

The equation above is the reaction rate constant as a function of frequency factor, activation energy and temperature. The activation energy of a UOP copper oxide sorbent is reported to be 20.1 KJ/gmole (15).

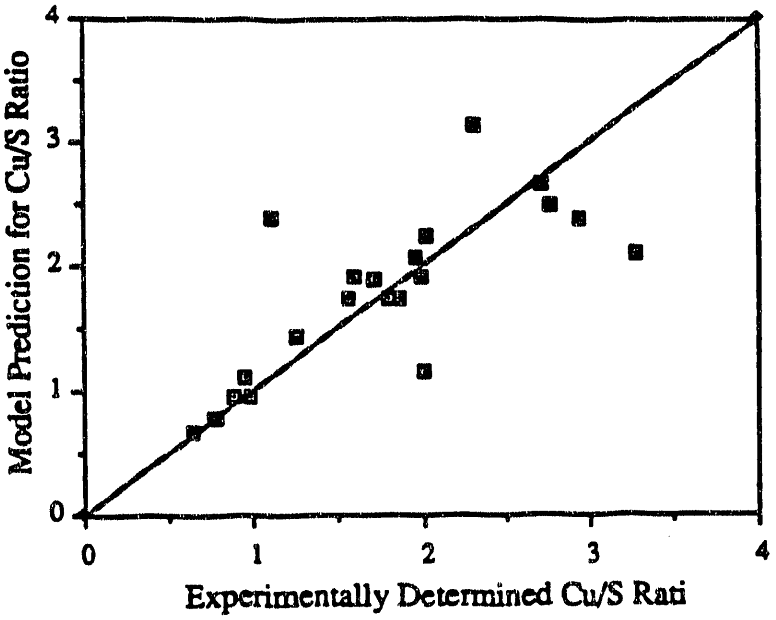
PETC report three values of the frequency factor as a function of the sorbent copper loading in terms of the percent copper in fresh sorbent (14). An equation for the frequency factor was developed using regression analysis. The three data points show a non-linear relationship between frequency factor and sorbent copper loading. The following equation was found to provide good agreement with the data.

$$Ff = 94{,}400\ 10^{-6.18x_{Cu}} \qquad R^2 = 0.998$$

In the above equation, the sorbent copper loading is the weight fraction of copper as copper oxide in the sorbent, to maintain consistency with the model.

Figure 3-2 shows model predictions for the copper-to-sulfur molar ratio based on experimental data by PETC (14). The model is a function of eight variables, each of that is subject to measurement error. Thus, scatter in the plotted data is expected. The scatter in the predicted Cu/S ratio can be represented statistically by a standard error, which is an indicator of the variance in the observed Cu/S ratio that is not explained by the analytical model.

Figure 3-2: Comparison of Experimental and Predicted Copper-to-Sulfur Ratio



3.4 Enthalpy Functions

In the original copper oxide model described in Reference (1), the enthalpy functions were approximated with linear equations. In the current copper oxide model, the enthalpy functions are approximated with polynomial equations, which are described in Section 2.2. This change increases the accuracy of the energy balances in the model. However, it modifies the equations used to determine the energy difference of a stream between two temperatures, the heat capacity of a stream and the temperature of a stream exiting a device. Any energy difference between two known temperatures in the current model is found by using the new enthalpy functions. Any heat capacity in the current model is found using the form (3.16). The change in the algorithm to determine the temperature of a stream exiting a device is described below.

Since the enthalpy functions were linear, the temperature of a stream exiting a device could be determined explicitly. For example, Figure 3-3 shows two streams with known temperatures entering a device and undergoing an exothermic reaction. The energy balance of the device is shown in Equation (3.10). If the enthalpy functions are of the form shown in Equation (3.11), then Equation (3.10) can be solved for the exit temperature as shown in Equation (3.12).

$$M_1\, h_1(T_1) + M_2\, h_2(T_2) + Q_{reac} = M_3\, h_3(T_3) \tag{3.10}$$

$$h(T) = a\,T + b \tag{3.11}$$

$$T_3 = \frac{M_1[a_1 T_1 + b_1] + M_2[a_2 T_2 + b_2] + Q_{reac}}{M_3 a_3} - \frac{b_3}{a_3} \tag{3.12}$$

In the current copper oxide model, the enthalpy functions are of the form shown in Equation (3.13)[12]. Because of the form of the enthalpy functions, Equation (3.10) cannot be solved for the exit temperature explicitly. Instead a two step iteration replaces the equations in the original copper oxide model which determined temperatures from an energy balance. In the first step, an initial estimate of the temperature is made using Equation (3.14)[13]. For the second step, the exit temperature is determined with Equation (3.15). In Equation (3.15), the inlet stream that has the greatest effect on the exit temperature is used for T_1. This two step iteration is very accurate for a variety of cases studies.

$$h(T_R) = AT_R + \frac{Be^{-3}T_R^2}{3.6} - \frac{3.24Ce^5}{T_R} + \frac{De^{-6}T_R^3}{9.72} - 1.8H_{298.15} \tag{3.13}$$

$$T_{guess} = \frac{M_1 h_1(T_1) T_1 + M_2 h_2(T_2) T_2}{M_1 h_1(T_1) + M_2 h_2(T_2)} \left(1 + \frac{Q_{reac}}{Q_{total}}\right) \tag{3.14}$$

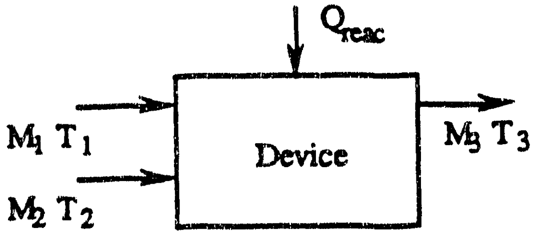
$$T_3 = \frac{Q_{total} - M_3 h_3(T_1)}{Cp_{3,avg}} + T_1 \tag{3.15}$$

where

$$Q_{total} = M_1 h_1(T_1) + M_2 h_2(T_2) + Q_{reac}$$

$$Cp_{3,avg} = \frac{M_3[h_3(T_{guess}) - h_3(T_1)]}{T_{guess} - T_1} \tag{3.16}$$

Figure 3-3: Typical Device in Copper Oxide Process



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[12] The constants A, B, C, D, and $H_{298.15}$ are given in Table 2.3.

[13] In the current copper oxide model, the temperature of the flue gas exiting the absorber is determined with Equation (3.14), since the correction determined by Equation (3.15) is insignificant.

4 NOXSO PROCESS MODEL

4.1 Nomenclature

English Letter Symbols

A_k	area of device, k (ft^2)
$C_{categorie}$	capital charges associated with startup ($)
C_{idx}	chemical engineering cost index
C_o	molar gas concentration of SO_2 in the flue gas entering the adsorber (lb•mole/ft^3)
CF	capacity factor of power plant (fraction)
DCC_k	capital cost for device, k (M$)
$e^{\#}$	notation for specifying power of 10.
$E_{j,k}$	energy flow rate of specie, j, at device, k (lb•mole/hr)
EC_k	electricity consumption of the device, k (kW)
f_{makeup}	attrition rate of sorbent (fraction)
$f_{j,wet\ air}$	amount of specie, j, in ambient moist air (fraction)
$fp_{j,k}$	quantity of specie, j, produced in device, k (fraction)
F_{oil}	constant used to estimate amount of sulfur from oil (fraction)
FOC	fixed operating cost ($/yr)
G_k	gas flow rate for device, k (ft^3/min)
$h_{j,temperature}$	molar enthalpy of specie, j, at specified temperature (Btu/lb•mole)
H	fluidized bed height in adsorber (ft)
HHV_j	higher heating value of specie, j, (Btu/lb)
HR	heat rate of power plant (kW-Hr/MBtu)
i	inflation rate (fraction)
K_a	apparent rate constant ($atm^{-1}\ sec^{-1}$)
$LMTD_k$	log mean temperature difference of device, k (°F)
m_j	mass flow of specie, j, (lbs/hr or tons/hr)
$M_{j,k}$	molar flow rate of specie, j, for device, k (lb•mole/hr)
M'_j	Pound mole per pound of coal entering furnace of species, j. (lb•mole/lb coal)
MW_g	gross electrical capacity of power plant (MW)
N_t	initial loading of the active Na on sorbent (lb•mole/lb)
NOP	number of operating adsorbers
NRD	number of spare adsorbers
$OC_{catagorie}$	annual operating cost ($/yr)
Q_k	heat load across heat exchanger device, k (Btu/hr)
p	interest rate (fraction)
P_k	pressure of the device, k (" water or atm)
RT_k	residence time of sorbent in device, k (hours)
R	Ratio of SO_2 removal efficiency to NO_x removal efficiency (fraction)
$T_{sj,k}$	temperature of specie, j, for the device, k (°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 ($/yr)
U_k	universal heat transfer coefficient for device, k (Btu/hr-ft^2 °F)
UC_j	unit cost of specie, j, ($/unit)
Ut_j	utilization constant for specie, j, 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	molar fraction of SO_2 in the flue gas (fraction)

Greek Letter Symbols

δ_{NOx}	fraction of NOx returned to boiler that is destroyed (fraction)
ΔH_k	heat of reaction in device, k (Btu/hr)
$\eta_{j,k}$	efficiency of device, k (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 a device, k
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_2S
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, H_2S, S_2, SO_2 and SO_3
SD	sulfur dioxide, SO_2
SOX	sulfur dioxide and sulfur trioxide
ST	sulfur trioxide, SO_3
W	water, H_2O

Equipment:

aph	air preheater
AD	adsorber
AH	air heater for sorbent heater

AP	acid plant
B	boiler of power plant
GB	gas burner
R	regenerator
R&S	regenerator and steam treatment vessel
SC	sorbent cooler
SH	sorbent heater
STV	steam treatment vessel

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

4.2 Introduction

This chapter describes improvements to the NOXSO process model originally developed by Barrett (1). Most of these changes have been reported in previous reports to PETC. (16, 17). Other minor improvements change how sulfur from the air heater is handled and modify Equations (4.1), (4.2), (4.3), (4.7) and (4.8). Another improvement couples the SO_2 and NO_x removal efficiencies in the absorber by an input parameter, R. This change modifies Equations (4.4) and (4.5).

The basic NOXSO model is based on designs by NOXSO Corporation (18-21) and Stearns-Rogers (22). The design of the process has changed over time to incorporate other potential improvements. The current process design for this model is based on a study for EPRI (22), with one modification suggested by NOXSO Corp (23), 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 SO_x are returned to the boiler, while the remaining sulfur compounds are sent either to a sulfuric acid or Claus plant. The NO_x returned to the boiler is expected to decompose partially into nitrogen leading to a steady-state NO_x concentration.

A proposed process diagram is shown in Figure 4-1. 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:

- 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

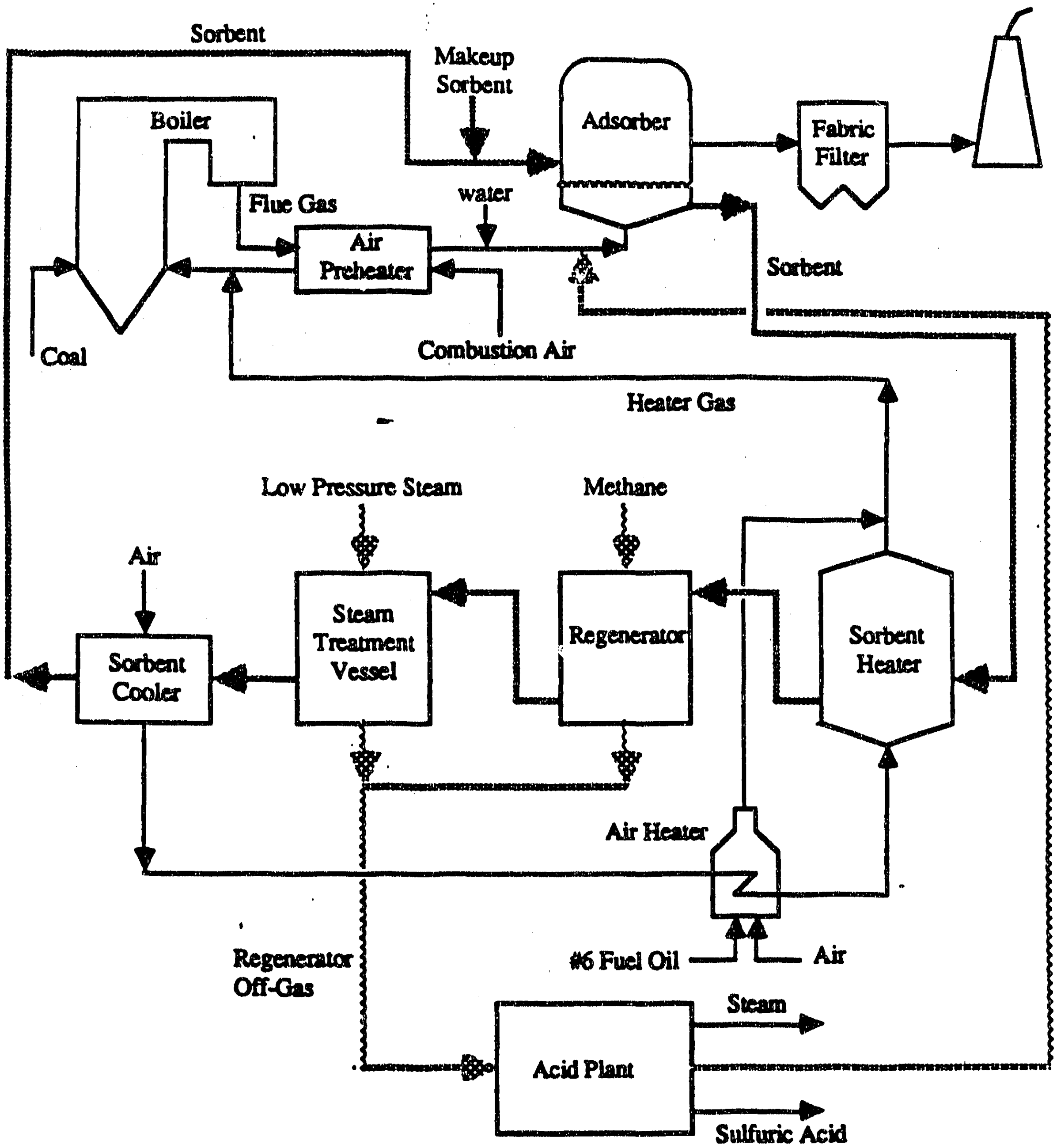
Figure 4-1 is best understood by examining each major mass flow separately. The first mass flow is the sorbent stream. The sorbent entering the adsorber contains some residual sulfur compounds. The sorbent removes NO_x and SO_x from the flue gas while raising the temperature of the flue gas. When inside the sorbent heater, 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 another 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 on the type and quantity of reducing gas used and the design of the regenerator and steam treatment vessels. In communications with NOXSO Corporation 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 (24). 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, SO_x and 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 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 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.

Figure 4-1: NOXSO Process Diagram



The adsorption and regeneration chemistry of NO_x and SO_x are explained in detailed in manyreports 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 on several 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 dependent on 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 that releases COS, H_2S, S_2 and SO_2. These gases are sent to the acid plant. Finally the sorbent is treated with steam to convert as many sulfites to H_2S as possible. NO_x is regenerated by heating the sorbent to 1000°F.

4.3 Performance Model

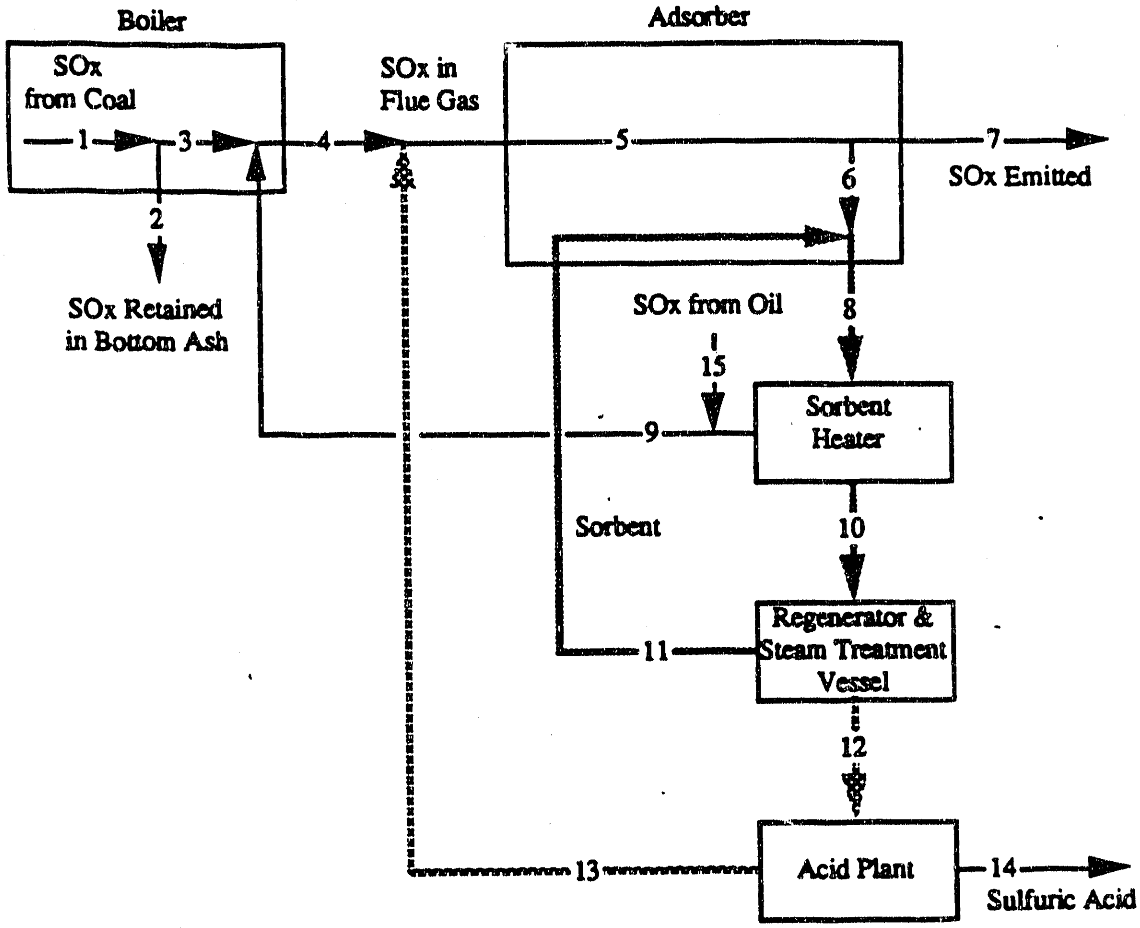
The primary purpose of the process performance model is to characterize the major flow rates defined in the previous section and to predict the NO_x and SO_x removal efficiencies in the adsorber. The NOXSO process recycles some NO_x and SO_2 removed by the adsorber. This requires the adsorber to have 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. 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 and that the ratio of the NO_x removal efficiency to SO_2 removal efficiency is given by a constant input parameter, R. The following procedure is then used to determine the sorbent flow rate:

- The required SO_2 removal efficiency, η_{SO2}, in the adsorber needed to meet the emission standard is determined. It includes the effects of recycled SO_2 and SO_2 from the air heater.
- The required NO_x removal efficiency, η_{NOx}, in the adsorber needed to meet the emission standard is determined. It includes the effects of recycled NO_x and the NO_x 'destroyed' in the boiler.
- If R is less than or equal to 1, the actual SO_2 removal efficiency, $\eta_{SO2,A}$, is the maximum of either η_{NOx} / R or η_{SO2}.
- If R is greater than 1, the actual SO_2 removal efficiency, $\eta_{SO2,A}$, is the maximum of either η_{NOx} or $\eta_{SO2} * R$.
- The actual NO_x removal efficiency, $\eta_{NOx,A}$, is $\eta_{SO2,A} * R$.

Figure 4-2 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. The sulfur dioxide from the oil burned in the air heater is dependent on the sorbent flow rate, which depends on the sulfur removal efficiency in the adsorber. Since this is an iterative problem, the approach taken is to increase the removal of the sulfur dioxide in the absorber by a constant. This constant is called the oil factor and usually is about 1% of the sulfur from the coal. Because the SO_2 emission standard remains the same, all the sulfur from the oil must exit the process as acid. The performance of the NOXSO process is not very sensitive to the value of the oil factor, so it is not necessary to estimate this value precisely. 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 4-2: Simplified Diagram of Mass Flows for Sulfur Compounds



The objective is to derive the actual SO_2 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 SO_2 returned to the boiler from the sorbent heater is retained in the bottom ash. These mass conservation equations (Equations 4.1) are needed to calculate the apparent and actual SO_x removal efficiencies in the adsorber:

$$M_6 = M_8 - M_{11} \qquad M_{12} = \frac{M_{14}}{\eta_{AP}} \tag{4.1}$$

$$M_8 = \frac{M_{10}}{\eta_{SH}} \qquad\qquad M_{14} = (\eta_{std} + F_{oil})\, M_3\ .$$

$$M_{11} = (1 - \eta_{R\&S})\, M_{10} \qquad\qquad M_5 = M_6 + M_7$$

$$M_{10} = \frac{M_{12}}{\eta_{R\&S}} \qquad\qquad M_7 = (1 - \eta_{std})\, M_3$$

where $\eta_{R\&S} = \eta_R + (1 - \eta_R)\, \eta_{STV}$

The apparent removal efficiency is the SO_x removed by the adsorber, M_6, divided by the SO_x from the coal, M_3. Substituting for M_6 and simplifying yields Equations 4.2 which determines the apparent removal efficiency based on known values:

$$\eta_{app} = \frac{M_6}{M_3} = \frac{M_8 - M_{11}}{M_3} = \frac{\frac{M_{10}}{\eta_{SH}} - M_{10}(1 - \eta_{R\&S})}{M_3} = \frac{M_{10}\left(\eta_{R\&S} - 1 + \eta_{SH}^{-1}\right)}{M_3} \tag{4.2}$$

$$\eta_{app} = \frac{M_{12}\left(\eta_{R\&S} - 1 + \eta_{SH}^{-1}\right)}{M_3\, \eta_{R\&S}} = \frac{M_{14}\left(\eta_{R\&S} - 1 + \eta_{SH}^{-1}\right)}{M_3\, \eta_{R\&S}\, \eta_{AP}} = \frac{M_3\,(\eta_{std} + F_{oil})\left(\eta_{R\&S} - 1 + \eta_{SH}^{-1}\right)}{M_3\, \eta_{R\&S}\, \eta_{AP}}$$

$$\eta_{app} = \frac{(\eta_{std} + F_{oil})\left(\eta_{R\&S} - 1 + \eta_{SH}^{-1}\right)}{\eta_{R\&S}\, \eta_{AP}}$$

The actual SO_2 removal efficiency in the adsorber is the SO_x removed, M_6, divided by the SO_x entering the adsorber, M_5. Substituting $\eta_{app}M_3$ for M_6 and simplifying, yields the actual removal efficiency.

$$\eta_{SOX} = \frac{M_6}{M_5} = \frac{\eta_{app}\, M_3}{M_6 + M_7} = \frac{\eta_{app}\, M_3}{\eta_{app}\, M_3 + (1 - \eta_{std})\, M_3} = \frac{\eta_{app}}{\eta_{app} + 1 - \eta_{std}} \tag{4.3}$$

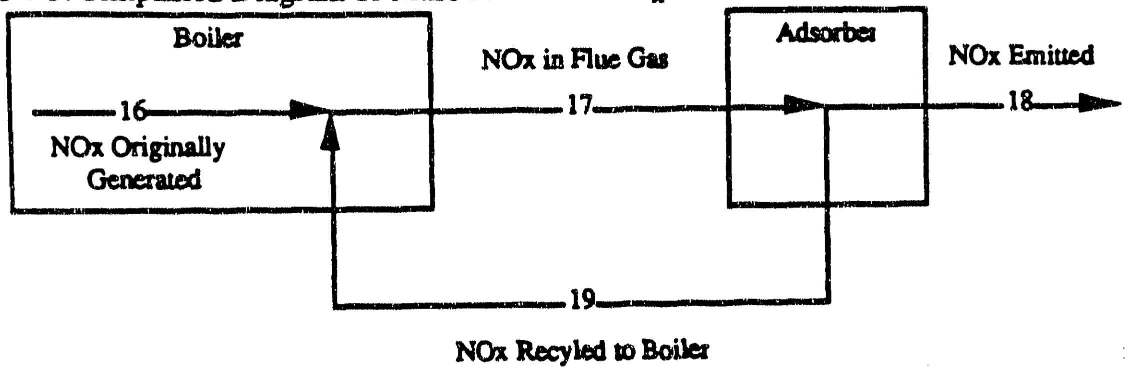
The next step is to determine the NO_x removal efficiency required by the emission standard (including the effects of recycling NO_x to the boiler). Figure 4-3 shows a simplified NO_x flow diagram. The following parameters are known: the NO_x produced originally, M_{16}, the emission constraint, M_{18}, and the fraction of NO_x "destroyed" in the boiler, δ_{NOX}. The actual NO_x removal efficiency is the NO_x removed, M_{19}, divided by the NO_x entering the adsorber, M_{17}. Substituting for M_4 and M_2 and simplifying yields:

$$\eta_{NOX} = \frac{M'_{19}}{M'_{17}} = \frac{M'_{19}}{M'_{16} + (1 - \delta_{NOX})M'_{19}} = \frac{\dfrac{\eta_{NOX} M'_{18}}{1 - \eta_{NOX}}}{M'_{16} + \dfrac{(1 - \delta_{NOX})\eta_{NOX} M'_{18}}{1 - \eta_{NOX}}} \tag{4.4}$$

Solving the above equation for η_{NOX} yields

$$\eta_{NOX} = \frac{M'_{16} - M'_{18}}{M'_{16} - (1 - \delta_{NOX})M'_{18}} \tag{4.5}$$

Figure 4-3: Simplified Diagram of Mass Flows for NO_x



NOXSO has reported that the actual NO_x removal efficiency is related to the SO_x removal efficiency. However, a steady state relationship between η_{NOX} and the SO_x removal efficiency could not be determined from the available data, so this relationship is modeled as an input parameter, R, which is the ratio of NO_x removal efficiency to the actual SO_2 removal efficiency. Since the actual SO_2 removal efficiency equals R times the actual NO_x removal efficiency, the actual SO_x removal efficiency is chosen so that both the SO_2 and NO_x emission constraints are satisfied. the actual NO_x removal efficiency is R times the actual SO_2 removal efficiency.

if R > 1 then

$$\eta_{SOX,A} = \text{maximum}(\eta_{NOX}, R\,\eta_{SOX})$$

else

$$\eta_{SOX,A} = \text{maximum}(\eta_{NOX} / R, \eta_{SOX})$$

$$\eta_{NOX,A} = R\,\eta_{SOX,A} \tag{4.6}$$

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

$$M_{17} = M_{16} + (1 - \delta_{NOX})M_{19} = M_{16} + (1 - \delta_{NOX})\eta_{NOX,A}\,M_{17} \tag{4.7}$$

$$M_{17} = \frac{M_{16}}{1 - (1 - \delta_{NOX})\eta_{NOX,A}} \tag{4.8}$$

$$M_{19} = \eta_{NOX,A} M_{17}$$

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. Equations 4.6, 4.7 and 4.9 are easily derived from Figure 4-2. The derivation of Equation 4.8 is quite involved and is not presented here. The ratio of sulfur exiting the absorber to the sulfur removed by the absorber is

$$c = \frac{M_6}{M_8} = 1 - (1 - \eta_{R\&S})\,\eta_{SH} \tag{4.9}$$

$$M_7 = M_5\,(1 - \eta_{SO2,A})$$

$$M_6 = \frac{M_3\,\eta_{SO2,A}\,c\,(1 + F_{oil})}{c - \eta_{SO2,A}\,(1 - \eta_{SH} + (1 - \eta_{AP})\,\eta_{R\&S}\,\eta_{SH})}$$

$$M_8 = \frac{M_6}{c}$$

The sorbent flow rate is determined by an algorithm developed by NOXSO (24). The numerator in Equation 4.10 is the SO_x removed by the adsorber, M_6. λ is the stoichiometric ratio of sulfur removed to available sodium and is assumed to be unity (23). The parameter X can be determined by existing algorithms (24).

$$m_{sorb} = \frac{A_A V C_o (y_i - y_o)}{\lambda N_t X} = \frac{M_6}{\lambda N_t X} \tag{4.10}$$

$$X = \frac{\ln\left(\frac{y_o}{y_i}\right) V}{k_a P H} + 1 = \frac{\ln(1 - \eta_{SOX,A}) V}{k_a P H} + 1$$

H, K_a, P and λ are input parameters. K_a is currently set to 3.7 according to (24), 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:

$$N_t = \frac{w_{Na}}{23\,\eta_{R\&S}}$$

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 (22):

$$m_{makeup} = f_{makeup}\, m_{sorb}$$

$$EC_{sorb} = 1795 \text{ kW} / 1.3486e^{6} \text{ lb/hr} * m_{sorb} = 1.32e^{-3}\, m_{sorb}$$

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 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.

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

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

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.

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

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

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 (8). The actual composition is not extremely critical, yet the components are in place in case another fuel, such as coal, is used.

$$m_{oil} = \frac{E_{air,SH}}{HHV_{oil}\, \eta_{AH}}$$

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

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 (25). 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.

$$M_{SC,R,i} = M_{SC,A,o}\,\eta_{SH}$$

$$M_{M,R,i} = 3690 / 575 * 0.1585 M_{SC,R,i}$$

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

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 used 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.

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

$$M_{SD,R,o} = fp_{SD,R}\,\eta_R M_{SD,R,i}$$

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

$$M_{S,R,o} = (1 - fp_{SD,R} - fp_{HS,R})\eta_R M_{SD,R,i} / 2$$

$$M_{M,R,o} = (1 - Ut_M)\,M_{M,R,i}$$

$$M_{CD,R,o} = Ut_M\,M_{M,R,i}$$

$$M_{W,R,o} = (1 - Ut_W)M_{W,STV,i} + 2M_{CD,R,o} - fp_{HS,R}\,\eta_R\,M_{SD,R,i}$$

The next step is to determine the composition of the gas returned to the boiler. This gas stream consists 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. Since it is a small stream and to simplify the calculations, it is treated as SO_2 returned to the boiler. It is assumed that only SO_2 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 (22).

$$M_{N,B,i} = f_{N,\text{wet air}} M_{air,SH} + 0.0014 / 28\ M_{oil}$$

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

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

$$M_{CD,B,i} = 0.8787 / 12\ M_{oil}$$

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

$$M_{NO,B,i} = fp_{NO,B} M_{NOX,A,o}$$

$$M_{ND,B,i} = (1 - fp_{NO,B})M_{NOX,A,o}$$

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 Chapter 2 for more details on how the variables, $M_{B,i}$, are determined. Once these parameters are known, the composition of the flue gas exiting the boiler can be determined:

$$M_{O,AP,i} = M_{O,required} - M_{O,B,i}$$

$$M_{CD,B,o} = M_{C,coal} + M_{CD,B,i}$$

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

$$M_{SD,B,o} = fp_{SD,B}\ \eta_{ash}\ M_{S,coal} + M_{SD,B,i}$$

$$M_{ST,B,o} = (1 - fp_{SD,B})\ \eta_{ash}\ M_{S,coal}$$

$$M_{ND,orig} = \frac{NO_{x_{ef}} m_{coal}}{46 + \dfrac{30 fp_{NO,B}}{1 - fp_{NO,B}}}$$

$$M_{NO,orig} = \frac{fp_{NO,B} M_{ND,orig}}{1 - fp_{NO,B}}$$

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

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

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

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

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:

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

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

$$G_{A,o} = G_{A,i} \frac{250 + 460}{210 + 460}$$

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 (22). The algorithm to determine the number of redundant trains is retained from Reference (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.

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

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

$$A_A = \frac{G_{A,i}}{60\ NOP\ V}$$

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

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

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:

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

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

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 the air required for the coal consumed.

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

$$\text{if } EC_{steam} < 0 \text{ then } ECr_{steam} = -EC_{steam} \text{ else } 0$$

$$ECr_{total} = ECr_{recycled} + EC_{steam}$$

4.4 Economic Model

The current economics model for the NOXSO process is based primarily on the recent case study by EPRI (22). 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 ft^2 and 7200 lb/hr. The area of the adsorber, 2545 ft^2, 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 it chosen, is also included as a part of the capital cost for the NOXSO process.

4.4.1 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 4-1. 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 4-1. 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 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 rates 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:

$$DCC_{10} = \frac{1,651,777}{880^{0.7}} m_{makeup}^{0.7} + \frac{965,006}{7200^{0.7}} m_{oil}^{0.7} = 14,350 m_{makeup}^{0.7} + 1.925 m_{oil}^{0.7} \qquad (4.11)$$

Table 4-1: Area Cost Multipliers for NOXSO Process

Area	Description	Equipment Costs	Total Cost	Multiplier
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 are sized for 30" of water, the NOXSO process is charged for 73% of the I.D. fans and dampers. The capital cost for the duct work associated with the multicyclones and ESP are not included. The second component is the adsorber, which is in the SO_2 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:

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

$$DCC_{30} = 530 G_{A,i}^{0.7} + 2,188\,(NOP + NRD)\, A_A^{0.7} \qquad (4.12)$$

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:

$$DCC_{40} = \frac{15,132,844}{1,358,600^{0.7}} m_{sorb}^{0.7} = 770 m_{sorb}^{0.7} \qquad (4.13)$$

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

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

The total direct capital cost is the sum of Equations 4.11 through 4.14, 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.

$$DCC_{total} = DCC_{10} + DCC_{30} + DCC_{40} + DCC_{70} + DCC_{APH}$$

$$DCC_{gf} = 0.10DCC_{total}$$

$$DCC_{eng} = 0.125DCC_{total}$$

$$DCC_{proj} = 0.212DCC_{total}$$

$$DCC_{proc} = 0.134DCC_{total}$$

$$TPC = DCC_{total} + DCC_{gf} + DCC_{eng} + DCC_{proj} + DCC_{proc} + TCC_{acid}$$

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 (12). 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:

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

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

$$C_{misc} = 0.005DCC_{total} + 4.97e^{-5}MW_{g}$$

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.

$$C_{work} = (2.5m_{makeup} + 0.378UC_{M}M_{M,R,i} + UC_{oil}HHV_{oil}m_{oil})24 * 60$$

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 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:

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

$$TCC = TPI + C_{startup} + C_{work} + C_{inv} + C_{misc}$$

4.4.2 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 (12). 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:

$$OC_{oper} = 5.2 * 19.7 * 8766$$

$$OC_{maint\text{-}labor} = 0.40 * 0.048\,(TPC - TCC_{acid})$$

$$OC_{maint\text{-}matl} = 0.60 * 0.048\,(TPC - TCC_{acid})$$

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

$$FOC = OC_{oper} + OC_{maint\text{-}labor} + OC_{maint\text{-}matl} + OC_{admin}$$

$$OC_{sorb} = 2.5 * 8{,}766\ CF\ m_{makeup}$$

$$OC_M = 0.378 * 8{,}766\ CF\ UC_M\ M_{M,R,i}$$

$$OC_{oil} = 8{,}766\ CF\ HHV_{oil}\ UC_{oil}\ m_{oil}$$

$$OC_{misc} = 0.019 DCC_{total}$$

$$VOC = OC_{sorb} + OC_M + OC_{oil} + OC_{misc}$$

The NOXSO process typically produces an energy credit. In the IEC model, energy credits are account 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 if the NOXSO process decreases the amount of coal burned in the boiler. Since the energy credit and the cost of the NOXSO are dependent on the coal consumption, it becomes an iterative problem.

$$TCC_{BP,incre} = \frac{ECr_{total}}{MWg*1000} TCC_{BP}$$

$$TVC_{BP,incre} = \frac{ECr_{total}}{MWg*1000} TVC_{BP}$$

$$OCr_{coal} = 8766\ CF\ UC_{coal} \frac{ECr_{total}\ HR}{2000\ HHV_{coal}}$$

The total capital and operating cost of the power plant are increased by $TCC_{BP,incr}$ + $TVC_{BP,incr}$. 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:

$$TVC = FOC + VOC - OCr_{coal} - OC_{credit,acid}$$

$$Util = 8766\ CF\ UC_{elec}\ EC_{total}$$

Table 4-2: Properties of Illinois No. 6 Coal Used for Case Studies (As-Fired Basis)

Coal Property	Run-of-Mine Coal	Washed Coal[a]
Btu/lb	10,190	10,330
% Sulfur	4.4	3.1
% Carbon	57.0	57.7
% Hydrogen	3.7	4.0
% Oxygen	7.2	8.4
% Nitrogen	1.1	1.1
% Moisture	12.3	17.5
$/ton (at mine)[b]	28.10	32.70
$/ton (transport)[b]	5.90	5.90

[a] Model results for a 30% reduction on lbs/MBtu basis using conventional coal cleaning (Level 3 plant design).

[b] 1985 dollars, assuming a midwestern plant and mine location.

4.5 Deterministic Analysis for the NOXSO Process

This section presents a deterministic analysis of the NOXSO process and compares it to a conventional plant design with wet flue gas desulfurization (FGD) and selective catalytic reduction (SCR) and to the advanced copper oxide process design. The NOXSO process diagram is shown in Figure 4-1. This case study assumed a new 522 MW power plant burning an Illinois #6 coal. The properties of this coal are shown in Table 4-2, while key input assumptions for the NOXSO process are shown in Table 4-3. The financial assumptions and emission standards are shown in Table 4-4. Current federal New Source Performance Standards (NSPS) for SO_2 and stringent than the current NSPS and requires an emission reduction of 85 to 90 percent below current U.S. requirements. This represents current NO_x control requirements in Japan, West Germany and California.

Table 4-3: NOXSO Performance and Economic Assumptions

Parameter	Value	Parameter	Value
Air Preheater Enlargement	no	Regenerator Utilization of:	
Bed Height (in)	36	Methane (%)	90
Bed Pressure Drop (in water)	22	Steam (%)	30
Bed Temperature (°F)	250	Residence Time of Sorbent in:	
Flue Gas Bed Velocity (ft/s)	2.95	Cooler (min)	18
Gas Burner for Regenerator Gas	yes	Heater (min)	28
K_a, Rate Constant (atm^{-1} s^{-1})	3.7	Regenerator (min)	35
Methane Cost ($/MSCF)	4.50	Sodium Loading (% of weight)	3.8
NO_x "destruction" efficiency (%)	65	Sorbent Characteristics:	
Oil Cost ($/MBtu)	4.50	Attrition Rate (% of sorbent flow)	0.07
Oil Sulfur Correction Factor	0.6	Cost ($/lb)	2.57
Regenerator Gas Sulfur Composition:		Density (lbs/ft^3)	30
H_2S (% of S regenerated)	30	Sorbent Regeneration Efficiency by:	
S_2 (% of S regenerated)	5	Methane (%)	81.4
SO_2 (% of S regenerated)	65	Steam (%)	90.7
		Overall Calc. (%)	98.3

4.5.1 Cost Results

Table 4-5 shows the calculated capital and levelized total revenue requirement for the assumptions shown in Tables 4-2 to 4-4. The assumptions for the wet FGD and Copper Oxide process are shown in Reference (26). As shown, the NOXSO process has the lowest capital and revenue requirements for the unwashed coal. The revenue requirement is 8% and 15% lower than the conventional and Copper Oxide designs, respectively. For the washed coal, its capital cost is still 13% less than the Copper Oxide process, while the total revenue requirement is 5% higher. Table 4-6 shows the cost breakdown for the capital and operating cost for the NOXSO process. For the unwashed coal, the direct capital cost is divided somewhat equally between the equipment associated with the sorbent, flue gas and acid plant. Most of the indirect costs, including startup costs, working and inventory capital are attributed to the sorbent flow rate. Approximately 40% of the total variable cost, excluding sulfuric acid sales and coal energy credits, is for sorbent makeup, while oil and gas consumption account for 25% and 18%, respectively. The fixed operating costs (12%), acid plant variable cost (4%) and miscellaneous cost (1%) account for the rest.

Table 4-4: Financial and Emission Assumptions for Case Studies

Model Parameter	Nominal Value
<u>Emission Constraints</u>	
Nitrogen Oxides	0.08 lbs/MBtu
Sulfur Dioxide	90% Removal
Particulates	0.03 lbs/MBtu
<u>Power Plant Parameters</u>	
Gross Capacity	522 MW
Gross Heat Rate	9500 Btu/kWh
Capacity Factor	65%
Excess Air (boiler / total)	20% / 39%
Ash to Flue Gas	80%
Sulfur to Flue Gas	97.5%
Preheater Inlet Temperature	700 °F
Preheater Outlet Temperature	300 °F
<u>Financial Parameters</u>	
Inflation Rate	0%
Debt Fraction / Real Return	50% / 4.6%
Common Stock Fraction / Real Return	35% / 8.7%
Preferred Stock Fraction / Real Return	15% / 5.2%
Federal Tax Rate	36.7%
State Tax Rate	2.0%
Ad Valorem Rate	2.0%
Investment Tax Credit	0%
Book Life	30 years
Real Escalation Rates	0%
Real Discount Rate (calc)	6.13%
Fixed Charge Factor (calc)	10.34%
Levelization Factors	1.000

Table 4-5: Summary of Total Pollution Control Costs
(4.4%S Illinois No. 6 Coal)
All Costs in Constant 1985 Dollars

	No Coal Cleaning		Washed Coal[a]	
Process Configuration	Capital ($/net kW)	Level Rev Req (mills/kWh)	Capital ($/net kW)	Level Rev Req (mills/kWh)
Conventional Plant Design				
Coal Cleaning	-	-	(6)[b]	1.9
SCR System	69	3.7	70	3.7
Cold-Side ESP	43	0.9	40	0.8
Wet FGD System	197	9.0	192	8.3
Solid Waste Disposal	56	2.0	43	1.6
Total	365	15.6	339	16.3
Copper Oxide Design				
Coal Cleaning	-	-	(3)[b]	1.9
Copper Oxide Process	244	14.4	180	8.5
Fabric Filter	62	1.4	62	1.4
Solid Waste Disposal	25	1.1	21	1.0
Total	332	16.9	260	12.8
NOXSO Design				
Coal Cleaning	-	-	(4)[b]	1.9
NOXSO Process	178	11.9	149	9.2
Fabric Filter	60	1.4	59	1.4
Solid Waste Disposal	25	1.1	21	0.9
Total	263	14.4	225	13.4

[a] 30% sulfur reduction on lbs/MBtu basis.

[b] These costs (or credits) result from changes in the base plant cost.

Table 4-6: Breakdown of Costs for NOXSO Process

Component	Capital Cost (85 M$)
Feed Equipment	1.8
Flue Gas Equipment	15.6
Sorbent Equipment	15.4
General Support Equipment	0.2
Acid Plant	18.0
Total Direct Capital	51.0
General Facilities	3.3
Engineering Fees	4.1
Project Contingency	7.0
Process Contingency	4.4
Total Plant Cost	69.9
AFUDC	6.6
Total Plant Investment	76.5
Royalties	0.2
Startup Costs	4.3
Working Capital	7.1
Initial Catalyst Cost	7.2
Total Capital Cost	95.2

Component	Operating and Maintenance Cost (85 M$/yr)
Fixed Operating	4.0
Methane	6.0
Oil	8.6
Makeup Sorbent	13.6
Miscellaneous	0.6
Acid Plant O&M	1.5
Sulfuric Acid Sales	-8.3
Coal Credit	-2.5
Total Variable Cost	23.4

Table 4-7: NOXSO Performance Parameters

Parameter	Unwashed Coal	Washed Coal
Concentration of Pollutants entering Absorber (ppm)		
NO_x	806	811
SO_2	3300	2350
Energy Consumption (-) or Production (+)		
Acid Plant		
Electricity (MW)	-2.0	-1.4
Steam (10^6 Btu/hr)	+84.4	+59.0
NOXSO Process		
Electricity (MW)	-12.1	-10
Methane Consumption (10^6 Btu/hr)	-234	-164
Oil Consumption (10^6 Btu/hr)	-334	-230
Recycled Gas to Boiler (10^6 Btu/hr)	+172	+132
Steam (10^6 Btu/hr)	-7.9	-5.5
Total Electricity Consumption (MW)	-14.2	-11.4
Coal Credit (tons/hr)[a]	12.7	9.3
Flue Gas Flow Rate (10^6 acfm)	1.78	1.74
Makeup Sorbent Flow Rate (lbs/hr)	929	641
Molar Stoichiometry (Na/S removed)	3.31	3.27
Net Capacity (MW)	533	529
Number of Operating Trains	4	4
Required Removal Efficiency of Absorber		
NO_x	92.8	92.7
SO_2	91.1	87.0
Actual (larger value of SO_2 and NO_x)[b]	92.8	92.7
Sorbent Flow Rate (10^6 lbs/hr)	1.33	0.92

[14a] This value is the sum of the steam requirements of the NOXSO process and acid plant divided by the boiler efficiency (88%), plus the energy sent to the boiler in the recycled gas. This net energy requirement is divided by the higher heating value of the coal and converted to tons/hr.

[14b] The SO_2 and NO_x removal efficiency are assumed to be equal, so the larger of these two values is used to determine the molar stoichiometry.

Sulfuric acid sales reduce the total variable cost by 24%, while the coal energy credit reduces the cost by 7%. For the washed coal the same general trends appear. On the other hand, the capital cost associated with the flue gas remains constant, while the direct capital costs associated with the sorbent and acid plant decrease by approximately 20%. The variable operating cost and washed coal, the capital cost is 30 \$/kW and the sulfuric acid sales are 5.8 M\$/yr. The net result is a savings of 1.1 mills/kWh or 28 \$/ton.

4.5.2 NO_x Removal Efficiency

Originally, NOXSO believed that the NO_x removal efficiency was a function of the SO_2 concentration and the bed temperature (20). In Reference (1), it was estimated that at a bed temperature of 248°F the NO_x and SO_2 removal efficiencies would be equal. However, in the process developmental unit test at the Pittsburgh Energy Technology Center (PETC), the experimental data did not show any clear correlation between NO_x removal efficiency and bed temperature (27). However, there was clear evidence that the NO_x removal efficiency was depended on the regeneration gas. Methane was found to improve the NO_x removal efficiency compared to hydrogen. Four experimental tests were conducted using methane at a bed temperature of approximately 245°F. The SO_2 and NO_x concentrations were held at approximately 2300 and 630 ppm, respectively. Three test were conducted at an 18 inch bed height, the other was at 42 inches. For three of the tests with removal efficiencies were greater than 84%, the SO_2 and NO_x removal efficiencies were within ± 2. For the other test, the removal efficiencies were much lower (SO_2 equalled 69%, while NO_x equalled 78%). For the reason shown above the SO_2 and NO_x removal efficiencies are assumed to be equalled.

In Reference (27), NOXSO also showed that the NO_x removal efficiency was correlated to the ratio of SO_2 to NO_x by a factor of 0.80. However, all the data came from experiments which used hydrogen as a regeneration gas and it is not clear if the same trend would hold if methane is used as a regeneration gas. NOXSO also showed a significant transient effect of increasing the ratio of SO_2 to NO_x from 3.1 to 4.1. The steady-state effect was small, approximately 3.5 removal points. Since this is a steady-state model, the transient change is not useful. Yet, it could be very useful to a power plant operator. These test were also conducted using hydrogen, so the steady-state effect may not be applicable using methane—especially if removal efficiencies of 90% or greater are required.

4.5.3 Effects of Stoichiometry

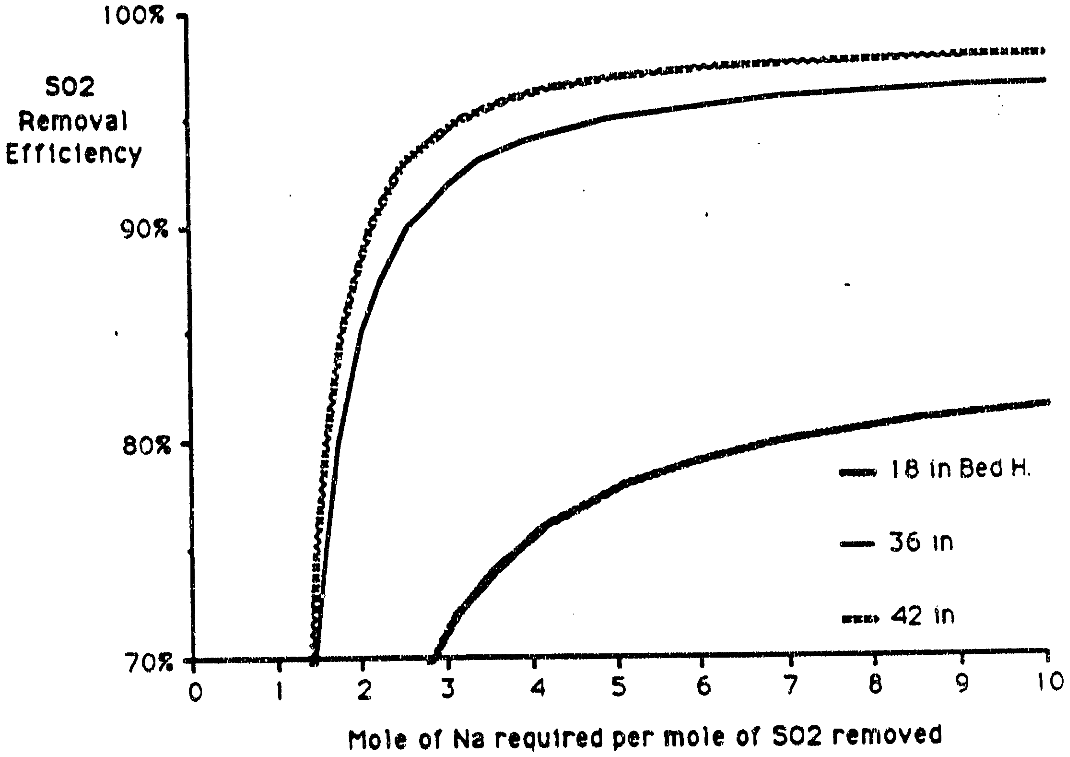
Table 4-7 gives a breakdown of the important performance parameters for the washed and unwashed coals. For both cases the required NO_x removal efficiency, (92.8%) is higher than the SO_2 efficiency, (91.1%). This is caused by the inefficient destruction of NO_x which is recycled to the boiler. Since the NO_x and SO_2 efficiencies are assumed to be equal, the molar stoichiometry is determined by the NO_x removal efficiency. As shown, the sorbent flow rate decreases by 30% for the washed coal. However, if the molar stoichiometry was driven by the SO_2 removal efficiency, its value for the unwashed and washed coals would be 2.8 and 2.2 respectively, instead of 3.3. These stoichiometries would produce sorbent flow rates of 1.1 x 10^6 lbs/hr and 0.57 x 10^6 lbs/hr, respectively. The NOXSO process capital cost would decrease from 178 to 166 \$/kW for the unwashed coal and from 149 to 129 \$/kW for the washed and the total NOXSO process revenue requirement would fall to 10.4 mills/kWh and 6.8 mills/kWh, respectively. Thus, if the NO_x "destruction" efficiency was improved substantially or the NO_x emission constraint was relaxed, the cost of the NOXSO process would decrease more substantially with coal cleaning.

Figure 4-4 shows the SO_2 removal efficiency versus molar stoichiometry for three different bed heights with the flue gas velocity and rate constant, K_a, held constant at 2.95 ft/s and 3.7 respectively. The molar stoichiometry is the moles of sodium required to remove one mole of SO_2. This value is equal to the inverse of the average conversion factor of sodium, X, times the effective molar ratio of sodium to sulfur removed. According to NOXSO (23, 28), the effective molar ratio of sodium to sulfur removed is one. Therefore, the equation shown below is the molar stoichiometry of sodium to sulfur removed.

$$msr = \frac{1}{\frac{\ln(1-\eta)V}{K_a H} + 1}$$

where H = Bed height (inches)
K_a = Reaction rate constant ($atm^{-1}\ s^{-1}$)
msr = molar stoichiometry (Na to S removed)
V = Flue gas velocity (inches s^{-1})
η = SO_2 removal efficiency (fraction)

Figure 4-4: Sulfur Removal Efficiency versus Molar Stoichiometry



For a fixed value of K_a, increasing the bed height or decreases the flue gas velocity will decrease the molar stoichiometric ratio. While this equation is very useful for understanding and predicting the performance of the absorber, it is only an approximation. A limitation of this equation is that the molar stoichiometry goes to infinity if the following conditions occur.

$$\eta = 1 - e^{-\frac{K_aH}{V}}$$

For Ka = 3.7 $\text{atm}^{-1}\text{sec}^{-1}$, H = 36 in and V = 2.95 ft/s, the molar stoichiometry goes to infinity at η = 97.7%. At 18 and 42 inches and the same values of Ka and V, the asymptotic values are 84.8% and 98.8%, respectively. It is important to known this asymptotic value since the molar stoichiometry increase rapidly as this value is approached. For the 36 inch bed height, the molar stoichiometry increases rapidly for values above 90% removal, since it is approaching its asymptotic value. For the unwashed coal, the molar stoichiometry is 3.31. If the bed height was increased to 42 inches, the molar stoichiometry would decrease by 25%. It was not possible to determine if this would be economical since pressure drop data does not exist for the 42 inch bed height.

4.5.4 Process Energy Requirements

The NOXSO process consumes and produces large quantities of energy as shown in Table 4-7. About half the energy from the fuel oil consumption is recovered by recycling the heater gas to the boiler. Also, 35% of the energy from the methane and steam consumed in the regenerator is converted to steam in the acid plant. Approximately 50% of the electricity consumption for the NOXSO process is used to overcome the pressure drop across the absorber. The sorbent cooler compressor and the pneumatic conveying blowers consume about 35% and 13%, respectively. The acid plant consumes some additional electricity (2MW), while producing steam which can be used to regenerate the sorbent in the steam treatment vessel or sent to the steam cycle to produce electricity.

4.6 Sensitivity Analysis for the NOXSO Process

Beginning with the results shown above, a sensitivity analysis was performed to determine the effects of important parameters affecting the NOXSO process. The process parameters which were varied are the molar stoichiometry, sorbent attrition rate, regenerator efficiency, NO_x "destruction" efficiency, sorbent cost, methane cost, oil cost and sulfuric acid cost. System effects of coal cleaning, air preheater size and the use of a gas burner for the acid plant inlet gas also were examined. Since pressure drop data are not available for different bed height and flue gas velocities, these parameters were held constant.

4.6.1 Combustion of Acid Plant Gases

The default assumption for the NOXSO process is to use a gas burner for the regenerator, since it appeared in the EPRI report (22). However, it was not clear if it was needed since it was never mentioned in previous reports by NOXSO. Using a gas burner for the regenerator gas is useful if there are sufficient combustible gases in the gas stream entering the acid plant. This is because:

- the energy in the combustible gases is released before the boiler and superheater so it can be captured and turned into steam

- any hydrogen or gases containing hydrogen are oxidized to water before the dryers so there is less moisture in the converter
- the gas flow rate entering the converter is lower, so the capital and power costs are lower for the converter and any downstream equipment

The disadvantages are additional capital and power costs for the gas burner equipment and a larger gas flow through the boiler, superheater and gas humidification and cooling tower. This often increases the cost of these components, so the overall economics depends on the composition of the gas. Table 4-8 summaries the important performance and cost changes of a gas burner. If a gas burner is not used, the acid plant capital cost doubles and the acid plant uses more than three times more electricity while producing no steam. The total revenue requirement for the NOXSO process increases by 1.8 mills/kWh and the net capacity of the power plant decreases 15 MW. Thus, the advantages of using a gas burner for the gas entering the acid plant are substantial. If the washed coal is used, the magnitude of the effects is smaller, but it is still advantages to use a gas burner. Another feature of a gas burner is that the it minimizes the effects of varying gas composition on the acid plant.

Table 4-8: Effects of Gas Burner for Sulfuric Acid Plant with the Unwashed Coal

Parameter	With Gas Burner	No Gas Burner
Acid Plant		
Capital Cost ($/kW)	37	72
Total Variable Cost (M$/yr)	1.52	1.63
Utility Cost (M$/yr)	0.43	1.43
Levelized Rev. Requirement (mills/kWh)	-1.72	-0.46
Acid Profit ($/ton of acid)	31	8
Electricity Consumption (kW)	2030	6770
Steam Production (kW)	0	10,020
Total Process		
Capital Cost ($/kW)	263	305
Levelized Rev. Requirement (mills/kWh)	14.4	16.1
Net Capacity (MW)	533	519

4.6.2 Air Preheater Effects

The NOXSO process recycles NO_x to the boiler via the gas stream used to heat the sorbent. This stream contains about 18% oxygen, which reduces by 37% the required combustion air entering the air preheater. Since the combustion air stream entering the air preheater is smaller, the air preheater cannot transfer as much heat, resulting in an exit temperature of the flue gas higher than the nominal value of 300°F. This results in an energy penalty for the NOXSO process. Building a larger air preheater would reduce the energy penalty. Yet, it is not possible to eliminate the energy penalty since the combustion air stream is much smaller. Table 4-9 the energy credit by 19 MBtu/hr or 1 ton/hr of coal. The larger air preheater costs 8.4 \$/kW, while increasing the coal credit by 0.2 M\$/yr. The effect on the total process including the cost of the fabric filter is to increase the total revenue requirement by 0.3 mills/kWh. For the washed coal the energy credit increases by 54 MBtu/hr or 2.5 tons/hr of coal. The capital cost increases to 12 \$/kW, while the total revenue requirement still increases by 0.3 mills/kWh. This value is within the error of the model, so it is uncertain whether a larger air preheater is economical.

Table 4-9: Effects of the Air Preheater for the Unwashed Coal

Parameter	w/o NOXSO	Original Size	Larger Size
Flue Gas Flow Rate (acfm)			
Inlet Temperature (°F)	700	700	700
Exit Temperature (°F)	300	382	370
Combustion Air (10^3 acfm)	1041	655	655
Inlet Temperature (°F)	80	80	80
Exit Temperature (°F)	515	634	660
Energy Flow Flow Rate (10^6Btu/hr)			
Across Air Preheater	497	400	419
From Recycled Air	0	269	269
Total to Boiler	497	669	688
Coal Energy Credit (tons/hr)[a]	0	8.4	9.4
NOXSO Process			
Additional Capital Cost (\$/kW)	--	0	8.4
Coal Credit (M\$/yr)	--	1.63	1.82
Total Process			
Capital Cost (\$/kW)	--	263	271
Levelized Rev. Requ. (mills/kWh)	--	14.4	14.5
Net Capacity (MW)	--	533	535

[a] This is the difference between the total energy flow to the boiler minus the energy flow to the boiler without the NOXSO process divided by the higher heating value of the coal and converted to tons/hr

Air preheaters of different sizes also were examined. This resulted in the same conclusion: the cost change was within the error of the model. Other options for capturing more energy from the flue gas, such as a second economizer after the air preheater, were not explored. However, if the flue gas temperature could be reduced to 300°F, an additional coal credit of 6.6 tons/hr could be achieved. This would save an additional 1.3 M\$/yr.

4.6.3 Other Process Parameters

The next sensitivity test was to multiply the nominal values (shown in Table 4-3) of the molar stoichiometry, attrition rate, sorbent cost, methane cost, oil cost and acid price by 0.5, 0.75, 1, 1.5 and 2. Each parameter was varied individually while all other parameters were held

Apparently the most important parameter is the molar stoichiometry, since the both the capital and total revenue requirement change drastically with minor changes in the stoichiometry. The capital cost and revenue requirement increase by 13% and 32%, respectively, for a 50% increase in the molar stoichiometry. There are several reasons for this:

- The sorbent flow rate is directly proportional to the molar stoichiometry. Higher sorbent flow increases the electricity used for sorbent transportation and the size of the equipment, except the absorber and acid plant.
- The gas quantity returned to the boiler is also proportional to the sorbent flow rate. This stream increases the flue gas flow rate entering the absorber and the fabric filter. The capital cost for the absorber increases slightly. Doubling the molar stoichiometry increases the capital cost of the fabric filter by 7%.
- Most of the indirect costs, working capital, startup costs and inventory capital are proportional to either the total process capital, which is proportional to the sorbent flow rate or to the sorbent flow rate directly.
- Most of the variable costs are proportional to the sorbent flow rate either directly or indirectly. The only exceptions are the variable cost for methane and sulfuric acid sales. The oil cost increases since the heat required for the sorbent heater is proportional to the sorbent flow rate. Most of the fixed operating cost are related to the total process capital.

The next most important parameters are the sorbent cost and the attrition rate. These two are closely related, since they effect the makeup sorbent cost, working capital and startup cost in the same manner. The only difference is that the sorbent cost affects the inventory capital while the attrition rate does not. This difference is shown most distinctly in Figure 4-5.

Figure 4-5: Capital Cost Sensitivity Analysis for Unwashed Coal

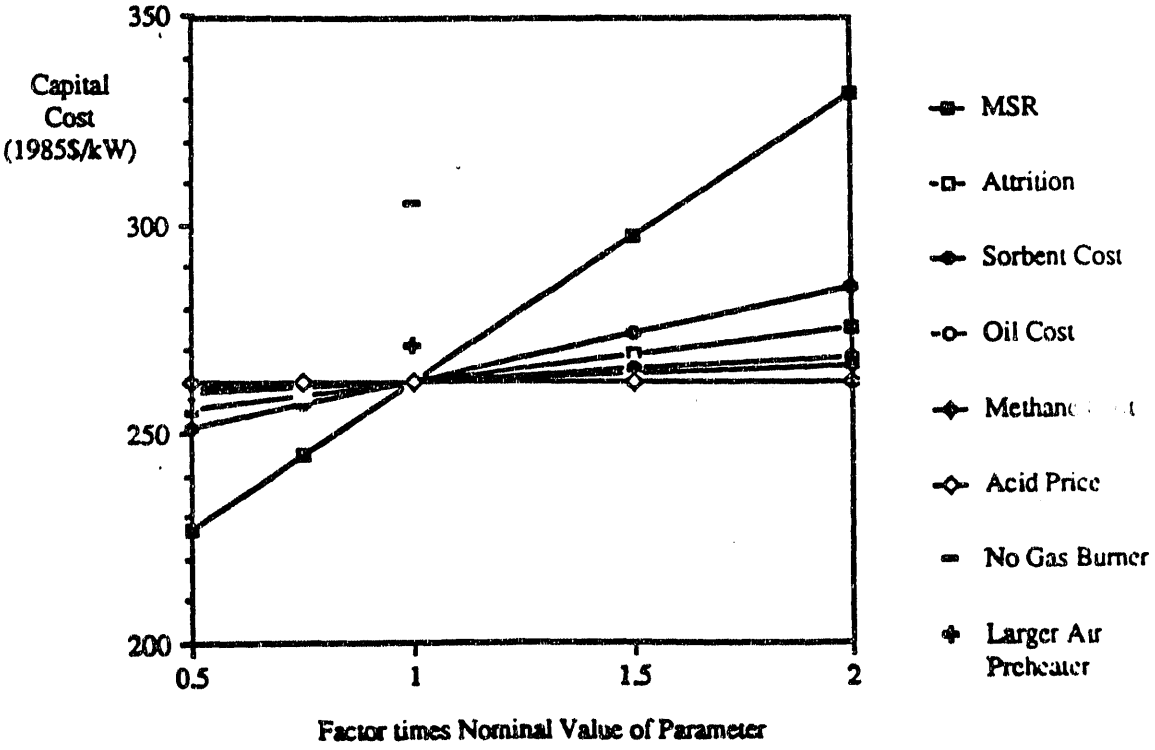
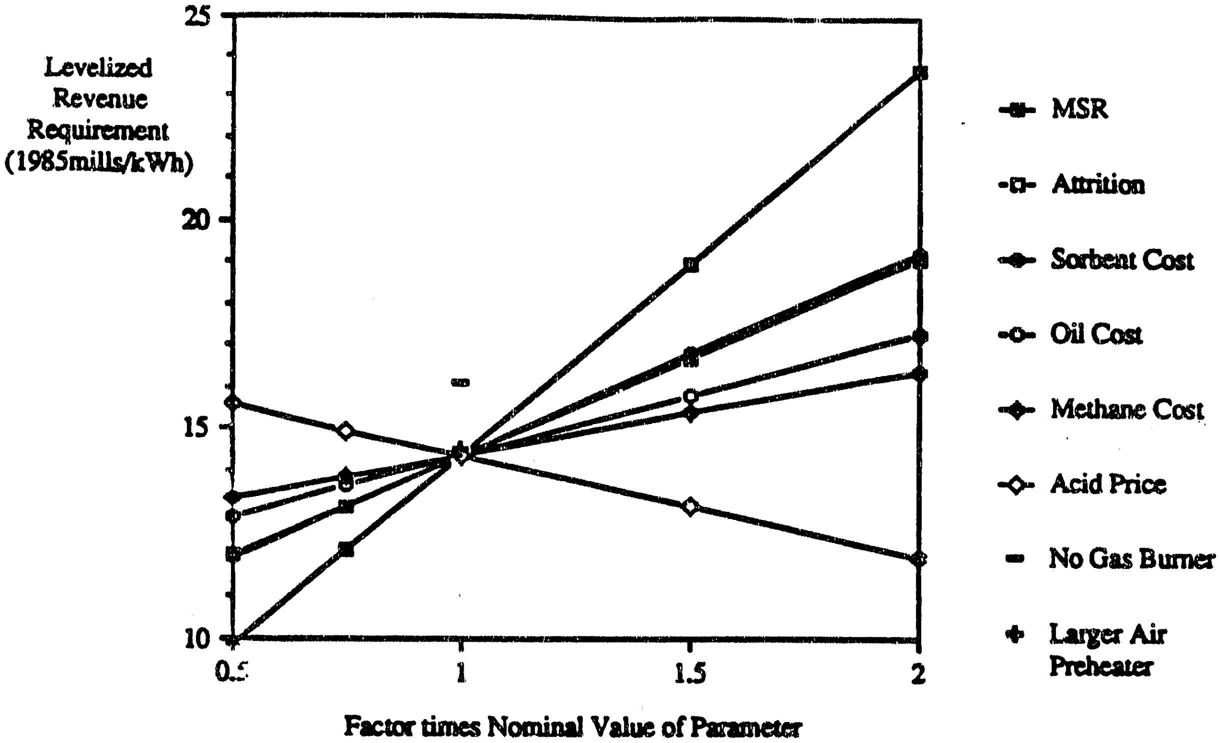


Figure 4-6: Total Revenue Requirement Sensitivity Analysis



Of the remaining parameters, the price of methane, fuel oil and sulfuric acid, the total revenue requirement is most sensitive to the price of oil and least sensitive to the price of methane. A 50% increase in the price of oil increases the total revenue requirement by 10%, while the same increase in methane cost, results in a 7% increase. These two parameters also affect the capital cost since they affect the startup and working capital. The price of sulfuric acid has no effect on the capital cost, while having a significant effect on the total revenue requirement. A 50% increase in the price of sulfuric acid decreases the total revenue requirement by 8.5%.

4.6.4 NO_x Reduction Efficiency

Figure 4-7 shows the capital and revenue requirements for different values of the NO_x being destroyed in the boiler. The NO_x "destruction" efficiency determines the NO_x removal efficiency required in the adsorber to meet the emission standard. As this value decreases the removal efficiency increases since there is a more NO_x entering the adsorber. Between destruction efficiencies of 50% and 80%, the NO_x removal efficiency in the adsorber is higher than the required SO_2 removal efficiency, so any change in this parameter changes the molar stoichiometry, which has a significant effect on the overall cost. Above a NO_x "destruction" efficiency of 80% the SO_2 removal efficiency is greater, so the molar stoichiometry is not affected. For the washed coal, the NO_x removal efficiency is always greater so the cost always decreases with improvements in the destruction efficiency.

4.6.5 Sorbent Regenerator Efficiency

Figure 4-8 shows the capital and revenue requirements versus the overall regeneration efficiency. The overall regeneration efficiency is a function of the efficiencies of both the regenerator and the steam treatment vessel:

$$\eta_{R\&S} = \eta_R + (1 - \eta_R)\eta_{STV}$$

where

η_R the efficiency of removing sulfur from the sorbent with methane in the

η_{STV} the efficiency of removing sulfur from the sorbent with steam in the steam treatment vessel

$\eta_{R\&S}$ the overall regeneration efficiency of both vessels

To analyze the sensitivity of the NOXSO process to the overall regeneration efficiency, η_R and η_{STV} were given the following values: 55%, 60%, 70%, 80%, 90%, 95%. This produced the overall efficiencies of 79.75%, 84%, 91%, 96%, 99% and 99.75% shown plotted in Figure 4-8. The nominal value is 98.27%, which was estimated from an EPRI report (22). The utilization of methane and steam was assumed to remain constant at their nominal values of 90% and 30%, respectively. The efficiency of the regenerator using methane was not set to 50%, because this would have created a gas composition which the acid plant was not designed to handle.[14] As shown, the capital and revenue requirement cannot be improved significantly, since the nominal value for the regeneration efficiency is high. However, if the regeneration efficiency drops to 91%, then the capital and revenue requirement increase by 2.7% and 6.7%, respectively.

4.7 Conclusion

From this analysis it is obvious that the most significant parameter affecting the design and cost of the NOXSO process is the sorbent flow rate needed to achieve a given removal efficiency. Therefore, the relationship between NO_x and SO_2 removal efficiencies, the molar stoichiometry and regeneration process should be studied further, since they affect the sorbent flow rate directly and have a high degree of uncertainty. Data on NO_x removal and destruction in the boiler is the most critical, since it is the most uncertain of any of the parameters. More experimental data is needed to confirm the analytical model for SO_2 removal efficiency. However, the results of the performance model are consistent with previous studies.

Experiments using a continuous regenerator should be performed since only batch test have been performed. These experiments should be designed to develop a performance curve relating methane and steam consumption to regeneration efficiency and predict the regenerated gas composition. If a performance curve existed, the IEC model could be used to optimize the NOXSO process, since the tradeoffs between the sorbent flow rate, oil consumption, methane consumption and acid plant are modeled explicitly.

The analysis of the air preheater showed that an additional that an energy credit worth 1.3 M$/yr can be achieved if the temperature in the flue gas is reduced to 300°F. Other options for

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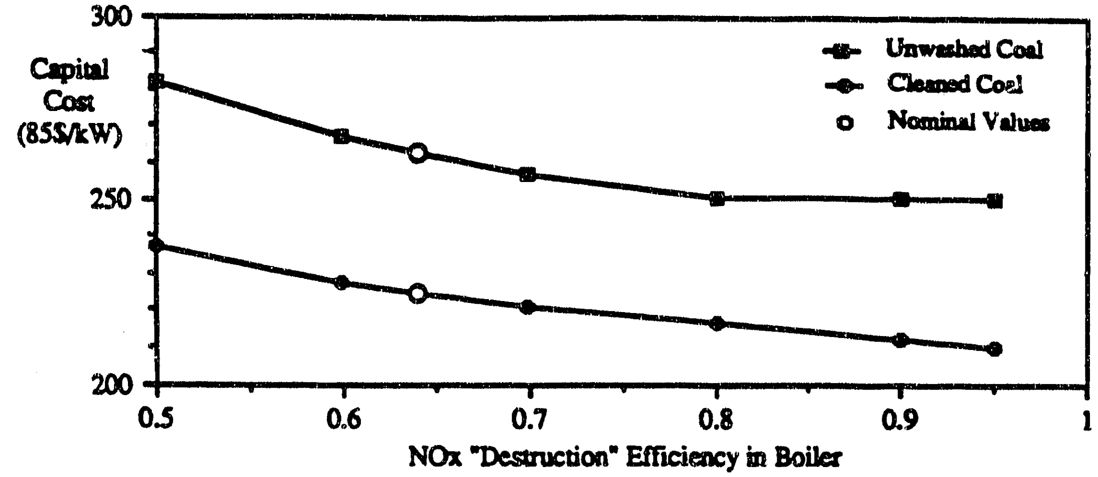
[14] The inlet sulfur dioxide concentration was too low for this design, so the capital and operating cost would not be valid.

capturing this energy should be explored. A second economizer after the air preheater may be economical.

Figure 4-7: Effect of NO_x Destruction Efficiency in Boiler



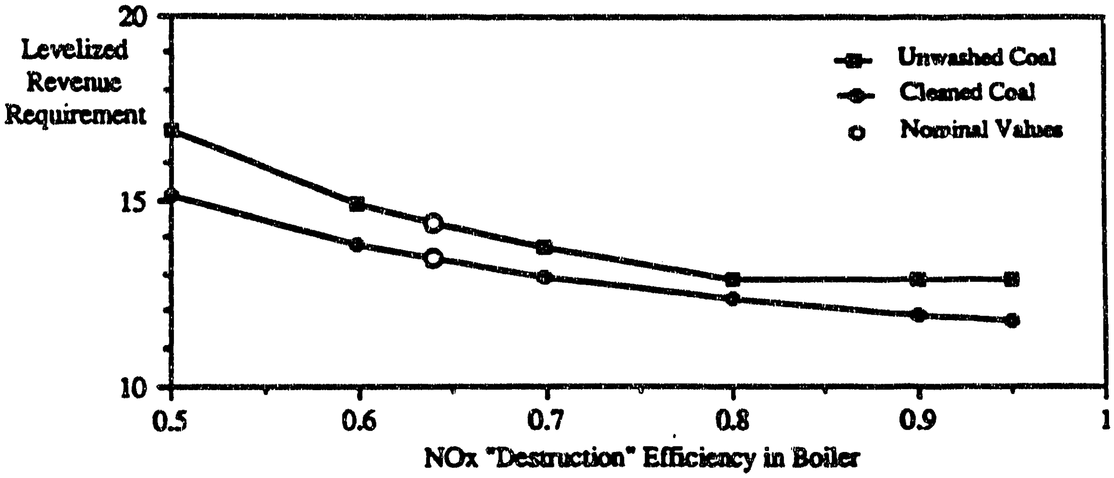
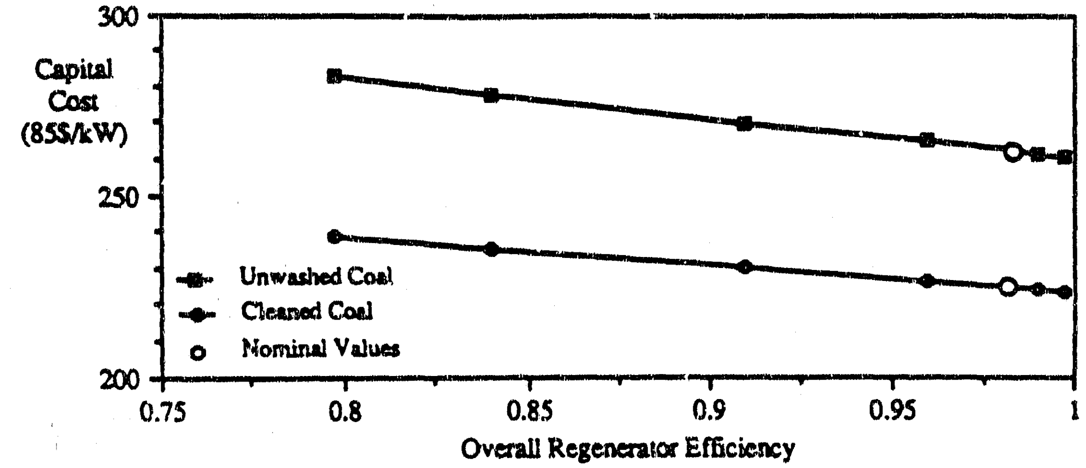
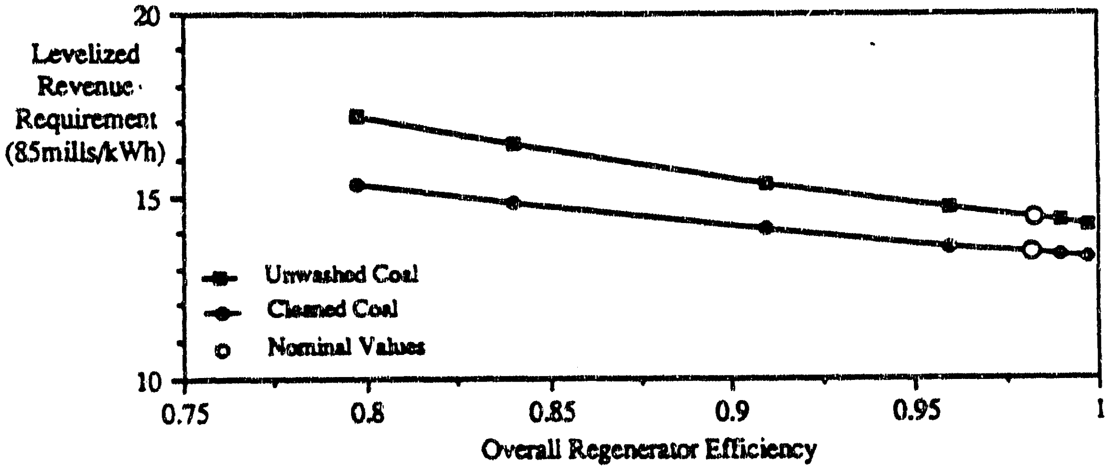


Figure 4-8: Effect of Overall Regenerator Efficiency





5 ELECTRON BEAM PROCESS MODEL

5.1 Nomenclature

English Symbols

Byp	Bypass (fraction)
C_j	Concentration of j in flue gas (ppm)
D	Electron beam dosage (Mrads)
ES	Emission standard (lb/million Btu into furnace)
Hhv	Higher heating value of fuel (Btu/lb)
$\dot{m}_{\#,j}$	Molar flow rate of component j at point # (lb•mole/hr)
$\dot{M}_{\#,j}$	Mass flow rate of component j at point # (tons/hr)
R_{purity}	Purity of reagent (fraction)
$T_{\#}$	Temperature at point # (°R)

Greek Symbols

ΔT	Temperature difference (°F)
η	Efficiency (fraction)
σ	Molar stoichiometry (fraction)

Subcategories for Combustion Air and Flue Gas Components

CO	Carbon monoxide
CO_2	Carbon dioxide
H_2O	Moisture
N_2	Nitrogen
NO	Nitrogen oxide
NO_2	Nitrogen dioxide
O_2	Oxygen
SO_2	Sulfur dioxide
SO_3	Sulfur trioxide

Subcategories for Solid Stream Components

Ash	Ash
CaO	Lime
$CaCO_3$	Limestone
$CaSO_3 \cdot .5H_2O$	Hydrated calcium sulfite
$CaSO_4$	Calcium Sulfate
$CaSO_4 \cdot 2H_2O$	Hydrated calcium sulfate
H_2O	Water or Moisture
Misc	Miscellaneous

General Subcategories

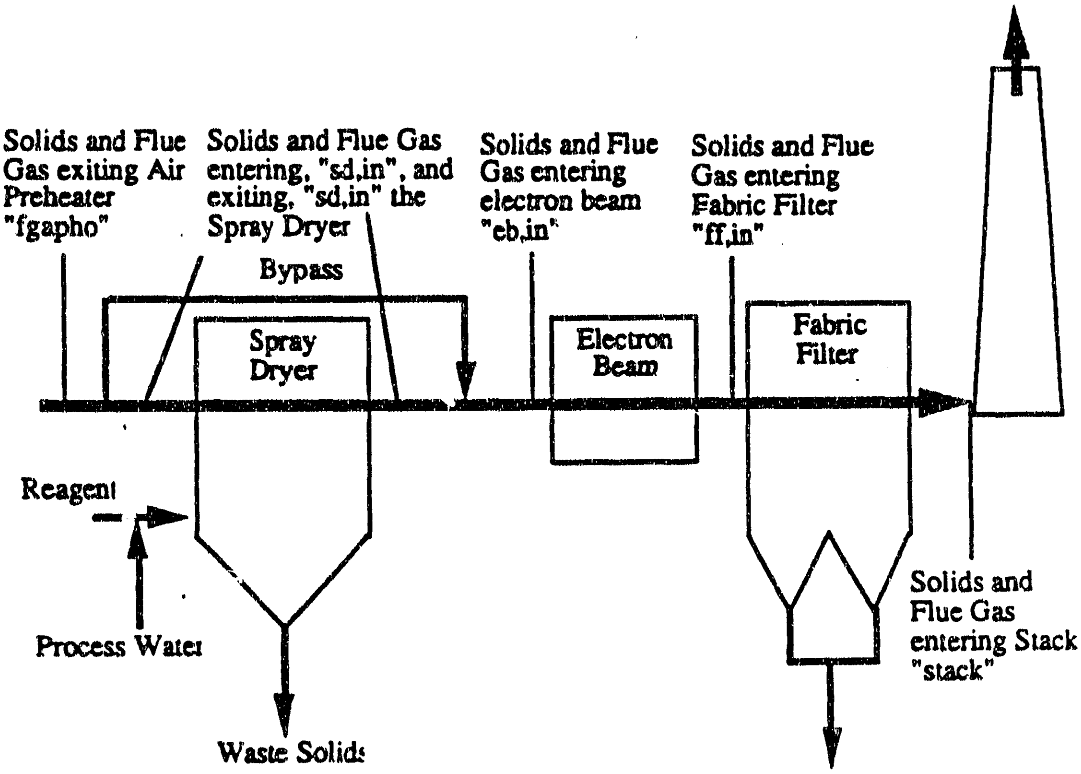
eb	Electron beam chamber
exit	Exiting device
fgapho	Exiting air preheater on flue gas side
fuel	Fuel stream
in	Entering device
NO_x	Nitrogen oxide
sat	Saturation

sd	spray dryer
SO_2	Sulfur dioxide
std	Based on emission standard

5.2 Introduction

This section describes several improvements to the electron beam (E-beam) process model, developed previously (1). The areas which were updated are the electron beam dose, flue gas composition and solids composition exiting the electron beam chamber. A schematic diagram of the electron beam process is shown in Figure 5-1. In the configuration, a spray dryer is employed upstream of the electron beam chamber to remove SO_2, to add moisture and lime to the flue gas and to lower the flue gas temperature.[15] A fabric filter is downstream to collect the flyash and solids which form in the electron beam chamber. The electron beam process model uses a modified spray dryer model. The modifications to the spray dryer model are described in Section 5.3, while the original spray dryer model is described in Section 2.6.

Figure 5-1: Schematic Diagram of Electron Beam Process



5.3 Spray Dryer Model Modifications

Because the spray dryer used with the electron beam process does not have a reheater, equations (2.24), (2.25) and (2.27) through (2.31) are not used. For the electron beam process,

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[15] This is the configuration initially of interest to DOE/PETC. More recently, an E-beam process using ammonia injection without a spray dryer was tested at the pilot plant level. While the IECM can be modified to simulate the latter configuration, the current model code retains the original design developed by Research-Cottrell.

the flue gas exiting the spray dryer enters the electron beam process instead of a fabric filter. The result of modifying equations (2.22) and (2.23) are shown below:

$$\dot{m}_{eb,in,j} = \dot{m}_{sd,exit,j} + Byp\ \dot{m}_{fgapho,j}$$

$$T_{eb,in} = Byp\ T_{fgapho} + (1 - Byp)\ T_{sd,exit}$$

In the original spray dryer model, the reagent and molar stoichiometry was determined using Equations (2.18) and (2.19). For the electron beam model, they are determined with the equations below. The molar stoichiometry of the E-beam, σ_{eb}, is an input parameter and is the molar ratio of lime to sulfur dioxide plus one-half the NO_x entering the spray dryer.

$$\dot{M}_{reag} = \frac{56.08\,(\dot{m}_{sd,in,SO_2} + \dot{m}_{sd,in,SO_3} + 0.5\dot{m}_{sd,in,NO} + 0.5\dot{m}_{sd,in,NO_2})\,\sigma_{eb}}{2000\ R_{purity}}$$

$$\sigma_{sd} = \frac{2000\ \dot{M}_{reag}\ R_{purity}}{56.08\,(\dot{m}_{sd,in,SO_2} + \dot{m}_{sd,in,SO_3})}$$

In the spray dryer model, the amount of bypass and SO_2 removal was determined using Equations (2.16) and (2.16). For the electron beam model, the amount of bypass is an input parameter and the SO_2 removal is determined by solving Equation (2.18) for η_{SO_2}.

$$\eta_{SO_2} = \frac{\ln \sigma_{sd} - 0.025\Delta T_{sat} + 2.9}{3.322}$$

5.4 Electron Beam Dose

The sulfur dioxide and NO_x removal efficiencies required for the ebeam process to meet their respective emission standards are determined by

$$\eta_{SO_2,std} = 1 - \frac{2000\ ES_{SO_2}\ \dot{M}_{fuel}\ Hhv_{fuel}}{64.06 * 1{,}000{,}000\ (\dot{m}_{eb,in,SO_2} + \dot{m}_{eb,in,SO_3})} \tag{5.1}$$

$$\eta_{SO_2,std} = 1 - \frac{2000\ ES_{NO_x}\ \dot{M}_{fuel}\ Hhv_{fuel}}{46.01 * 1{,}000{,}000\ (\dot{m}_{eb,in,NO} + \dot{m}_{eb,in,NO_2})} \tag{5.2}$$

Helfritch and Feldman determined an algorithm for predicting the outlet concentration of SO_2 and NO_x versus the dose of electron directed into the flue gas (29). Their algorithm is based on the rates of reactions of the principal chemical reactions and experimental data and is shown below.[16]

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[16] In Reference (29), there is a typographical error for Equation 5.3. The constant "2.5" is typed as "0.25."

$$\frac{C_{SO_2}}{C_{SO_2,in}} = \exp\left\{\frac{-2.5\,D}{1 + 0.0058\ C_{SO_2,in}}\right\} \tag{5.3}$$

$$\frac{C_{NO_x}}{C_{NO_x,in}} = \exp\left\{\frac{-0.12\,D\left(1 + 0.058\ C_{SO_2,in}\right)}{1 + 0.0058\ C_{SO_2,in}}\right\} \tag{5.4}$$

Typically when the IECM is used, the emission constraints are specified and the pollution control equipment has to meet these constraints. Therefore, Equations (5.3) and (5.4) are solved for the electron beam dose and the ratios of the outlet to inlet concentrations are replaced by one minus the removal efficiencies specified in Equations (5.1) and (5.2).

$$D_{SO_2} = \frac{\left(1 + 0.0058\ C_{SO_2,in}\right) * \ln\left(1 - \eta_{SO_2,std}\right)}{-2.5} \tag{5.5}$$

$$D_{NO_x} = \frac{\left(1 + 0.0058\ C_{SO_2,in}\right) * \ln\left(1 - \eta_{NO_x,std}\right)}{-0.12\left(1 + 0.058\ C_{SO_2,in}\right)} \tag{5.6}$$

where

$$C_{SO_2,in} = \frac{1{,}000{,}000\left(\dot{m}_{eb,in,SO_2} + \dot{m}_{eb,in,SO_3}\right)}{\sum_{j=1}^{9} \dot{m}_{eb,in,j}}$$

Since the electron beam process has to meet both the NO_x and SO_2 emission constraints, the larger dose determined by Equations (5.5) and (5.6) is used and the actual NO_x and SO_2 removal efficiencies are determined by the equations below. Thus,

if $D_{SO_2} \geq D_{NO_x}$ then $D = D_{SO_2}$ else $D = D_{NO_x}$

$$\eta_{SO_2} = 1 - \exp\left\{\frac{-2.5\,D}{1 + 0.0058\ C_{SO_2,in}}\right\}$$

$$\eta_{NO_x} = 1 - \exp\left\{\frac{-0.12\,D\left(1 + 0.058\ C_{SO_2,in}\right)}{1 + 0.0058\ C_{SO_2,in}}\right\}$$

5.5 Flue Gas Composition

The composition of the flue gas changes in the electron beam chamber. The two most significant changes are the reduction in the sulfur dioxide content and nitrogen oxide content. The sulfur dioxide and nitrogen oxide are removed from the flue gas by a complex set of chemical reactions (29). These chemical reactions have been greatly simplified in the IECM and are shown below.

$$
\begin{aligned}
&SO_2 + CaO + 2H_20 + 0.5O_2 \dashrightarrow CaSO_4{\cdot}2H_20 \qquad (5.7)\\
&SO_3 + CaO + 2H_20 \dashrightarrow CaSO_4{\cdot}2H_20\\
&2NO + CaO + H_20 + 0.5O_2 \dashrightarrow Ca(NO_2)_2{\cdot}H_20\\
&2NO + CaO + 1.5O_2 \dashrightarrow Ca(NO_3)_2\\
&2NO_2 + CaO + H_20 \dashrightarrow Ca(NO_2)_2{\cdot}H_20 + 0.5O_2\\
&2NO_2 + CaO + 0.5O_2 \dashrightarrow Ca(NO_3)_2
\end{aligned}
$$

Using these chemical reactions the composition of the flue gas exiting the electron beam chamber can be determined from a molar balance as shown below. The symbol, Ox, represents the fraction of calcium nitrite oxidized to calcium nitrate.

$$\dot{m}_{eb,exit,j} = \dot{m}_{eb,in,j} \quad \text{for } j = N_2,\ CO_2,\ CO$$

$$\dot{m}_{eb,exit,O_2} = \dot{m}_{eb,in,O_2} - \{0.5\, \dot{m}_{eb,in,SO_2}\, \eta_{SO_2} +$$

$$[(0.5\, Ox + 0.25)\, \dot{m}_{eb,in,NO} + (0.5\, Ox - 0.25)\, \dot{m}_{eb,in,NO_2}]\, \eta_{NO_x}\}$$

$$\dot{m}_{eb,exit,H_2O} = \dot{m}_{eb,in,H_2O} - \{2\, [\dot{m}_{eb,in,SO_2} + \dot{m}_{eb,in,SO_3}]\, \eta_{SO_2} +$$

$$(1 - Ox)\, [\dot{m}_{eb,in,NO} + \dot{m}_{eb,in,NO_2}]\, \eta_{NO_x}\}$$

$$\dot{m}_{eb,exit,SO_2} = \dot{m}_{eb,in,SO_2} - \dot{m}_{eb,in,SO_2}\, \eta_{SO_2}$$

$$\dot{m}_{eb,exit,SO_3} = \dot{m}_{eb,in,SO_3} - \dot{m}_{eb,in,SO_3}\, \eta_{SO_2}$$

$$\dot{m}_{eb,exit,NO} = \dot{m}_{eb,in,NO} - \dot{m}_{eb,in,NO}\, \eta_{NO_x}$$

$$\dot{m}_{eb,exit,NO_2} = \dot{m}_{eb,in,NO_2} - \dot{m}_{eb,in,NO_2}\, \eta_{NO_x}$$

5.6 Waste Composition

A major environmental flow stream emanating from the electron beam system is the stream of dry waste solids. The basic chemistry for the creation of these solids is shown in Equation

(5.7). The difference in the composition and mass flow rates of electron beam waste depends on the extent of oxidation of calcium nitrite to calcium nitrate, Ox. Other constituents of the electron beam solids stream include unreacted reagent (which depends on the molar stoichiometry), inert materials introduced with the reagent (as dictated by the level of reagent purity) and the solid waste from the spray dryer system. The total mass flow rate of the solids exiting the electron beam is shown below.

$$\dot{M}_{eb,exit,j} = \dot{M}_{eb,in,j} \text{ for } j = \text{Ash}, CaCO_3, CaSO_4, CaSO_3 \cdot 0.5H_2O$$

$$\dot{M}_{eb,exit,CaO} = \dot{M}_{eb,in,CaO} - \frac{56.08}{2000}\left([\dot{m}_{eb,in,SO_2} + \dot{m}_{eb,in,SO_3}]\,\eta_{SO_2} + \right.$$

$$\left. 0.5\,[\dot{m}_{eb,in,NO} + \dot{m}_{eb,in,NO_2}]\,\eta_{NO_x}\right)$$

$$\dot{M}_{eb,CaSO_4 \cdot 2H_2O} = \dot{M}_{eb,in,CaSO_4 \cdot 2H_2O} + \frac{172.17\,(\dot{m}_{eb,in,SO_2} + \dot{m}_{eb,in,SO_3})\,\eta_{SO_2}}{2000}$$

$$\dot{M}_{eb,exit,Misc} = \dot{M}_{eb,in,Misc} + \frac{[150.1\,(1\text{-}Ox) + 164.09\,Ox]\,0.5\,(\dot{m}_{eb,in,NO} + \dot{m}_{eb,in,NO_2})\,\eta_{NO_x}}{2000}$$

5.7 Economics Algorithm

The economic algorithm for the electron beam process has remained unchanged except one item. The single indirect charge factor for capital cost has been split into different categories of indirect charges following the nomenclature of the TVA (see baseline plant section).

6 SULFURIC ACID PLANT MODEL

6.1 Nomenclature

English Letter Symbols

A_k	area of device, k (ft^2)
$C_{categorie}$	capital charges associated with startup ($)
C_{idx}	chemical engineering cost index
C_o	molar gas concentration of SO_2 in the flue gas entering the adsorber (lb•mole/ft^3)
CF	capacity factor of power plant (fraction)
DCC_k	capital cost for device, k (M$)
$e^{\#}$	notation for specifying power of 10.
$E_{j,k}$	energy flow rate of specie, j, at device, k (lb•mole/hr)
EC_k	electricity consumption of the device, k (kW)
f_{makeup}	attrition rate of sorbent (fraction)
$f_{j,wet\ air}$	amount of specie, j, in ambient moist air (fraction)
$fp_{j,k}$	quantity of specie, j, produced in device, k (fraction)
F_{oil}	constant used to estimate amount of sulfur from oil (fraction)
FOC	fixed operating cost ($/yr)
G_k	gas flow rate for device, k (ft^3/min)
$h_{j,temperature}$	molar enthalpy of specie, j, at specified temperature (Btu/lb•mole)
H	fluidized bed height in adsorber (ft)
HHV_j	higher heating value of specie, j, (Btu/lb)
HR	heat rate of power plant (kW-Hr/MBtu)
i	inflation rate (fraction)
K_a	apparent rate constant ($atm^{-1}\ sec^{-1}$)
$LMTD_k$	log mean temperature difference of device, k (°F)
m_j	mass flow of specie, j, (lbs/hr or tons/hr)
M_{jk}	molar flow rate of specie, j, for device, k (lb•mole/hr)
MW_g	gross electrical capacity of power plant (MW)
N_t	initial loading of the active Na on sorbent (lb•mole/lb)
NOP	number of operating adsorbers
NRD	number of spare adsorbers
$OC_{catagorie}$	annual operating cost ($/yr)
Q_k	heat load across heat exchanger device, k (Btu/hr)
p	interest rate (fraction)
P_k	pressure of the device, k (" water or atm)
RT_k	residence time of sorbent in device, k (hours)
$T_{sj,k}$	temperature of specie, j, for the device, k (°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 ($/yr)
U_k	universal heat transfer coefficient for device, k (Btu/hr-ft^2 °F)
UC_j	unit cost of specie, j, ($/unit)
Ut_j	utilization constant for specie, j, 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	molar fraction of SO_2 in the flue gas (fraction)

Greek Letter Symbols

δ_{NOx}	fraction of NOx returned to boiler which is destroyed (fraction)
ΔH_k	heat of reaction in device, k (Btu/hr)
$\eta_{j,k}$	efficiency of device, k (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 a device, k
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_2S
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, H_2S, S_2, SO_2 and SO_3
SD	sulfur dioxide, SO_2
SOX	sulfur dioxide and sulfur trioxide
ST	sulfur trioxide, SO_3
W	water, H_2O

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

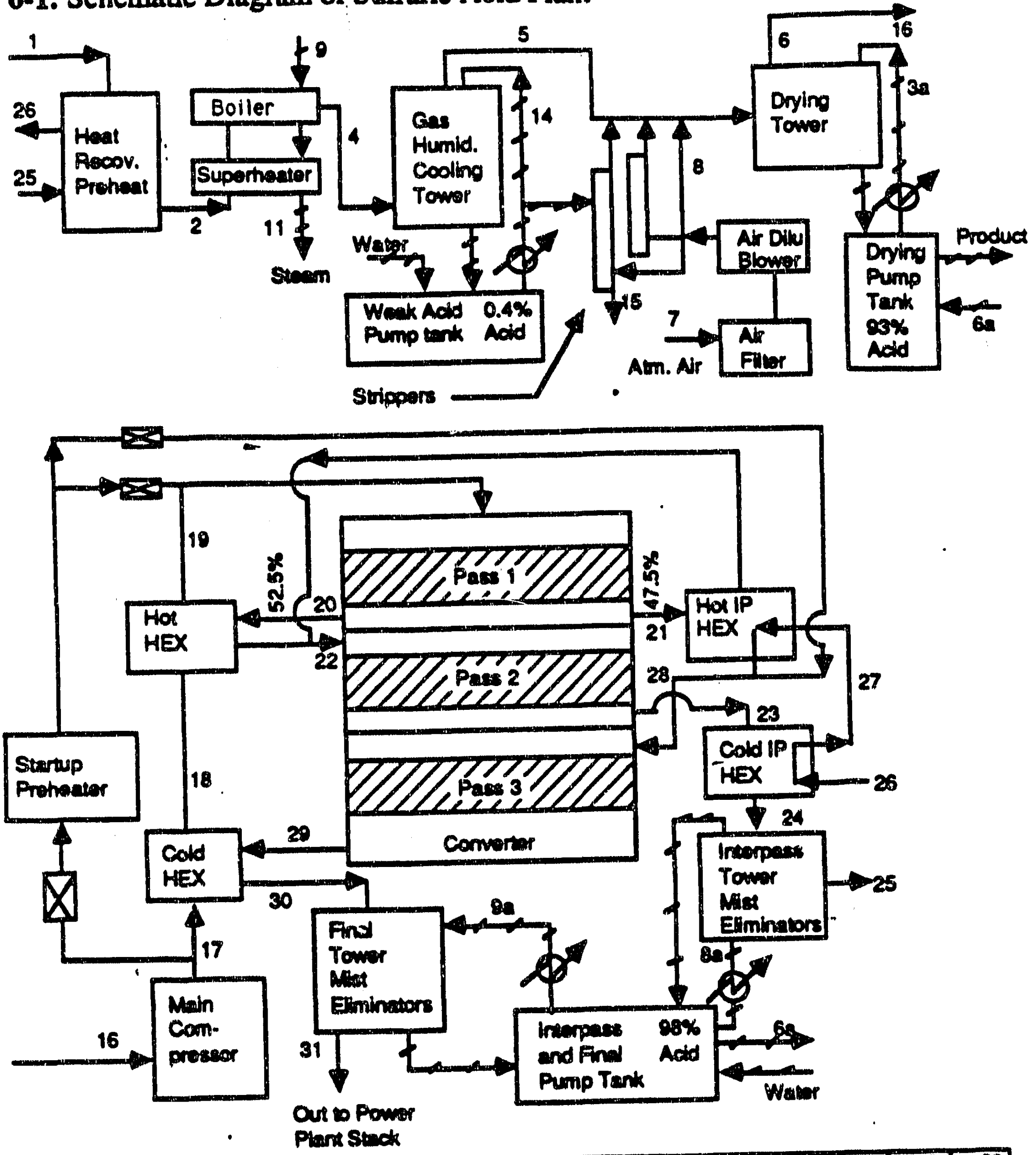
Categories for capital and operating cost:

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

6.2 Introduction

This chapter describes a sulfuric acid plant model developed by Frey (30). This model has been incorporated into the IECM to more carefully analyze the economics of processes producing a sulfuric acid byproduct. The original IECM models of the NOXSO and copper oxide processes treated the acid plant as a simple system, based on earlier studies for DOE/PETC. The new acid plant performance and economic models were developed based on an interpass absorption (2/1) contact acid plant design by Monsanto for SMC (31, 32). Subsequent information from Monsanto (33, 34) and other studies (22) also were used for this model.

Figure 6-1: Schematic Diagram of Sulfuric Acid Plant

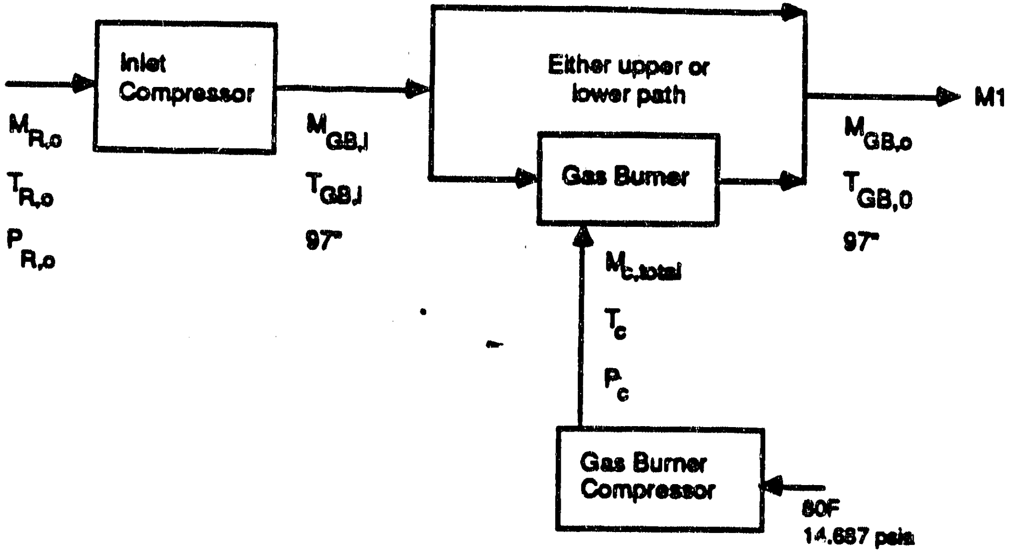


Stream	1	2	4	5	6	7	8	9	11	14	16	17	18	19	20
Temp. F	824	609	506	169	120	85	115	226	450	163	120	171	603	779	1158
" Water	97			67	51	0	67	100	100		51	167		155	

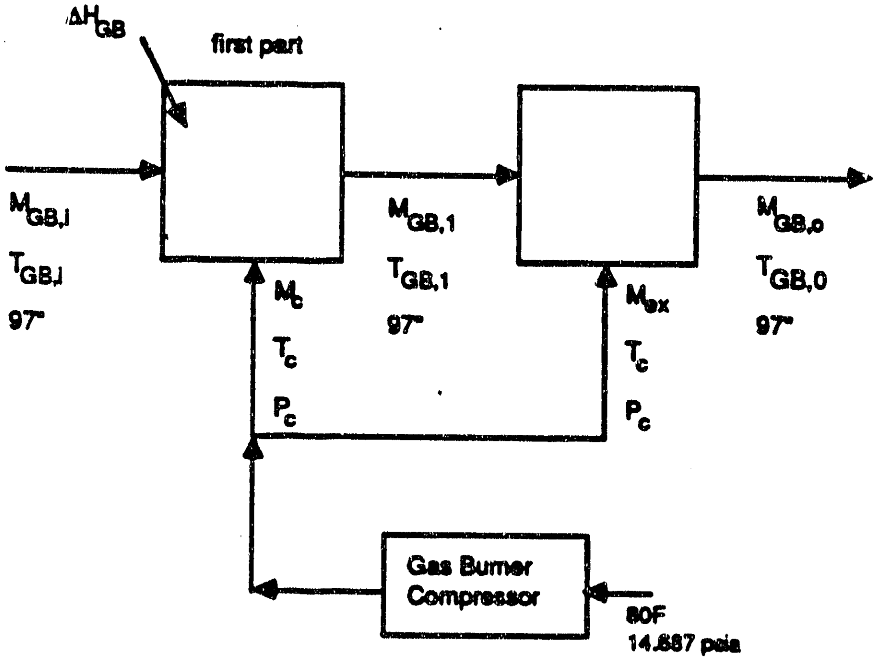
Stream	21	22	23	24	25	26	27	28	29	30	31	3a	6a	8a	9a
Temp. F	1158	828	918	570	180	256	667	850	877	380	180	120	180	180	180
" Water				97				37			1				

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 6-1, was modified to fit 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 6-2.

Figure 6-2: Schematic Diagrams of Inlet Compressor and Gas Burner



Break down of Gas Burner



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 IECM. 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 on 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 fluorine. 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.

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 6-1 and 6-2 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 on 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 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 somewhat expensive and have a significant pressure drop. To prevent moisture from entering the converter, drying towers are used upstream. 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. Yet, the conversion efficiency decreases with increasing temperature. Because of this, a three pass converter design is used to achieve a 99.5% conversion efficiency. The first stage oxides 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 6.1) 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 is not used. This occurs when substantial combustible gases enter 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. It is assumed that the natural gas to fire these burners 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 done 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.

6.3 Performance Model

The sulfuric acid plant model developed is meant to respond to several factors that affect sulfuric acid plant cost. These include the volume flow rate, moisture content, temperature, pressure, combustible gases and SO_2 content of the inlet gas stream. To achieve this, mass and energy balances are performed on 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 (5) and Barin, Knacke and Kubaschewski (6). These polynomial equations are functions in this model, as explained earlier in Chapter 2 (Section 2.2). When the 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 assumptions for this model are (1) that the inlet gas is free of aust, arsenic, chlorine and fluorine, (2) the inlet pressure entering the heat recovery preheater is 95 - 97" inches of water and (3) 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 (31). 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. Although these values appear as constants in this report, they are 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 on the pressure difference. If the pressure difference is greater than 50" of water, a compressor is used with an efficiency of 75% (35). Otherwise, a blower is used with an efficiency of 85% (36). 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.

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

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

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

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

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

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 affects 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. It is 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 oxide all the combustible gases. To prevent the gas burner from operating above 2000°F, additional air is added above the stoichiometric requirement to oxides the combustible gases. To solve for the additional air requirement, the gas burner is assumed to be divided into two parts, shown in Figure 6-2. 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

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

The additional air needed for 5% excess air is

if $1.05M_{O,c,1} > M_{O,R,o}$ then

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

else $M_{O,c} = 0$

$M_{N,c} = 3.76M_{O,c}$

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

Since combustion air has to be raised to 97" of water, its temperature into the gas burner is

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

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.

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

$M_{SD,GB,1} = M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o}$

$M_{W,GB,1} = M_{W,R,o} + M_{W,c} + 2M_{M,R,o} + M_{H,R,o} + M_{HS,R,o}$

$M_{CD,GB,1} = M_{CD,R,o} + M_{M,R,o} + M_{CM,R,o} + M_{CS,R,o}$

$M_{N,GB,1} = M_{N,R,o} + M_{W,c}$

if $M_{O,R,o} > 1.05M_{O,c,1}$ then

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

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

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

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

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

Now an energy balance is performed on 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 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, with the energy consumed by the gas burner combustion air compressor.

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

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

$$E_{GB,total} = E_{BG,i} + E_c + \Delta H_{GB}$$

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

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

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

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

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

else $M_{O,ex} = 0$

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

$$M_{N,ex} = 3.76M_{O,ex}$$

$$M_{W,ex} = 1.611*0.018*4.76M_{O,ex}$$

$$M_{c,total} = M_{O,c} + M_{N,c} + M_{W,c} + M_{O,ex} + M_{N,ex} + M_{W,ex}$$

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

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

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 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

$$M_{k,HP,i} = M_{k,R,o}$$

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

else

$$M_{j,HP,i} = 0$$

$$M_{SD,HP,i} = M_{SD,GB,1}$$

$$M_{CD,HP,i} = M_{CD,GB,1}$$

$$M_{W,HP,i} = M_{W,GB,1} + M_{W,ex}$$

$$M_{N,HP,i} = M_{N,GB,1} + M_{N,ex}$$

$$M_{O,HP,i} = M_{O,GB,1} + M_{O,ex}$$

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

$$M_{HP,i} = \sum_{k=1}^{11} M_{k,HP,i}$$

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

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 have followed the gas stream into the acid plant and it seems 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 on 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. Another 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, with the oxygen needed for oxidation all the combustible gases and converting all the SO_2 to SO_3 is calculated below. This ensures that enough oxygen is available to convert the SO_2 to SO_3. 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:

$M_{O,CS,1} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.35M_{SD,PH,i} + 1.85M_{CS,PH,i} +$

$1.85M_{HS,PH,i} + 2.7M_{S,PH,i}$

$M_{O,CS,all} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.5M_{SD,PH,i} + 2M_{CS,PH,i} +$

$2M_{HS,PH,i} + 3M_{S,PH,i}$

if $M_{O,CS,all} > M_{O,PH,i}$ then $M_{O,CS,c} = M_{O,CS,all} - M_{O,PH,i}$

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

$M_{N,CS,c} = 3.76M_{O,CS,c}$

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

if $M_{O,CS,all} > M_{O,PH,i}$ then $M_{O,CS,1,o} = M_{O,CS,all} - M_{O,CS,1}$

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

$M_{N,CS,1,o} = M_{N,PH,i} + M_{N,CS,c}$

$M_{CD,CS,1,o} = M_{CD,PH,i} + M_{M,PH,i} + M_{CM,PH,i} + M_{CS,PH,i}$

$M_{W,CS,1,o} = M_{H,PH,i} + 2M_{M,PH,i} + M_{HS,PH,i}$

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

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

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

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

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 the species entering the heat recovery preheater at 779°F, except 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 6.69 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.

$$E_{CS,1} = \sum_{k=1}^{10} \hat{h}_j(779)M_{k,PH,i} + 5{,}235.7M_{O,CS,c} + 5{,}028.4M_{N,CS,c} + \Delta H_{CS,1} \tag{6.1}$$

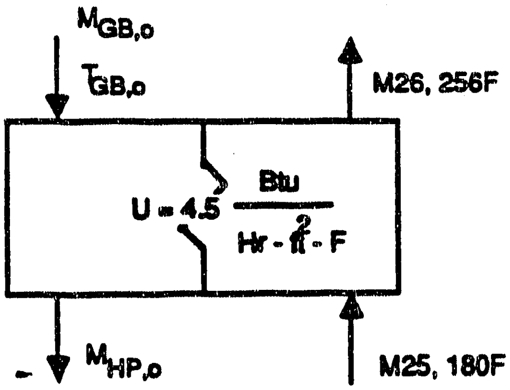
$$E_{CS,1,max} = \sum_{j=1}^{6} \hat{h}_j(1158)M_{j,CS,1,o}$$

$$M_{air,CS,ex} = \frac{E_{CS,1} - E_{CS,1,max}}{2{,}864.2} \tag{6.2}$$

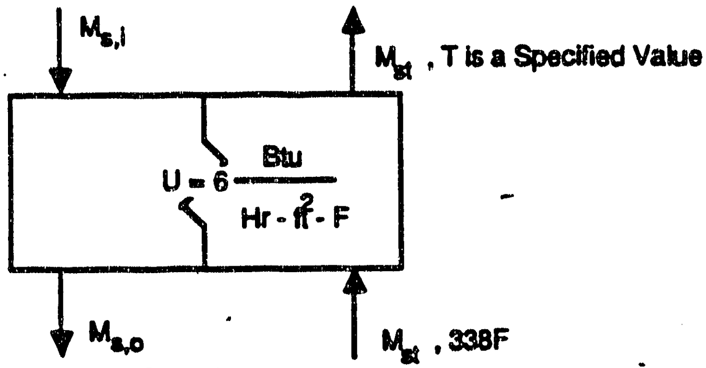
$M_{BF} = (1 + 1.611 * 0.018)M_{air,CS,ex} + M_{O,CS,c} + M_{N,CS,c} + M_{W,CS,c}$

where k = CD,CM,CS,H,HS,M,N,O,S,SD and j = CD,N,O,SD,ST,W

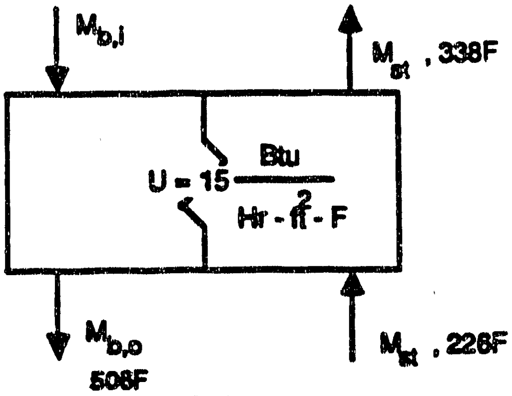
Figure 6-3: Inlet Gas Cooling Heat Exchangers



(a) Heat Recovery Preheater



(b) Superheater



(c) Boiler

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.

$$M_{D,i} = M_{PH,i} + M_{BF} - 0.3M_{W,PH,i}$$

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

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

$$M_{CD,25} = M_{CD,CS,1,o}$$

$$M_{N,25} = M_{N,CS,1,o} + 0.79M_{air,CS,ex}$$

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

$$M_{SD,25} = 0.17M_{SD,CS,1,o}$$

$$M_{25} = \sum_{j=1}^{4} M_{j,25}$$

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 6-3. 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.

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

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

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

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

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

$$T_{HP,o} = -Q_{HP}\frac{T_{HP,i} - T_{guess}}{E_{HP,i} - E_{guess}} + T_{HP,i}$$

$$LMTD_{HP} = \frac{(T_{HP,i} - 256) - (T_{HP,o} - 180)}{\ln\left(\frac{T_{HP,i} - 256}{T_{HP,o} - 180}\right)}$$

$$A_{HP} = \frac{Q_{HP}}{4.5 LMTD_{HP}}$$

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. 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.[17]

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

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[17] 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 determine more accurately by subtracting the heat load from the energy entering the preheater.

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.

$$E_{HP,o} = E_{HP,i} - Q_{HP}$$

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

```
if $E_{HP,o} > E_{506}$ then
    $E_{GC,i} = E_{506}$
    $T_{GC,i} = 506$
else
    $E_{GC,i} = E_{HP,o}$
    $T_{GC,i} = T_{HP,o}$
```

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

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 similarly 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.

$$Q_b = 17,929M_{st}$$

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

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

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

$$T_{bi,i} = -Q_s \frac{T_{HP,o} - T_{guess}}{E_{HP,o} - E_{guess}} + T_{HP,o}$$

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.

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

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

$$A_s = \frac{Q_s}{6\mathrm{LMTD}_s}$$

$$A_b = \frac{Q_b}{15\mathrm{LMTD}_b}$$

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.

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

$$M_{WA} = \frac{E_{GC,i} - E_{GC,o} + 0.3(\hat{h}_W(T_{GC,i}) - 840.6 + 17{,}813}{324.6}$$

The electricity usage for the main and dilution compressors and also 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.

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

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

The total acid produced can be determined 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 efficiencies 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*.93 + 1*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.

$$m_{acid} = 0.995\,(M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o}) * 98\ \text{lbm/lb-mole}$$

$$/\ 2000\ \text{tons/lbm}$$

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

which simplifies to

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

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

which simplifies to

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

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

which simplifies to

$$EC_{PA} = \frac{80\frac{\text{lbf}}{\text{in}^2} m_{acid}}{1017\frac{\text{tons/hr lbf/in}^2}{\text{kW}} * 0.70}$$

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.

$$EC_{total} = EC_{IC} + EC_{GB} + EC_{BF} + EC_{MC} + EC_{WA} + EC_{SS} + EC_{PA}$$

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

6.4 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 costs are in mid-83 dollars, except 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.

6.4.1 Capital Cost

The cost of the inlet compressor depends on the pressure drop and the inlet gas flow rate. The cost is pro-rated by pressure drop since the capital cost of blowers and compressors increase with increasing pressure. The cost estimates come from the NOXSO chapter in the EPRI Economic Evaluation of FGD Systems (22). For both estimates, it is assumed that there are two operating and one spare. The algorithm is:

if $P_{R,o} < 47$" of water

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

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

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

The capital gas of the gas burner is also taken from reference (22). It is assumed that there are two operating and one spare and that the cost includes the cost of the combustion air compressor.

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

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.

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

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

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

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

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

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.

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

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 lb•mole/hr of gas.

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

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 lb•mole/hr.

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

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.

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

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}.

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

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.

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

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

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.

$$DCC_{total} = \sum_{k=1}^{3} DCC_k$$

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

6.4.2 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 (33, 34). The maintenance personnel are assumed to only work 1/3 of the total number of hours in a year. 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.

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

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

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

The maintenance material cost 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 lb-mole/hr of gas flow (1985\$) (34). The marketing and shipping cost are estimated to be 10% of the sulfuric acid credit (12). Sulfuric acid is assumed to sell for \$50/ton (1985\$). (12).

$$OC_{maint\text{-}matl} = 0.009 * DCC_{total}$$

$$OC_{makeup} = 0.02 * 35.2\ 85\$/lb\text{-}mole/hr * M_6 * C_{idx}/325.3$$

$$OC_{credit} = 50\ 85\$/ton * CF * 8766 * m_{acid} * C_{idx}/325.3$$

$$OC_{marketing} = 0.1 * OC_{credit}$$

$$OC_{total} = OC_{oper} + OC_{maint\text{-}labor} + OC_{admin} + OC_{main\text{-}mater} + OC_{makeup}$$

$$+ OC_{marketing} - OC_{credit}$$

6.5 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 6-1. 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 consists of the species with which this model has been designed for except nitrogen and oxygen.[18] 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 6.3, 6.4, 6.5 and 6.6 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.

$$T_{IC,o} = (T_{R,o} + 460)\left(\frac{14.687 + 3.612e^{-2}*97}{14.687 + 3.612e^{-2}P_{R,o}}\right)^{\frac{1.4-1}{1.4}} - 460 \tag{6.3}$$

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

$$T_{IC,i} = 958.5°F$$

$$G_{IC,i} = \frac{1545\ M_{R,o}(T_{R,o} + 460)}{60*144\ (14.687 + 3.612e^{-2}\ P_{R,o})} \tag{6.4}$$

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

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[18] 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.

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

$$G_{IC,o} = \frac{1545\ M_{R,o}\ (T_{IC,o} + 460)}{60*144(14.687 + 3.612e^{-2}*97)} \qquad (6.5)$$

Table 6-1: 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 lb•mole/hr
$P_{R,o}$	28" of water	$M_{N,R,o}$	0 lb•mole/hr
$T_{specified}$	550°F	$M_{O,R,o}$	0 lb•mole/hr
$M_{CD,R,o}$	500 lb•mole/hr	$M_{S,R,o}$	41 lb•mole/hr
$M_{CO,R,o}$	50 lb•mole/hr	$M_{SD,R,o}$	200 lb•mole/hr
$M_{COS,R,o}$	17 lb•mole/hr	$M_{W,R,o}$	500 lb•mole/hr
$M_{H,R,o}$	100 lb•mole/hr	$M_{R,o}$	1,568 lb•mole/hr
$M_{HS,R,o}$	150 lb•mole/hr		

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

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

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

$$EC_{IC} = \left(\frac{1545 M_{R,o}}{0.75*60*44{,}240}\right)\left(\frac{1.4}{1.4-1}\right)\left[\left(\frac{14.687 + 3.612e^{-2}*97}{14.687 + 3.612e^{-2}P_{R,o}}\right)^{\frac{1.4-1}{1.4}} - 1\right]\left(T_{R,o} + 460\right) \qquad (6.6)$$

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

Since 28" is less than 97"

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

$EC_{IC} = 249.3$ kW

The gas burner is used since the inlet gas contains many combustible gases. The algorithm of the gas burner divides it into two parts, see Figure 6-3. 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.

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

$$M_{O,c,1} = 2*10 + 0.5*100 + 0.5*50 + 1.5*17 + 1.5*150 + 2*41 = 42\ .5 \text{ lb•mole/hr}$$

since $1.05*427.5 > 0$

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

$$M_{N,c} = 3.76M_{O,c} = 3.76*448.88 = 1{,}688 \text{ lb•mole/hr}$$

$$M_{W,c} = 1.611*0.018(448.88 + 1{,}687.77) = 61.96 \text{ lb•mole/hr}$$

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

$$T_c = 114.1°\mathrm{F}$$

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

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

$$M_{SD,GB,1} = M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o}$$

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

$$M_{W,GB,1} = M_{W,R,o} + M_{W,c} + 2M_{M,R,o} + M_{H,R,o} + M_{HS,R,o}$$

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

$$M_{CD,GB,1} = M_{CD,R,o} + M_{M,R,o} + M_{CM,R,o} + M_{CS,R,o}$$

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

$$M_{N,GB,1} = M_{N,R,o} + M_{W,c}$$

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

since $0 > 1.05*427.5$ is false

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

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

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

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

$$222{,}900*150 + 236{,}000*17$$

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

The total energy exiting the first part of the gas burner is calculated next, 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 with the electricity consumed by the compressor for the combustion air.

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

$$E_{GB,i} = 9,567*500 + 6,414*50 + 10.34e^3*17 + 6,166*100 + 7,950*150 +$$

$$10,33e^3*10 + 6,359*0 + 7.426*41 + 9,833*200 + 7,576*500$$

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

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

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

$$E_{GB,total} = E_{BG,i} + E_c + \Delta H_{GB}$$

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

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

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

$$17.92e^3*832.0$$

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

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

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

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

if $E_{GB,total} > E_{GB,max}$ then

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

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

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 $81.68e^6 > 63.24e^6$

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

$M_{O,ex} = 260.9$ lb•mole/hr

$T_{GB,o} = 2000°F$

$M_{N,ex} = 3.76 M_{O,ex} = 3.76*260.9 = 981.1$ lb•mole/hr

$M_{W,ex} = 1.611*0.018*4.76 M_{O,ex} = 1.611*0.018*4.76*260.9 = 36.02$ lb•mole/hr

$M_{c,total} = M_{O,c} + M_{N,c} + M_{W,c} + M_{O,ex} + M_{N,ex} + M_{W,ex}$

$M_{c,total} = 448.9 + 1,688 + 61.96 + 260.9 + 981.1 + 36.02 = 3,477$ lb•mole/hr

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

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

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

$EC_{GB} = 321.8$ 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 upstream of the superheater and boiler, the energy released in the gas burner can be partially recovered by the superheater and boiler.

MCO,HP,i = MCOS,HP,i = MH,HP,i = MHS,HP,i = MM,HP,i = MS,HP,i = 0 lb•mole/hr.

MSD,HP,i = MSD,GB,1 = 449 lb•mole/hr

MCD,HP,i = MCD,GB,1 = 577 lb•mole/hr

MN,HP,i = MN,GB,1 + MN,ex = 1,688 + 981.1 = 2669 lb•mole/hr

MO,HP,i = MO,GB,1 + MO,ex = 21.38 + 260.9 = 282.3 lb•mole/hr

MW,HP,i = MW,GB,1 + MW,ex = 832.0 + 36.02 = 868.0 lb•mole/hr

THP,i = TGB,o = 2000°F

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

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

$G_{HP,i} = 117.2e^3$ 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 dilution air. The first part burns any combustibles and converts above 70% of the SO_2 to SO_3.

$M_{O,CS,1} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.35M_{SD,PH,i} + 1.85M_{CS,PH,i} +$

$1.85M_{HS,PH,i} + 2.7M_{S,PH,i}$ lb•mole/hr

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

$M_{O,CS,all} = 2M_{M,PH,i} + 0.5M_{CM,PH,i} + 0.5M_{H,PH,i} + 0.5M_{SD,PH,i} + 2M_{CS,PH,i} +$

$2M_{HS,PH,i} + 3M_{S,PH,i}$

$M_{O,CS,all} = 20 + 0.5*0 + 0.5*0 + 0.5*449 + 2*0 + 2*0 + 3*0 = 224.5$ lb•mole/hr

if $M_{O,CS,all} > M_{O,PH,i}$ then $M_{O,CS,c} = M_{O,CS,all} - M_{O,PH,i}$

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

since 224.5 is not greater than 282.3 then

$M_{O,CS,c} = 0$ lb•mole/hr

$M_{N,CS,c} = 3.76M_{O,CS,c} = 3.76*0 = 0$ lb•mole/hr

$M_{W,CS,c} = 1.611*0.018(M_{O,CS,c} + M_{O,CS,c}) = 1.611*0.018(0 + 0) = 0$ lb•mole/hr

if $M_{O,CS,all} > M_{O,PH,i}$ then $M_{O,CS,1,o} = M_{O,CS,all} - M_{O,CS,1}$

else MO,CS,1,o = MO,PH,i - MO,CS,1

since 224.5 is not greater than 282.3 then

$M_{O,CS,1,o} = M_{O,PH,i} - M_{O,CS,1} = 282.3 - 157.2 = 125.2$ lb•mole/hr

$M_{N,CS,1,o} = M_{N,PH,i} + M_{N,CS,c} = 2{,}669 + 0 = 2{,}669$ lb•mole/hr

$M_{CD,CS,1,o} = M_{CD,PH,i} + M_{M,PH,i} + M_{CM,PH,i} + M_{CS,PH,i}$

$M_{CD,CS,1,o} = 577 + 0 + 0 + 0 + 0 = 577$ lb•mole/hr

$M_{W,CS,1,o} = M_{H,PH,i} + 2M_{M,PH,i} + M_{HS,PH,i} = 0 + 0 + 2*0 = 0$ lb•mole/hr

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

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

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

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

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

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

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

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

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 with the molar flow rates exiting the drying tower (M_6), second stage (M_{23}) and entering the heat recovery preheater (M_{25}).

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

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

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

$13.38e^{6}$

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

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

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

$$+9{,}439*0$$

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

where k = CD,CM,CS,H,HS,M,N,O,S,SD and j = CD,N,O,SD,ST,W

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

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

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

$$M_{D,i} = M_{PH,i} + M_{BF} - 0.3M_{W,PH,i} = 4845 + 43.76 - 0.3*868.0 = 4{,}629 \text{ lb-mole/hr}$$

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

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

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

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

$$M_{23} = 3{,}807 \text{ lb-mole/hr}$$

$$M_{CD,25} = M_{CD,CS,1,o} = 577 \text{ lb-mole/hr}$$

$$M_{N,25} = M_{N,CS,1,o} + 0.79M_{air,CS,ex} = 2{,}669 + 0.79*42.53 = 2{,}702 \text{ lb-mole/hr}$$

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

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

$$M_{O,25} = 78.19 \text{ lb-mole/hr}$$

$$M_{SD,25} = 0.17M_{SD,CS,1,o} = 0.17*134.7 = 22.90 \text{ lb-mole/hr}$$

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

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 6.7 and 6.8, the molar flow rates of the combustible gases are zero and weren't shown in the calculation.

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

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

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

$$E_{HP,i} = \sum_{k=1}^{11} \hat{h}_k(T_{HP,i})M_k = \sum_{k=1}^{11} \hat{h}_k(2000)M_k \tag{6.7}$$

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

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

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

$$E_{guess} = \sum_{k=1}^{11} \hat{h}_k(T_{guess})M_k = \sum_{k=1}^{11} \hat{h}_k(1{,}953)M_k \tag{6.8}$$

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

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

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

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

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

$$A_{HP} = \frac{Q_{HP}}{4.5 LMTD_{HP}} = \frac{1.943e^6}{4.5*1{,}761} = 245.1 \text{ ft}^2$$

The amount of steam generated with the heat and area of the boiler and superheater, are determined similarly 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.

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

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

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

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

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

```
if $E_{HP,o} > E_{506}$ then
    $E_{GC,i} = E_{506}$
    $T_{GC,i} = 506$
else
    $E_{GC,i} = E_{HP,o}$
    $T_{GC,i} = T_{HP,o}$
```

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

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

$$T_{GC,i} = 506°\text{F}$$

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

$$M_{st} = 3215\ \text{lb}\bullet\text{mole/hr}$$

Now the boiler and superheater heat loads and also 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 the model 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.

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

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

$$T_{guess} = T_{HP,o}\left(1 - \frac{Q_s}{E_{HP,o}}\right) = 1{,}959\left(1 - \frac{5.768e^6}{80.07e^6}\right) = 1{,}817°F$$

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

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

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

$$T_{bi,i} = -Q_s \frac{T_{HP,o} - T_{guess}}{E_{HP,o} - E_{guess}} + T_{HP,o} = -5.786e^6 \frac{1{,}959 - 1{,}817}{80.07e^6 - 73.49e^6} + 1{,}959 = 1{,}834°F$$

$$LMTD_s = \frac{(T_{HP,o} - T_{specified}) - (T_{b,i} - 338)}{\ln\left(\dfrac{T_{HP,o} - 338}{T_{b,i} - 338}\right)} = \frac{(1{,}959 - 550) - (1{,}834 - 338)}{\ln\left(\dfrac{1{,}959 - 550}{1{,}834 - 338}\right)} = 1{,}452°F$$

$$LMTD_b = \frac{(T_{b,i} - 338) - (506 - 226)}{\ln\left(\dfrac{T_{b,i} - 338}{506 - 226}\right)} = \frac{(1{,}834 - 338) - (506 - 226)}{\ln\left(\dfrac{1{,}834 - 338}{506 - 226}\right)} = 725.8°F$$

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

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

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

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

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

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

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

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

$M_{WA} = 57,710$ lb•mole/hr.

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

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

$EC_{BF} = 2.862$ kW

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

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

$EC_{MC} = 422.7$ kW

$m_{acid} = 0.995(M_{SD,R,o} + M_{CS,R,o} + M_{HS,R,o} + 2M_{S,R,o})$ 98 lbm/lb•mole

/2000 tons/lbm

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

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

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

$$EC_{SS} = \frac{202.4\frac{\text{ga;,om}}{\text{tons/hr}}*80 \text{ ft } m_{acid}}{2955\frac{\text{gal/min*f}}{\text{kW}}*0.80}$$

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

$$EC_{PA} = \frac{80\frac{lbf}{in^2}m_{acid}}{1017\frac{tons/hr\ lbf/in^2}{kW}*0.70}$$

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

$$EC_{total} = EC_{IC} + EC_{GB} + EC_{BF} + EC_{MC} + EC_{WA} + EC_{SS} + EC_{PA}$$

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

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

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

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

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

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

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

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

since $P_{R,o} > 47$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Now the operating costs are calculated.

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

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

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

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

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

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

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

$OC_{makeup} = 0.02 * 35.2 \text{ 85\$/lb•mole/hr} * M_6 * C_{idx}/325.3$

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

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

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

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

$OC_{total} = OC_{oper} + OC_{maint\text{-}labor} + OC_{admin} + OC_{main\text{-}mater} + OC_{makeup}$

$+ OC_{marketing} - OC_{credit}$

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

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

7 CLAUS PLANT MODEL

7.1 Nomenclature

AC	Annual cost (M$/yr)
C_{idx}	Chemical Engineering Plant cost index for current year
$C_{idx,\#}$	Chemical Engineering Plant cost index for year #
C_f	Capacity factor (fraction)
DC	Direct capital cost (M$)
EC	Electric power consumption (kW)
ICF	Indirect charge factor (fraction)
$\dot{m}_{\#,j}$	Molar flow rate of component j at point # (lb-mole/hr)
$\dot{M}_{\#,j}$	Mass flow rate of component j at point # (tons/hr)
P	Price ($/ton)
TDC	Direct capital cost (M$)
TCC	Total capital cost (M$/yr)
η	Efficiency (fraction)

Subcategories for Inlet Gas Components

CH_4	Methane
CO_2	Carbon dioxide
COS	
H_2	Hydrogen
H_2O	Moisture
H_2S	Hydrogen Sulfide
S_2	Sulfur
SO_2	Sulfur dioxide

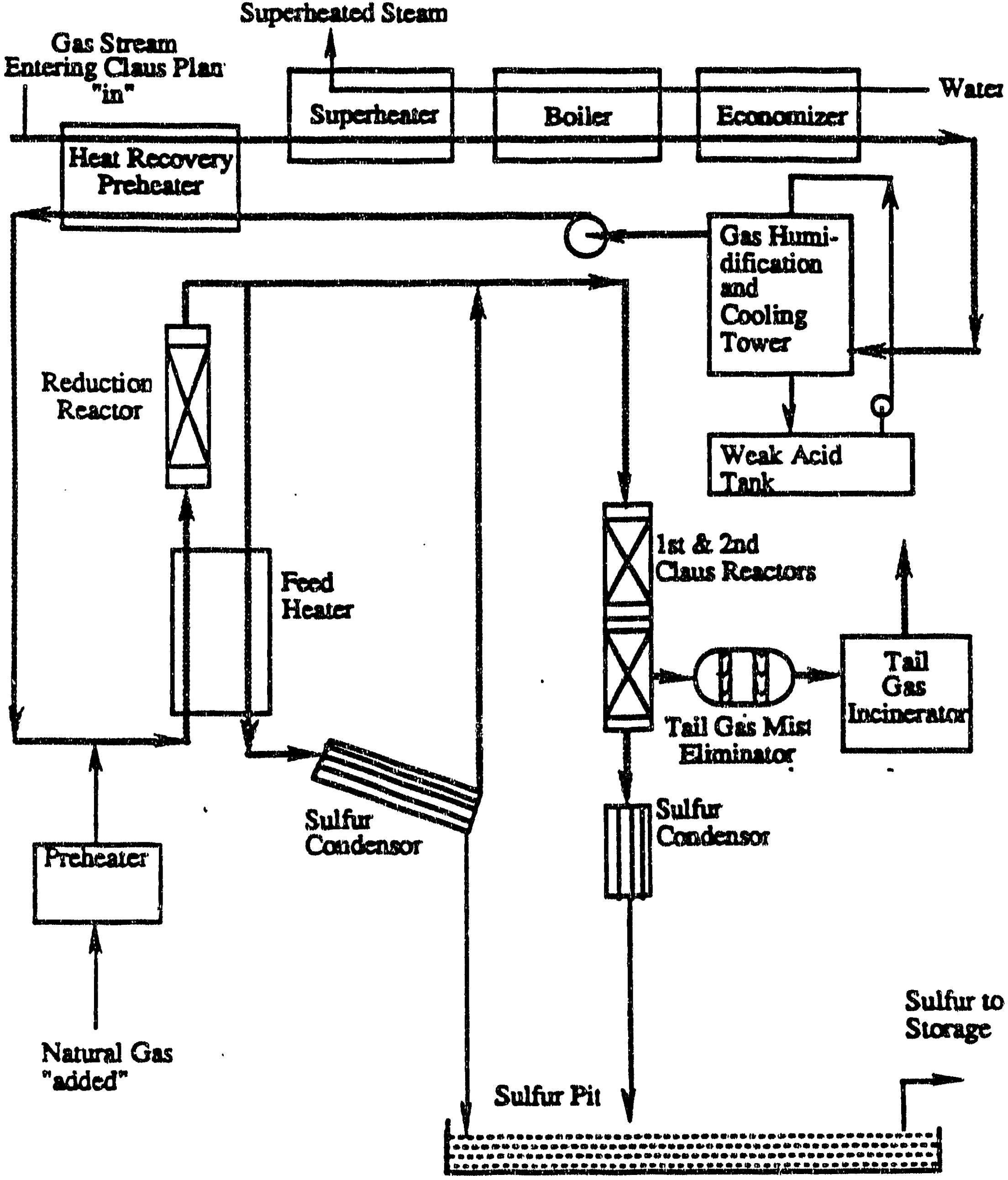
General Subcategories

added	Added to inlet gas stream
claus	Claus reduction system
credit	Credit
in	Entering Claus plant
pret	Inlet gas pretreatment system
S	sulfur

7.2 Introduction

This chapter describes a Claus sulfur plant model originally developed by Frey (30). The purpose of the Claus sulfur plant is to convert the off-gas from the regenerators in the copper oxide and NOXSO processes into elemental sulfur (as an alternative to sulfuric acid recovery). The original IECM treated the sulfur recovery system in a somewhat simple fashion, consistent with available studies then. The more detailed Claus sulfur plant performance and economic models now developed were based on a design by Allied Chemical Corporation documented by Ratafia-Brown (32). The performance and cost information for this design was developed by Allied Chemical for a specified gas composition, temperature, pressure and flow rate. The Allied Chemical design had a conversion efficiency of 95% and was based on an inlet gas composition which consisted of CH_4, CO_2, H_2O and SO_2. The current model has been modified to accommodate additional inlet gases: COS, H_2, H_2S and S_2. These additional gases change the process methane requirement. A schematic diagram of the Claus sulfur plant is shown in Figure 7-1.

Figure 7-1: Schematic Diagram of Claus Sulfur Plant



7.3 Performance Model

A standard Claus plant usually processes a gas stream containing hydrogen sulfide, a portion of which is combusted to form sulfur dioxide. The hydrogen sulfide and sulfur dioxide are converted to elemental sulfur via the Claus reaction.

$$2H_2S + SO_2 \longrightarrow 3S + 2H_2O$$

However, if the inlet gas does not contain hydrogen sulfide a portion of the SO_2 in the inlet gas must be reduced with natural gas to produce the required quantity of hydrogen sulfide. This is accomplished via the following reaction:

$$2CH_4 + 3SO_2 \dashrightarrow S + 2H_2S + 2CO_2 + 2H_2O$$

Thus, some elemental sulfur is obtained via the reducing reaction, while the remainder is obtained via the Claus reaction. The overall reaction is:

$$CH_4 + 2SO_2 \dashrightarrow 2S + 2H_2O + CO_2$$

Thus, the required molar flow rate of methane is one-half the molar flow rate of sulfur dioxide in the inlet gas. Since the inlet gas may contain COS, H_2 and H_2S, the methane requirement is modified to account for the effects of these chemical compounds. Any H_2 is assumed to react with SO_2 to produce H_2S and H_2O as shown in Equation (7.1). The COS content of the inlet gas is very small and it is assumed that sufficient water is available to convert COS into CO_2 and H_2S as shown in Equation (7.2).

$$3H_2 + 3SO_2 \dashrightarrow H_2S + 2SO_2 + 2H_2O \tag{7.1}$$

$$COS + H_2O \dashrightarrow CO_2 + H_2S \tag{7.2}$$

The methane requirement is based on a molar balance and the requirement that 2 moles of hydrogen sulfide are needed for each mole of sulfur dioxide entering the Claus reactor. The derivation of the methane requirement is shown below. In Equation (7.3), the a, b, c, d, e and f are the number of moles of SO_2, CH_4, H_2S, COS and H_2 and x represents the additional methane that must be added to the inlet gas.

$$aSO_2 + (b+x)CH_4 + cH_2S + dCOS + dH_2O + eH_2 \dashrightarrow \tag{7.3}$$

$$(b+x+d)CO_2 + (c+b+x+d+e/3)H_2S + (b+x+2/3e)H_2O + 0.5(b+x)S + (a-s.5(b+x)-e/3)SO_2$$

want the molar ratio of H_2S to SO_2 equal 2.

$$\frac{H_2S}{SO_2} = \frac{c+b+x+d+e/3}{a-1.5(b+x)-3/e} = 2$$

solving for x yields

$$x = 0.5a - b - 0.25c - 0.25d - 0.25e$$

or expressing the methane requirement with the symbols list in Figure 7-1.

$$\dot{m}_{added,CH_4} = 0.5\dot{m}_{in,SO_2} - \dot{m}_{in,CH_4} - 0.25\dot{m}_{in,H_2S} - 0.25\dot{m}_{in,COS} - 0.25\dot{m}_{in,H_2}$$

The Allied Chemical sulfur recovery plant design includes a reduction stage using two packed-bed, cyclic heat exchangers and a catalyst packed reactor. The gas stream then flows through a two-stage Claus plant, where sulfur is recovered for byproduct sale. Allied recommended that the inlet gas have a very low water content prior to treatment in the sulfur recovery plant. Therefore, gas cooling and water removal prior to the sulfur recovery plant is assumed in the design reported by Ratafia-Brown. This pretreatment system removes 91.2% of the moisture in the inlet gas.

Most of the electricity is consumed in an inlet gas compressor and air blowers. The electric power consumption is assumed to be proportional to the inlet molar flow rate. The constant of proportionality for the electric power consumption is determined by dividing the power consumption, 0.104 kW, by the inlet gas molar flow rate, 1063 mole/hr, reported in Reference (32). The electricity consumption is determined with

$$EC = \frac{0.104}{1{,}063} \sum_{j=1}^{8} \dot{m}_{in,j}$$

The amount of sulfur recovered by the process is estimated based on the total inlet sulfur compounds and the sulfur recovery efficiency of the byproduct plant. This efficiency is approximately 95 percent, so the total mass flow rate of byproduct sulfur is

$$\dot{M}_S = (\dot{m}_{in,SO_2} + \dot{m}_{in,H_2S} + \dot{m}_{in,COS} + 2\dot{m}_{in,S_2})\,\eta_S \,\frac{32.06}{2000}$$

7.4 Economic Model

The cost of the sulfur recovery system is estimated based on the direct cost of the sulfur plant gas pretreatment equipment and the Allied Chemical SO_2 Reduction and Claus plant system. The cost of the pretreatment section is based on an "exponential scaling rule" with the inlet gas flow rate as the predictive parameter. The cost of Claus plants has been shown to scale with mass flow rates using an exponent of approximately 0.7 in other studies. In Reference (32), the direct capital cost of pretreatment was reported to be \$903,000 in 1984 and the total inlet flow rate was 1,063 moles/hr. The direct capital cost of pretreatment is determined with

$$DC_{pret} = 0.903\left(\sum_{j=1}^{8} \frac{\dot{m}_{in,j}}{1{,}063}\right)^{0.7} \frac{C_{idx,\#}}{C_{idx,1984}}$$

The cost of the Allied Chemical SO_2 Reduction and Claus plant system is scaled to the inlet flow of gas to the reduction unit of the plant after gas treating. In Reference (32), the direct capital cost of the reduction system was reported to be \$9,500,000 in 1984 and the inlet flow rate was 637 moles/hr. The direct capital cost of the reduction system is determined with

$$DC_{claus} = 9.53\left(\sum_{j=1}^{8} \frac{\dot{m}_{in,j} - 0.918\dot{m}_{in,H_2O}}{637}\right)^{0.7} \frac{C_{idx,\#}}{C_{idx,1984}}$$

The total direct cost is the sum of the above direct costs discussed. The total capital cost is the sum of the total direct cost and the indirect costs. The indirect costs include general facilities, engineering and home office fees and project and process contingency and are expressed as a fraction of the total direct cost.

$$TDC = DC + DC$$

$$TCC = TDC\,(1 + ICF)$$

The annual costs of the sulfur recovery plant include methane and power consumption and sulfur by-product credit. The annual costs for methane and power consumption are accounted for in either the copper oxide or NOXSO process. The credit from the sale of the by-product sulfur is:

$$AC_{S,credit} = 8766\text{x}10^{-6}\, C_f\, P_S\, \dot{M}_S$$

The model does not include costs for catalyst replacement. A typical annual replacement cost is only a few thousand dollars, negligible compared to the annual totals. However, the initial catalyst charge is included in the capital costs.

8 FROTH FLOTATION PROCESS MODEL

8.1 Nomenclature

A = Ash content coal (fraction)
AC = Annual operating cost (78\$/dry ton of clean coal)
c_k = Chemical cost for k^{th} level plant (78\$/dry ton of cleaned coal)
CS = Concentration of solids (fraction)
DC = Direct capital cost (78\$)
DCC = Cost coefficient for cleaning equipment (78\$/dry ton of raw coal)
e_k = Electricity cost for k^{th} level plant (78\$/dry ton of cleaned coal)
E_d = Energy needed for thermal drier (Btu/lb of dry coal)
f = Weight fraction of coal (fraction)
HHV = Average higher heating value of coal (Btu/lb)
K_{specie} = Rate constant of specie (min^{-1})
l_k = Labor cost for k^{th} level plant (78\$/dry ton of cleaned coal)
LHV = Lower heating value of coal (Btu/lb)
m' = Total moisture content of coal (fraction)
mi' = Inherent moisture content of coal (fraction)
ms' = Surface moisture content of coal (fraction)
m = Dry mass flow rate of coal (tons/hr)
MIBC = MIBC consumption of froth flotation circuit (lb/raw dry ton)
O = #2 fuel oil consumption of froth flotation circuit (lb/raw dry ton)
r_{specie} = Recovery of species (fraction)
R_{specie} = Ultimate recovery constant of species (fraction)
S = Sulfur content of coal (fraction)
T = Residence time of flotation vessels (minutes)
v = Volume of flotation cells (ft^3)
V_{ef} = Effective volume of flotation equipment (fraction)
w' = Weight of water evaporated in thermal drier per pound of dry coal processed (fraction)
w'_e = Weight of water evaporated in thermal drier (tons/hr)
w_k = Water cost for k^{th} level plant (78\$/dry ton of cleaned coal)
Y_d = Mass yield of the thermal drier (fraction)
Y_p = Mass yield of coal cleaning plant excluding the thermal drier yield (fraction)
Y_t = Mass yield of the entire coal cleaning plant (fraction)
Yo_d = Ratio of coal mass exiting wash streams to coal mass exiting plant (fraction)

Greek Letter Symbols

ε = Efficiency of thermal drier (fraction)
δ_i = Equals 0 if wash stream i is not thermally dried and 1 if it is thermally dried.
ρ_c = density of coal (lb/ft^3)
ρ_w = density of water (lb/ft^3)

Subscripts:

c = clean coal exiting wash streams
d = thermal drier
i = (1) coarse, (2) medium or (3) fine streams
in = entering thermal drier
j = oil or MIBC

k = level of plant (2,3,4 or 5)
l = clean, thermal, raw, refuse, sample
o = clean coal exiting plant
out = exiting thermal drier
ref = refuse coal
ROM = raw coal

species:
a = ash
afc = ash-free coal
s = sulfur content

8.2 Introduction

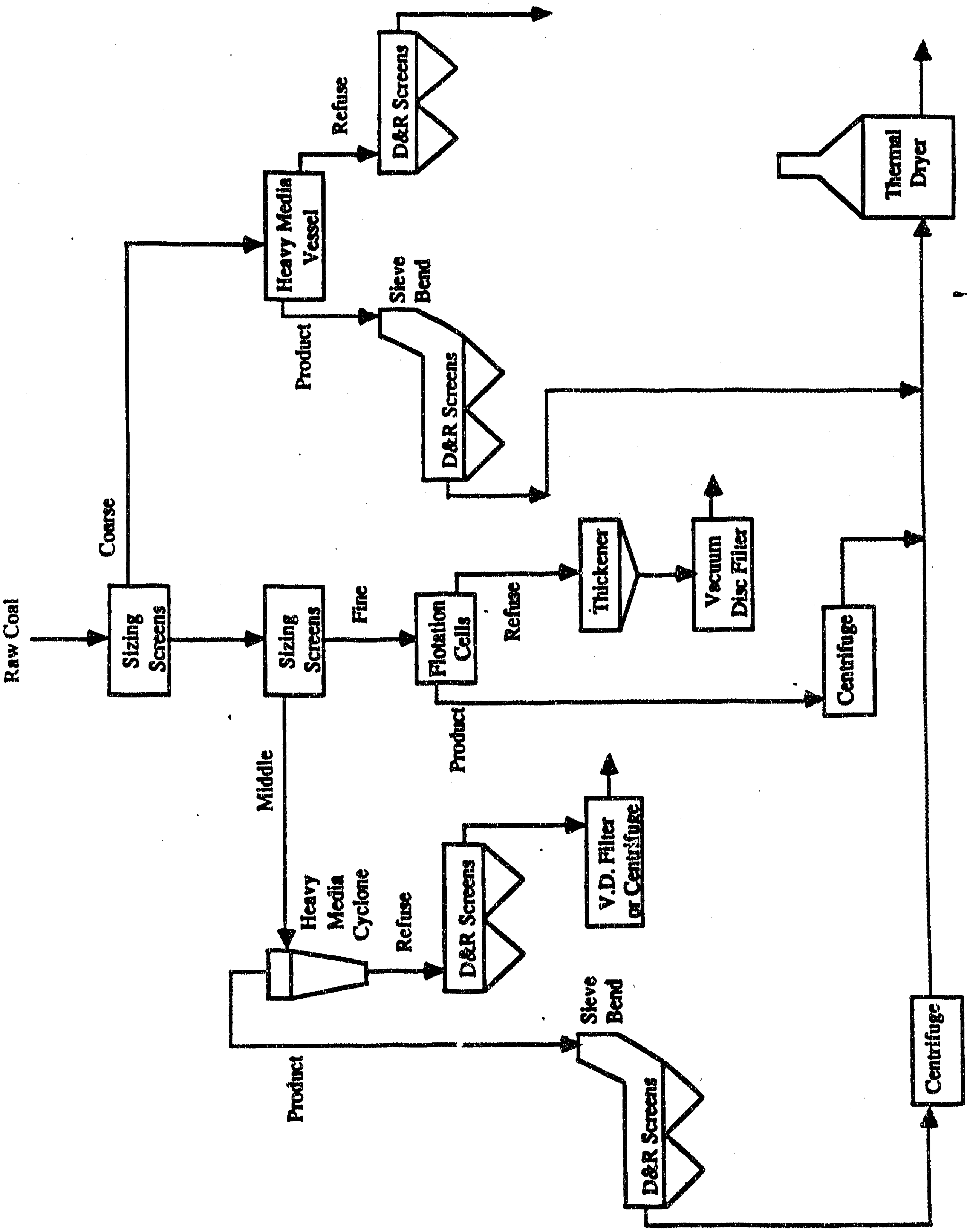
This chapter describes the addition of a conventional froth flotation circuit into the coal cleaning module of the IECM. The purpose of this modification is to include froth flotation as an option to clean the fine coal stream. The original model (1) has three beneficiation levels (2, 3 and 4) in which different streams are washed by specific gravity equipment. Level 2 washes only the coarse stream. Level 3 washes the coarse and medium streams. Level 4 washes the coarse, medium and fine streams. The new modification adds a fifth level, which uses specific gravity equipment to wash the coarse and medium streams and froth flotation equipment for the fine stream. The specific size fractions in each stream are specified by the model user. As before, the model optimizes the yield of each circuit To achieve a target coal quality for the cleaned coal product.

8.3 Process Description

This section only briefly describes froth flotation of coal. For a more detailed descriptions of the froth flotation process see References (37-41). Most coal cleaning processes use the difference between the specific gravity of coal, ash and pyrite to separate the coal from the ash and pyrite (40). Froth flotation, however, uses the difference between the adhesion of small air bubbles to coal, ash and pyrite to achieve separation. Usually small air bubbles are passed through a fine coal slurry stream. Air attaches itself to coal and floats to the surface, where it is removed. Since the air does not attach itself to the ash it remains in the slurry and is carried off. Particles which stick to air bubbles are called hydrophobic, while those which are easily wetted are called hydrophilic.

Coal is inherently hydrophobic, but the degree of floatability depends on several parameters, including particle size, pulp density, coal rank, extent of oxidation, quantity and type of chemicals used, slurry pH, aeration and agitation, retention time. Three theories which broadly try to predict the floatability of coal are the carbon-hydrogen ratio theory, the carbon content theory and the surface-components theory. All three theories have advantages and disadvantages in predicting the floatability of coal. Yet, none of the theories predicts the quality and yield of coal for a specific set of flotation parameters. Although they are not applicable for this model, they can be used to estimate the performance of a new coal from existing floatability data.

Figure 8-1: Coal Cleaning Plant with Froth Flotation of Fine Stream



Usually chemicals, called frothers, are added to the coal slurry to prolong the life of the air bubbles, which enhances the stability of the froth. MIBC (methyl isobutyl carbinol) is a common frother used for coal froth flotation. Collectors increase the adhesion of air to coal and are needed for highly oxidized or lower rank coals. A common collector used for froth flotation of coal is fuel oil. Other chemicals can be added which perform a variety of functions. The most common are depressing agents, activating agents, pH regulators, dispersing agents and protective colloids.

Figure 8-1 shows the a process diagram for a conventional coal cleaning plant with froth flotation for the fine size stream. Although it is widely used, the process is not understood as well as specific gravity based beneficiation. Because less is known about froth flotation, it is difficult to predict full scale performance from laboratory batch data. Although there are algorithms for scaling up laboratory data (42), they have not been implemented in this model until they can be further evaluated. It is also generally accepted that flotation washability data cannot be predicted from specific gravity washability data (43, 44).

8.4 Froth Flotation Performance Model

A complete description of the conventional coal cleaning model is found in Reference (1). This report only discusses the improvements that have been added. The model uses a Lagrange multiplier technique to maximize the yield (mass or energy) for a given coal and plant configuration. The algorithm needs discrete data points of the yield and coal quality at different specific gravities for three wash streams (coarse, medium, fine). For froth flotation of the finesize stream, the user can specify washability data in one of three different ways:

- Actual yield and quality data at different residence times
- Rate and ultimate recovery constants for ash-free yield, ash and sulfur content
- Mass yield and coal quality of the cleaned coal for the flotation circuit

For all three options the following information is also needed:

- The quantity of MIBC and #2 fuel oil,
- Inlet slurry concentration
- Effective volume of the cells

For option one, the froth flotation data is substituted for the conventional fine stream data and the model optimizes the yield for all three streams as usual. Data in this form can be found in Reference 9. But, this is batch data and has not been scaled to full size. The only difference is that the residence time is determined instead of a specific gravity for the fine stream. The only restriction currently is that the number of coal quality data points for froth flotation must equal the number of specific gravity data points.

For the second option, the rate and ultimate recovery constants are used in the Klimpel model (Equation 8.1) to predict the recovery of ash-free coal, ash and sulfur at different residences times (42, 43):

$$r_i = R_i\left[1 - \frac{1}{K_i T}\left(1 - e^{-K_i T}\right)\right] \tag{8.1}$$

The total mass yield is equal to the sum of the ash-free coal and ash recovered (Equation 8.2). The ash content of the cleaned coal is equal to the recovery of ash times the raw coal ash content divided by the mass yield (Equation 8.3). The sulfur content of the cleaned coal is determined similarly (Equation 8.4). The higher heating value is estimated by Equation 8.5.

$$Y_{p,3} = (1 - A_{ROM})\, r_{afc} + A_{ROM} r_a \tag{8.2}$$

$$A_{o,3} = \frac{A_{ROM} r_a}{Y_{p,3}} \tag{8.3}$$

$$S_{o,3} = \frac{S_{ROM} r_s}{Y_{p,3}} \tag{8.4}$$

$$HHV_{o,3} = HHV_{ROM} \left(\frac{1 - A_{o,3}}{1 - A_{ROM}} \right) \tag{8.5}$$

The coal yield and quality in the froth circuit at different residence intervals can be determined with Equations 8.2 - 8.5. The residence times intervals are determined by specifying a maximum residence time and dividing by the number of specific gravity data points.[19] This data is then substituted into the fine size washability data and the model proceeds as usual.

For the third option, the yield and quality of the froth flotation circuit is specified at a given residence time. This data is passed into the optimization algorithm, where the model optimizes the mass yields of the coarse and medium streams to achieve the overall target coal quality.

For all three options, once the residence time is determined the total volume of the cells can be determined from Equation 8.6:

$$v = m_{ROM}\; f_{ROM,3}\; T \frac{2000 \text{ lb/ton}}{60 \text{ min/hr}} \left[\frac{1}{r_c} + \left(\frac{1}{CS} - 1 \right) \frac{1}{r_w} \right] \frac{1}{V_{ef}} \tag{8.6}$$

The densities of water and coal are assumed to be 84 and 62 lb/ft^3, respectively. The effective volume, V_{ef}, is used to account for the volume occupied by the air-ingestion equipment and air bubbles.

8.5 Process Economics

The general coal cleaning plant economic model is based on several studies (45-50) and is described in Reference (1). All cost are computed in 1978 dollars then escalated to a current year using a plant cost index. The same method is used to estimate the cost of the new level five plant

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[19] This will be changed to the maximum number of data points possible in the next version of the model.

with froth flotation. The capital cost is divided into five different sections: (1) raw coal handling, (2) cleaning equipment, (3) thermal drying, (4) refuse handling and (5) coal sampling system. The direct capital cost of each section other than the coal sampling system is related to its characteristic mass flow and is assumed to have an economy of scale of 0.7 for plant sizes in the range of 500 to 2000 clean tons per hour (tph) (46). Only the cost of the cleaning equipment section is assumed to vary with different levels of coal cleaning. The capital cost related to clean coal handling (which includes the cost of conveyors, storage and loading equipment) is included in the raw coal handling cost since the cleaning plant is assumed to be at the mine site. It is assumed that the cost of the coal sampling system does not vary with plant capacity.

The economics of froth flotation depend on the residence time, chemical usage and process yield. The direct capital for the cleaning equipment for a level 5 plant is estimated by Equation 8.7:

$$DC_{clean} = DCC_5 \, m_{ROM}^{0.7} + 6780 \, v^{0.4} \tag{8.7}$$

where $DCC_5 = 43{,}700$

The first term of Equation 8.7 is the capital cost of the cleaning equipment excluding the flotation cells. The second term is the capital cost of the flotation cells. The value for the first term was obtained from Reference (46). It represents the average cost of cleaning equipment excluding the flotation cells scaled to the raw coal mass flow rate. The direct capital cost for the froth flotation equipment is scaled to the total volume of the vessels (46, 47). An exponential scaling factor of 0.4 is used as the best fit to available data (46, 47).

The indirect and annualized capital costs are calculated as shown in Reference (1). The operating and maintenance costs of a level five plant are calculated similarly to the other levels. The cost factors for labor, maintenance, refuse and taxes are the same as a level four plant (46). The cost factor for chemicals (excluding oil and MIBC), electricity and water are, respectively, 0.064, 0.15 and 0.0015 in 1978$/ton of raw coal (45). The amounts of MIBC and #2 fuel oil used are input parameters in the model. Therefore, the cost per ton of cleaned coal is estimated by the following equations:

$$AC_{oil} = \frac{0.072 \, O \, f_{ROM,3}}{Y_t}$$

$$AC_{MIBC} = \frac{0.60 \, MIBC \, f_{ROM,3}}{Y_t}$$

9 SELECTIVE AGGLOMERATION PROCESS MODEL

9.1 Nomenclature

English Symbols

A_{clean}	Ash content of the clean coal going to thermal drier (fraction)
A_r	Ash content of the raw coal input (fraction)
A_{ref}	Ash content of the refuse coal (fraction)
AC_{elect}	Annual cost of electricity ($ / dry ton of cleaned coal)
AC_{labor}	Annual cost of labor ($ / dry ton of cleaned coal)
AC_{agg}	Annual cost of agglomerant ($ / dry ton of cleaned coal)
AC_{maint}	Annual cost of maintenance ($ / dry ton of cleaned coal)
AC_{payovh}	Annual cost of payroll overheads ($ / dry ton of cleaned coal)
AC_{plovh}	Annual cost of plant overheads ($ / dry ton of cleaned coal)
AC_{tax}	Annual cost of taxes, insurance, etc ($ / dry ton of cleaned coal)
AC_{waste}	Annual cost of waste disposal ($ / dry ton of cleaned coal)
AC_{water}	Annual cost of water ($ / dry ton of cleaned coal)
c	Cost of agglomerant used ($/lb agglomerant)
C_{idx}	Chemical engineering cost index
$C_{idx, 1984}$	Chemical engineering cost index for 1984 for current year
C_{sol}	Degree of agglomerant solubility in water (fraction)
$C_{capital}$	Total capital cost ($ /dry ton of cleaned coal)
$C_{operating}$	Total operating cost ($ /dry ton of cleaned coal)
C_r	Cost of raw coal ($ /dry ton of raw coal)
C_{ref}	Cost of refuse coal ($ /dry ton of cleaned coal)
C_{total}	Total cost of clean coal ($ /dry ton of cleaned coal)
CRF	Capital Recovery factor (dimensionless)
d	Real discount rate for capital cost (fraction)
DC	Direct capital cost ($)
$DC_{aggequip}$	Direct capital cost of the selective agglomeration plant equipment ($)
DC_{aggrec}	Direct capital cost of agglomerant recovery equipment ($)
DC_r	Direct capital cost of the refuse handling ($)
DC_{ref}	Direct capital cost of the refuse handling ($)
$DC_{thermal}$	Direct capital cost of thermal drying system ($)
e	Cost of electricity ($/dry ton of raw coal)
E_{drier}	Energy needed for thermal drier (Btu)
h	Annual operating hours of coal cleaning plant (hrs/yr)
HHV_r	Higher heating value of raw coal (Btu/lb dry coal)
HHV_{clean}	Higher heating value of raw coal (Btu/lb dry coal)
i	Nominal interest rate (fraction)
l	Labor cost ($/hr)
LHV	Lower heating value of cleaned coal (Btu/lb dry coal)
m_{dry}	Dry mass flow rate of clean coal entering the thermal drier (tons/hr)
$m_{evapwater}$	Mass flow rate of water evaporated in thermal drier (tons/hr)
$m_{evapwater}'$	Weight of water evaporated in thermal drier per pound of clean coal (fraction)
m_{inmois}'	Moisture content of clean coal entering thermal drier (fraction)
$m_{aggclean}$	Mass flow rate of agglomerant entering the evaporator system (tons/hr)
$m_{agglosttoatmtot}$	Mass flow rate of total agglomerant lost to the atmosphere (tons/hr)
$m_{agglosttowater}$	Mass flow rate of agglomerant lost to water (tons/hr)

$m_{agglosttosolid}$	Mass flow rate of agglomerant lost to solid(tons/hr)
m_{aggnew}	Mass flow rate of new agglomerant (tons/hr)
m_{aggrec}	Mass flow rate of recovered agglomerant (tons/hr)
$m_{aggtotal}$	Mass flow rate of recovered agglomerant mixed with raw coal (tons/hr)
m_o	Dry mass flow rate of clean coal leaving the plant (tons/hr)
$m_{outmois}'$	Moisture content of clean coal leaving thermal drier (fraction)
m_r	Dry mass flow rate of raw coal input (tons/hr)
m_{ref}	Dry mass flow rate of refused coal (tons/hr)
m_{steam}	Total mass flow rate of steam required for stripping system (tons/hr)
m_{water}	Total mass flow rate of cooling water required for stripping system (tons/hr)
m_t	Cost of maintenance (fraction)
n	Life of coal cleaning plant (years)
p	Inflation rate (fraction)
PS_{clean}	Pyritic sulfur in the clean coal removed from the raw input (%)
r	Cost of refuse coal disposal ($/wet ton)
R	Ratio of dry mass agglomerant to dry mass of raw coal (dimensionless)
s	Cost of steam ($/1000 tons)
t	Annual rate of taxes and insurance costs for plant (fraction)
TCC	Total capital cost ($)
TDC	Total direct capital cost
w	Cost of water ($/1000 tons)
W	Water loss in the process (tons/hr)
W_c	Working capital ($/dry of clean coal)
Y_{clean}	Mass yield of clean coal going to the thermal drier (fraction)
Y_{drier}	Thermal drier mass yield (fraction)
Y_{total}	Mass yield of entire coal cleaning plant (fraction)

Greek letter symbols

ε	Efficiency of thermal drier (fraction)

9.2 Introduction

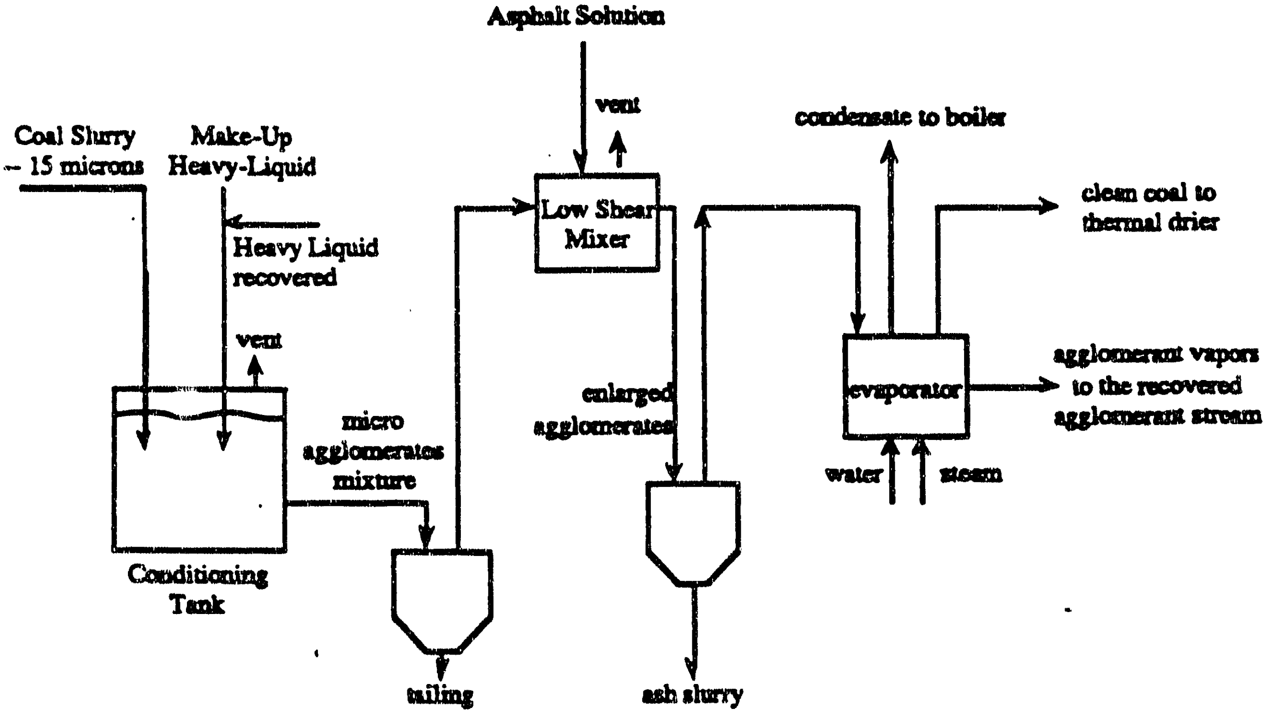
This chapter presents new performance and economic models simulating the operation of a coal beneficiation plant using the selective agglomeration process. The primary function of this model is to estimate the cost and ability of the process to remove the pyritic sulfur and ash to help meet power plant emission standards. This section presents a brief overview of the selective agglomeration process, a description of the economic algorithms and an assessment of this process' ability to reduce sulfur dioxide emissions of coal fired power plants. Performance models are based on bench-scale tests on a one ton per hour (tph) Proof-of-Concept (POC) unit performed by Bechtel for the U.S Department of Energy, Pittsburgh Energy Technology Center under Contract No. DE-AC-22-84PC79867 (51). An assessment of capital investment and operating costs for a selective agglomeration process with plant size of 300 tph proposed by Burns and Roe Services Corporation is adopted in developing the economic model (52).

In selective coalescence (also known as selective agglomeration), an agglomerating liquid such as chlorofluorocarbons (e.g., Freon 113) or hydrocarbons (e.g., n-pentane and n-heptane) is contacted with an agitated, aqueous suspension of the feed coal. The coal particles agglomerate into a large floc in the non-aqueous phase. The mineral matter particles which remain dispersed in the aqueous phase are then separated by screening the flocs.

9.3 Process Description

A conceptual flow scheme for a selective agglomeration process is shown in Figure 9-1. This design is adopted from the Bechtel 1tph proof of concept selective agglomeration process and forms the basis for the economic model discussed below. The coal feed capacity of this design is 300 tons per hour. The process comprises three steps: raw coal particle size reduction near 15 microns, agglomeration and separation of the product coal from mineral matter which remains dispersed in the aqueous phase and recovery of the agglomerating agent for recycling in the process.

Figure 9-1: Schematic Diagram of Selective Agglomeration Process



9.3.1 Grinding Operation

The first step includes the grinding operation where the feed is ground to an extremely fine size to render most of the coal and the impurities (and pyritic minerals) into discrete particles. Unlike heavy liquid cyclones, the selective agglomeration process can treat coal-water slurries. Therefore, pre-drying of the coal is not necessary. In grinding the raw coal particles to 15 microns, a stirred ball mill also can be used.

Grinding is an important step since, depending on the method of grinding, the surface properties of pyrites will change. This will have very important implications on the sulfur removal potential of the process.

9.3.2 Agglomeration and Separation

In the second step, slurry is intensely mixed with a hydrocarbon bridging agent (agglomerant) for example normal heptane or normal pentane. Under these conditions the agglomerant selectively wets and agglomerates the coal under high shear for 1 to 4 minutes. The coal forms small spherical agglomerates, while the mineral matter remains dispersed in the aqueous phase and thus is rejected as tailings. The agglomerates approximately 50-100 mesh size are grown to larger sizes by adding a solution to the binder material, typically asphalt dissolved in agglomerant. Mixing is continued under less severe conditions to allow the agglomerates to grow 2-3 mm in size. The ash-laden water is then drained or screened from the agglomerates. The agglomerant is then recovered for reuse by steam stripping. The residual asphalt serves to maintain the physical stability of the agglomerates, easing their dewatering, storage and handling.

The second step process could be operated under a slight negative pressure or the process equipment could be vented to a vapor collection system.

Table 9-1: Properties of n-heptane and n-pentane (52)

Liquid	Boiling Point, ^{o}C	Density gm/cm3	Heat of Vaporization cal/gm	Viscosity cp
n-heptane (C_7H_{16})	98.4	0.684	76.5	0.40
n-pentane (C_5H_{12})	36.1	0.626	91.6	0.21

Table 9-1 compares the properties of n-heptane and n-pentane. Compared to n-heptane, n-pentane is a highly volatile liquid. It has a low boiling point (36.1C or 97F) and high vapor pressure (at 30C, 670mm Hg). n-pentane is highly flammable. The lower and upper limits of flammability for n-pentane in air are 1.40 and 7.80 percentage (by volume) respectively. The design of the plant controls excessive n-pentane losses due to vaporization.

The limit for human exposure to n-pentane contaminated air is 500 ppm (52). To avoid human exposure to n-pentane, the equipment in the system should be air tight, the piping should be leak proof.

The n-pentane based plant required a refrigeration system to provide cooling water during hot weather (ambient greater than 25C or 77F). No such refrigeration system was required for n-heptane (boiling point 98.4C) based plant (52). The only difference between n-pentane and n-heptane based plants was the absence of a refrigeration system in the n-pentane based plant.

9.3.3 Solvent Recovery and Refuse Thickening

The product coal-agglomerant-water mixture is fed to an evaporator, where almost all the agglomerant is evaporated. The agglomerant vapors are cooled in a heat exchanger. Vapors that are not condensed are compressed by a compressor. The resulting liquid is circulated to the conditioning tank. The product coal may retain as little as 50 to 100 ppm of the agglomerant.

The product coal can be obtained as a somewhat dry product containing 10% moisture or as a pulp containing 40% water. This will depend on the type of evaporator used to vaporize the agglomerant.

The mineral matter-water slurry contains very small amount of agglomerant (50 to 100 ppm). This slurry is thickened in a static thickener and the clarified water is recirculated to the circuit and the refuse is sent to the refuse disposal circuit.

9.4 Performance Model

The selective agglomeration process was evaluated by Bechtel for three coals. They are Pittsburgh No.8, Illinois No.6 and Upper Freeport seams. The average ROM coal characteristics for these coals are shown in Table 9-2. Using Bechtel's 1tph POC, the average clean coal performance for coal plants of 300 tph (dry) coal feed is estimated and shown in Table 9-2.

It was not possible to develop a generalized algorithm which would determine the quality and yield of the clean coal based on the experimental data. Therefore, the model uses experimental data of the cleaned coals quality (i.e. ash and sulfur content) and mass yield directly to determine the cost of the cleaned coal. The input parameters for the performance and economic models are:

- Ash, sulfur, inherent moisture and surface moisture contents of raw coal
- Higher heating value of raw coal
- Ash, sulfur, surface moisture of cleaned coal
- Mass yield of process
- Moisture content entering thermal drier
- Mass ratio of agglomerant to dry raw coal
- Solubility of agglomerant in water
- Efficiency of thermal drier
- Cost of agglomerant in dollars per ton

As noted above, the basic performance parameters characterizing the change in coal quality are determined from experimental data for a particular coal. Because data for the selective agglomeration process are currently limited, only three coals are represented here.

If the higher heating value of the clean coal is not provided then the following algorithm is used

$$HHV_{clean} = (HHV)_r\,[1-A_{clean}]/[1-A_{raw}]$$

Estimates of plant operating and capital costs typically are scaled to various mass flow rates within the coal cleaning plant. Those developed below are the rate of raw coal and agglomerant into the plant, the rate of dry and wet refuse coal out of the plant, the rate of agglomerant recovered and lost from the plant, the rate steam and water required for stripping the agglomerant and the rate of water evaporated in the thermal drier. The process flow scheme with respective mass flows shown in Figure 9-2.

Table 9-2: Feed Coal and Clean Coal Quality(1)

Performance Parameter	Pittsburgh No.8	Illinois No.6	Upper Freeport
ROM coal Quality			
Ash %	39.16	15.71	57.31
Sulfur %	4.71	4.54	2.11
Pyritic sulfur %	3.39	2.46	1.93
Organic sulfur %	1.24	2.03	0.16
Sulfate sulfur, %	0.08	0.05	0.03
Heating Value (Btu/lb)	8,528	11,837	5,947
Performance (ROM basis)*			
% Yield	56.5	72.5	39.5
% Ash removal	93.3	81.1	94.6
% Ash reduction	92.8	77.6	94.3
% Sulfur removal	59.5	51.3	70.4
% SO_2 reduction	56.9	42.3	68.9
% Pyritic sulfur removal	82.3	79.1	82.6
% Pyritic sulfur reduction	79.0	78.1	75.3
% Btu Recovery	92.2	84.8	91.3

* The calculations on a ROM basis for ash reduction, sulfur dioxide reduction, pyritic sulfur reduction are based on analytical values for ROM coal for the feed and those of clean coal agglomerates for the individual tests. The ROM basis energy (Btu) recovery is calculated as follows:

ROM basis Btu recovery, % = (Bench-scale test of Bechtel's 1tph POC, Btu recovery, %) x Btu recovery, % for precleaning operation, i.e prior to the Bechtel's 1tph POC bench scale test)

The amount of agglomerant dosage needed for this process is obtained from experiments. The ratio of mass of agglomerant to the dry mass of raw coal is denoted by R, or

$$R\, m_r = [\, m_{aggnew} + m_{aggrec}\,] = m_{aggtotal}$$

R = 1 to 2 or up are recommended for Pittsburgh No.8, Illinois No.6 and Upper Freeport (52).

The amount of steam and cooling water needed in coal stripping system is calculated by

$$m_{steam} = 0.127\, (\, m_{aggnew} + m_{aggrec}\,) = 0.127\, m_{aggtotal}$$

$$m_{water} = 6.061\, (\, m_{aggnew} + m_{aggrec}\,) = 6.061\, m_{aggtotal}$$

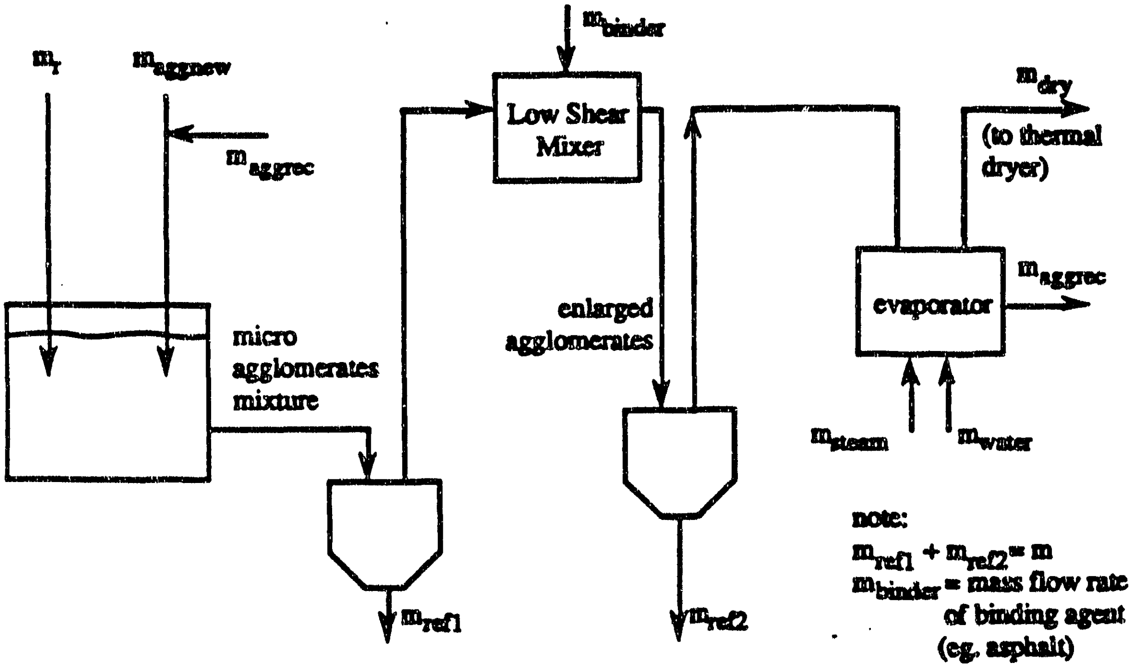
Details of the calculation can be found later in the numerical example section.

Not all the agglomerant will be recovered. Depending on the degree of solubility of agglomerant in water, some will be lost to the water. The amount of agglomerant that is lost to the water is estimated to be

$$m_{agglosttowater} = C_{sol} \times W$$

where W is the total water loss in the process.

Figure 9-2: Schematic Diagram of Selective Agglomeration Process with Flow Rates



note:
$m_{ref1} + m_{ref2} = m$
m_{binder} = mass flow rate of binding agent (eg. asphalt)

Besides the loss of agglomerant to the water in the stripping system, some agglomerant is also lost to the atmosphere. To find the agglomerant that is lost to the atmosphere, we have to consider all components of the subcircuits. The formula obtained is shown below:

$$m_{agglosttoatmtot} = 3 \times 10^{-4}\, m_r$$

The agglomerant is also lost with the solids. To find the agglomerant lost with the clean coal and the refuse, we have assumed the following formula:

$$m_{agglosttosolid} = 5 \times 10^{-4}\, m_r$$

Therefore, the new or makeup agglomerant is

$$m_{aggnew} = m_{agglosttowater} + m_{agglosttoatmtot} + m_{agglosttosolid}$$

Normally, it is necessary to thermally dry the fine sizes of coal-hot water slurry. It is assumed that product coal is used to fire the thermal drier, thus reducing the overall plant yield. It is also assumed that drying alters only the coal moisture content, with all the other coal properties (measured on a dry basis) remain the same. Since the moisture content of coal entering and leaving the thermal drier is specified, the weight of the water evaporated per pound of precleaned coal into the thermal drier is (1):

$$m_{evapwater}' = m_{inmois}' - m_{outmois}' / [\,(1 - m_{inmois}')\,(1 - m_{outmois}')\,]$$

The amount of energy needed to evaporate this water is

$$E_d = 1020\, m_{evapwater}' / \varepsilon$$

The lower heating value can be approximated by

$$LHV = 0.96\, HHV_{clean} - [\, 1020\, m_{outmois}' / (\, 1 - m_{outmois}'\,)\,]$$

Therefore, the drier yield and total plant yield are given by

$$Y_{drier} = 1 - E_d / LHV$$

and

$$Y_{total} = Y_{clean} Y_{drier}$$

The weight of water evaporated is

$$m_{evapwater} = m_{evapwater}' \, [\, m_{dry} / Y_{drier}\,]$$

Once the drier is determined, the dry mass flow rates for the raw coal stream, refuse stream and drier stream can be calculated by the following equations:

$$m_r = m_o / Y_{total}$$

$$m_{dry} = m_o / Y_{drier}$$

$$m_{ref} = m_r - m_{dry}$$

The water loss in the coal cleaning plant is

$$W = mdry\, [\, (\, 1 / (\, 1 - minmois'))\, -1] + mref\, [\, (\, 1 / RC\,) - 1\,]$$

9.5 Economic Model

The total cost in dollars per ton of dry cleaned coal can be divided into four separate costs categories.

- cost of raw coal
- cost of rejected coal
- annual operating and maintenance costs
- annualized capital costs

The cost of raw coal is an input parameter. The cost of the refuse coal is a function of the plant yield and can be calculated from

$$C_{ref} = C_r\, [(1/Y_{total}\,) - 1] \tag{9.1}$$

9.5.1 Capital Cost

The capital cost is divided into five different sections: raw coal handling, selective agglomeration process equipment, agglomerant handling, refuse handling and thermal driers. The capital costs related to clean coal storage is included in the raw coal cost, since the coal cleaning equipment is assumed to be at the mine site. This include the cost for conveyors, storage and loading equipment.The raw coal cost also includes the cost of grinding the ROM feed coal. The direct capital cost for refuse handling includes refuse sump and explosion proof pump. The direct capital cost is determined by these equations:

$$DC_r = \$\ 91{,}963\ m_r^{0.7} \text{ x } C_{idx} / C_{idx,1984} \tag{9.2}$$

$$DC_{aggequip} = \$10{,}521 m_r^{0.7} \text{ x } C_{idx} / C_{idx,1984} \tag{9.3}$$

$$DC_{aggrec} = \$\ 102{,}005\ m_r^{0.7} \text{ x } C_{idx}/C_{idx,\ 1984}$$

$$= \$\ 102{,}005 \text{ x } [\ (m_{aggnew} + m_{aggrec}\ ) / R\ ]^{0.7} \text{ x } C_{idx}/C_{idx,\ 1984}$$

$$= \$\ 102{,}005\ R^{-0.7}(m_{aggnew} + m_{aggrec}\ )^{0.7} \text{ x } C_{idx}/C_{idx,\ 1984} \tag{9.4}$$

$$DC_{ref} = \$19{,}100\ m_{ref}^{0.7} \text{ x } C_{idx}/C_{idx,\ 1984} \tag{9.5}$$

$$DC_{coalsampling} = \$324{,}000 \text{ x } C_{idx}/C_{idx,\ 1984} \tag{9.6}$$

$$DC_{drier} = \$153,\ 000\ m_{evapwater}^{0.7} \text{ x } C_{idx}/C_{idx,\ 1984} \tag{9.7}$$

The direct capital cost for the selective agglomeration subcircuit equipment covers the cost for the 18,000 gallon conditioning tank with a carbon steel agitator of 100 horsepower, explosion proof feed pump, 12,000 gallon high shear mixer with stainless steel agitator of 400 horsepower, enclosed sieve bend and a stainless steel horizontal-tube evaporator. The direct cost for agglomerant recovery subcircuit equipment consists of the costs for 12,000 and 500 gallon weathered carbon steel tanks, explosion proof pumps, adsorption tower, blower, sump and 8900 ton refrigeration system.

The total direct capital cost is found by adding Equation (9.2) through (9.7)

$$TDC = DC_r + DC_{aggequip} + DC_{aggrec} + DC_{ref} + DC_{drier} + DC_{coal\ sampling}$$

The indirect capital and contingencies costs are estimated to be 54% of the direct capital cost. Therefore, the total capital cost, which is depreciated over the life of the plant is

$$TCC = 1.54\ TDC$$

The total capital cost is annualized as follows:

$$d = [\ (\ 1 + i\ ) / (\ 1 + p\ ) - 1\ ]$$

Where i is the interest rate and p is the inflation rate. Therefore, capital recover factor is

$$CRF = d / [\ 1 - (\ 1 + d\ )^{-n}\ ]$$

Working capital is estimated to be 25% of the labor, maintenance, electricity, water, waste disposal and chemical(agglomerant) costs as in the conventional plant model described in Chapter 2.

$$W_c = 0.25\ (\ AC_{labor} + AC_{maint} + AC_{elect} + AC_{water} + AC_{waste} + AC_{agg}\ )$$

As in Chapter 2, the capital cost in ($ per dry ton of cleaned coal) is

$$C_{capital} = dW_c + [\ (\ TCC \text{ x } CRF\ ) / (\ m_o \text{ x } h\ )\ ] \tag{9.8}$$

9.5.2 Operating and Maintenance Cost

The annual operating and maintenance costs comprise several cost elements, including labor, maintenance, raw material and waste disposal costs, also taxes, insurance and general administrative overhead. The operating and maintenance cost is broken down into the components shown in Table 9-3. The total annual cost of agglomerant in \$/ton of clean coal is then estimated to be:

$$AC_{agg} = cm_{aggnew} / m_0$$

The cost of labor is estimated to be dependent of plant size. Maintenance costs, taxes and insurance are estimated to be proportional to the total capital cost of the plant. The cost of electricity is linked to the mass flow rate of the coal entering the plant, while the cost of waste disposal is proportional to the quantity of coal rejected. The cost for water is proportional to the amount of water in the clean coal and refuse streams. Overhead costs are based on labor, maintenance and agglomerant costs. The equations for these costs are:

$$AC_{elect} = e / Y_{tot} \cdot C_{idx} / C_{idx,1980}$$

$$AC_{labor} = l / m_0 \cdot C_{idx} / C_{idx,1980}$$

$$AC_{maint} = [\, mt.\ TCC \,] / [\, m_0\, h \,]$$

$$AC_{payovh} = 0.30\ AC_{labor}$$

$$AC_{pltovh} = 0.26\ [\, AC_{labor} + AC_{maint} + AC_{agg} \,]$$

$$AC_{steam} = sm_{steam} / Y_{tot} \cdot C_{idx} / C_{idx,1980}$$

$$AC_{tax} = [\, t\ TCC \,] / [\, m_0\, h \,]$$

$$AC_{waste} = [\, r\ m_{ref} \,] / m_0\ RC \cdot C_{idx} / C_{idx,1980}$$

$$AC_{water} = [\, w\ 240\ W \,] / m_0 \cdot C_{idx} / C_{idx,1980}$$

where e, l, m, r and w are taken from Table 9-3. Adding the above equations yields and converting to a base year yield

$$C_{operating} = (AC_{agg} + AC_{elect} + AC_{labor} + AC_{maint} + AC_{payovh} + AC_{pltovh} + AC_{tax} + AC_{waste} + AC_{water}) \tag{9.9}$$

The total cost for cleaned coal is found by adding Equations (9.1), (9.8), (9.9) and the raw coal cost

$$C_{total} = C_r + C_{ref} + C_{operating} + C_{capital}$$

Table 9-3: Operating Cost Factors (1980 $)

Variable Cost Elements	Symbol Definition	Value
Electricity	e ($/raw ton)	1.560
Labor	l ($/hr)	268.000
Maintenance	mt (fraction)	0.045
Refuse Disposal	r ($/wet ton)	1.200
Taxes	t (fraction)	0.040
Water	w ($/1000 gallon)	0.180
Agglomerant	c ($/lb)	0.800

9.6 Illustrative Example

Here we present a numerical example to illustrate the model calculations. The following assumptions are made:

Coal type = Illinois #6
Size = 9.8microns[20]
Agglomerant = n-pentane
R = 1.30
p = 0.06
i = 0.13
n = 25
$C_{idx,\,1984}$ = 261.5
C_{sol} = 1%
m_o = 500 tons/hr
h = 5500 hrs/yr

9.6.1 Performance Model

Clean coal characteristics:

$\%A_{clean}$ = 3.52
$\%S$ = 2.46
$\%Y_{clean}$ = 72.5
HHV_{clean} = 11.837 x [1-0.0352] /[1 - 0.1571]
= 13,549
$m_{outmois}'$ = 0.05

---

[20] Please refer to Table 9-2.

Assume m_{inmois}' = 0.24 . Then, the weight of water evaporated per pound of dry into thermal coal drier:

$m_{evapwater}'$ = $[m_{inmois}' - m_{outmois}'] / [(1 - m_{inmois}')(1 - m_{outmois}')]$
= $0.24 - 0.05 / [(1 - 0.24)(1 - 0.05)]$
= 0.26

The amount of energy needed to evaporate this water is

E_d = $1020\, m_{evapwater}' / \varepsilon$
= $[1020 \times 0.26] / 0.55$ = 482.2 Btu/lb

The lower heating value:

LHV = $0.96\, HHV_{clean} - [(1020\, m_{outmois}') / (1 - m_{outmois}')]$
= $0.96 \times 13{,}549 - [(1020 \times 0.05) / (1 - 0.05)]$
= 12,953 Btu/lb

The drier yield:

Y_{drier} = $1 - E_d / LHV$
= $1 - (482.2 / 12{,}953)$
= 0.963

The plant yield:

Y_{total} = $Y_{clean} Y_{drier}$
= 0.725×0.963
= 0.698

The weight of water evaporated:

$m_{evapwater}$ = $m_o [m_{evapwater}' / Y_{drier}]$
= $500 \times (0.26 / 0.963)$
= 135.0 tons/hr

Dry mass flow rate of raw coal input:

m_r = m_o / Y_{total}
= $500 / 0.698$
= 716.3 tph

Mass flow rate of n-pentane input (dry basis)

$m_{aggnew} + m_{aggrec}$ = $1.3\, m_r$
= 1.3×716.3
= 931.2 tph

Dry mass flow rate of cleaned coal entering the thermal drier:

m_{dry} = m_o / Y_{drier}
= $500 / 0.963$
= 519.2 tph

Dry mass flow rate of refuse coal:

m_{ref} = $m_r - m_{dry}$
= $716.3 - 519.2$
= 197.1 tph

Water loss in the coal cleaning plant:

W = $m_{dry} [(1 / (1 - m_{inmois}')) - 1] + m_{ref} [(1 / RC) - 1]$

$= 519.2\,[\,(1/(1-0.24))-1] + 197.1\,[\,(1/0.35)-1\,]$

$= 530.0$ tph

Mass flow rate of agglomerant lost to water

$m_{agglosttowater} = C_{sol} \times W$

$= 0.01 \times 530.0$

$= 5.30$ tph

Mass flow rate of agglomerant lost to atmosphere

$m_{agglosttoatm} = 0.0003 \times m_r$

$= 0.0003 \times 716.3$

$= 0.21$ tph

Mass flow rate of agglomerant lost with refuse

$m_{agglosttosolid} = 0.0005 \times m_r$

$= 0.0005 \times 716.3$

$= 0.35$ tph

Mass flow rate of new agglomerant makeup

$m_{aggnew} = 5.30 + 0.21 + 0.35$

$= 5.87$ tph

9.6.2 Economic Model

$d = [\,(1+i)/(1+p)-1\,]$

$= [\,(1+0.13)/(1+0.06)-1\,]$

$= 0.066$

$CRF = 0.066/[\,1-(1+0.066)^{-25}\,]$

$= 0.083$

Capital Cost:

$DC_r = \$\,91{,}963\; m_r^{0.7} \times [\,C_{idx}/C_{idx,1984}\,]$

$= \$\,91{,}963 \times (716.3)^{0.7} \times [216.5/216.5]$

$= \$9{,}165{,}995$

$DC_{aggequip} = \$10{,}521\; m_r^{0.7} \times [\,C_{idx}/C_{idx,1984}\,]$

$= \$10{,}521 \times 716.3^{\,0.7} \times [\,216.5/216.5]$

$= \$1{,}048{,}633$

$DC_{aggrec} = \$102{,}005\; m_r^{0.7} \times [\,C_{idx}/C_{idx,1984}\,]$

$= \$\,102{,}005 \times 716.3^{\,0.7} \times [\,216.5/216.5\,]$

$= \$10,\,166{,}885$

$DC_{ref} = \$19{,}100\; m_{ref}^{0.7} \times [\,C_{idx}/C_{idx,1984}\,]$

$= \$19{,}100 \times 197^{\,0.7} \times [\,216.5/216.5\,]$

$= \$771{,}461$

$DC_{drier} = \$153{,}000\; m_{evapwater}^{0.7} \times [\,C_{idx}/C_{idx,1984}\,]$

$= \$153,\,000 \times 135.0^{\,0.7} \times [\,216.5/216.5\,]$

$= \$4{,}741{,}602$

$DC_{coalsampling} = \$324{,}000 \times [\,C_{idx}/C_{idx,1984}\,]$

$= 324{,}000 \times [\,216.5/216.5\,] = \$\,387{,}230$

$\mathrm{TDC} = \$9{,}165{,}995 + \$1{,}048{,}633 + \$10,\ 166{,}885 + \$771{,}461 +$
$\$4{,}741{,}602 + \$\ 387,\ 230$
$= \$26{,}281{,}806$

$\mathrm{TCC} = 1.54 \times \mathrm{TDC}$
$= 1.54 \times \$26{,}281{,}806$
$= \$40{,}473{,}982$

Annual Cost

$AC_{agg} = [c\ x[\ m_{agglosttowater} + m_{agglosttoatmtot} + m_{agglosttosolid}\ ]\ ] / m_o$
$= (0.8 \times 5.87\ ) / 500$
$= \$0.0094/\mathrm{ton}$

$AC_{elect} = e / Y_{tot}\ [\ C_{idx}/C_{idx,1980}\ ]$
$= 1.56 / 0.698\ [\ 261.5/218.8]$
$= \$2.67/\mathrm{ton}$

$AC_{labor} = 1 / m_o\ [\ C_{idx}/C_{idx,1980}\ ]$
$= 268 / 500\ [\ 261.5/218.8]$
$= \$0.65/\mathrm{ton}$

$AC_{maint} = [\ mt.\ \mathrm{TCC}\ ] / [\ m_o\ h\ ]$
$= [\ 0.045 \times \$40{,}473{,}982\ ] / [\ 500 \times 5500\ ]$
$= \$0.66/\mathrm{ton}$

$AC_{payovh} = 0.30\ AC_{labor}$
$= 0.30 \times \$0.65$
$= \$0.20/\mathrm{ton}$

$AC_{pltovh} = 0.26\ [\ AC_{labor} + AC_{maint} + AC_{agg}\ ]$
$= 0.26\ (\ \$0.65 + \$0.66 + \$0.0094\ )$
$= \$0.34/\mathrm{ton}$

$AC_{tax} = [\ t\ \mathrm{TCC}\ ] / [\ m_o\ h\ ]$
$= [\ 0.04 \times \$40{,}473{,}982\ ] / [\ 500 \times 5500\ ]$
$= \$0.59/\mathrm{ton}$

$AC_{waste} = [\ r\ m_{ref}\ ] / m_o\ RC \cdot C_{idx}/C_{idx,1980}$
$= [\ 1.2 \times 197\ ] / [\ 500 \times 0.35\ ] \cdot 261.5/218.8$
$= \$1.61/\mathrm{ton}$

$AC_{water} = [\ w\ 240\ W\ ] / m_o \cdot C_{idx}/C_{idx,1980}$
$= (0.18/1000) \times 240 \times 521.7/500 \times 261.5/218.8$
$= \$0.055/\mathrm{ton}$

Working Capital

$W_c = 0.25\ (\ AC_{labor} + AC_{maint} + AC_{elect} + AC_{water} + AC_{waste} + AC_{agg}\ )$
$= 0.25\ (\ \$0.65 + \$0.66 + \$2.67 + \$0.055 + \$1.61 + \$0.0094\ )$
$= \$1.41/\mathrm{ton}$

Cleaning Cost is then:

$C_T = \$28.60/\mathrm{ton}$ (see Table 9-4)
$C_{ref} = C_T\ [(1/Y_{total}) - 1]$
$= \$28.60\ [\ (1/ 0.709) - 1]$

$$\begin{aligned}
& = \$11.74/\text{ton} \\
C_{operating} & = (AC_{agg} + AC_{elect} + AC_{labor} + AC_{maint} + AC_{payovh} + AC_{pltovh} + \\
& \quad AC_{tax} + AC_{waste} + AC_{water}) \\
& = (\$0.0094 + \$2.67 + \$0.65 + \$0.66 + \$0.20 + \$0.34 + \$0.59 + \\
& \quad \$1.61 + \$0.055) \\
& = \$6.78/\text{ton} \\
C_{capital} & = dW_c + [(TCC \times CRF) / (m_o \times h)] \\
& = [0.066 \times \$1.41] + [(\$40{,}473{,}982 \times 0.083) / (500 \times 5500)] \\
& = \$1.31/\text{ton} \\
C_{total} & = C_r + C_{ref} + C_{operating} + C_{capital} \\
& = \$25.00 + \$10.82 + \$6.78 + \$1.31 \\
& = \$43.91/\text{ton}
\end{aligned}$$

Tables 9-4, 9-5 and 9-6 summarize the results of the case study and present similar results for two additional coals: Pittsburgh #8 and Upper Freeport. The results for these three coals also are summarized graphically in Figures 9-3 and 9-4.

Table 9-4: Components of Cleaning Cost (1984$ / dry ton of clean coal)

Components	Illinois #6	Pittsburgh	Upper Freeport
Raw*	28.60	21.80	13.60
Capital	1.31	1.55	1.97
O&M	6.78	8.95	12.84
Refuse	11.74	18.27	22.16
Total	48.43	50.57	50.57

* The raw coal price is a model input parameter. The base prices assumed were taken from the (1986) report. However, since two of the coals reported by Bechtel had extraordinarily high ash contents (see Table 9-2), the base prices were adjusted for the higher ash levels. For example, the Pittsburgh coal price is assumed to be $32.49/ton with an ash content of 9.30%. However, at 39.16% ash the price is:

$$32.49 \cdot \frac{1 - 0.3916}{1 - 0.093} = \$21.80/\text{ton}.$$

Base prices for Illinois #6 and Lower Freeport are $26.91/ton (20.70% ash) and $28.29/ton (11.20% ash) respectively.

Table 9-5: Breakdown of Operating and Maintenance Costs (1984$ / dry ton of clean coal)

Component	Illinois #6	Pittsburgh	Upper Freeport
Heavy Liquid	0.0094	0.0157	0.028
Electricity	2.67	3.43	4.11
Labor	0.65	0.65	0.65
Maintenance	0.66	0.77	0.97
Payroll Overhead	0.20	0.20	0.20
Plant Overhead	0.34	0.37	0.43
Taxes & Insurance	0.59	0.69	0.85
Waste Disposal	1.61	2.74	5.46
Water	0.055	0.08	0.14

Table 9-6: Breakdown of Capital Cost (Million 1984$)

Component	Illinois #6	Pittsburgh	Upper Freeport
Raw Coal Processing	9.166	10.905	14.030
Sel. Agg. Cleaning Equip.	1.049	1.248	1.605
Sel. Agg. Recovery Equip.	10.167	12.104	15.562
Refuse Coal	0.771	1.266	2.051
Thermal Drier	4.741	4.741	4.741
Coal Sampling Equipment	0.387	0.387	0.387

Figure 9-3: Components of Total Coal Cost (1984$/dry ton of cleaned coal)

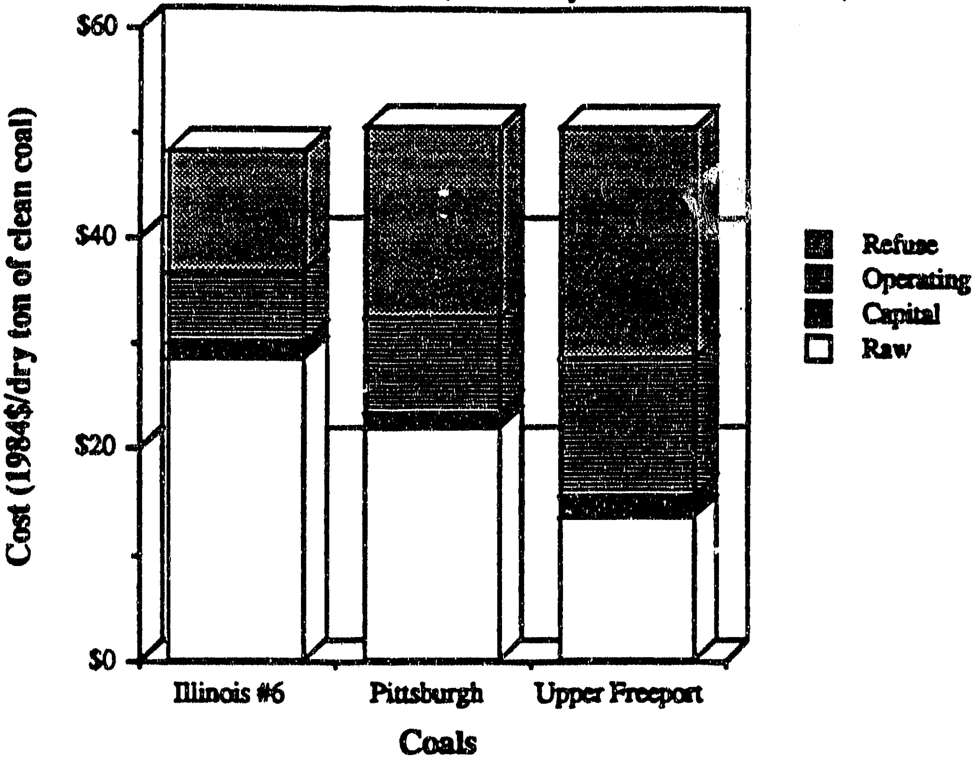
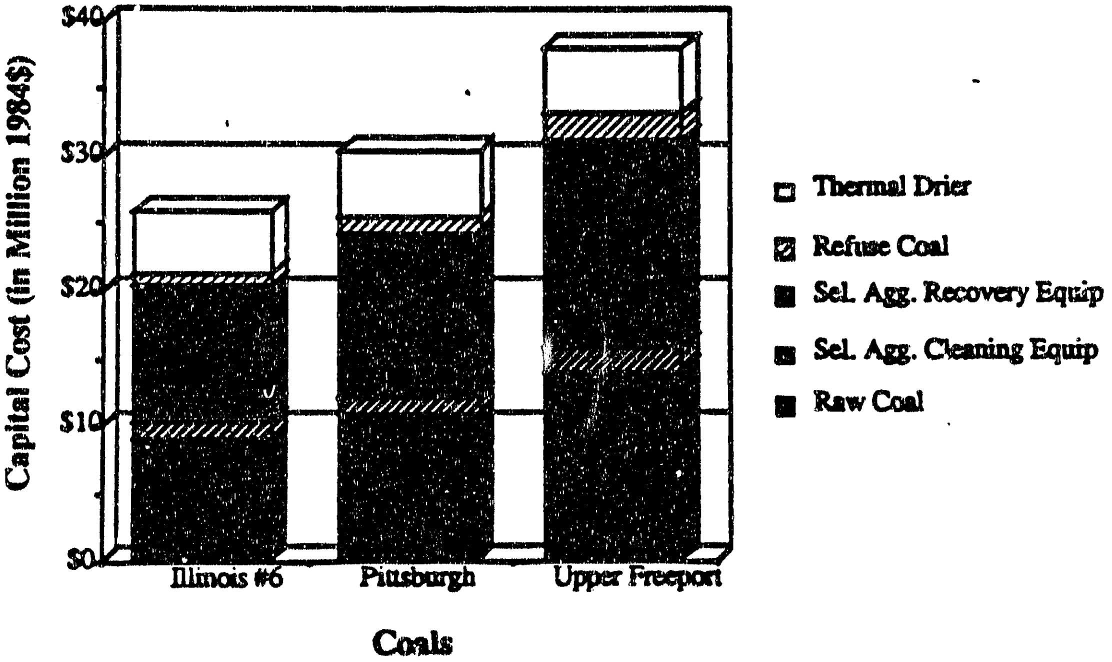


Figure 9-4: Breakdown of Capital Cost (Million 1984$)



9.7 Sensitivity Analysis

Tests to identify the key design and operating parameters for the selective agglomeration process were conducted by Bechtel in its 1 tph POC bench scale test(51). Among the variables examined were:

1. coal grind (to determine the minimum size of coal input that produces greater yield)
2. pulp density
3. effects of oxidation and aging
4. speed of reactors
5. agglomerant dosage (in high shear reactor)
6. asphalt dosage (in low shear reactor)

It is assumed that the key design and operating parameters identified in these tests will also be the key design and operating parameters for selective agglomeration for a 300 tph coal feed. The results of the tests were as follows.

9.7.1 Coal Grind

Pittsburgh No. 8

The tests yielded clean coal with ash contents between 3.4% and 5.4%, while the sulfur dioxide emission potential per million Btu of the ROM coal was reduced by 48 to 56 percent. This means a reduction in pyritic sulfur between 67 and 77 percent. Interestingly, in all the tests more than 90% Btu recovery in the clean coal was obtained.

Table 9.7: Bechtel Test Results on Pittsburgh #8 Coal (51)

	Fine Grind	Coarse Grind:		
		Typical	Mean	Std. Dev.
Agglomerated Clean Coal:-				
Test No.	I-12-B	P-10-B	23 tests	
Grind Size (microns)	3.70	12.10	12.10	ND
% Ash	3.30	4.80	4.93	0.19
% Total Sulfur	3.48	3.61	3.78	0.11
Heating Value (Btu/lb)	14251	14014	14003	48
ROM Performance:-				
% Energy Recovery	92.90	92.70	92.30	0.80
% Ash Reduction	95.00	92.50	92.30	0.30
% Sulfur Reduction	58.70	56.50	54.60	1.50
% SO_2 Reduction	55.60	53.20	51.00	1.50
% Pyritic Sulfur Red.	77.30	73.90	70.80	2.20

Better ash reduction was obtained from finer particle size (see Table 9-7). When the particle size was reduced from 12.4 microns to 3.7 microns (50% passing), the clean coal ash was lowered from 4.8 to 3.3 percent at the same high energy recovery. The reduction in the sulfur content was less pronounced, however, due to the high organic sulfur content of this coal. Clean coal sulfur content was only reduced from 3.6% to 3.5%. The comparative results are shown in Table 9-7.

The mean values of several tests with different process conditions, all at a grind size of 12.1 microns are also shown in Table 9-7. These are compared to results obtained with reduced size feed. The small standard deviations of results at the same grind size despite variations in process conditions are taken as indications that none of the variables other than the size of the grind affected process performance to any significant degree.

Illinois No.6

The tests yielded clean coal with ash reductions between 78% and 84%. The ROM sulfur dioxide reduction varied between 46% and 54%. The ROM pyritic sulfur was reduced to about 90 percent.

Table 9-8: Bechtel Test Results on Illinois #6 Coal (51)

	Fine Grind	Coarse Grind:		
		Typical	Mean	Std. Dev.
Agglomerated Clean Coal:-				
Test No.	1-9-A	1-9-A	18 tests	-
Grind Size (microns)	3.7	9.8	9.8	ND
% Ash	2.9	3.5	3.7	0.27
% Total Sulfur	2.56	2.75	2.72	0.09
Heating Value (Btu/lb)	13857	13780	13744	38
ROM Performance:-				
% Energy Recovery	84.90	84.60	84.60	0.30
% Ash Reduction	84.20	80.90	79.70	1.50
% Sulfur Reduction	59.70	56.50	56.80	1.50
% SO_2 Reduction	51.80	48.00	48.30	1.70
% Pyritic Sulfur Red.	95.60	88.50	89.20	3.20

The effects of grind size on performance with Illinois No. 6 coal are shown in Table 9-8. Finer grinding to 3.7 microns, from 9.8 microns (50 percent passing) resulted in improvement in the clean coal ash and sulfur contents. The mean values of 18 tests with different process conditions, all at a grind size of 9.8 microns and their standard deviation are also shown in Table

9-8. These are compared to results obtained with reduced size feed. The minimal standard deviations of results at the same grind size, despite variations in process conditions, are taken as indications that none of the variables other than the size of the grind affected process performance to any significant degree.

Upper Freeport Coal

The results showed that the coal could be cleaned with ROM energy recoveries between 89% and 92% and the clean coal ash could be reduced to between 9.0% and 6.1%. Very fine grinding to 2.9 microns (50 percent passing) did not improve the results. The ash reductions obtained were between 74 to 95 percent. As can been seen in Table 9-9, the Upper Freeport ROM coal's sulfur content is mostly in the pyritic form. This would indicate high sulfur reduction potential. In fact, the total SO_2 reductions achieved varied from 56% to as high as 72%. The ash content in the tailing was high 88.1 to 92.4%, showing a good carbon capture efficiency.

Comparative results with coarse and finely ground Upper Freeport coal are shown in Table 9-9. As with the other two coals, all tests with the coarser grind produced similar results. However, when the feed was reground to a finer size of 2.9 microns from 4.5microns (50 percent passing), an increase in the clean coal ash content occurs accompanied by a slight reduction in the sulfur content.

Table 9-9: Bechtel Test Results on Upper Freeport Coal (51)

	Fine Grind	Coarse Grind:		
		Typical	Mean	Std. Dev.
Agglomerated Clean Coal:-				
Test No.	F-8-A	F-6-B	12 tests	
Grind Size (microns)	2.9	4.3	4.3	ND
% Ash	8.5	7.8	8.1	0.85
% Total Sulfur	1.40	1.56	1.58	0.05
Heating Value (Btu/lb)	14106	14206	14168	143
ROM Performance:-				
% Energy Recovery	92.0	91.7	91.7	0.1
% Ash Reduction	93.8	94.3	94.1	0.7
% Sulfur Reduction	73.5	70.8	70.3	1.2
% SO_2 Reduction	72.0	69.1	68.6	1.3
% Pyritic Sulfur Red.	78.8	75.5	75.0	1.4

9.7.2 Pulp Density

Tests were run at 10, 15, 20 and 25 percent solids by weight. At 25 percent solids, the sample slurries of the fine ground coal all became too strongly non-Newtonian under high shear to agglomerate properly. Illinois No. 6 and Pittsburgh No. 8 samples were run at 20 percent solids, where their fluid mechanical properties were marginal. The results indicated that Pittsburgh No. 8 performed marginally worse at 20 percent solids, but that Illinois No. 6 showed no significant change. No detectable change in performance was seen for any of the samples agglomerated at 10 percent as compared to 15 percent. These results led to the selection of a solids concentration of 15 percent in the nominal selective agglomeration process design.

9.7.3 Agglomerant Dosage

In a high shear reactor (where the agglomerate is added to the slurry), the approximate speed is 12,000 rpm. Given an adequate quantity to sustain agglomeration, the agglomerant dosage affects only the size of the agglomerates and not the product quality or energy recovery. Agglomerant dosages (by weight percent of dry coal feed) of 25% or up are recommended for Pittsburgh No.8 and Illinois No.6 and agglomerant dosages 35% or up for Upper Freeport.

9.7.4 Asphalt Dosage

In low shear reactor (where asphalt binder is added to the mixture of agglomerate and slurry), the approximate speed is 6,000 rpm. Asphalt dosage affects product size and strength. Agglomerates of adequate strength are required to avoid carbon losses during product screening. Asphalt dosages (by weight percent of dry coal feed) of 4% or up are recommended for Pittsburgh No.8, Illinois No.6 and Upper Freeport. Since the cost of adding the asphalt to the process is marginal compared to other costs, we dropped it in calculating the cost of the entire coal cleaning process.

9.7.5 Effects on Economics

The cleaning cost (excluding the raw coal cost) for Illinois #6 coal for the two different grind sizes of coal input noted earlier was investigated. The results of this sensitivity analysis suggest that as 9.8 microns coal was ground to 3.7 microns, the sulfur content of cleaned coal was reduced by 5%. Still, the cleaning cost increased by $1 per dry ton of cleaned coal (Figure 9-5).

The cleaning cost for Illinois #6 coal for the two different solids concentrations (pulp density) was also investigated. The results of this sensitivity analysis suggested that an increase of 5% solid concentration could lead to about a 0.3% increase in sulfur reduction and an additional $0.30 increase in clean cost per dry ton of cleaned coal (Figure 9-6). The results support the selection of 15% solid concentration in the selective agglomeration process.

Figure 9-5: Cleaning Cost (1984$/dry ton of cleaned coal) vs. Sulfur Reduction for Different Grind Sizes (Illinois #6 coal).

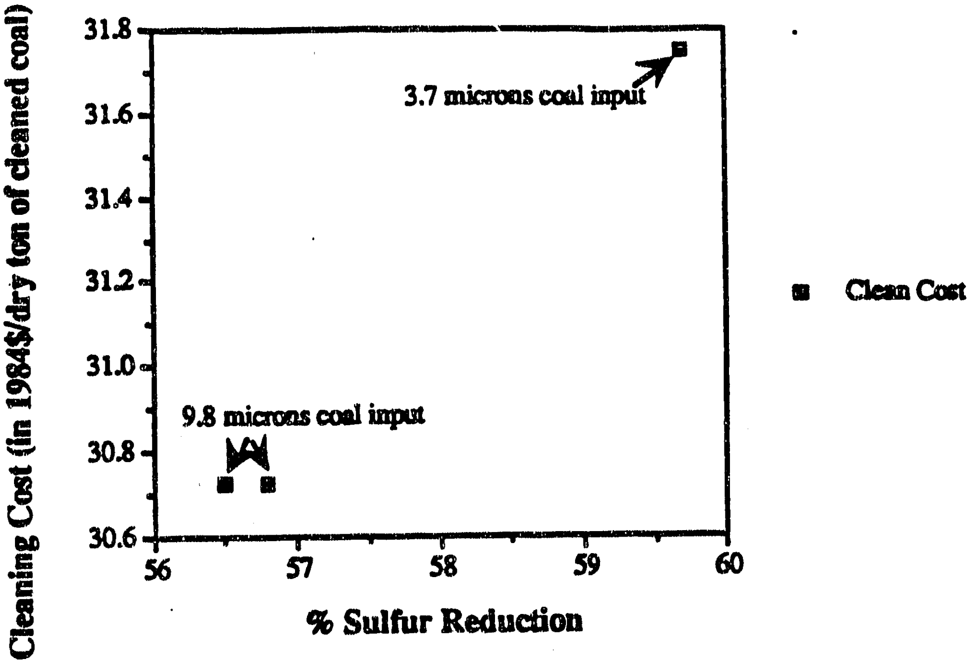
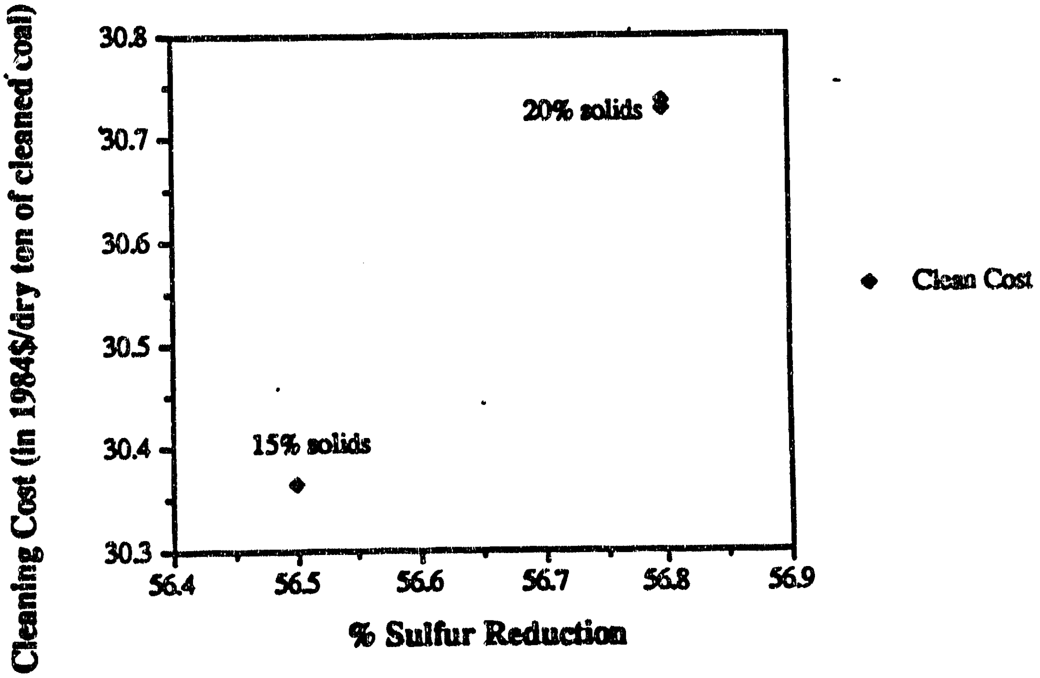


Figure 9-6: Cleaning Cost (1984$/dry ton of cleaned coal) vs. Sulfur Reduction for on Different Pulp Density (Illinois #6 coal).



10 HEAVY LIQUID SEPARATION PROCESS MODEL

10.1 Nomenclature

English letter symbols

A_{clean}	Ash content of the clean coal going to cleaning circuit and eventually thermal drier (fraction)
$A_{precleaned}$	Ash content of precleaned coal (fraction)
A_{preref}	Ash content of the refuse coal from the precleaning subcircuit (fraction)
A_r	Ash content of the raw coal input (fraction)
A_{ref}	Ash content of the refused coal going to refuse circuit (fraction)
AC_{elect}	Annual cost of electricity ($ / dry ton of clean coal)
AC_{labor}	Annual cost of labor ($ / dry ton of clean coal)
AC_{liq}	Annual cost of heavy liquids ($ / dry ton of clean coal)
AC_{maint}	Annual cost of maintenance ($ / dry ton of clean coal)
AC_{payovh}	Annual cost of payroll overheads ($ / dry ton of clean coal)
AC_{plovh}	Annual cost of plant overheads ($ / dry ton of clean coal)
AC_{steam}	Annual cost of steam ($ / dry ton of clean coal)
AC_{tax}	Annual cost of taxes, insurance, etc ($ / dry ton of clean coal)
AC_{waste}	Annual cost of waste disposal ($ / dry ton of clean coal)
AC_{water}	Annual cost of water ($ / dry ton of clean coal)
c	Cost of heavy liquid used ($/lb heavy liquid)
C_{idx}	Chemical Engineering Cost Index for current year
$C_{idx,\ 1984}$	Chemical Engineering Cost Index for 1984
C_{sol}	Degree of heavy liquid solubility in water (fraction)
$C_{capital}$	Total capital cost ($ /dry ton of clean coal)
$C_{operating}$	Total operating cost ($ /dry ton of clean coal)
C_r	Cost of raw coal ($ /dry ton of raw coal)
C_{ref}	Cost of refuse coal ($ /dry ton of clean coal)
C_{total}	Total cost of clean coal ($ /dry ton of clean coal)
CRF	Capital Recovery factor (dimensionless)
d	Real discount rate for capital cost (fraction)
DC	Direct capital cost ($)
$DC_{hlcequip}$	Direct capital cost of the heavy liquid cyclone plant equipment ($)
DC_{liqrec}	Direct capital cost of heavy liquid recovery equipment ($)
DC_r	Direct capital cost of the refuse handling ($)
DC_{ref}	Direct capital cost of the refuse handling ($)
$DC_{coal\ sampling}$	Direct capital cost of sampling the clean coal ($)
$DC_{thermal}$	Direct capital cost of thermal drying system ($)
e	Cost of electricity ($/dry ton of raw coal)
E_{drier}	Energy needed for thermal drier (Btu)
h	Annual operating hours of coal cleaning plant (hrs/yr)
HHV_r	Higher heating value of raw coal (Btu/lb dry coal)
HHV_{clean}	Higher heating value of clean coal (Btu/lb dry coal)
i	Nominal interest rate (fraction)
l	Labor cost ($/hr)
LHV	Lower heating value of clean coal (Btu/lb dry coal)
m_{clean}	Dry mass flow rate of clean coal entering the cleaning circuit (tons/hr)
m_{dry}	Dry mass flow rate of clean coal leaving the cleaning plant (tons/hr)

$m_{evapwater}$	Mass flow rate of water evaporated in thermal drier (tons/hr)
$m_{evapwater}'$	Weight of water evaporated in thermal drier per pound of clean coal (fraction)
m_{inmois}'	Moisture content of clean coal entering thermal drier (fraction)
$m_{liqclean}$	Mass flow rate of heavy liquid from the overflows of cleaner and scavenger cyclones, entering the cleaning circuit (tons/hr)
$m_{liqeffluentref}$	Mass flow rate of heavy liquid leaving as effluent from solid bowl centrifuge (tons/hr)
$m_{liqfiltclean}$	Mass flow rate of heavy liquid leaving as filtrate from the drum filter (tons/hr)
$m_{liqlosttoatmtot}$	Mass flow rate of total heavy liquid lost to the atmosphere (tons/hr)
$m_{liqlosttowater}$	Mass flow rate of heavy liquid lost to water (tons/hr)
m_{liqnew}	Mass flow rate of new heavy liquid (tons/hr)
m_{liqrec}	Mass flow rate of recovered heavy liquid (tons/hr)
m_{liqref}	Mass flow rate of heavy liquid from the overflows of cleaner and scavenger cyclones, entering the refuse coal circuit (tons/hr)
$m_{liqstripclean}$	Mass flow rate of heavy liquid entering the clean coal stream stripping system (tons/hr)
$m_{liqstripref}$	Mass flow rate of heavy liquid entering the refused coal stripping system (tons/hr)
$m_{liqthicclean}$	Mass flow rate of underflow heavy liquid leaving the coal thickening cyclone(tons/hr)
$m_{liqthicref}$	Mass flow rate of overflow heavy liquid leaving the refuse thickening cyclone(tons/hr)
m_o	Dry mass flow rate of clean coal leaving the plant (tons/hr)
$m_{outmois}'$	Moisture content of clean coal leaving thermal drier (fraction)
$m_{precleaned}$	Dry mass flow rate of precleaned coal (tons/hr)
m_r	Dry mass flow rate of raw coal input (tons/hr)
m_{ref}	Dry mass flow rate of refused coal entering the refuse circuit (tons/hr)
m_{steam}	Total mass flow rate of steam required for stripping system (tons/hr)
$m_{steamclean}$	Mass flow rate of steam required for clean coal stream stripping system (tons/hr)
$m_{steamref}$	Mass flow rate of steam required for refused coal stream stripping system (tons/hr)
m_t	Cost of maintenance (fraction)
n	Life of coal cleaning plant (years)
p	Inflation rate (fraction)
PS_{clean}	Pyritic sulfur in the clean coal removed from the raw input (%)
r	Cost of refuse coal disposal ($/wet ton)
R	Ratio of dry mass heavy liquid to dry mass of clean coal from the precleaning subcircuit (dimensionless)
t	Annual rate of taxes and insurance costs for plant (fraction)
TCC	Total capital cost ($)
TDC	Total direct capital cost
w	Cost of water ($/1000 tons)
W	Water loss in the process (tons/hr)
W_c	Working capital ($/dry of clean coal)
Y_{clean}	Mass yield of clean coal exiting from the HLR subcircuit (fraction)
Y_{drier}	Thermal drier mass yield (fraction)
$Y_{precleaned}$	Mass yield of clean coal from the precleaning subcircuit (fraction)
Y_{total}	Mass yield of entire coal cleaning plant (fraction)

Greek letter symbols

ε	Efficiency of thermal drier (fraction)

10.2 Introduction

This chapter describes new performance and economic models simulating the operation of a coal beneficiation plant using the heavy liquid cyclone process. The primary function of these models is to estimate the cost and ability of the process to remove pyritic sulfur and ash content to help meet power plant emission standards. This report presents a brief overview of heavy liquid cyclones, a description of the economic algorithms and an assessment of this process' ability to reduce sulfur dioxide emissions of coal fired power plants. Models are adopted from bench-scale test on a one ton per hour (tph) Proof-of-Concept (POC) units performed by Process Technology Institute (PTI)[21] (53). An assessment of capital investment and operating costs for a heavy liquid cyclone process for a plant size of 300 tph proposed by Burns and Roe Services Corporation (52) is adopted in developing the economic model.

The heavy liquid cyclone process uses the differences in specific gravity (s.g.) between the coal and liberated pyrites to achieve separation. In this process, coal (s.g. ~ 1.30) is mixed with a heavy liquid of specific gravity between 1.33 to 1.60 and passed through a cyclone. The high centrifugal forces experienced by the coal and the liberated pyrites in the heavy liquid promote separation by moving the lighter coal particles to the center and the heavier pyrites particles to the wall of the cyclone. The clean coal reports as overflow and the heavy impurities as underflow.

The process design is based on 2" to 4" diameter cyclones. Because of the small throughput capacity of these cyclones, a large number of cyclones is required. Effective distribution of the feed material to the cyclones is a challenging problem. Because of these uncertainties in the performance of cyclones, the operating cost of cyclones is a cost-sensitive area. Another cost-sensitive area is recovery of the heavy liquid.

10.3 Process Description

A conceptual flow scheme for an HLC process is shown in Figure 10-1 and 10-2. The HLC process comprises of two subcircuits: heavy liquid cyclone subcircuit and heavy liquid recovery subcircuit. Two other subcircuits also contributed to the HLC process discussed here. They are the precleaning subcircuit and the comminution subcircuit.

10.3.1 Precleaning Subcircuit

The objective of the precleaning circuit (flowsheet not shown) was to remove the out-of-seam dilution rock that is collected during the normal course of mining operations. Because most of this rock is coarse, it is advantageous to remove the rock prior to grinding to avoid energy intensive grinding process and fine particle separation difficulties. Heavy medium cyclone circuit would be used to remove the most coarse rock and maintain high thermal recovery.

In this subcircuit, the ROM feed was crushed to 3/8" and screened at 8 mesh. The 3/8" x 8 mesh material was subjected to cleaning in the heavy medium cyclone while the -8 mesh material was saved for recombination with the precleaned +8 mesh material.

The 3/8" x 8 mesh coal was fed continuously into a sump where it was mixed with the water. A 5" kreb cyclone was used to make separation. The clean coal and refuse products were collected off the drain and rinse screens into 55 gallon barrels. These 55 gallon barrels were removed to storage alongside the -8 mesh material. The +8 mesh and the -8 mesh material were

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[21] There are four other groups involved in the project: Michigan Technological University (MTU); Bateman Engineer, Inc (BE); Norton, Hambleton Engineering Inc. (NHE); and, American Electric Power (AEP).

then proportionally combined as needed to provide the feed to the grinding circuit for heavy liquid cyclone (HLC) test work.

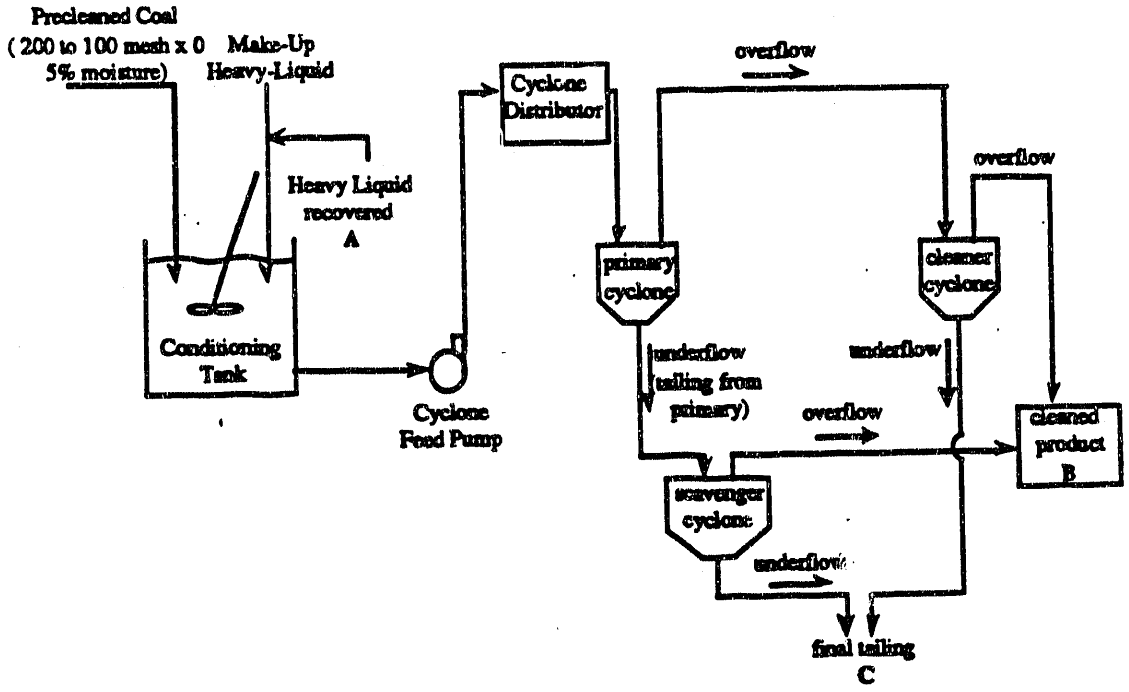
10.3.2 Comminution Subcircuit

Precleaned feed is crushed in an open circuit to a top size of 28 mesh in a dry roll crusher. It is then slurred and fed to an attrition mill operating in closed circuit which simplifies grinding to various topsizes typically ranging from 100-325 mesh. There is no flowsheet for this subcircuit.

10.3.3 Heavy Liquid Cyclone (HLC) Subcircuit

This subcircuit shown in Figure 10-1 comprises the various stages of HLC separation. It involves a 2" diameter cyclone acting as a primary stage of separation and 1" diameter cyclones acting as cleaner and scavenger stage. The cleaner stage is used for cleaning the primary cyclone or clean coal flow stream. The scavenger cyclone was used for recovering misplaced clean coal in the tailings stream from the primary cyclone.

Figure 10-1: Heavy Liquid Cyclone Subcircuit (HLC)



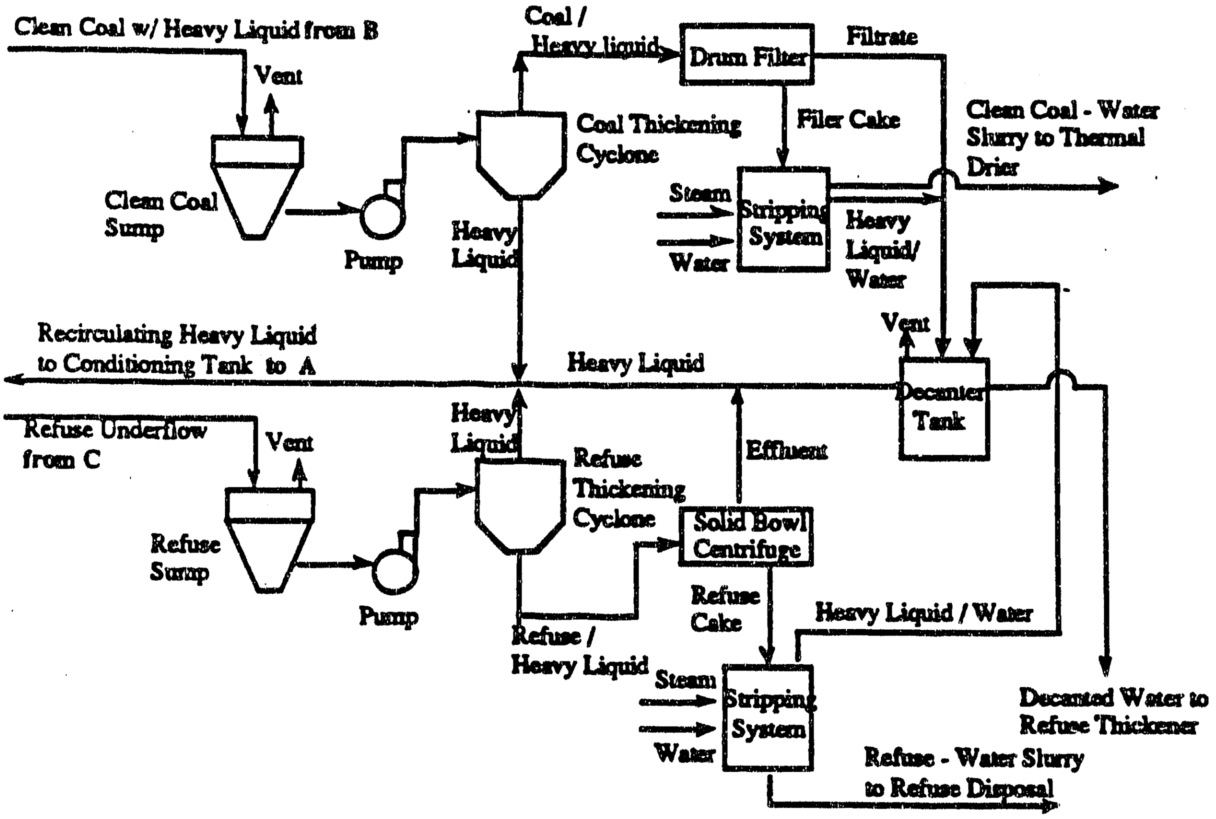
In this configuration, the overflow from the cleaner and the scavenger cyclones normally combine to constitute a clean coal product of 4% - 5% ash at 80% Btu recovery when run near optimum. A middlings stream is produced from the cleaner cyclone underflow. Ash values often occur in the 8% - 12% range with this flow stream which represents 7% - 10% of the total feed to the circuit. Final tailings are removed from the scavenger and cleaner underflows. These are generally 10% -20% of the plant feed with ash in the 50%-60% range when run near optimum (52).

PTI also tested a three stage cyclone circuit where the scavenger was removed and used as a recleaning stage reprocessing the overflow stream from the cleaner cyclone. It was found that marginal improvements in coal quality with the recleaner cyclone generally did not warrant the corresponding loss in Btu recovery.

10.3.4 Heavy Liquid Recovery Subcircuit

This subcircuit shown in Figure 10-2 comprises of two streams: the clean coal stream and the refuse stream. The original design of the clean coal stream showed a pressure filter as a mechanical deliquoring stage followed by a turbo dryer as a thermal recovery stage for stripping the heavy liquid from the surface of the coal and refuse. In the Dow Organic Heavy Liquid (OHL) process (52), the coal heavy-liquid slurry is deliquored by the hooded vacuum filter and the filter cake is washed with hot water to displace residual heavy liquid. Final heavy-liquid removal is achieved in a proprietary stripping system. The stripping system is believed to consist of a direct contact evaporator. The coal is discharged from the stripping system as a coal/hot-water slurry. The amount of moisture (water) in coal-hot water slurry is depended on the amount of steam required to remove the heavy liquid from the clean coal and the amount of water discharged with the heavy liquid in the other exit stream. The water is removed in the thermal drier.

Figure 10-2: Heavy Liquid Recovery Subcircuit (HLR)



In the refuse stream, the refuse is thickened in a solids bowl centrifuge and then stripped of any remaining heavy liquid in a stripping system similar to the clean coal stripping system. The heavy liquid and water are allowed to separate under quiescent conditions in decanter. The heavy liquid from the decanter is mixed with other recovered heavy liquid and recirculated to the conditioning tank.

It is recommended that when designing the HLC and HLR subcircuits, all the equipment in the circuit be vented to a collection system to minimize the heavy liquid losses. All the equipment should be air tight. The piping should be designed to prevent losses of the heavy liquid vapors. Basides the losses to the atmosphere, the heavy liquid also lost to the water. The detailed calculation of heavy liquid losses are discussed later in illustrative results.

10.4 Performance Model

The algorithm for the determining the higher heating value is as follows:

$$HHV_{clean} = HHV_r [1 - A_{clean} / 1 - A_r]$$

Estimates of plant operating and capital costs typically are scaled to various mass flow rates within the coal cleaning plant. Those developed below are the rate of raw coal and heavy liquid into the plant, the rate of dry and-wet refuse coal out of the plant, the rate of heavy liquid recovered and lost from the plant, the rate steam and water required for stripping the heavy liquid and the rate of water evaporated in the thermal drier.

In approaching the performance models developed, we will look at one subcircuit at a time.

10.4.1 Precleaning Subcircuit

The yield of the clean coal going into the Communition subcircuit is calculated as follows:

$$Y_{precleaned} = [A_{preref} - A_r] / [A_{preref} - A_{precleaned}] \qquad (10.1)$$

10.4.2 Communition Subcircuit

We assume the grinding process does not significantly affect the percentage yield of precleaned coal. $Y_{precleaned}$ obtained from Equation (10.1) remains as the ground precleaned coal enters the HLC subcircuit.

10.4.3 HLC Subcircuit

The amount of heavy liquid needed for this process related to the specific gravity of the coal and the specific gravity of the heavy liquid. The ratio of mass of heavy liquid to the dry mass of precleaned coal is denoted by R, or

$$m_{liq} = R_{m\ precleaned}$$

The value of R is determined from experiments.

The yield of the clean coal going into the HLR subcircuit is calculated as follows:

$$Y_{clean} = [A_{ref} - A_{precleaned}] / [A_{ref} - A_{clean}]$$

10.4.4 HLR Subcircuit

As was mentioned earlier, we have divided this subcircuit into two streams -- the clean coal and refuse coal streams. We will look at the clean coal stream first.

Clean Coal Stream

The mass flow rate of the heavy liquid entering this stream, $m_{liqclean}$, is the sum of the mass flow rate of the underflow of the coal thickening cyclone, $m_{liqthicclean}$ and the heavy liquid exiting from the drum filter ($m_{liqfiltclean} + m_{liqstripclean}$):

$$m_{liqclean} = m_{liqthicclean} + m_{liqfiltclean} + m_{liqstripclean}$$

The amount of stream needed in clean coal stripping system was

$$m_{steamclean} = 0.149\ m_{liqstripclean} \tag{10.2}$$

Refuse Coal Stream

The approach in developing the following equations for the refuse coal stream is similar to the one discussed in the clean coal stream. The mass flow rate of the heavy liquid entering this stream, m_{liqref}, is the sum of the mass flow rate of the overflow of the refuse thickening cyclone, $m_{liqthicref}$ and the heavy liquid exiting from the solid bowl centrifuge ($m_{liqeffluentref}$ and $m_{liqstripref}$):

$$m_{liqref} = m_{liqthicref} + m_{liqeffluentref} + m_{liqstripref}$$

The amount of steam and cooling water needed in refuse stripping system is calculated by equations follows:

$$m_{steamref} = 0.149\ m_{liqstripref} \tag{10.3}$$

Combining equations (10.2) and (10.3), the total steam consumption is therefore

$$m_{steam} = m_{steamclean} + m_{steamref} = 0.149\ (m_{liqstripclean} + m_{liqstripref})$$

By tabulating the experimental data

$$m_{liqstripclean} + m_{liqstripref} = 0.436\ m_{liq}$$

Therefore,

$$m_{steam} = 0.149 \times 0.436 \times m_{liq}$$

$$= 65.0 \times 10^{-3}\ m_{liq}$$

Not all the heavy liquid will be recovered. Depending on the degree of solubility of heavy liquid in water, some will be lost to the water. The amount of heavy liquid that is lost to the water is estimated to be

$$m_{liqlosttowater} = C_{sol} \times W$$

where W is the total water loss in the process

Besides the losses of the heavy liquid to the water in both stripping system, some heavy liquid is also lost to the atmosphere. To find the heavy liquid that is lost to the atmosphere, we have to consider the entire components of HLC and HLR subcircuits. The formula obtained is shown below:

$$m_{liqlosttoatmtot} = 3.5 \times 10^{-4}\ m_{precleaned}$$

Hence, the recovered heavy liquid (methylene chloride) from this stream is

$$(m_{liqrec}) = m_{liqclean} + m_{liqref} - m_{liqlosttowater} - m_{liqlosttoatmtot} \tag{10.4}$$

Since the sum of $m_{liqclean} + m_{liqref}$ is also the sum of $m_{liqnew} + m_{liqrec}$, equation (10.4) is reduced to

$$m_{liqrec} = (\ m_{liqnew} + m_{liqrec}\ ) - m_{liqlosttowater} - m_{liqlosttoatmtot}$$

or

$$m_{liqnew} = m_{liqlosttowater} + m_{liqlosttoatmtot}$$

10.4.5 Thermal Drier Subcircuit

Normally, it is necessary to thermally dry the fine sizes of coal-hot water slurry. It is assumed that product coal is used to fire the thermal drier, thus reducing the overall plant yield (this subcircuit is not shown in the flowsheet). It is also assumed that drying alters only the coal moisture content, with all the other coal properties (measured on a dry basis) remain the same. Since the moisture content of coal entering and leaving the thermal drier is specified, the weight of the water evaporated per pound of precleaned coal into the thermal drier is

$$m_{evapwater}' = [m_{inmois}' - m_{outmois}'] / [(1 - m_{inmois}') (1 - m_{outmois}')]$$

The amount of energy needed to evaporate this water is

$$E_d = 1020\, m_{evapwater}' / \varepsilon$$

The lower heating value can be approximated by

$$LHV = 0.96\, HHV_{clean} - [1020\, m_{outmois}' / (1 - m_{outmois}')]$$

Therefore, the drier yield and total plant yield are given by

$$Y_{drier} = 1 - E_d / LHV$$

and

$$Y_{total} = Y_{precleaned} Y_{clean} Y_{drier}$$

The weight of water evaporated is

$$m_{evapwater} = m_{evapwater}' [m_o / Y_{drier}]$$

Once the drier is determined, the dry mass flow rates for the raw coal stream, refuse stream and drier stream can be calculated by the following equations:

$$m_r = m_o / Y_{total}$$

$$m_{precleaned} = m_o \times Y_{precleaned}$$

$$m_{dry} = m_o / Y_{drier}$$

$$m_{ref} = m_o - m_{dry}$$

The water loss in the coal cleaning plant is

$$W = m_{dry} [(1 / (1 - m_{inmois}')) - 1] + m_{ref} [(1 / RC) - 1)$$

10.5 Economic Model

The total cost in dollars per ton of dry clean coal can be divided into four separate costs categories.

- cost of raw coal
- cost of rejected coal

- annual operating and maintenance costs
- annualized capital costs

The cost of raw coal is an input parameter. The cost of the refuse cost is a function of the plant yield and can be calculated from

$$C_{ref} = C_r\,[(1/Y_{total}) - 1] \tag{10.5}$$

10.5.1 Capital Cost

The capital cost is divided into five different sections: raw coal handling, heavy liquid cyclone equipment, heavy liquid handling, refuse handling and thermal driers (if needed). The capital costs related to clean coal storage is included in the raw coal cost, since the coal cleaning equipment is assumed to be at the mine site. This includes the cost for conveyors, storage and loading equipment. The raw coal cost also includes the related capital cost from the precleaning process. This includes heavy mediums cyclones, sieve bends, coal screens and coal centrifuges. The cost of handling the refuse from the precleaning process is combined with the cost of handling the refuse from the HLR subcircuit. This direct capital cost for refuse handling includes refuse sump, explosion proof pump, refuse thickening cyclone, centrifuges and refuse stripping system. The direct capital cost is determined by these equations:

$$DC_r = \$\ 22,524\ m_r^{0.7} \times [C_{idx} / C_{idx,1984}] \tag{10.6}$$

$$DC_{hlcequip} = \$22,528\ m_{precleaned}^{0.7} \times [C_{idx} / C_{idx,1984}] \tag{10.7}$$

$$DC_{liqrec} = \$\ 30,643\ (m_{liqnew} + m_{ligrec})^{0.7} \times [C_{idx} / C_{idx,1984}]$$

$$= \$\ 30,643 \times (Rm_r)^{0.7} \times [C_{idx} / C_{idx,1984}] \tag{10.8}$$

$$DC_{ref} = \$33,514\ m_{ref}^{0.7} \times [C_{idx} / C_{idx,1984}] \tag{10.9}$$

$$DC_{drier} = \$153,000\ m_{evapwater}^{0.7} \times [C_{idx} / C_{idx,1984}] \tag{10.10}$$

$$DC_{coalsampling} = \$324,000 \times [C_{idx} / C_{idx,1980}] \tag{10.11}$$

The direct capital cost for the HLC subcircuit equipment covers the cost for the 20,000 gallon cast iron conditioning tank, agitator of 200 horsepower, cyclone feed pump and three set of cyclones -- primary, cleaner and scavenger. Clean coal sump, pump, coal thickening cyclone, drum filter and clean coal stripping system are included in DC_{clean}.

The total direct capital cost is found by adding Equation (10.6) through (10.11)

$$TDC = DC_r + DC_{hlcequip} + DC_{liqrec} + DC_{ref} + DC_{drier} - DC_{coalsampling}$$

The indirect capital and contingencies costs are estimated to be 56% of the direct capital cost. Therefore, the total capital cost, which is depreciated over the life of the plant is

$$TCC = 1.56\ TDC$$

The total capital cost is annualized as follows:

$$d = [(1 + i)/(1 + p) - 1]$$

where i is the interest rate and p is the inflation rate. Therefore, capital recover factor is

$$CRF = d / [1 - (1 + d)^{-n}]$$

Working capital is estimated to be 25% of the labor, maintenance, electricity, water, waste disposal and heavy liquid costs as in the conventional plant model described in Chapter 2.

$$W_c = 0.25 (AC_{labor} + AC_{maint} + AC_{elect} + AC_{water} + AC_{waste} + AC_{liq} + AC_{steam})$$

As in Chapter 2, the capital cost in ($ per dry ton of clean coal) is

$$C_{capital} = [dW_c + [(TCC \times CRF) / (m_o \times h)]] \tag{10.12}$$

10.5.2 Operating and Maintenance Cost

The annual operating and maintenance costs comprise several cost elements, including labor, maintenance, raw material and waste disposal costs, also taxes, insurance and general administrative overhead. The operating and maintenance cost is broken down into nine components.

- heavy liquid
- electricity
- labor
- maintenance
- payroll overhead
- taxes and insurance
- waste disposal
- water
- steam

Table 10-1 shows the cost factors for various components. The total annual cost of heavy liquid in $/ton of clean coal is estimated to be

$$AC_{liq} = [c \times m_{liqnew}]] / m_o$$

The cost of labor is estimated to be dependent of plant size. Maintenance costs, taxes and insurance are estimated to be proportional to the total capital cost of the plant. The cost of electricity is linked to the mass flow rate of the coal entering the plant, while the cost of waste disposal is proportional to the quantity of coal rejected. The cost for water is proportional to the amount of water in the clean coal and refuse streams. Overhead costs are based on labor, maintenance and heavy liquid costs. The equations for these costs are

$$AC_{elect} = e / Y_{tot} \times [C_{idx} / C_{idx,1980}]$$

$$AC_{labor} = l / m_o \times [C_{idx} / C_{idx,1980}]$$

$$AC_{maint} = [m_L \ TCC] / [m_o h]$$

$$AC_{payovh} = 0.30 \ AC_{labor}$$

$$AC_{pltovh} = 0.26 [AC_{labor} + AC_{maint} + AC_{liq}]$$

$$AC_{tax} = [t \ TCC] / [m_o h]$$

$$AC_{waste} = [r \ m_{ref}] / m_o RC \times [C_{idx} / C_{idx,1980}]$$

$$AC_{water} = [\, w\ 240\ W\,] / m_o \times [C_{idx} / C_{idx,1980}]$$

$$AC_{steam} = s \times m_{steam} / m_o \times [C_{idx} / C_{idx,1980}]$$

where e, l, m, r, s and w are taken from Table 10-1. Adding the above equations and converting to a base year yields:

$$C_{operating} = C_{idx} (AC_{liq} + AC_{elect} + AC_{labor} + AC_{maint} + AC_{payovh} + AC_{pltovh} + AC_{tax} + AC_{waste} + AC_{water} + AC_{steam} \qquad (10.13)$$

The total cost for clean coal is found by adding Equations (10.5), (10.12), (10.13) and the raw coal cost

$$C_{total} = C_{raw} + C_{ref} + C_{operating} + C_{capital}$$

Table 10-1: Operating Cost Factors (1980 $)

Variable Cost Elements	Symbol Definition	Value
Electricity	e ($/raw ton)	1.560
Labor	l ($/hr)	268.000
Maintenance	mt (fraction)	0.045
Refuse Disposal	r ($/wet ton)	1.200
Taxes	t (fraction)	0.040
Water	w ($/1000 gallon)	0.180
Heavy Liquid	c ($/lb)	0.800

10.6 Illustrative Results

Experimental HLC process done by PTI on Pittsburgh coal and Illinois No.6 coal is shown in Table 10-2. In this process the heavy liquid used is methylene chloride. Methylene chloride is chosen over Freon-113 (another heavy liquid considered) since the lower specific gravity of methylene chloride (s.g. 1.33) will give better product quality than the process based on Freon-113 (s.g. 1.57). The relevant properties of methylene chloride and Freon-113 are listed in Table 10-3.

Table 10-2: HLC Feed Coal and Clean Coal Quality (53)

Performance parameter	Pittsburgh No. 8	Illinois No.6
Feed Product Quality		
Ash %	40.9	25.30
Sulfur %	3.66	4.53
Pyritic sulfur %	2.83	2.24
Heating value (Btu/lb)	8260	10580.
lb $SO_2/10^6$Btu	8.86	8.56
Product Quality		
Ash %	1.67	2.52
Pyritic sulfur %	0.45	0.55
Heating value (Btu/lb)	14150.	13520.
lb $SO_2/10^6$Btu	2.37	3.72
Performance		
% Ash removal	94.70	82.80
% Ash reduction	89.50	81.80
% Sulfur removal	76.20	64.80
% Sulfur reduction	54.40	44.40
% Pyritic sulfur removal	90.60	81.00
% Pyritic sulfur reduction	84.10	75.40
% Btu Recovery	80.40	87.60

Table 10-3: Properties of Heavy Liquids

Liquid	Formula	Boiling Point, °C	Density, gm/cm^3	Heat of Vapor., cal/gm	Viscosity, cp	Toxicity	Solubility in Water, gm/gm
Freon-113	CCl_2F- $CClF_2$	47.6	1.57	35.0	0.68	non-toxic	insoluble
Methylene Chloride	CH_2Cl_2	40.0	1.33	89.0	0.45	High	0.02

PTI had also performed experiments of the HLC process without the precleaned subcircuit for the Pittsburgh coal. The product qualities found could not come close to meeting the quality requirements for clean coal products. It was found necessary to have the precleaned subcircuit. Table 10-4 shows the comparisons between the quality product coal of HLC process with and without precleaned subcircuit.

10.7 Sensitivity Results

The key design and operating parameters for HLC process considered were:

1. Coal Grind—minimum size that could be run without degradation in cyclone performance.
2. Solids Concentration—maximum capacity of the 2" and 1" cyclones before pulp density became a hindrance in the separation.

Analyzing PTI's experimental result of the HLC process we found that the value of the parameters vary with coal type. It can be summarized as follows:

10.7.1 Illinois Coal

A much lower reduction in ash values was obtained with the 200 mesh grind than with the 100 mesh grind. However, the ash reduction did not come without a loss in thermal recovery. For example, it was possible to achieve ash reductions in excess of 80% with corresponding thermal recoveries of 72% - 74%. It is realized that ash values in clean coal product of less than 4% are not theoretically possible, even if the coal is ground below 325 mesh.

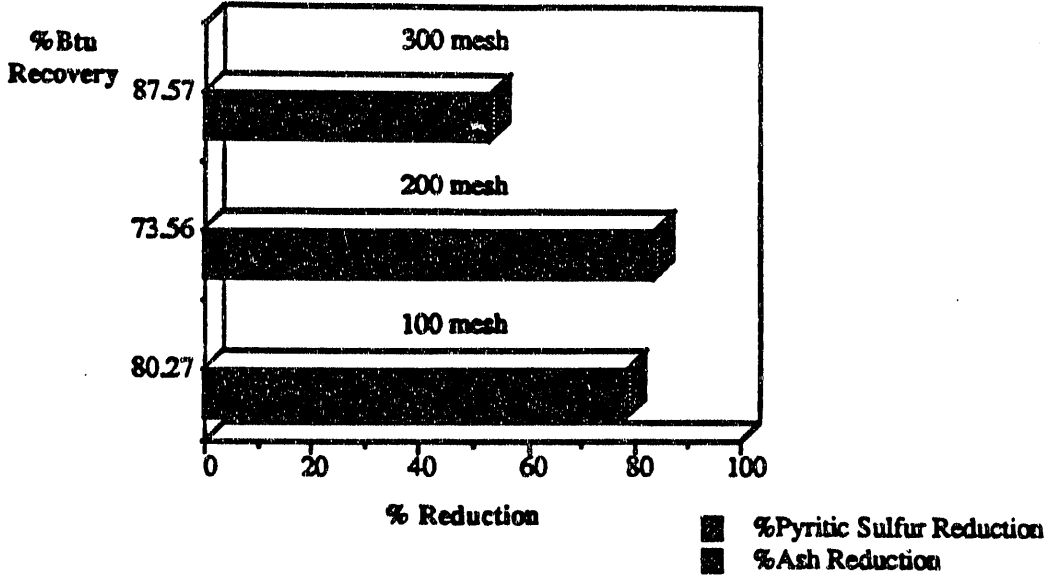
When the coal was ground to pass 325 mesh, the cyclone efficiency degraded. The ash values achieved in the clean coal product was 11% -12% at a resultant thermal recovery of 88%. Since it is theoretically possible to achieve somewhat lower ash levels at 80% recovery, this result indicates that the cyclone efficiency began deteriorating at 325 mesh. Table 10-3 shows the experimental results of grind size on product performance. The results are graphically displayed in Figures 10-3 and 10-4.

Table 10-4: The Effect of Precleaned Subcircuit on Pittsburgh coal(53)
100 mesh grind size, 5% solids, inlet pressure of 15 psi

Performance Parameter	Pittsburgh No. 8	Illinois No.6
Feed Product Quality		
Weight %	100.00	72.50
Ash %	40.90	24.56
Sulfur %	3.66	3.52
Pyritic sulfur %	2.83	2.60
lb $SO_2/10^6$Btu	8.86	6.44
Heating value (Btu/lb)	8260.	10937.
Product Quality		
Weight %	35.08	46.72
Ash %	22.03	5.33
Sulfur %	not determined	1.72
Pyritic sulfur %	not determined	0.41
lb $SO_2/10^6$Btu	not determined	2.46
Heating value (Btu/lb)	11342	13980
% Btu Recovery	49.00	80.44
% Ash reduction	46.10	84.96
% Sulfur reduction	not determined	53.01
% Pyritic sulfur reduction	not determined	85.51
% Ash red./10^6Btu	61.42	92.43
% Sulfur red./10^6Btu	not determined	72.71
% Pyritic sulfur red./10^6Btu	not determined	91.59
% Ash removal	83.07	93.37
% Pyritic sulfur removal	not determined	91.96

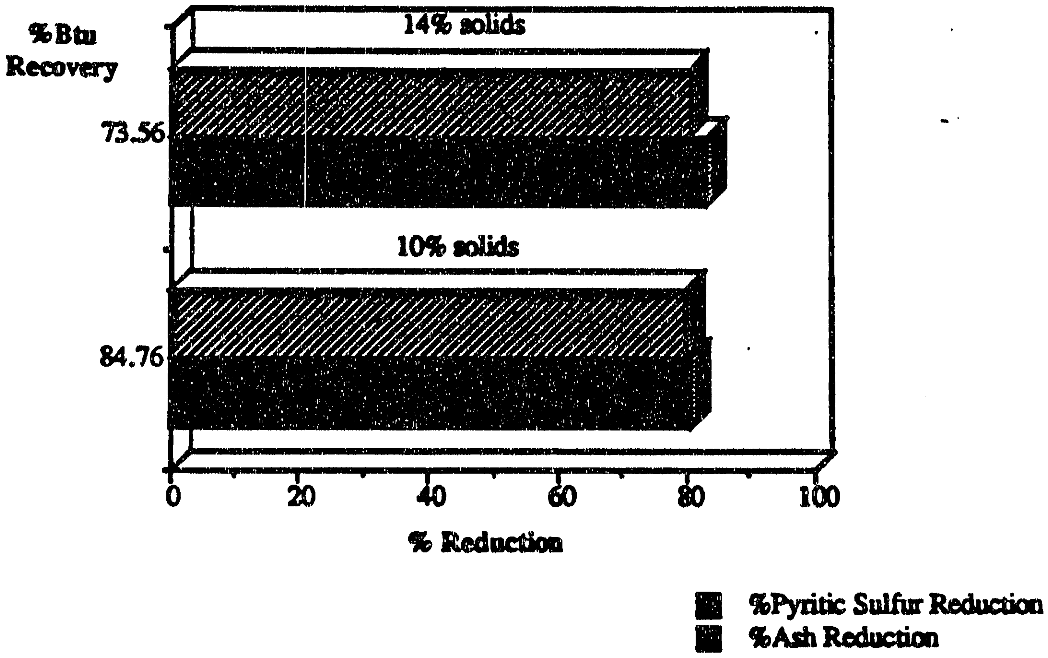
The effect of solids concentration using 10, 15, 20 and 25 percent solids by weight on the heavy cyclones showed that thermal recovery is optimum at medium solids (i.e. 10% by weight). However, there also is a trade-off in that lower ash values are achieved at lower concentrations.

Figure 10-3: Illinois #6: Grind Size vs. Grade Recovery
(% Btu rec., %Ash red., %Pyritic Sulfur red.)



note: % Pyritic Sulfur reduction for 300 mesh
is not Available
Clean coal product based on ROM coal

Figure 10-4: Illinois #6: Effect of Solid Concentration on Performance



note: Clean coal product based on ROM coal

A most encouraging results in this test work occurred with respect to the pyritic sulfur removal. Usually, the pyritic sulfur removals were greater than 79%. The most important aspect of these results was that they were consistent irrespective of thermal recoveries. Pyritic sulfur removals were consistently between 80-90% while Btu recoveries ranged from under 29% to over 77%. These results are encouraging in that the efficiency of the cyclone appears to remain high with respect to pyritic sulfur removal, even when ash removal may suffer. Pyritic sulfur removal always exceeded ash removal showing that the cyclone is more selective with respect to pyrites.

Table 10-5: Coal Quality vs. Coal Size (Illinois No. 6 Coal)(53)
Process: HLC - 15 psi
Coal type: precleaned Illinois #6 ; 5% solids

Feed Quality	Wt %	A%	S%	PS%	lb $SO_2/10^6$	Btu	%Btu Rec
Rom Feed	100.00	25.29	4.53	2.24	8.56	10580.	100.00
Precleaned Feed	89.50	17.40	3.28	1.65	5.66	11582.	97.98

Coal size:	100 mesh	200 mesh	300 mesh
Product Quality			
Weight %	63.38	57.27	74.48
Ash %	5.43	4.14	11.97
Sulfur %	2.33	2.50	2.77
Pyritic sulfur %	0.28	0.43	not available
Heating value (Btu/lb)	13399.00	13589.	12438.
% Btu Recovery	80.27	73.56	87.57
% Ash reduction	78.52	83.64	52.66
% Sulfur reduction	48.65	44.85	38.76
% Pyritic sulfur red.	87.31	80.74	not available

note: Clean coal products based on ROM coal

10.7.2 Pittsburgh No. 8 Coal

During the test program, the previous 100 mesh grind tests were compared to additional tests run at 200 mesh grinds. Specifically, tests were run at smaller apex diameters in an attempt to increase thermal recoveries. Although the ash in the clean coal product remained low, hovering around 4.5% -5.5%, thermal recoveries did not dramatically improve. When the coal was ground to pass 200 mesh, slightly better thermal recoveries were achieved. However, a considerable amount of ash reported to the cyclone overflow when the apex was constricted in this manner. This can be observed in Table 10-6 and Figures 10-5 and 10-6.

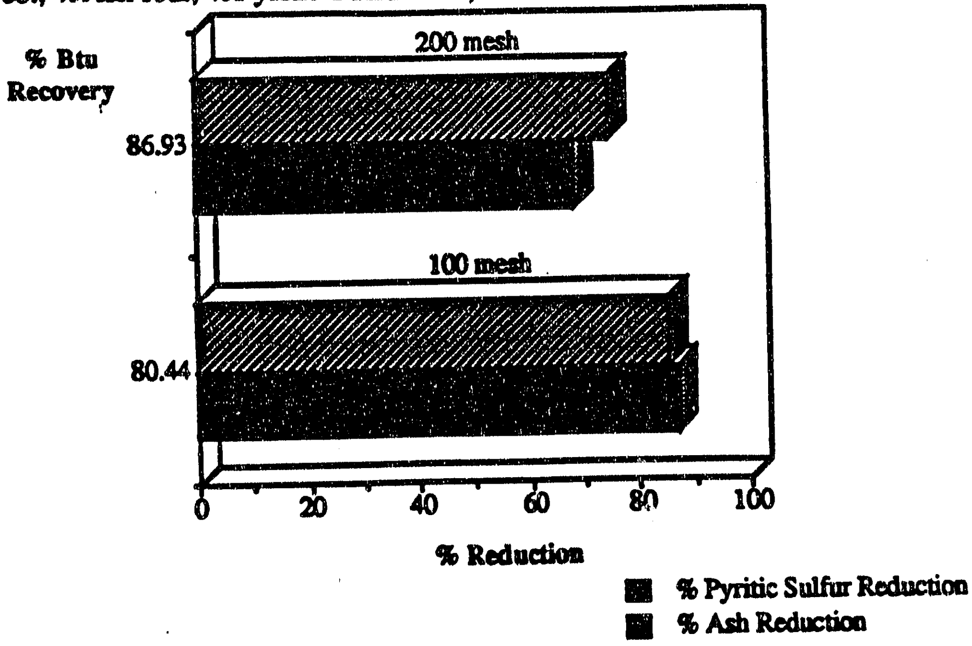
Table 10-6: Coal Quality vs. Coal Size (Pittsburgh No. 8 Coal)(53)
Process: HLC - 15 psi
Coal type: precleaned Pittsburgh ; 5% solids

Feed Quality	Wt %	A%	S%	PS%	lb $SO_2/10^6$	Btu	%Btu Rec
ROM Feed	100.00	40.80	3.66	2.83	9.02	8119	100.00
Precleaned Feed	72.50	24.56	3.52	2.60	6.44	10937	97.67

Coal size:	100 mesh	200 mesh
Product Quality		
Weight %	46.72	54.68
Ash %	5.33	12.78
Sulfur %	1.72	1.94
Pyritic sulfur %	0.41	0.71
Heating value (Btu/lb)	13980.	12906.
% Btu Recovery	80.44	86.93
% Ash reduction	86.96	68.73
% Sulfur reduction	53.01	46.98
% Pyritic sulfur reduction	85.51	74.98

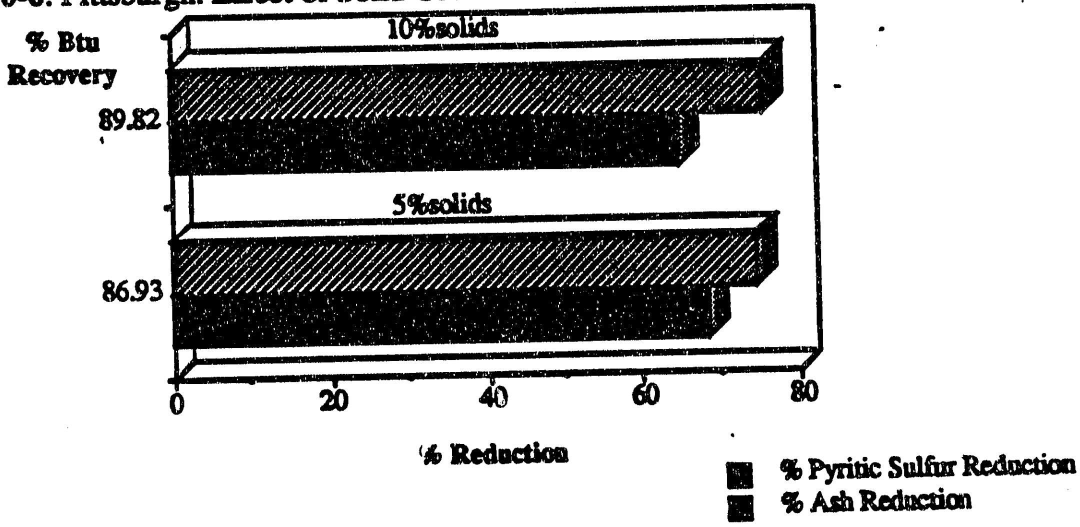
note: Clean coal products based on ROM coal

Figure 10-5: Pittsburgh: Grind Size vs. Grade Recovery
(% Btu rec., %Ash red., %Pyritic Sulfur red.)



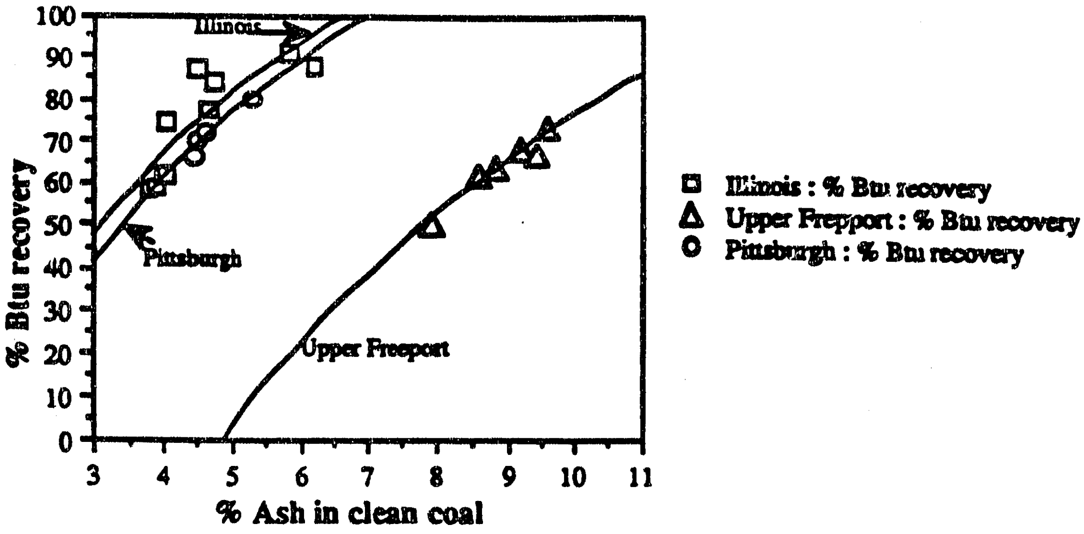
note: Clean coal product based on ROM coal

Figure 10-6: Pittsburgh: Effect of Solid Concentration on Performance



note: Clean coal product based on ROM coal

Figure 10-7: Grade / Recovery vs. A_{clean}



Illinois:
% Btu recovery = -25.387 + 152.33*log(Aclean) R^2 = 0.727
Upper Freeport:
% Btu recovery = -167.11 + 243.38*log(Aclean) R^2 = 0.942
Pittsburgh:
% Btu recovery = -35.353 + 159.77*log(Aclean) R^2 = 0.927

A grade recovery plots of %Btu recovery vs. % ash content of clean coal shown in Figure 10-7. A similar grade recovery plot between the Btu recovery and pyritic sulfur removal is presented in Figure 10-8. Regressing both plots, relationships between Btu recovery and clean ash and Btu recovery and pyritic sulfur removal were obtained :

Illinois No. 6:

$$\% \text{ Btu recovery} = -25.387 + 152.33 \times \log(A_{clean})$$

$$\% \text{ Btu recovery} = 96.439 + 0.1337 \times PS_{clean} - 0.004 \times PS_{clean}^2$$

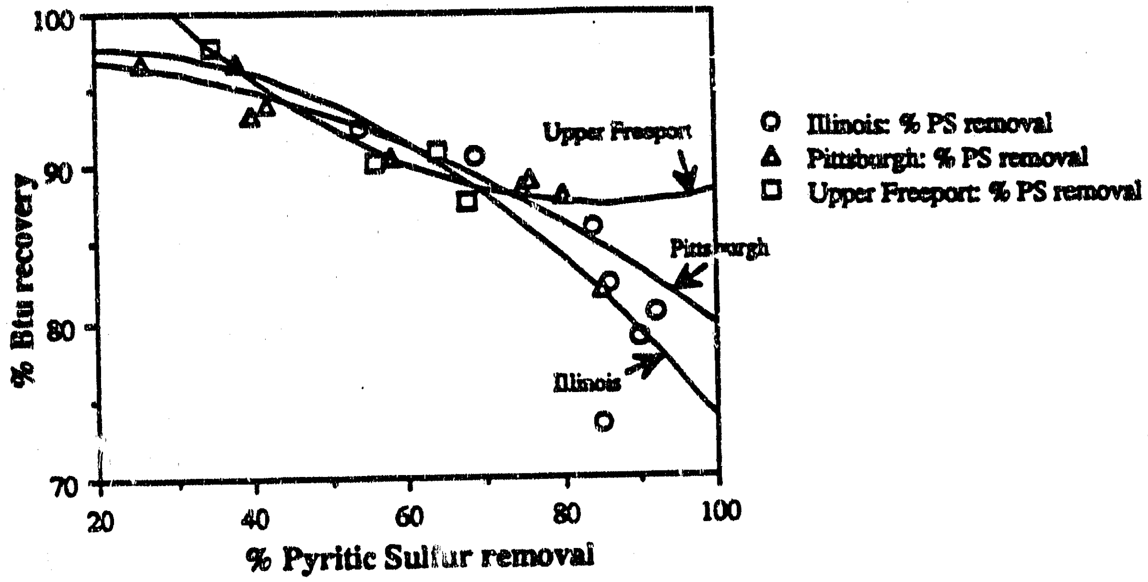
Pittsburgh No. 8:

$$\% \text{ Btu recovery} = -35.353 + 159.77 \times \log(A_{clean})$$

$$\% \text{ Btu recovery} = 97.119 + 0.023 \times PS_{clean} - 0.020 \times PS_{clean}^2$$

In incorporating the economic model for Illinois #6 and Pittsburgh #8 to predict the cost of cleaning the coal, the performance data of 10% solid concentration and 100 mesh grind size of the two types of coal is used. A summary of performance and costs for Illinois #6 and Pittsburgh coals to produce an output of 500 tons per hour is presented in Table 10-7, 10-8 and 10-9.

Figure 10-8: Grade / Recovery vs. PS_{clean}



Illinois:
% Btu recovery = 96.439 + 0.134*PSclean - 0.004*PSclean^2 R^2 = 0.650
Pittsburgh:
% Btu recovery = 97.119 + 0.023*PSclean - 0.020*PSclean^2 R^2 = 0.884
Upper Freeport:
% Btu recovery = 116.73 - 0.682*PSclean + 0.004*PSclean^2 R^2 = 0.921

10.8 Numerical Example

Type of coal = Illinois #6
Size = 100 mesh (5% solids)
Heavy Liquid = Methylene Chloride
R = 5.60
p = 0.06
i = 0.13
n = 25
C_{sol} = 2%
m_o = 500 tons/hr
h = 5500 hrs/yr

10.8.1 Performance Model

Clean coal characteristics:

%Ash clean = 5.43

$Y_{precleaned} = 0.895$

$\% \text{ Btu recovery} = -25.387 + 152.33 \times \log(A_{clean})$

$\% \text{ Btu recovery} = -25.387 + 152.33 \times \log 5.43 = 86.5\%$

$\% \text{ Btu recovery} = 96.439 + 0.1337 \times PS_{clean} - 0.004 \times PS_{clean}^2$

or

$0 = 0.004 \times PS_{clean}^2 - 0.1337 \times PS_{clean} - 96.439 + 86.5$

$0 = 0.004 \times PS_{clean}^2 - 33.425 \times PS_{clean} - 9.939$

$0 = PS_{clean}^2 - 33.425 \times PS_{clean} - 2484.75$

$PS_{clean} = \{(33.425) + [(33.425^2) + (4 \times 1 \times 2484.75)]^{1.5}\} / 2 \times 1$

$= 69.3\%$ pyrites removed

$HHV_{clean} = HHV_r [1 - A_{clean} / 1 - A_r]$

$= 10,580 [1 - 0.0543 / 1 - 0.2529]$

$= 13,392$ Btu

The weight of water evaporated per pound of dry into thermal coal drie

$m_{evapwater}' = m_{inmois}' - m_{outmois}' / [(1 - m_{inmois}')(1 - m_{outmois}')]$

$= 0.28 - 0.05 / [(1 - 0.28)(1 - 0.05)]$

$= 0.336$

The amount of energy needed to evaporate this water is

$E_d = 1020 m_{evapwater}' / \varepsilon$

$= [1020 \times 0.336] / 0.55$

$= 623.6$ Btu/lb

The lower heating value:

$LHV = 0.96\, HHV_{clean} - [(1020\, m_{outmois}') / (1 - m_{outmois}')]$

$= 0.96 \times 13,392 - [(1020 \times 0.05) / (1 - 0.05)]$

$= 12,803.1$ Btu/lb

The drier yield:

$Y_{drier} = 1 - E_d / LHV$

$= 1 - (623.6 / 12,803.1)$

$= 0.9513$

The plant yield:

$Y_{total} = Y_{precleaned} Y_{clean} Y_{drier}$

$= 0.895 \times 0.634 \times 0.951$

$= 0.540$

The weight of water evaporated:

$m_{evapwater} = m_o [m_{evapwater}' / Y_{drier}]$

$= 500 \times (0.336 / 0.9513)$

$= 176.7$ tph

Dry mass flow rate of raw coal input:

$m_r = m_o / Y_{total}$

$= 500 / 0.540$

$= 925.9$ tph

Dry mass flow rate of precleaned coal to HLC process:

$$\begin{aligned} m_{precleaned} &= Y_{precleaned} \times m_r \\ &= 0.895 \times 925.9 \\ &= 829.3 \text{ tph} \end{aligned}$$

Mass flow rate of methylene chloride input (dry basis)

$$\begin{aligned} m_{liq} &= 5.60\ m_{precleaned} \\ &= 5.60 \times 829.3 \\ &= 4644.0 \text{ tph} \end{aligned}$$

Dry mass flow rate of cleaned coal entering the thermal drier:

$$\begin{aligned} m_{dry} &= m_o / Y_{drier} \\ &= 500 / 0.951 \\ &= 525.6 \text{ tph} \end{aligned}$$

Dry mass flow rate of refuse coal:

$$\begin{aligned} m_{ref} &= m_{precleaned} - m_{dry} \\ &= 829.3 - 525.6 \\ &= 401 \text{ tph} \end{aligned}$$

Water loss in the coal cleaning plant:

$$\begin{aligned} W &= m_{dry} [(1 / (1 - m_{inmois'})) -1] + m_{ref} [(1 / RC) - 1] \\ &= 525.6 [(1 / (1 - 0.28)) -1] + 401 [(1 / 0.35) - 1] \\ &= 949.1 \text{ tph} \end{aligned}$$

Total mass flow rate of steam for the stripping system in (tons/hr)

$$\begin{aligned} m_{steam} &= 65.0 \times 10^{-3} \cdot m_{liq} \\ &= 65.0 \times 10\text{-}3 \cdot 4644.0 \\ &= 301.9 + ph \end{aligned}$$

Total mass flow rate of coolant for the stripping system in (tons/hr)

$$\begin{aligned} m_{water} &= m_{waterclean} + m_{water\ ref} \\ &= 2.37\ m_{liqstripclean} + 2.37\ m_{liqstripref} \\ &= 2.37\ (m_{liqstripclean} + m_{liqstripref}) \\ &= 2.37 \times 2024.8 \\ &= 4{,}798.8 \text{ tph} \end{aligned}$$

Mass flow rate of methylene chloride lost to water

$$\begin{aligned} m_{liqlosttowater} &= C_{sol} \times W \\ &= 0.02 \times 949.1 \\ &= 18.98 \text{ tph} \end{aligned}$$

Mass flow rate of methylene chloride lost to atmosphere

$$\begin{aligned} m_{liqlosttoatm} &= 0.00035 \times m_{precleaned} \\ &= 0.00035 \times 829.3 \\ &= 0.29 \text{ tph} \end{aligned}$$

Mass flow rate of new heavy liquid in tons per hour

$$\begin{aligned} m_{liqnew} &= 18.98 + 0.29 \\ &= 19.27 \text{ tph} \end{aligned}$$

10.8.2 Economic Model

Capital Cost:

$$\begin{aligned}
DC_r &= \$\,22,524\ m_r^{0.7} \\
&= \$\,22,524 \times (926.575)^{0.7} \\
&= \$2,688,202
\end{aligned}$$

$$\begin{aligned}
DC_{hlcequip} &= \$22,528\ m_{precleaned}^{0.7} \\
&= \$22,528 \times 829.3^{0.7} \\
&= \$2,487,798 \\
DC_{liqrec} &= \$\,30,643\ R^{0.7} m_r^{0.7} \\
&= \$\,30,643 \times 5.66^{0.7} \times 926.575^{0.7} \\
&= \$19,153,152 \\
DC_{ref} &= \$33,514\ m_{ref}^{0.7} \\
&= \$33,514 \times 401^{0.7} \\
&= \$2,225,399 \\
DC_{drier} &= \$153,000\ m_{evapwater}^{0.7} \\
&= \$153,000 \times 176.74^{0.7} \\
&= \$153,037 \\
TDC &= \$2,688,202 + \$2,487,798 + \$19,153,152 + \$2,225,399 + \$153,037 \\
&= \$41,663,840 \\
TCC &= 1.56 \times TDC \\
&= 1.56 \times \$41,663,840 \\
&= \$41,663,840
\end{aligned}$$

Annual Cost

$$\begin{aligned}
AC_{liq} &= [\,(Rcm_{precleaned}) + [\,c \times (m_{liqnewt})]\,] / m_o \\
&= (\,5.60 \times 0.8 \times 829.3 + 0.8 \times 18.981\,) / 500 \\
&= \$7.54/\text{ton} \\
AC_{elect} &= e / Y_{tot} \\
&= 1.56 / 0.540 \\
&= \$2.89/\text{ton} \\
AC_{labor} &= l / m_o \\
&= 268 / 500 \\
&= \$0.54/\text{ton} \\
AC_{maint} &= [\,m_t.\ TCC\,] / [\,m_o\, h\,] \\
&= [\,0.045 \times \$41,663,840\,] / [\,500 \times 5500\,] \\
&= \$0.68/\text{ton} \\
AC_{payovh} &= 0.30\ AC_{labor} \\
&= 0.30 \times \$0.536 \\
&= \$0.16/\text{ton} \\
AC_{pltovh} &= 0.26\,[\,AC_{labor} + AC_{maint} + AC_{liq}\,] \\
&= 0.26\,(\,\$0.536 + \$0.6818 + \$7.5404\,) \\
&= \$2.28/\text{ton}
\end{aligned}$$

$$\begin{aligned}
AC_{tax} &= [\,t\,TCC\,] / [\,m_o\,h\,] \\
&= [\,0.04 \times \$41{,}663{,}840\,] / [\,500 \times 5500\,] \\
&= 0.61/\text{ton} \\
AC_{waste} &= [\,r\,m_{ref}\,] / m_o\,RC \\
&= [\,1.2 \times 401\,] / [\,500 \times 0.35\,] \\
&= \$2.75/\text{ton} \\
AC_{water} &= [\,w\,240\,W\,] / m_o \\
&= (0.18/1000) \times 240 \times 949.1/500 \\
&= \$0.08/\text{ton}
\end{aligned}$$

Working Capital

$$\begin{aligned}
W_c &= 0.25\,(\,AC_{labor} + AC_{maint} + AC_{elect} + AC_{water} + AC_{waste} + AC_{liq}\,) \\
&= 0.25\,(\,\$0.54 + \$0.82 + \$2.89 + \$0.08 + \$2.75 + \$7.54\,) \\
&= \$3.66/\text{ton}
\end{aligned}$$

Cleaning Cost is then:

$$\begin{aligned}
C_r &= \$25.35 \text{ (see Table 10-7)} \\
C_{ref} &= C_r\,[(1/Y_{total}) - 1] \\
&= \$25.35\,[\,(1/\,0.540) - 1] \\
&= \$21.60/\text{ton} \\
C_{operating} &= C_{idx}\,(AC_{liq} + AC_{elect} + AC_{labor} + AC_{maint} + AC_{payovh} + AC_{pltovh} \\
&\quad + AC_{tax} + AC_{waste} + AC_{water}\,) \\
&= 1.193\,(\$7.54 + \$2.89 + \$0.54 + \$0.82 + \$0.16 + \$2.31 \\
&\quad + \$0.73 + \$2.75 + \$0.082\,) \\
&= \$21.27/\text{ton} \\
C_{capital} &= dW_c + [\,(\,TCC \times CRF\,) / (\,m_o \times h\,)\,] \\
&= [\,0.066 \times \$3.66] + [\,(\,\$50{,}357{,}033 \times 0.083\,) / (\,500 \times 5500\,)\,] \\
&= \$2.10/\text{ton} \\
C_{total} &= C_r + C_{ref} + C_{operating} + C_{capital} \\
&= \$25.00 + \$21.33 + \$21.27 + \$2.10 \\
&= \$69.70/\text{ton}
\end{aligned}$$

A summary of total cleaned coal cost components appears in Table 10-7 for both the Illinois and Pittsburgh coals. Breakdowns of O&M costs and total capital costs appear in Tables 10-8 and 10-9, respectively. Graphical comparisons of total coal cost and capital cost appear in Figures 10-9 and 10-10.

Table 10-7: Components of Total Coal Cost (1984$ / dry ton of clean coal)

Components	Illinois #6	Pittsburgh
Raw*	25.35	21.17
Capital	2.10	2.69
Operating	21.27	32.65
Refuse	21.60	43.20
Total	70.32	99.71

* See footnote to Table 9-4 for explanation of input coal prices.

Table 10-8: Breakdown of the Operating and Maintenance Cost (1984$ / dry to of clean coal)

Components	Illinois #6	Pittsburgh
Heavy Liquids	7.54	9.94
Electricity	2.89	4.74
Labor	0.54	0.54
Maintenance	0.82	1.02
Payroll Overhead	0.16	0.16
Plant Overhead	2.31	2.99
Taxes & Insurance	0.73	0.90
Waste Disposal	2.75	6.89
Water	0.08	0.18

Table 10-9: Breakdown of the Capital Cost (Million 1984$)

Components	Illinois #6	Pittsburgh #8
Raw Coal	2.688	3.802
HLC Equip.	2.488	3.036
HLR Equip.	19.153	23.128
Refuse Coal	2.225	4.235
Thermal Drier	5.726	5.645

Figure 10-9: Components of Total Coal Cost
(1989$ / dry ton of clean coal)

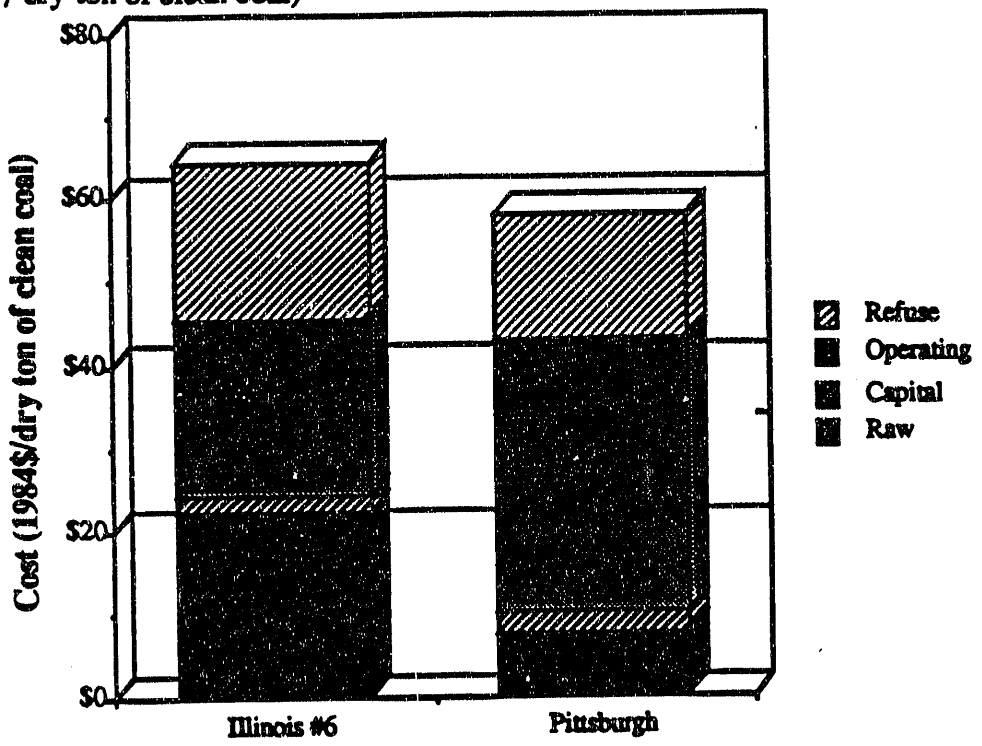
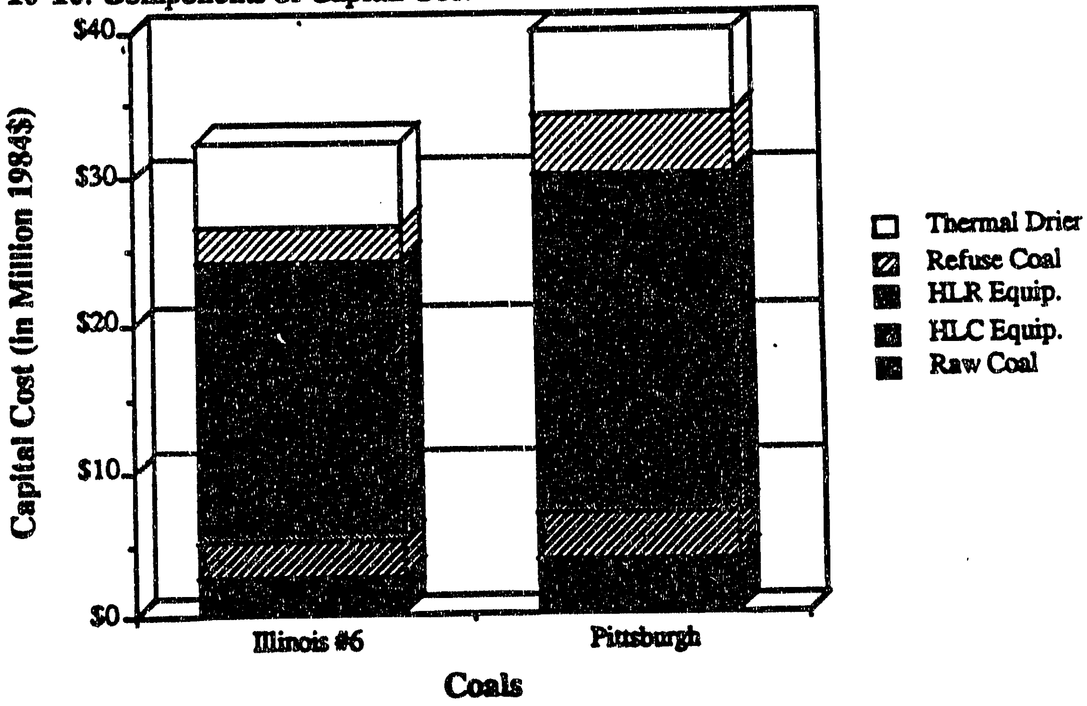


Figure 10-10: Components of Capital Cost



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APPENDIX

Illustrative Case Studies

PROBABILISTIC MODELING OF ADVANCED SO_2/NO_x CONTROL TECHNOLOGY

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Presented at:
1990 AIChE Summer National Meeting
August 19-22, 1990

INTRODUCTION

The purpose of research is to provide and improve information regarding the feasibility, optimal designs, promising applications, uncertainties and risks associated with a new process. The information generated from research can be used by process developers to refine a technology and ultimately by potential process adopters to make a decision about whether, and under what circumstances, to use the new technology. Of concern to process developers is the prioritization of research needs and an understanding of the barriers that exist between a conceptual design and commercial adoption of an environmental control technology. Which technologies are the most promising for further process development? What conditions favor the selection of the new technology? What specific technical areas require more research? What economic and cost uncertainties affect the economic feasibility of the technology? How much funding should reasonably be committed to further research?

This paper presents a research planning method that can be used to help answer these questions. The salient features of the method include:

- Development of engineering performance and cost models
- A probabilistic modeling capability to incorporate uncertainties
- Judgments regarding uncertainties, likely applications, and the outcome of additional research
- Exercising of the models to answer these questions:
  - What are the key process design trade-offs?
  - What uncertainties most affect the overall costs?
  - What are the potential pay-offs and risks vis-a-vis conventional technology?
  - What is the likely effect and value of additional research?
- Decision analysis to select a course of action

SCOPE OF THIS PAPER

An example of a technology innovation for pollution control of a coal-fired power plant is used to illustrate the research planning method outlined above. The purpose of the method is to provide a systematic approach to evaluating research priorities and the value of additional research. An engineering process model is required to characterize key performance and cost interactions. Because many performance and cost parameters are uncertain during the early research phase of a technology, a probabilistic modeling capability is required to analyze the effects of these uncertainties on process feasibility. Judgments about the possible outcomes of additional research provide a basis for estimating the value of such activity and, therefore, for bounding research funding. A decision analysis for one case study is discussed. Finally, the costs of a demonstration plant are considered.

INTEGRATED ENVIRONMENTAL CONTROL

With the prospect of increasingly stringent emission control has evolved the concept of integrated environmental control. The concept has several dimensions. One is to consider interactions among control methods for air, water, and solid waste emissions control. Another is the integrated use of pre-combustion, combustion, and post-combustion control methods (as distinct from one approach alone). A third dimension is the development of new processes for combined pollutant removal in lieu of separate processes for individual pollutants. Thus, integrated environmental control represents good design practice and provides opportunities to minimize costs for a given set of emission reduction requirements (Carr, 1986).

A conventional emission control system for a new coal-fired power plant typically consists of a wet limestone flue gas desulfurization (FGD) system for 90 percent SO_2 control, an electrostatic precipitator (ESP) for over 99 percent particulate matter (PM) removal, and combustion controls for about 50 percent NO_x reduction. The spent limestone reagent used in the FGD system is disposed of with the power plant solid waste. These systems are all commerically available and well-demonstrated. However, recent commercial experience in Japan and Germany with selective catalytic reduction (SCR) indicates that 80 to 90 percent NO_x removal may be feasible, although SCR has not yet been applied with U.S. coals (Robie, Ireland, and Cichanowicz, 1989).

The DOE Pittsburgh Energy Technology Center (PETC) has conducted research on a number of technologies that combine SO_2 and NO_x removal into a single reactor, and that reduce the solid waste produced by air pollution control systems. One of these technologies, which is used as a case study in this research, is the fluidized bed copper oxide process. Key features of the copper oxide process are that, unlike a wet FGD/SCR system, (1) it combines SO_2 and NO_x removal in a single reactor vessel; (2) it is regenerative (i.e. the reagent is reused rather than disposed of); and (3) it produces a saleable sulfur or sulfuric acid byproduct, in contrast to the sludge produced by FGD systems (Drummond et al, 1985). Schematic diagrams of a baseline FGD/SCR and an advanced, integrated copper oxide based system are shown in Figures 1 and 2, respectively.

Figure 2 illustrates some of the features of the copper oxide process. Briefly, a copper impregnated sorbent, consisting of small diameter aluminum spheres, circulates between a fluidized bed reactor, where SO_2 in the flue gas is removed by reaction with copper oxide in the sorbent, and a regenerator, in which SO_2 is evolved in a reaction of the sulfated sorbent with methane. The SO_2-rich gas from the regenerator is sent to an elemental sulfur or a sulfuric acid plant for byproduct recovery. The regenerated sorbent is returned to the absorber for another cycle. Factors such as the fluidized bed height and the amount of copper in the sorbent influence the sorbent mass flow rate. NO_x is removed from the flue gas by reaction with ammonia, which is injected into the flue gas upstream of the absorber. The absorber reactions are exothermic, increasing the temperature of the flue gas. This energy can be recovered in the power plant furnace, through additional preheating of the furnace combustion air by the power plant air preheater.

A PROBABILISTIC ENGINEERING MODEL

The copper oxide process is a technology in an early phase of development, for which limited test data and no commercial design or operating experience are available. Uncertainties in system performance at the commercial scale lead to uncertainties in capital and operating costs, which are the ultimate measures of interest for comparative analysis. Furthermore, even if process performance were known with certainty, uncertainties regarding the costs of equipment and

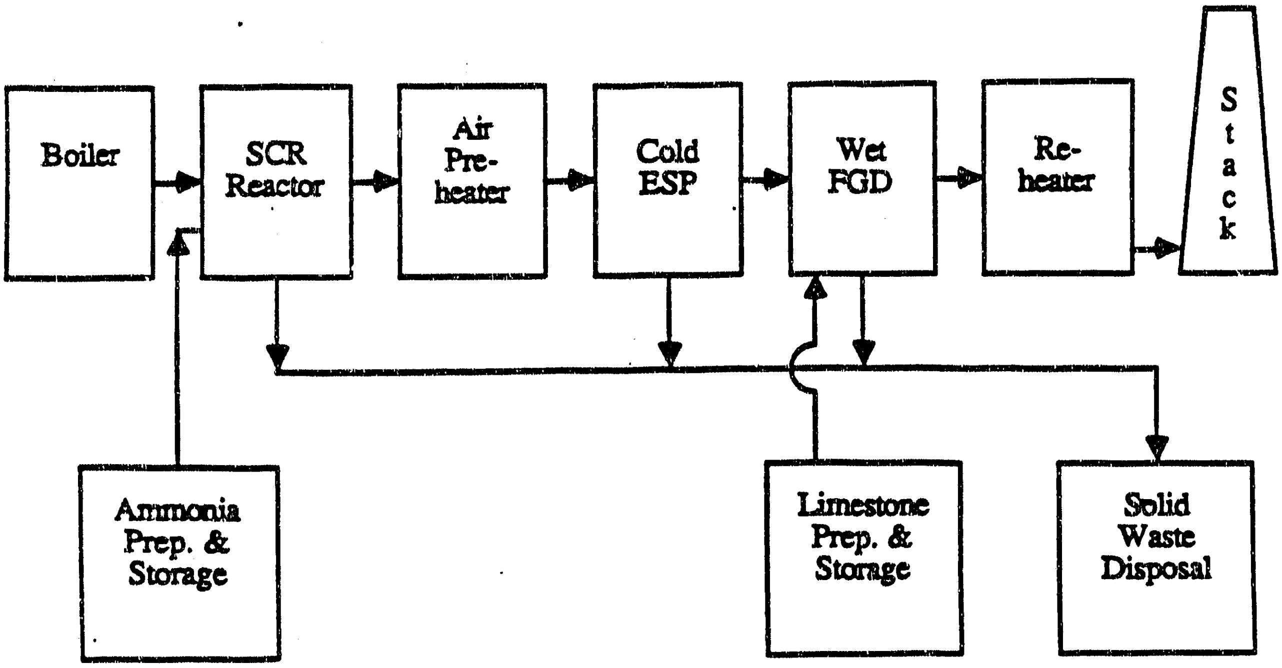

Figure 1. Power Plant Design with a FGD/SCR Emission Control System

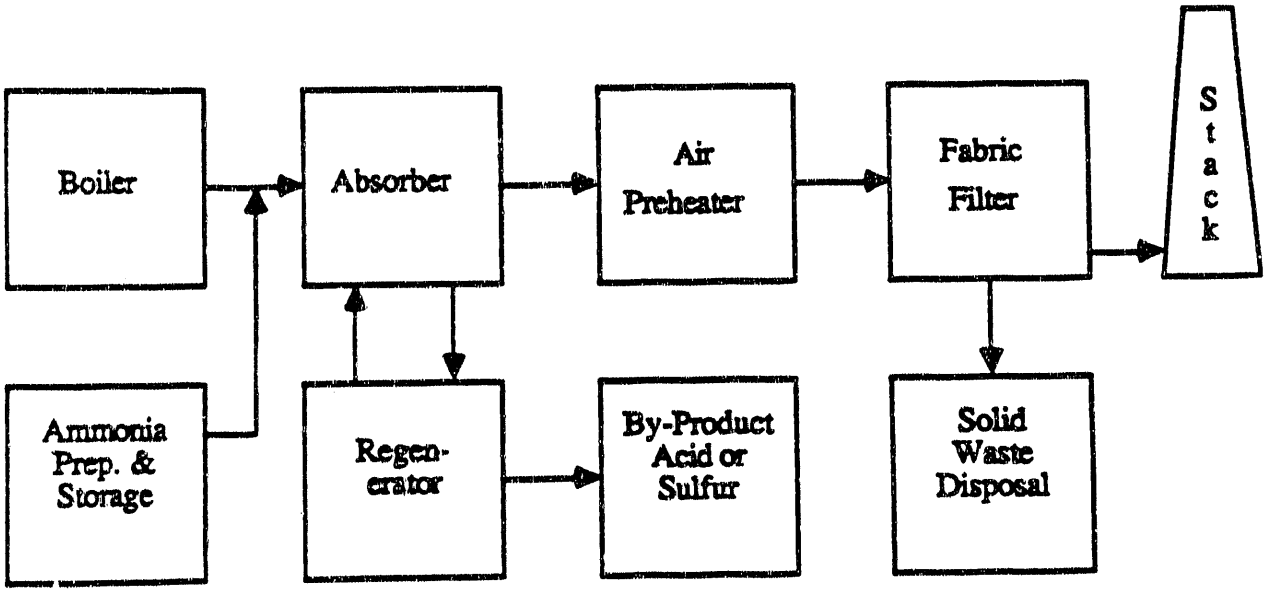

Figure 2. Power Plant Design with a Copper Oxide Emission Control System

reagents would remain. To explicitly characterize these uncertainties, and to evaluate the overall uncertainty in process costs, a probabilistic engineering modeling framework has been developed.

Analytic models for a conventional PC power plant, pre-combustion coal cleaning processes, and the components of conventional and advanced post-combustion pollution control systems are available as part of the Integrated Environmental Control Model (IECM), developed under contract to PETC by Rubin et al. (1986). Details of the copper oxide process model, plus models of the power plant air preheater and a sulfuric acid recovery plant, are described elsewhere (Frey, 1987).

The analytic models are based on mass and energy balances for key process equipment. The capital cost models are based on equipment cost estimates available in the literature, adjusted for plant size using key process stream flow rates and exponential scaling factors. Indirect costs are calculated based on the direct equipment costs. Variable and fixed operating costs are also calculated. The IECM has a capability to report costs in either constant or current dollars. Constant 1985 dollars, which are exclusive of inflation, are used in this analysis.

To characterize uncertainties in advanced emission control systems, the IECM is implemented in a modeling environment developed by Henrion for performing probabilistic analysis (Henrion, 1982; Henrion and Wishbow, 1987). The key uncertainties in process parameters can therefore be characterized using a variety of user-specified probability distribution functions. The resulting uncertainty distributions for model outputs are calculated using median Latin hypercube sampling, a variant of Monte Carlo simulation.

CASE STUDY: COPPER OXIDE VS. FGD/SCR

To illustrate the application of the research planning method, an integrated emission control system consisting of the copper oxide process with integrated coal cleaning, byproduct recovery, and energy recovery via the power plant air preheater, was compared with a conventional system consisting of wet FGD and SCR. Table 1 summarizes some of the key parameters, including emission constraints, base plant design, and financial parameters, assumed for this analysis. Both deterministic (nominal point-estimate) values and probability distributions are indicated in the table. Table 2 summarizes the different coals considered, including both unwashed and cleaned (30 percent sulfur reduction on an energy basis) coals. Table 3 summarizes key input values and distributions for the conventional wet FGD/SCR emission control system, which is taken as a technological baseline in this analysis. The main emphasis of this research will be on applying the research prioritization methodology to the copper oxide process, assuming the FGD/SCR system as benchmark. The key inputs and distributions assigned to the copper oxide emission control system are summarized in Table 4.

The selection of parameters for probabilistic representation was based on a review of reported information, statistical analysis, and judgments by process developers and the authors (Rubin et al., 1986; Frey, 1987; Rubin, Salmento, and Frey, 1988). The uncertainties are intended to represent the possible ranges that could be obtained in mature (i.e. fifth-of-a-kind) commercial units. The specification of uncertainties requires information or technical judgments about the possible range of values for a parameter and the likelihood of obtaining values within the range.

IDENTIFICATION OF KEY UNCERTAINTIES

The primary advantage of probabilistic simulation over traditional sensitivity analysis is the simultaneous incorporation of uncertainties in multiple model inputs. The resulting interactions among uncertain variables results in uncertainties in total costs, which are the basis for comparative analysis. Research can provide additional information about the uncertain input variables, resulting

Table 1: Selected Input Parameter Assumptions for Case Studies

Model Parameter	Deterministic (Nominal) Value	Probability Distribution	Values (or σ as % of mean)
Emission Constraints			
Nitrogen Oxides	90% Reduction		
Sulfur Oxides	90% Reduction		
Particulates	0.03 lb/MBtu		
Power Plant Parameters			
Gross Capacity	522 MW		
Gross Heat Rate	9500 Btu/kWh	-1/2 Normal	(1.8 %)
Capacity Factor	65 %	Normal	(7 %)
Excess Air (boiler/total)	20 %/39 %	Normal	(2.5 %)
Ash to Flue Gas	80 %		
Sulfur to Flue Gas	97.5 %		
Economizer Outlet Temp	700 °F		
Preheater Outlet Temp	300 °F		
Financial Parameters			
Inflation Rate	0 %		
Debt Fraction	50 %		
Common Stock Fraction	35 %		
Preferred Stock Fraction	15 %		
Real Return on Debt	4.6 %	Normal	(10 %)
Real Return on Com. Stock	8.7 %	Normal	(10 %)
Real Return on Pref. Stock	5.2 %	Normal	(10 %)
Federal Tax Rate	36.7 %		
State Tax Rate	2.0 %		
Ad Valorem Rate	2.0 %		
Investment Tax Credit	0 %		
Book Life	30 years		
Real Fuel Escalation	0 %	1/2 Normal	σ = 0.06 %

Table 2. Selected Properties of Coals Used for Case Studies (As-Fired Basis)

Coal Property	Illinois No. 6 Coal		Pittsburgh Coal	
	Run-of-Mine	Washed[a]	Run-of-Mine	Washed[a]
Heating Value, Btu/lb	10,190	10,330	13,400	12,900
Sulfur, wt %	4.36	3.09	2.15	1.66
Carbon, wt %	57.0	57.7	74.8	72.1
Hydrogen, wt %	3.7	4.0	4.6	4.5
Oxygen, wt %	7.2	8.4	5.3	5.4
Nitrogen, wt %	1.1	1.1	1.4	1.3
Moisture, wt %	12.3	17.5	2.7	7.9
$/ton (at mine)	26.10	30.68	33.40	34.99
$/ton (transport)	7.90	7.90	7.90	7.90

[a] Model results for a 30 % sulfur reduction on a lb/MBtu basis using conventional coal cleaning (Level 3 plant design)

Table 3. Nominal Parameter Values and Uncertainties for the Conventional Environmental Control System

Model Parameter	Deterministic (Nominal) Value	Probability Distribution	Values (or σ as % of mean)[a]
<u>Wet FGD System</u>			
Molar Stoichiometery	(calc)	Normal	(5 %)
No. Operating Trains	4	Chance	10 % @ 1; 20 % @ 2; 40 % @ 3; 30 % @ 4
No. Spare Trains	1	Chance	75 % @ 0; 25 % @ 1
Reheat Energy	(calc)	Chance	75 % @ 0; 25 % @ x
Total Energy Use	(calc)	Normal	(10 %)
Limestone Cost	$15/ton	Uniform	$10-15/ton
Direct Capital Costs	(calc)	Normal	(10 %)
Operating Costs	(calc)	Normal	(10 %)
<u>Selective Catalytic Reduction</u>			
Space Velocity	2,850/hr	Normal	(10 %)
NH_3 Stoichiometry	(calc)	Normal	(10 %)
Catalyst Life	15,000 hrs	Chance	5 % @ 1,275 hrs 30 % @ 5,700 hrs 50 % @ 11,400 hrs 14 % @ 17,100 hrs 1 % @ 28,500 hrs
Energy Requirement	(calc)	Normal	(10 %)
Ammonia Cost	$150/ton	Uniform	$150-225/ton
Catalyst Cost	$460/ft^3	Normal	(7.5 %)
Direct Capital Cost	(calc)	Triangular	0.8x, x, 2x
Operating Cost (excl. Cat.)	(calc)	Normal	(10 %)
<u>Cold-Side Electrostatic Precipitator</u>			
Specific Collection Area	(calc)	Normal	(5 %)
Energy Requirement	(calc)	Normal	(10 %)
Total Capital Cost	(calc)	Normal	(10 %)
Operating Cost	(calc)	Normal	(10 %)
<u>Solid Waste Disposal</u>			
Land Cost	$6,500/acre	Normal	(10 %)
Direct Cost	(calc)	Normal	(10 %)
Operating Cost	(calc)	Normal	(10 %)

[a] For uniform distributions actual values are shown. For triangular distributions, endpoints and median are shown. For chance distributions, the probabilities of obtaining specific values are shown.

Table 4. Nominal Parameter Values and Uncertainties for the Advanced Environmental Control System

Model Parameter	Deterministic (Nominal) Value	Probability Distribution	Values (or σ as % of mean)[a]
Copper Oxide Process[b]			
Fluidized Bed Height	48 inches		
Sorbent Copper Loading	7 wt-%		
Regeneration Efficiency	99.2 %	-1/2 Normal	(20 %)
Fluidized Sorbent Density	400 kg/m^3	Normal	(10 %)
Standard Error, Cu/S Ratio	0	Normal	σ = 0.39
Sorbent Attrition	0.06 %	Normal	(41 %)
Ammonia Stoichiometry	(calc)	Normal	(6.25 %)
Regeneration Temp	900 °F	Normal	(2 %)
No. Operating Trains	4	Chance	10 % @ 1; 20 % @ 2; 40 % @ 3; 30 % @ 4
No. Spare Trains	1	Chance	50 % @ 0; 50 % @ 1
Sorbent Cost	$5.00/lb	-1/2 Normal	(25 %)
Methane Cost	$4.50/mscf	1/2 Normal	(25 %)
Ammonia Cost	$150/ton	Uniform	$150-225/ton
Sulfuric Acid Cost	$40/ton	-1/2 Normal	(30 %)
Sulfur Cost	$125/ton	-1/2 Normal	(30 %)
Absorber Direct Cap. Cost	(calc)	Uniform	1.0x - 1.5x
Solids Heater DCC	(calc)	Uniform	1.0x - 1.5x
Regenerator DCC	(calc)	Uniform	1.0x - 1.5x
Solids Transport DCC	(calc)	Uniform	1.0x - 2.0x
Sulfur Recovery DCC	(calc)	Uniform	1.0x - 1.2x
Total Capital Cost	(calc)	1/2 Normal	(10 %)
Fabric Filter			
Air-to-Cloth Ratio	2.0 acfm/ft^2	-1/2 Normal	(10 %)
Bag Life	(calc)	Normal	(25 %)
Energy Requirement	(calc)	Normal	(10 %)
Bag Cost	$0.80/ft^2	Normal	(5 %)
Operating Cost	(calc)	Normal	(15 %)
Total Capital Cost	(calc)	Normal	(15 %)
Solid Waste Disposal			
Land Cost	$6,500/acre	Normal	(10 %)
Direct Cost	(calc)	Normal	(10 %)
Operating Cost	(calc)	Normal	(10 %)

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[a] For uniform distributions actual values are shown. For triangular distributions, endpoints and median are shown. For chance distributions, the probabilities of obtaining specific values are shown.

[b] As part of integration of the copper oxide process with the base power plant, the plant air preheater is resized to maintain an exit flue gas temperature of 300 °F.

in changes in their uncertainty distributions (such as the mean or standard deviation) and, in turn, in the overall uncertainties of the technology. Therefore, it may be fruitful to reduce the uncertainties of key variables that contribute most to the risk of technology failure.

The key parameter uncertainties have been identified primarily by estimating correlations between the primary cost results, such as total levelized revenue requirement, and the copper oxide process input uncertainties included in Table 4. Correlations provide a measure of the linear dependence of one distribution on another; however, there are some non-linear relationships in the model, such as between sorbent flow rate and regeneration efficiency. Scatter plots can be used to visually identify non-linear dependencies that may not be well-characterized by correlation coefficients.

The factors which contributed most to uncertainty in the total levelized process cost were uncertainties in sorbent attrition, regeneration efficiency, and copper-to-sulfur molar ratio, with correlations of 0.55, -0.41, and 0.41, respectively. Uncertainties in sorbent cost and plant capacity factor also were significant. Scatter plots did not reveal any strong non-linear dependencies. These results suggest that further research on the copper oxide process should focus on improving understanding of sorbent attrition, regeneration efficiency, and the variability in the copper-to-sulfur molar ratio required to achieve a given SO_2 removal efficiency.

CHARACTERIZING UNCERTAINTY IN CAPITAL COSTS

In deterministic costs estimates, a contingency is used to represent additional costs that are expected to occur, but that are not included explicitly in the cost estimate. Contingency factors are typically simple multipliers that are applied to installed equipment costs after process area costs have been estimated without regard to their uncertainty. The Rand Corporation conducted a survey of 18 companies in the chemical and petroleum industries to determine the actual methods used to develop contingency factors (Milanese, 1987). The study indicates that contingency factors are often badly under-estimated. Rand recommends greater and more formalized use of experience, the use of a "delphi" technique to get multiple expert inputs, and the inclusion of costs associated with risks and innovation.

A probabilistic modeling approach supplants the traditional contingency factor approach by incorporating expert knowledge about uncertainties explicitly and at a more disaggregated level (e.g., for specific performance and cost parameters). Furthermore, while simple contingency factors provide no explicit insights into the specific performance or cost parameters that contribute most to the process technical and economic risks, a probabilistic approach permits identification and ranking of the uncertain parameters that contribute most to the overall uncertainty, as discussed above. Because the uncertainties contributing to "contingencies" are considered at a disaggregated level, more realistic estimates of performance and cost will generally result.

The Electric Power Research Institute (EPRI) uses two types of contingency factors: project and process contingency (EPRI, 1986). The "project" contingency is intended to cover the costs of additional equipment or other costs that would result from a more detailed design of a definitive project at a specific site. This implies that as costing proceeds from a preliminary to a detailed final estimate, the project contingency factor should be reduced. In the present analysis, a project contingency of 25 percent is assumed for the copper oxide process, based on an estimate by Science Management Corporation (1983). The "process" contingency is intended to quantify the additional costs expected due to uncertainty in the technical performance and commercial scale cost of a new technology. This contingency factor is reduced as a technology proceeds from bench scale to full commercial use. However, there is little substantive discussion of how these factors should be derived.

The contingency factor can be defined as the value that adjusts the deterministic estimate (without contingency) to some specified fractile of the probabilistic estimate. Typically, some "best estimate" value from the probabilistic analysis, such as the mean or the median, would be used. However, if there is significant risk aversion on the part of an investor, who may want to minimize the chance of a cost over-run, then an upper fractile from the probability distribution (e.g., 90th percentile) may be used.

An example of this type of analysis is shown graphically in Figure 3, which shows the results of a probabilistic analysis of the capital cost of the copper oxide process. The mean value of the distribution was $111 million. For a completely deterministic case using nominal values with no contingencies the cost was $74 million. Thus, the mean value of the probabilistic analysis corresponds to a deterministic overall contingency factor of 80 percent or a 55 percent process contingency, assuming a 25 percent project contingency, as illustrated in Figure 4. The probability of an overrun at this contingency factor was 45 percent.

The contingency factor estimated in this fashion is significantly higher than assumed in previous analyses (SMC, 1983). Contributing factors to the difference are the uncertainties assigned to the regeneration efficiency and the capital costs for each major process section, which are skewed. The difference is not surprising, since the previous contingency was based on a rule-of-thumb, rather than a detailed probabilistic risk assessment. The fact that the original estimate seems to be low is also supported by the results of the Rand study, which indicates that contingency factors are generally grossly under-estimated, especially early in process development.

SELECTING DESIGNS FOR COMPARATIVE ANALYSIS

Before comparing the copper oxide process to an FGD/SCR system, an analysis of performance and cost trade-offs was done to select values of key design parameters such as fluidized bed height, air preheater size, weight percent of copper in the sorbent, and sulfur recovery option. Furthermore, the model was used to identify potential market niches where process costs are likely to be low, such as for certain coal characteristics (including coal cleaning).

The evaluation of design trade-offs must consider performance and cost interactions between the control technology and the balance of the power plant system, in addition to interactions within the technology itself. Thus, comparisons between copper oxide design alternatives were made on the basis of total pollution control system costs, which are exclusive of the base plant and include SO_2, NO_x, and PM removal, solid waste handling, and coal cleaning. Any emission control system-related changes to the base plant are charged to the pollution control system. As a result, interactions between components of the pollution control system and between the pollution control system and the base plant are integrated into the analysis. Furthermore, because design decisions may be affected by process uncertainties, the analysis was based on probabilistic estimates of the costs associated with various design decisions. The details of this analysis have been reported elsewhere (Frey, Rubin, and Salmento, 1989). Two examples will be summarized here.

One process integration issue is the recovery of energy added to the flue gas by the exothermic reactions in the fluidized bed absorber. A deterministic "best guess" analysis indicated that there was an overall cost penalty to enlarging the air preheater. However, a probabilistic analysis indicates that an enlarged air preheater does provide an overall cost savings. The difference in results is due to the skewness of many of the distributions assigned to key parameters in the probabilistic model. Furthermore, the model accounts for downstream effects, such as the size of the fabric filter, which are often neglected by process developers. The cost of the fabric filter is reduced by the larger air preheater, because the fabric filter inlet flue gas temperature, and the corresponding volumetric flue gas flow rate, are reduced.

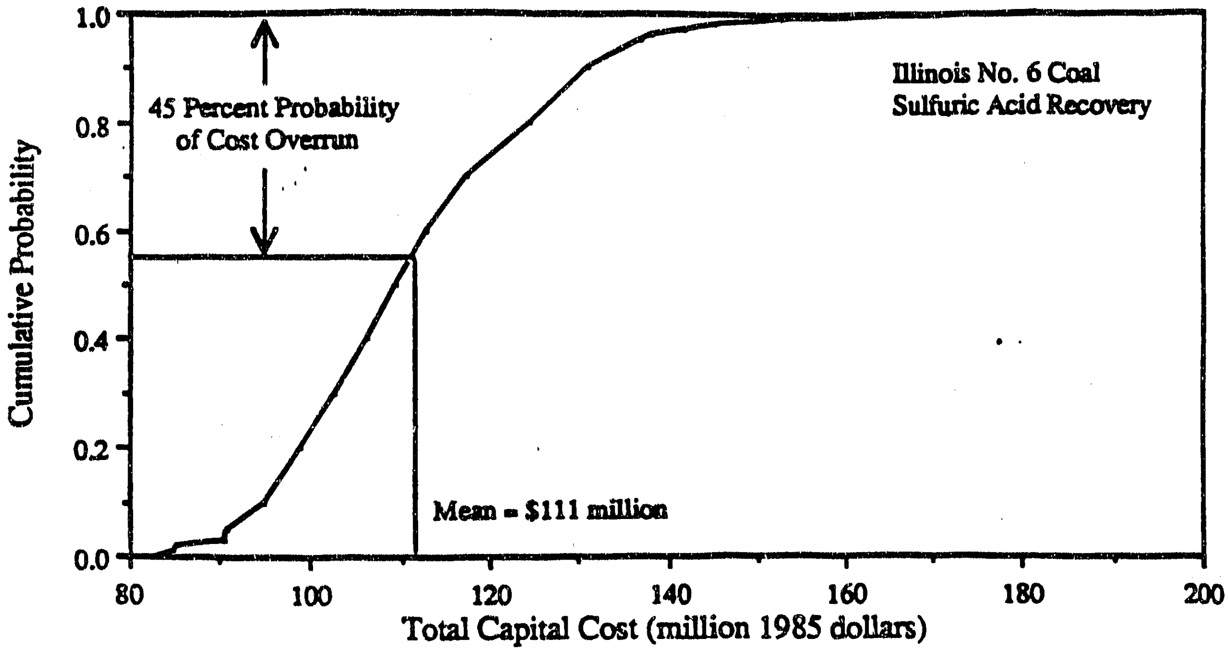

Figure 3. Uncertainty in Total Capital Cost for the Copper Oxide Process

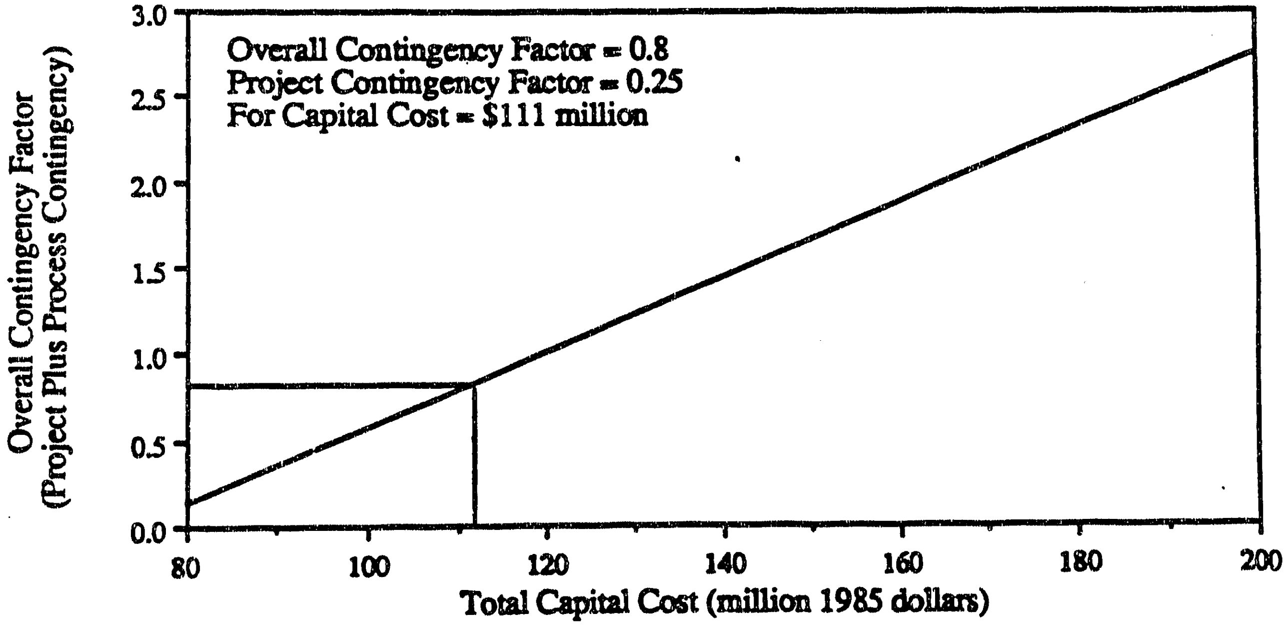

Figure 4. Overall Contingency Factor and Total Capital Cost

The effect of coal cleaning on process costs also is an important consideration in comparative analysis. Because many of the costs of the copper oxide process are sensitive to sorbent flow rate, which in turn is proportional to the coal sulfur content, a reduction in the coal sulfur content through coal cleaning can reduce the costs of the process. In contrast, the FGD/SCR system is comprised of two separate reactor vessels for SO_2 and NO_x control, both of which are proportional in cost primarily to the flue gas flow rate and not significantly influenced by coal cleaning. Figure 5 shows the mean levelized pollution control costs of each component of the copper oxide emission control system associated with various levels of coal preparation for an Illinois No. 6 coal. The figure illustrates the strong relationship between copper oxide process costs and coal sulfur content, and the incremental costs associated with coal cleaning. For medium and low sulfur coals, the increased costs of coal cleaning are larger than the reduction in process costs.

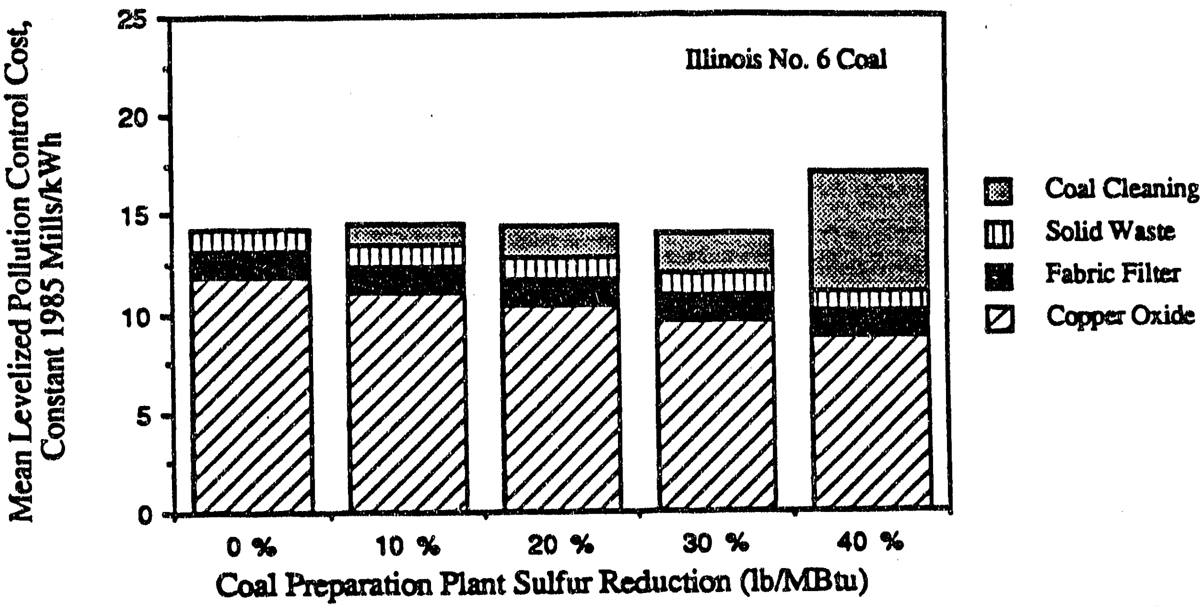

Figure 5. Mean Levelized Pollution Control Cost vs. Sulfur Reduction From Coal Cleaning

In the remaining comparisons of FGD/SCR and copper oxide systems, optimal levels of coal cleaning for both will be used. These are no coal cleaning for FGD/SCR systems and copper oxide systems with the Pittsburgh coal, and 30 percent coal sulfur reduction for copper oxide systems with the Illinois No. 6 coal.

COMPARATIVE ANALYSIS: COPPER OXIDE VS. FGD/SCR

Based on the identification of copper oxide process design issues, four case studies involving probabilistic comparison of copper oxide and conventional environmental control systems were made. These comparisons were made for optimal levels of coal cleaning and for both sulfuric acid and sulfur recovery options. Probabilistic comparison of the pollution control systems provides information about the likely cost savings that can be achieved by the new process, as well as the risks that the new technology may be more expensive than existing technology.

Because many of the input parameter distributions are common to both systems (e.g., financial parameters, base plant characteristics, solid waste disposal, and ammonia cost), there is in general positive correlation between the cost distributions for the two systems.[1] Therefore, in determining the distribution for the cost differences between the copper oxide and FGD/SCR systems, the samples for the distributions of the costs of each system were paired.

Figure 6 shows differences in levelized pollution control costs between FGD/SCR and copper oxide systems for two coals and the two sulfur recovery options. In all cases, the copper oxide process is most likely to be less expensive than the FGD/SCR system; however, for the higher sulfur coal there is a substantial risk that the copper oxide process will be more expensive. Taking the case with sulfur recovery as an example, there is nearly a 30 percent probability than the new process will be more expensive than conventional technology, based on the levelized costs.

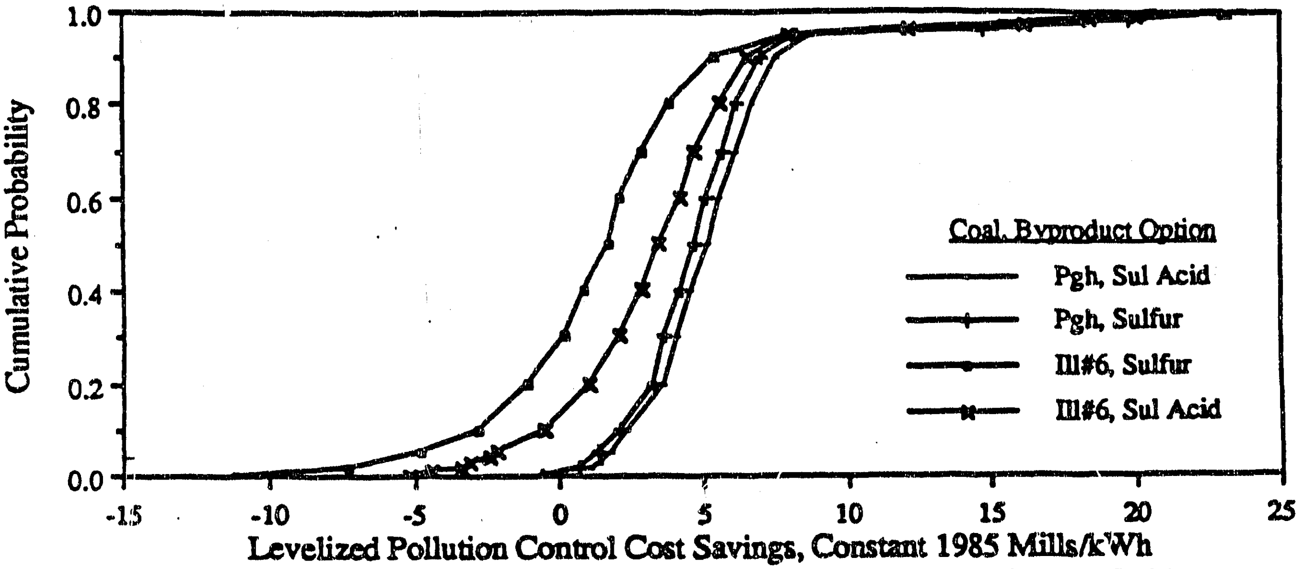

Figure 6. Comparison of Levelized Pollution Control Cost Savings for Copper Oxide versus FGD/SCR Systems: Effect of Coal and Byproduct Recovery Option

The risk that the new technology will be more expensive can be quantified using the partial mean of the cost difference distribution for all negative values. The downward and upward partial means are defined as (Buck and Askin, 1986):

$$\mu_d(x) \equiv \int_{-\infty}^{0} x\, f(x)\, dx \tag{1}$$

$$\mu_u(x) \equiv \int_{0}^{\infty} x\, f(x)\, dx \tag{2}$$

where f(x) is the probability density function for the random variable x. In our example, the downward partial mean is -0.8 mills/kWh and the upward partial mean is 2.5 mills/kWh. These

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[1] In this example, the correlation between the uncertainty distributions of levelized pollution control costs for conventional FGD and advanced copper oxide/sulfuric acid systems is estimated to be 11 percent for optimal levels of coal cleaning with the Illinois No. 6 coal.

sum to the distribution mean. Buck and Askin define the conditional partial mean based on the partial mean and the probability that a loss or gain has occured. The expected value of a loss, given that a loss has occured, is:

$$\mu_{d|x<0}(x) = \frac{\mu_d(x)}{P(x<0)} \tag{3}$$

where $P(x<0)$ is the probability that the random variable x has a value less than zero. The expected value of a gain, given that a gain has occured, is defined similarly. For our example, the expected value of a loss is 2.8 mills/kWh if a loss occurs, and the expected value of a gain is 3.5 mills/kWh if a gain occurs.

The information provided by this analysis can be used to answer questions about the risks and potential pay-offs of the new technology compared to conventional technology. While the copper oxide process is unlikely to be commercialized for another 5 to 15 years, process research will ultimately be used by potential adopters to make a decision about what emission control system to use for a specific application. Therefore, it is reasonable to look at the decision a hypothetical adopter would make with currently available information vis-a-vis information expected to be yielded from research over the next several years.

The opportunity loss from a hypothetical decision to adopt the copper oxide process is given by the downward partial mean (Moore and Chen, 1984). The downward partial mean is the same as the expected value of perfect information (EVPI) for the case where the loss function, L(x), of a potential adopter is represented as linear for all negative outcomes and zero for all postive outcomes, i.e.:

$$E[L(x)] = \int_{-\infty}^{\infty} L(x)\, f_x(x)\, dx \tag{4}$$

where,

$$L(x) = \begin{Bmatrix} x, & x<0 \\ 0, & x>0 \end{Bmatrix} \tag{5}$$

The downward partial mean is the maximum amount that a decision-maker (with the given loss function) would be willing to pay to obtain perfect information that would be used to avoid the downward risk. Although research is unlikely to completely resolve uncertainties, research which leads to a reduction in the probability of a loss through process improvements, or which provides insight into situations in which FGD/SCR systems are less expensive, has value as "information" to a potential process adopter. The value of information is one measure by which to bound the expenditures on research, development, and demonstration.

CONDITIONAL EXPECTED VALUE OF ADDITIONAL RESEARCH

While additional research may reduce the downward risk of a new technology, it can also lead to incremental improvements in the new technology which would, in turn, increase the expected value of cost savings compared to conventional technology. The value of research may thus be estimated based on the incremental increase in the expected cost savings of the new technology compared to current information, rather than based on the reduction in downside risk.

Several factors must be considered in determining the value of research. First, judgment is required to estimate the likely results from a research effort. The value of research depends also on the circumstances of actual adoption of the new technology, which determines the ultimate cost savings compared to other technology. Judgment is required regarding the likely plant sizes, byproduct markets, coal characteristics, and other influencing factors that will face the new technology. It is unlikely that any single cost estimate can be used for such an analysis; rather, several case studies representative of different applications may be required. A third factor influencing the value of research is the possibility of simultaneous improvement in information about or design of competing processes. Therefore, any prior estimate of the value of research is conditioned on the judgments regarding research results, technology diffusion, and improvements in competing processes.

In this analysis, the primary emphasis is on estimating the effect of possible research results on the comparative costs of the copper oxide process versus FGD/SCR systems. It is assumed that research can reduce the uncertainties about several key process variables, and thus provide "imperfect information"[1] about the technology. Because the key uncertainties in process cost have been identified to be related to regeneration, solids transport, and the stoichiometric copper-to-sulfur ratio, it is assumed that new research would be focused on these areas. Table 5 shows illustrative assumptions made about the possible reduction in uncertainties in several variables from new research. More study of the regenerator, solids transport system, and absorber could reasonably be expected to reduce uncertainties regarding regeneration efficiency, regeneration temperature, the equipment costs for the regenerator and solids transport system, sorbent attrition, and the copper-to-sulfur molar ratio.

Four case studies are used to illustrate that the value of research results is conditional on actual applications, although no attempt is made to actually forecast the diffusion of the copper oxide process into commercial use. For the sake of simplicity, it is assumed that the FGD/SCR pollution control system is relatively mature, and that, as an approximation, there will be no incremental improvements in FGD/SCR system costs.

Table 5. Case Studies for Reduction in Copper Oxide Process Uncertainties Due to Research

			Values (or σ as % of mean)	
Model Parameter	Nominal Value	Probability Distribution	Prior to Research	After Research
<u>Regenerator</u>				
Regeneration Efficiency	99.2 %	-1/2 Normal	(20 %)	(5 %)
Regeneration Temp.	900°F	Normal	(2 %)	(1 %)
Regen. Direct Capital Cost	(calc)	Uniform	1.0x - 1.5x	1.1x - 1.4x
<u>Solids Transport</u>				
Sorbent Attrition	0.06 %	Normal	(41 %)	(10 %)
Solids Trans. Dir. Cap. Cost	(calc)	Uniform	1.0x - 2.0x	1.1x - 1.8x
<u>Absorber</u>				
Standard Error, Cu/S Ratio	0	Normal	$\sigma = 0.39$	$\sigma = 0.2$

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[1] As opposed to perfect information, which would remove all uncertainties and would allow a potential process adopter to avoid any loss in selecting between FGD and copper oxide systems.

Results for the case study involving the Illinois No. 6 coal and elemental sulfur recovery are shown graphically in Figure 7 for levelized total pollution control costs. The figures show the cost differences for copper oxide versus FGD/SCR systems based on current information, and selected results for the difference based on information from further research. The assumptions about additional research reduced the variance of the cost difference distributions, but also reduced the skewness (due to assumptions about the regeneration efficiency). Thus, the assumed research outcomes have reduced the downside risk of the new technology and increased the expected cost savings.

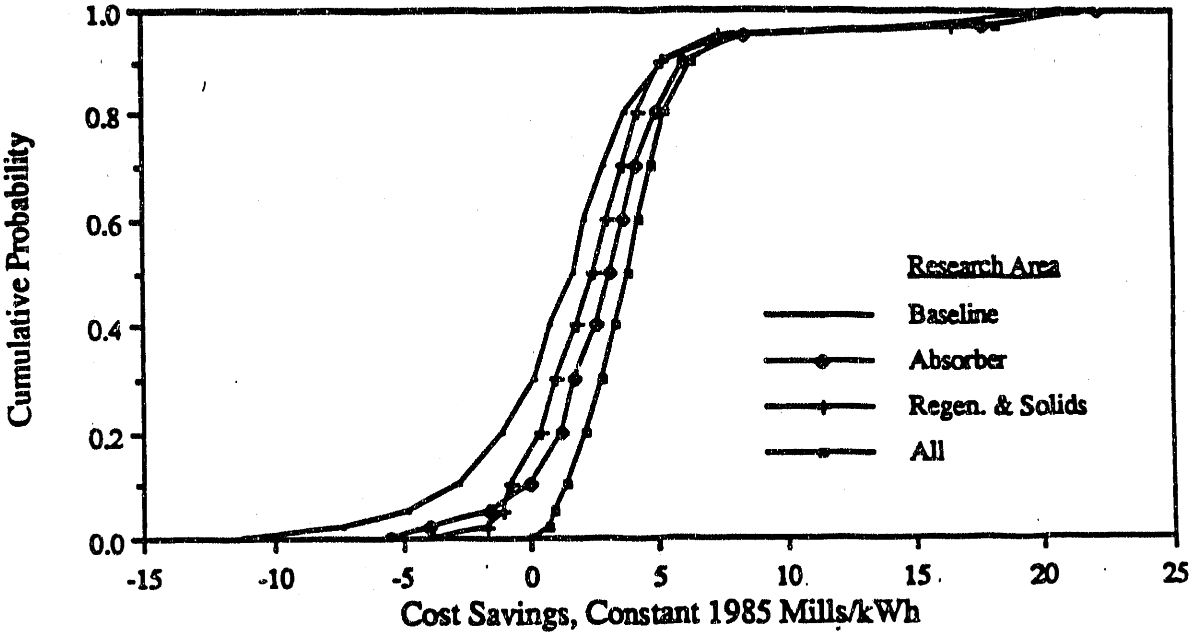


Figure 7. Levelized Pollution Control Cost Savings for Copper Oxide/Sulfur Plant System, Washed Illinois No. 6 Coal: Effect of Illustrative Research Outcomes

The results from additional research for all four cases are summarized in Table 6. Note that while the cost difference between the copper oxide process and the FGD/SCR system were obtained as continuous probability distributions, the uncertainties in cost savings were represented in Table 6 as discrete outcomes (i.e. loss or gain) using the statistics discussed previously. These statistics include the probability that the copper oxide process was more expensive than an FGD/SCR system, the downward partial mean, the downward and upward conditional partial means, and the mean for the entire cost difference distribution. The hypothesized research results reduced the downward partial mean of the cost differences for all cases, and therefore reduced the risk of an opportunity loss to a potential process adopter.

The mean cost difference with more research for all targeted process areas was higher than for current estimates. It can be seen in Table 6 that the value of research in terms of cost improvements was significantly greater than the reduction in downside risk. Thus, the value of research may be greater than the EVPI discussed previously because of improvement in expected cost savings, as well as reduction in downside risk.

To complete an estimate of the value of research requires some forecasting of technology diffusion. The four case studies indicate the variability of the value of research for different types

Table 6. Results of Research Information Case Studies: Comparison of Levelized Total Pollution Control Costs for Copper Oxide versus Conventional FGD/SCR

Research Area	Probability of a Loss (%)	Downward Partial Mean	Expected Value of a Loss	Expected Value of a Gain	Mean	Reduction in Risk	Value of Research
		(mills/kWh)					
Sulfuric Acid Recovery, Washed Illinois No. 6 Coal							
Baseline	15	-0.27	-1.7	4.6	3.6	--	--
Solids Transport	10	-0.13	-1.4	4.2	3.6	0.14	0.0
Absorber	9	-0.16	-1.8	4.8	4.2	0.11	0.6
Regeneration	7	-0.09	-1.3	4.8	4.4	0.19	0.8
Regen. and Solids Trans.	2	-0.02	-1.1	4.5	4.4	0.25	0.8
All	0	0	0	5.1	5.1	0.27	1.5
Sulfur Recovery, Washed Illinois No. 6 Coal							
Baseline	29	-0.81	-2.8	3.5	1.7	--	--
Solids Transport	17	-0.25	-1.5	3.7	2.8	0.56	1.1
Absorber	11	-0.23	-2.0	4.1	3.4	0.58	1.7
Regeneration	18	-0.28	-1.6	3.8	2.8	0.53	1.1
Regen. and Solids Trans.	17	-0.17	-1.0	3.7	2.9	0.64	1.2
All	0	0	0	4.3	4.3	0.81	2.6
Sulfuric Acid Recovery, Unwashed Pittsburgh Coal							
Baseline	1	> -0.01	-0.3	5.6	5.5	--	--
Solids Transport	1	> -0.01	-0.3	5.6	5.5	0	-0.0
Absorber	1	> -0.01	-0.5	5.9	5.9	0	0.4
Regeneration	0	0	0	6.0	6.0	< 0.01	0.5
Regen. and Solids Trans.	0	0	0	6.0	6.0	< 0.01	0.5
All	0	0	0	6.4	6.4	< 0.01	0.9
Sulfur Recovery, Unwashed Pittsburgh Coal							
Baseline	2	> -0.01	-0.4	5.2	5.1	--	--
Solids Transport	1	> -0.01	-0.4	5.2	5.1	0	-0.0
Absorber	2	> -0.01	-0.3	5.6	5.5	0	0.4
Regeneration	< 1	> -0.01	> -0.1	5.6	5.6	0	0.5
Regen. and Solids Trans.	0	0	0	5.6	5.6	< 0.01	0.5
All	0	0	0	6.0	6.0	< 0.01	0.9

of applications. Other factors discussed in previous sections, including plant size and capacity factor, will also influence the level of funding that can reasonably be committed to research.

IMPLICATIONS FOR RESEARCH PLANNING

The data summarized in Table 6 can be used to answer a number of questions such as:

- Is one technology preferred over another?
- Is additional research merited?
- What should be the research strategy?
- How much is additional research worth?
- Under what conditions does the decision strategy change? (How robust is the decision strategy?)

These questions can be answered using decision analysis as an analytical tool for evaluating alternative technology options and research strategies. The discretization of the continuous probability distributions for the cost savings of the copper oxide process compared to an FGD/SCR system, given in Table 6, facilitates the use of relatively simple decision trees to evaluate research strategies. An example of such a decision tree, based on the case with high sulfur coal and elemental sulfur recovery, is given in Figure 8. In this example, the decision analysis is based on a single attribute of cost savings compared to the conventional FGD/SCR system. First, we will consider decisions based on expected cost savings, and then briefly consider a more detailed decision model incorporating the risk attitudes of a decision maker and the time value of research outcomes.

The tree in Figure 8 includes three general decisions. The first is a choice between the copper oxide process based on current knowledge of the process and the FGD/SCR system. In this example, the copper oxide process without additional research is shown to have a positive expected cost savings compared to the conventional FGD/SCR system, based on current information. A second decision is regarding obtaining perfect information that would resolve all downside risks of the new process. The elimination of downside risk increased the expected value by 0.81 mills/kWh, and this is the measure of the EVPI. A third type of decision is that regarding further research and development of the process as discussed previously. As can be seen in Figure 8, and as summarized in Table 6, the expected values of the research options are larger than for the current state of knowledge, indicating that additional research is merited. The most fruitful research strategy in this case appeared to be for all three major process areas considered in the analysis. Such a strategy increased the expected value of the process, compared to current information by 2.6 mills/kWh; this is the basis for bounding the amount of money that should be spent on further research. These differences are summarized in Table 6 as the "value of research."

The decision model can easily be refined to consider the risk attitude of a particular decision maker using expected utility, rather than expected cost savings, as the basis for decision making. Utility is a measure of the personal value a decision maker places on a specific outcome, and it may differ from the monetary value of the outcome (Dawes, 1988). Furthermore, because the results of research may not be obtained for 5 to 15 years, the time value of the outcomes can be modeled using discounting. One possible utility function for such a decision model is thus:

$$u(x) = \left\{ \frac{x(i,n) - x_l(i,n)}{x_h(i,n) - x_l(i,n)} \right\}^b \tag{6}$$

where,

x = discounted outcome of a given alternative
i = discount rate
n = time period (years)

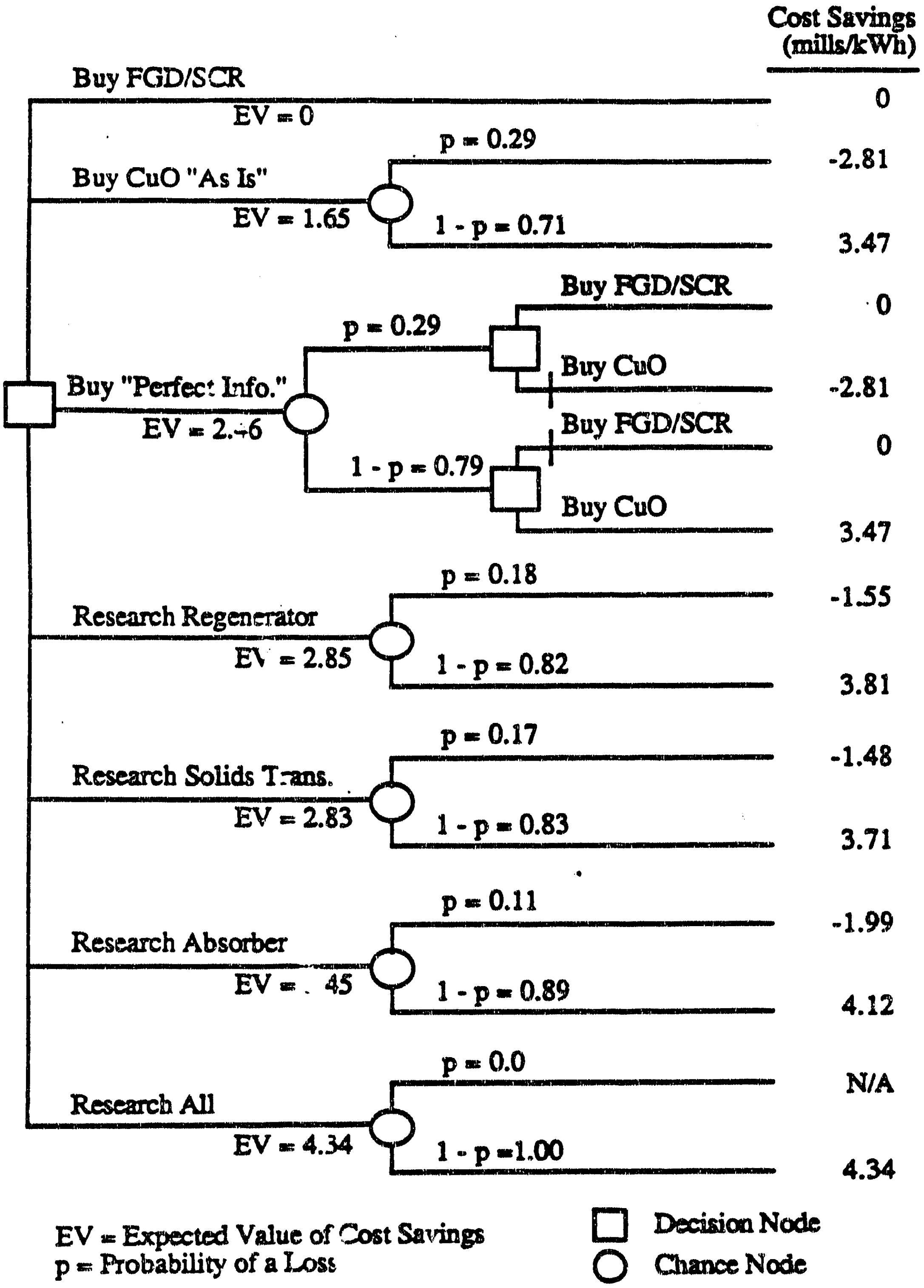
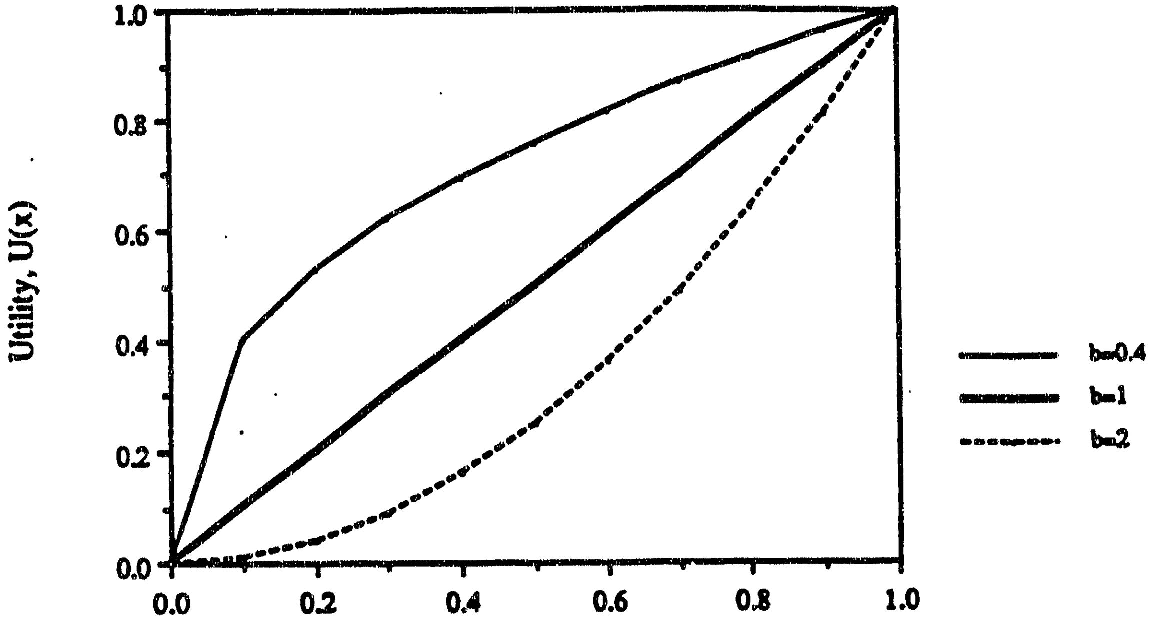


Figure 8. Decision Tree for Copper Oxide Process Research Planning: Example for Illinois No. 6 Coal and Elemental Sulfur Recovery

x_l = discounted lower limit of x for all alternatives
x_h = discounted upper limit of x for all alternatives
b = risk attitude exponent

For a risk neutral decision-maker, b=1. A risk averse decision maker prefers a sure outcome over an alternative with a slightly higher expected value and a risk of a loss. Thus, a risk averse decision maker tends to be "conservative." For a risk averse decision maker, b<1. Conversely, a risk seeking decision maker is willing to forfeit an increase in expected value to play a riskier game, and in this case b>1. The utility function is plotted for normalized values of x and selected values of b in Figure 9. A nominal value of b=0.6 (risk averse) was used in the expected utility analysis.



Normalized Value of Outcome, x

Figure 9. Power Utility Function

The effect of discounting the outcomes of research is to reduce the expected utility of these outcomes. For the Illinois No. 6 coal and elemental sulfur recovery case, the research option for all areas is preferred by a risk averse decision maker if the pay-off from research is obtained within 10 years at a discount rate less than about 20 percent. If the pay-off from research is not available for another 20 years, the discount rate would have to be less than 10 percent for the strategy to have the highest expected utility. Research results for the copper oxide process could reasonably be expected in the next 5 to 15 years. Thus, the best research strategy for high sulfur coal applications is to wait for the results of further research. Only an extremely risk seeking decision maker would choose to accept the copper oxide process "as is". For the medium sulfur coal, the robust strategy, considering risk attitude, discount rate, and time until research pay-off, is to accept the copper oxide process "as is".

For high sulfur coal/elemental sulfur recovery applications, the decision model can be used to bound research expenditures. Using expected value as the basis for the decision, the expected value of research in all areas is 2.7 mills/kWh higher than the expected value of the process as is.

This is equivalent to a savings of about $7 million per year for 500 MW power plant at a capacity factor of 65 percent. For the decision analysis based on expected utility, the equivalent value of research is about $5 million per year. The actual amount to be spent on research depends on how many and what size power plants would be expected to use the copper oxide process with a high sulfur coal and elemental sulfur recovery.

The above example indicates the sensitivity of decisions not only to the outcomes from the engineering process models, but also to the assumptions made in the decision model.

COSTS OF DEMONSTRATION

A remaining question is whether the types of results expected from research can be achieved at a cost consistent with the estimated value of the research. Therefore, it is important to consider the costs incurred in developing a technology from an idea to a demonstrated system. Of all the costs of research, development, and demonstration (RD&D), the first-of-a-kind plant costs are by far the most expensive. The Rand Corporation has conducted a number of studies regarding cost growth for first-of-a-kind plants based on a database containing 106 cost estimates prepared, at various stages of development, for 44 chemical process plants. From the database, a regression equation for capital cost growth from the cost estimate to actual plant costs was developed, based on factors such as the detail of the cost estimate, and the complexity and newness of the technology (Hess, Merrow, and Pei, 1987). Application of the regression equation to the copper oxide process indicates capital cost growth of a factor of 2.3 can be expected for the first plant compared to a deterministic cost estimate without contingency. The implication of this result is that any cost differences between different process applications will be magnified for the demonstration plant. For example, using the nominal deterministic performance and cost assumptions in Table 4 and the capital cost growth factor derived from the Rand model, the capital cost of a 125 MW copper oxide demonstration unit with an unwashed Illinois No. 6 coal was estimated to be $56 million. For an unwashed Pittsburgh coal, the estimated capital cost of a demonstration unit of the same size was $9 million less expensive. The value of research must be weighed against research costs, including the first-of-a-kind demonstration plant.

CONCLUSIONS

A probabilistic engineering model can be used during the research phase of a technology to provide insights into important design trade-offs and key uncertainties. Application of such a model for the fluidized bed copper oxide process was discussed, which captures interactions among key process areas, and between the copper oxide process and other components of the power plant and emission control system. In some cases, the integrated model provided insights into performance trade-offs that were contrary to common assumptions, and the incorporation of uncertainty resulted in different results that deterministic analysis in the case of power plant air preheater sizing.

Probabilistic cost comparisons between conventional and advanced technology can be used to estimate the likely cost savings and the risks of a new technology. Judgments about the outcome of further process research can be combined with probabilistic modeling to estimate the value of research information to a potential process adopter, and to estimate the cost-savings from process improvement. The value of the research, coupled with judgment about the extent and nature of technology diffusion, can be used to bound research expenditures. Whether research is feasible depends also on the costs of the first commercial scale demonstration plant. Because these costs are potentially large, care must be exercised in the selection of an appropriate first application.

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