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DEVELOPMENT OF THE INTEGRATED ENVIRONMENTAL CONTROL MODEL:

Performance and Cost Models for the NOXSO Process

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Quarterly Progress Report

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Nomenclature for Section 1 (Performance Models)

A = available surface area of sorbent

A_a = cross sectional area of adsorber

A_0 = available surface area of fresh sorbent

C_0 = molar gas concentration of flue gas, kmole/m^3

F_g = flue gas flow rate, kmole/sec

F_s = sorbent circulation rate, kg/sec

H = height of fluidized bed

ΔH_i = heat of reaction for regeneration, Btu/lb sulfur

K_i = rate constant of ith gas species, 1/(atm sec)

n = sodium content on sorbent, kmole/kg sorbent

n_{Na} = sodium content on sorbent, %wt

n_{SiO_2} = silicon content on sorbent, %wt

P = gas pressure, atm

r = sulfur regeneration rate, (lb sulfur)/hr/(lb sorbent)

R_{NO_x} = fraction of NO_x converted to N in combustor

R_{SO_2} = fraction of SO_2 retained on sorbent after heating in sorbent heater

S = sulfur fraction of regenerated sorbent, %wt

S_a = sulfur fraction of spent sorbenr, %wt

t_i = sorbent residence time in regenerator for gas i

T_a = temperature of adsorber, °C

V = superficial gas velocity

W = sorbent inventory, kg

$\overline{X}_a$ = mean conversion factor of active sorbent

X_a = conversion factor of active sorbent at adsorber inlet

X_r = conversion factor for sorbent regeneration

X_{shift} = conversion factor at which regeneration shifts

X_{final} = total temp. conversion for sorbent regeneration

y_{oi} = mole fraction of ith gas species, $z = 0$

y_{fi} = mole fraction of ith gas species, $z = H$

$\overline{y}$ = mean mole fraction

Greek Symbols

ρ = sorbent density in fluid bed, kg/m^3

λ_i = stochiometric ratio of ith gas species to active sorbent,

ϕ = removal fraction

Nomenclature for Section 2 (Cost Models)

A_i	=	fluidized bed area, ft^2
C_i	=	process area cost, 1993$
EC_i	=	electricity consumption, kW
F_s	=	sorbent feed rate at absorber inlet, fresh sorbent basis, lb/min
G_{FG}	=	volumetric flue gas flow rate at absorber inlet, ft^3/min
h_i	=	height of vessel, ft
I_b	=	bed inventory, lb
m_i	=	mass flow rate, lb/hr
M_i	=	molar flow rate of species i, lbmole/hr
P	=	absorber inlet pressure, atm
r_i	=	radius of vessel, ft
$SA_{absorber}$	=	surface area of absorber vessel, ft^2
t_{ir}	=	thickness of inner or base refractory, ft
t_A	=	absorber solids residence time, min
t_R	=	regenerator residence time, min
t_{SH}	=	solids heater residence time, min
R_{cost}	=	refractory cost, $/$ft^2$
R_{elec}	=	electricity cost, $/MWh
S_{cost}	=	sorbent cost, $/lb
T	=	absorber bed temperature, °K
UA_i	=	product of heat transfer coefficient and heat transfer area
V_s	=	superficial flue gas velocity at absorber inlet, ft/sec
x	=	molar fraction of copper as copper sulfate at the regenerator inlet
x_1	=	molar fraction of copper oxide converted to copper sulfite just inside regenerator
y_i	=	SO_2 inlet flue gas concentration, lbmoles SO_2/lbmole flue gas
y_o	=	SO_2 outlet flue gas concentration, lbmoles SO_2/lbmole flue gas
Z_i	=	fluidized bed height, ft
<u>Subscripts</u>		
A	=	absorber
air	=	air flow in preheater with NOXSO process
orig	=	air flow in preheater without NOXSO process
contact	=	height of vessel in contact with sorbent
CH_4	=	methane
d	=	ductwork
ID	=	induced draft fans
s	=	sorbent
ms	=	makeup sorbent
O	=	operating train
S	=	spare train
SO_2	=	sulfur dioxide
T	=	total trains
R	=	regenerator
SH	=	sorbent heater
V	=	vessel
<u>Greek Symbols</u>		
ρ_s	=	Sorbent density (expanded bed), lb/ft^3

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1-1 INTRODUCTION

This Quarterly Report documents research efforts carried out under Contract No. DE-AC22-92PC91346 from the U.S. Department of Energy. The purpose of this contract is to develop and refine the Integrated Environmental Control Model (IECM) created and enhanced by Carnegie Mellon University (CMU) for the U.S. Department of Energy's Pittsburgh Energy Technology Center (DOE/PETC) under contract Numbers DE-FG22-83PC60271 and DE-AC22-87PC79864.

In its current configuration, the IECM provides a capability to model various conventional and advanced processes for controlling air pollutant emissions from coal-fired power plants before, during, or after combustion. The principal purpose of the model is to calculate the performance, emissions, and cost of power plant configurations employing alternative environmental control methods. The model consists of various control technology modules, which may be integrated into a complete utility plant in any desired combination. In contrast to conventional deterministic models, the IECM offers the unique capability to assign probabilistic values to all model input parameters, and to obtain probabilistic outputs in the form of cumulative distribution functions indicating the likelihood of different costs and performance results.

The most recent version of the IECM, implemented on a Macintosh II computer, was delivered to DOE/PETC at the end of August 1995. The current contract continues the model development effort to provide DOE/PETC with improved model capabilities, including new software developments to facilitate model use and new technical capabilities for analysis of environmental control technologies. Integrated environmental control systems involving pre-combustion, combustion, and post-combustion control methods will be considered.

The work in this contract is divided into two phases. Phase I deals with further developing the existing version of the IECM and training PETC personnel on the effective use of the model. Phase II deals with creating new technology modules, linking the IECM with PETC databases, and training PETC personnel on the effective use of the updated model. The present report summarizes recent progress on the Phase I effort during the period July 1, 1995 through September 30, 1995. This report presents additional details on the new performance models of the NOXSO process. For convenience, the complete description of the NOXSO performance model is presented here, including information previously presented in the Quarterly Report submitted in April 1995. Also included in this report is a newly developed cost model for the NOXSO process. Illustrative results are presented using the new performance and cost models as implemented in the IECM.

Section 1: Performance Model

1-2 BACKGROUND TO THE NOXSO PROCESS

The NOXSO process is an advanced technology that removes both SO_2 and NO_x simultaneously using a sorbent prepared by spraying sodium carbonate on the surface of γ-alumina spheres. It is designed to achieve SO_2 removal efficiencies above 90% and NO_x removal at levels above 80%. The main features of this process are:

- Simultaneous SO_2 and NO_x removal in a single absorber vessel;
- Regenerative use of sorbent, thereby avoiding the production of liquid or solid waste
- Production of a saleable byproduct in the form of sulfur or sulfuric acid.

The NOXSO process was developed in the early 1980s and successfully demonstrated at the small-scale (0.17 MW) in 1983-85 at TVA's Shawnee Steam Plant facility (Haslbeck & Neal, 1985; Yates, 1983). This was followed by Process Development Unit (PDU) tests on a slightly larger scale (0.75 MW) in cooperation with DOE/PETC in the mid-eighties. A Life-Cycle Test Unit (LCTU) was built (0.06 MW) in 1988 to examine the NOXSO process in an integrated continuous mode operation (Yeh, Drummond, Haslbeck, & Neal, 1987; Yeh, Ma, Pennline, Haslbeck, & Gromicko, 1990). Finally a Proof-of-Concept (POC) unit was built in the early 1990s at a 5 MW scale as the last test before full-scale demonstration (Black, Woods, Friedrich, & Leonard, 1993; Ma, 1994-95; Ma, Haslbeck, et. al., 1993). Based on these tests, conceptual designs of commercial scale units are now being developed.

There are several similarities between the NOXSO process and the fluidized bed copper oxide process another integrated emission control technology supported by DOE/PETC and modeled in the IECM. The key *differences* between these processes are twofold:

i) NOXSO uses a sorbent that consists of sodium carbonate sprayed on the surface of γ-alumina spheres while the CuO process uses copper oxide as a sorbent. The latter requires operation at high temperatures upstream of the air preheater, where the NOXSO catalyst operates at lower temperatures downstream of the preheater.

ii) NOXSO recycles the NO_x removed from the flue gas back to the furnace along with combustion air. By injecting it into the fuel-rich high temperature combustion zone it is decomposed to N_2 and O_2. The CuO process, on the other hand, requires the use of ammonia as an additional reagent to reduce NO_x to N_2.

1-2.1 Study Scope and Objectives

This report provides a description of the NOXSO process and refines the existing performance models in the literature and in the IECM computer model. Special attention is given to the fact that no installations currently exist at a commercial size of 200 MW or greater. This lack of information at a large scale introduces additional uncertainty and requires that models parametrized using data from pilot plants of about 5 MW be

extrapolated. The process model presented in this report uses principles of thermodynamics and mass transfer for unit operations of the NOXSO process. These models are then parametrized using data from pilot scale studies and subsequently used for conceptual design of planned commercial size plants.

The accuracy of model predictions depends in large part on how completely all the relevant processes have been modeled. Past experience in industry has shown that mass transfer units, especially for solid-gas and liquid-gas exchange, are difficult to scale up. This can lead to uncertainty in predicting the performance of commercial-scale installations. In this report, process performance models developed by NOXSO Corporation, which have been parametrized against Proof-of-Concept (POC) data have been used. These process models were then integrated into the IECM framework to provide an overall system model for the NOXSO process in which uncertainties can be modeled explicitly.

1-2.2 Organization of Report

The discussion of performance models is organized as follows: Section 1-3 provides a description of the unit operations used in the NOXSO process. Section 1-4 provides some theoretical background for modeling fluidized beds. Section 1-5 provides mass balance models for all NOXSO process areas along with emission control design equations for the adsorber and regenerator. Section 1-5 also provides a numerical example illustrating the use of these models for conceptual design of a commercial scale NOXSO plant.

1-3 PROCESS DESCRIPTION

A schematic of the NOXSO process is shown in Figure 1. It consists of four main units: the adsorber, sorbent heater, regenerator, and the sorbent cooler. SO_2 and NO_x are adsorbed from the flue gas onto the surface of the sorbent at 320° F in a single-stage fluidized bed adsorber. The SO_2 reacts with the sodium bicarbonate on the sorbent surface to form sodium sulfates. The sorbent is then transported into the three-stage fluidized bed sorbent heater using a dense-phase conveyer, where it is heated to 1150° F to desorb NO_x. The desorbed NO_x is recycled to the furnace where about 65% is reduced to N_2. Following NO_x desorption, the sorbent is transported via a J-valve to a regenerator where natural gas and steam are used to reduce the sulfate on the sorbent to SO_2 and H_2S which are also desorbed. These offgases are sent to a Claus plant or a sulfuric acid plant to recover the sulfur. Finally, sorbent is transported to a three-stage fluidized bed cooler (via a second J-valve) where it is cooled to 320° F and transported back to the adsorber via a third J-valve.

Provided in the following sections is a brief description of each unit operation along with its associated process chemistry. Discussion regarding the modeling of the mass transfer operations for each unit can be found in Section 1-5.

1-3.1 Adsorber

The adsorber consists of a single-stage fluidized bed containing the Na_2CO_3 covered γ-alumina beads of 1/16 inch diameter. The operating temperature of the bed is 320° F at

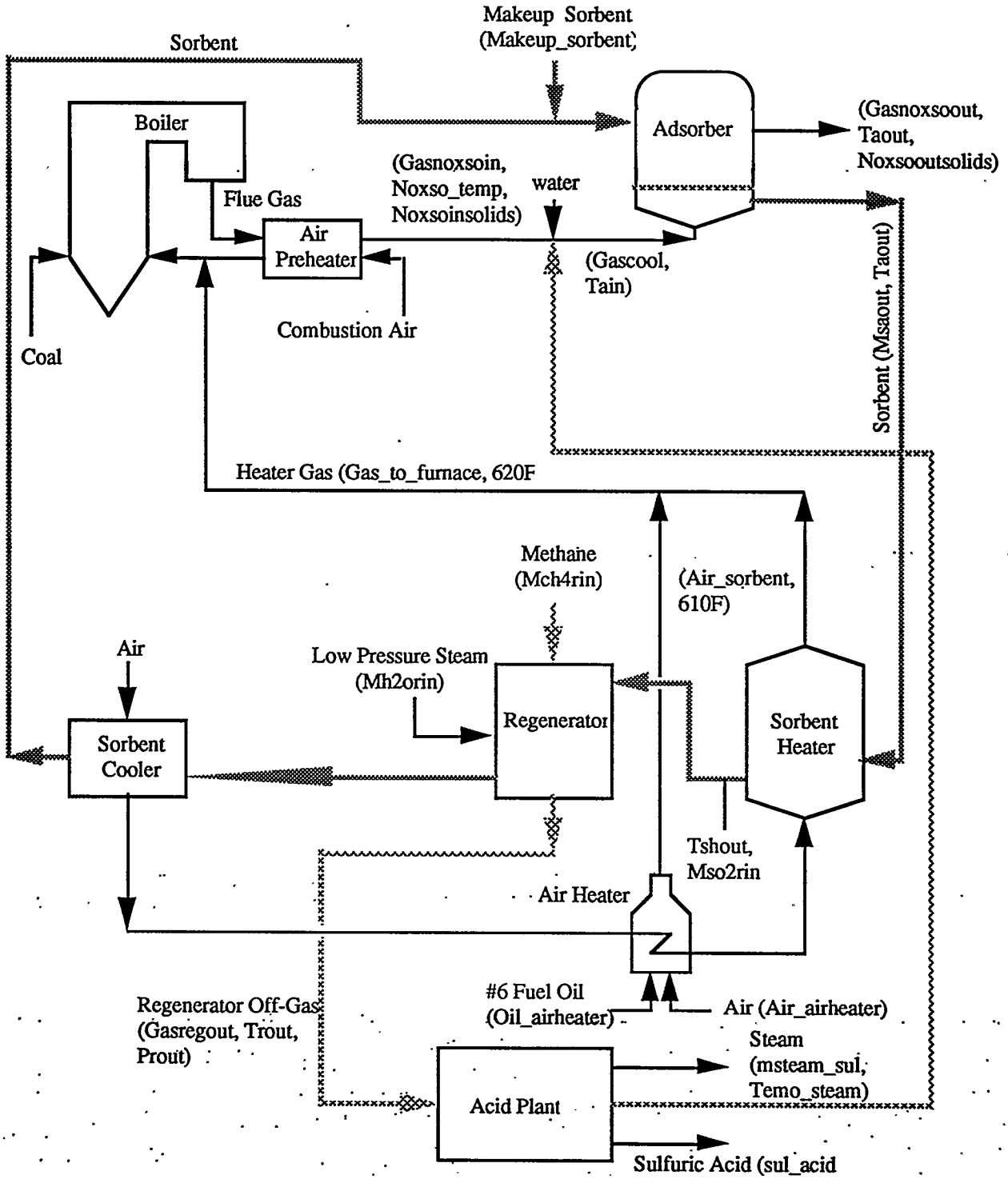

Figure 1. A Schematic of the NOXSO Process Flowsheet

which temperature Na_2CO_3 is reduced to Na_2O. If necessary, the flue gas is first cooled to 320° F by spraying water into the flue gas ducts. It then passes through the adsorber at a superficial velocity at least as large as the minimum fluidization velocity. The SO_2 and NO_x in the flue gas are adsorbed onto the surface of the alumina beads via solid-gas mass transfer.

Based on laboratory experiments and the results obtained from the POC tests the proposed mechanism for the SO_2/NO_x adsorption is as follows:

$$Na_2O + SO_2 \Leftrightarrow Na_2SO_3 \quad (1\text{-}1)$$

$$Na_2SO_3 + 1/2\ O_2 \Leftrightarrow NaSO_4 \quad (1\text{-}2)$$

$$Na_2O + SO_2 + NO + O_2 \Leftrightarrow Na_2SO_4 + NO_2 \quad (1\text{-}3)$$

$$Na_2O + 3\ NO_2 \Leftrightarrow 2\ NaNO_3 + NO \quad (1\text{-}4)$$

The overall reaction summarizing (1-1) and (1-2) is given by:

$$Na_2O + SO_2 + 1/2\ O_2 \Leftrightarrow NaSO_4 \quad (1\text{-}5)$$

The overall reaction summarizing (1-3) and (1-4) is given by:

$$4\ Na_2O + 3\ SO_2 + 2\ NO + 3\ O_2 \Leftrightarrow 3\ Na_2SO_4 + 2\ NaNO_3 \quad (1\text{-}6)$$

Examining reactions (1-5) and (1-6), we see that 2 moles of SO_2 are adsorbed for every mole of NO. The rate of reactions for both SO_2 and NO_x adsorption have been established as first-order based on experimental data. Therefore, the reaction rate is:

$$\frac{dC_i}{dt} = -k_i [C_i] S$$

where k_i is the reaction rate constant, $[C_i]$ is the concentration of SO_2 or NO_x, and S is the available surface area of the sorbent. The available surface area depends on the gas-solid mixing and flow conditions in the fluidized bed. Modeling the flow in a fluidized bed is quite complex and often difficult, therefore, the available surface area is usually experimentally determined.

1-3.2 Sorbent Heater

The saturated sorbent from the bottom bed of the adsorber is transported to the top of the sorbent heater using a dense phase conveyor system. The sorbent heater is a three-stage fluidized bed reactor. A natural gas fired air heater supplies hot air to heat the sorbent to 1150° F. During the heating process all of the NO_x (65%-75% NO_2, balance NO) and some of the SO_2 desorbs from the sorbent. In commercial applications the heater off-gas, which is rich in NO_x, is returned to the furnace. The introduction of NO_x recycle into the

furnace results in: (a) inhibited NO_X production due to higher NO_X concentrations, and (b) reduction of NO_X to N_2. As noted earlier, about 65% of the recycled NO_X is reduced to N_2.

NO_X desorbtion in the sorbent heater produces both NO and NO_2, where the latter is about 65-75% of the total NO_X. The type of gas used (i.e., the constituents of hot air plus combustion byproducts) to heat the sorbent does not affect the ratio of NO to NO_2 (in NO_X) significantly. A small fraction of SO_2 is also desorbed. Based on experimental findings the following reaction mechanisms have been proposed to explain the desorbtion process:

$$2\,NaNO_3 \rightarrow Na_2O + 2\,NO_2 + 1/2\,O_2 \qquad (1\text{-}7)$$

$$2\,NaNO_3 \rightarrow Na_2O + NO_2 + NO + O_2 \qquad (1\text{-}8)$$

$$Na_2SO_3 \Leftrightarrow Na_2O + SO_2 \qquad (1\text{-}9)$$

Fluidized bed reactors have excellent heat transfer properties, and it has been experimentally observed that all of the adsorbed NO_X is desorbed in the sorbent heater. In this work, the sorbent heater is modeled purely as a heat and mass transfer device resulting in 100% NO_X removal and 0-5% SO_2 removal.

1-3.3 Regenerator

The regenerator is of a moving bed type, i.e., the sorbent continuously moves from the top to the bottom of the regenerator bed. The hot sorbent from the bottom of the sorbent heater is transported to the top of the regenerator via J-valves. Natural gas is used to treat the hot sorbent and reduce the sulfate to SO_2, H_2S, and sulfide. In the lower part of the regenerator bed steam is used to hydrolyze any residual sulfide to H_2S. The off-gas streams from the natural gas treater and steam treater are mixed and fed either to a Claus plant, which converts gases to elemental sulfur, or to a sulfuric acid plant.

The reaction mechanisms for regeneration of the sorbent based on POC results are as follows:

$$1/4\,CH_4 + Na_2SO_4 \rightarrow 1/4\,CO_2 + SO_2 + 1/2\,H_2O + Na_2O \qquad (1\text{-}10)$$

$$SO_2 + Na_2O \rightarrow Na_2SO_3 \qquad (1\text{-}11)$$

$$3/4\,CH_4 + Na_2SO_3 \rightarrow 3/4\,CO_2 + H_2S + 1/2\,H_2O + Na_2O \qquad (1\text{-}12)$$

$$Na_2S + H_2O \Leftrightarrow H_2S + Na_2O \qquad (1\text{-}13)$$

$$CO_2 + Na_2S \rightarrow COS + Na_2O \qquad (1\text{-}14)$$

$$1/2\ CO_2 + Na_2S \rightarrow 1/2\ CS_2 + Na_2O \qquad (1\text{-}15)$$

Equations 1-10, 1-11, and 1-12 represent the regeneration in the upper part of the moving bed, and can be summarized as follows:

$$CH_4 + Na_2SO_4 \rightarrow CO_2 + H_2S + H_2O + Na_2O \qquad (1\text{-}16)$$

The residual sulfide is hydrolized in the lower part of the moving bed:

$$3\ Na_2S + H_2O + 1.5\ CO_2 \rightarrow 3\ Na_2O + H_2S + COS + 1/2\ CS_2 \qquad (1\text{-}17)$$

The reaction rates are governed by the available surface area and the reaction rate constants can be determined experimentally.

1-3.4 Sorbent Cooler

The sorbent from the regenerator flows into a three-stage fluidized bed sorbent cooler via a second J-valve. The sorbent is cooled to 320 F using ambient air supplied by a fan. The heat is recovered by using the air for combustion in the air heater. The cooled and regenerated sorbent is recycled back to the adsorber via a third J-valve. The cooling of the regenerated sorbent does not involve any chemical reactions and is modelled purely as a heat transfer operation.

1-4 FLUIDIZED BED REACTORS

Fluidizing a bed of solid particles with gas provides a means of bringing the two into intimate contact and thus enhancing mass and heat transfer. The heat transfer properties of fluidized beds are excellent and even when accommodating strongly exothermic or endothermic reactions, the beds remain isothermal due to good solids mixing. Additionally, because of their liquid-like properties, fluidized beds can be mechanically transferred by pumping from one container to another. In many industrial processes the gas mixing in a fluidized bed often is not good due to gas bubbles, which can severely reduce the contact between gas and solids. There can also be problems with particle attrition and break-up caused by the vigorous agitation of particles and their impingement on vessel walls. Often, however, the advantages outweigh the disadvantages and the use of fluidization in industrial processes is fairly common.

In designing a fluidized bed reactor two main factors are considered: (1) the formation of bubbles in the fluidized bed, which is determined by the minimum fluidization velocity U_{mf}, and (2) reactive mass transfer in the fluidized bed. In the following paragraphs models for the calculation of U_{mf} and for reactive mass transfer for fluidized bed reactors are described (Davidson & Harrison, 1971; Kunii & Levenspiel, 1969; Yates, 1983).

1-4.1 Minimum Fluidization Velocity

Fluidization of a bed with solid particles occurs when the superficial gas velocity in a vessel is large enough so that the drag force on the particles equals the gravitational pull of the particle. At this velocity, called the minimum fluidization velocity, U_{mf}, the bed takes on

the appearance of a fluid with a flat surface responding in the same way as a fluid to stirring or pouring. If the superficial gas velocity increases above U_{mf}, bubbles form in the bed and rise to the surface where they burst through in the same way as gas bubbles in a boiling liquid. At these velocities the bed is essentially divided into two phases — the dense or emulsion phase where the gas percolates through as in a packed bed, and the lean or bubble phase where much of the gas is not in contact with the solids. If the superficial velocity is increased further the gas bubbles increase in size and might become as large as the diameter of the container itself. The bed is then said to be "slugging" and is characterized by considerable heaving of the surface.

The expressions available for estimating U_{mf} in terms of the physical properties of the solid particles and the fluidizing gas are based on the principle of taking a gas velocity-pressure drop relationship and extending it to the point where particles become fluidized and the gas velocity is U_{mf}. The Ergun equation (Yates, 1983) provides an expression for pressure drop through a vertical bed of particles (for size > 150 μm) of height H_{mf}:

$$\frac{\Delta p}{H_{mf}} = \frac{150\,(1-\varepsilon)^2}{\varepsilon^3} \times \frac{\mu \times V}{(\psi d_p)^2} + \frac{1.75\,(1-\varepsilon)}{\varepsilon^3} \times \frac{\rho_g V^2}{\psi d_p} \qquad (1\text{-}18a)$$

where

$\Delta p \equiv$ pressure drop through the bed
$H_{mf} \equiv$ bed height
$\varepsilon \equiv$ voidage fraction of bed
$\mu \equiv$ fluid viscosity
$V \equiv$ gas velocity
$\psi \equiv$ sphericity factor
$d_p \equiv$ particle diameter
$\rho_g \equiv$ density of gas
$\rho_s \equiv$ density of solid

At the point of minimum fluidization the force exerted by the upward flowing fluid is equal to the gravitational force of the particles, i.e.,

$$\frac{\Delta p}{H_{mf}} = (1-\varepsilon_{mf})\,(\rho_s - \rho_g)\,g \qquad (1\text{-}18b)$$

The minimum fluidization velocity can then be estimated by substituting Equation 1-18b for the pressure drop in Equation 1-18a:

$$(1-\varepsilon_{mf})\,(\rho_s - \rho_g)\,g = \frac{150\,(1-\varepsilon_{mf})^2}{\varepsilon_{mf}^3} \times \frac{\mu \times V}{(\psi d_p)^2} + \frac{1.75\,(1-\varepsilon_{mf})}{\varepsilon_{mf}^3} \times \frac{\rho_g V^2}{\psi d_p} \qquad (1\text{-}19)$$

Usually the voidage fraction at fluidization velocity is unknown. Wen and Yu (Yates, 1983) found that for a range of particle types and sizes the following empirical relationships were valid:

$$\frac{1-\varepsilon}{\psi^2 \varepsilon_{mf}^3} \approx 11; \quad \frac{\varepsilon}{\psi \varepsilon_{mf}^3} \approx 14$$

Using the Ergun equation with the above empirical relations, a generalized correlation for the estimation of minimum fluidization velocity can be written as:

$$Re_{mf} = [(33.7)^2 + 0.0408Ga]^{1/2} \tag{1-20}$$

where

$$Re_{mf} \equiv \frac{V_{mf}\, d_p\, \rho_g}{\mu}$$

$$Ga \equiv \frac{d_p\, \rho_g\, (\rho_s - \rho_g)\, g}{\mu^2}$$

1-4.2 Fluidized Bed Reactor Modeling

Modeling a fluidized bed reactor is critical for evaluating design parameters such as sorbent residence time and sorbent flow rate. The performance of the fluidized bed reactor is determined by a combination of chemical factors and hydrodynamic factors. The chemical factors are determined by the reaction kinetics and the stochiometry of the reaction. The hydrodynamic factors are determined by the gas distribution, bubble size and residence time, and the interphase exchange rate. In order to quantify the way in which these factors affect the reactor performance we present a model based on the theory of two-phase flow in fluidized beds which makes explicit the contribution of these factors.

Most reactor models assume that if the superficial velocity is greater than U_{mf} then the gas entering the bed divides into two streams, one flowing through the emulsion phase and the other flowing as bubbles. Gas flowing in the emulsion phase is in intimate contact with the solid particles so the reaction can proceed efficiently. Bubbles, however, are essentially empty of particles and gas within them can only react at the walls of the bubble. However, there is an exchange of gas between the emulsion and bubble phase, the bubbles thereby acting as a secondary source of fresh reactant as they rise through the bed. A general one-dimensional two-phase flow model is shown in Figure 2.

For an irreversible, first-order gas-solid reaction with no accompanying volume change, a mass balance for the emulsion phase (Equation 1-21) and bubble phase (Equation 1-22) is written as follows:

$$V_e \frac{dy_{Ae}}{dz} + K_{be}\,(y_{Ae} - y_{Ab}) + k_e\, y_{Ae}\, S = 0 \tag{1-21}$$

$$V_b \frac{dy_{Ab}}{dz} + K_{be} (y_{Ab} - y_{Ae}) = 0 \qquad (1\text{-}22)$$

where

$V \equiv$ velocity
$y_A \equiv$ concentration of species A
$K_b \equiv$ interphase mass transfer rate per unit volume of bubble gas
$k \equiv$ reaction rate constant
$S \equiv$ surface area of solid available for reaction

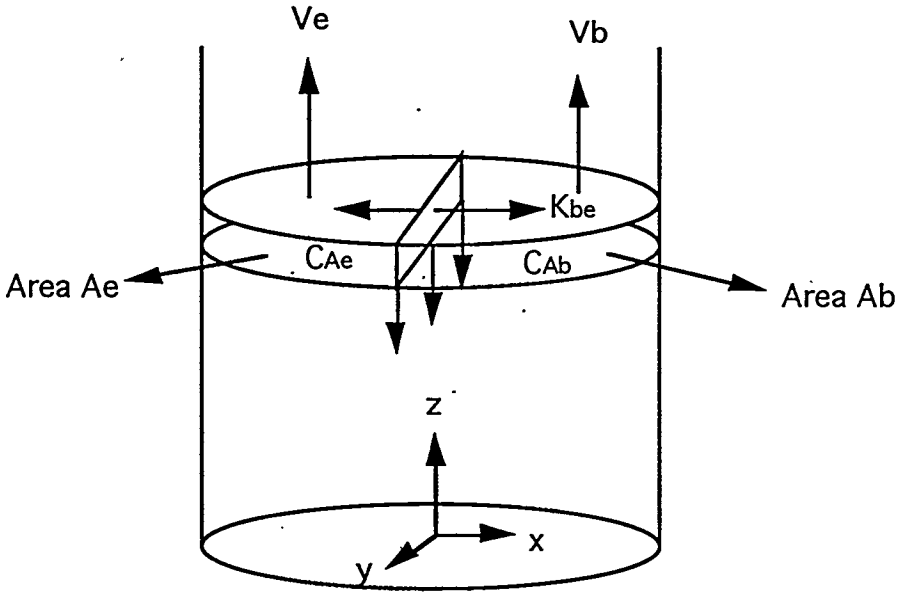

Figure 2. The General One-Dimensional Two-Phase Flow

The subscript 'e' is used for emulsion phase and subscript 'b' is used for bubble phase. These equations have been simplified using the following assumptions: (i) the reactor operates in steady state, (ii) the gas is in plug flow in both phases and hence there is no back flow, and (iii) no chemical reaction occurs in the bubble phase.

These model formulations provide an alternative form to the models described below in Section 1-5. An advantage is that this formulation explicitly recognizes the two separate phases, especially the bubble phase which may limit performance in future process scale-up. Further development of Equations 1-21 and 1-22, however, remains a subject for future research.

1-5 NOXSO PROCESS PERFORMANCE MODEL

The four main process areas for the NOXSO process were described in Section 1-3. Across these areas, the adsorber, sorbent heater, and sorbent cooler use a fluidized bed for improved gas-solid contact. The sorbent heater and sorbent cooler utilize a fluidized bed mainly for efficient heat transfer between gas and solid sorbent particles. As discussed in Section 1-3, the fluidized bed provides excellent heat transfer properties and provides

isothermal conditions. The adsorber, on the other hand, is used primarily for reactive mass transfer, involving pollutant removal. The modeling of the adsorber performance will be discussed in some detail. The regenerator is a moving bed reactor which is used for regenerating sulfur. The reactive mass transfer model for this unit also is treated in some detail.

The performance models that are developed in this section are based on principles of thermodynamics and mass/energy transfer for unit operations of the NOXSO process. Data from various pilot studies has been used to parameterize these models.

1-5.1 Fluid Bed Adsorber Model

A mathematical model based on first principles has been developed by NOXSO Corporation for the design of future commercial installations (Ma and Haslbeck, 1993). The reaction rate constants for SO_2 and NO_x sorption were derived using data from the process development unit (PDU), life cycle-test unit (LCTU), and proof of concept (POC) tests. The rate constants have been lumped to treat the hydrodynamics of the gas-solid contact and the reaction kinetics in one variable. The main purpose of this model is to provide design equations for calculating key design parameters such as sorbent inventory and sorbent residence time for a desired level of SO_2 and NO_x removal. We have rewritten the equations developed by NOXSO Corporation to provide explicit relations for the design variables. Since the equations are quite detailed, and it is easy to get lost in the nomenclature, we first provide an overview of the equations.

Equations 1-23 to 1-26 express the pollutant removal efficiency in terms of the operating parameters of the fluidized bed (W, Fs) and physical constants (K_i, ρ, etc). The main objective here is to progressively rewrite the equations in terms of variables and functions which are readily measured and can be provided as inputs to the model. Equation 1-27 and 28 provide a set of equations for removal efficiencies, operating parameters and physical constants. Equations 1-29 to 1-32 provide a set of relations for the physical constants determined from experimental data. Finally, Equation 1-33 provides the design equations for the operating parameters of the fluidized bed absorber.

The fluid bed mass balance in the vertical direction is derived using the following assumptions: (i) there is no bubbling in the fluidized bed, (ii) the gas is in plug flow, (iii) the solids are in mixed flow, and (iv) SO_2 and NO_x absorption are first-order reactions with respect to their concentrations. Therefore the mass balance is written as follows:

$$- V C_0 (y_{oi} - y_{fi}) = \rho \lambda_i n K_i P \bar{y}_i (1 - \bar{X}) H \qquad (1\text{-}23)$$

Notice that unlike Equation 1-21, the mass balance has been written for the total bed by using a mean value for the concentration of gas species 'i'.

Defining the removal fraction as:

$$\phi_i = \left(1 - \frac{y_{fi}}{y_{oi}}\right)$$

Equation 1-23 can be rewritten as follows:

$$\phi_i = \frac{W}{F_g}\lambda_i \, n \, K_i \, P \, \frac{\overline{y}_i}{y_{oi}} \, (1 - \overline{X}) \tag{1-24}$$

When sorption takes place in the adsorber, both SO_2 and NO_x compete for active sites on the sorbent. A mass balance on the sorbent material in a mixed flow reactor results in:

$$F_s \, (\overline{X} - X_0) = W \, P \, (K_1 \, \overline{y}_1 + K_2 \, \overline{y}_2) \, (1 - \overline{X}) \tag{1-25}$$

Combining Equations 1-24 and 1-25, the removal efficiency for the ith gas species can be rewritten as:

$$\phi_i = \frac{W \, E_i}{F_g} K_i \, P \, \frac{\overline{y}_i}{y_{oi}} \, \frac{1}{1 + \dfrac{W}{F_s} P \, (K_1 \, \overline{y}_1 + K_2 \, \overline{y}_2)} \tag{1-26}$$

where $E_i = \lambda_i \, n \, (1 - X_0)$

Since the alumina substrate also adsorbs SO_2 and NO_x from the flue gas, the stochiometric ratio of reactant gas to active sorbent must include contributions from both sodium and alumina. In order to avoid having to make this distinction, an empirical relationship has been developed to calculate the stochiometry as a ratio of adsorber temperature:

$$\text{For } SO_2 : \frac{1}{\lambda_1} = 0.3761 + 0.0052 \, T_a$$

$$\text{For } NO_x : \frac{1}{\lambda_2} = -4.789 + 0.075 \, T_a \tag{1-26a}$$

where T_a is in degrees Celcius.

Since the gas flow in the fluidized bed is assumed to be plug flow and the reaction is first-order, $\overline{y}_i$ can be taken as the logarithmic mean expressed in terms of the removal efficiency as follows:

$$\overline{y}_i = \frac{-y_{oi} \, \phi_i}{\ln(1 - \phi_i)}$$

Substituting for $\overline{y}_i$ in Equation 1-26, the removal efficiencies can be written as follows:

For SO_2:

$$\ln(1 - \phi_1) - \frac{W}{F_s} P \frac{A}{A_0} \left(K_1 \, y_{01} + K_2 \, y_{02} \, \frac{\phi_2}{\ln(1 - \phi_2)} \, \frac{\ln(1 - \phi_1)}{\phi_1} \right) \phi_1 + \frac{W \, E_1}{F_g} P \, K_1 \, \frac{A}{A_0} = 0 \tag{1-27}$$

For NO_x:

$$\ln(1-\phi_2)-\frac{W}{F_s}P\frac{A}{A_0}\left(K_2\, y_{02}+K_1\, y_{01}\,\frac{\phi_1}{\ln(1-\phi_1)}\,\frac{\ln(1-\phi_2)}{\phi_2}\right)\phi_2+\frac{W\,E_2}{F_g}P\,K_2\frac{A}{A_0}=0 \quad (1\text{-}28)$$

Note that since removal is a sorption reaction, the rate constant is proportional to sorbent surface area which has been introduced into the equations (refer to Section 1-3.1). Equations 1-27 and 1-28 can be solved simultaneously for the removal efficiencies in terms of the following exogenously specified variables :

(i) The key operating parameters of the fluidized bed, i.e., sorbent residence time (W/F_S) and sorbent inventory (W),
(ii) Key inlet conditions including the mole fractions of SO_2 and NO_x (y_{oi}) entering the adsorber, and the flue gas flow rate (F_g),
(iii) Key physical constants including the lumped kinetic constants (K_i), the available surface area (A/A_o), and the available unused sorbent capacity (E_i).

The physical constants have been determined by NOXSO Corporation using experimental data from the PDU, LCTU, and POC tests. In the following paragraphs we describe the parametrizations used for solving the above equations.

The sorbent's SO_2 and NO_x capacities are calculated as follows:

$$\text{For } SO_2\text{: } E_1 = \left(\lambda_1\, n + \frac{0.8 - S_r}{3200}\right)\frac{A}{A_0} \quad (1\text{-}29)$$

$$\text{For } NO_x\text{: } E_2 = \left(\lambda_2\, n + \frac{0.8 - S_r}{3200}\right)\frac{\lambda_2}{\lambda_1} \quad (1\text{-}30)$$

where $n = \frac{n_{Na}}{2300} - \frac{n_{SiO_2}}{6000}$

Typically the sorbent contains 3.5-5% sodium and 6-7% silicon by weight.

The factor 0.8 in Equations 1-29 and 1-30 is the average sulfur content (% wt) of the regenerated sorbent in the PDU tests used as a reference for the above parametrization. The temperature dependent rate constants were derived by NOXSO Corporation by using PDU data along with Equations 1-27 and 1-28 to solve for K_i at different temperatures. A least squares fit was used to obtain the following relations:

$$\text{For } SO_2\text{: } K_1 = 52.15 \exp\left(\frac{-1840.2}{T_s + 273}\right) \quad (1\text{-}31)$$

$$\text{For } NO_x\text{: } K_2 = 14.75 \exp\left(\frac{-912.14}{T_s + 273}\right) \qquad (1\text{-}32)$$

The available surface area A/A_0 has a value of 0.6 based on PDU test data collected after sorbent surface area had stabilized.

For designing the adsorber, we need to estimate the operating parameters of the fluidized bed for given removal efficiencies for SO_2 and NO_x. The key parameters are the sorbent circulation rate, sorbent inventory, sorbent residence time and fluidized bed height. Equations 1-27 and 1-28 can be solved for sorbent inventory and sorbent circulation rate. Note that sorbent residence time also can be calculated from these two variables. The result is:

$$\frac{W}{F_s} = \frac{a_1 b_3 + a_3 b_1}{a_2 b_3 + a_3 b_2} \qquad (1\text{-}33a)$$

$$W = \frac{b_1(a_2 b_3 + a_3 b_2) - b_2(a_1 b_3 + a_3 b_1)}{b_3(a_2 b_3 + a_3 b_2)} \qquad (1\text{-}33b)$$

where

$$a_1 = \ln(1 - \phi_1);\ b_1 = (\ln(1 - \phi_2);$$

$$a_2 = P\frac{A}{A_0}\left(K_1 y_{01} + K_2 y_{02} \frac{\phi_2}{\ln(1-\phi_2)} \frac{\ln(1-\phi_1)}{\phi_1}\right);$$

$$b_2 = P\frac{A}{A_0}\left(K_2 y_{02} + K_1 y_{01} \frac{\phi_1}{\ln(1-\phi_1)} \frac{\ln(1-\phi_2)}{\phi_2}\right);$$

$$a_3 = \frac{E_1}{F_g} P K_1 \frac{A}{A_0};\ b_3 = \frac{E_2}{F_g} P K_2 \frac{A}{A_0};$$

The height of the fluidized bed is calculated as follows:

$$H = \frac{W}{\rho A_s} \qquad (1\text{-}33c)$$

The total sorbent inventory is calculated by adding the sorbent in the regenerator and the solids heater and cooler as follows:

$$S_{inv} = W + F_s\left(t_{CH_4} + t_{H_2O}\right) + 2\, A_{SH/SC}\, H_{SH/SC}\, \rho$$

where $A_{SH/SC}$ is the cross-sectional area of the sorbent heater/cooler and $H_{SH/SC}$ is the height of the sorbent. It has been assumed that the cross-sectional area for solids heater and the solids cooler is the same. The total pressure drop in the fluidized bed is easily calculated by considering the total weight of sorbent that is fluidized by the flue gas, i.e.

$$\Delta p = \frac{W}{A_s}$$

Sorbent attrition is caused by physical and thermal stresses that the sorbent experiences as it is transported through the processing loop. These stresses can fracture the sorbent beads and erode the surface of the beads. Sorbent makeup is then required to maintain a constant sorbent inventory. The attrition rate has been measured experimentally at the pilot plant and is equivalent to 0.026% of the inventory per hour. The makeup sorbent is calculated as follows:

$$m_{makeup} = AR_{sorbent} \times S_{inv}$$

where $AR_{sorbent}$ is the sorbent attrition rate.

Figures 3a and 3b graph the sensitivity of the two design variables (W and W/F_S) to different SO_2 and NO_x removal efficiencies. These sensitivities are plotted for a medium sulfur (2.6%S) Appalachian coal. The sorbent residence time (W/F_S) increases with the required NO_x and SO_2 removal (Figure 3a). Similarly, the sorbent inventory (W) also increases with NO_x and SO_2 removal (Figure 3b).

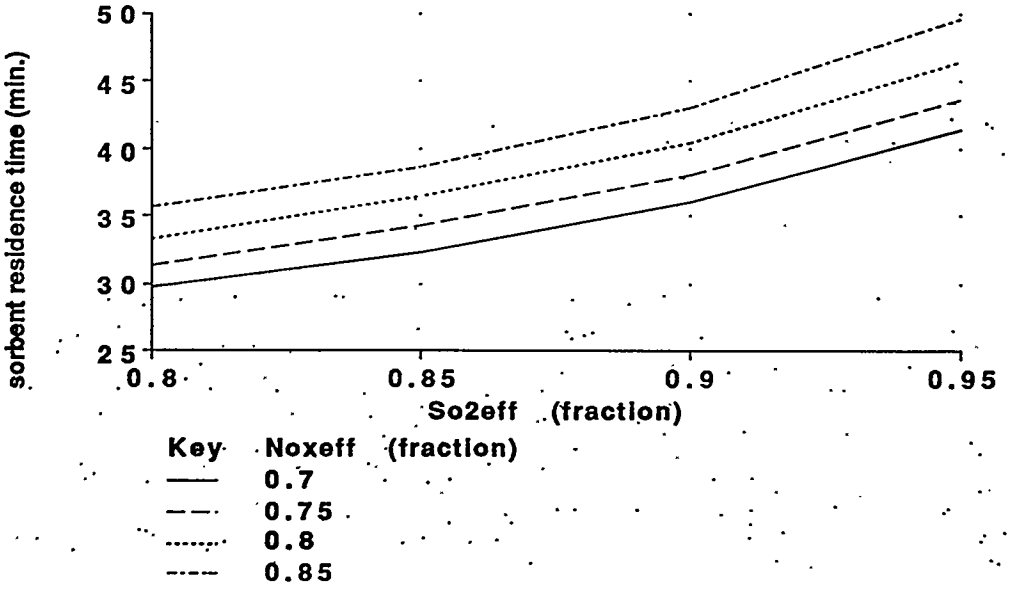

Figure 3a. Sorbent Residence Time in Adsorber (Medium Sulfur Appalachian Coal)

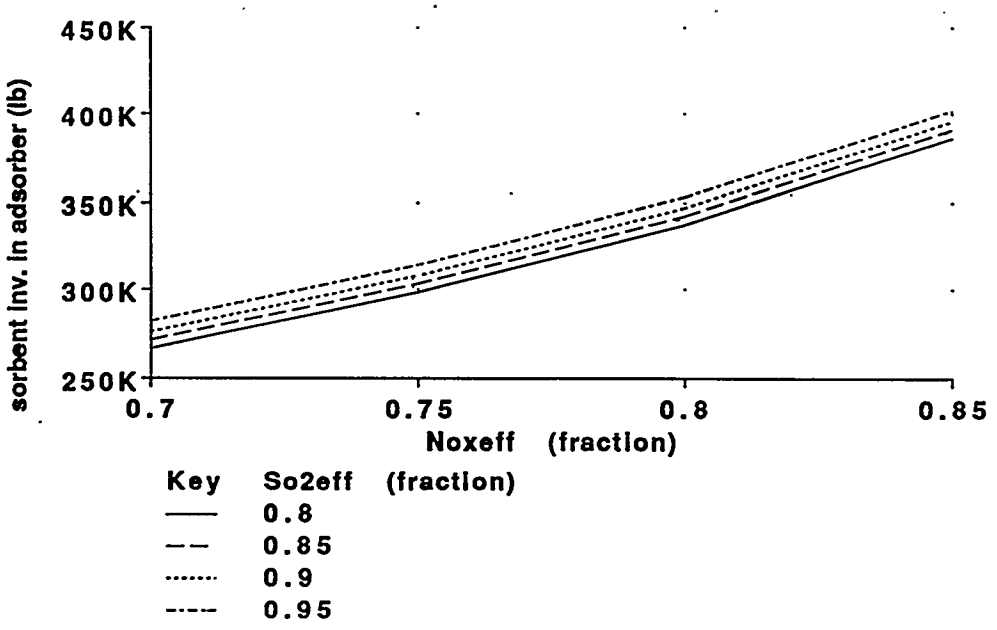

Figure 3b. Sorbent Inventory in Adsorber (Medium Sulfur Appalachian Coal)

A promising alternative to the single-stage fluidized bed design described above is a design featuring two fluidized beds in series. A schematic of the two-stage fluidized bed absorber is shown in Figure 4. In the two-stage design, regenerated sorbent enters a first stage fluidized bed, where the sorbent reacts with flue gas which has already passed through a second stage sorbent bed. The partially sulfated sorbent from the first bed then goes to a second bed, where it contacts inlet flue gas. Each of the two beds can have different bed heights and removal efficiencies. The overall removal efficiency is given by:

$$\phi_i = \phi_i^2 + \left(1 - \phi_i^2\right) \phi_i^1 \qquad i = SO_2, NO_x$$

where the subscripts 1,2 refer to the stage-1 and stage-2 fluidized beds. For each of the two beds, the general models given in Equation (1-33) apply. However, the input conditions for each bed is different. Since the output flue gas from the first stage enters the second stage, the SO_2 and NO_x concentrations are lower. Conversely, the regenerated sorbent enters the first stage and adsorbs SO_2 and NO_x before it enters the second stage. This is shown schematically in Figure 4.

The calculation procedure for a 2-stage bed requires the specification of the overall SO_2 (or NO_x removal efficiency) and a second stage removal efficiency. The removal efficiency for the 1st-stage is calculated as follows:

$$\phi_i^1 = \frac{\phi_i - \phi_i^2}{1 - \phi_i^2}$$

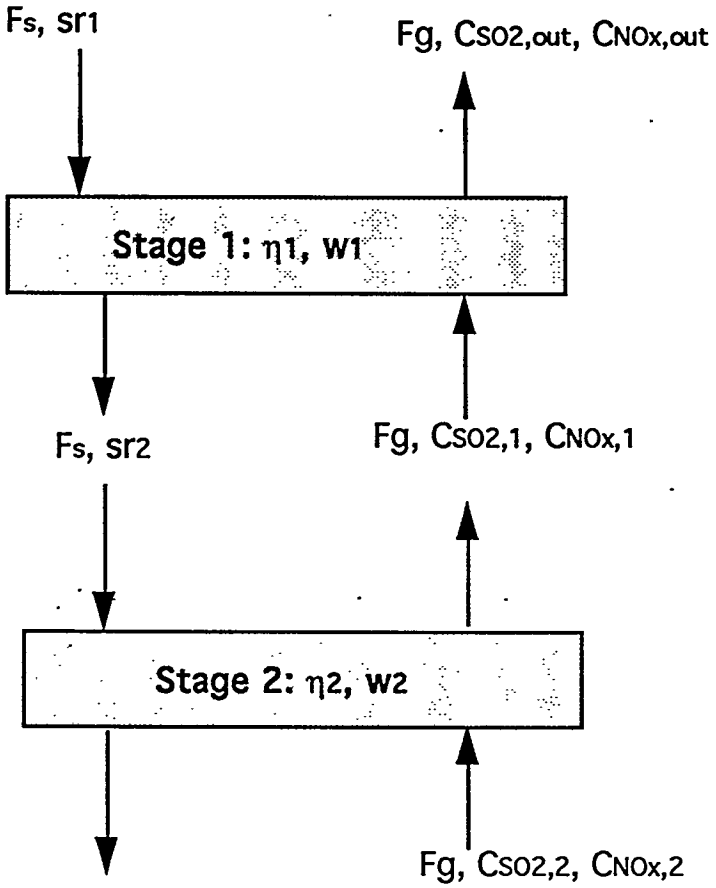

Figure 4. A Two-Stage Adsorber

The corresponding fluidized bed height (or sorbent inventory) and the sorbent circulation rate for stage-1 and stage-2 is calculated using Equations 1-33 as before. The larger sorbent circulation is used for costing purposes. It is assumed that SO_2 and NO_x removal are distributed between the two stages in a similar fashion.

1-5.2 Regenerator Model

The regenerator consists of two sections as shown in Figure 5. The sorbent moves down in a moving bed, while the regenerating gases move upward. The flow is assumed to be approximately plug flow. Natural gas enters the bottom of the upper section of the regenerator and reduces the sulfate on the sorbent to SO_2, H_2S, and sulfide. SO_2 and H_2S evolve as gases and sulfide remains on the sorbent surface. Steam is introduced in the lower section of the regenerator and hydrolyzes the sulfide to H_2S.

The models presented here determine the main operating parameters of the regenerator which are the sorbent residence times for natural gas reduction and steam reduction. The total residence time in the regenerator is used to size the regenerator and to estimate the

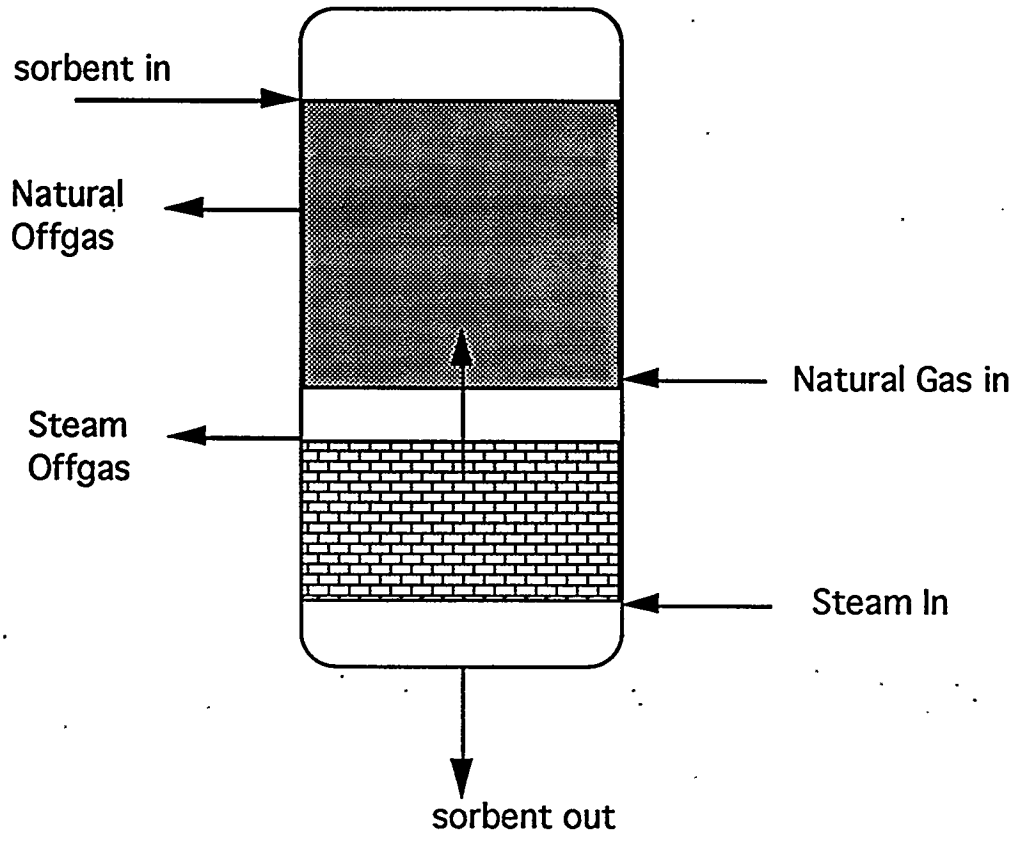

Figure 5. Schematic of the NOXSO Regenerator

sorbent inventory required for the regenerator. Moreover, the total height of the regenerator is calculated based on the respective residence times for natural gas and stream reduction. Equation 1-34 provides a mass balance for sulfur which has been used as a basis for interpreting experimental data. Equation 1-35 provides the rate constants for the two reduction reactions given by Equations 1-16 and 1-17. Finally, Equation 1-35 provides the design equations for sorbent residence times.

The sulfur molar balance provides the rate of sulfur regeneration as a function of sorbent flow rate and sorbent inventory as follows:

$$F_s S_a dX_r = r_s dW \Rightarrow X_r = \frac{W}{F_s S_a} r_s \qquad (1\text{-}34)$$

where $X = 1 - S/S_a$

The sulfur regeneration rate has been studied extensively in the POC plant. The experimental results indicate that regeneration consists of two main reactions and both are first-order with respect to sorbent sulfur content. The first set of reactions, corresponding to Equation 1-16, uses natural gas to reduce the sulfate. The second reaction corresponds to Equation 1-17 and uses steam to hydrolyze sulfide on the sorbent surface. Data from the POC plant was plotted as X_r vs. $W/(F_S S_a)$ based on Equation 1-30. This plot consists

of two straight lines with different slopes. The lines correspond to the reaction rates of Equations 1-16 and 1-17, respectively. The reaction rate of Equation 1-16 is eight times higher than that of Equation 1-17. The reaction rates have been parametrized using experimental data from the POC tests, and are given as follows (Ma and Haslbeck, 1993):

$$r_{s_1} = k_1 \exp\left(-\frac{E_1}{RT}\right) S_a$$
$$r_{s_2} = k_2 (1-0.6)\, S_a \qquad (1\text{-}35)$$
$$\text{where, } \frac{E}{R} = 34554.0;\ \ln(k_1) = 38.97;\ k_2 = 0.85;\ S_a = 0.01$$

Another result of these experimental studies is that 60% of the sulfur on the spent sorbent is regenerated by natural gas, while the steam treatment regenerates 20-30% of the remaining sulfides on the sorbent. The shift in sulfur regeneration from reaction 1 to reaction 2 at $X_{shift} = 0.6$ is independent of the inlet sorbent temperature. However, the amount of sulfur that is regenerated by the steam treater (X_{final}) depends on the inlet sorbent temperature. Typically, varying the inlet temperature from 1100-1250°F increases the sulfur regeneration from 20% to 30%. Assuming a linear relationship, this is written as:

$$X_{final} = (0.001\,T - 0.35 - X_{shift}) \qquad (1\text{-}36)$$

The heat of regeneration for both reactions also has been estimated from experimental data:

$$\Delta H_1 = 917.2 \text{ Btu/lb sulfur}$$

$$\Delta H_2 = 2032 \text{ Btu/lb sulfur}$$

The design equations for sorbent residence times are now straightforward:

$$t_{CH_4} = \frac{X_{shift}\, S_a}{r_{s_1}} \qquad (1\text{-}37a)$$

$$t_{H_2O} = \frac{(X_{final} - X_{shift})\, S_a}{r_{s_2}} \qquad (1\text{-}37b)$$

Figure 6 plots the sensitivities of the total regenerator residence time ($t_{CH4}+t_{H2O}$) as a function of the SO_2 and NOx removal efficiencies. The regenerator residence time increases with increasing SO_2 removal. However, with increasing NO_x removal, the total SO_2 removed decreases and this decreases the residence time required in the regenerator. The regenerator temperature is assumed to be 1150°F. Figure 7 examine the sensitivity of the total regenerator residence time to the regenerator temperature and the fraction of sulfur on the sorbent removed by methane reduction reactions, for 90% SO_2 removal and 80%

NOx removal. A 2.6% sulfur Appalachian coal is assumed. The residence time decreases with increasing temperature of the sorbent since the rate of the reduction reactions increases with temperature.

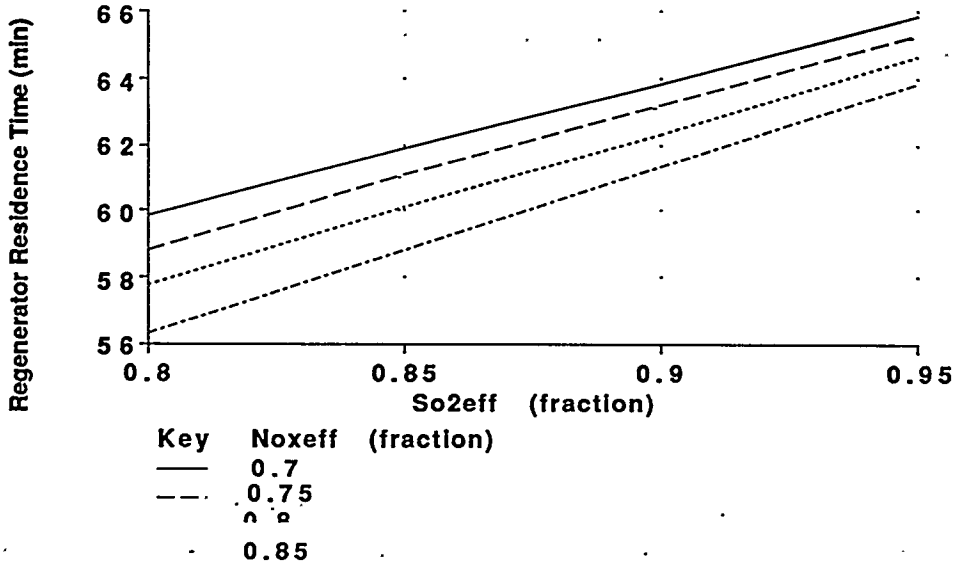

Figure 6. Sorbent Residence Time for Methane Reduction in Regenerator

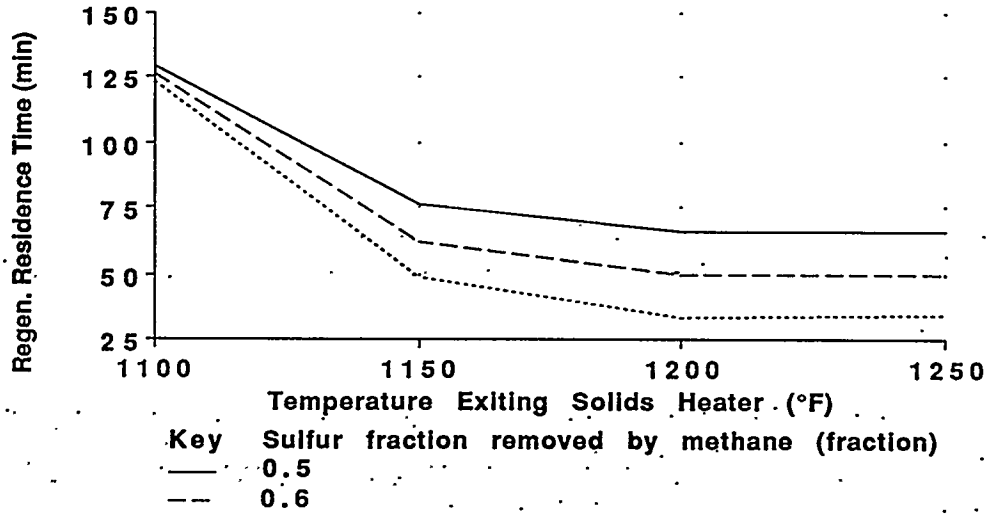

Figure 7. Regenerator Residence Time vs. Temperature and Sulfur Removal

1-5.3 Sorbent Heater and Cooler

Models of the sorbent heater and cooler are limited to simple mass and energy balances. The heat exchange between the sorbent and the hot air is treated as a simple energy balance. Similarly, the cooling of the sorbent is also treated as a simple energy balance as follows:

$$\mp F_g C_p (T - T_0) = \pm F_s c_{ps} (T_s - T_{s0}) \qquad (1\text{-}38)$$

where the subscript "0" refers to initial condition, and

F_g = gas flow rate (kmole/sec)
c_p = gas specific heat kcal/mole (°C)
F_s = sorbent flow rate (kg/sec)
c_{p_s} = sorbent heat capacity (kcal/kg°C)
T_s = sorbent temperature (°C)

The $\pm$ signs are chosen depending on whether sorbent is being cooled or heated. These heat exchange models are used to calculate the energy requirement for sorbent heating and the related calculation of natural gas consumption.

The mass balance equations are used to evaluate the amount of NO_x and SO_2 that are recycled to the boiler as part of the combustor gas. The NO_x from the sorbent is completely desorbed in the sorbent heater and about 5-10% of the SO_2 is desorbed. Since this extra amount of SO_2 and NO_x is recycled back to the flue gas, the absorber needs to actually remove a large fraction of these species in order to achieve the same levels of emissions as if there were no recycle. Mass balance equations are used to calculate the actual removal efficiencies for a desired level of emissions. A schematic of the recycle loop is shown in Figure 8 below.

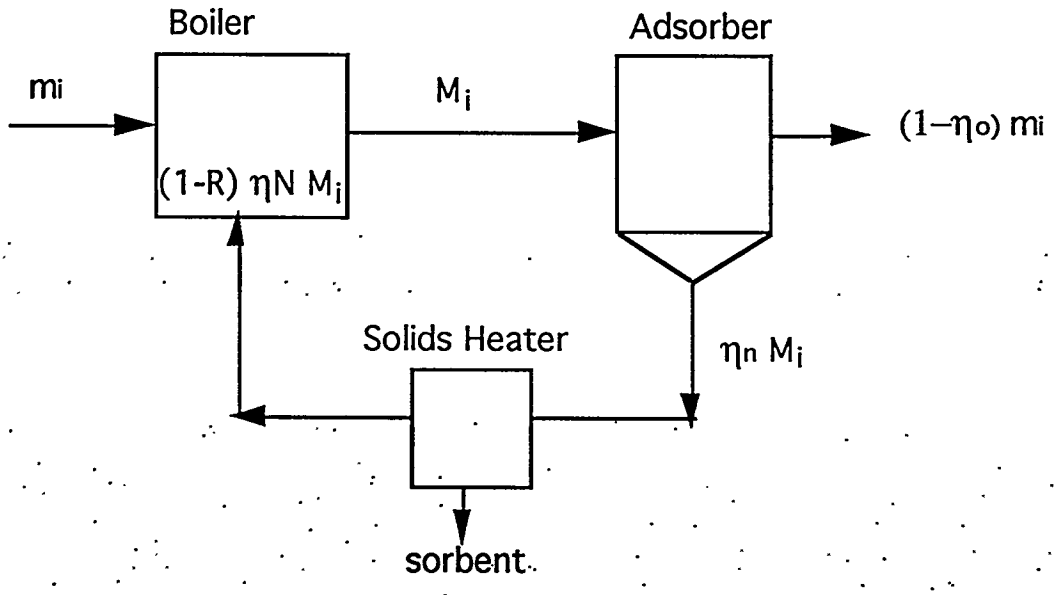

Figure 8. Schematic of the Recycle Loop

The initial mass flow rate for each species (SO_2, NO_x) is denoted by m_i and the mass flow rate with recycle is denoted by M_i. The desired emission level of $(1-\eta_o)\, m_i$ is specified with respect to m_i and let us assume that the required removal efficiency is η_o. Since the emission levels should not change with recycle, the actual removal efficiency η_N required to achieve this is given by

$$M_i (1 - \eta_N) = m_i (1 - \eta_O) \quad (1\text{-}39)$$

Moreover, from mass balance the recycle mass flow for species i (M_i) is related to original mass flow rate m_i as shown below:

$$M_i = m_i + (1 - R_i)\, \eta_N\, M_i \quad (1\text{-}40)$$

Solving these equations for η_N we get

$$\eta_N = \frac{\eta_O}{1 - (1 - \eta_O)(1 - R_i)} \quad (1\text{-}41)$$

where R_i is the recycle fraction for each species (94% for SO_2 and 65% for NO_x).

1-5.4 A Numerical Example

Provided here is a conceptual design of a commercial NOXSO plant of size 300 MW achieving 90% SO_2 removal and 80% NO_x removal. The coal used is a medium sulfur Appalachian coal (2.6% sulfur, and 1.12% nitrogen). The design specifications are:

Plant Size	300 MW, 842 Kacfm (at 320°F)
Temp. of flue gas entering adsorber	320°F
SO_2 removal requirement	90%
NO_x removal requirement	80%
Inlet SO_2 conc. (η_{SO2})	1516 ppm (calculated by IECM)
Inlet NO_x conc. (η_{NOx})	400 ppm (calculated by IECM)
Sorbent	Na_2CO_3 on γ-alumina spheres

Actual Removal Efficiencies

Since some NO_x and SO_2 are recycled back to the boiler, we need to calculate the actual absorber removal efficiencies required to achieve the desired design. This can be calculated by a simple mass balance of SO_2 and NO_x around the power plant once the recycle fractions are known. Based on the current NOXSO design, these fractions are 94% for SO_2 and 65% for NO_x. Thus,

$$\phi_{N,1} = \frac{\eta_{SO_2}}{1 - (1 - \eta_{SO_2})(1 - R_{SO_2})} = \frac{0.9}{1 - (1 - 0.9) \times (1 - 0.06)} = 0.905$$

$$\phi_{N,2} = \frac{\eta_{NO_x}}{1 - (1 - \eta_{NO_x})(1 - R_{NO_x})} = \frac{0.8}{1 - (1 - 0.8) \times (1 - 0.35)} = 0.86$$

Adsorber

Physical parameters required for the calculations are first estimated. Substituting the adsorber temperature of 275°F in Equation 1-26a we estimate the stochiometric ratios

$\lambda_1 = 0.93;\ \lambda_2 = 0.19.$

Similarly, the temperature-dependent rate constants obtained from Equations 1-31 and 1-32 are:

$$K_1 = 0.5734\ (\text{atm sec})^{-1};\ K_2 = 1.577\ (\text{atm sec})^{-1}.$$

The sorbent capacities are calculated using Equations 1-29 and 1-30. Based on pilot plant data, the weight fraction of sodium in the sorbent is taken to be 3.8%, silicon content is about 5.2%, the sulfur content of regenerated sorbent is 0.25%, and the available surface area fraction is 0.6. Thus,

$$\text{For } SO_2: E_1 = \left(\lambda_1 n + \frac{0.8 - S_r}{3200}\right)\frac{A}{A_0} = \left(0.93\times1.65\times10^{-3} + \frac{0.8-0.25}{3200}\right)\times 0.6 = 1.02\times10^{-3}$$

$$\text{For } NO_x: E_2 = \left(\lambda_2 n + \frac{0.8 - S_r}{3200}\right)\frac{\lambda_2}{\lambda_1} = \left(0.19\times1.65\times10^{-3} + \frac{0.8 - 0.25}{3200}\right)\times\frac{0.93}{0.19} = 0.3\times10^{-3}$$

Now the key operating parameters, sorbent residence time and sorbent inventory, can be calculated using Equation 1-33. The calculation of the intermediate variables is not shown.

$$\frac{W}{F_s} = -\frac{a_1 b_3 + a_3 b_1}{a_2 b_3 + a_3 b_2} = -\frac{-2.36\times11.5\times10^{-6} - 12.4\times10^{-6}\times1.97}{0.95\times10^{-3}\times11.5\times10^{-6} + 12.4\times10^{-6}\times0.84\times10^{-3}} = 2416 \text{ sec.}$$

$$W = \frac{b_1 - b_2\times W/F_s}{b_3} = -\frac{-1.97 - 0.84\times10^{-3}\times2416}{11.5\times10^{-6}} = 347{,}780 \text{ lbs of sorbent required}$$

Therefore, the sorbent flow rate F_S is 347,780 / (2416/3600) = 518,210 lbs/hr.

Regenerator

Once again the reaction rates are evaluated using Equation 1-35.

$$r_{s_1} = k_1 \exp\left(-\frac{E_1}{RT}\right) S_a = \exp(38.97 - 34554/895)\ 0.0136 = 0.0188$$

$$r_{s_2} = k_2 (1 - 0.6)\ S_a = 0.85\times0.4\times0.0136 = 0.0046$$

The shift in the reducing reaction from methane to water is at X_{shift}=0.6 and X_{final}=0.8. Therefore the residence time of the sorbent is calculated as follows using Equation 1-37:

$$t_{CH_4} = \frac{X_{shift}\, S_a}{r_{s_1}} = \frac{0.6 \times 0.0136}{0.0185} \times 60 = 26.5 \text{ min}$$

$$t_{H_2O} = \frac{(X_{final} - X_{shift})\, S_a}{r_{s_2}} = \frac{0.2 \times 0.0136}{0.0045} \times 60 = 36.3 \text{ min}$$

The total residence time in the regenerator is used to determine the sorbent inventory. This is used to estimate the cost of startup inventory.

$$\text{Inventory} = (F_S / 60)\,(t_{CH4} + t_{H2O})$$

$$\frac{518{,}210}{60}\,(26.5 + 36.3)$$

$$= 536{,}600 \text{ lbs}$$

DISCLAIMER

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Section 2: NOXSO Cost Models

2-1 OVERVIEW OF COST MODELING METHODS

Because the NOXSO process is a new technology still under development, cost information is still extremely limited. Recent published reports (Leonard et al 1994, Haslbeck et al 1993, Cichanowicz et al 1991) have provided estimates of the total capital requirement, but with little supportive detail. Prior to the present study, a 1986 EPRI study remains the only published cost estimate of the NOXSO process with process area detail. That study was the basis for the NOXSO cost model originally developed for the IECM (CMU, 1986). Thus, unlike other IECM components, for which detailed engineering cost studies have been completed more recently, little recent information for NOXSO process costs is available in the open literature.

For this reason, two approaches to cost modeling are presented in this report. The first method is based on the earlier economic evaluation of the NOXSO process performed for EPRI. This 1986 cost analysis is useful since it is the only study based on detailed equipment costing which is available in the open literature. Moreover, recent NOXSO reports continue to report capital cost estimates which are virtually identical to the cost estimate provided in the 1986 EPRI study.

A new (1995) cost model also has been developed for the NOXSO process, and implemented in the IECM. The new model is based on a detailed cost model of the fluidized bed copper oxide process recently developed for the IECM (Frey and Rubin, 1994). The rationale for this approach is twofold:

1) The NOXSO process and the fluidized bed copper oxide process are structurally similar. Both processes use a regenerable sorbent which is cycled through a fluidized bed adsorber, sorbent heater, a combustor for the sorbent heater, a regenerator, sorbent cooler and a dense phase conveyor system for transporting the sorbent. As a result of this structural similarity, both processes use largely the same set of equipment. A key difference is that NOXSO, unlike the CuO process, does not require ammonia injection for NO_x removal. However, it does require recycle of NO_x to the furnace.

2) The difference in capital cost between these processes arises primarily from differences in the sizing of equipment since the operating conditions for the two processes are different. In particular, the NOXSO adsorber is operated at 320°F while the CuO process operates at 700°F. However, since the equipment cost models developed for the CuO process are sensitive to differences in operating parameters, these same models can be used to estimate costs for the NOXSO process conditions. Allowances also can be made for other cost items that distinguish these two processes.

The remainder of this report is organized as follows: Section 2-2 presents the new capital cost models for the NOXSO process, together with a comparison with results from the earlier EPRI study. Section 2-3 provides models of fixed and variable operating and maintenance (O&M) costs. Section 2-4 combines the capital costs with annual O&M costs to calculate a levelized revenue requirement or cost of electricity. Section 2-5 provides a numerical example of costing the NOXSO process, and compares current results with earlier EPRI studies. Finally, Section 2-6 outlines a list of issues that need to be addressed to further improve the current models.

2-2 CAPITAL COST MODEL

In this section we provide a detailed description of two capital cost models developed for the NOXSO process. Section 2.1 first reviews the cost model originally developed for the IECM based on the 1986 EPRI report. We refer to this as the 1986 model. Section 2-2.2 then develops a new cost model based on the recent modeling of the fluidized bed copper oxide (CuO) process. We refer to this as the 1995 model. Section 3.3 provides a comparison of results from the two models to illustrate the difference in the cost estimates generated by each model.

2-2.1 1986 Capital Cost Model

This model is based on a case study by EPRI (1986), and is similar to the original IECM cost model for NOXSO, except that a number of plant components have been updated. Capital costs were estimated for a base plant of 1000 MW with 4% sulfur coal. The main operating parameters for this base case design, which are used for scaling capital cost estimates, are provided in Table 1.

Table 1. Base Case Design Parameters (1000 MW plant)

Parameters	Values
Flue gas flow rate, acfm	3.6×10^6
Sorbent flow rate, lb/hr	1.36×10^6
Makeup sorbent flow rate, lb/hr	880
Surface area of adsorber, ft^2	2542
Methane consumption, lb/hr	7200

The EPRI report lists plant components by section with itemized delivered equipment costs. The cost of components for each process area has been summed to obtain the process facilities capital cost, as shown in Table 2. Two major changes were made to the EPRI assumptions regarding the process facilities cost:

(i) The EPRI report assumed the use of synthesis gas produced on site for regeneration. This has been replaced with the use of methane which is treated as one of the consumables. In order to account for this we eliminated the capital cost for a Texaco gasifier that was used in the original design as part of the regenerator (process area 40).

(ii) The original design used oil in the solids combustor. This, too, has been replaced with the use of methane. We assumed that the capital costs for storing and pumping methane would be similar to that of oil. However, the capital cost equations are now scaled by the amount of methane used rather than oil.

Table 2. Process Facilities Cost Based on 1986 EPRI Report

Area	Description	Equipment Cost (10^6 1986$)
10	Reagent Feed System	2.6
20	SO_2 Removal System	5.3
30	Flue Gas Handling System	20.6
40	Sorbent Regenerator System	15.13
70	General Support Equipment	0.29
80	Air Preheater Modification	-
90	Sulfur Byproduct Recovery	-
100	Initial Sorbent Inventory	-

The cost model for each process area was parameterized on one or more of the main operating parameters enumerated in Table 1. Coefficients were estimated by adding all component costs associated with each parameter and normalizing them to the base case. As a conservative estimate, an exponential scaling factor of 0.7 was used in the 1986 model to estimate costs for designs different from the EPRI base case. Thus, the canonical form used for all process area cost models is as follows:

$$C_i = \sum_i a_i x_i^{0.7} \qquad (2\text{-}1)$$

where x_i is the operating parameter used for scaling and a_i is the cost coefficient for each parameter.

2-2.1.1 Reagent Feed System

The reagent feed system consists of equipment for the preparation and transportation of the makeup sorbent to the adsorber. The pumps and storage tanks required for methane are also included in this process area. The capital cost for the reagent feed system is based on the makeup sorbent flow rate and methane consumption as shown below:

$$C_{10} = 14350\, m_{ms}^{0.7} + 1.925\, m_{CH4}^{0.7} \qquad (2\text{-}2)$$

2-2.1.2 SO_2 Removal System

The SO_2 removal system includes the absorber vessels and the sorbent pneumatic conveying system. The capital cost is scaled based on the cross sectional area of the adsorber vessels and is provided as:

$$C_{20} = 2188 \left(N_{towers} + N_{spares}\right) A_{absorber} \qquad (2\text{-}3)$$

2-2.1.3 Flue Gas Handling System

The flue gas handling system includes equipment for transporting flue gas such as I.D. fans, ductwork and inlet/outlet manifolds. The cost models are scaled based on flue gas flow rate as follows:

$$C_{30} = 530\ G_{FG}^{0.7} \tag{2-4}$$

2-2.1.4 Sorbent Regeneration System

The regeneration system includes the regenerator vessels, and regenerated sorbent handling equipment. The capital costs are based on sorbent flow rate and are given as follows:

$$C_{40} = 770\ m_{sorbent}^{0.7} \tag{2-5}$$

2-2.1.5 General Support Equipment

This process area accounts for all the miscellaneous equipment required for process areas 10, 20, 30, and 40. The cost model is defined as a fraction of the other process facilities cost as shown:

$$C_{70} = 0.007\ (C_{10} + C_{20} + C_{30} + C_{40}) \tag{2-6}$$

2-2.1.6 Air Preheater Modifications

Capital cost for air preheater, modifications to allow off-gas from the solids heater to preheat incoming combustion air is based on the change in the heat transfer in the air preheater. The IECM air preheater model is used for this purpose. The capital cost is scaled based on the UA product (Btu/K, a product of the heat transfer coefficient and the heat transfer area) of the heat exchanger. The capital cost is given as a function of the change in UA as follows:

$$C_{80} = 2.6\times10^{-3}\left(UA_{air}^{0.6} - UA_{orig}^{0.6}\right) \tag{2-7}$$

2-2.1.7 Sulfur Byproduct Recovery

A performance and cost model of a sulfur byproduct recovery process (Claus plant) has been developed for the IECM and is documented in an earlier reort to DOE (Rubin, et al., 1991). That model has been employed here.

2-2.1.8 Sorbent Inventory

The initial sorbent requirement is governed by the amount of sorbent hold up in the fluidized bed adsorber, the regenerator, and the solids heater. It is assumed that the sorbent hold up in the transport system is small. The cost for initial sorbent is given as follows:

$$C_{100} = \left(\rho_s Z_A A_A + m_s t_R + 2\,\rho_S Z_{SH} A_{SH}\right) S_{cost} \tag{2-8}$$

2-2.1.9 Total Process Facilities Cost

The total process facilities cost is the total of all process area costs and is given by:

$$PFC = C_{10} + C_{20} + C_{30} + C_{40} + C_{70} + C_{80} + C_{90} + C_{100} \quad (2\text{-}9)$$

Figure 9 graphs the sensitivity of the process facility cost to power plant size and coal type. Only medium to high sulfur coals are considered since the NOXSO process has not been tested for low sulfur coals. The Chemical Engineering plant cost index has been used to convert 1986 dollars to 1993 costs. The graph illustrates the economy of scale as plant size increases for a particular coal. Capital costs also are sensitive to coal properties. Higher sulfur content increases cost (e.g., 4%S Illinois coal vs. 2.6% Appalachian coal). However, other coal properties such as heating value that affect the flue gas volumetric flow also are important. Thus, although the North Dakota lignite has a lower sulfur content than the Appalachian coal, its heating value also is substantially lower; this generates a larger gas volume per MW of power produced, resulting in larger equipment sizes and higher cost. All of these interactions are captured in the IECM.

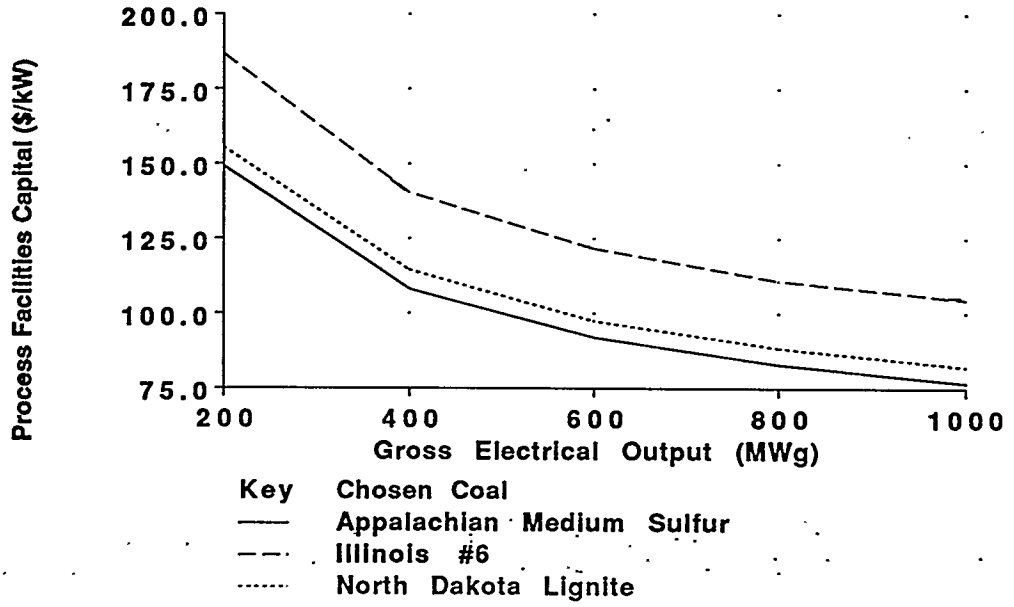

Figure 9. Total Process Facilities Cost (1993$) Based on the 1986 Model

2-2.2 1995 Capital Cost Model

The capital cost model presented in this section is based on a new cost model recently developed for the fluidized bed CuO process (CMU 1994). Appropriate changes have been made to tailor the models to the NOXSO process. Compared to the 1986 model, the new cost model is more highly disaggregated by process area.

2-2.2.1 Fluidized Bed Adsorbers

The process capital cost of the fluidized bed absorbers includes the absorber vessel, structural supports, dampers, isolation valves, refractory lining for the inside of the absorber, ductwork, instrumentation and control, and installation costs.

The absorber vessels are refractory-lined carbon steel of minimum one-half inch thickness. Each absorber vessel may be approximated as a cylinder. The internal diameter of the absorber vessel is determined based on the superficial gas velocity requirement. The materials cost of the absorber is proportional to the surface area of the absorber vessel. The absorber vessel internal radius is given by:

$$r_A = \sqrt{\frac{G_{FG}}{60\,\pi\,V_s\,N_{towers}}} \qquad (2\text{-}10)$$

The diameter of the absorber vessel must be larger than this internal radius to accommodate the thickness of refractory lining. The design basis developed by A.E. Roberts and Associates (AERA) for the copper oxide absorber includes a two-inch thick base or inner refractory covering the internal surface of the absorber vessel. This two-inch base or inner refractory lining also is assumed to be sufficient for the NOXSO process. The CuO process has an additional "hot base" refractory layer which is approximately six inches thick. However, since the adsorber temperature for the NOXSO process is only 320°F (as compared to 700°F for the CuO process), the "hot base" is assumed to be unnecessary for the NOXSO vessel. Thus, the vessel internal diameter is:

$$r_{V,A} = r_A + t_{ir} \qquad (2\text{-}11)$$

The surface area of the absorber vessel is approximated by the following equation for the surface area of a cylinder:

$$SA_A = 2\,\pi\left(r_{V,A}\right)^2 + 2\,\pi\,r_{V,A}\,h_A \qquad (2\text{-}12)$$

The design height of the copper oxide absorber vessel is approximately 70 feet. The total height of the absorber assembly is larger when flue gas outlet ductwork is taken into consideration. The straight wall portion of the absorber vessel that is covered with refractory lining is approximately 35 feet.

The direct cost for the steel absorber vessel is estimated based on the ratio of surface areas referenced to a base case design. The copper oxide design is predicated on a flue gas volumetric flow rate of approximately 500,000 scfm at 705 °F and a superficial gas velocity of 4.5 ft/sec. For this case, the approximate surface area of the absorber vessel is 24,875 ft^2. The base cost estimate is $1,434,000 (in 1993 dollars) for a single absorber vessel of this size. Therefore, the direct cost model for the cost of the NOXSO steel absorber vessel is given by:

$$C_{A,V} = 1434\,N_{total}\left(\frac{SA_A}{24{,}875}\right)\frac{PCI}{1993\,PCI} \qquad (2\text{-}13)$$

where the smaller surface area for the NOXSO process is calculated from Equations 2-10 to 12. Typically, there will be two 50% capacity absorber vessels with no spares.

The cost of refractory is given by the refractory surface area, required to cover the sides of the absorber vessel, and a unit cost for refractory per square foot:

$$C_{A,R} = 2\,\pi\, r_A\, h_{A,S}\, N_{towers}\, R_{cost} \qquad (2\text{-}14)$$

In 1993 dollars, the unit cost of the total of 8 inches of refractory required for the absorber was approximately $\$55/ft^2$.

Each absorber requires structural supports. In the copper oxide design, these are estimated at $100,000 per vessel. The structural support is assumed here to have some economy of scale with respect to size. A six-tenths scaling rule traditionally used in the process technology and chemical engineering literature is assumed:

$$C_{A,S} = 100\, N_{total} \left(\frac{SA_A}{24{,}875}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}15)$$

The surface area of the absorber vessel is used as a surrogate variable for the size of the absorber system and, hence, the proportional size of the structural supports.

The Costs for flue gas ductwork, flue gas isolation valves, and dampers are assumed to be proportional to the flue gas volumetric flow rate. Moreover, economies of scale are assumed. In the absence of more detailed information, the following direct cost model was adapted based on the copper oxide study:

$$C_{A,d} = 300\, N_{total} \left(\frac{G_{FG}}{1.1\times10^6\, N_{towers}}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}16)$$

In this model, the cost of ductwork, isolation valves, and dampers is estimated for a single absorber vessel, and is multiplied by the total number of absorber vessels. The total direct cost for the absorber process area is then given by:

$$C_A = (1 + f_{ic,a})\,(C_{A,V} + C_{A,R} + C_{A,S} + C_{A,d}) \qquad (2\text{-}17)$$

where $f_{ic,a}$ is an installation cost factor for the absorber process area. A default value of 0.45 is suggested for the CuO process and adopted as well for the NOXSO process.

In addition to these direct costs, there is a cost associated with using a new induced draft fan to overcome the pressure drop of the flue gas in the adsorber. The fan efficiency is typically 85 percent. The cost of the ID fan differential is:

$$C_{ID} = 180\, N_{A,t} \left(\frac{EC_{ID}}{4600}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}18)$$

2-2.2.2 Regenerator

The regenerator cost model assumes a carbon steel cylindrical vessel sized to accommodate sorbent storage for a specified sorbent residence time. The base case copper oxide design

has a regenerator with a sorbent hold-up volume of 8,800 ft^3. The regenerator design features a 28 foot straight wall height. Here, it is assumed that the straight wall height is held fixed, and the radius is adjusted to accommodate various residence times. Usually, columns that are higher than 28-30 feet require buildings with high roofs which increase construction costs. The required regenerator radius for the NOXSO process is therefore given by:

$$r_R = \sqrt{\frac{m_{s,R}\, t_R}{60\, \rho_s\, N_{towers}\, \pi\, h_{R,S}}} \tag{2-19}$$

The total height of the regenerator is the straight wall height plus inlet and outlet clearances for gas flows. These clearances add approximately 17 feet to the straight wall height. The inside of the regenerator vessel walls are covered with two layers of refractory totaling 8 inches in thickness. Therefore, the steel vessel diameter is:

$$r_{V,R} = r_R + t_{ir} \tag{2-20}$$

The surface area of the regenerator vessel is approximated by the surface area of a cylinder:

$$SA_R = 2\, \pi \left(r_{V,R}\right)^2 + 2\, \pi\, r_{V,R}\, h_R \tag{2-21}$$

For the copper oxide process, the regenerator has an equivalent overall height of 78 feet and a radius of 10 feet, yielding a surface area of 5530 ft^2. The direct cost of the NOXSO regenerator vessel is then estimated as:

$$C_{R,d} = 475\, N_{total} \left(\frac{SA_R}{5530\, N_{R,t}}\right)^{0.6} \frac{PCI}{1993\, PCI} \tag{2-22}$$

The additional direct cost of refractory is given by:

$$C_{R,R} = 2\, \pi\, r_R\, h_{R,S}\, N_{R,t}\, R_{cost} \tag{2-23}$$

Each regenerator requires structural supports. In the base case design, this cost is estimated at $42,500 per vessel. The structural support is assumed here to have some economy of scale with respect to size. A six-tenths scaling rule again is assumed:

$$C_{R,s} = 42.5\, N_{total} \left(\frac{SA_R}{5530\, N_{R,t}}\right)^{0.6} \frac{PCI}{1993\, PCI} \tag{2-24}$$

The surface area of the absorber vessel is used as a surrogate variable for the size of the regenerator system and, hence, the proportional size of the structural supports.

The costs for ductwork, isolation valves, and dampers are assumed to be proportional to the regenerator off-gas volume flow rate. Moreover, economies of scale are assumed. In the base case analysis, approximately 626 lbmole/hour of off-gas is evolved from each of

the two copper oxide regenerator vessels. At 900°F, the volumetric flow rate is 21,900 ft^3/min. Thus, in the absence of more detailed information, the following direct cost model was developed:

$$C_{R,d} = 350\, N_{total} \left(\frac{G_{FG}}{626\, N_{R,t}} \right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}25)$$

In this model, the cost of ductwork, isolation valves, and dampers is estimated for a single absorber vessel, then multiplied by the total number of absorber vessels.

A methane feed system, a booster compressor and motor are required for the inlet methane to overcome the pressure drop through the regenerator. The booster compressor cost is assumed to be proportional to the methane flow rate. Again scaling costs from the copper oxide model gives:

$$C_{R,CH4} = 350\, N_{total} \left(\frac{M_{R,CH4}}{187\, N_{R,t}} \right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}26)$$

The total direct cost for the absorber process area is given by:

$$C_R = (1 + f_{ic,R})\,(C_{R,V} + C_{R,R} + C_{R,S} + C_{R,d} + C_{R,CH4}) \qquad (2\text{-}27)$$

where $f_{ic,R}$ is an installation cost factor for the absorber process area. A default value of 0.45 again is suggested.

2-2.2.3 Solids Heater

The solids heater is assumed to be a carbon steel cylindrical vessel. For the copper oxide process, AERA has designed a solids heater with an internal radius of 10 feet and a height of 50 feet. The side walls of the heater are lined with refractory material. The internal diameter of the solids heater is proportional to the mass flow of sorbent entering the vessel. The vessel contains two sorbent beds in which hot combustion gases from a methane combustor contact the sorbent in counter-current flow. Thus, for fixed bed heights in each stage, the solids heater internal radius varies with the sorbent mass flow rate as follows:

$$r_{SH} = \sqrt{\frac{m_{s,SH}\, t_{SH}}{400{,}000\, N_{SH,t}}} \qquad (2\text{-}28)$$

The inside of the solids heater vessel walls are covered with two layers of refractory totaling 8 inches in thickness. Therefore, the steel vessel diameter is:

$$r_{V,SH} = r_{SH} + t_{ir} \qquad (2\text{-}29)$$

The surface area of the solids heater vessel is approximated by the surface area of a cylinder. Thus, for a single vessel, the surface area is:

$$SA_{SH} = 2\,\pi\left(r_{V,SH}\right)^2 + 2\,\pi\, r_{V,SH}\, h_{SH} \qquad (2\text{-}30)$$

In the base case, the solids heater has an equivalent overall height of 50 feet and an internal radius of 10 feet. Scaling results for the copper oxide process, the direct cost of the NOXSO regenerator vessel is:

$$C_{SH,V} = 360\, N_{total}\left(\frac{SA_{SH}}{4060\, N_{SH,t}}\right)^{0.6}\frac{PCI}{1993\ PCI} \qquad (2\text{-}31)$$

The additional direct cost of refractory is given by:

$$C_{SH,V} = 2\,\pi\, r_{SH}\, h_{SH,S}\, N_{SH,t}\, R_{cost} \qquad (2\text{-}32)$$

Each solids heater requires structural supports. In the copper oxide design, these are estimated at $72,500 per vessel. The structural support is assumed here to have some economy of scale with respect to size. A six-tenths scaling rule gives:

$$C_{SH,s} = 72.5\, N_{SH,t}\left(\frac{SA_{SH}}{4060\, N_{SH,t}}\right)^{0.6}\frac{PCI}{1993\ PCI} \qquad (2\text{-}38)$$

The surface area of the solids heater vessel is used as a surrogate variable for the size of the NOXSO solids heater system and, hence, the proportional size of the structural supports.

The costs for ductwork, isolation valves, dampers, booster fans and motors are assumed to be proportional to the solids heater exit gas volumetric flow rate. Again, economies of scale are assumed. In the copper oxide process, approximately 6,500 lbmole/hour of gas exits the solids heater at 830 °F. Thus, the following direct cost model was developed:

$$C_{SH,d} = 608\, N_{total}\left(\frac{G_{SH,off}}{6467\, N_{SH,t}}\right)^{0.6}\frac{PCI}{1993\ PCI} \qquad (2\text{-}39)$$

In this model, the cost of ductwork, isolation valves, dampers, booster fans, and booster fan motors is estimated for a single solids heater vessel, and multiplied by the total number of absorber vessels.

The total direct cost for the solids heater is:

$$C_{SH} = (1 + f_{ic,SH})\,(C_{SH,V} + C_{R,r} + C_{SH,S} + C_{SH,d}) \qquad (2\text{-}40)$$

where $f_{ic,R}$ is an installation cost factor for the absorber process area. A default value of 0.45 is suggested.

2-2.2.5 Sorbent Transport System

A dense phase pneumatic transport system is employed to transport sorbent from the regenerator outlet to the absorber inlet. The transport system includes valves, compressors, piping, filters, and surge bins. The dense phase transport system was sized for a sorbent circulation rate of 1,000,000 lb/hr. The total cost for this system for the copper oxide process is $6,580,000. The cost of the NOXSO transport system is assumed to be proportional to the sorbent circulation rate. Thus, the equipment cost for the dense phase transport system is:

$$C_{ST,e} = 6580 \left(\frac{m_{sorbent}}{1,000,000}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}41)$$

In addition, a sorbent storage silo is required. The cost of these silos is proportional to the sorbent circulation rate and the sorbent attrition rate, which determine the sorbent make-up rate. The nominal sorbent makeup rate is 500 lb/hr in the base case design. Therefore, the cost of the storage silos with air locks is:

$$C_{ST,s} = 330 \left(\frac{m_{makeup}}{500}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}42)$$

The total direct cost for the sorbent transport system is:

$$C_{ST} = (1 + f_{ic,ST})\,(C_{ST,e} + C_{ST,s}) \qquad (2\text{-}43)$$

where $f_{ic,ST}$ is an installation cost factor for the solids transport process area. A default value of 0.45 is suggested.

2-2.2.6 Solids Heater Combustor

The cost of the combustor for the solids heater is assumed to be proportional to the methane requirement: Scaling results for the copper oxide combustor gives:

$$C_{SH,s} = 330\ (1 + f_{ic,SH,c}) \left(\frac{m_{CH4,SH}}{225}\right)^{0.6} \frac{PCI}{1993\ PCI} \qquad (2\text{-}44)$$

where $f_{ic,SH,c}$ is an installation cost factor for the solids heater combustor process area. A default value of 0.45 is suggested.

2-2.2.7 Byproduct Recovery

A performance and cost model (C_{By}) of a byproduct sulfur recovery plant has been developed previously (Rubin et al., 1991). This model has been adapted for the NOXSO process.

2-2.2.8 Air Preheater Modifications

The NOXSO process produces off-gas from the solids heater at temperatures of about 610°F. This can be used to preheat the combustion air going into the boiler. The cost of air preheater modifications (C_{APH}) to allow this was shown previously in Section 2-2.1.6.

2-2.2.9 Initial Sorbent Inventory

The initial sorbent requirement is governed primarily by the amount of sorbent hold up in the fluidized bed absorber, the regenerator, and the solids heater. It is assumed that the quantity of sorbent hold up in the transport system is small by comparison. The cost for initial sorbent fill is therefore:

$$C_{S,I} = \left(\rho_s Z_A A_A + m_s t_R + 2 \rho_S Z_{SH} A_{SH}\right) S_{cost} \qquad (2\text{-}45)$$

2-2.2.10 Total Process Facilities Cost

The total process facilities cost is the sum of the plant section direct costs. The cost of initial catalyst charge is also included in the direct costs because it is a large and integral part of the NOXSO system. Therefore, the total direct cost is given by:

$$PFC = C_A + C_{ID} + C_R + C_{SH} + C_{ST} + C_{SH,s} + C_{By} + C_{APH} + C_{S,I} \qquad (2\text{-}46)$$

Figure 10 graphs the sensitivity of process facilities cost for different coals as a function of plant size. As in Figure 9 shown earlier, this graph illustrates the economy of scale achieved in capital costs with increasing size, as well as sensitivity to fuel properties.

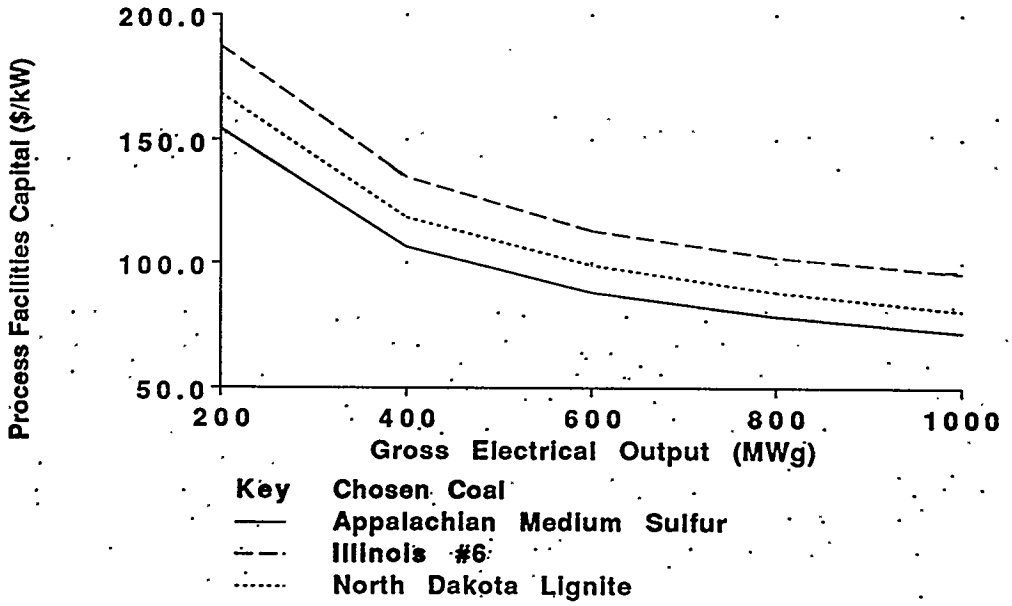

Figure 10. Total Process Facilities Cost (1993$) for the 1995 Model

2-2.3 Total Capital Requirement

All IECM cost models employ a standard set of "indirect" cost factors based on the EPRI costing methodology. These are model parameters that can be set by the user. Most of these factors are expressed as fractions of the total process facilities cost (PFC).The default values of all indirect cost factors associated with the NOXSO process have been adopted from the CuO study since both technologies are at similar stages of development. We enumerate the various indirect cost factors in Table 3 below with the default values used.

Table 3. Indirect Cost Factors

Indirect Cost Factor	Default Value	Formula
General Facilities Cost	10%	$C_{GFC} = f_{GFC}$ (PFC)
Engineering & Home Office Fees	15%	$C_{EHO} = f_{EHO}$ (PFC)
Project Contingency	20%	$C_{ProjC} = f_{ProjC}$ (PFC)
Process Contingency	20%	$C_{ProcC} = f_{ProcC}$ (PFC)
Total Plant Cost		$TPC=PFC+C_{GFC}+C_{EHO}+C_{ProjC}+C_{ProcC}$
Royalties	2%	$C_{Royal} = f_{Royal}$ (TPC)
Preproduction Costs	2%	$C_{PP}=f_{PP}$ (TPI)
Inventory Capital	0.5%	$C_{IC} = f_{IC}$ (TPC)

The total plant cost (TPC) is the overnight construction cost. An allowance for funds used during construction (AFUDC) is calculated based on the TPC as a function of the time to construct the NOXSO system. A 36 month construction period for a new plant is assumed. Methods for computing the AFUDC are documented elsewhere (e.g., EPRI, 1993) and are not repeated here. The total plant investment (TPI) represents the sum of the total plant cost and the AFDC.

The final measure of capital cost is the total capital requirement (TCR). The TCR includes the total plant investment plus costs for royalties, startup costs, and initial inventories of feedstocks. Preproduction costs typically include one month of both fixed operating costs (FOC) and variable operating costs (VOC) plus two percent of total plant investment. Inventory capital is estimated as 0.5 percent of total process capital excluding catalyst. For the NOXSO process, the costs for initial catalysts and chemicals is zero. The NOXSO initial sorbent requirement is included in the process capital costs. Thus, the total capital requirement for the NOXSO system is:

$$TCR = \frac{VOC + FOC}{12} + \left(1 + f_{PP} + f_{R}\right)(TPI) + f_{IC}(TPC) \qquad (2\text{-}47)$$

2-2.4 Comparison of Capital Cost Models

This section presents a numerical example which compares the new model cost estimates for the NOXSO process to the earlier 1986 model estimate based on the EPRI study. The comparison demonstrates the behavior of the NOXSO cost models and highlight parts of

the models that need to be further refined. We compare costs for a design with the performance characteristics shown in Table 4. The various performance parameters in Table 4 have been calculated using the NOXSO performance model which has been implemented in IECM.

Since the process area descriptions are different in the two models we present the cost estimates separately in Tables 5 and 6 below. Both models have been adjusted to report costs in 1993 dollars. Only the process facility costs are shown since this is the only source of differences between the two models.

It is interesting to note that the total process facilities cost estimates from the two models are within 5 percent of each other, when put on a common basis, with the 1995 model estimates being slightly higher. Thus, although the new model has been developed from a different basis it provides cost estimates similar to those reported earlier in the literature. For different plant sizes, the new model yields slightly greater economies of scale than the earlier 1986 model.

Table 4. NOXSO Process Design Assumptions for a 500 MW Plant

Parameter	Value
Required SO_2 Removal Efficiency, %	90
Actual SO_2 Removal Efficiency, %	90.5
Required NOx Removal Efficiency, %	80
Actual NOx Removal Efficiency, %	86
Flue Gas Inlet Temp. at Adsorber, ^oF	300
Absorber Sorbent Inventory, lbs	579,000
Regenerator Sorbent Inventory, lbs	894,000
Solids Heater Sorbent Inventory, lbs	931,000
Sorbent Circulation Rate, lb/hr	432,000
Makeup Sorbent, lb/hr	624
Train Size per Adsorber, acfm	425,000
Number of Absorbers (spares)	1(0)
Sorbent Absorber Residence Time, min	40
Superficial Flue Gas Velocity, ft/s	2.8
Expanded Bed Height, inches	32
Fluidized Bed Pressure Drop, in. H_2O	27
Solids Heater Outlet Temp., ^oF	1150
Methane Consumption, lb/hr	1952
Steam Consumption, lb/hr	2192
Sorbent Regenerator Residence Time, min	62
Sulfur Content of Spent Sorbent, wt %	2.7
Sulfur Content of Regenerated Sorbent, wt %	0.25

Table 5. NOXSO Process Capital Costs Using 1995 Model

Process Area* and Equipment	(1993 M$)
Adsorber (Area 10)	6.57
Adsorber Vessel	2.95
Refractory lining	0.90
Structural support	0.20
Ductwork	0.48
ID Fan Differential (Area 20)	0.39
Regenerator (Area 40)	4.71
Regenerator Vessel	1.16
Refractory lining	0.61
Structural support	0.10
Ductwork	0.43
Boosterfan	0.96
Solids Heater (Area 50)	7.45
Adsorber Vessel	0.78
Refractory lining	0.37
Structural support	0.15
Ductwork	3.83
Sorbent Transport System (Area 60)	9.18
Dense Phase Transport	6.0
Sorbent storage	0.3
Solids Heater Combustor (Area 70)	7.15
Sulfur Byproduct Recovery (Area 90)	8.40
Initial Sorbent Inventory (Area 100)	2.73
Adsorber inventory	0.87
Regenerator inventory	1.3
Solids heater inventory	0.52
Total Process Facilities Cost (M $)	46.57

*An installation cost factor of 0.45 is assumed for each process area. Thus, the total installed cost is 1.45 times the total equipment cost shown for each process area.

Table 6. NOXSO Process Capital Costs Using 1986 Model

Process Areas	(1993 M$)
Reagent Feed System (10)	1.62
SO_2 Removal System (20)	1.57
Flue Gas Handling System (30)	11.16
Sorbent Regenerator System (40)	18.4
General Support Equipment (70)	0.23
Sulfur Byproduct Recovery (90)	8.40
Initial Sorbent Recovery (100)	2.73
TOTAL	44.11

2-3 ANNUAL O&M COST MODEL

The annual operating and maintenance (O&M) costs for the NOXSO process consist of fixed operating and maintenance cost and variable operating costs. Cost models for these two components are summarized below.

2-3.1 Fixed Operating Costs

Fixed operating costs include operating labor, maintenance labor and materials, and overhead costs associated with administrative and support labor. The operating labor cost is based on an estimate of the number of personnel hours required to operate the NOXSO process multiplied by an average labor rate. It is common to assume that four shifts per day are required for plant operation, allowing two hours overlap for transition between shifts. Furthermore, an allowance for personnel on sick leave or vacation can be incorporated into the "shift factor." A shift factor of 4.75 is assumed as a default in this study, based on Bechtel (1988). For the NOXSO process we do not have any independent estimates for the labor, material and overhead costs. Therefore we have assumed the same set of default values as used for the CuO process.

The number of operators required per shift is assumed to be five. The total operating labor cost is estimated by summing the number of plant operators per shift for all process areas, applying the shift factor, and applying the average labor rate as follows:

$$OC_L = ALR \frac{2{,}080 \text{ hrs}}{\text{yr}} SF (1 + 2 N_{A,O}) \qquad (2\text{-}48)$$

The cost for maintenance material and labor for new technologies is typically estimated as a percentage of the installed capital cost for each process section. The total maintenance cost for the plant is given by:

$$OC_M = f_M (TPC) \qquad (2\text{-}49)$$

where a typical value of the maintenance cost multiplier, f_M, is 0.045 for a solids handling system. The total maintenance operating cost may be disaggregated into material and labor components using fractions suggested by EPRI:

$$OC_{MM} = 0.60\ OC_M \quad (2\text{-}50)$$

$$OC_{ML} = 0.40\ OC_M \quad (2\text{-}51)$$

The administrative and support labor cost is assumed to be 30 percent of the operating and maintenance labor cost:

$$OC_{AS} = 0.30\ (OC_L + OC_{ML}) \quad (2\text{-}52)$$

The total fixed operating and maintenance costs is:

$$FOC_{Total} = FOC_L + FOC_M + FOC_{As} \quad (2\text{-}53)$$

The total fixed O&M costs for different coals and plant size is graphed in Figure 11. This graph shows a nearly linear increase in the total fixed O&M cost with gross power plant size. As the plant becomes larger, the labor and maintenance costs exhibit a slight economy of scale. Since some of the fixed O&M costs are estimated as fractions of plant capital cost, total fixed cost also exhibits a sensitivity to fuel type, reflecting the cost differences seen earlier in Figure 10.

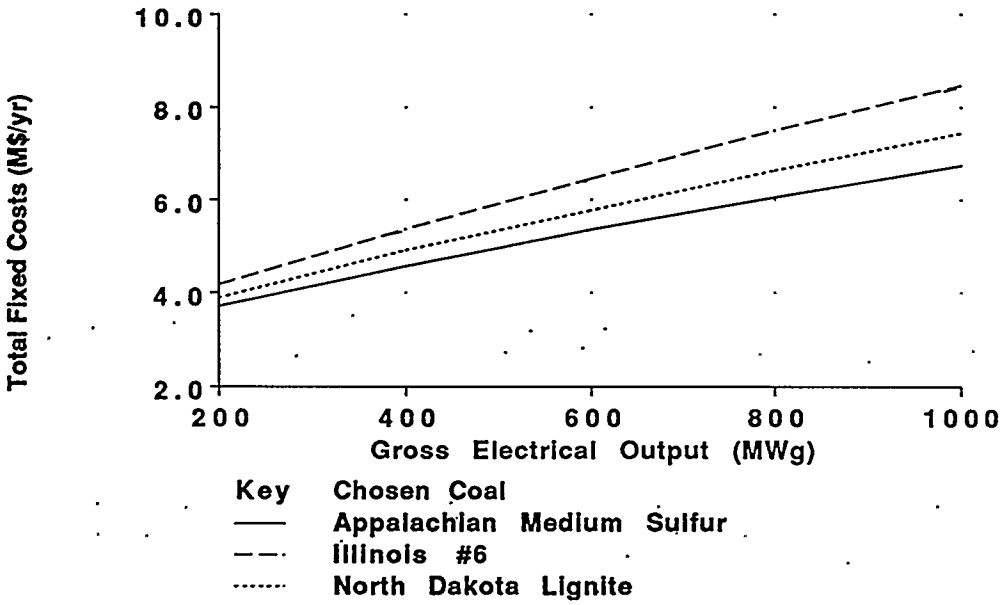

Figure 11. Fixed O&M Costs for Different Plant Configurations (1993$)

2-3.2 Variable Operating Costs

Variable operating costs include all consumable materials required for operation of the process. These include the costs of sorbent for makeup of attrition losses, the cost of methane and steam required for regeneration and solids heating. In addition, the electricity and steam consumption of the NOXSO process results in an energy penalty.

The annual costs for sorbent makeup, methane and steam consumption are given by:

$$VOC_{sorbent} = 8760\ cf\ m_{makeup}\ R_{sorbent} \quad (2\text{-}53)$$

$$VOC_{CH4} = 8760\ cf\left(m_{CH4,SH} + m_{CH4,R} + m_{CH4,By}\right) R_{CH4} \quad (2\text{-}54)$$

$$VOC_{steam} = 8760\ cf\left(m_{steam,R}\right) R_{steam} \quad (2\text{-}55)$$

Note that methane is required for solids heating, as a reducing gas for the regeneration reactions, and also as a reducing gas for off-gas pretreatment in the Claus plant.

The energy required to overcome the absorber flue gas pressure drop is:

$$EC_{ID} = \frac{G_{FG}\ \Delta P_A\ N_{A,O}}{8512\ \eta_{fan}} \quad (2\text{-}56)$$

Additional energy requirements for sorbent transport and for overcoming the pressure drop in the solids heater are calculated as follows:

$$EC_{sorbent} = \frac{1795\ (kW)}{1.36\times10^6\ (lb/hr)}\ m_{sorbent} \quad (2\text{-}57)$$

$$EC_{AH} = \frac{G_{Offgas}\ \Delta P_{AH}}{8512\ \eta_{fan}} \quad (2\text{-}58)$$

where the pressure drop ΔP_{AH} in the solids heater is typically about 4 inches of H_2O, and the fan efficiency is in the range of 50-85%, combining the three equations above yields the overall electrical energy operating cost:

$$VOC_{Elec} = 8760\ cf\left(EC_{sorbent} + EC_{AH} + EC_{ID}\right) R_{Elec} \quad (2\text{-}59)$$

Note that in the IECM the internal cost of electricity either can be specified by the user or calculated by the model based on generating costs for a new power plant.

Finally, the variable operating costs also include a byproduct credit for the sale of elemental sulfur produced by the Claus plant. The amount of this credit is given by:

$$VOC_{By} = 8760\ cf\ \eta_{By}\left(\frac{32\ M_{SO2,R}}{2000}\right) R_S \quad (2\text{-}61)$$

Summarizing the above terms, the total variable operating cost is:

$$VOC_{Total} = VOC_{sorbent} + VOC_{CH4} + VOC_{steam} + VOC_{Elec} - VOC_{By} \quad (2\text{-}62)$$

The total variable cost for different coals and plant sizes is graphed in Figure 12. As with fixed O&M cost, the total variable cost also increases in a nearly linearly fashion with plant size, reflecting larger input and output flows of plant materials and energy requirements. In this case, however, there is a slight upward curvature, indicating slightly higher variable

costs with increasing plant size. This is primarily due to nonlinearities that result in higher sorbent requirements and attrition losses with larger vessel sizes. Overall, however, this is not a significant factor affecting economics of scale.

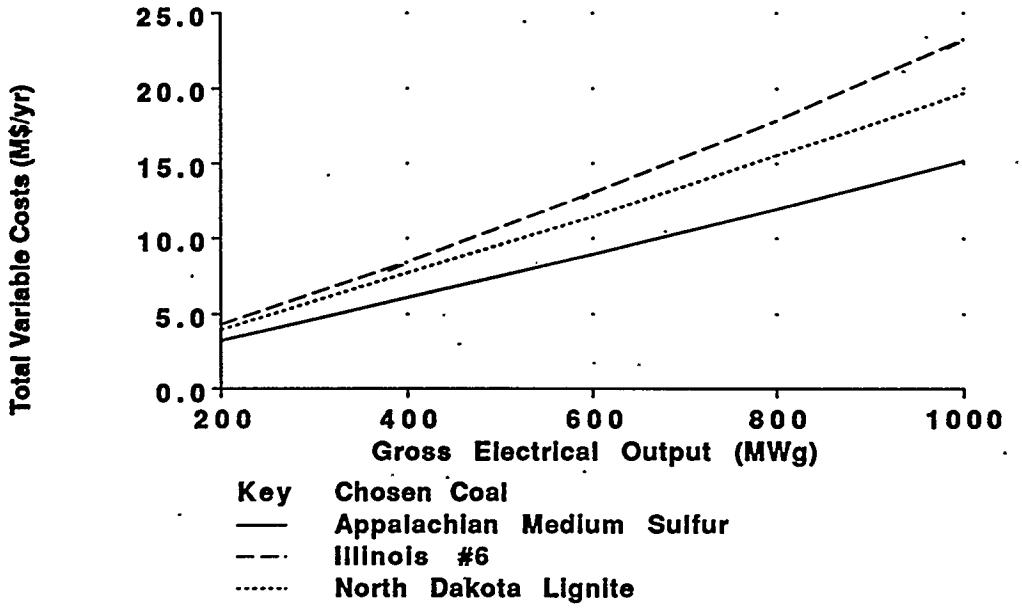

Figure 12. Variable O&M Costs for Different Plant Configurations (1993$)

2-4 TOTAL LEVELIZED COST MODEL

Typically, the capital and O&M costs are combined to determine a total annualized or levelized cost based on various financial parameters and the book life of the technology. A detailed discussion of levelized cost calculations can be found in EPRI TAG V3 (1989). The levelized cost is calculated as follows:

$$C_{NOXSO,\,Lev}\ (\$/MWh) = \frac{(fcf)\ (TCR) + (FOC + VOC)\ vclf}{8760\ (cf)\ (MW)} \qquad (2\text{-}63)$$

The IECM already contains a routine for calculating the levelized cost given the various input factors for a specific technology.

REFERENCES

Black, J. B., M. Woods, J.J. Friedrich and C. A. Leonard (1993). "The NOXSO Clean Coal Technology Project: Commercial Plant Design." *Proceedings of The Thirteenth EPRI/EPA/DOE SO2 Control Symposium*, Boston, MA.

Cichanowicz, J.E., C.E. Dene, W. DePriest and R.P. Gaikwad (1991). "Engineering Evaluation of Combined NO_x/SO_2 Controls for Utility Application," *Proceedings of the 1991 SO_2 Control Symposium*, EPRI/EPA, Miami, FL.

Davidson, J. F. and D. Harrison (Ed.) (1971). *Fluidization*. London, UK: Academic Press.

DePriest, W., R.P. Gaikwad and J. Jarvis (1986). "Technical and Feasibility Assessment of Combined SO_2/NO_x Processes," EPRI Report, TR-102820, V1, EPRI, Palo Alto, CA.

Frey, H.C. and E.S. Rubin (1994). "Performance and Cost Models for the Fluidized Bed Copper Oxide Process", Report No. DE-AC22-92PC91346-8, U.S. Department of Energy, Pittsburgh energy Technology Center, Pittsburgh, PA.

Haslbeck, J. L. and L.G. Neal (1985). "The NOXSO Process Development: An Update." *Ninth EPA/EPRI Symposium on Flue Gas Desulfurization*, Cincinnati, OH.

Haslbeck, J.L., M.C. Woods, W.T. Ma, S.M. Harkins and J.B. Black (1993). "NOXSO SO2/NOx Flue Gas Treatment: Proof-of-Concept Test", *Proceedings of 1993 SO_2 Control Symposium*, EPRI/DOE, Boston, MA.

Kunii, D. and O. Levenspiel (1969). *Fluidization Engineering*. New York: Wiley.

Leonard, C.A., J.L. Haslbeck, J.J. Friedrich and M.C. Woods (1994). "NOXSO Economics," Technical Report prepared by NOXSO Corp., Unpublished Manuscript.

Ma, W. T., J.L. Haslbeck, et al. (1993). "Proof-of-Concept Testing of the Advanced NOXSO Flue Gas Cleanup Process," Report of Contract No. DE-AC22-89PC88889, U.S. Dept. of Energy, Pittsburgh Energy Technology Center, Pittsburgh, PA.

Rubin, E.S., J.S. Salmento, H.C. Frey, A. Abu-Baker and M. Berkenpas (1991). "Modeling of Integrated Environmental Control Systems for Coal-Fired Power Plants," Report DE-AC22-87PC79864, DOE/PETC, Pittsburgh, PA.

Yates, J. G. (1983). *Fundamentals of Fluidized-Bed Chemical Processes*. Boston, MA: Butterworths.

Yeh, J. T., Drummond, C. J., Haslbeck, J. L. and L.G. Neal (1987). "The NOXSO Process: Simultaneous Removal of SO_2 and NO_x from Flue Gas." *Proceedings of Spring National Meeting of the AIChE*, Houston, TX.

Yeh, J. T., Ma, W. T., Pennline, H. W., Haslbeck, J. L. and F.N. Gromicko (1990). Integrated Testing of the NOXSO Process: Simultaneous Removal of SO_2 and NO_x from Flue Gas, *Proceedings of AIChE Spring National Meeting*, Orlando, FL.