Development and Application of Optimal Design Capability for Coal Gasification Systems - Task 1 (Volumes 1, 2, and 3)

Topical Report
July 1995

September 1995

Work Performed Under Contract No.: DE-AC21-92MC29094

For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

By
Carnegie Mellon University
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Performance and Cost Models For The Direct Sulfur Recovery Process - Task 1, Volume 3

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Task 1 Topical Report, Volume 3

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September 1995
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PREFACE

Insert one page introduction to the METC project, to be provided by Dr. E.S. Rubin.
## Nomenclature

### English Letter Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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</thead>
<tbody>
<tr>
<td><code>[A]_i</code></td>
<td>concentration of species A entering Stage I reactor (volume %)</td>
</tr>
<tr>
<td><code>[A]_o</code></td>
<td>concentration of species A leaving Stage I reactor (volume %)</td>
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<tr>
<td><code>[A]_G</code></td>
<td>concentration of species A generated in Stage I reactor by a certain reaction (volume %)</td>
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<td><code>[A]_{II,i}</code></td>
<td>concentration of species A entering Stage II reactor (volume %)</td>
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<td><code>[A]_{II,o}</code></td>
<td>concentration of species A leaving Stage II reactor (volume %)</td>
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<tr>
<td><code>[A]_{II,G}</code></td>
<td>concentration of species A generated in Stage II reactor by a certain reaction (volume %)</td>
</tr>
<tr>
<td>AFDC</td>
<td>Allowance for funds during construction, $1,000</td>
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<tr>
<td>C_{ProcC}</td>
<td>Process contingencies costs, $1,000</td>
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<td>Project contingencies costs, $1,000</td>
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<td>C_{EHO}</td>
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<td>C_{GF}</td>
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<td>C_{Roy}</td>
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<td>Direct capital cost of the DSRP, $1,000</td>
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<tr>
<td>DC_{GH,1}</td>
<td>Direct capital cost of the gas handling system for Stage I, $1,000</td>
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<td>DC_{S,1}</td>
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<td>Direct capital cost of the solids handling system for Stage II, $1,000</td>
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<tr>
<td>f_{InvC}</td>
<td>Inventory capital cost factor</td>
</tr>
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<td>f_{p}</td>
<td>Pressure correction factor (ratio)</td>
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<td>f_{ProjC}</td>
<td>Project contingency factors for each process area (fraction of direct cost)</td>
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<td>f_{Roy}</td>
<td>Royalties cost factor</td>
</tr>
<tr>
<td>FOC</td>
<td>Fixed operating cost, $1,000/yr</td>
</tr>
<tr>
<td>L_{cat}</td>
<td>Catalyst life, years</td>
</tr>
</tbody>
</table>
Greek Letter Symbols

\( \eta_{SO2,I} \) = fraction of \( SO_2 \) entering Stage I which is converted to elemental sulfur in that reactor

\( \eta_{SO2,II} \) = fraction of \( SO_2 \) entering Stage II which is converted to elemental sulfur in that reactor

\( \eta_# \) = portion of \( \eta_{SO2,I} \) accounted for by reaction (#)
1.0 INTRODUCTION

The purpose of this project is to develop performance and cost models of the Direct Sulfur Recovery Process (DSRP). The DSRP is an emerging technology for sulfur recovery from advanced power generation technologies such as Integrated Gasification Combined Cycle (IGCC) systems. In IGCC systems, sulfur present in the coal is captured by gas cleanup technologies to avoid creating emissions of sulfur dioxide to the atmosphere. The sulfur that is separated from the coal gas stream must be collected. Leading options for dealing with the sulfur include byproduct recovery as either sulfur or sulfuric acid. Sulfur is a preferred byproduct, because it is easier to handle and therefore does not depend as strongly upon the location of potential customers as is the case for sulfuric acid.

Many concepts for coal gasification power generation systems have been modeled using the ASPEN chemical process simulator. The U.S. Department of Energy (DOE) is among many organizations that have used process simulation tools to evaluate and optimize power generation concepts. The work described here is in support of DOE efforts to: (1) develop improved performance models for key components of the power generation systems; (2) develop new engineering-economic models; and (3) apply the models to gain insights into research priorities for future technology development and the comparison of technology alternatives.

In this report, the need for new sulfur recovery technologies for IGCC systems is reviewed. The DSRP is identified as one of the leading alternatives sulfur recovery. It offers the potential of low cost and high efficiency sulfur recovery. Technical background information is used to provide a basis for the development of a performance model of the DSRP. A new engineering-economic model of the DSRP is developed and documented. The performance and cost models are illustrated through several case studies. Needs for future work regarding model refinement and model applications are discussed. Because the DSRP has not yet been proven at full-scale, one key area for future work is the quantification of uncertainties inherent in making estimates of DSRP performance and cost for advanced IGCC systems. Thus, future case studies will feature a probabilistic approach to technology assessment.
2.0 ENVIRONMENTAL CONTROL IN IGCC SYSTEMS

IGCC systems offer the potential of lower environmental discharges than conventional coal-fired power plants. First, general features of IGCC technology are reviewed, followed by more detailed discussion of cold gas cleanup, hot gas cleanup, and sulfur recovery options.

2.1 IGCC Systems

The major components of coal are carbon and hydrogen. In conventional combustion, coal reacts with oxygen to produce carbon dioxide and water. The heat released from coal combustion is used to power a steam cycle with a steam turbine generator. During the coal gasification process, coal reacts with steam and a substoichiometric amount of oxygen, typically one-fifth to one-third the amount needed for complete combustion, at high temperature (e.g., 2000°C) and pressure (e.g., 400 psi) to produce a gas containing carbon monoxide and hydrogen. The partial combustion of the coal provides thermal energy required for the endothermic gasification reactions. The coal gas is highly combustible and can serve as fuel to gas turbines. However, the raw fuel gas contains contaminants such as particulate matter and hydrogen sulfide that can damage the turbines and result in unacceptable environmental discharges. Therefore, fuel gas cleanup steps are required to remove these containants. The cleaned coal gas is employed as a fuel for a gas turbine combined cycle (GTCC) system. A GTCC is composed of a simple cycle gas turbine and a bottoming steam cycle used to extract additional energy from the hot exhaust gases of the gas turbine. When a GTCC is integrated with a coal gasifier, the resulting process is known as an Integrated Gasification Combined Cycle (IGCC) (Simbeck, 1983). This system is shown schematically in Figure 1. This report focuses on the development of an analytic performance model for a component of an advanced IGCC system.

Coal contains components such as carbon, hydrogen, oxygen, nitrogen, sulfur, and ash. Sulfur and ash in particular are of key environmental and operational concern in coal gasification systems. When coal is gasified, sulfur-containing species such as hydrogen sulfide (H₂S) and carbonyl sulfide (COS) are formed. Sulfur species combusted in the gas turbine are converted to sulfur dioxide (SO₂) and are released into the atmosphere. Particulate matter or "fly ash" from the gasifier is also a source of emissions. Both sulfur and particulate matter emissions must be controlled to comply with federal, state, and local emission regulations and environmental permit agreements. For example, the Environmental Protection Agency (EPA) has regulations regarding industrial utility
Figure 1. Schematic Diagram of an Integrated Gasification Combined Cycle (IGCC) System
emissions, embodied in New Source Performance Standards (NSPS) for coal-fired boilers and gas turbines. While it is not clear which of these regulations would apply to IGCC systems, it is likely that state or local restrictions would be more stringent than others. In addition to environmental concerns, there are operational reasons to reduce emissions. Sulfur and ash contribute to corrosion, erosion, and fouling of turbine blades. For these reasons, it is essential to remove a high percentage (typically 95-99 percent) of the sulfur and more than 99 percent of the fly ash from the syngas before it is combusted to produce electricity.

2.2 Cold Gas Cleanup

Sulfur-containing species are typically removed from the coal gas by either hot gas desulfurization or cold gas desulfurization. The methods of cold gas desulfurization in use commercially can be divided into the two main categories of chemical and physical absorption. Chemical absorption involves reaction of acid gases (H$_2$S and CO$_2$) in the syngas with various solutions of alkanolamines or alkaline salts in water. In the absorber, the lean solution is contacted with the acid gas at high pressure. The temperature is typically between 80°F (27°C) and 120°F (49°C). The sulfur-rich solution is then reduced to low pressure and heated in the stripper to reverse the reaction and regenerate the absorbent solution. The temperature in the regenerator is the boiling temperature of the solution, usually 220-260°F (105-127°C). This solution is then cooled, pressurized, and recycled back to the absorber. This process removes acid gas from the syngas at low to moderate pressures, but the selectivity of H$_2$S absorption over CO$_2$ absorption is low (SFA, 1987).

The physical absorption processes rely on the solubility of the acid gases in certain organic solvents and are generally favored at high pressures (Simbeck, 1983). The hot coal gas from the gasifier is first cooled to approximately 100°F (38°C) using a series of shell and tube heat exchangers. The cooled gas is then cleaned through counter-current contact with the organic solvent in a packed bed. The removed sulfur is stripped from the solvent by lowering the pressure and raising the temperature. The cleaned gas is then sent on to the gas turbines and the sulfur-laden gas is sent to byproduct recovery (Fluor, 1985). Two popular methods of physical cold gas desulfurization are Selexol, which uses dimethyl ether of polyethylene glycol as a solvent, and Rectisol, which uses methanol as a solvent. These processes can effectively remove up to 95 percent or more of the H$_2$S in the coal gas (SFA, 1987). The offgas from cold gas desulfurization processes usually has a high sulfur concentration (in the form of H$_2$S).
2.3 Hot Gas Desulfurization

Since gas usually leaves the coal gasifier at an elevated temperature, hot gas desulfurization would be more efficient and economical than cold gas desulfurization. It would eliminate the need for heat exchangers to cool the hot gases, thereby potentially reducing the capital cost of the plant. Furthermore, hot gas cleanup enables more of the sensible heat of the fuel gas to be delivered to the gas turbine, where it can be efficiently converted to electricity. Thus, hot gas cleanup also offers the potential benefit of higher plant efficiency.

Mixed-metal oxide sorbents, such as zinc ferrite (ZnFe$_2$O$_4$) and zinc titanate (ZnTiO$_3$), are proposed to remove H$_2$S from the raw coal gas (e.g., Gangwal, 1991). As an example of hot gas desulfurization systems, we consider a fixed bed design as illustrated by Figure 2. Two parallel reactor vessels each contain a fixed bed of mixed-metal oxide sorbent pellets. As the diagram shows, each vessel cycles between absorption and regeneration phases. In Figure 2, the reactor on the left is in the absorption mode while the reactor on the right is in the regeneration mode. The reactors usually operate at pressures between 300 psia (20 atm) and 400 psia (27 atm) and inlet gas temperature of about 1100°F (600°C). The relevant reaction mechanisms occurring during absorption, using zinc ferrite sorbent, are:

$$6 \text{ZnFe}_2\text{O}_4 + \text{CO} + \text{H}_2 \leftrightarrow 6 \text{ZnO} + 4 \text{Fe}_3\text{O}_4 + \text{CO}_2 + \text{H}_2\text{O} \quad (1)$$

$$\text{ZnO} + \text{H}_2\text{S} \leftrightarrow \text{ZnS} + \text{H}_2\text{O} \quad (2)$$

$$\text{Fe}_3\text{O}_4 + 3 \text{H}_2\text{S} + \text{H}_2 \leftrightarrow 3 \text{FeS} + 4 \text{H}_2\text{O} \quad (3)$$

$$\text{COS} + \text{H}_2\text{O} \leftrightarrow \text{H}_2\text{S} + \text{CO}_2 \quad (4)$$

This yields an overall absorption phase reaction of:

$$6 \text{ZnFe}_2\text{O}_4 + \text{CO} + 5 \text{H}_2 + 17 \text{H}_2\text{S} + \text{COS} \leftrightarrow 6 \text{ZnS} + 12 \text{FeS} + 22 \text{H}_2\text{O} + 2 \text{CO}_2 \quad (5)$$

As this reaction illustrates the sorbent, sulfur species, and reducing gases (CO and H$_2$) react to form carbon dioxide, water, and two sulfated sorbent species (ZnS and FeS).

Once the absorption of hydrogen sulfide is complete, the cleaned syngas is sent onward to be used as fuel for gas turbines. The sorbent must then be regenerated so it can be reused. The sulfated sorbent is reacted with a stoichiometric amount of oxygen. This produces regenerated sorbent and an offgas stream typically containing one to three percent SO$_2$ for fixed-bed systems, although concentrations as high as 12 percent have been
Figure 2. Absorption/Regeneration System for Hot Gas Desulfurization.

○ = open valve

● = closed valve
observed for moving bed systems. Because the regeneration reactions are highly exothermic, a thermal diluent such as steam must be added to control temperature. Temperatures above 650 °C may cause sintering of the sorbent, so steam is necessary to keep the temperature below this level (Frey, 1991). Note that the sulfur concentration of the offgas is much lower than that occurring in conventional cold gas desulfurization systems. The relevant reaction mechanisms occurring during regeneration of zinc ferrite sorbent are (METC, 1987):

\[
2 \text{FeS} + 7/2 \text{O}_2 \leftrightarrow \text{Fe}_2\text{O}_3 + 2 \text{SO}_2 \tag{6}
\]

\[
\text{ZnS} + 3/2 \text{O}_2 \leftrightarrow \text{ZnO} + \text{SO}_2 \tag{7}
\]

\[
\text{ZnO} + \text{Fe}_2\text{O}_3 \leftrightarrow \text{ZnFe}_2\text{O}_4 \tag{8}
\]

This yields an overall regeneration phase reaction of:

\[
2 \text{FeS} + \text{ZnS} + 5 \text{O}_2 \leftrightarrow \text{ZnFe}_2\text{O}_4 + 3 \text{SO}_2 \tag{9}
\]

The reactor vessels for absorption and regeneration are generally vertical cylinders with a maximum diameter of 12.5 feet to enable rail shipment and a maximum length-to-diameter ratio of four (Kasper, 1988). Research has indicated that maximum absorption occurs at temperatures between 1000°F (540°C) and 1200°F (650°C) (Underkoffler, 1986). For best results, a maximum space velocity of 2,000/hr should also be observed. Space velocity is defined as the volume of gas fed to the reactor at standard temperature and pressure (0°C, 1 atm) per volume of sorbent per unit time. The sorbent should be replaced periodically under normal operating conditions due to attrition (Kasper, 1988).

2.4 Sulfur Recovery

The sulfur dioxide-containing offgas from hot gas desulfurization systems must be handled in an environmentally acceptable manner. The sulfur dioxide is typically converted to elemental sulfur or to sulfuric acid. Historically, between 85 and 90 percent of all elemental sulfur consumed in the United States has been converted first to sulfuric acid. However, the market for sulfuric acid appears to be diminishing. Sulfuric acid is very expensive to store and can be costly and dangerous to transport. Therefore, unless the energy plant needs sulfuric acid on-site or the demand is high at a nearby site, it is more advantageous and profitable to convert the SO₂ to elemental sulfur (BRSC, 1987).

Sulfur is the second most consumed mineral in the world (after coal). Conversion of SO₂ to elemental sulfur is both environmentally and economically desirable. Elemental sulfur is easily stored and transported, and it is a valuable industrial commodity. The most
A common method of converting hydrogen sulfide and sulfur dioxide to elemental sulfur is use of a Claus plant. Elemental sulfur is typically produced by reacting H_2S and SO_2 in the presence of a catalyst via the Claus reaction:

\[ 2 \text{H}_2\text{S} + \text{SO}_2 \leftrightarrow 3 \text{S} + 2 \text{H}_2\text{O} \quad (10) \]

Since the regeneration offgas from conventional cold gas desulfurization processes contains H_2S at fairly high concentrations and contains no SO_2, part of the feed stream is usually combusted to form SO_2 by the following reaction:

\[ 2 \text{H}_2\text{S} + 3 \text{O}_2 \leftrightarrow 2 \text{H}_2\text{O} + 2 \text{SO}_2 \quad (11) \]

Thus, the overall reaction in a typical Claus plant is:

\[ 2 \text{H}_2\text{S} + \text{O}_2 \leftrightarrow 2 \text{H}_2\text{O} + 2 \text{S} \quad (12) \]

A typical Claus plant consists of two reactors, each followed by a sulfur condenser to remove elemental sulfur. The first reaction is rapid and occurs at a high temperature of 2300-2500°F (1260-1370°C). The second reaction is much slower and requires several stages of catalytic reactors at 400-500°F (205-260°C). Sulfur recovery in a Claus plant is usually between 91 and 98 percent (SFA, 1987).

Claus plants are adept at handling feed streams with high sulfur concentrations, but they are ineffective for feed streams with less than about 15 percent H_2S. There are some modified Claus processes, such as Selectox, which can handle low sulfur concentrations, but the conversion to elemental sulfur is typically too low (70 to 90 percent). Other processes, such as wet oxidation, produce elemental sulfur in water-based solutions. These processes yield very high conversion rates for low-sulfur feed streams, but they require special reagents such as vanadium salts and anthraquinone disulfonic acid (ADA). They are also quite expensive, especially if the reagent consumption is high. Therefore, wet oxidation processes are used mostly to further clean tail-gases from Claus plants if the sulfur recovery is not high enough to meet environmental and operational standards. The most widely used wet oxidation processes are Stretford, Takahax, Unisulf, and LO-CAT (SFA, 1987).
3.0 DIRECT SULFUR RECOVERY PROCESS

Since 1988, researchers at the Research Triangle Institute (RTI) have been developing a process to convert feed streams with low sulfur concentration to elemental sulfur. The Direct Sulfur Recovery Process (DSRP) appears to be capable of effectively converting the \( \text{SO}_2 \) in the regenerator offgas from a zinc ferrite-based hot gas desulfurization unit to elemental sulfur. Figure 3 is a schematic diagram of the DSRP unit. The DSRP promises to be an efficient way to lower sulfur emissions, but to date it has only been tested on a bench-scale. The major advantage of the DSRP over conventional Claus processes is the match in operating conditions between the DSRP and the hot gas cleanup portions of an IGCC plant. The DSRP operates at the same temperature and pressure as the zinc-ferrite desulfurization process. Using a proprietary catalyst, the DSRP can accommodate feed streams with low sulfur concentrations (as low as 0.85 percent by volume) with no pre-concentration necessary. This makes it especially attractive since the regenerator offgas from many hot gas desulfurization systems typically contains only one to three percent \( \text{SO}_2 \). The capital and operating costs for a two-stage DSRP unit also appear to be low compared with conventional elemental sulfur recovery processes (Notestein, 1990).

3.1 DSRP Bench Scale Experimental Apparatus

RTI has been conducting bench-scale testing on the DSRP since 1990. The DSRP bench-scale unit consists of four subunits: gas delivery, Reactor No. 1, Reactor No. 2, and gas conditioning/pressure control. Each reactor is followed by a sulfur condenser to remove elemental sulfur, and a re heater follows the first condenser to heat the gas back to an appropriate temperature for Reactor No. 2. The gas delivery system is capable of simulating regeneration offgas mixtures of up to 12 percent \( \text{SO}_2 \), and it is also capable of simulating typical gasifier effluent streams. Up to one liter of catalyst may be contained within each reactor. The reactors may be configured with space velocities up to 10,000 scf/(cc-hr).

The fixed-bed reactors for the bench-scale DSRP unit are built from four inch schedule 160 316H stainless pipe. The reactors are approximately 24 inches in height. The catalyst is held in a removable catalyst cage made of stainless steel. The catalyst bed is supported by a porous ceramic or perforated plate gas distribution. One liter of catalyst occupies nine inches of packing height. Figure 4 shows the structure of the DSRP reactors (Gangwal, 1990). Typical sulfur recovery values for the fixed-bed reactors are approximately 95 percent in Stage I and 80 to 90 percent in Stage II. Recent tests have also
Figure 3. Simple Schematic Diagram of the Direct Sulfur Recovery Process (DSRP) Bench-Scale Unit
Figure 4. Cross-Sectional View of a DSRP Bench-Scale Reactor
been conducted using a fluidized-bed reactor for Stage I and a fixed bed reactor in Stage II. Fluidization of the catalyst bed provides better temperature control over the exothermic SO₂ reduction reactions. Overall sulfur recoveries as high as 99.1 percent have been obtained with this reactor configuration and interstage water removal (Gangwal, 1993).

Once the elemental sulfur-laden gas leaves Reactor No. 1, it enters a sulfur condenser (see Figure 5) where it is cooled by surrounding steam at about 250°F (120°C) in a coil. The cooled gas is then flashed into the sulfur collection pot where gas and sulfur are separated. The elemental sulfur may then be drained. The separated gas goes to the re heater where its temperature is raised to a level required for the reactions in Reactor No. 2. Sulfur recovery as high as 96 percent has been observed after the first reactor. However, the overall percent recovery is often decreased in Reactor No. 2. This is due to insufficient separation of gas and sulfur in the condensers. If all the elemental sulfur exiting Reactor No. 1 is not removed before the gas enters Reactor No. 2, the reverse Claus reaction may occur and the process can become counter-productive. Improvements need to be made to the condensers to achieve sufficient sulfur recovery of more than 99 percent (Gangwal, 1992). The researchers at RTI have recently devised a technique that can be used to completely condense the sulfur interstage, but information regarding this technique has not yet been disclosed (Gangwal, 1993).

Once the gas has been through both Claus reactors and the elemental sulfur has been recovered, the gas enters the gas conditioning subsystem. This system is unique to the bench scale test apparatus, and is required to remove pollutants from the gas stream prior to discharge to the atmosphere. First a high pressure Dryrite trap removes essentially all water vapor from the stream. Particulate matter is removed by a Balston filter, then the gas enters a back pressure regulator to reduce pressure. Finally, the nearly atmospheric pressure gas will pass through a two-stage NaOH scrubber to remove any remaining H₂S and SO₂ prior to venting. If the mass output of sulfur dioxide in the vented stream is still too high, this tail-gas may need further treatment (Gangwal, 1990). The goal for the DSRP is to achieve high enough conversions such that tail-gas treatment will be unnecessary. As part of integration with an IGCC system, the DSRP tail gas may be combined with the coal gas stream prior to gas turbine combustion (e.g., Robin et al., 1993).

More recent experimental work has focused on the development of a skid-mounted bench scale zinc titanate fluidized bed desulfurization and DSRP reactor system. The skid-mounted system will be employed in testing with coal gas slip streams from larger scale coal gasification facilities. Future plans include the design, fabrication, and commissioning of a larger, pilot-plant scale DSRP reactor system. The pilot-plant system will be designed
Figure 5. DSRP Bench-Scale Sulfur Condenser

A, G: 1/2" Female Weld Fitting
B: SS 3/8' Tubing, 0.035" Wall
C: Blind Flange
D, F: 3/8" Weld Fitting
E, H, I: 3/8" Bored-through Union
for gas volume flow rates six times larger than for the bench-scale design (Gangwal et al., 1994).

3.2 DSRP Process Chemistry

In bench-scale tests, the feed to the DSRP typically consisted of a simulated SO₂ offgas from the regenerator of a zinc ferrite desulfurization process and a stream of reducing gas (H₂S, H₂, CO). The flowrates were adjusted so that there was a 2 to 1 ratio of reducing gas to SO₂. Since the raw coal gas effluent from a gasifier contains H₂S, a slip stream of this gas could be used as the source of the reducing gas. This mixture of offgas and reducing gas was reacted in the presence of a catalyst at a pressure of 20 atm and temperature of 450-700°C in Reactor No. 1, which can operate as either a fixed-bed or fluidized-bed catalytic reactor. In the tests reported to date, only the fixed-bed mode has been used extensively. Under these conditions, the following reactions network is postulated:

\[
\begin{align*}
\text{CO} + \text{H}_2\text{O} & \leftrightarrow \text{CO}_2 + \text{H}_2 \quad (13) \\
\text{SO}_2 + 2 \text{H}_2 & \rightarrow \frac{1}{x} \text{S}_x + 2 \text{H}_2\text{O} \quad (14) \\
\text{SO}_2 + 3 \text{H}_2 & \rightarrow 2 \text{H}_2\text{O} + \text{H}_2\text{S} \quad (15) \\
\text{SO}_2 + 3 \text{CO} & \rightarrow \text{COS} + 2 \text{CO}_2 \quad (16) \\
\text{SO}_2 + 2 \text{CO} & \rightarrow 2 \text{CO}_2 + \frac{1}{x} \text{S}_x \quad (17) \\
\text{SO}_2 + 2 \text{COS} & \leftrightarrow 3\text{x} \text{S}_x + 2 \text{CO}_2 \quad (18)
\end{align*}
\]

Reaction (13) is the water gas shift reaction. It is presumed to be at equilibrium as the gas streams enter the reactor. Reaction (14) is a desired conversion of SO₂ to elemental sulfur via reaction with hydrogen. Reaction (15) is desired because it produces the H₂S needed to react with SO₂ in Stage II. Reactions (16) and (17) are governed by catalyst space velocity. At high space velocities (greater than about 6×10⁵ cc/hr·g), only reaction (16) occurs (See Section 4.1.1 for complete explanation). At lower space velocities, both reactions (16) and (17) occur. Reaction (17) becomes more prominent as space velocity is lowered, thus increasing sulfur conversion and lowering the amount of COS that is sent on to Stage II. Reaction (18) is clearly desirable because it converts two gaseous sulfur species to elemental sulfur.

After interstage sulfur condensation, the gas streams were sent to Reactor No. 2. This reactor was always operated in the fixed-bed mode, typically at temperatures between
250 and 300°C and a pressure of about 20 atm. Under these conditions, the following reactions are believed to occur:

\[
2 \text{H}_2\text{S} + \text{SO}_2 \leftrightarrow 3/x \text{S}_x + 2 \text{H}_2\text{O} \tag{19}
\]

\[
\text{COS} + \text{H}_2\text{O} \leftrightarrow \text{H}_2\text{S} + \text{CO}_2 \tag{20}
\]

Recall that reaction (19) is the Claus reaction. The "x" is typically between 2 and 8 depending on temperature and residence time. Reaction (20) converts any remaining COS to hydrogen sulfide, which is then converted to elemental sulfur via the Claus reaction. Bench-scale tests indicate that reaction (20) proceeds to completion. Due to the reaction mechanism for Stage II, the inlet stream should contain a 2 to 1 ratio of H\text{2}S and COS to SO\text{2} (Gangwal, 1993).

### 3.3 DSRP Design Studies

There have been two major published design studies that feature a performance and cost evaluation of the DSRP as applied to several IGCC flowsheets. The first of these is a 1993 study by Texaco which was published in May 1993 (Robin et al., 1993). In this study, the DSRP was evaluated as part of two different hot gas cleanup systems as applied to a Texaco gasifier-based IGCC system. In one case, a moving bed zinc titanate desulfuration system was evaluated, while in the other case a fluidized bed zinc titanate desulfurization system was studied. In both cases, detailed performance and cost data were reported. The performance data are summarized in Tables 1 and 2 for the two Texaco design cases. The tables reference stream numbers which are depicted in Figure 6.

The second design study was developed by Gilbert/Commonwealth, Inc (Buchanan et al., 1994). This study focused on evaluation of gas stream cleanup systems as applied to KRW gasifier-based IGCC systems. The DSRP was evaluated in conjuction with two IGCC designs that featured fluidized bed zinc titanate desulfurization. The difference in the two cases was that one was for an oxygen-blown gasifier, while the other was for an air-blown system. The report by Buchanan et al. does not provide as much detail regarding the DSRP performance and cost as does the report by Robin et al. Therefore, much of the model development effort benefited primarily from the latter report.
Figure 6. Simple Schematic Diagram of the Direct Sulfur Recovery Process (DSRP).

Table 1. DSRP Mass Balance for a Texaco IGCC with a Moving Bed Zinc Titanate Desulfurization System (Robin et al., 1993)a

<table>
<thead>
<tr>
<th>Stream Number</th>
<th>Description</th>
<th>Temperature (°F)</th>
<th>Pressure (psia)</th>
<th>Flow Rate (lb/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Regenerator Off-Gas</td>
<td>1,500</td>
<td>423</td>
<td>88,250</td>
</tr>
<tr>
<td>2</td>
<td>Coal Gas Slip Stream</td>
<td>1,496</td>
<td>476</td>
<td>10,420</td>
</tr>
<tr>
<td>3</td>
<td>Reactor No. 1 Inlet</td>
<td>962</td>
<td>411</td>
<td>98,650</td>
</tr>
<tr>
<td>4</td>
<td>Reactor No. 1 Outlet</td>
<td>1,292</td>
<td>386</td>
<td>95,900</td>
</tr>
<tr>
<td>5</td>
<td>Condenser No. 1 Outlet</td>
<td>320</td>
<td>376</td>
<td>95,900</td>
</tr>
<tr>
<td>6</td>
<td>Reheater Outlet</td>
<td>544</td>
<td>376</td>
<td>96,100</td>
</tr>
<tr>
<td>7</td>
<td>Reactor No. 2 Outlet</td>
<td>550</td>
<td>351</td>
<td>95,900</td>
</tr>
<tr>
<td>8</td>
<td>Condenser No. 2 Outlet</td>
<td>320</td>
<td>341</td>
<td>95,900</td>
</tr>
<tr>
<td>9</td>
<td>DSRP Off-Gas to Gas Turbine</td>
<td>320</td>
<td>341</td>
<td>61,750</td>
</tr>
<tr>
<td>10</td>
<td>DSRP Off-Gas to Other Areas</td>
<td>320</td>
<td>341</td>
<td>34,100</td>
</tr>
<tr>
<td>11</td>
<td>Elemental Sulfur from Cond. No. 1</td>
<td>320</td>
<td>376</td>
<td>2,750</td>
</tr>
<tr>
<td>12</td>
<td>Elemental Sulfur from Cond. No. 2</td>
<td>320</td>
<td>341</td>
<td>220</td>
</tr>
<tr>
<td>13</td>
<td>Total Elemental Sulfur</td>
<td></td>
<td></td>
<td>2,970</td>
</tr>
</tbody>
</table>

a The regenerator off-gas and coal gas slip stream are cooled in a heat recovery steam generator prior to going to the DSRP system.
Figure 6 (repeated). Simple Schematic Diagram of the Direct Sulfur Recovery Process.

Table 2. DSRP Mass Balance for a Texaco IGCC with a Fluidized Bed Zinc Titanate Desulfurization System (Robin et al., 1993)\textsuperscript{a}

<table>
<thead>
<tr>
<th>Stream-Number</th>
<th>Description</th>
<th>Temperature (°F)</th>
<th>Pressure (psia)</th>
<th>Flow Rate (lb/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Regenerator Off-Gas</td>
<td>1400</td>
<td>473</td>
<td>45,140</td>
</tr>
<tr>
<td>2</td>
<td>Coal Gas Slip Stream</td>
<td>1250</td>
<td>454</td>
<td>7,810</td>
</tr>
<tr>
<td>3</td>
<td>Reactor No. 1 Inlet</td>
<td>791</td>
<td>444</td>
<td>52,950</td>
</tr>
<tr>
<td>4</td>
<td>Reactor No. 1 Outlet</td>
<td>1292</td>
<td>419</td>
<td>50,190</td>
</tr>
<tr>
<td>5</td>
<td>Condenser No. 1 Outlet</td>
<td>350</td>
<td>409</td>
<td>50,190</td>
</tr>
<tr>
<td>6</td>
<td>Reheater Outlet</td>
<td>547</td>
<td>409</td>
<td>50,190</td>
</tr>
<tr>
<td>7</td>
<td>Reactor No. 2 Outlet</td>
<td>550</td>
<td>384</td>
<td>50,040</td>
</tr>
<tr>
<td>8</td>
<td>Condenser No. 2 Outlet</td>
<td>350</td>
<td>374</td>
<td>50,040</td>
</tr>
<tr>
<td>9</td>
<td>DSRP Off-Gas to Gas Turbine</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>DSRP Off-Gas to Other Areas</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Elemental Sulfur from Cond. No. 1</td>
<td>350</td>
<td>409</td>
<td>2,750</td>
</tr>
<tr>
<td>12</td>
<td>Elemental Sulfur from Cond. No. 2</td>
<td>350</td>
<td>374</td>
<td>150</td>
</tr>
<tr>
<td>13</td>
<td>Total Elemental Sulfur</td>
<td></td>
<td></td>
<td>2,900</td>
</tr>
</tbody>
</table>

\textsuperscript{a} The regenerator off-gas and coal gas slip stream are cooled a heat recovery steam generator prior to going to the DSRP system.
4.0 PERFORMANCE MODEL

There are several key factors which must be fully understood in order to create a model to simulate the operation of the DSRP. The most obvious of these are the specific reaction mechanisms which occur in the Stage I and Stage II reactors. Understanding the reaction mechanisms makes it possible to predict outlet compositions given a certain feed stream. Another important design consideration is the catalyst requirement of the reactors. It is necessary to understand the dependence of catalyst volume on key design and performance characteristics. Since space velocity is a key measure of catalyst size, an analysis of variables affecting space velocity is required to develop simple models for estimating catalyst requirements. This performance model will focus on these areas.

4.1 Modeling Reaction Mechanisms

One of the most important steps in modeling the performance of any chemical process is understanding reaction mechanisms and conversion rates. A typical DSRP inlet stream contains a mixture of hot gas desulfurization off-gas products and a slip stream of coal gas to supply the reducing agents required for the DSRP reactions. Thus, the components included in the mixed gas stream are SO₂, H₂, CO, CO₂, H₂O, COS, H₂S, O₂, and N₂ in varying amounts. The goal of the reaction model is to estimate the effluent composition given a certain inlet composition and reaction conditions.

The water gas shift reaction, Equation (13), is assumed to be at equilibrium at the entrance to Reactor No. 1. This condition can be modeled using standard features of the ASPEN chemical process simulator.

The reaction model described here concentrates on the other five Stage I reactions. RTI developed an equilibrium model for the DSRP reactors. This model predicted experimental reaction results extremely poorly. With this in mind, RTI also developed an equilibrium-modified kinetic reaction model. This model assumed the water gas shift reaction to be at equilibrium and the other Stage I reactions to be governed by kinetics. This model fell close to the experimental results, especially for the pressure range of interest (around 20 atm). An even more rigorous model including water gas shift kinetics would likely further improve model predictions (Gangwal, 1993). Unfortunately, only the results of the RTI model were reported and not the data acquired through kinetic testing. Due to lack of kinetic reaction data, a kinetic-based model was not a plausible approach for model development here. Therefore, a parametric stoichiometric reaction model was
created to enable the examination of the relative conversions of all relevant DSRP reactions through sensitivity analyses.

Several assumptions were made in order to create a simplified model. Key parameters of the model are the conversion efficiency of SO$_2$ to elemental sulfur in each reactor. Most of the testing done indicated a typical sulfur capture fraction of .90 to .95 for the Stage I reactor and .80 to .90 for the Stage II reactor. Research also indicates that there should be a 2 to 1 ratio of H$_2$S and COS to SO$_2$ at the entrance to Stage II, so this constraint was applied to the reaction model. Since no reactions are assumed to occur between the outlet of Reactor 1 and the inlet of Reactor 2, the Stage I effluent and Stage II inlet stream are used interchangeably. All elemental sulfur captured in Stages I and II is assumed to be completely condensed at the reactor outlets. The validity of this assumption is examined in a later section.

### 4.1.1 Reactor 1 Mass Balance

The concentration of SO$_2$ leaving Reactor 1 is estimated based on the inlet concentration and SO$_2$ removal efficiency (please see Nomenclature section):

$$[SO_2]_o = (1-\eta_{SO_2,1}) [SO_2]_i$$  \hspace{1cm} (21)

However, because of the reagent requirements of the Stage II reactor, the following constraint applies:

$$2 [SO_2]_o = [H_2S]_o + [COS]_o$$  \hspace{1cm} (22)

As a result of this constraint, the Stage I outlet H$_2$S requirement is:

$$[H_2S]_o = 2 (1-\eta_{SO_2,1}) [SO_2]_i - [COS]_o$$  \hspace{1cm} (23)

The concentration of H$_2$S leaving the Stage I reactor is given by:

$$[H_2S]_o = [H_2S]_i + [H_2S]_G$$  \hspace{1cm} (24)

where [H$_2$S]$_G$ is the concentration of H$_2$S generated by Reaction (15). It is assumed that all of the COS that enters the reactor is converted to elemental sulfur via reaction (18). Therefore, any COS leaving the reactor is produced within the reactor by Reaction (16):

$$[COS]_o = [COS]_G$$  \hspace{1cm} (25)

The molar CO$_2$/COS ratio, R, at the outlet of Reactor No. 1 is an indication of the relative importance of Reactions (16) and (17). In kinetic and thermodynamic studies of the DSRP process chemistry, RTI estimated the molar CO$_2$/COS ratio as a function of catalyst space velocity for an SO$_2$-CO reaction system (Gangwal, 1993). The relationship
of this ratio to space velocity is shown in Figure 7. For low space velocities, which are indicative of large catalyst volumes, the ratio is high. For space velocities above about 6 x 10^5 cc/hr-g, the ratio becomes nearly constant at a value near two.

By combining reactions (16) and (17), the following reaction is obtained:

\[ a \text{ SO}_2 + b \text{ CO} \rightarrow d \text{ COS} + e \text{ CO}_2 + f/x S_x \]  

(26)

where a, b, d, e, f are functions of the ratio R. The resulting stoichiometric equation, expressed as a function of R, is:

\[ \frac{R}{2} \text{ SO}_2 + (R+1) \text{ CO} \rightarrow \text{ COS} + R \text{ CO}_2 + \frac{[(R-2)/2]}{x} S_x \]  

(27)

Given a value of the CO₂/COS ratio, Reaction (27) makes it possible to determine the contributions of reactions (16) and (17).

Although the data in Figure 7 may be useful for identifying qualitative trends, it is uncertain how applicable these results are to a large scale system due to the testing conditions used. The data were obtained from kinetic testing in a quartz-lined micro reactor containing approximately .5 g of catalyst. The reaction system contained only CO and SO₂ rather than a typical DSRP feed stream. The space velocities also may differ from those used in a large scale commercial system. For comparison, the space velocities on the curve can be converted to the same units as those used in bench-scale tests. This was accomplished by converting the reported space velocity from a catalyst mass basis (e.g., cc/hr-g) to a catalyst volume basis, assuming a catalyst density of about 0.5 g/cc (estimate obtained through personal communication with RTI). Using this conversion factor and adjusting for standard temperature and pressure, the space velocities tested were considerably higher (greater than about 200,000 scc/cc-hr) than those typical for DSRP bench-scale testing (less than about 5,500 scc/cc-hr). Thus, the results of Figure 7 are not directly applicable to commercial scale designs. Therefore, the CO₂/COS ratio is treated as a performance model parameter that can be adjusted by the user.

Reaction (27) can be used to determine the amount of COS generated in Stage I. Assuming that all inlet CO reacts in this system, since it is the only reaction system which consumes CO in the Stage I reactor, the amount of COS generated is:

\[ [\text{COS}]_G = \frac{1}{R+1} [\text{CO}]_i - [\text{COS}]_0 \]  

(28)

Using the mass above, it is possible to determine the contributions of reactions (14) through (18) to the overall SO₂ conversion. The amount of SO₂ converted by reaction (15) should be equal to the amount of H₂S generated by this reaction. Since this reaction is
Figure 7. Plot of $R$ vs. SV for CO-SO2 System

![Graph showing the relationship between $R$ (CO2/COS Ratio) and Space Velocity (x 10^5 cc/hr·g).](image-url)
the only reaction generating \( H_2 S \) in the mechanism, this amount must be equal to the required \( H_2 S \) outlet concentration minus the inlet concentration. Combining equations (23), (24), and (27), the efficiency of reaction (15) in removing \( SO_2 \) can be written as:

\[
\eta_{15} = \frac{2(1-\eta_{SO_2})[SO_2]_i - [H_2 S]_i - \frac{1}{R+1}[CO]_i}{[SO_2]_i}
\] (29)

In a similar manner, the efficiency for the system of reactions (16) and (17) can be written as:

\[
\eta_{16-17} = \frac{R[CO]_i}{2(R+1)[SO_2]_i}
\] (30)

Reaction (18) converts all inlet \( COS \) to elemental sulfur. The concentration of \( SO_2 \) consumed by this reaction will be equal to half of the inlet \( COS \) concentration as dictated by stoichiometry. The contribution of reaction (18) to the overall conversion of \( SO_2 \) to elemental sulfur in Stage I is:

\[
\eta_{18} = \frac{\frac{1}{2}[COS]_i}{[SO_2]_i}
\] (31)

Thus, the contribution of reaction (14) can be determined by difference:

\[
\eta_{14} = \eta_{SO_2,I} - (\eta_{15} + \eta_{16-17} + \eta_{18})
\] (32)

### 4.1.2 Stage I Sulfur Condenser

The hot gas stream (typically 450 to 650°C) leaving the Stage I reactor enters a sulfur condenser where it is cooled in a heat exchanging coil surrounded by steam at about 120°C. There are no chemical reactions in this unit, but there is a change in the content of the stream. The elemental sulfur produced in the Stage I reactor is condensed and removed from the stream. Some of the water content is often also removed by this process. In the DSRP bench-scale tests, sulfur condensation has been less than 100 percent efficient. However, recent work at RTI has focused on developing a new technique which appears to be capable of condensing and removing all of the elemental sulfur before the stream is sent to Stage II. Information regarding this technique has not yet been disclosed. However, based on this development, it is assumed that 100 percent of the elemental sulfur exiting both the Stage I and Stage II reactors is condensed.
4.1.3 Interstage Reheater

The gas stream leaving the condenser is typically at a temperature of 150 to 200°C. It must be reheated to an appropriate temperature for the Stage II reactor, which generally operates most effectively at 250 to 300°C. This is accomplished by contacting the gas stream with superheated steam in a heat exchanger. There are no chemical or physical changes to the gas stream.

4.1.4 Reactor II Mass Balances

Modeling Stage II is considerably less complex because only two reactions are of concern. Testing has indicated that reaction (20) proceeds to completion, so all COS entering Stage II is converted to H₂S. This H₂S and entering H₂S react with entering SO₂ via the Claus reaction (19) to form elemental sulfur. In most of the bench-scale testing 80 to 90 percent of SO₂ entering Stage II was converted. As stated earlier, it is assumed that no interstage chemical reactions occur. Therefore, the SO₂ concentration at the entrance of the Stage II reactor is the same as the SO₂ concentration at the exit of the Stage I reactor:

\[ [\text{SO}_2]_{\text{II},i} = [\text{SO}_2]_{\text{I},o} \]  

Assuming a conversion efficiency \( \eta_{\text{SO}_2,\text{II}} = .8 \) to \( .9 \), the outlet SO₂ concentration from Stage II is:

\[ [\text{SO}_2]_{\text{II},o} = (1-\eta_{\text{SO}_2,\text{II}})[\text{SO}_2]_{\text{II},i} \]  

All inlet COS reacts to generate an equal concentration of H₂S:

\[ [\text{H}_2\text{S}]_{\text{II},G} = [\text{COS}]_{\text{II},i} \]  

\[ [\text{COS}]_{\text{II},o} = 0 \]  

Reaction (19) shows that H₂S reacts with SO₂ at a 2:1 mole ratio to form elemental sulfur. Enough H₂S will react to produce the required conversion efficiency. Using this knowledge, the outlet concentration of H₂S is:

\[ [\text{H}_2\text{S}]_{\text{II},o} = 2(1-\eta_{\text{SO}_2,\text{II}})\{[\text{H}_2\text{S}]_{\text{II},i} + [\text{H}_2\text{S}]_{\text{II},G}\} \]  

Using these mass balances and the mass balances for the Stage I reactor, the stoichiometric model was implemented using the Excel spreadsheet program. This model can process a given inlet stream composition and reaction specifications and predict the outlet concentrations of key reaction species for both Stages I and II. Table 3 shows an analysis of a possible sample DSRP inlet stream (after the water gas shift has reached
Table 3. Reaction Model Using Hypothetical Inlet Composition

<table>
<thead>
<tr>
<th>Performance Model Input Parameters (must be specified)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage I Inlet Concentrations (vol %)</td>
</tr>
<tr>
<td>[SO2] 1.64%</td>
</tr>
<tr>
<td>[CO] 0.50%</td>
</tr>
<tr>
<td>[H2] 2.80%</td>
</tr>
<tr>
<td>[COS] 0.10%</td>
</tr>
<tr>
<td>[H2S] 0.08%</td>
</tr>
<tr>
<td>Ratio: [CO2]/[COS]=R 2</td>
</tr>
<tr>
<td>Efficiency of SO2 Conversion (Stage I) 0.92</td>
</tr>
<tr>
<td>Efficiency of SO2 Conversion (Stage II) 0.85</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stage I Calculated Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fraction of Inlet SO2 Consumed by:</td>
</tr>
<tr>
<td>Reaction 14 0.778</td>
</tr>
<tr>
<td>Reaction 15 0.010</td>
</tr>
<tr>
<td>Reactions 16-17 0.102</td>
</tr>
<tr>
<td>Reaction 18 0.030</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stage II Inlet Variables (calculated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage I Outlet = Stage II Inlet (vol %)</td>
</tr>
<tr>
<td>[SO2] 0.1312%</td>
</tr>
<tr>
<td>[COS] 0.1667%</td>
</tr>
<tr>
<td>[H2S] 0.0957%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stage II Calculated Outlet (vol %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[SO2] 0.0197%</td>
</tr>
<tr>
<td>[H2S] 0.0787%</td>
</tr>
<tr>
<td>[COS] 0.0000%</td>
</tr>
</tbody>
</table>
equilibrium). No DSRP outlet concentrations were reported from the bench-scale testing, so it is not possible to compare these results with actual experimental data at this time.

4.1.5 Stage II Sulfur Condenser

This condenser is the same as the condenser following the Stage I reactor. As noted above, it is assumed that the condensation and removal of elemental sulfur from the gas stream is complete.

4.1.6 Gas Conditioning/Pressure Control

Very little physical information or test data are available for these final DSRP units. All bench-scale testing has concentrated on the operation of the reactors and condensers. It is even possible that these units are unique to the bench-scale DSRP unit and would not be applicable to or necessary for a commercial scale unit.

4.2 Estimating Space Velocities

In the early stages of this project, an effort was made to develop an empirical statistical model that relates catalyst space velocity to key performance variables. The results of this work are reported in Section 4.2.1. The statistical analysis provides some insight into factors that may need to be considered in choosing a space velocity as part of the design of a new system. However, due to the evolving nature of this technology, and particularly due to improvements in catalyst formulation, assumptions regarding space velocity are changing. Therefore, the performance model that is implemented in ASPEN includes space velocity as a user-specified parameter. The basis for selecting a parameter value, based on currently available information, is described in Section 4.2.2.

4.2.1 Statistical Models for Space Velocity

In order to size a catalytic reactor for the Stage I and Stage II reactors, it is necessary to know the dependence of catalyst volume on key design or performance characteristics. Space velocity is a key measure of catalyst size. To gain insight into the key factors which influence the catalyst size, space velocity data for bench-scale tests were analyzed. Using data reported by McMichael and Gangwal (1991) for bench-scale tests with both Stage I and Stage II reactors in the fixed-bed mode, a number of alternative linear regression models were evaluated using the StatWorks program with catalyst space velocity as the dependent variable. The independent variables explored for both reactors included SO2 removal efficiency (%), temperature (°C), pressure (atm), and inlet concentrations of relevant reaction species. For Stage I the species used were SO2, CO, and H2. For Stage

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II the species used were SO$_2$ and H$_2$S. Although COS plays a key role in the Stage II reactor, none of the reported data sets included COS as a component of the inlet gas stream. RTI evaluated several catalysts for use in both the Stage I and Stage II reactors. Tests showed that Catalyst A provided the best results for Stage I and Catalysts B and C were preferred for Stage II. Therefore only test runs using these catalysts were analyzed.

Regression analyses were performed for space velocity as a function of each independent variable taken individually, as well as for groups of independent variables. The scatter plots of space velocity versus each independent variable for all three catalysts are given in Appendix A. The Stage I plots seemed to show two clusters of points, one for space velocities of about 2,000 scc/cc-hr (low SV) and the other for space velocities of about 5,000 scc/cc-hr (high SV). These groups of data points were re-analyzed separately (see Table 4). The low space velocity data indicated that space velocity depends most heavily on the inlet concentrations of SO$_2$, CO, and H$_2$. The statistical results for a linear regression model of space velocity versus these three independent variables gave a coefficient of determination (R$^2$ value) of 0.47 and a standard error of about 426 scc/cc-hr. The equation for this linear regression model is:

$$SV_{IA,L} = 5270 - 2390[SO_2]_i + 1350[H_2]_i - 856[CO]_i$$ \hspace{1cm} (38)

This model is statistically significant at the .006 confidence level based on the F-test. However, the low value of R$^2$ and high standard error indicate that there is a large portion of variance in space velocity that cannot be explained by the linear model. Figure 8 contains a parity plot of results predicted by this model versus experimental values of space velocity. This plot illustrates the shortcomings of this particular model. If the model was perfect, all points would lie on the 45° line. Figure 8 shows that most of the data points are close to this line, but that there is considerable scatter.

At high space velocities, the regression analyses indicated that space velocity depends most heavily on SO$_2$ removal (%) and the inlet concentrations of SO$_2$ and CO. The statistical results for a linear regression model of space velocity versus these three independent variables gave a coefficient of determination (R$^2$ value) of 0.92 and a standard error of about 91 scc/cc-hr. The equation for this linear regression model is:

$$SV_{IA,H} = 11,000 - 10.1(\eta_{SO_2,t}) - 1490[SO_2]_i - 1100[CO]_i$$ \hspace{1cm} (39)

This model is statistically significant at the .000 confidence level based on the F-test. The higher R$^2$ value and considerably lower standard error indicate that this is a much better
Table 4. Data for Stage I Regression Analyses

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<th>[SO2] (vol. %)</th>
<th>[H2] (vol. %)</th>
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Data for Catalyst A at High Space Velocity

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Figure 8. Comparison Between Experimental Values and Values of Space Velocity Predicted by the Model for Stage I at Low Space Velocities

Figure 9. Comparison Between Experimental Values and Values of Space Velocity Predicted by the Model for Stage I at High Space Velocities
model than for the low space velocity case above. Figure 9 contains a parity plot of results predicted by this model versus experimental values of space velocity. This plot reinforces the validity of this model. All data points lie quite close to the 45° line, indicating that the model is good at predicting experimental values.

Similar to the Stage I data, the data for Stage II test runs indicated clusters for low and high space velocities. However, there were not enough high velocity data points to create a statistical model. Therefore only low space velocities (around 2000-2300 scc/cc·hr) were used in the regression models (see Table 5). For the tests using Catalysts B and C at low space velocities, it appears that space velocity is strongly correlated with the inlet concentrations of SO₂ and H₂S. Since these values are collinear ([H₂S] = 2[SO₂]), it is not meaningful to create a model in which space velocity is a function of both. Therefore only inlet SO₂ concentration was used for the model. Space velocity is plotted as a function of SO₂ concentration in Figure 10 for Catalyst B and Figure 11 for Catalyst C. Also shown in the figures are the linear regression models. In Figure 10 there are essentially only two clusters of data. Thus, it is uncertain if a linear model is appropriate in this case. In Figure 11, there are three clusters of data which fall on the line, indicating greater confidence in the use of a linear model. The model using Catalyst B gave a coefficient of determination of 0.93 and standard error of about 43 scc/cc·hr. The equation for this linear regression model is:

\[ SV_{IB} = 3950 - 30.850[SO₂]_{II,i} \] (40)

The model using Catalyst C gave a coefficient of determination of 0.997 and standard error of about 8.7 scc/cc·hr. The equation for this linear regression model is:

\[ SV_{IC} = 4090 - 32.600[SO₂]_{II,i} \] (41)

Both of these models are statistically significant to the .000 confidence level based on the t-test. The high R² values and low values for standard error indicate that these models are good representations of space velocity dependence in Stage II.

4.2.2 Recent Space Velocity Estimates

As part of on-going work, Research Triangle Institute is conducting a series of slipstream tests at METC's fluidized bed gasifier using actual coal gas. The objectives of the tests are to demonstrate the operation of fluidized bed desulfurization sorbents, the DSRP, and high-temperature catalytic ammonia decomposition. The test apparatus is a mobile laboratory which is comprised of a trailer containing a small-scale DSRP unit. The DSRP is reported to convert SO₂ in actual or synthetic tail-gas to elemental sulfur, achieving 95.1
Table 5. Data for Stage II Regression Analyses

**Data for Catalyst B at Low Space Velocity**

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**Data for Catalyst C at Low Space Velocity**

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Figure 10. Regression Plot for Stage II Using Catalyst B at Low SV

Figure 11. Regression Plot for Stage II Using Catalyst C at Low SV
to 99.5 percent conversion after the first stage of a two-stage system. As part of tests to be conducted later in 1995, a single-stage DSRP reactor system will be used in long-term testing. The purpose of the long-term testing is to assess new control logic and to evaluate the longer-term effect of trace contaminants in the coal gas. A larger pilot-scale DSRP unit is also planned. The pilot-scale unit will be six times larger than the mobile laboratory unit, and will be tested at Enviropower's 15 MW (thermal) gasifier, beginning in late 1995.

The mobile laboratory DSRP system has been operated with a Stage I space velocity of 4,560 scc/(cc-hr), in a temperature range of 550 to 610 °C, and at a pressure of 260 psi. The conversion of SO₂ to sulfur has been high, while the conversion of SO₂ to H₂S has been low (e.g., 1.2 to 4.9 percent of the inlet sulfur). In Stage II of the mobile laboratory system, it is believed that the reverse Claus reaction may be occurring, thereby reducing the overall sulfur production of the DSRP. For this reason, a one-stage design is preferred for future testing (Portzer, 1995).

4.2.3 Discussion

The regression analyses of space velocity provided insight regarding key parameters that affect space velocity. For example, the statistical analysis confirms that SO₂ removal efficiency decreases with increased space velocity. RTI tests indicated that temperature had little effect over a range of about 500 to 650°C for Stage I.

There are some questions raised by the regression analyses which cannot be answered at this time. It is unknown why the system appears to behave differently at low space velocities than it does at high space velocities. Also, space velocity is expected to be dependent on pressure. There were not enough data available to test this dependence, as almost all test runs were conducted at 20 atm of pressure.

Furthermore, space velocity also depends on catalyst formulations. The parametric test data which were used in the regression analyses represent one set of alternative catalyst formulations. The regression analysis results cannot be applied to other catalyst formulations. However, they do provide useful qualitative insights into the behavior of the DSRP system.

Because catalyst formulation is changing, and due to the limited availability of parametric data which can be used to related catalyst space velocity to other performance variables, catalyst space velocity for each stage of the DSRP is treated as a user-specified input variable.
4.3 Implementation of the Performance Model in ASPEN

The performance model of the DSRP has been implemented into ASPEN. A listing of the performance model code is given in Appendix B. ASPEN is a Fortran-based deterministic steady-state chemical process simulator developed by the Massachusetts Institute of Technology (MIT) for DOE to evaluate synthetic fuel technologies (MIT, 1987). The ASPEN framework includes a number of generalized unit operation "blocks", which are models of specific process operations or equipment (e.g., chemical reactions, pumps). By specifying configurations of unit operations and the flow of material, heat, and work streams, it is possible to represent a process plant in ASPEN. In addition to a varied set of unit operation blocks, it is possible to include Fortran programs within the simulation models as "Fortran blocks," or to call external Fortran subroutines. ASPEN contains an extensive physical property database, which allows a modeler to include a wide range of chemical species in the model. ASPEN also includes convergence algorithms for calculating results in closed loop systems, which are modeled using "design specification." A design specification causes part or all of the simulation model to be executed iteratively, varying the value of a selected flowsheet input variable to achieve a specified value of a key design variable within a given tolerance. These combinations of features make ASPEN a powerful tool for process simulation.

Many advanced coal-based power generation technologies have been modeled by DOE using ASPEN. The DSRP performance model has been implemented as part of a previously developed and modified flowsheet for an air-blown Lurgi-gasifier-based IGCC system (Frey and Rubin, 1990, 1991, 1992).

The DSRP performance model consists of 15 unit operation blocks and three FORTRAN blocks, as illustrated in Figure 12. The key features of this model are described here.

The offgas from the high temperature, high pressure gas cleanup system enters the DSRP system via stream SO2PROD. This gas may typically have a temperature of approximately 1,200 °F to 1,500 °F. A portion of the clean fuel gas from the gas cleanup system, ZF-CLFL (which stands for "Zinc Ferrite-CLean Fuel"), is split in unit operation block REDUSPLT into a slip stream DSLIP and a fuel gas stream TOGTMIXR. The fuel gas stream later joins with the tail gas from the DSRP system before being fired in the gas turbine combustor. The slip stream mass flow is determined by FORTRAN block SET-RSPLT. This FORTRAN block ensures that the molar flow rate of the sum of CO and H₂ in the slip stream will be twice the molar flow rate of SO₂ in the offgas. The slipstream
Figure 12. Schematic Diagram of the ASPEN Performance Model for the DSRP
DSLIP is mixed with SO2PROD in a mixer unit operation block DSRP-MIX. The outlet of this block is DCOOLIN.

The stream DCOOLIN enters a heater unit operation block DSRP-COL, which represents an inlet gas precooler. The heat released by cooling the gas may be used to heat high temperature streams such as in a superheater. As noted in Section 3.2, it is expected that the water-gas shift reaction will be at equilibrium as the gas stream enters the first DSRP reactor. Thus, the water-gas shift equilibrium reaction is modeled using the Gibbs free energy minimization optimization code contained in the RGIBBS unit operation block labelled DSRP-SH. The outlet stream from this block, DR1IN, enters the first reactor, which is modeled as a stoichiometric chemical reaction in block DSRP-R1. The outlet temperature of the reactor is set to a specified temperature of 1,292 °F, which matches the maximum values assumed in a design study of the DSRP as applied to Texaco gasifier-based IGCC systems with hot gas cleanup (Robin et al., 1993). The specified temperature may be changed by the user. The specified reactor outlet temperature is achieved by varying the outlet temperature from the inlet gas precooler such that the heat transferred from the first reactor is set to zero. The variation of outlet temperature for the precooler is achieved using the design-specification DS-DSRPC. The design specification allows for the temperature change of the gas stream associated with the water-gas shift reaction in DSRP-SH and with the exothermic chemical reactions in DSRP-R1 to be accounted for to ensure that sintering of the catalyst does not occur.

The FORTRAN block SET-DCNV is used to calculate the reaction conversion rates for the reactions that occur in both of the DSRP reactor vessels, which are modeled using the stoichiometric reaction blocks DSRP-R1 and DSRP-R2. The user may specify the SO2 conversion efficiency for each of the reactors. Using the relationships developed in Equations (29) through (32), the conversion rates of each of five reactions occurring in DSRP-R1 and each of two reactions occurring in DSRP-R2 are calculated.

The gas leaving Reactor No. 1, DC1IN, enters a heater unit operation block, DSRP-C1, which represents the first condenser. The outlet temperature for this condenser may be specified by the user, and typically would have a value of approximately 350 °F. The heat stream from the condenser, QDSRP-C1, is used in an economizer. The separation of elemental sulfur is represented by a separate unit operation block, DSRP-SP1, in which the solid elemental sulfur is removed in stream DES1 and the remaining gas is contained in stream DRHIN. The stream DRHIN enters reheater, which is modeled by the heater unit operation block DSRP-RHX. Design studies by Robin et al. (1993) suggest that a temperature of approximately 550 °F would be typical of the reheater outlet.
temperature. The user may set the reheater outlet temperature by changing its value in the unit operation block parameter sentence.

The reheated gas stream, DR2IN, enters the second reactor, DSRP-R2. As previously noted, the reaction conversion rates for this stoichiometric reactor model are determined by the FORTRAN block SET-DCNV. The reactions that occur in DSRP-R2 have only a minor effect on the gas temperature. As an approximation, it is assumed that the outlet gas temperature is the same as the inlet gas temperature. By comparison, studies by Robin et al. (1993) indicate a temperature change of approximately three to six degrees Fahrenheit. The gas stream that leaves the second reactor, DC2IN, enters the unit operation block DSRP-C2, which represents the second condenser. The heat released by the condenser is represented by the heat stream QDSRP-C2. The heat released by the second condenser is assumed to be available as input to the low pressure economizer.

The sulfur removed in the DSRP second condenser is modeled in unit operation block DSRP-SP2, in which the elemental sulfur stream DES2 is separated from the gas stream TAILGAS. The TAILGAS is compressed to a sufficient pressure in the compressor TAILCOMP for mixing with the clean fuel gas in stream TOGTMIXR in unit operation block GTMIXR, which produces the outlet fuel gas stream FUELIN.

The elemental sulfur streams from the two condensers are mixed together in a mixer block DSRP-SM and then cooled to an appropriate product exit temperature in the heater block DSRP-PRD.

The pressures of the gas streams are determined by the inlet pressure of the fuel gas slip stream and specified pressure drops in the gas precooler, Reactors Nos. 1 and 2, Condensers Nos. 1 and 2, and the reheater between Condenser 1 and Reactor 2. These pressure drops were estimated based upon design studies by Robin et al. (1993). They are summarized in Table 6.

The ASPEN performance model is used to estimate the energy requirements for the tailgas booster compressor. All of the work streams for the DSRP are grouped together for integration with the balance of the power systems model.

The heat streams from the DSRP performance model have been grouped into three categories, based upon the approximate temperature at which heat is transferred. There are four heat streams which are grouped as high temperature streams that are associated with an approximate outlet temperature of 1,200 °F. Three heat streams are grouped together as
Table 6. Typical Pressure Drop Assumptions for Key Components of the DSRP

<table>
<thead>
<tr>
<th>Unit Operation</th>
<th>Typical Gas Stream Pressure Drop (psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Gas Precooler</td>
<td>2</td>
</tr>
<tr>
<td>Reactor No. 1</td>
<td>25</td>
</tr>
<tr>
<td>Condenser No. 1</td>
<td>10</td>
</tr>
<tr>
<td>Reheater</td>
<td>1</td>
</tr>
<tr>
<td>Reactor No. 2</td>
<td>25</td>
</tr>
<tr>
<td>Condenser No. 2</td>
<td>10</td>
</tr>
</tbody>
</table>

medium temperature streams (approximately 500 °F). One stream is included in the category of low temperature streams (approximately 300 °F).
5.0 DSRP COST MODEL

In this section, analytical models of direct, indirect, and total capital costs are developed for DSRP systems applied to IGCC systems.

5.1 Direct Capital Costs

Direct capital cost models for key components of the DSRP were developed based upon data presented by Robin et al. (1993). Total installed capital costs were reported for components that include Reactors No. 1 and 2, Condensers No. 1 and 2, gas precooling, gas reheat, and sulfur handling. These components can be categorized into two major groups: (1) gas handling; and (2) sulfur handling. Most of the components fall into the gas handling group. For the Case 11F cost estimate as described in Robin et al. (1993), the direct cost for the gas handling components is $13.1 million, while the direct cost for the sulfur handling components is $0.4 million. To a first order, the costs of the gas handling components are proportional to the volume flow rate of the gas streams, which in turn depend on pressure and temperature. In addition, the costs of the pressure vessels depend upon the thickness of the pressure vessel walls, which in turn are proportional to pressure. For the sulfur handling systems, the costs are proportional to the mass flow rate of molten sulfur.

A capacity-exponent cost model formulation is employed. Because few cost data are available, it was necessary to make a reasonable assumption regarding the appropriate functional form of the cost model. The capacity-exponent model is widely used for the purposes of developing preliminary, budgetary cost estimates of chemical processes. An exponential scaling factor of two-thirds is typically employed.

To enable evaluation of the costs of both one-stage and two-stage DSRP systems, the costs of the DSRP are broken into separate stages.

A listing of the DSRP cost model code is given in Appendix C.

5.1.1 Adjusting for Pressure

To adjust for differences in cost due to the thickness of pressure vessel walls, a correction factor developed by Frey and Rubin (1990) based upon data presented in Ulrich (1984) is employed:

\[
f_p = 2.5 + 0.093 P^{0.54}
\]

(42)
In the direct cost model for the gas handling section of the DSRP, the correction factor is normalized with respect to the value for the Reactor No. 1 pressure in the base case cost estimate obtained from Robin et al (1993), which is 444 psi. At this pressure, the correction factor has a value of 7.1.

5.1.2 Direct Costs for the First Stage of the DSRP

For each of the two DSRP reactor stages, the costs are divided into gas handling and sulfur handling. For the first stage, gas handling equipment costs include the gas cooler, reactor vessel, and sulfur condenser. The sulfur handling section includes equipment required to handle the sulfur once it has been condensed.

For the gas cooler and sulfur condenser, the costs are assumed to be proportional to the gas volumetric flow rate. The reported costs are $3.38 million per train of equipment to handle a volume flow rate of 77,000 ft³/hr at 444 psi (Robin et al., 1993). Of this amount, $1.75 million is attributable to gas cooling upstream of Reactor No. 1, and the balance is due to the sulfur condenser. To adjust for differences in pressure, the pressure correction factor is employed. Because costs are reported in 1993 dollars, the costs are normalized using the Chemical Engineering magazine 1993 plant cost index of 361.2.

\[
DC_{GH,1} = N_{T,DSRP} \left( \frac{2.5 + 0.093 P_{g,R1,1}^{0.64}}{7.1} \right) \left( 3.380 \left( \frac{V_{g,R1,1}}{77,000 N_{O,DSRP}} \right)^{0.67} \right) (PCI)_{361.2}
\] (43)

For the Stage I reactor vessel, the cost per vessel is reported to be $1.02 million in 1993 dollars based upon a gas flow rate of 77,000 ft³/hr and a space velocity of approximately 2,000 scc/cc-hr. Unlike the gas cooler and sulfur condenser costs, the cost of the reactor vessel is proportional not only to the volumetric flow rate of the gas, but also to the volume required for the catalysts. Thus, all other things being equal, a pressure vessel which must hold a larger quantity of catalyst is presumed to cost more than one that must handle the same gas flow rate but with a smaller catalyst volume. Since catalyst volumes are typically expressed using "space velocity", the catalyst volume is typically normalized to the gas flow rate. Therefore, as a measure of reactor vessel size, both the gas volumetric flow rate and the catalyst space velocity are used. The purpose here is to develop a ratio of catalyst volumes, rather than gas flow rate, as the sizing variable for the reactor vessel. The resulting equation is:
The sulfur handling system includes heaters to maintain the sulfur in a molten state. The costs for these are reported to be $80,000 per unit for a unit capable of handling 2,900 lb/hr of sulfur. Thus, the cost of the solids handling system for the first stage of the DSRP are:

$$DC_{S,1} = N_{T,DSRP} \left[ \frac{m_{s,R1,o}}{2,900 N_{O,DSRP}} \right]^{0.67} \left( \frac{PCI}{361.2} \right)$$

(45)

5.1.3 Direct Costs for the Second Stage of the DSRP

For a two-stage system, there are additional direct costs for a reheater, reactor vessel, sulfur condenser, and sulfur handling systems. The reheater is reported to have a 1993 cost of $480,000 based on a gas volumetric flow rate of 69,000 ft³/hr. The sulfur condenser, which costs $726,000 per unit, is also sized for the same gas volumetric flow rate. Thus, the total cost for the reheater and sulfur condenser is:

$$DC_{GH,2} = N_{T,DSRP} \left( \frac{2.5 + 0.093 P_{g,R2,1}^{0.64}}{7.1} \right) \left[ \frac{V_{g,R2,i}}{69,000 N_{O,DSRP}} \right]^{0.67} \left( \frac{PCI}{361.2} \right)$$

(46)

For the Stage II reactor vessel, the 1993 cost is $960,000, based upon a gas flow rate of 69,000 ft³/hr and a space velocity of 2,000 scc/cc-hr. The direct cost, adjusted for other gas flow rates and space velocities, is:

$$DC_{R,2} = N_{T,DSRP} \left( \frac{2.5 + 0.093 P_{g,R2,1}^{0.64}}{7.1} \right) \left[ \frac{V_{g,R2,i}}{77,000 N_{O,DSRP}} \right]^{0.67} \left( \frac{SV_{R2,ref}}{SV_{R2,actual}} \right)^{0.67} \left( \frac{PCI}{361.2} \right)$$

(47)

The sulfur handling system has approximately the same costs as for Stage II. Thus, the direct cost equation is:

$$DC_{S,2} = N_{T,DSRP} \left[ \frac{m_{s,R2,o}}{2,900 N_{O,DSRP}} \right]^{0.67} \left( \frac{PCI}{361.2} \right)$$

(48)
5.1.4 Total Direct Costs for the DSRP

The total direct cost of the DSRP is given by the sum of all of the direct cost equations for the gas handling, reactors, and solids handling components:

\[ DC_{DSRP} = DC_{GH,1} + DC_{R,1} + DC_{S,1} + DC_{GH,2} + DC_{R,2} + DC_{S,2} \]  \hspace{1cm} (49)

For a one-stage DSRP system, the direct costs for all second stage components are modeled as being zero.

5.2 Other Capital Costs for the DSRP

Other capital costs include general facilities, engineering and home office fees, contingencies, various indirect capital costs, preproduction costs associated with startup, and inventory costs associated with providing initial stocks of chemicals and fuels. For more details on other capital cost models, please see Frey and Rubin (1990).

General facilities include roads, office buildings, shops, laboratories, and other equipment or facilities that are not part of other process areas but that are associated with the process technology. General facilities costs are typically estimated as a percentage of the direct capital cost of all other process areas. These costs are handled by the power systems cost model. Like general facilities costs, engineering and home office fees are typically estimated as a percentage of the total direct cost. A typical value of 10 percent of the total direct cost is often assumed for engineering and home office fees.

Project contingency cost is estimated for the entire power plant as a multiplier of total direct cost (e.g., EPRI, 1986). Process contingency costs are typically evaluated separately for each process area. The total process contingency is given by:

\[ C_{Proc} = \sum f_{Proj} DC_i \]  \hspace{1cm} (50)

For the DSRP, a typical value for process contingency would be 25 percent, based upon the state of development of the technology. As shown in Table 7, contingency factors of 20 to 35 percent are often employed for technologies for which small pilot plant data are available.

The total plant cost, or overnight construction cost, is given by:

\[ TPC = TDC + C_{GF} + C_{EHO} + C_{Proj} + C_{Proc} \]  \hspace{1cm} (51)

An allowance for funds during construction (AFDC) is calculated based on the TPC as a function of the amount of time it would take to construct a power plant system. A
Table 7. Process Contingency Factors Recommended by EPRI\(^a\)

<table>
<thead>
<tr>
<th>State of Technology Development</th>
<th>Percentage of Process Area Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>New concept with limited data</td>
<td>≥ 40</td>
</tr>
<tr>
<td>Concept with bench scale data available</td>
<td>30 to 70</td>
</tr>
<tr>
<td>Small pilot plant data (e.g., 1 MW) available</td>
<td>20 to 35</td>
</tr>
<tr>
<td>A full-size module has been operated (e.g., 20-100 MW)</td>
<td>5 to 20</td>
</tr>
<tr>
<td>The process is used commercially</td>
<td>0 to 10</td>
</tr>
</tbody>
</table>

\(^a\) Cost estimates using these contingency factors are intended to represent the cost of commercialized (e.g., fifth of a kind) process plants. Source: EPRI (1986)

three-to-five year construction period for a new plant is often assumed. Methods for computing the AFDC are documented elsewhere (e.g., EPRI, 1986; Frey and Rubin, 1990) and are not repeated here. The total plant investment (TPI) represents the sum of the total plant cost and the AFDC.

\[
TPI = TPC + AFDC
\] (52)

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.

The royalty cost is typically estimated as a multiplier of total direct cost:

\[
C_{Roy} = f_{Roy} \times TDC
\] (53)

However, in this case, no costs are assumed for royalties ($f_{Roy} = 0$).

Preproduction costs are intended to cover operating, training, equipment checkout, changes in plant equipment, extra maintenance, and inefficient use of fuel, chemicals, catalysts, and other materials during plant startup. Pre-production costs typically include one month of both fixed and variable operating costs and two percent of total plant investment.

\[
C_{PP} = \frac{N_{m,FOC} \times FOC + N_{m,VOC} \times VOC}{12} + f_{pp} \times TPI
\] (54)

where $N_{m,FOC}$ is the number of months of fixed operating cost to be included in the pre-production cost estimate, $N_{m,VOC}$ is the number of months of variable operating cost to be included, and $f_{pp}$ is the pre-production cost factor, typically assigned a value of 0.02.
The inventory capital cost accounts for inventories of consumables required to be on-site and is typically estimated as 0.5 percent of total process capital excluding catalyst.

\[ C_{\text{InvC}} = f_{\text{InvC}} \cdot \text{TDC} \]  

(55)

For the DSRP, the costs for initial catalysts and chemicals is based upon the initial catalyst requirements for each reactor vessel. The initial catalyst requirement is calculated based upon the molar flow rate of the gas in each reactor stage and the user-specified space velocity for each reactor stage. Because space velocity is expressed on a standard cubic centimeter (scc) basis, the molar flow rate of the gas in each reactor can be converted to a volumetric flow rate. The conversion factor is 10.762 million scc/lbmole. Because available cost data for the DSRP catalyst are on a $/lb basis, it is necessary to convert from catalyst volume to catalyst weight. This is done by assuming a typical catalyst density of 0.72 g/cc, or 0.00159 lb/cc, based upon data reported by McMichael et al. (1991). Thus, the expression for the total weight of initial catalysts is:

\[ m_{\text{cat}} = \left( \frac{M_{g,R1,\text{in}}}{SV_{R1,\text{act}}} \right) + \left( \frac{M_{g,R2,\text{in}}}{SV_{R2,\text{act}}} \right) \times 10.762 \times 10^6 \times 0.00159 \]  

(56)

The cost for the initial catalyst is:

\[ C_{\text{IC}} = \frac{m_{\text{cat}} \cdot UC_{\text{cat}}}{1000} \]  

(57)

The total capital requirement for a system that includes the DSRP is therefore:

\[ \text{TCR} = \text{TPI} + C_{\text{PP}} + C_{\text{InvC}} + C_{\text{IC}} + C_{\text{Roy}} \]  

(58)

5.3 Annual Costs

Fixed operating costs include operating labor, maintenance labor and materials, and overhead costs associated with administrative and support labor. Cost models for these items have previously been developed by Frey and Rubin (1990). The fixed operating costs are developed based upon the direct costs for each process area. A maintenance cost factor is used to estimate the annual maintenance costs as a fraction of direct capital costs for each process area. For the DSRP, a maintenance cost factor of 0.02 is assumed. The annual maintenance cost is divided into materials and labor components. It is assumed that the DSRP does not require any operators in addition to those already present at the power plant site or that would otherwise be needed to operate a conventional sulfuric acid byproduct recovery plant.
The major component of the variable operating cost is for catalyst replacement. Based upon data in Robie et al (1993), it is assumed that the DSRP catalyst is replaced every three years. Therefore, the annual cost for the DSRP catalyst replacement is:

\[
OC_{\text{cat}} = \left( \frac{m_{\text{cat}}}{L_{\text{cat}}} \right) UC_{\text{cat}}
\]

(59)

where \( L_{\text{cat}} = 3 \) years.

The performance model of the DSRP is fully integrated with the power plant model with respect to internal auxiliary loads, including electricity and steam. Any incremental water or fuel consumption due to the DSRP is modeled as part of the integrated power plant model simulation.
6.0 MODEL APPLICATIONS

The new performance and cost models of the DSRP have been implemented as part of previously developed performance and cost models of the air-blown Lurgi-gasifier-based IGCC system with hot gas cleanup. This system features a fixed bed zinc ferrite process operating at a pressure of approximately 300 psia.

6.1 Modeling IGCC Systems

The performance, emissions, and cost of the IGCC system are modeled using detailed engineering models. Performance models of a Lurgi-based system were developed by DOE/METC using the ASPEN chemical process simulator. These performance models have been significantly modified to more completely and accurately represent process performance and emissions (Frey, 1991; Frey and Rubin 1991). For example, gas cleanup and gas turbine performance and emissions are more completely characterized in the modified models. A new performance and cost model of selective catalytic reduction (SCR) NOx control has been added to these IGCC models (Frey, 1994).

The cost models for the IGCC system are based on approximately 30 design studies of IGCC systems (Frey and Rubin, 1990). Direct capital costs are estimated for approximately one dozen major process areas. Typically, several performance and design variables are included in the direct cost models. Indirect and other capital costs are estimated based on approximately 60 cost model parameters. These include process area contingencies, project contingency, indirect construction costs, sales tax, allowance for funds used during construction, environmental permitting costs, spare parts inventory costs, costs for initial inventories of fuels and chemicals, land cost, and startup costs. Fixed and variable operating costs are estimated based on 40 to 50 parameters. Fixed operating costs include maintenance material and labor for each process area, plant operating labor, and administrative and support labor. Variable operating costs include consumables (e.g., water treatment chemicals, zinc ferrite sorbent), ash disposal, fuel, and byproduct credit. Total levelized costs are calculated using the methodology of EPRI (1986).

6.2 Modeling Assumptions

The case studies developed here are based on system performance and cost assumptions which have been documented elsewhere (Frey and Rubin, 1991; 1992; Frey, 1994). Here, we focus on assumptions that are unique to the DSRP process area. These assumptions are given in Table 8. These assumptions include performance and cost inputs
Table 8. Modeling Assumptions for DSRP Systems

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DSRP Performance Assumptions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stage I SO₂ Removal Efficiency</td>
<td>%</td>
<td>95</td>
</tr>
<tr>
<td>Stage I SO₂ Removal Efficiency</td>
<td>%</td>
<td>90</td>
</tr>
<tr>
<td>Stage I Space Velocity</td>
<td>sc/ce-hr</td>
<td>5,000</td>
</tr>
<tr>
<td>Stage II Space Velocity</td>
<td>sc/ce-hr</td>
<td>5,000</td>
</tr>
<tr>
<td>Stage I Reference Space Velocity</td>
<td>sc/ce-hr</td>
<td>2,000</td>
</tr>
<tr>
<td>Stage II Reference Space Velocity</td>
<td>sc/ce-hr</td>
<td>2,000</td>
</tr>
<tr>
<td><strong>DSRP Cost Assumptions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of Units</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Process Contingency</td>
<td>% of direct cost</td>
<td>25</td>
</tr>
<tr>
<td>Maintenance Cost</td>
<td>% of direct cost</td>
<td>2</td>
</tr>
<tr>
<td>DSRP Catalyst Cost</td>
<td>$/lb</td>
<td>12.28</td>
</tr>
<tr>
<td>Catalyst Layer Replacement Interval</td>
<td>Years</td>
<td>3</td>
</tr>
<tr>
<td>Sulfuric Acid Sale Price</td>
<td>$/ton</td>
<td>40</td>
</tr>
<tr>
<td>Sulfur Sale Price</td>
<td>$/ton</td>
<td>125</td>
</tr>
</tbody>
</table>

to the DSRP models. The sulfur removal efficiency assumptions are based upon typical values obtained in small scale testing of the DSRP. The space velocity assumptions are based in part on recently presented results for the DSRP (Portzer, 1995). The reference space velocity numbers are based upon data used in previous design studies (Robin et al., 1993). It is assumed that there are two parallel trains of equipment with no spares. The process contingency and maintenance cost factors have been previously presented. The DSRP catalyst cost is based upon data from Robin et al. (1993), as is the assumption regarding the catalyst life. The sulfuric acid and sulfur price assumptions are from Frey and Rubin (1990).

*For pressure drop assumptions, please see Table 6.*

### 6.3 Running the Model

The engineering models were exercised to characterize key measures of plant performance, emissions, and cost. The IGCC model was run on a DEC VAXStation 3200 mini-computer using the public version of ASPEN. Model results are reported in Tables 9, 10, and 11. The model assumptions include a current heavy duty gas turbine with a pressure ratio of 15 and a firing temperature of 2,350 °F.

### 6.4 Modeling Results

Results from application of the new performance and cost model of the DSRP are presented in this section. A total of three cases are considered. One is a base case in which a Lurgi-gasifier-based IGCC system is configured with a conventional sulfuric acid byproduct recovery plant. The second case features a one-stage DSRP system for sulfur
recovery, in place of the sulfuric acid plant. The third case features a two-stage DSRP. A complete listing of the model results for all three cases is given in Appendix D.

The performance model results for the one and two stage DSRP systems are presented in Tables 9 and 10, respectively. These tables identify the major gas streams in the DSRP, and include data on the calculated mass flows, temperatures, and pressure drops for each stream.

For both systems, a slip stream of coal gas is calculated based upon the requirements for the sum of the molar flow of carbon monoxide and hydrogen to be twice that of the sulfur dioxide in the off-gas from the hot gas desulfurization (HGD) system. The off-gas from the HGD system undergoes a pressure drop from 305.5 to 286.72 psia, which is the pressure level of the coal gas. The mixture of HGD off-gas and the coal gas slip steam enters the DSRP gas cooler at a temperature of approximately 1,228 °F. The gas is cooled to reactor inlet temperature of 1,160 °F, and the maximum gas temperature in the reactor is limited to 1,292 °F. During gas cooling, the water-gas shift reaction is modeled as going to equilibrium. The gas cooler has a pressure drop of approximately 2 psi, while Reactor No. 1 has a pressure drop of approximately 25 psi. For both the one and two stage systems, the gas exiting Reactor No. 1 is cooled to 350 °F, resulting in the condensation of elemental sulfur. In the one-stage system, the outlet gas from the first condenser is also the DSRP tailgas. This gas is recompressed to the pressure of the gas turbine fuel gas, and it is mixed with the fuel gas prior to combustion in the gas turbine.

For the two-stage system, the outlet gas from Condenser No. 1 enters a re heater, where it is increased in temperature to 550 °F. The gas then passes through Reactor No. 2

---

### Table 9. Modeling Results for a One-Stage DSRP System: Mass Flow Rates, Temperatures, and Pressures of Key Gas Streams

<table>
<thead>
<tr>
<th>Description</th>
<th>Mass Flow (lb/hr)</th>
<th>Temp. (deg F)</th>
<th>Pres. (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HGD OFF-GAS</td>
<td>647,878</td>
<td>1234</td>
<td>305.50</td>
</tr>
<tr>
<td>COAL GAS</td>
<td>3,091,798</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>SLIP STREAM</td>
<td>156,108</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>COOLER INLET</td>
<td>783,786</td>
<td>1228</td>
<td>286.72</td>
</tr>
<tr>
<td>SHIFT INLET</td>
<td>783,786</td>
<td>1147</td>
<td>285.72</td>
</tr>
<tr>
<td>REACTOR 1 INLET</td>
<td>783,786</td>
<td>1160</td>
<td>284.72</td>
</tr>
<tr>
<td>CONDENSER 1 INLET</td>
<td>763,901</td>
<td>1292</td>
<td>259.72</td>
</tr>
<tr>
<td>CONDENSER 1 OUTLET</td>
<td>763,901</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>DSRP TAILGAS</td>
<td>763,901</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>COMPRESSED TAILGAS</td>
<td>763,901</td>
<td>360</td>
<td>286.72</td>
</tr>
<tr>
<td>FUEL TO GAS TURB.</td>
<td>3,662,061</td>
<td>801</td>
<td>286.72</td>
</tr>
</tbody>
</table>
Table 10. Modeling Results for a Two-Stage DSRP System: Mass Flow Rates, Temperatures, and Pressures of Key Gas Streams

<table>
<thead>
<tr>
<th>Description</th>
<th>Mass Flow (lb/hr)</th>
<th>Temp. (deg F)</th>
<th>Pres. (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HGD OFF-GAS</td>
<td>637,315</td>
<td>1233</td>
<td>305.50</td>
</tr>
<tr>
<td>COAL GAS</td>
<td>2,982,200</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>SLIP STREAM</td>
<td>133,882</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>COOLER INLET</td>
<td>771,198</td>
<td>1228</td>
<td>286.72</td>
</tr>
<tr>
<td>SHIFT INLET</td>
<td>771,198</td>
<td>1148</td>
<td>285.72</td>
</tr>
<tr>
<td>REACTOR 1 INLET</td>
<td>771,198</td>
<td>1161</td>
<td>284.72</td>
</tr>
<tr>
<td>CONDENSER 1 INLET</td>
<td>752,777</td>
<td>1292</td>
<td>259.72</td>
</tr>
<tr>
<td>CONDENSER 1 OUTLET</td>
<td>752,777</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>REHEATER INLET</td>
<td>752,777</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>REACTOR 2 INLET</td>
<td>752,777</td>
<td>550</td>
<td>248.72</td>
</tr>
<tr>
<td>CONDENSER 2 INLET</td>
<td>749,874</td>
<td>550</td>
<td>223.72</td>
</tr>
<tr>
<td>CONDENSER 2 OUTLET</td>
<td>749,874</td>
<td>350</td>
<td>213.72</td>
</tr>
<tr>
<td>DSRP TAILGAS</td>
<td>749,874</td>
<td>350</td>
<td>213.72</td>
</tr>
<tr>
<td>COMPRESSED TAILGAS</td>
<td>749,874</td>
<td>372</td>
<td>286.72</td>
</tr>
<tr>
<td>FUEL TO GAS TURB.</td>
<td>3,601,418</td>
<td>852</td>
<td>286.72</td>
</tr>
</tbody>
</table>

and Condenser No. 2. The tailgas is recompressed to the pressure of the gas turbine fuel gas.

The one-stage DSRP is assumed to have a Reactor No. 1 sulfur capture efficiency of 95 percent. The two-stage system is assumed to have an overall sulfur capture efficiency of approximately 99 percent. As noted earlier, there is uncertainty as to the effectiveness of a second stage. In particular, the reverse Claus reaction may occur in the second stage, which would substantially penalize, rather than enhance, the overall sulfur capture efficiency.

A comparison of results for the base case, one stage DSRP, and two stage DSRP is given in Table 11. The results include power plant performance, cost, byproduct, and emissions.

The DSRP appears to offer significant advantages over a conventional sulfuric acid plant with respect to plant performance. The plant thermal efficiency is approximately six-tenths of a percentage point higher for the two DSRP cases than for the base case system with sulfuric acid recovery. The DSRP system is highly integrated with the IGCC plant, particularly with respect to heat streams and the DSRP tailgas. The DSRP returns a pressurized gas to the gas turbine, enabling recovery of energy through the hot gas path of the gas turbine. The mass flow of fuel to the gas turbine is increased by approximately 20 percent for this reason. In contrast, the tail gas from the sulfuric acid plant is assumed to be vented to the atmosphere. Thus, for the DSRP cases, the ratio of fuel gas to inlet air is slightly greater than 0.4 lb/lb, compared to only 0.26 lb fuel gas per lb of inlet air for the
The higher mass flow for the high pressure fuel stream enables greater energy recovery from the gas turbine.

The steam turbine energy recovery is higher for the DSRP cases due to a combination of factors. The gas turbine exhaust temperature is slightly higher for the DSRP cases, thereby enabling more energy recovery through the heat recovery steam generator. In addition, the integration of the DSRP with the steam cycle enables efficient use of steam, especially the steam generated due to gas cooling and condensation in the DSRP.

Thus, the net power produced by the IGCC systems with the DSRP is substantially higher than for the base case with sulfuric acid recovery.

The capital cost of the IGCC systems with the DSRP is lower than for the base case. The capital cost of the two-stage DSRP is comparable to that for the sulfuric acid plant (approximately $25 million). However, the increased power available from the gas turbines, due to an increase in the flow of pressurized fuel gas, leads to a reduced cost on a per kilowatt basis. This is even though the IGCC system with the two-stage DSRP has a larger coal throughput and, hence, higher absolute costs for coal handling, oxidant feed, gasification and associated subsystems, hot gas desulfurization, heat recovery steam generator, and steam turbine.

The comparison of the capital costs of the one-stage DSRP to the base case is similar to the comparison of the two-stage DSRP to the base case, except that the direct

| Table 11. Comparison of Modeling Results for One-Stage and Two-Stage DSRP Systems |
|---------------------------------|-----------------|-----------------|-----------------|
| **Description**                 | **Base Case**   | **1-Stage DSRP**| **2-Stage DSRP**|
| Thermal Efficiency, % HHV basis| 38.31           | 38.93           | 38.96           |
| Net Plant Output, MW            | 709             | 851             | 838             |
| **Cost (January 1989 dollars)**|                 |                 |                 |
| Capital Cost, $/kW              | 1,357           | 1,235           | 1,277           |
| Fixed Operating Cost, $/kW-yr   | 41.41           | 36.69           | 37.22           |
| Variable Operating Cost, mills/kWh| 19.23           | 19.15           | 19.18           |
| Cost of Electricity, mills/kWh  | 51.14           | 48.01           | 48.91           |
| **Byproduct**                   |                 |                 |                 |
| Sulfuric Acid, tons/yr          | 173,230         | 58,918          | 60,710          |
| Sulfur, tons/yr                 |                 |                 |                 |
| **Emissions**                   |                 |                 |                 |
| SO₂, lb/10⁶ BTU                 | 0.041           | 0.350           | 0.090           |
capital cost for the one-stage DSRP is approximately 35 percent less than for the two-stage design. Therefore, there is an additional cost savings for the one-stage design when compared to the two-stage design.

The cost comparisons are similar for fixed operating, variable operating, and levelized costs. The one-stage design offers the lowest costs for all of these categories.

The byproduct mass flow rates are significantly different for the base case versus the DSRP cases. The key shortcomings of sulfuric acid production are the large mass of acid that is produced, and the difficulty in storing and handling the acid. In contrast, elemental sulfur is easier to handle, store, and ship, and is produced in smaller mass quantities for the same amount of recovered sulfur.

A potential advantage of the sulfuric acid recovery option is the high sulfur capture efficiency and correspondingly low plant sulfur dioxide emission rate. The two-stage DSRP design has an estimated sulfur dioxide emission rate twice that of the sulfuric acid recovery option. This presumes that the second stage of the DSRP would be effective in removing sulfur, rather than in producing sulfur gases through the reverse Claus reaction. The one-stage DSRP is shown to have the highest SO₂ emission rate of the three options.
7.0 SUMMARY

Detailed performance and cost models of DSRP systems have been developed. These models have been implemented as computer code to augment previously developed performance, emissions, and cost models of selected IGCC systems.

The DSRP models allow the implications of alternative sulfur control strategies to be explored, and also permit sensitivity and optimization case studies to minimize the total cost of environmental control for advanced power generation systems. The illustrative case studies presented here indicate that there may be substantial performance and cost benefits to the use of the DSRP in lieu of more conventional approaches for sulfur byproduct recovery.

Because DSRP systems have not yet been applied to many of the advanced power generation systems, it is critically important to consider the role of uncertainties in making predictions of DSRP performance and cost. Because many of these technologies are of interest to research and development (R&D) planners and to electric utilities, it is necessary to fully understand their environmental characteristics and the costs of complying with current and future regulations. Thus, the use of probabilistic modeling techniques, as described by Frey and Rubin (1991), to evaluate the DSRP will be a key area for future work.

The DSRP performance and cost models developed here will need to be revised as new data and technologies become available. As experience is gained regarding long-term catalyst durability, model input assumptions may be revised. As better understanding is gained regarding the factors that affect catalyst sizing, perhaps more detailed mechanistic models can be developed to characterize catalyst requirements. Therefore, the models developed here should be viewed as a first step in an iterative model development and adaptation process, as new data become available and as the need emerges to adapt these models for applications to new types of systems not currently envisioned.
8.0 REFERENCES


Appendix A
Regression Plots for Stage I Using Catalyst A for Low Space Velocities

SO2 Removal (%)

Experimental Data
Regression Model

SO2 Removal (Vi)

Experimental Data
Regression Model

Temp. (°C)

Experimental Data
Regression Model

Pressure (atm)

Experimental Data
Regression Model
Regression Plots for Stage I Using Catalyst A for Low Space Velocities

- Experimental Data
- Regression Model

Space Velocity (sec/°C/hr)

[SO2] (vol. %)

Space Velocity (sec/°C/hr)

[H2] (vol. %)

Space Velocity (sec/°C/hr)

[CO] (vol. %)
Regression Plots for Stage I Using Catalyst A for High Space Velocities

1. SO2 Removal (%) vs. Temperature (°C)
   - Experimental Data
   - Regression Model

2. Pressure (atm) vs. Space Velocity (sec/cc/hr)
   - Experimental Data

3. SO2 Removal (%) vs. Pressure (atm)
   - Experimental Data
   - Regression Model
Regression Plots for Stage I Using Catalyst A for High Space Velocities

- [SO2] (vol. %) vs. Space Velocity (scf/cc-hr)
- [H2] (vol. %) vs. Space Velocity (scf/cc-hr)
- [CO] (vol. %) vs. Space Velocity (scf/cc-hr)

Data

- Experimental Data
- Regression Model
Regression Plots for Stage II Using Catalyst B for Low Space Velocities

![Graph 1: SO2 Removal (%) vs. Space Velocity (sec/cc-hr)]

- Experimental Data
- Regression Model

![Graph 2: Temp. (°C) vs. Space Velocity (sec/cc-hr)]

![Graph 3: Pressure (atm) vs. Space Velocity (sec/cc-hr)]
Regression Plots for Stage II Using Catalyst B for Low Space Velocities

- Experimental Data
- Regression Model

Space Velocity (sec/ce-hr)

[S02] (vol. %)

[H2S] (vol. %)
Regression Plots for Stage II Using Catalyst C for Low Space Velocities

- Experimental Data
- Regression Model

Space Velocity (sec/cc-hr)

SO2 Removal (%)

Temp. (°C)

Pressure (atm)
Regression Plots for Stage II Using Catalyst C for Low Space Velocities

- Experimental Data
- Regression Model

[SO₂] (vol. %)

[H₂S] (vol. %)
Appendix B

DSRP PERFORMANCE MODEL CODE
This appendix contains a listing of the ASPEN input file code for the DSRP flowsheet section. This code can be included with a model of an Integrated Gasification Combined Cycle (IGCC) system. The key input and output variables are identified in the comments at the beginning of the code.

```plaintext
;* IN-UNITS are assumed to be ENG
;*
;///////////////////////////////////////////////////////////////
;///////////////////////////////////////////////////////////////
;///////////////////////////////////////////////////////////////
; /// DIRECT SULFUR RECOVERY PROCESS ///
;///////////////////////////////////////////////////////////////
;///////////////////////////////////////////////////////////////
;
; Date: June 15, 1995
; Author: H.C. Frey, NC State Univ.
; Developed originally for air-blown Lurgi flowsheet.
; Key Input Variables:
; FUELGAZ is the clean fuel gas exiting the high temperature
desulfurization system.
; SO2GAS is the regenerator off-gas. If the inlet gas variable is
different, be sure to search for it and change it
(e.g., in SET-RSPLT)
; Key Output Variables
; FUELGAZ2 is what goes to the gas turbine

Integration of heat streams:
High temperature streams (approx 1200 deg F outlet temps)
  QDSRP-CL QDSRP-SF QDSRP-R1 QDSRP-C1
  These can be integrated with the superheater (SUPERHTR)
  These are combined into one stream: QDSRP-H
Medium temperature streams (approx 500 deg outlet temps)
  QDSRP-RH QDSRP-R2 QDSRP-C2
  These can be integrated with the low pressure boiler (LPBOILER)
  These are combined into one stream: QDSRP-M
Low temperature streams (approx 300 deg outlet temps)
  QDSRP-SL
  This can be integrated with LPBCON (note, while the inlet
temp of LPBCON is less than 300 deg, the outlet is not.
  Therefore, this is an approximation.
  These are combined into one stream: QDSRP-L

Integration of work streams
All work streams are mixed to form WDSRP. The work from WDSRP
should be included in the cost model subroutine in determining
the plant efficiency.

Integration of pressure specifications
Pressure drops are specified throughout the DSRP model.
The tail gas which returns to the fuel gas stream must be
compressed back up to the fuel gas pressure. This is done
in TAILCOMP

******************************************************************************
;* DSRP STREAM DATA
******************************************************************************
```

70
DEF-STREAMS &
MIXCISLD DSRP / CONVEN FUELGAZ2 TAILCNV HPTCNV /
HEAT QDSRP-CL QDSRP-SF QDSRP-R1 QDRSP-C1 QDSRP-RH &
QDSRP-R2 QDRSP-C2 QDSRP-SL &
QDSRP-H QDSRP-M QDSRP-L /
WORK TAILWK WDSRP

;******************************************************************************
;* DSRP FLOWSHEET
******************************************************************************
;
FLOWSHEET DSRP
DSRP-CLC IN = FUELGAZ OUT = TODSRP
DSRP-CL2 IN = SO2GAS OUT = SO2PROD
REDUSPLT IN = TODSRP OUT = DSLIP TOGMIXR
DSRP-MIX IN = DSLIP SO2PROD OUT = DCOLIN
DSRP-COL IN = DCOLIN OUT = DSHFIN QDSRP-CL
DSRP-SHIF IN = DSHFIN OUT = DR1IN D-DUMMY QDSRP-SF
DSRP-R1 IN = DR1IN OUT = DC1IN QDSRP-R1
DSRP-CL IN = DC1IN OUT = DC1OUT QDRSP-C1
DSRP-SP1 IN = DC1OUT OUT = DHIN DES1
DSRP-RHIN IN = DHIN OUT = DR2IN QDSRP-RH
DSRP-R2 IN = DR2IN OUT = DC2IN QDSRP-R2
DSRP-C2 IN = DC2IN OUT = DC2OUT QDSRP-R2
DSRP-SP2 IN = DC2OUT OUT = TAILGAS DES2
DSRP-CL4 IN = TAILGAS OUT = TAILCNV
TAILCOMP IN = TAILCNV OUT = HPTCNV TAILWK
DSRP-CL5 IN = HPTCNV OUT = HPTAIL
GTMIXR IN = TOGMIXR HPTAIL OUT = FUELTEMPP
DSRP-CL3 IN = FUELTEMPP OUT = FUELGAZ2
DSRP-SM IN = DES1 DES2 OUT = DSPIN
DSRP-PRD IN = DSPIN OUT = SULPROD QDSRP-SL
DSRP-WK IN = TAILWK OUT = WDSRP
DSRP-HTM IN = QDSRP-CL QDSRP-SF &
QDSRP-R1 QDRSP-C1 OUT = QDSRP-H
DSRP-MTM IN = QDSRP-RH QDSRP-R2 QDSRP-C2 OUT = QDSRP-M
DSRP-LTM IN = QDSRP-SL OUT = QDSRP-L

;******************************************************************************
;* DSRP BLOCKS
******************************************************************************
;
BLOCK DSRP-CLC CLCHNG
; changes the class of the fuel gas from conventional to mixcisld
;
BLOCK DSRP-CL2 CLCHNG
; changes the class of the SO2GAS from conven to mixcisld
;
BLOCK REDUSPLT FSPLIT ; ACTUAL MOLE FLOW SET BY FORTRAN BLOCK SET-RSPLT
DESCRIPTION 'SPLIT SLIP STREAM OF REDUCING GAS'
MOLE-FLOW DSLIP 50.5 1
DEF-KEY ID=1 SUBS=MIXED COMP=CO H2
;
BLOCK DSRP-MIX MIXER
DESCRIPTION 'CONTACT REDUCING GAS AND REGENERATOR OFF-GAS'

71
; BLOCK DSRP-COL HEATER
DESCRIPTION ' DSRP INLET GAS PRECOOLER'
PARAM PRES=-1 TEMP=800.
; Cooler outlet temperature is set by Design Spec DS-DSRPC
;
BLOCK DSRP-SHF REQUAL
DESCRIPTION ' DSRP WATER-GAS SHIFT EQUILIBRIUM'
BLOCK-OPTIONS RESTART=0
PARAM PRES=-1 NR=1 NPK=1 MXOL=90 MXIL=90 KODE=1 TEST=800.
STOI  1  CO  -1 0 / H2O  -1 0 / H2  1 0 / CO2  1 0
;
BLOCK DSRP-R1 RSTOIC
DESCRIPTION ' DSRP REACTOR NO. 1'
;
; RATE OF CONVERSION CONTROLLED BY FORTRAN BLOCK SET-DCNV
;
PARAM PRES = -25. TEMP = 1292.
STOI  1  MIXED  SO2  -1 / COS  -2 / CO2  2 / CISOLID  SULFUR  3 /  
  2  MIXED  SO2  -1 / H2  -2 / H2O  2 / CISOLID  SULFUR  1 /  
  3  MIXED  SO2  -1 / H2  -3 / H2O  2 / H2S  1 /  
  4  MIXED  SO2  -1 / CO  -3 / CO2  2 / COS  1 /  
  5  MIXED  SO2  -1 / CO  -2 / CO2  2 / CISOLID  SULFUR  1
CONV  1  MIXED  SO2  0. /  
  2  MIXED  SO2  0. /  
  3  MIXED  SO2  0. /  
  4  MIXED  SO2  0. /  
  5  MIXED  SO2  0. /  

; BLOCK DSRP-C1 HEATER ; HEAT STREAM SENT TO HPECON
DESCRIPTION ' ELEMENTAL SULFUR CONDENSER #1'
PARAM PRES=-10. TEMP=350.
;
BLOCK DSRP-SPL SSPLIT
DESCRIPTION ' SPLIT OUT THE CONDENSED ELEMENTAL SULFUR'
FRAC CISOLID DES1 1.0 / MIXED DRHIN 1.0
;
BLOCK DSRP-RHX HEATER
DESCRIPTION ' DSRP REHEATER'
PARAM PRES=-1. TEMP=550.
;
BLOCK DSRP-R2 RSTOIC
DESCRIPTION ' DSRP REACTOR NO. 2'
;
; RATE OF CONVERSION CONTROLLED BY FORTRAN BLOCK SET-DCNV
;
PARAM PRES = -25. TEMP = 550.
STOI  1  MIXED  COS  -1 / H2O  -1 / CO2  1 / H2S  1 /  
  2  MIXED  SO2  -1 / H2S  -2 / H2O  2 / CISOLID  SULFUR  3
CONV  1  MIXED  COS  1.0 /  
  2  MIXED  SO2  0.
;
BLOCK DSRP-C2 HEATER ; HEAT STREAM SENT TO HPECON
DESCRIPTION ' ELEMENTAL SULFUR CONDENSER #2'
PARAM PRES=-10. TEMP=350.
;
BLOCK DSRP-SP2 SSPLIT
DESCRIPTION ' SPLIT OUT THE CONDENSED ELEMENTAL SULFUR'

72
FRAC CISOLID DES2 1.0 / MIXED TAILGAS 1.0
;
BLOCK DSRP-CL4 CLCHNG
;
BLOCK TAILCOMP COMPR
   DESCRIPTION ' DSRP TAIL GAS COMPRESSOR ' PARAM TYPE=1 PRES=286.72 EP=0.9 GFLAG=0
;
BLOCK DSRP-CL5 CLCHNG
;
BLOCK GTMIXR MIXER ; MODELS LINE LOSSES OF GAS STREAM TO GT
   DESCRIPTION ' MIX DSRP GAS EFFLUENT AND MAIN STREAM FOR GT FEED ' PARAM PRES=286.72
;
BLOCK DSRP-CL3 CLCHNG
; Changes FUELTEMP (MIXCISLD) to FUELGAZ2 (CONVEN), which goes to GT
;
BLOCK DSRP-SM MIXER
   DESCRIPTION "MIX SULFUR FROM CONDENSERS 1 AND 2"
;
BLOCK DSRP-PRD HEATER
   PARAM PRES=14.7 TEMP=300.
;
BLOCK DSRP-WK MIXER
;
   Combine similar temperature heat streams for integration with
   the steam cycle
;
BLOCK DSRP-HTM MIXER
;
BLOCK DSRP-MTM MIXER
;
BLOCK DSRP-LTM MIXER
;
******************************************************************************

   DSRP SEQUENCING
******************************************************************************

CONVERGENCE DS-COOL ONE-VAR
   SPEC DS-DSRPC

SEQUENCE DSRP-SEQ &
   DSRP-CLC DSRP-CL2 SET-RSPLT REDUSPLT &
   DSRP-MIX DS-COOL DSRP-COL &
   DSRP-SHF SET-DCNV &
   DSRP-R1 (RETURN DS-COOL) DSRP-C1 DSRP-SP1 &
   DSRP-RHX DSRP-R2 DSRP-C2 DSRP-SP2 &
   DSRP-CL4 TAILCOMP DSRP-CL5 GTMIXR DSRP-CL3 &
   DSRP-SM DSRP-PRD DSRP-WK &
   DSRP-HTM DSRP-MTM DSRP-LTM &
   DSRP-SUM

******************************************************************************

   DSRP FORTRAN BLOCKS
******************************************************************************

FORTRAN SET-RSPLT ; FLOWRATE SET AT 0% ABOVE STOICHIOMETRIC
   DESCRIPTION ' SET REDUCING GAS FLOWRATE TO DSRP PLANT'
DEFINE SFLOW MOLE-FLOW STREAM=SO2PROD SUBSTREAM=MIXED COMPONENT=SO2
DEFINE RFRAC BLOCK-VAR BLOCK=REDUSPLT SENTENCE=MOLE-FLOW &
VARIABLE=FLOW ID1=DSLIP

F       RFRAC=2.00*SFLOW
;       EXECUTE BEFORE REDUSPLT
;
FORTRAN SET-DCNV
F       COMMON /USRDSR/ DSRSV1, DSRSV2,
F &       FDSPRE, VGR1IN, DCDSG1, DCDSS1,
F &       FDSPR2, VGR2IN, DCDSG2, DCDSS2,
F &       DCDS, TDSCAT, ADSCAT, XMSULF
F &       EFSO21, EFSO22, DSRPR
F
COMMON /USRDSI/ NSTGDS
DESCRIPTION "SET CONVERSION RATES FOR REACTORS 1 AND 2"
DEFINE XS02I MOLE-FLOW STREAM=DR1IN SUBSTREAM=MIXED COMPONENT=SO2
DEFINE XH2SI MOLE-FLOW STREAM=DR1IN SUBSTREAM=MIXED COMPONENT=H2S
DEFINE XC01 MOLE-FLOW STREAM=DR1IN SUBSTREAM=MIXED COMPONENT=CO
DEFINE XCOSI MOLE-FLOW STREAM=DR1IN SUBSTREAM=MIXED COMPONENT=COS
DEFINE XTOTI SUBSTREAM-VAR STREAM=DR1IN SUBS=MIXED VAR=MOLEFLOW
;
DEFINE CNV11 BLOCK-VAR BLOCK=DSRP-R1 SENTENCE=CONV VAR=CONV ID1=1
DEFINE CNV12 BLOCK-VAR BLOCK=DSRP-R1 SENTENCE=CONV VAR=CONV ID1=2
DEFINE CNV13 BLOCK-VAR BLOCK=DSRP-R1 SENTENCE=CONV VAR=CONV ID1=3
DEFINE CNV14 BLOCK-VAR BLOCK=DSRP-R1 SENTENCE=CONV VAR=CONV ID1=4
DEFINE CNV15 BLOCK-VAR BLOCK=DSRP-R1 SENTENCE=CONV VAR=CONV ID1=5
DEFINE CNV21 BLOCK-VAR BLOCK=DSRP-R2 SENTENCE=CONV VAR=CONV ID1=1
DEFINE CNV22 BLOCK-VAR BLOCK=DSRP-R2 SENTENCE=CONV VAR=CONV ID1=2
;
DEFINE YSO2I MOLE-FLOW STREAM=TODSRP SUBSTREAM=MIXED COMPONENT=SO2
DEFINE YH2SI MOLE-FLOW STREAM=TODSRP SUBSTREAM=MIXED COMPONENT=H2S
DEFINE YC01 MOLE-FLOW STREAM=TODSRP SUBSTREAM=MIXED COMPONENT=CO
DEFINE YCOSI MOLE-FLOW STREAM=TODSRP SUBSTREAM=MIXED COMPONENT=COS
DEFINE YTOTI SUBSTREAM-VAR STREAM=TODSRP SUBS=MIXED VAR=MOLEFLOW
;
DEFINE ZS02I MOLE-FLOW STREAM=DSHFIN SUBSTREAM=MIXED COMPONENT=SO2
DEFINE ZH2SI MOLE-FLOW STREAM=DSHFIN SUBSTREAM=MIXED COMPONENT=H2S
DEFINE ZC0I MOLE-FLOW STREAM=DSHFIN SUBSTREAM=MIXED COMPONENT=CO
DEFINE ZCOSI MOLE-FLOW STREAM=DSHFIN SUBSTREAM=MIXED COMPONENT=COS
DEFINE ZTOTI SUBSTREAM-VAR STREAM=DSHFIN SUBS=MIXED VAR=MOLEFLOW
;
DEFINE TDSRC1 BLOCK-VAR BLOCK=DSRP-C1 VAR=TEMP
DEFINE PDSRC1 BLOCK-VAR BLOCK=DSRP-C1 VAR=PRES
DEFINE TDSREH BLOCK-VAR BLOCK=DSRP-RHX VAR=TEMP
DEFINE PDSREH BLOCK-VAR BLOCK=DSRP-RHX VAR=PRES
DEFINE TDSRR2 BLOCK-VAR BLOCK=DSRP-R2 VAR=TEMP
DEFINE PDSRR2 BLOCK-VAR BLOCK=DSRP-R2 VAR=PRES
DEFINE TDSRC2 BLOCK-VAR BLOCK=DSRP-C2 VAR=TEMP
DEFINE PDSRC2 BLOCK-VAR BLOCK=DSRP-C2 VAR=PRES
;
INITIALIZE KEY DSRP VARIABLES HERE FOR THE TIME BEING
;
        EFSO21 = SO2 Removal Efficiency for Reactor 1
        EFSO22 = SO2 Removal Efficiency for Reactor 2
        DSRPR = CO2/COS molar ratio
;
F       EFSO21 = 0.95
F       EFSO22 = 0.90
DSRPR = 2.
NDSSTG = 2
IF (NDSSTG.EQ.1) THEN
   EFSo22 = 0.0
   TDSREH = TDSRC1
   PDSREH = PDSRC1
   TDSRR2 = TDSRC1
   PDSRR2 = PDSRC1
   TDSRC2 = TDSRC1
   PDSRC2 = PDSRC1
ENDIF

; echo input variables to the history file for debugging purposes
WRITE(NHSTRY, 201) YSO2I, YH2SI, YCOI, YCOSI, YTOTI
F 201 FORMAT(/' Sampled Variables for stream TODSRP ',/,
F & 'SO2 Flow Rate ',F10.2,/
F & 'H2S Flow Rate ',F10.2,/
F & 'CO Flow Rate ',F10.2,/
F & 'COS Flow Rate ',F10.2,/
F & 'Total Flow Rate ',F10.2,/) ;
WRITE(NHSTRY, 202) ZSO2I, ZH2SI, ZCOI, ZCOSI, ZTOTI
F 202 FORMAT(/' Sampled Variables for stream DSHFIN ',/,
F & 'SO2 Flow Rate ',F10.2,/
F & 'H2S Flow Rate ',F10.2,/
F & 'CO Flow Rate ',F10.2,/
F & 'COS Flow Rate ',F10.2,/
F & 'Total Flow Rate ',F10.2,/) ;
WRITE(NHSTRY, 203) XSO2I, XH2SI, XCOI, XCOSI, XTOTI,
F & CNV11, CNV12, CNV13, CNV14, CNV15, CNV21, CNV22
F 203 FORMAT(/' Sampled Variables for stream DR1IN ',/,
F & 'SO2 Flow Rate ',F10.2,/
F & 'H2S Flow Rate ',F10.2,/
F & 'CO Flow Rate ',F10.2,/
F & 'COS Flow Rate ',F10.2,/
F & 'Total Flow Rate ',F10.2,/
F & 'Reaction 11 cnv ',F10.4,/
F & 'Reaction 12 cnv ',F10.4,/
F & 'Reaction 13 cnv ',F10.4,/
F & 'Reaction 14 cnv ',F10.4,/
F & 'Reaction 21 cnv ',F10.4,/
F & 'Reaction 22 cnv ',F10.4,/) ;

ETA1 = 0.
ETA2 = 0.
ETA3 = 0.
ETA4 = 0.
IF (XSO2I.LE.0) GOTO 101
ETA1 = 0.5*XCOSI/XSO2I
IF (ETA1.LT.0.) ETA1=0.
IF (ETA1.GT.1.) ETA1=1.
ETA2 = (2*(1-EFSO2I)*XSO2I-XH2SI-1/(DSRPR+1)*XCOI)/XSO2I
IF (ETA2.LT.0.) ETA2=0.
IF (ETA2.GT.1.) ETA2=1.
ETA3 = (DSRPR/(2*(DSRPR+1))*XCOI)/XSO2I
IF (ETA3.LT.0.) ETA3=0
IF (ETA3 .GT. 1.) ETA3 = 1.
ETA4 = EFSO21 - (ETA1 + ETA2 + ETA3)
IF (ETA4 .LT. 0.) ETA4 = 0
IF (ETA4 .GT. 1.) ETA4 = 1.

WRITE (NHSTRY, 204) ETA1, ETA2, ETA3, ETA4
FORMAT (/ 'Reaction Conversion Efficiencies ',' /,
', ETA1', 'F10.4,/',
', ETA2', 'F10.4,/',
', ETA3', 'F10.4,/',
', ETA4', 'F10.4,/')

CNV11 = ETA1
CNV12 = ETA4
CNV13 = ETA2
CNV14 = ETA3*0.5
CNV15 = ETA3*0.5

CNV21 = 1.
CNV22 = EFSO22
IF (NSTGDS .EQ. 1) THEN
  CNV21 = 0.
  CNV22 = 0.
ENDIF
FORTRAN DSRP-SUM
CHARACTER TIM*8
CHARACTER*3 MONTH(12)
DATA MONTH(1)/'JAN'/, MONTH(2)/'FEB', MONTH(3)/'MAR'/,
+ MONTH(4)/'APR'/, MONTH(5)/'MAY', MONTH(6)/'JUN'/,
+ MONTH(7)/'JUL'/, MONTH(8)/'AUG', MONTH(9)/'SEP'/,
+ MONTH(10)/'OCT'/, MONTH(11)/'NOV', MONTH(12)/'DEC'/
COMMON/USRDSRP/ EFSO21, EFSO22, DSRPR
DESCRIPTION ' DSRP SUMMARY BLOCK ' IN UNITS ENG
DEFINE XSO2GA SUBSTREAM-VAR STREAM=S02PROD SUBS=MIXED VAR=MASSFLOW
DEFINE XZFCLF SUBSTREAM-VAR STREAM=ZF-CLFL SUBS=MIXED VAR=MASSFLOW
DEFINE XGTM SUBSTREAM-VAR STREAM=TOGTMIXR SUBS=MIXED VAR=MASSFLOW
DEFINE XSLIP SUBSTREAM-VAR STREAM=DSLIP SUBS=MIXED VAR=MASSFLOW
DEFINE XCOOLI SUBSTREAM-VAR STREAM=DCOOLIN SUBS=MIXED VAR=MASSFLOW
DEFINE XSHFIN SUBSTREAM-VAR STREAM=DSHFIN SUBS=MIXED VAR=MASSFLOW
DEFINE XR1IN SUBSTREAM-VAR STREAM=DR1IN SUBS=MIXED VAR=MASSFLOW
DEFINE XC1IN SUBSTREAM-VAR STREAM=DC1IN SUBS=MIXED VAR=MASSFLOW
DEFINE XC1OUT SUBSTREAM-VAR STREAM=DC1OUT SUBS=MIXED VAR=MASSFLOW
DEFINE XRHIN SUBSTREAM-VAR STREAM=DRHIN SUBS=MIXED VAR=MASSFLOW
DEFINE XR2IN SUBSTREAM-VAR STREAM=DR2IN SUBS=MIXED VAR=MASSFLOW

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DEFINE XC2IN SUBSTREAM-VAR STREAM=DC2IN SUBS=MIXED VAR=MASSFLOW
DEFINE XC2OUT SUBSTREAM-VAR STREAM=DC2OUT SUBS=MIXED VAR=MASSFLOW
DEFINE XTLGAS SUBSTREAM-VAR STREAM=TAILGAS SUBS=MIXED VAR=MASSFLOW
DEFINE XHPTL SUBSTREAM-VAR STREAM=HPTAIL SUBS=MIXED VAR=MASSFLOW
DEFINE XFUELT SUBSTREAM-VAR STREAM=FUELT SUBS=MIXED VAR=MASSFLOW

DEFINE TS02GA SUBSTREAM-VAR STREAM=S02PROD SUBS=MIXED VAR=TEMP
DEFINE TZFCLF SUBSTREAM-VAR STREAM=ZF-CLFL SUBS=MIXED VAR=TEMP
DEFINE TGTIM SUBSTREAM-VAR STREAM=TOGMIXR SUBS=MIXED VAR=TEMP
DEFINE TLSLIP SUBSTREAM-VAR STREAM=DSLIP SUBS=MIXED VAR=TEMP
DEFINE TCOOLI SUBSTREAM-VAR STREAM=DCOOLIN SUBS=MIXED VAR=TEMP
DEFINE TSHFIN SUBSTREAM-VAR STREAM=DSHFIN SUBS=MIXED VAR=TEMP
DEFINE TR1IN SUBSTREAM-VAR STREAM=DR1IN SUBS=MIXED VAR=TEMP
DEFINE TC1IN SUBSTREAM-VAR STREAM=DC1IN SUBS=MIXED VAR=TEMP
DEFINE TR2IN SUBSTREAM-VAR STREAM=DR2IN SUBS=MIXED VAR=TEMP
DEFINE TC2IN SUBSTREAM-VAR STREAM=DC2IN SUBS=MIXED VAR=TEMP
DEFINE TC20UT SUBSTREAM-VAR STREAM=DC2OUT SUBS=MIXED VAR=TEMP
DEFINE TTLGAS SUBSTREAM-VAR STREAM=TAILGAS SUBS=MIXED VAR=TEMP
DEFINE THPTL SUBSTREAM-VAR STREAM=HPTAIL SUBS=MIXED VAR=TEMP
DEFINE TFUELT SUBSTREAM-VAR STREAM=FUELT SUBS=MIXED VAR=TEMP

DEFINE PS02GA SUBSTREAM-VAR STREAM=S02PROD SUBS=MIXED VAR=PRES
DEFINE P2FCLF SUBSTREAM-VAR STREAM=ZF-CLFL SUBS=MIXED VAR=PRES
DEFINE PGTIM SUBSTREAM-VAR STREAM=TOGMIXR SUBS=MIXED VAR=PRES
DEFINE PSLIP SUBSTREAM-VAR STREAM=DSLIP SUBS=MIXED VAR=PRES
DEFINE PCOOLI SUBSTREAM-VAR STREAM=DCOOLIN SUBS=MIXED VAR=PRES
DEFINE PSHFIN SUBSTREAM-VAR STREAM=DSHFIN SUBS=MIXED VAR=PRES
DEFINE PR1IN SUBSTREAM-VAR STREAM=DR1IN SUBS=MIXED VAR=PRES
DEFINE PC1IN SUBSTREAM-VAR STREAM=DC1IN SUBS=MIXED VAR=PRES
DEFINE PC1OUT SUBSTREAM-VAR STREAM=DC1OUT SUBS=MIXED VAR=PRES
DEFINE PRHIN SUBSTREAM-VAR STREAM=DRHIN SUBS=MIXED VAR=PRES
DEFINE PR2IN SUBSTREAM-VAR STREAM=DR2IN SUBS=MIXED VAR=PRES
DEFINE PC2IN SUBSTREAM-VAR STREAM=DC2IN SUBS=MIXED VAR=PRES
DEFINE PC20UT SUBSTREAM-VAR STREAM=DC2OUT SUBS=MIXED VAR=PRES
DEFINE PTLGAS SUBSTREAM-VAR STREAM=TAILGAS SUBS=MIXED VAR=PRES
DEFINE PHPTL SUBSTREAM-VAR STREAM=HPTAIL SUBS=MIXED VAR=PRES
DEFINE PFUELT SUBSTREAM-VAR STREAM=FUELT SUBS=MIXED VAR=PRES

; INLET SULFUR
;
DEFINE XGOSO2 MOLE-FLOW STREAM=S02PROD SUBS=MIXED COMP=SO2
DEFINE XSLSO2 MOLE-FLOW STREAM=DSLIP SUBS=MIXED COMP=SO2
DEFINE XSLH2S MOLE-FLOW STREAM=DSLIP SUBS=MIXED COMP=H2S
DEFINE XSLCOS MOLE-FLOW STREAM=DSHFIN SUBS=MIXED COMP=COS

; OUTLET SULFUR
;
DEFINE XES1 MOLE-FLOW STREAM=DES1 SUBS=CISOLID COMP=SULFUR
DEFINE XES2 MOLE-FLOW STREAM=DES2 SUBS=CISOLID COMP=SULFUR
DEFINE XSPROD MOLE-FLOW STREAM=SULPROD SUBS=CISOLID COMP=SULFUR
DEFINE XTLSO2 MOLE-FLOW STREAM=HPTAIL SUBS=MIXED COMP=SO2
DEFINE XTLH2S MOLE-FLOW STREAM=HPTAIL SUBS=MIXED COMP=H2S

; Print only after flowsheet simulation is completed.
;
F IF (IPASS.EQ.1) RETURN
;
F CALL IDATE(IM,ID,IY)
F CALL TIME(TM)
F WRITE(NRPT,101) MONTH(IM),ID,IY,TIM(1:5)
F 101 FORMAT('/19X,'DIRECT SULFUR RECOVERY PROCESS',/
+ 19X,'RESULTS GENERATED ON ',A,I3', 19'12' AT ',A/)
F WRITE(NRPT,102)
F 102 FORMAT(26X,'** DSRP MASS BALANCE (LB/HR) **',/
);
F WRITE(NRPT,103) XSO2GA, TSO2GA, PSO2GA,
F 1 XZFCLF, TZFCLF, PZFCLF,
F 2 XSLIP, TSLIP, PSLIP,
F 3 XCOOLI, TCOOLI, PCOOLI,
F 4 XSHFIN, TSHFIN, PSHFIN,
F 5 XR1IN, TR1IN, PR1IN,
F 6 XC1IN, TC1IN, PC1IN
F 103 FORMAT(26X,'DSRP GAS STREAMS',/
& 10X,' Description (lb/hr) (deg F) (psia)',/
1 10X,'------------------',/
2 10X,'HGD OFF-GAS ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'COAL GAS ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'SLIP STREAM ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'COOLER INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'SHIFT INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'REACTOR 1 INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'CONDENSER 1 INLET ',3X,F11.2,4X,F9.0,1X,F9.2)
F WRITE(NRPT,104) XC1OUT, TC1OUT, PC1OUT,
F 1 XRHIN, TRHIN, PRHIN,
F 2 XR2IN, TR2IN, PR2IN,
F 3 XC2IN, TC2IN, PC2IN,
F 4 XC2OUT, TC2OUT, PC2OUT,
F 5 XTLGAS, TTLGAS, PTLGAS,
F 6 XHPTL, THPTL, PHPTL,
F 6 XFUELT, TFUELT, PFUELT
F 104 FORMAT(
F & 10X,'CONDENSER 1 OUTLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'REHEATER INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'REACTOR 2 INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'CONDENSER 2 INLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'CONDENSER 2 OUTLET ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'DSRP TAILGAS ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'COMPRESSED TAILGAS ',3X,F11.2,4X,F9.0,1X,F9.2,/
F & 10X,'FUEL TO GAS TURB. ',3X,F11.2,4X,F9.0,1X,F9.2)
F WRITE(NRPT,105)
F 105 FORMAT('/19X,'** DSRP SULFUR MASS BALANCE (LBMOLE/HR) **',/
F XSITOT = XOGS02 + XSLS02 + XSLH2S + XSLCOS

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WRITE(NRPT,106) XCGS02, XSLSO2, XSLH2S, XSLCOS, XSITOT
WRITE(NRPT,106) XCGS02, XSLSO2, XSLH2S, XSLCOS, XSITOT
F 106 FORMAT(
   & 20X,'INLET SULFUR: SO2 IN OFF-GAS ',F10.2,/, 
   & 20X,' SO2 IN SLIP STREAM ',F10.2,/
   & 20X,' H2S IN SLIP STREAM ',F10.2,/
   & 20X,' COS IN SLIP STREAM ',F10.2,/
   & 20X,' TOTAL INLET SULFUR----->',F10.2,/
   ;
F SFCAP = (XSPROD/XSITOT)*100.
F XSOTOT = XES1+XES2+XTLS02+XTLH2S
WRITE(NRPT,107) XES1, XES2, XTLS02, XTLH2S, XSOTOT, FSCAP
F 107 FORMAT(
   & 20X,'OUTLET SULFUR: CONDENSER NO. 1 ',F10.2,/
   & 20X,' CONDENSER NO. 2 ',F10.2,/
   & 20X,' SO2 IN TAILGAS ',F10.2,/
   & 20X,' H2S IN TAILGAS ',F10.2,/
   & 20X,' TOTAL OUTLET SULFUR----->',F10.2,/
   & 20X,'DSRP SULFUR CAPTURE EFFICIENCY: ',F6.2,' PERCENT')
;
WRITE(NRPT,100) XSO2GA, XZFCLF, XSLIP, XCOOL1, XSHFIN,
F 1 XR1 IN, XC1 IN
C F 100 FORMAT(26X,'DSRP GAS STREAMS',/,
   & ' HGD Off-gas: ',F14.2,/
   & ' Coal Gas: ',F14.2,/
   & ' Coal Gas Slip Stream: ',F14.2,/
   & ' Gas Into Cooler: ',F14.2,/
   & ' Gas Into Shift: ',F14.2,/
   & ' Reactor No. 1 Inlet: ',F14.2,/
   & ' Condenser No. 1 Inlet: ',F14.2,/)  ;

;******************************************************************************
 ; DSRP DESIGN SPECIFICATIONS
 ;******************************************************************************

DES-SPEC DS-DSRPC
DEFINE QR1 STRM-ATTR-VAR ATTR=HEAT VAR=Q STREAM=QDSRP-R1
SPEC QR1 TO 0.
TOL-SPEC 1000.
VARY BVAR BLOCK=DSRP-COL SENTENCE=PARAM VAR=TEMP
LIMITS 500. 1292.

;
Appendix C

DSRP COST MODEL CODE
This appendix contains a listing of the FORTRAN code from the cost model subroutine for a Lurgi-based IGCC system which includes the DSRP. Only the code specific to the DSRP is included here.

**Direct Capital Cost of the DSRP**

```
C Direct capital cost of the DIRECT SULFUR RECOVERY PROCESS
C
C NTDS = Number of total trains of DSRP units
C NODS = Number of on-line (operating) trains of DSRP units
C NDSSTG = Number of DSRP stages (reactors): 1 or 2
C RSV1DR = Reference space velocity for Reactor No. 1 (scc/(cc-h))
C RSV2DR = Reference space velocity for Reactor No. 2 (scc/(cc-h))
C FDSPRE = DSRP Pressure correction factor for pressure vessel cost
C XPR1IN = Reactor No. 1 inlet gas pressure, psia
C XTR1IN = Reactor No. 1 inlet gas temperature, F
C VGR1IN = Reactor No. 1 inlet gas volume flow rate, ft^3/hr
C FDSPR2 = DSRP Pressure correction factor for pressure vessel cost
C XPR2IN = Reactor No. 2 inlet gas pressure, psia
C XTR2IN = Reactor No. 2 inlet gas temperature, F
C VGR2IN = Reactor No. 2 inlet gas volume flow rate, ft^3/hr
C DCDSG1 = Direct cost for stage 1 gas handling equipment, $1,000
C DCDSG2 = Direct cost for stage 2 gas handling equipment, $1,000
C DCDSSL = Direct cost for stage 1 sulfur handling equipment, $1,000
C DCDSS2 = Direct cost for stage 2 sulfur handling equipment, $1,000

NTDS = 2
NODS = 2
NDSSTG = 2
RSV1DR = 2000.
RSV2DR = 2000.

also define space velocities. units are scc/(cc-h).

DSRSV1 = 5000.
DSRSV2 = 5000.

pressure correction factor for pressure vessel cost

FDSPRE = (2.5 + 0.093 * XPR1IN ** 0.64)/7.1

calculate gas volume flow through DSRP, units are ft^3/hr

VGR1IN = XTR1IN * 0.73 * (XTR1IN+460)/(XPR1IN/14.7)

calculate cost for the 1st stage of the DSRP

The first term represents the gas cooler and sulfur condenser
The second term represents the reactor vessel. The latter is sensitive to the gas volume flow rate and the space velocity

DCDSG1 = NTDS*FDSPRE*(3380.*VGR1IN/(77000.*NODS))**0.67
```
& + 1020.*(VGR1IN/(77000.*NODS)*(RSV1DR/DSRSV1))**0.67
& *(CI/361.2)
DCDSS1 = 80.*NTDS*(XSPROD/(2900.*NODS))**0.67*(CI/361.2)

calculate cost for the 2nd stage of the DSRP

DCDSG2 = 0.
DCDSS2 = 0.

IF (NDSSSTG.EQ.2) THEN
  VGR2IN = XR2IN * 0.73 * (XTR2IN+460)/(XPR2IN/14.7)
  FDSPR2 = (2.5 + 0.093 * XPR2IN ** 0.64)/7.1
  DCDSG2 = NTDS*FDSPR2*(1205.*(VGR2IN/(69000.*NODS))**0.67
& + 960.*(VGR2IN/(69000.*NODS)*(RSV2DR/DSRSV2))**0.67)
& *(CI/361.2)
  DCDSS2 = 80.*NTDS*(XSPROD/(2900.*NODS))**0.67*(CI/361.2)
ENDIF

DCDS = DCDSG1 + DCDSG2 + DCDSS1 + DCDSS2

Other Capital Costs

Direct capital cost of general facilities

DCGF=FGF*(DCCH+DCL +DCOF+DCG +DCSS+DCCY+DCZF+DCSA+DCS +DCBF
& +DCGT+DCHR+DCDS+DCCR+DCST)

CAPITAL COSTS: TOTAL PLANT INVESTMENT

The total plant investment is estimated in this section. The
total capital requirement, which includes items dependent on
operating costs, is not calculated until after the operating
costs are estimated.

Total Direct Cost (TDC)

TDC= DCCH+DCL +DCOF+DCG +DCSS+DCCY+DCZF+DCSA+DCS +DCBF
& +DCGT+DCHR+DCDS+DCCR+DCST+DCGF

Total Indirect Cost (TIC)

CICC=FICC*TDC
CTAX=RTAX*(0.8*TDC+0.1*CICC)
CEHO=FMO*(TDC+CICC+CTAX)
TIC=CICC+CTAX+CEHO+CEP

Process Contingency Costs

CPCDS = FPCDS*DCDS*(1.+TIC/TDC)

CPC=CPCCH+CPCCL+CPCOF+CPCSS+CPCCY+CPCG+CPCS+CPCZF+CPCSA
& +CPCBF+CPCGT+CPCHR+CPCDS+CPCCR+CPCST+CPCGF

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Project contingency cost

\[ CPJ=FPJ \times (TDC+TIC+CPC) \]

Total Plant Cost (TPC)

\[ TPC=TDC+TIC+CPC+CPJ \]

Total plant investment (TPI)

\[ Z = \frac{(1+INTRST)/(1+EREAL)}{\text{IF}(Z \leq 1)\ \text{THEN}\ \text{AF} = 1\ \text{ELSE} \ AF = (Z^{\text{NOYEARS}-1})/(\text{NOYEARS}^{Z-1})\ \text{ENDIF} } \]
\[ TPI=AF\times TPC \]
\[ AFDC=TPI-TPC \]

Net Plant Electrical Output (including DSRP auxiliary loads)

--- NET PLANT ELECTRICAL OUTPUT ---

The net electrical output must be estimated in order to estimate a number of plant costs. The gross power plant electrical output is reduced by plant auxiliary loads, including coal handling, the oxygen plant, the gasification section, limestone handling, sulfation, general facilities, and power consumption in the steam cycle. The pump and compressor power consumption is estimated directly from the ASPEN simulation. The other areas are estimated from regression relationships taken from Frey and Rubin (1990).

Gas Turbine Output: \( WGTE \)
Steam Turbine Output: \( WSTE \)

The auxiliary loads have been converted to MW from Frey and Rubin (1990).

\[ WCHE = 1.89D-06 \times MCFGI + ERRWCH \]
\[ WLE = 0.0 \]
\[ \text{IF}(NTL.GT.0) \ WLE = (-13.3 + 0.00461*MLGI)/1000. \]
\[ WOFE = WCME/1000. \]
\[ WGE = (0.005*MCFGI)/1000. \]
\[ WSE = 0.0 \]
\[ \text{IF}(NTS.GT.0) \ WSE = (-3.7 + 0.0102*(MDISP1+MDISP2))/1000. \]
\[ WSCR = 3.47D-5 \times XNH3IN \times 2000. / (8760. \times CF) \]
\[ WDSRP = WKDSRP/1000000. \]
\[ WBFE = STAUXE/1000000.0 \]
\[ WGFE = 1.64 + 0.0877\times(WCHE+WLE+WOFE+WGE+WSE+WBFE) \]
\[ WAXE = WCHE+WLE+WOFB+WGE+WSE+WSAE+WBFE+WGFE+WDSRP+WSCR \]
\[ WNETE = WGTE+WSTE-WAXE \]
Initial Catalyst for the DSRP

--- INITIAL CATALYSTS AND CHEMICALS ---

DSRP: the total catalyst charge is:

NOTE: need to convert from lbmole/hr to scc/hr

\[
\text{lbmole/hr} \times 0.73 \text{ (atm-ft}^3)/(\text{lbmole-R}) \times 520 \text{ R} / 1 \text{ atm} = \text{ ft}^3/\text{hr}
\]

Thus, lbmole/hr * 379.6 ft^3/lbmole * 28,350 cc/ft^3

or lbmole/hr * 10,762,000 cc/lbmole = scc/hr

Space velocity is scc/(cc-hr), thus cat volume is cc.

Convert to weight basis to be consistent with cost data.

cc * (0.72 g/cc (typical density) * 1lb/454 g) = lb

or cc * 0.00159 = lb

TDSCAT has units of lb.

\[
\text{TDSCAT} = (\text{XR1IN/DSRSV1} + \text{XR2IN/DSRSV2}) \times 10762000 \times 0.00159
\]

Fixed Operating Cost for the DSRP

Fixed Operating Costs: Maintenance

\[
\text{OCMDS} = \text{FMCDS} \times (\text{DCDS} \times (1 + (\text{TIC} + \text{CPJ}) / \text{TDC}) + \text{CPCDS})
\]

Variable Operating Cost for the DSRP

Annual DSRP Catalyst Requirement

\[
\text{ADSCAT} = \text{TDSCAT}/3.
\]

\[
\text{OCDSCA} = \text{UCDSCA} \times \text{ADSCAT}
\]
Appendix D

COST MODEL OUTPUTS

a) Base Case
(Lurgi IGCC with sulfuric acid recovery)
b) One-Stage DSRP
c) Two-Stage DSRP
**Computer Model Output for Base Case Analysis: Lurgi-based IGCC with conventional sulfuric acid recovery**

Air-Blown Fixed-Bed Gasifier IGCC w/SCR: Deterministic Analysis

### System Summary

**GASIFIER CONDITIONS**

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>COAL FLOW RATE</td>
<td>0.562244E+06 LB/HR</td>
</tr>
<tr>
<td>SOURBENT FLOW RATE</td>
<td>0.378160E-00 LB/HR</td>
</tr>
<tr>
<td>AIR FLOW RATE</td>
<td>0.138042E-06 LB/HR</td>
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<tr>
<td>REQUIRED STEAM</td>
<td>0.690210E-06 LB/HR</td>
</tr>
<tr>
<td>SUPPLIED STEAM</td>
<td>0.999983E-03 LB/HR</td>
</tr>
<tr>
<td>SOX FLOW RATE</td>
<td>0.610123E-03 LB/HR</td>
</tr>
<tr>
<td>ASH FLOW RATE</td>
<td>0.000000E+00 LB/HR</td>
</tr>
<tr>
<td>GASIFIER PRESSURE</td>
<td>307.5 PSI</td>
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<tr>
<td>GASIFIER TEMPERATURE</td>
<td>1100.0 °F</td>
</tr>
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</table>

**Air-Blown Fixed-Bed Gasifier IGCC w/SCR: Deterministic Analysis**

### System Summary

**ZINC FERITE SULFUR REMOVAL PROCESS**

RESULTS GENERATED ON OCT 17, 1994 AT 17:37

<table>
<thead>
<tr>
<th>Name</th>
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<tr>
<td>H2S IN RAMGAS</td>
<td>19720.09</td>
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<tr>
<td>H2S IN FUELGAS</td>
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<tr>
<td>SO2 IN FUELGAS</td>
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<tr>
<td>PMV OF H2S IN FUELGAS</td>
<td>11.</td>
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**FLOW RATES (LB/HR)**

<table>
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<tbody>
<tr>
<td>RAMGAS</td>
<td>0.260E+07 Mw = 23.11</td>
</tr>
<tr>
<td>FUELGAS</td>
<td>0.260E+07 Mw = 23.08</td>
</tr>
<tr>
<td>SO2GAS</td>
<td>548541.39 Mw = 20.35</td>
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</table>

**STEAM REQUIRED TO MAINITAIN**

<table>
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<tr>
<td>REGENERATOR TEMPERATURE</td>
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<tr>
<td>AIR FLOW TO REGENERATOR</td>
<td>110.00 F</td>
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**GENERAL**

<table>
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<th>Value</th>
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</thead>
<tbody>
<tr>
<td>CO/(CO+CO2 RATIO (SHFT-STM)</td>
<td>0.281</td>
</tr>
<tr>
<td>SULFUR CAPTURE EFFICIENCY</td>
<td>0.998</td>
</tr>
<tr>
<td>TEMPERATURE OF THE REGENERATED GAS</td>
<td>1450.2</td>
</tr>
<tr>
<td>VOLUME PERCENT AIR IN REGENERATION GAGS</td>
<td>16.765</td>
</tr>
</tbody>
</table>

**MS7000F GAS TURBINE CONDITIONS**

<table>
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<tbody>
<tr>
<td>FUEL FLOW RATE</td>
<td>0.250743E-07 LB/HR</td>
</tr>
<tr>
<td>AIR FLOW RATE</td>
<td>0.138042E-06 LB/HR</td>
</tr>
<tr>
<td>AIR DIVERTED TO GASIFIER</td>
<td>0.138042E-06 LB/HR</td>
</tr>
<tr>
<td>AIR DIVERTED TO ZINC. FER</td>
<td>0.133546E-06 LB/HR</td>
</tr>
<tr>
<td>FUEL HW (NET BASIS)</td>
<td>1726.5 Btu/LB, 105.5 Btu/SCF</td>
</tr>
<tr>
<td>FUEL HW (NET BASIS)</td>
<td>1938.9 Btu/LB, 117.9 Btu/SCF</td>
</tr>
<tr>
<td>FUEL FLOW RATE</td>
<td>0.250743E-07 LB/HR</td>
</tr>
<tr>
<td>COMBUSTOR EXIT TEMPERATURE</td>
<td>2436.7 °F</td>
</tr>
<tr>
<td>TURBINE EXHAUST TEMPERATURE</td>
<td>1131.1 °F</td>
</tr>
<tr>
<td>THERMAL EFFICIENCY (H/JV)</td>
<td>0.6308</td>
</tr>
<tr>
<td>GASIFIER AIR INTERCOOLER DUTY</td>
<td>0.000000E+00 Btu/HR</td>
</tr>
</tbody>
</table>

**Ratio of Inlet Air to Exhaust Gas:** 0.901
**Ratio of Boost Air to Inlet Air:** 0.153
**Ratio of Gasif Air to Inlet Air:** 0.143
**Ratio of Regen Air to Inlet Air:** 0.014
**Ratio of Fuel Gas to Inlet Air:** 0.260

**CO2 Emissions:** 194.3 lb/MMBTU
**CO Emissions:** 0.32281 lb/MMBTU
**SO2 Emissions:** 0.166.60 ppmv
**NOx Emissions:** 0.54707 lb/MMBTU
**Oxygen in Exhaust:** 9.8814 percent
**Vapor in Exhaust:** 16.5838 percent
**CO2 in Exhaust:** 7.1489 percent

**STEAM TURBINE CONDITIONS**

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEAM DIVERTED TO GASIFIER</td>
<td>0.690210E+06 LB/HR</td>
</tr>
<tr>
<td>STEAM DIVERTED TO ZINC. FER</td>
<td>0.408896E+06 LB/HR</td>
</tr>
<tr>
<td>STEAM TURBINE FLOW RATE</td>
<td>0.129455E+07 LB/HR</td>
</tr>
<tr>
<td>STEAM TURBINE TEMPERATURE</td>
<td>1000.0°F</td>
</tr>
</tbody>
</table>

**Summary of Sampled Aspen Flowsheet Performance Parameters**

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLANT SECTION</td>
<td>FLOWSHEET PERFORMANCE PARAMETERS</td>
</tr>
<tr>
<td>Coal Feed</td>
<td>Mass flow of coal to gasifier</td>
</tr>
<tr>
<td>Limestone Feed</td>
<td>Mass flow of limestone (mixed)</td>
</tr>
<tr>
<td>Oxidant Feed</td>
<td>Mass flow of limestone (ciscoid)</td>
</tr>
<tr>
<td>C02 in Exhaust</td>
<td>Work to boost air compressor</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>First precon gas to inlet temp.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>First precon gas to outlet temp.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>First precon gas to BFW temp.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Heat transfer in first precon</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Heat trans. to BFW from HRSG</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Heat trans. to BFW from Regen.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Gasifier output syngas pres.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Gasifier output syngas temp.</td>
</tr>
<tr>
<td>C02 Divisions</td>
<td>Gasifier output syngas density</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>Gasifier recycle fines flow rate</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>Off-gas to sulfuric acid plant</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>SO2 to sulfuric acid plant</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>Off-gas temp. to sul. acid plant</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>Zinc ferrite inlet H2O flow</td>
</tr>
<tr>
<td>Zinc Fertire</td>
<td>Zinc ferrite inlet COS flow</td>
</tr>
<tr>
<td>Ash in coal</td>
<td>Gasifier ash removal</td>
</tr>
<tr>
<td>Ash in coal</td>
<td>Gasifier ash removal</td>
</tr>
<tr>
<td>Ash in coal</td>
<td>Gasifier fines removal</td>
</tr>
<tr>
<td>Water to power plant</td>
<td>Raw water to power plant</td>
</tr>
</tbody>
</table>

**Miscellaneous**

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam turbine condensate</td>
<td>750596.08 lb/hr</td>
</tr>
<tr>
<td>Gas Turbine</td>
<td>Gas turbine inlet air flow</td>
</tr>
<tr>
<td>Steam Cycle</td>
<td>HRSG outlet HP steam pres.</td>
</tr>
<tr>
<td>Gas Turbine</td>
<td>Gas turbine net shaft work</td>
</tr>
<tr>
<td>Steam Cycle</td>
<td>Steam turbine net shaft work</td>
</tr>
<tr>
<td>Steam Cycle</td>
<td>Steam turbine cycle auxiliary</td>
</tr>
<tr>
<td>Steam Cycle</td>
<td>Acid gas auxiliary power</td>
</tr>
<tr>
<td>Moisture in coal feed</td>
<td>0.12 wt%</td>
</tr>
<tr>
<td>SCR Inlet Gas Pressure</td>
<td>12747.00 BTU/lb</td>
</tr>
<tr>
<td>SCR Inlet Gas Temperature</td>
<td>390773.89 lb/hr</td>
</tr>
<tr>
<td>SCR Inlet Gas Pressure</td>
<td>717.00 lb/hr</td>
</tr>
<tr>
<td>SCR Inlet Gas Pressure</td>
<td>15.33 lb/hr</td>
</tr>
</tbody>
</table>
A. KEY INPUT ASSUMPTIONS

**Economic Assumptions:**
- Cost Year: January 1989
- Inflation Rate: 0.00%
- Plant Cost Index: 351.5
- Chemicals Cost Index: 411.3
- Plant Capacity Factor: 0.65
- Indirect Construction Factor: 0.20
- Average Operating Labor Rate: 19.70
- Years of Construction: 4

**Process Contingency and Maintenance Cost Factors:**
- Process Contingency Factor: 0.17
- Maintenance Cost Factor: 1.00

**Performance Assumptions:**
- Gasifier Availability: 0.87
- Sorb. Sulfur Loading: 0.168
- Max. Desulf. Vessel Diameter: 12.50
- L/D Ratio: 3.00
- Maximum Space Velocity (l/hr): 2000
- Sorb. Attrition Rate/80 cycles: 0.800
- Gasifier Coal Throughput: 1.01

**Process Data:**
- SCR Inlet NO loading: 357.29 l/hole/hr
- SCR Inlet NO2 loading: 16.80 l/hole/hr
- SCR Ammonia Requirement: 304.78 l/hole/hr
- SCR Dilution Steam Requirement: 5790.83 l/hole/hr

**Environmental High Pressure Blowdown:**
- CO2 from gas turbine: 27936.17 l/hole/hr
- CO from gas turbine: 72.92 l/hole/hr
- NO2 from gas turbine: 1.20 l/hole/hr
- NO from gas turbine: 0.00 l/hole/hr
- NO from gas turbine: 0.00 l/hole/hr
- NH3 to gas turbine: 397.41 l/hole/hr
- NO from gas turbine: 74.16 l/hole/hr

**Cost Summary:**
- Actual coal heating value: 11248.73 Btu/lb

**COST VAR WARNING**
- Variable MCFP1 value of 56252.961 in DCSS above the upper limit of 433000.000
- Variable VSNF1 value of 9218.250 in DCXV above the upper limit of 60000.000
- Variable MRF value of 1247373.267 in DCBF above the upper limit of 6140000.000

B. CALCULATED DIRECT CAPITAL AND PROCESS CONTINGENCY COSTS ($1,000)

<table>
<thead>
<tr>
<th>Plant Section</th>
<th>Operating Total Capital Cost</th>
<th>Contingency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Handling</td>
<td>114670.5 Ib/yr</td>
<td>18.2 ton/yr</td>
</tr>
<tr>
<td>Limestone Handling</td>
<td>160.00 $/ton</td>
<td>17536.95</td>
</tr>
<tr>
<td>Oxidant Feed</td>
<td>14451.6 l/bf</td>
<td>24298.00</td>
</tr>
<tr>
<td>Gasification</td>
<td>20201.2 lb/yr</td>
<td>24298.00</td>
</tr>
<tr>
<td>Coke, Ash, &amp; Bent. Subsystems</td>
<td>111137.0 $/ton</td>
<td>111137.0</td>
</tr>
<tr>
<td>High Temp. Cyclones</td>
<td>26604.5 $/ton</td>
<td>26604.5</td>
</tr>
<tr>
<td>Sulfuric Acid Plant</td>
<td>29585.4 $/ton</td>
<td>29585.4</td>
</tr>
<tr>
<td>Selective Catalytic Reduction</td>
<td>150.00 $/ton</td>
<td>150.00</td>
</tr>
<tr>
<td>Steam Turbine</td>
<td>11628.7 $/ton</td>
<td>11628.7</td>
</tr>
<tr>
<td>General Facilities</td>
<td>38.38 $/ton</td>
<td>38.38</td>
</tr>
</tbody>
</table>

C. CALCULATED TOTAL CAPITAL REQUIREMENT ($1,000)

<table>
<thead>
<tr>
<th>Description</th>
<th>Capital Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Direct Cost</td>
<td>409741.00</td>
</tr>
<tr>
<td>Indirect Construction Cost</td>
<td>81948.00</td>
</tr>
<tr>
<td>Sales Tax</td>
<td>16799.00</td>
</tr>
<tr>
<td>Engineering and Home Office Fees</td>
<td>50849.00</td>
</tr>
<tr>
<td>Hydrargyn</td>
<td>50000.00</td>
</tr>
<tr>
<td>Total Indirect Costs</td>
<td>150596.00</td>
</tr>
<tr>
<td>Total Process Contingencies</td>
<td>78143.00</td>
</tr>
<tr>
<td>Project Contingency</td>
<td>311769.00</td>
</tr>
<tr>
<td>Total Plant Cost</td>
<td>750449.00</td>
</tr>
<tr>
<td>Initial Catalysts and Chemicals</td>
<td>20751.00</td>
</tr>
<tr>
<td>Land dial</td>
<td>35511.00</td>
</tr>
<tr>
<td>Total CAPITAL REQUIREMENT ($1,000)</td>
<td>962589.00</td>
</tr>
</tbody>
</table>

D. CALCULATED FIXED OPERATING COSTS ($/year)

<table>
<thead>
<tr>
<th>Description</th>
<th>Annual Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating Labor</td>
<td>853352.00</td>
</tr>
<tr>
<td>Maintenance Costs</td>
<td>162500.00</td>
</tr>
<tr>
<td>Administration and Supervision</td>
<td>451897.00</td>
</tr>
<tr>
<td>TOTAL FIXED OPERATING COST ($/year)</td>
<td>297723.00</td>
</tr>
</tbody>
</table>

E. CALCULATED VARIABLE OPERATING COSTS

1. CONSUMABLES ($/year)
   - Assumed Material Requirement
   - Calc. Annual Operating Cost
### Bentonite
- **Cost:** $0.03/lb
- **Usage:** 4577299.7 lb/yr
- **Total:** $132742.

### Fuel Oil
- **Cost:** $42.00/bbl
- **Usage:** 40245.9 bbl/yr
- **Total:** $1690328.

### Plant Air Ads.
- **Cost:** $2.80/lb
- **Usage:** 3018.4 lb/yr
- **Total:** $8452.

### Raw Water
- **Cost:** $0.73/Kgal
- **Usage:** 851394.6 Kgal/yr
- **Total:** $621518.

### Waste Water
- **Cost:** $840.00/gpm
- **Usage:** 0 lb/hr
- **Total:** $0.

### LPG Flare
- **Cost:** $11.70/bbl
- **Usage:** 3521.5 bbl/yr
- **Total:** $41202.

### Total Consumables ($/year)
- **Total:** $16401766.

### Fuel, Ash Disposal, and Byproduct Credit ($/year)
- **Coal:** $1.61/MMBtu
- **Usage:** 562253.0 lb/hr
- **Total:** $65841846.

### Sulfuric Acid
- **Cost:** $40.00/ton
- **Usage:** 173231.5 ton/yr
- **Total:** $6236336.

### Total Variable Operating Cost ($/year)
- **Total:** $77687668.

### Power Summary (MWe)

<table>
<thead>
<tr>
<th>Description</th>
<th>Calculated KWe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas Turbine Output</td>
<td>562.85</td>
</tr>
<tr>
<td>Steam Turbine Output</td>
<td>173.33</td>
</tr>
<tr>
<td>Total Auxiliary Loads</td>
<td>26.71</td>
</tr>
<tr>
<td>Net Electricity</td>
<td>709.46</td>
</tr>
</tbody>
</table>

### Fixed Operating Cost
- **Total:** $1356.78/kW

### Incremental Variable Costs
- **Fixed:** $41.41/kWh

### Byproduct Credit
- **Total:** $1.54/kWh

### Capital Cost
- **Total:** $51.14/kWh

### Cost of Electricity
- **Total:** $51.14/kWh

### Environmental Summary

#### Inputs
- **Coal:** 0.7925 lb/kWh
- **Water:** 1.7382 lb/kWh

#### Outputs
- **Blowdown:** 0.0745 lb/kWh
- **Ash:** 0.0432 lb/kWh
- **Sulfuric Acid:** 0.0858 lb/kWh
- **CO2 emissions:** 1.7326 lb/kWh
- **CO emissions:** 0.0029 lb/kWh
- **SO2 emissions:** 0.0414 lb/MMBtu
- **COS emissions:** 0.0000 lb/MMBtu
- **CH4 emissions:** 0.0000 lb/MMBtu
- **H2S emissions:** 0.0000 lb/MMBtu
- **NOX emissions:** 0.5471 lb/MMBtu

#### Notes on NOX emissions:
- NOX emissions are based on fuel bound ammonia

### SCR Summary

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference Removal Efficiency</td>
<td>0.80 fraction</td>
</tr>
<tr>
<td>Actual Removal Efficiency</td>
<td>0.80 fraction</td>
</tr>
<tr>
<td>Ammonia Slip</td>
<td>10.00 ppmv</td>
</tr>
<tr>
<td>Reference NOX Concentration</td>
<td>42.00 ppmv</td>
</tr>
<tr>
<td>Minimum Relative Cat. Activ.</td>
<td>842.12 ratio</td>
</tr>
<tr>
<td>Activity Time Constant</td>
<td>1263.01</td>
</tr>
<tr>
<td>Replacement Interval</td>
<td>11300.00 hrs</td>
</tr>
<tr>
<td>Reference Temperature</td>
<td>717.00 F</td>
</tr>
<tr>
<td>Actual Temperature</td>
<td>717.00 F</td>
</tr>
<tr>
<td>Dilution Steam/NH3 Ratio</td>
<td>19.00 Ib mole/lb mole</td>
</tr>
<tr>
<td>NH3/NOX Ratio</td>
<td>0.81 Ib mole/lb mole</td>
</tr>
<tr>
<td>Fraction NOX on NH3</td>
<td>0.75</td>
</tr>
<tr>
<td>Reference Replacement Interval</td>
<td>17082.00 hrs</td>
</tr>
<tr>
<td>SO2 Oxidation Rate</td>
<td>0.01 fraction</td>
</tr>
<tr>
<td>SCR Pressure Drop</td>
<td>0.14 psig</td>
</tr>
<tr>
<td>Reference Space Velocity</td>
<td>10000.00 lb/hr</td>
</tr>
<tr>
<td>Calculated Space Velocity</td>
<td>4150.95 lb/hr</td>
</tr>
</tbody>
</table>

### Total Catalyst Layers
- **Initial:** 3
Computer Model Output for One-Stage DSRP Analysis:
Lurgi-based IGCC with One-Stage DSRP

Air-Blown Fixed-Bed Gasifier IGCC w/SCR: Deterministic Analysis

**SYSTEM SUMMARY**

<table>
<thead>
<tr>
<th>Description</th>
<th>Mass Flow (lb/hr)</th>
<th>Temp. (deg F)</th>
<th>Pres. (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HzD Off-Gas</td>
<td>647678.12</td>
<td>1234</td>
<td>305.50</td>
</tr>
<tr>
<td>Coal Gas</td>
<td>3031798.68</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>Slip Stream</td>
<td>136108.52</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>Oxidizer Inlet</td>
<td>783786.64</td>
<td>1228</td>
<td>286.72</td>
</tr>
<tr>
<td>Shift Inlet</td>
<td>783786.64</td>
<td>1347</td>
<td>285.72</td>
</tr>
<tr>
<td>Reactor 1 Inlet</td>
<td>783786.47</td>
<td>1160</td>
<td>284.72</td>
</tr>
<tr>
<td>Condenser 1 Inlet</td>
<td>763091.87</td>
<td>1292</td>
<td>284.72</td>
</tr>
<tr>
<td>Condenser 1 Outlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>Regenerator Inlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>Condenser 2 Inlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>Condenser 2 Outlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td><strong>DSRP TAILGAS</strong></td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td><strong>COMPRESSION</strong></td>
<td>763091.87</td>
<td>360</td>
<td>286.72</td>
</tr>
<tr>
<td><strong>FUEL TO GAS TURB.</strong></td>
<td>3662061.73</td>
<td>801</td>
<td>286.72</td>
</tr>
</tbody>
</table>

**DSRP SULFUR MASS BALANCE (LB/MOLE/HR)**

**INLET SULFUR:**
- SO2 in Off-Gas: 681.86
- H2S in Slip Stream: 0.00
- CO2 in Slip Stream: 0.06
- TOTAL INLET SULFUR: 681.93

**OUTLET SULFUR:**
- Condenser No. 1: 645.42
- Condenser No. 2: 0.00
- H2S in Tailgas: 13.64
- TOTAL OUTLET SULFUR: 677.53

**DSRP SULFUR CAPTURE EFFICIENCY:** 94.65 PERCENT

**TOTAL DSRP GAS STRAINGS**

<table>
<thead>
<tr>
<th>Description</th>
<th>Mass Flow (lb/hr)</th>
<th>Temp. (deg F)</th>
<th>Pres. (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HGD Off-gas</td>
<td>647678.12</td>
<td>1234</td>
<td>305.50</td>
</tr>
<tr>
<td>Coal Gas</td>
<td>3031798.68</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>Coal Gas Slip Stream</td>
<td>136108.52</td>
<td>1206</td>
<td>286.72</td>
</tr>
<tr>
<td>Gas into Cooler</td>
<td>783786.64</td>
<td>1228</td>
<td>286.72</td>
</tr>
<tr>
<td>Gas into Shift</td>
<td>783786.64</td>
<td>1347</td>
<td>285.72</td>
</tr>
<tr>
<td>Reactor 1 Inlet</td>
<td>783786.47</td>
<td>1160</td>
<td>284.72</td>
</tr>
<tr>
<td>Condenser 1 Inlet</td>
<td>763091.87</td>
<td>1292</td>
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<td>Condenser 1 Outlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>Regenerator Inlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td>Condenser 2 Inlet</td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
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<tr>
<td><strong>DSRP TAILGAS</strong></td>
<td>763091.87</td>
<td>350</td>
<td>249.72</td>
</tr>
<tr>
<td><strong>COMPRESSION</strong></td>
<td>763091.87</td>
<td>360</td>
<td>286.72</td>
</tr>
<tr>
<td><strong>FUEL TO GAS TURB.</strong></td>
<td>3662061.73</td>
<td>801</td>
<td>286.72</td>
</tr>
</tbody>
</table>

**ZINC FERRITE SULFUR REMOVAL PROCESS**

RESULTS GENERATED ON JULY 6, 1995 AT 22:19

**SO2 BALANCE (LB/HR)**

- H2S in Rawgas: 23286.81
- H2S in Fuelgas: 48.90
- SO2 in SO2gas: 43682.21

**SO2 FLOW RATE**

- H2S in Rawgas: 0.30E+07 MW = 23.11
- H2S in Fuelgas: 0.30E+07 MW = 23.08
- SO2 in SO2gas: 647678.12 MW = 20.35

**FIRING TEMPERATURE**

1392.2 BTU/LB, 83.0 BTU/SCF

**THERMAL EFFICIENCY (LHV)**

0.4272

**GENERATOR EFFICIENCY**

0.9850

**SUMMARY OF SAMPLED ASPEN FLOW SHEET PERFORMANCE PARAMETERS**

**DSRP GAS STREAMS**

- HGD Off-gas: 647678.12
- Coal Gas: 3031798.68
- Coal Gas Slip Stream: 136108.52
- Gas into Cooler: 783786.64
- Gas into Shift: 783786.64
- Reactor No. 1 Inlet: 763091.87
- Condenser No. 1 Inlet: 763091.87

**SO2 IN OFF-GAS**: 681.86

**SO2 IN SLIP STREAM**: 0.00

**TOTAL INLET SULFUR**: 681.93

**SO2 IN TAILGAS**: 13.64

**TOTAL OUTLET SULFUR**: 677.53

**DSRP SULFUR CAPTURE EFFICIENCY**: 94.65 PERCENT
### PLANT SECTION

<table>
<thead>
<tr>
<th>Flowsheet Performance Parameters</th>
<th>Value Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Feed Mass flow of coal to gasifier</td>
<td>663880.32 lb/hr</td>
</tr>
<tr>
<td>Limestone Feed Mass flow of limestone (mixed)</td>
<td>172.7 lb/hr</td>
</tr>
<tr>
<td>Oxidant Feed Work to boost air compressor</td>
<td>0.16393785 × 10^5 Watts</td>
</tr>
<tr>
<td>Gasifier fines removal</td>
<td>330.39 lb/hr</td>
</tr>
<tr>
<td>Gasifier output syngas density</td>
<td>0.1000 ft/ft^3</td>
</tr>
<tr>
<td>Zinc Ferrite inlet H2S flow</td>
<td>681.86 lb/hr</td>
</tr>
<tr>
<td>HRSG outlet HP steam flow</td>
<td>230.45 lb/hr</td>
</tr>
<tr>
<td>Heat leaving from economizer</td>
<td>13518.33 lb/hr</td>
</tr>
<tr>
<td>Gasifier outlet syngas pres.</td>
<td>1307.50 psia</td>
</tr>
<tr>
<td>Gasifier recycle fines flow rate</td>
<td>4871.50 lb/hr</td>
</tr>
<tr>
<td>SO2 to sulfuric acid plant</td>
<td>325.40 lb/hr</td>
</tr>
<tr>
<td>Zinc ferrite inlet H2S flow</td>
<td>0.00 lb/hr</td>
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<td>Sulfuration</td>
<td>0.10 wt %</td>
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<tr>
<td>Gas turbine inlet air flow</td>
<td>330.39 lb/hr</td>
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<tr>
<td>Steam cycle</td>
<td>0.12 wt %</td>
</tr>
<tr>
<td>Miscellaneouss</td>
<td>0.10 wt %</td>
</tr>
<tr>
<td>SCR</td>
<td>0.12 wt %</td>
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<tr>
<td>Air Blow Lurgi-Based IGCC System with Hot Gas Cleanup</td>
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</tr>
<tr>
<td>Cost Year: January 1989</td>
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</tr>
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<tr>
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<tr>
<td>Gas Turbine Inlet Air Flow: 663880.32 lb/hr</td>
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<tr>
<td>Boiler Feedwater Temperature: 500.00 °F</td>
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<tr>
<td>Boiler Feedwater Pressure: 200.00 psia</td>
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<tr>
<td>Limestone Feed Mass flow of limestone (CaCO3)</td>
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<tr>
<td>Oxidant Feed Work to boost air compressor</td>
<td>0.16393785 × 10^5 Watts</td>
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<td>Gasifier fines removal</td>
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<tr>
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<td>0.1000 ft/ft^3</td>
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<td>SCR</td>
<td>0.12 wt %</td>
</tr>
</tbody>
</table>

### A. KEY INPUT ASSUMPTIONS

**Performance Assumptions:***
- Gasifier Availability: 0.87
- Sorb. Sulfur Loading: 0.168
- Max. Desulf. Vessel Diameter: 12.50 ft
- Superficial Velocity: 2.00 ft/sec
- Indirect Construction Factor: 0.20
- Byproduct Marketing Factor: 0.10
- Project Contingency Factor: 0.17
- General Facilities Factor: 0.20
- Coke, Ash, CO2 from gas turbine: 16.97 m mole/hr
- Sulfuric Acid Plant: 31825.97 lb/hr
- Heating value of coal: 12777.00 BTU/lb
- Average Operating Labor Rate: 19.70
- DCHR Cost Model Version 1.63 Rev. Date: June 24, 1995

**Economic Assumptions:***
- Cost Year: January 1989
- Real Escalation Rate: 0.000
- Plant Book Value: 433000.000
- Inflation Rate: 0.000
- Real Return on Equity: 0.015
- Real Return on Debt: 0.046
- Debt Ratio: 0.500
- Investment Tax Credit: 0.000
- Number of Shifts: 4.25
- Average Operating Labor Rate: 19.70
- Fed. & State Taxes: 0.380
- Years of Construction: 4

**Process Contingency and Maintenance Cost Factors:***
- Plant Section Contingency
- Process Contingency
- Maintenance Cost Factor
- Coal Handling: 0.050
- Limestone Handling: 0.000
- Oxidant Feed: 0.100
- Gasification: 0.200
- Coke, Ash, & Bent. Subsystems: 0.050
- High Temp. Cyclones: 0.050
- Zinc Ferrite: 0.400
- Sulfuric Acid Plant: 0.100
- General Facilities: 0.050
- Boiler Feedwater Treatment: 0.000
- Gas Turbine: 0.250
- Heat Recovery Steam Generator: 0.025
- Direct Sulfur Recovery Process: 0.250
- Selective Catalytic Reduction: 0.100
- Gas Turbine: 0.250
- General Facilities: 0.050

**COST SUMMARY:**

- Air Blow Lurgi-Based IGCC System with Hot Gas Cleanup
- Cost Model Version 1.63 Rev. Date: June 24, 1995
- Gas Turbine: 0.250
- Oxidant Feed: 0.100
- Gasification: 0.200
- Coke, Ash, & Bent. Subsystems: 0.050
- High Temp. Cyclones: 0.050
- Zinc Ferrite: 0.400
- Sulfuric Acid Plant: 0.100
- General Facilities: 0.050
- Boiler Feedwater Treatment: 0.000
- Gas Turbine: 0.250
- Heat Recovery Steam Generator: 0.025
- Direct Sulfur Recovery Process: 0.250
- Selective Catalytic Reduction: 0.100
- Gas Turbine: 0.250
- General Facilities: 0.050
- B. CALCULATED DIRECT CAPITAL AND PROCESS CONTINUITY COSTS ($1,000) ---

**Plant Section**

<table>
<thead>
<tr>
<th>Number of Units</th>
<th>Direct Process</th>
<th>Operating Total Capital Cost</th>
<th>Contingency</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

---

COST VAR WARNING --- Variable MCFG1 value of 663880.324
Coal Handling: 1 1 1 2474.3 1692.
Limestone Handling: 0 0 0 5284.2 752.
Oxidant Feed: 1 1 1 5284.2 752.
Classification: 13 15 1 99270. 27147.
Coke, Ash, & Bent. Subsystems: 13 15 1 18716. 12600.
High Temp. Cyclones: 26 30 1 7406. 504.
Zinc Ferrite: 13 30 1 14484. 7922.
Sulfuric Acid Plant: 1 1 1 0. 0.
Sulfation: 0 0 0 0. 0.
Boiler Feedwater Treatment: 1 1 1 6727. 0.
Gas Turbine: 3 3 1 36000. 32816.
Heat Recovery Steam Generator: 2 2 1 13559. 1145.
Selective Catalytic Reduction: 3 3 1 10337. 1413.
Steam Turbine: 3 3 1 38630. 1321.
General Facilities: N/A N/A 74000. 5059.

C. CALCULATED TOTAL CAPITAL REQUIREMENT ($1,000) --------- Capital Cost

Description: Capital Cost
Total Direct Cost: 443998.
Direct Construction Cost: 88600.
Sales Tax: 16204.
Engineering and Home Office Fees: 55100.
Environmental Permitting: 10000.
Total Indirect Costs: 163104.
Total Process Contingencies: 86415.
Project Contingency: 123113.
Total Plant Cost: 814529.
AFDC: 130528.
Total Plant Investment: 945058.
Preproduction (Startup) Costs: 26787.
N/A: 88600.
Initial Catalysts and Chemicals: 41812.
Land: 5059.
TOTAL CAPITAL REQUIREMENT ($1,000) --------> 1050991.

D. CALCULATED FIXED OPERATING COSTS ($/year) ----------- Annual Cost

Description: Annual Cost
Operating Labor: 646944.
Maintenance Costs: 1717410.
Administration and Supervision: 4829942.
TOTAL FIXED OPERATING COST ($/year) --------> 31234697.

E. CALCULATED VARIABLE OPERATING COSTS

1. CONSUMABLES ($/year) ----------------------------------------

Description: Assumed Calc. Material Calc. Annual Operating Cost
Sulfuric Acid: 110.00 $/ton 2866.7 ton/yr 315340.
NaOH: 220.00 $/ton 592.7 ton/yr 130401.
Na2SO4: 0.70 $/lb 3534.5 lb/yr 2474.
Hydrazine: 1.20 $/lb 17019.9 lb/yr 54664.
Morpholine: 1.30 $/lb 15894.8 lb/yr 20463.
Lime: 8.00 $/ton 699.5 ton/yr 55961.
Soda Ash: 160.00 $/ton 771.5 ton/yr 123444.
Corrosion Inh.: 1.50 $/lb 139553.2 lb/yr 265151.
Sulfuric Acid: 1.25 $/lb 139553.2 lb/yr 174442.
Chlorine: 250.00 $/ton 21.4 ton/yr 5351.
Biocide: 3.60 $/lb 27360.8 lb/yr 95539.
DEHP Catalyst: 12.28 $/lb 43034.4 lb/yr 52849.
SCHR Catalyst: 250.00 $/ft³ 6250.5 ft³/day 1562635.
Ammonia: 150.00 $/ton 17214.3 ton/yr 2582182.
Zinc: 30.00 $/ton 345959.6 1 lb/yr 1048799.
Limestone: 18.00 $/ton 6.0 ton/yr 0.
Sul Acid Cat.: 1.90 $/fly 3508.6 lb/hr 66516.
Coke: 15.00 $/ton 1875.1 ton/yr 291209.
Hentolite: 0.03 $/lb 5404647.7 lb/yr 156735.
Fuel Oil: 42.00 $/lb 48098.7 lb/yr 2020833.
Plant Air Ads.: 2.80 $/lb 3621.6 lb/hr 20540.
Raw Water: 0.73 $/Kgal 1006185.9 Kgal/yr 734662.

Waste Water: 840.00 $/gpm WW 0.0 lb/hr 0.
LIQ. Flare: 11.70 $/gal 4225.2 bbl/yr 49435.
TOTAL CONSUMABLES ($/year) --------> 19721288.

2. FUEL, ASH DISPOSAL, AND BYPRODUCT CREDIT ($/year)

Coal: 1.61 S/MMBtu 66380.3 lb/hr 3122600.
Ash Disposal: 10.00 $/ton 8363.1 ton/day 7742777.
Sulfuric Acid: 40.00 $/ton 0.0 ton/yr 0.
Sulfur: 125.00 $/ton 58917.5 ton/yr 6628217.

TOTAL VARIABLE OPERATING COST ($/year) --------> 9281998.

F. CALCULATED COST OF ELECTRICITY

Power Summary (MWh) Auxiliary Loads (MWh)

Description: Annual Cost
Gas Turbine Output: 641.25 Coal Handling: 1.25 Sulfation: 0.00
Steam Turbine Output: 243.41 Limestone Hdlg: 0.00 EHRP: 1.09
Total Auxiliary Loads: 33.44 Oxidant Feed: 16.39 Steam Cycle: 5.23
G. ENVIRONMENTAL SUMMARY

Fuel, Ash Disposal: 10.00 $/ton 0.0 ton/yr

Incremental Variable Costs: 4.48 mills/kWh
Byproduct Credit: 1.37 mills/kWh
Fuel Cost: 16.04 mills/kWh
Variable Operating Cost: 19.15 mills/kWh

COST OF ELECTRICITY --------> 48.01 mills/kWh
Fixed Charge Factor: 0.1034 Variable Cost Levelization Factor: 1.0000

The plant heatrate (HHV) is: 8773. BTU/kWh. Efficiency: 0.3893
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
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<td>Initial Catalyst Volume</td>
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<td>Total Catalyst Volume</td>
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<td>Ammonia Flow, tons/yr</td>
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<tr>
<td>J. DSRP SUMMARY</td>
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<tr>
<td>Stage 1 Space Velocity</td>
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<tr>
<td>Sulfur Hyproduct</td>
<td>58917.49 tons/year</td>
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Computer Model Output for Two-Stage DSRP Analysis:
Lurgi-based IGCC with Two-Stage DSRP

Air-Blown Fixed-Bed Gasifier IGCC w/SCR: Deterministic Analysis

** SYSTEM SUMMARY **

** GASIFIER CONDITIONS- **

- COAL FLOW RATE: 0.653009E+06 LB/HR
- SORBENT FLOW RATE: 0.568698E+00 LB/HR
- AIR FLOW RATE: 0.160327E+07 LB/HR
- REQUIRED STEAM: 0.801634E+06 LB/HR
- SUPPLIED STEAM: 0.999993E-06 LB/HR
- ABF FLOW RATE: 0.160327E+07 LB/HR
- GASIFIER TEMPERATURE: 1100.0 F

** SO2 BALANCE (LB/HR) **

- H2S IN OFF-GAS: 22905.91
- H2S IN FUELGAS: 48.10
- SO2 IN S02GAS: 42967.71

** FUEL LHV (WET BASIS) **

- 1391.2 BTU/LB, 82.9 BTU/SCF
- 1562.0 BTU/LB, 92.6 BTU/SCF

** SULFUR CAPTURE EFFICIENCY **

- 0.998

** DIRECT SULFUR RECOVERY PROCESS **

- STEAM REQUIRED TO MAINTAIN
  - CO/CO2 RATIO (SHFT-STM ): 1.00
- RATIO OF INLET AIR TO EXHAUST GAS: 0.824
- RATIO OF BOOST AIR TO INLET AIR: 0.200
- RATIO OF GASIF AIR TO INLET AIR: 0.182
- RATIO OF REGEN AIR TO INLET AIR: 0.018
- RATIO OF FUEL GAS TO INLET AIR: 0.410
- CO2 EMISSIONS: 194.2 LB/MMBTU
- CO EMISSIONS: 0.30849 LB/MMBTU
- CO EMISSIONS: 201.56 ppmv
- SO2 EMISSIONS: 0.06098 LB/MMBTU
- NOX EMISSIONS: 0.54114 LB/MMBTU
- NOX EMISSIONS: 220.56 ppmv
- Oxygen in Exhaust: 6.6749 percent
- Vapor in Exhaust: 25.6962 percent
- CO2 in Exhaust: 8.2744 percent

** STEAM TURBINE CONDITIONS **

- STEAM DIVERTED TO GASIFIER: 0.801634E+06 LB/HR
- STEAM DIVERTED TO ZINC FER: 0.475114E+06 LB/HR
- STEAM TURBINE FLOW RATE: 0.224309E+07 LB/HR
- SUPERHEATED STEAM TEMPERATURE: 1000.0 F
- EXPANDED STEAM QUALITY: 0.92777
- ISOTHERMAL EFFICIENCY: 0.9000
- GENERATOR EFFICIENCY: 0.9850

** SUMMARY OF SAMPLED ASPEN FLOWSHEET PERFORMANCE PARAMETERS **

- PLANT SECTION: FLOWSHEET PERFORMANCE PARAMETERS
- VALUE UNITS

<table>
<thead>
<tr>
<th>Description</th>
<th>Mass Flow (lb/hr)</th>
<th>Temp. (deg F)</th>
<th>Pres. (psia)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HGD OFF-GAS</td>
<td>637315.78</td>
<td>1233</td>
<td>305.50</td>
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<tr>
<td>COAL GAS</td>
<td>2285200.85</td>
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<td>286.72</td>
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<td>SLIP STREAM</td>
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<td>COOLER INLET</td>
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<td>SHIFT INLET</td>
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<td>REACTOR 1 INLET</td>
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<td>284.72</td>
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<td>REHEATER INLET</td>
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<td>REACTOR 2 INLET</td>
<td>749874.02</td>
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<td>Value</td>
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<td>----------------------------------</td>
<td>--------</td>
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<tr>
<td>Coal Feed</td>
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<td>Mass flow of coal to gasifier</td>
<td>2.11059.87 lb/hr</td>
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<tr>
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<td></td>
<td>Mass flow of limestone (mixed)</td>
<td>0.00 lb/hr</td>
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<td>Mass flow of limestone (cisol)</td>
<td>0.57 lb/hr</td>
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<tr>
<td>Oxidant Feed</td>
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<td>Work to boost air compressor</td>
<td>0.16125500 Wtts</td>
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<td></td>
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<td>First precompressor inlet air temp.</td>
<td>750.33 F</td>
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<td>First precompressor outlet air temp.</td>
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<td>First precompressor inlet BPM temp.</td>
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<td>First precompressor outlet BPM temp.</td>
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<td>Heat transfer in first precompressor</td>
<td>0.32180768 Mtu/hr</td>
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<td>Heat trans. to BW from HRSG</td>
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<td>Heat trans. to BW from Regen.</td>
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<td>Heat leaving from economizer</td>
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<td>Gasification</td>
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<td>Gasifier output syngas pres.</td>
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<td>Gasifier output syngas temp.</td>
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<td>Gasifier output syngas density</td>
<td>0.18307689 lmole/ft^3</td>
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<td>Gasifier recycle fines flow rate</td>
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<td>Zinc Ferrite</td>
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<td>Zinc Ferrite inlet syngas flow</td>
<td>12936.78 lb/hr</td>
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<td>Off-gas to sulfuric acid plant</td>
<td>31318.26 lb/hr</td>
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<td>Sulfation to sulfuric acid plant</td>
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<td>Off-gas to sul. acid plant</td>
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<td>Zinc ferrite inlet H2S flow</td>
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<td>Zinc ferrite inlet CO2 flow</td>
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<td>Sulfation</td>
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<td>Gasifier ash removal</td>
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<td>Gasifier fines removal</td>
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<td>BFW Treatment Rain water to power plant</td>
<td>34496.28 lb/hr</td>
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<td>Steam turbine condensate</td>
<td>8543.66 lb/hr</td>
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<td>Gas turbine inlet air flow</td>
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<td>Steam turbine condensate</td>
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<td>HSGG outlet HP steam flow</td>
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<td>Steam turbine net shaft work</td>
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<td>Acid gas auxiliary power</td>
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<td>Moisture in coal feed</td>
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<td>Ash in coal</td>
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<td>Temp. of ambient air</td>
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<td>Heating value of coal</td>
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<td>DSRP Compressor Work</td>
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<td>DSRP Sulfur Product</td>
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<td>DSRP Gas Cooler Inlet</td>
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<td>DSRP Reactor 1 Inlet</td>
<td>5748.59 Wttes</td>
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<td>DSRP Condenser 1 Inlet</td>
<td>5748.59 Wttes</td>
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<td>DSRP Reheater Inlet</td>
<td>5748.59 Wttes</td>
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<td>DSRP Reactor 2 Inlet Handling</td>
<td>5748.59 Wttes</td>
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<td>DSRP Condenser 2 Inlet</td>
<td>5748.59 Wttes</td>
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<td>DSRP Compressor Work</td>
<td>0.29829397 Wtts</td>
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<td>DSRP Reactor 2 Inlet Pressure</td>
<td>284.20 lb/hr</td>
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<td>SCR Inlet Gas Flow</td>
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<td>SCR Inlet Gas Temperature</td>
<td>717.00 lb/hr</td>
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<td>SCR Inlet Gas Pressure</td>
<td>15.33 lb/hr</td>
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<td>SCR Inlet NO loading</td>
<td>410.47 lb/hr</td>
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<td>SCR Inlet NO2 loading</td>
<td>21.60 lb/hr</td>
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<td>SCR Ammonia Requirement</td>
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<td>SCR Dilution Steam Requirement</td>
<td>6641.96 lb/hr</td>
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<td>SCR High Pressure Blowdown</td>
<td>45778.19 lb/hr</td>
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<td>Low Pressure Blowdown</td>
<td>45778.19 lb/hr</td>
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<td>CO from gas turbine</td>
<td>23419.12 lb/hr</td>
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<td>CO from gas turbine</td>
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<td>CO2 from gas turbine</td>
<td>7.00 lb/hr</td>
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<td></td>
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<td>CH4 from gas turbine</td>
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<td>H2S from gas turbine</td>
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<td>H2 to gas turbine</td>
<td>461.56 lb/hr</td>
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<td>NO from gas turbine</td>
<td>82.69 lb/hr</td>
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<td>NO2 from gas turbine</td>
<td>4.32 lb/hr</td>
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<td>Actual coal heating value</td>
<td>0.11246772 Mtu/lb</td>
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<td>COST VAR WARNING - Variable MCGI value of</td>
<td>653019.868 in DCB above the upper limit of</td>
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<td>COST VAR WARNING - Variable VSNZP1 value of</td>
<td>9059.221 in DCB above the upper limit of</td>
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</table>

A. KEY INPUT ASSUMPTIONS

Cost Model Version 1.63 Rev. Date: June 24, 1995

B. CALCULATED DIRECT CAPITAL AND PROCESS CONTINGENCY COSTS ($1,000)

<table>
<thead>
<tr>
<th>Section</th>
<th>Number of Units</th>
<th>Direct Cost</th>
<th>Process Contingency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal Handling</td>
<td>1</td>
<td>24522.00</td>
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<tr>
<td>Limestone Handling</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>Oxidant Feed</td>
<td>3</td>
<td>5240.00</td>
<td>717.00</td>
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<tr>
<td>Gasification</td>
<td>13</td>
<td>99270.00</td>
<td>27147.00</td>
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<tr>
<td>Coke, Ash, &amp; Bent. Subsystems</td>
<td>13</td>
<td>18391.00</td>
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<tr>
<td>High Temp. Cyclones</td>
<td>26</td>
<td>7353.00</td>
<td>503.00</td>
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</table>
C. CALCULATED TOTAL CAPITAL REQUIREMENT ($1,000)

D. CALCULATED FIXED OPERATING COST ($/year)

Direct Sulfur Recovery Process 22 2350. 8033.
Heat Recovery Steam Generator 33 33484. 1145.
Selective Catalytic Reduction 2 25300. 8033.
Steam Turbine 1 1 37227. 1273.
General Facilities N/A N/A 76254. 5145.

TOTAL CAPITAL REQUIREMENT ($1,000) ———— 1069951.

TOTAL FIXED OPERATING COST ($/year) ———— 31392437.

E. CALCULATED VARIABLE OPERATING COSTS

1. CONSUMABLES ($/year)

- Description
- Assumed
- Calc. Material Requirement
- Calc. Annual Operating Cost

- Sulfuric Acid: 110.00 $/ton 2818.9 lb/yr 310065.
- NaOH: 220.00 $/ton 581.6 lb/yr 127953.
- Na2HPO4: 0.70 $/lb 3476.3 lb/yr 2433.
- Morpholine: 1.30 $/lb 15631.8 lb/yr 20321.
- Lime: 33.00 $/ton 668.0 lb/yr 55563.
- Soda Ash: 60.00 $/ton 1.75 lb/yr 1241675.
- Corrosion Inh.: 1.90 $/lb 137224.3 lb/yr 260726.
- Surfactant: 1.25 $/lb 137224.3 lb/yr 1713709.
- Chlorine: 225.00 $/ton 21.1 lb/yr 47279.
- Biocide: 3.60 $/lb 23427.0 lb/yr 84319.
- DEHP Catalyst: 12.28 $/lb 835635. 1013072.
- SCR Catalyst: 220.00 $/ft3 6219.9 ft3/yr 1556897.
- Ammonia: 150.00 $/ton 16494.9 ton/yr 2542152.
- Zinc Fer Sorb: 3.00 $/lb 348812.7 lb/yr 10316346.
- Sul Acid. Cat.: 1.90 $/l 34500.2 1.00 y/r 2509500.
- Coke: 150.00 $/ton 1845.8 ton/yr 2618785.
- Boric Acid: 0.03 $/lb 531823.8 lb/yr 1351701.
- Fuel Oil: 42.00 $/bbl 47535.0 bbl/yr 1996470.
- Plant Air Ads.: 2.00 $/lb 19565.1 lb/yr 99692.
- Raw Water: 0.73 $/gal 98944.4 gal/yr 72229.
- Waste Water: 840.00 $/gpm w 4193.3 lb/hr 48684.

TOTAL CONSUMABLES ($/year) ———— 19931464.

2. FUEL, ASH DISPOSAL, AND HYDROPRODUCT CREDIT ($/year)

Coal: 1.61 $/MMBtu 653019.9 lb/hr 76470978.
<table>
<thead>
<tr>
<th>J. DSRP SUMMARY</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stage 1 Space Velocity</td>
<td>5000.00 scc/(cc-h)</td>
</tr>
<tr>
<td>Stage 2 Space Velocity</td>
<td>5000.00 scc/(cc-h)</td>
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<td>USRP Work, MW</td>
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<tr>
<td>Number of total trains</td>
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<tr>
<td>Number of oper. trains</td>
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<tr>
<td>Rxr 1 Inlet Volume Flow Rate</td>
<td>2268228.8773 ft^3/hr</td>
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<tr>
<td>Rxr 1 Inlet Temperature</td>
<td>1161.29°F</td>
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<tr>
<td>Rxr 1 Inlet Pressure</td>
<td>284.72 psia</td>
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<td>Cost Index</td>
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<td>Pressure Correction Factor</td>
<td>0.84 $1,000</td>
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<td>Rxr 2 Inlet Volume Flow Rate</td>
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<td>Rxr 2 Inlet Pressure</td>
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<td>Pressure Correction Factor</td>
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<td>Heat Duty: Precooler</td>
<td>0.2822558E+08 BTU/hr</td>
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<td>Heat Duty: Condenser 1</td>
<td>0.631346E+09 BTU/hr</td>
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<td>Heat Duty: Reheater</td>
<td>-0.372399E+09 BTU/hr</td>
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<td>Direct Cost, gas handling 1</td>
<td>14331.69 $1,000</td>
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<tr>
<td>Direct Cost, gas handling 2</td>
<td>8236.84 $1,000</td>
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<td>Direct Cost, sulfur hand, 1</td>
<td>372.52 $1,000</td>
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<td>Direct Cost, sulfur hand, 2</td>
<td>558.77 $1,000</td>
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<td>Direct Cost, total</td>
<td>23499.82 $1,000</td>
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<td>Total Initial Catalyst</td>
<td>251890.49 lb</td>
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<tr>
<td>Annual Catalyst</td>
<td>83963.50 lb/yr</td>
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<tr>
<td>Sulfur Byproduct</td>
<td>60710.01 tons/year</td>
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This cover stock is 30% post-consumer waste and 30% pre-consumer waste, and is recyclable.