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Development and Evaluation of a Process to Produce Hydrogen from Coal

T.E. Colson* and S. Lynn

*(M.S. Thesis)

August 1989

APPLIED SCIENCE
DIVISION

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DEVELOPMENT AND EVALUATION OF A PROCESS TO PRODUCE HYDROGEN FROM COAL

by

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August 1989

This work was supported by the Morgantown Energy Technology Center, Assistant Secretary for Fossil Energy, Office of Coal Utilization, Advanced Research and Technology Development, Division of Surface Coal Gasification through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Acknowledgements

At the conclusion of my seven (?) years at Berkeley, I look back on many memorable experiences shared with some great friends. I can now claim two degrees from U.C. Berkeley, but the people I've become close to will always be foremost in my mind when I think of these years.

First, I would like to thank Professor Scott Lynn for his guidance and support over the years. His willingness to take me on as an inexperienced undergraduate and the fair hand that governed all my dealings with him were much appreciated. It was the opportunity to work with someone with his knowledge, insight and patience that led me to remain at Berkeley for my graduate work.

To Kay Ekman and Ferne Kasarda go my heartfelt thanks for their friendship and for making the university bureaucracy sit up and wag its tail. Without their help (and the endless supply of suggestions for great books to read), my Berkeley career would have been much less fun and infinitely more frustrating.

I want to thank my past and present lab mates, all members of that august body The Right and Noble Order of the Fez, 205 Gilman Lodge, for their help in keeping me sane and happy. Without the aid of Dan Neumann, I think I would still be tangled in a morass of computer code. I want to thank Craig Stevens and Jim Russell for the number of times they ran me ragged on the Frisbee field (I think). Thanks to Marshall Hix for making many a lunch break fun with stories of the sea and ships and those who sail them, not to mention the game nights that went all till all hours. And my thanks to Dannes Hutapea who showed me that those wretched Macintosh things aren't that bad after all. And finally, many thanks to Steve Sciamanna, Fez Brother Emeritus, who showed me that real nuts-and-bolts engineering really is compatible with all those fancy equations.

During my entire college career, one person has been responsible for keeping my spirits up and my efforts on track. Without the support and enthusiasm of my best friend and companion Tristan, I could never have made it this far. The credit for any success I've had is in a large part hers.

Finally, I wish to thank my parents for their efforts to help me in all I've done. Their willingness to give their all when needed and to let me make my own mistakes are responsible for making me the person I am today. Without them my life would be much poorer.

This work was supported by the Morgantown Energy Technology Center, Assistant Secretary for Fossil Energy, Office of Coal Utilization, Advanced Research and Technology Development, Division of Surface Coal Gasification, through the Department of Energy under contract DE AC03 76SF00098.

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Chapter 1 INTRODUCTION

1.1 Background

Hydrogen has been an important raw material for chemicals production and petroleum refinery processes since the early part of this century. Traditional methods of hydrogen production rely on carbonaceous fuels such as petroleum and natural gas as raw materials. In the future these are likely to become increasingly expensive and in short supply. In addition, an increasing fraction of these raw materials are imported, increasing the dependence of the domestic chemical and petroleum industries on foreign sources. Coal is an alternative source of carbonaceous raw materials for hydrogen manufacture. Domestic coal reserves are abundant and contain enough energy to satisfy domestic needs for centuries. This thesis is a study of a proposed process to produce hydrogen from coal via coal gasification and the water-gas shift (WGS) reaction. A novel aspect of the process is the use of the U. C. Berkeley Sulfur Recovery Process (UCBSRP) for removal of CO_2 and H_2S from the gasified coal (Neumann 1986 and Sciamanna 1986). The CO_2 is recovered as a purified product and the H_2S is recovered as elemental sulfur.

1.2 Uses Of Hydrogen

The largest industrial uses of hydrogen are in petroleum refining, ammonia synthesis, methanol synthesis, metals manufacture, and food processing. Hydrogen is used in a variety of petroleum refinery processes, such as hydrocracking of heavy hydrocarbons and hydrodesulfurization. To manufacture synthetic ammonia, hydrogen is catalytically reacted with nitrogen under very high pressure. Synthetic methanol is formed by the reaction of hydrogen with carbon monoxide. In metals manufacture, hydrogen is used primarily to reduce ores and in metals treatment. Hydrogen in the foods industry is used primarily to hydrogenate unsaturated oils.

Because most hydrogen for refinery and synthetic uses is produced captively, it is difficult to estimate the total market. It is estimated that merchant hydrogen accounts for 10% or less of total hydrogen production. In 1985, merchant hydrogen production was about 280 million kg (4.9 x 10^{12} ft^3) (C. & E. News, 1985).

1.3 Current Hydrogen Production Technology

Most hydrogen is produced via steam reforming of light hydrocarbons. In addition, some hydrogen is produced by partial oxidation of heavy hydrocarbons and a very small fraction by coal gasification. For a detailed review of process routes for hydrogen manufacture, see Supp and Jockel, 1975.

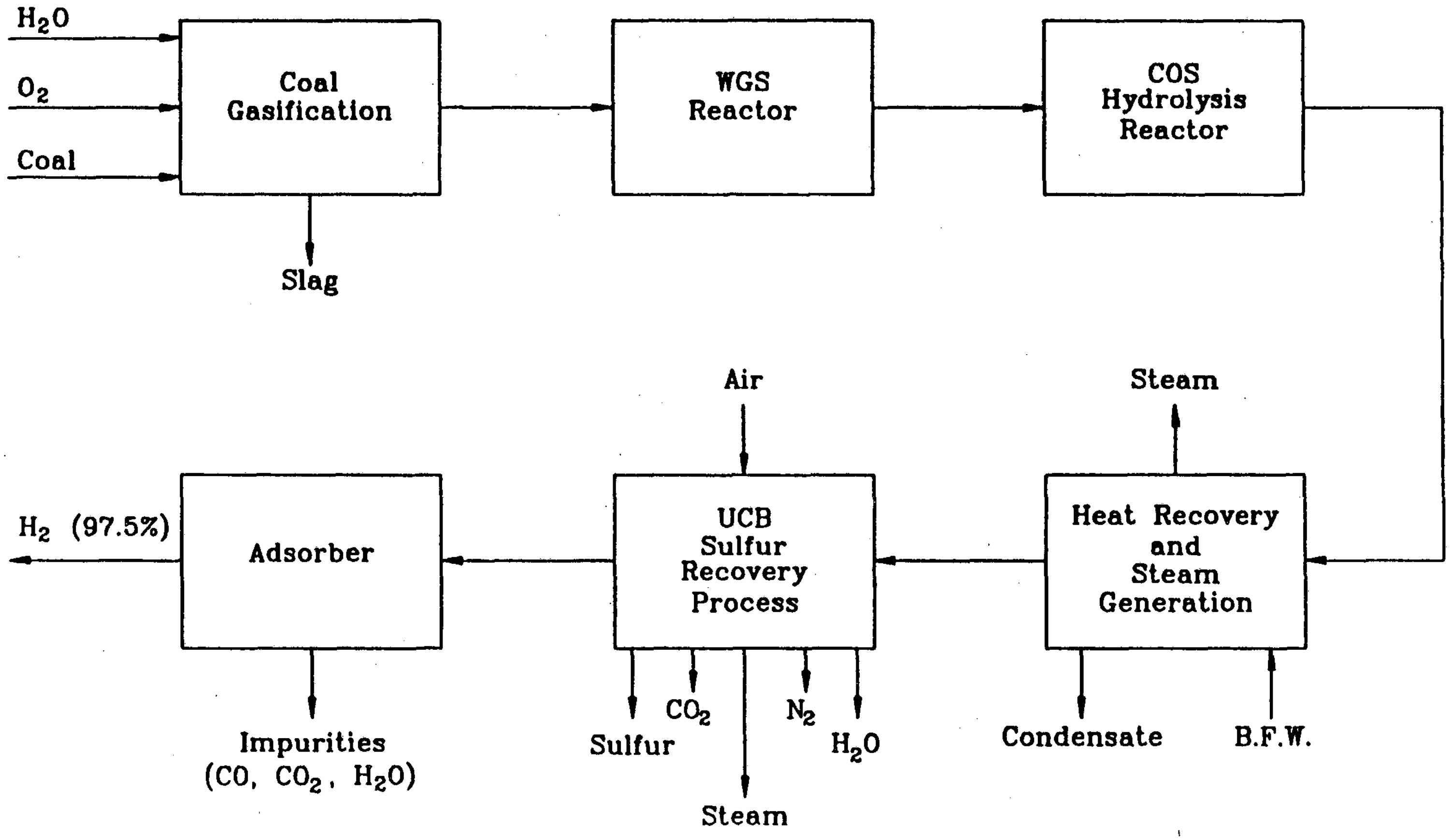
1.4 Proposed Process

Figure 1.1 shows a block flow diagram of the proposed process. The first step in the process is coal gasification. Following gasification, the hot gas is quenched by direct contact with water to cool the gas, saturate it with water and remove particulates, HCl and NH_3. The quenched gas is then heated to about 50^oF above its dew point and fed to the WGS reactor step. In this step, most of the CO in the gas is reacted with H_2O to form H_2 and CO_2. In addition, this reactor also converts some of the COS in the gas to H_2S via hydrolysis. After WGS, the gas is fed to a COS hydrolysis reactor to convert the remaining COS. The gas is then cooled and the recovered heat used to generate steam. The cooled gas is sent to the UCBSRP where H_2S and CO_2 are recovered as elemental sulfur and a purified (99+%) CO_2 stream. The sulfur-free gas is then sent to a fixed bed adsorber system to remove water, unreacted CO and any CO_2 not recovered in the UCBSRP step. The products from the adsorber system are a purified (97.5%) H_2 stream (major impurities: Ar and N_2), and an impurity stream containing H_2O, CO and CO_2.

1.5 Scope of Thesis Work

This study has a two-fold purpose: to demonstrate through computer simulation and traditional order-of-magnitude process design calculations that the proposed process is technically feasible, and to examine the economic feasibility of the proposed process.

Figure 1.1
Block Flow Diagram for Hydrogen Process


H_2O
O_2
Coal
Coal Gasification
Slag
WGS Reactor
COS Hydrolysis Reactor
Steam
Air
H_2 (97.5%)
Adsorber
UCB Sulfur Recovery Process
Heat Recovery and Steam Generation
Impurities (CO, CO_2, H_2O)
Sulfur
CO_2
Steam
N_2
H_2O
Condensate
B.F.W.

Chapter 2 PROCESS DEVELOPMENT

2.1 Design Basis and Problem Specification

2.1.1 Plant Size

The basis of the hydrogen plant design is the gasification of 910,000 kg/day (1000 ton/day) of Illinois #6 bituminous coal. Coal gasification at the above rate will produce 123,000 kg/day (136 ton/day) of H_2 (pure H_2 basis). This is equivalent to 49 MMSCFD of pure hydrogen (standard state 1 atm. and $70^{o}F$) or 12,200 MMBTUD (HHV). Production capacity for hydrogen plants such as those that supply the petroleum refining industry are in the range of 110,000 to 220,000 kg/day (120 to 240 ton/day) of hydrogen.

2.1.2 Hydrogen Product Specifications

Minimum hydrogen product purity for the design is 95%. Industrial hydrogen feedstocks range in purity from 90 to 99.99+% H_2. The hydrogen purity requirements and types of tolerable impurities vary greatly with the industrial application. For the design, the product is required to be free, to part-per-million (ppm) levels, of carbon oxides and water and, to sub-ppm levels, of sulfur compounds.

2.1.5 Carbon Dioxide Product Specifications

Minimum carbon dioxide purity for the design is 99% (dry basis). The carbon dioxide product is to contain less than one ppm sulfur compounds. The CO_2 is produced at 2500 kPa (360 psia).

2.1.4 Environmental Standards

Flue gases and waste-water streams are treated before discharge. These streams contain less than one ppm sulfur compounds and the gas streams are particulate-free.

2.2 Process Description

Figure 2.1 shows a block flow diagram of the hydrogen process. Compositions, temperatures and pressures for the process streams are given in Table 2.1. A detailed description of the process follows.

2.2.1 Coal Gasification

The first step in the hydrogen process is coal gasification. The gasifier chosen for use in this study was the Texaco oxygen-blown gasifier running in the total quench configuration. The Texaco gasifier is a high-pressure, entrained-flow gasifier. The coal feed is ground to about 200 mesh (74 micron) and slurried with water to yield a pumpable mixture of about 65 weight percent solids. The slurry is entrained in the oxidant feed and fed to the gasifier. The oxidant feed is supplied at high pressure from a cryogenic air separation plant. Oxidant purity is 95%, with argon (3.65%) and nitrogen (1.35%) as the major impurities. The gasifier outlet temperature is about 1600 K (2400 ^{o}F). At this temperature the mineral content of the coal is converted to a molten slag rather than ash. The gasifier effluent is quenched by direct contact with water to cool the gas to about 494 K (430 ^{o}F), saturate it with water, and remove fine particulates, HCl and NH_3. The molten slag is removed, dewatered, and sent to landfill.

The Texaco oxygen-blown gasifier was chosen for use in this study because of the large amount of detailed technical information available about the design and cost of the system (EPRI, 1984). In addition, the Texaco gasifier total quench configuration provides a high water content in the effluent gas, which can be used to drive the reaction equilibrium in the water-gas-shift (WGS) reaction as described below.

2.2.2 Water Gas Shift Reactor System

In order to enrich the gasifier effluent in hydrogen, the gas is fed to a water gas shift (WGS) reactor system where the following reaction occurs:

Figure 2.1
Process Flow Diagram for Hydrogen Process

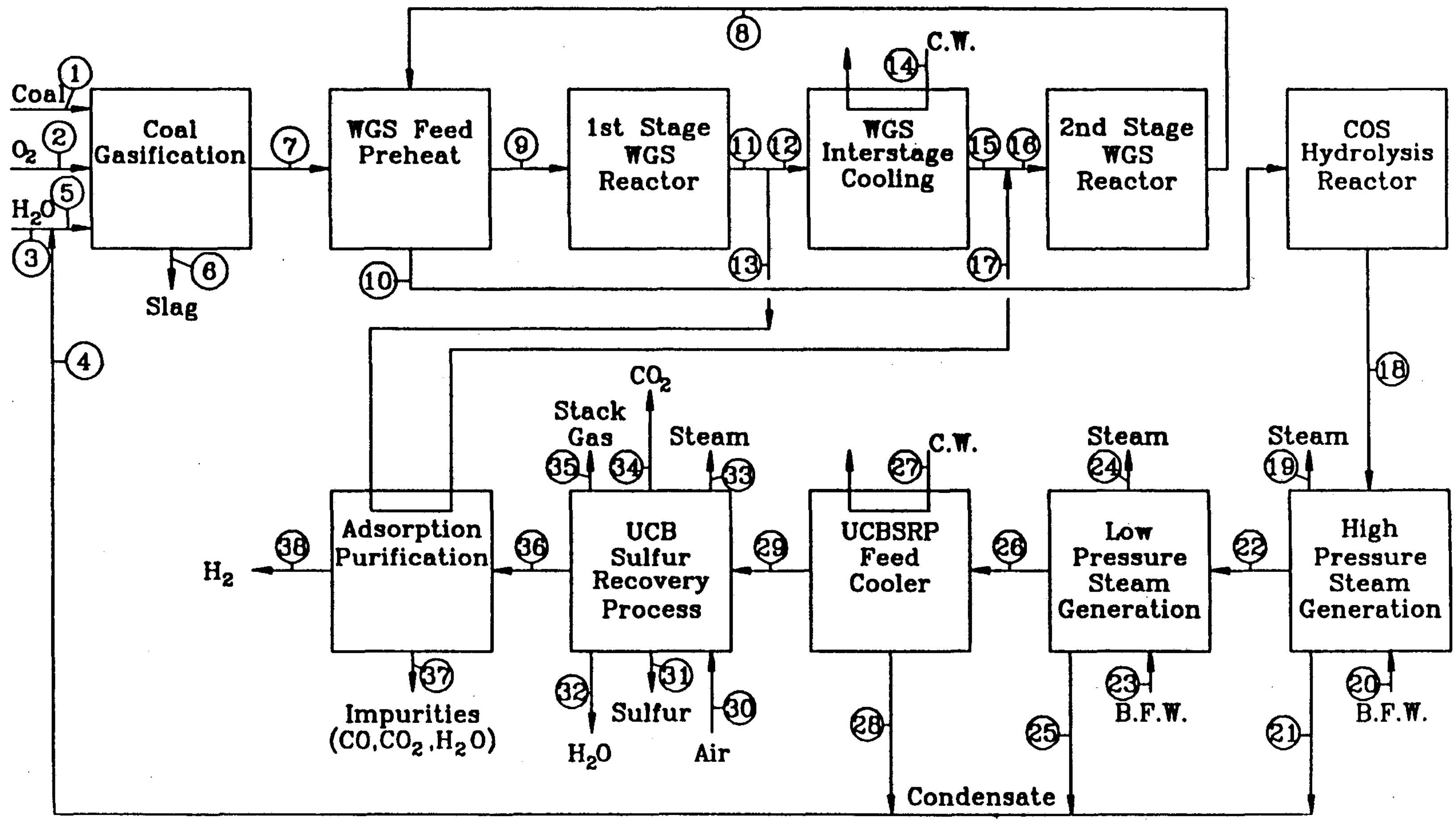

Coal
①
O_2
②
H_2O
⑤
③
④
Coal Gasification
⑥
Slag
⑦
WGS Feed Preheat
⑧
⑨
⑩
1st Stage WGS Reactor
⑪
⑫
⑬
WGS Interstage Cooling
⑭
C.W.
⑮
⑯
⑰
2nd Stage WGS Reactor
COS Hydrolysis Reactor
⑱
Steam
⑲
High Pressure Steam Generation
⑳
B.F.W.
㉑
㉒
Steam
㉔
Low Pressure Steam Generation
㉓
B.F.W.
㉕
㉖
C.W.
㉗
UCBSRP Feed Cooler
㉘
Condensate
㉙
CO2
Stack Gas
㉟
㉞
Steam
㉝
UCB Sulfur Recovery Process
㉜
H_2O
㉛
Sulfur
㉚
Air
㊱
Adsorption Purification
㊲
Impurities (CO, CO_2, H_2O)
㊳
H_2

Table 2.1
Stream Flows and Conditions for Hydrogen Process

Stream:	1	2	3	4	5	6	7	8	9	10	11
H2 (kmol/hr)	-	.	.	.	.	.	1,144.8	2,607.7	1,144.8	2,607.7	2,439.2
CO "	-	.	.	.	.	.	1,494.0	32.0	1,494.0	32.0	200.5
CO2 "	-	.	.	.	.	.	414.0	1,875.7	414.0	1,875.7	1,707.2
CH4 "	-	.	.	.	.	.	3.0	3.0	3.0	3.0	3.0
H2S "	-	.	.	.	.	.	41.0	41.2	41.0	41.2	41.2
COS "	-	.	.	.	.	.	2.3	2.3	2.3	2.3	2.3
N2 "	-	12.7	.	.	.	.	27.5	27.4	27.5	27.4	27.4
Ar "	-	34.5	.	.	.	.	35.1	35.1	35.1	35.1	35.1
H2O "	-	.	2,570.0	2,994.0	5,564.0	1,840 kg/hr	4,464.0	3,000.4	4,464.0	3,000.4	3,168.9
O2 "	-	897.0	.	.	.	.	.	.	.	.	.
Sulfur "	-	.	.	.	.	.	.	.	.	.	.
Coal (kg/hr)	37,800 kg/hr	.	.	.	.	.	.	.	.	.	.
Slag "	-	.	.	.	.	3,550 kg/hr	.	.	.	.	.
Flow (kmol/hr)	37,800 kg/hr	944.0	2,570.0	2,994.0	5,564.0	5,390 kg/hr	7,624.8	7,624.8	7,624.8	7,624.8	7,624.8
Temperature (K)	298	406	450	417	432	450	492	544	520	492	701
Pressure (kPa)	101	5,063	3,800	3,800	3,800	101	3,940	3,840	3,940	3,840	3,895

Stream:	12	13	14	15	16	17	18	19	20	21	22
H2 (kmol/hr)	2,306.7	132.4	.	2,306.7	2,439.2	132.4	2,607.7	.	.	.	2,607.7
CO "	189.6	10.9	.	189.6	200.5	10.9	32.0	.	.	.	32.0
CO2 "	1,614.5	92.7	.	1,614.5	1,707.2	92.7	1,875.7	.	.	.	1,875.7
CH4 "	2.9	0.2	.	2.9	3.0	0.2	3.0	.	.	.	3.0
H2S "	38.9	2.2	.	38.9	41.2	2.2	43.5	.	.	.	43.5
COS "	2.2	0.1	.	2.2	2.3	0.1	.	.	.	.	.
N2 "	26.0	1.5	.	26.0	27.4	1.5	27.4	.	.	.	27.4
Ar "	33.2	1.9	.	33.2	35.1	1.9	35.1	.	.	.	35.1
H2O "	2,996.8	172.1	25,700.0	2,996.8	3,168.9	172.1	3,000.4	10,300.0	10,300.0	1,595.0	1,405.4
O2 "	-	.	.	.	.	.	.	.	.	.	.
Sulfur "	-	.	.	.	.	.	.	.	.	.	.
Coal (kg/hr)	-	.	.	.	.	.	.	.	.	.	.
Slag "	-	.	.	.	.	.	.	.	.	.	.
Flow (kmol/hr)	7,210.8	414.0	25,700.0	7,210.8	7,624.8	414.0	7,624.8	10,300.0	10,300.0		6,030.0
Temperature (K)	701	701	298	520	520	520	492	443	298	450	450
Pressure (kPa)	3,895	3,895	101	3,895	3,895	3,895	3,800	790	790	3,800	3,800

Table 2.1 (continued)
Stream Flows and Conditions for Hydrogen Process

Stream:	23	24	25	26	27	28	29	30	31	32	33
H2 (kmol/hr)	.	.	.	2,607.7	.	.	2,607.7	.	.	.	.
CO "	.	.	.	32.0	.	.	32.0	.	.	.	.
CO2 "	.	.	.	1,875.7	.	.	1,875.7	.	.	.	.
CH4 "	.	.	.	3.0	.	.	3.0	.	.	.	.
H2S "	.	.	.	43.5	.	.	43.5	.	.	.	.
COS "	.	.	.	.	.	.	.	.	.	.	.
N2 "	.	.	.	27.4	.	.	27.4	81.7	.	.	.
Ar "	.	.	.	35.1	.	.	35.1	.	.	.	.
H2O "	1,410.0	1,410.0	1,098.0	307.4	14,300.0	301.4	6.0	.	.	65.2	200.0
O2 "	.	.	.	.	.		.	21.7	.	.	.
Sulfur "	.	.	.	.	.		.	.	43.5	.	.
Coal (kg/hr)	.	.	.	.	.		.	.	.	.	.
Slag "	.	.	.	.	.		.	.	.	.	.
Flow (kmol/hr)	1,410.0	1,410.0	1,098.0	4,932.0	14,300.0	301.4	4,630.0	103.4	43.5	65.2	200.0
Temperature (K)	298	394	400	400	298	313	313	298	393	373	490
Pressure (kPa)	205	205	3,800	3,800	101	3,800	3,800	101	200	101	4,240

Stream:	34	35	36	37	38
H2 (kmol/hr)	7.6	1.1	2,598.0	35.4	2,562.6
CO "	0.3	0.0	32.1	32.1	.
CO2 "	1,710.0	97.0	69.6	69.6	.
CH4 "	0.0	.	3.0	3.0	.
H2S "	.	.	.	.	.
COS "	.	.	.	.	.
N2 "	0.2	81.7	27.4	.	27.4
Ar "	.	.	35.0	.	35.0
H2O "	12.1	6.4	2.6	2.6	.
O2 "	.	.	.	.	.
Sulfur "	.	.	.	.	.
Coal (kg/hr)	.	.	.	.	.
Slag "	.	.	.	.	.
Flow (kmol/hr)	1,730.0	186.0	2,768.0	142.6	2,627.0
Temperature (K)	331	300	300	590	300
Pressure (kPa)	2,500	101	3,800	101	2,930

$$CO + H_2O = CO_2 + H_2 \qquad (1)$$

The WGS reaction is equilibrium-limited under the conditions of interest. A three-times stoichiometric excess of water is used to drive the equilibrium of Reaction 1 to the right. To enhance the rate of the reaction, a heterogeneous catalyst is used. The catalyst used in this study was C25-2-02, promoted Co/Mo on alumina, a catalyst manufactured by United Catalysts Inc. (UCI) of Louisville, Kentucky. This catalyst has good activity for the WGS reaction, can tolerate the presence of high levels of sulfur compounds, and has some activity for the COS hydrolysis reaction. This extra activity will help to decrease the size of the COS hydrolysis reactor, as described below.

The WGS reactor system is a two-stage, fixed-bed unit with feed preheater and interstage cooling. The feed must be preheated to at least 27 K (50 ^{o}F) above its dew point because the promoters present on the catalyst are water-soluble. Using two reactor stages, the feasible overall conversion of CO is at about 98%. Interstage cooling is necessary because the reaction is exothermic and equilibrium-limited. The first-stage reactor effluent will be cooled to 519 K (475 ^{o}F) against boiler feed water for the Heat Recovery and Steam Generation step. A portion of the hot gas will also be cooled against the adsorption bed regeneration gas to provide the hot purge gas (see below). The required feed preheat is provided by heat-exchanging the outlet gas from the second-stage reactor against the first-stage feed.

2.2.3 Carbonyl Sulfide (COS) Hydrolysis Reactor System

After the WGS step, the gas is fed to another fixed-bed catalytic reactor to convert COS to H_2S via hydrolysis:

$$COS + H_2O = CO_2 + H_2S \qquad (2)$$

The COS must be converted to H_2S to remove it in the UCBSRP step. This reaction is also equilibrium-limited under the conditions of interest. The equilibrium limitation requires that the second-stage WGS reactor effluent be cooled before the gas is fed to the COS hydrolysis reactor. This is accomplished by heat-exchanging the second-stage effluent against the first-stage WGS reactor feed, a step which serves a double purpose (see above).

The catalyst used in the COS hydrolysis step is UCI's G41-P, promoted chromia on alumina. With this catalyst it is feasible to reduce the COS concentration in the gas to about 2 ppm in one reactor stage.

2.2.4 Heat Recovery and Steam Generation

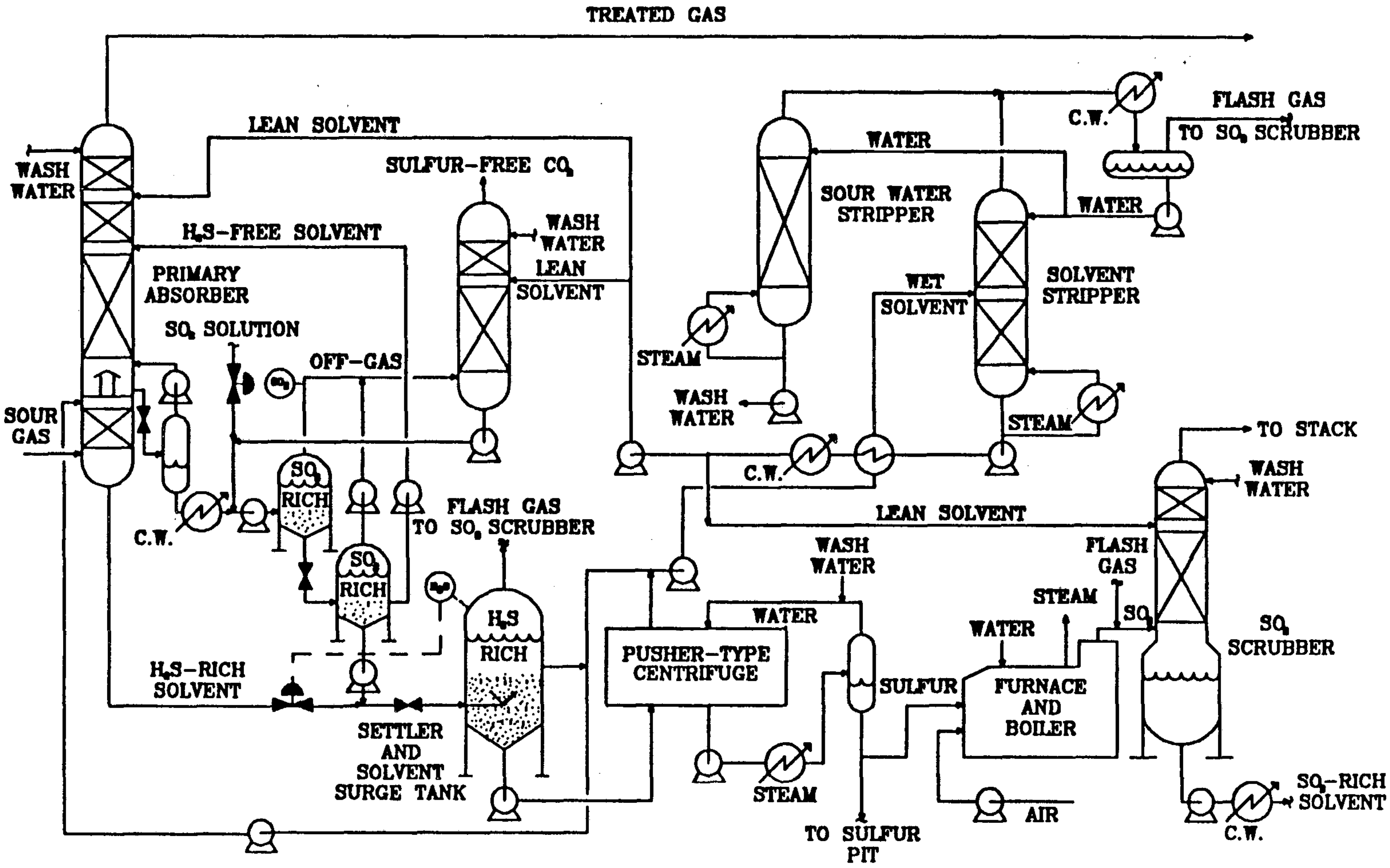
The feed to the UCBSRP must be cooled to about 313 K (100^oF) to condense excess water added in the total quench. Because the latent heat of the evaporated water represents a significant fraction of the heat generated in the coal-gasification step, this heat is recovered and used to generate steam at 790 kPa (100 psig) and 200 kPa (15 psig). For the purposes of this study, it is assumed that there is a ready use for this steam, either for use as process steam or for electric power generation. Final cooling to 313 K is done against cooling water.

2.2.5 U.C. Berkeley Sulfur Recovery Process (UCBSRP)

Figure 2.2 shows a process flow diagram for the UCBSRP in a configuration suitable for removing and recovering CO_2 *in addition* to H_2S from the gas being treated. For detailed process stream information, see Appendix A.2, section A.1.5.

In the main absorber CO_2 and H_2S are removed primarily by physical absorption. The column is separated into two sections by a chimney tray about 1/3 up the height of the column. The flow of solvent through the top section of the main absorber is set by the flow required for bulk removal of CO_2. Because H_2S is about seven times more soluble than CO_2, this easily provides removal of

Figure 2.2
Process Flow Diagram for U.C. Berkeley Sulfur Recovery Process


TREATED GAS
LEAN SOLVENT
WASH WATER
SULFUR-FREE CO_2
H_2S-FREE SOLVENT
WASH WATER
LEAN SOLVENT
PRIMARY ABSORBER
SO_2 SOLUTION
OFF-GAS
SOUR GAS
C.W.
SO_2 RICH
SO_2 RICH
FLASH GAS TO SO_2 SCRUBBER
H_2S RICH
H_2S-RICH SOLVENT
SETTLER AND SOLVENT SURGE TANK
WATER
SOUR WATER STRIPPER
STEAM
WASH WATER
C.W.
FLASH GAS TO SO_2 SCRUBBER
WATER
WET SOLVENT
SOLVENT STRIPPER
STEAM
TO STACK
WASH WATER
LEAN SOLVENT
WASH WATER
WATER
PUSHER-TYPE CENTRIFUGE
STEAM
SULFUR
TO SULFUR PIT
FLASH GAS
STEAM
WATER
SO_2
FURNACE AND BOILER
AIR
SO_2 SCRUBBER
SO_2-RICH SOLVENT
C.W.

H_2S in the treated gas to the part-per-million level. A water wash at the top of the absorber prevents loss of solvent vapor in the treated gas. At the bottom of the main absorber is a short section in which the solvent flow is set to provide a small stream of H_2S-rich solvent. In order to decrease the H_2 and CO content of the solvent (and thus that of the purified CO_2), the liquid off the chimney tray is flashed in a partial flash immediately downstream from the main absorber. The off-gas is recompressed and returned to the top section of the main absorber.

The solvent stream leaving the partial flash then enters a reactor/crystallizer that operates at the pressure of the CO_2 clean-up column. A second solvent stream containing SO_2 is metered into this reactor at a rate that keeps the SO_2 entering the reactor a few percent above stoichiometric relative to H_2S. (It is necessary to have an excess of one reactant or the other in the reactor to avoid excessive reactor volumes and the need for highly precise flow control.) The pressure of the SO_2-rich solvent stream is reduced in stages (only two are shown) to about one atmosphere. The off-gas from each stage is recompressed to the pressure desired for the CO_2 product and is contacted with a small amount of neat solvent to remove traces of SO_2, and then washed with water to recover solvent vapor. Most of the clarified H_2S-free solvent from the atmospheric flash can then be pumped directly back to the main absorber.

A small fraction of the underflow from the atmospheric flash carries the sulfur and water formed in the reaction between H_2S and SO_2. This stream is sized to keep the water content of the solvent from exceeding 5% and is directly proportional to the rate of H_2S removal. It is typically about 10% of the total flow of solvent through the main absorber. Sufficient H_2S-rich solvent, from the bottom section of the main absorber, is added to the stream to leave a small excess of H_2S after all of the residual SO_2 has reacted. This stream is then flashed to atmospheric pressure in a settler/surge tank and the off-gas sent to the SO_2 absorber where the remaining H_2S is reacted.

The sulfur made in the process forms a slurry in the underflow from the surge tank. The sulfur is recovered and washed in a centrifuge. About one-third of the sulfur will be burned in the furnace to make the SO_2 needed in the process. A significant fraction of the energy required by the process can be recovered in the waste-heat boiler. The furnace is operated under sulfur-rich conditions, with the excess sulfur being condensed in an economizer and recycled to the burner, to prevent SO_3 formation in the combustion gas.

The overflow streams for the surge tank and centrifuge are combined and sent to the solvent stripper. Boiling water out of the solvent provides a stripping vapor that also removes the unreacted H_2S and residual co-absorbed CO_2 and other gases from the solvent. The condensate from the stripper is used for wash water in the absorbers and centrifuge after passing through the sour water stripper. The net water of reaction is suitable for use as boiler feed water. The vent gas from the stripper is combined with the flash gas from the settler/surge tank and may be sent to the SO_2 absorber.

Some of the solvent leaving the solvent stripper is used in the SO_2 absorber where it absorbs SO_2 from the combustion gas leaving the furnace. The SO_2 content of this solvent is nil, and hence the SO_2 content of the stack gas leaving the absorber can readily be reduced to the part-per-million level. The remainder of the solvent from the solvent stripper is split between the main absorber and the CO_2 clean-up absorber, where it prevents loss of SO_2 in the treated gas and CO_2 product, respectively.

2.2.5 Adsorber System

The sulfur-free treated gas from the UCBSRP in this process will be sent to an adsorber system for final purification. Adsorptive purification exploits preferential adsorbance onto a porous substrate of one or more components in a mixture to effect a separation. Hydrogen can be recovered from gasified coal by selective adsorbance of the impurities (CO, CO_2, CH_4, and H_2O) from the gas stream. Under the conditions used in adsorptive separation, H_2 is essentially inert and will remain in the product gas.

Final product purification to 97.5% H_2 will be carried out in a three-module, temperature-swing adsorber system. The assumed adsorption cycle time is 4 hours. The three modules will cycle serially through adsorption, regeneration, and cooling, yielding a total cycle time of 12 hours. Each adsorber module was designed as three separate beds to minimize the total regeneration heat requirements. The beds will be regenerated by depressurizing them to atmospheric pressure and recirculating the off gases through heat exchangers where they will be heated against a portion of the first-stage WGS reactor effluent. The water removal bed will be regenerated at 590 K (600 ^{o}F) and the CO and CO_2 beds will be regenerated at 380 K (230 ^{o}F). The heated, regenerated beds will be cooled with a portion of the purified H_2 product. This product will be cooled against cooling water before being sent to storage.

2.3 Equipment Design Summary

2.3.1 Coal Gasification

The primary source of design information for the coal-gasification step was a report on the coal-gasification/combined-cycle power plants prepared by Fluor Engineers, Inc. (EPRI, 1984). The report contains mass and energy balances and construction cost data. Design details for individual pieces of equipment are not given in the report. However, construction cost data for integrated process blocks are included. To estimate equipment costs, the construction cost data were converted to equipment cost using a (Lang) factor of 4.1 for fluid/plants (see Peters and Timmerhaus, 1980).

The coal feed basis for the plant studied in the EPRI report is 6.11 million kg/day (6720 ton/day). In order to estimate costs for the present hydrogen plant, which uses 910,000 kg/day (1000 ton/day), costs for the coal handling and preparation, oxidant plant, and gasification, cooling and particulate/ash removal steps were scaled for plant capacity using a 0.6 power relationship. A cost summary for the coal gasification step is presented in the equipment cost summary (Chapter 3, section 3.4).

2.3.2 WGS Reactor System

WGS Reactor Feed Preheater

The WGS reactor feed preheater was designed as a gas-gas shell-and-tube exchanger with 1 shell pass and 2 tube passes. A constant overall heat-transfer coefficient (OHTC) of 280 W/m^2-K (50 BTU/hr-ft^2-^oF) was assumed. Exchanger area was estimated based on total heat transfer-duty. Total exchanger area was estimated at 28 m^2 (300 ft^2).

Water Gas Shift Reactors

Because the kinetic model for the WGS catalyst is proprietary, the WGS reactor design was based on information supplied by the catalyst manufacturer, United Catalyst, Inc. (UCI) of Louisville, KY. The two WGS reactor stages were designed as plug-flow reactors with a length-to-diameter ratio of about 3. The material of construction was carbon steel. The reactors were designed as cylindrical pressure vessels with hemispherical heads according to ASME pressure vessel codes. Parameter values used in the ASME code equations are given in Table 2.2. Design results are given in Table 2.3.

Table 2.2

Pressure Vessel Design Parameters

Safety Allowance:	10% of Operating Pressure
Hydrostatic Test Allowance:	3 kPa (0.43 psi) per foot of length
Corrosion Allowance:	0.25 cm (0.1 in)
Maximum Working Stress (carbon steel):	94,500 kPa (13700 psi)
Weld Efficiency:	100%
Min. Diameter Increment:	0.15 m (0.5 ft)
Min. Wall Thickness Increment:	0.32 cm (0.125 in)

Table 2.3

WGS Reactor Design Results

	1st-Stage	2nd-Stage
Volume (T-to-T) (m^3)	40	64
Inside Diameter (m)	2.9	3.7
Shell Length (T-to-T) (m)	6.1	6.1

Water Gas Shift Reactor Interstage Cooler

The WGS reactor interstage cooler was designed as a gas/liquid shell-and-tube exchanger with 1 shell pass and 2 tube passes. A constant OHTC of 390 W/m^2-K (70 BTU/hr-ft^2-^oF) was assumed. Exchanger area was estimated based on total heat transfer duty. Total exchanger area was estimated at 112 m^2 (1,210 ft^2).

2.3.3 COS Hydrolysis Reactor System

COS Hydrolysis Feed Cooler

See WGS reactor feed preheater.

COS Hydrolysis Reactor

As with the kinetic model for the WGS catalyst, the COS hydrolysis catalyst model is proprietary to UCI, and reactor volume and conditions were estimated based on information supplied by them. The reactor was sized as a pressure vessel according to the same procedure as the WGS reactors. Table 2.4 shows the design results.

Table 2.4

COS Hydrolysis Reactor Design Results

Volume (T-to-T) (m^3)	96
Inside Diameter (m)	3.7
Length (T-to-T) (m)	9.1

2.3.4 Heat Recovery and Steam Generation

The heat recovery and steam generation plants were sized as packed steam boiler units based on total heat duty. The heat recovered in each plant was determined by an isothermal flash of the gasified coal at the temperature of interest. The amount of steam produced was estimated from the total heat duty of the flash. Steam production rates for the 790 and 200 kPa (100 and 15 psig) plants were 185,000 and 25,400 kg/hr (408,000 and 56,000 lb/hr), respectively.

The trim cooler was designed according to the procedure for the WGS Reactor Interstage Cooler. Total heat-exchanger area was estimated at 226 m^2 (2,400 ft^2).

2.3.5 U. C. Berkeley Sulfur Recovery Process

Equipment design for the UCBSRP was based on results of a computer simulation of the flowsheet. For a detailed description of the simulation method, see Appendix 1. Table 2.5 gives a summary of the design results. Individual pieces of equipment for the UCBSRP were designed according to the following procedures.

Compressors

The compressors used for recompression of the CO_2 flash gases sized as multi-stage axial compressors with motor-gear drive. The first-stage flash compressor has 6 stages with intercooling to 313 K (100 ^oF) on all stages, including the last. The second-stage flash compressor has 10 stages with similar intercooling.

The light-gases flash compressor was sized as a 2-stage reciprocating compressor with intercooling as above.

Pumps

All pumps were sized as centrifugal pumps with size and cost based on the capacity factor [(gal/min)(psi)]. Pumping needs that required capacities too large for a single pump were sized as a set of similar pumps operating in parallel.

Steam Heaters

Steam heaters (reboilers and melter) were sized according to the procedure above for heat exchangers, with the additional assumption that the temperature driving force was constant. The OHTC was taken to be 470 W/m^2-K (83 BTU/hr-ft^2-^oF) for the reboilers and 700 W/m^2-K (125 BTU/hr-ft^2-^oF) for the melter.

Water-Cooled Exchangers

Water-cooled exchangers (compressor intercoolers, solvent coolers, and condensers) were sized as above. The cooling water outlet temperature was optimized with respect to total cost. For the purposes of the optimization, a pay-out period of three years (before taxes) was assumed to annualize the direct equipment cost and a Lang factor of 4.8 was used to convert the direct equipment cost to fixed capital cost. OHTC was taken as 560 W/m^2-K (100 BTU/hr-ft^2-^oF) for liquid cooling and 390 W/m^2-K (70 BTU/hr-ft^2-^oF) for gas cooling.

Refrigeration

The refrigeration system was sized for a 267 K (20 ^oF) evaporator. Design was estimated based on evaporator temperature and refrigeration duty.

Solvent- Solvent Heat Exchangers

The solvent-solvent exchangers (solvent-stripper feed preheater and sulfur-slurry preheater) were sized as liquid-liquid exchangers as above. OHTC was taken as 560 W/m^2-K (100 BTU/hr-ft^2-^oF).

Vessels

Vessels (reactors, stripper reflux drum, sulfur decanter, flash vessels, and sulfur settler) were sized as outlined above for the WGS reactors. The reactor vessels were sized with a length to diameter ratio of about 6. All other vessels were sized for a 5 min. liquid hold-up.

Centrifuge

The sulfur-recovery centrifuge was sized as a pusher-type, with the size based on solids production rate.

Absorber/Stripper Columns

The absorber/stripper columns were sized as pressure vessels using the same procedure as above. Weight of skirt, sieve trays, connections, and auxiliary equipment (ladders, platforms, etc.) was estimated and added to shell weight to determine total weight. All columns were designed with 0.6 m (2 ft) tray spacing.

2.3.6 Adsorber System

The adsorber system was designed assuming equilibrium removal of impurities. Required bed volume for each module was calculated based on an assumed adsorption cycle time of 4 hours. Equilibrium data for H_2O (Hersh, 1961), CO and CO_2 (Wakasugi et al., 1981) over Type 5A molecular sieves was used to predict bed length required to adsorb each impurity. Each adsorber module was sized as three separate beds to decrease the total regeneration heat requirements. Adsorber bed shells were designed as pressure vessels (see above). Compressors, intercoolers and heat exchangers for the system were designed as above. Design results are presented in Table 2.6.

Table 2.5
Major Equipment Summary: UCBSRP
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

Compressors

	Power (kW)	Capacity (m^3/min)
First Stage CO_2 Flash	1620	115
Second Stage CO_2 Flash	1450	252
Light Gases Flash	40.1	1.8

Pumps

	Power (kW)	Capacity (m^3/min)
Main Abs. Solv. Recycle	927	15.1
Main Abs. Side-draw to SO_2-rich Rxtor	184	22.2
SO_2-rich Slurry to H_2S-rich Rxtor	173	2.8
Lean Solv. CO_2 Column	53.4	1.3
SO_2 Solution to SO_2-rich Reactor	48.5	1.2
Lean Solv. to Main Abs.	10.8	0.5
2nd-Stg CO_2 Flash Comp. Drain	2.4	< 0.1
Sulfur/H_2O Slurry to Melt/Decant	1.8	1.10
1st-Stg CO_2 Flash Comp. Drain	0.5	< 0.1

Steam Heaters

	Heat Load (kW)	Area (m^2)
Reboiler, Solv. Stripper	1830	60.3
Reboiler, Sour Water Stripper	50.0	< 1
Melter, Sulfur/Water Slurry	31.1	< 1
Furnace/Waste Heat Boiler	1700	N/A

Water Cooled Exchangers

	Heat Load (kW)	Area (m^2)
Intercoolers, 1st-Stg. CO_2 Comp.	1880	286
Intercoolers, 2nd-Stg. CO_2 Comp.	1860	266
Intercoolers, Light-Gases Comp.	48.7	6.8

	Heat Load (kW)	Area (m^2)
Cooler, Main Abs. Side-draw	2000	300
Cooler, SO_2 Abs. Bottoms	103	23.6
Cooler, Main Abs. Bottoms	17.2	2.3
Condenser, Solv. Stripper	1370	22.5

Refrigeration System

	Heat Load (kW)
Chiller, Crystallizer Feed	161

Table 2.5 (continued)
Major Equipment Summary: UCBSRP
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

Heat Exchangers

	Area (m^2)
Exchanger, Solv. Stripper Feed Preheat	71.5
Exchanger, Sulfur Slurry Preheat	1.8

Vessels

	Volume (m^3)	Length T-to-T (m)	Diameter (m)
Reactor, SO_2-rich	2.32	4.57	0.76
Reactor, H_2S-rich	2.32	4.57	0.76
Reflux Drum*, Stripper	< 1	1.52	0.45
Decanter*, Sulfur Melter	< 1	0.305	0.45
Flash Vessel*, Light Gases	92.0	9.45	3.20
Flash Vessel*, 1st-Stage CO_2	103	9.45	3.45
Flash Vessel*, 2nd-Stage CO_2	103	9.45	3.45
Settler/Solvent Surge Tank	12.4	7.47	1.37

* 5 minute hold up

Absorber/Stripper Columns

	Trays	Diameter (m)
Absorber, Primary Top/Bot.	31	2.6/1.5
Absorber, SO_2	16	1.1
Absorber, CO_2 Clean Up	13	1.5
Stripper, Solv.	12	0.76
Stripper, Sour Water	3	0.15

Centrifuge

	Sulfur Production (kmol/hr)
Sulfur Recovery Cent. (Pusher Type)	73

Table 2.6
Adsorber System Design Results

Vessels

		Volume (m^3)	Length T-to-T (m)	Diameter (m)
H_2O	Removal Beds (3)	16.0	1.6	2.7
CO_2	Removal Beds (3)	377	4.9	3.1
CO	Removal Beds (3)	1410	23.8	3.1

Heat Exchangers

	Area (m^2)
Regeneration Gas Heaters (3)	< 1

Compressors

		Power (kW)	Capacity (m^3/min)
H_2O	Bed Regeneration Gas	0.3	5.6
CO_2	Bed Regeneration Gas	35.7	13.5
CO	Bed Regeneration Gas	1730	669

Water Cooled Exchangers

	Heat Load (kW)	Area (m^2)
CO Bed Regen. Comp. Intercooler	860	153
H_2 Product Cooler	503	181

3 ECONOMIC EVALUATION

3.1 Basis of Economic Analysis

The economic analysis of the hydrogen process is based on the results of the order-of-magnitude equipment design calculations. Major materials costs were estimated for all major pieces of equipment for the process. Two primary sources of data were used for equipment costs (Peters and Timmerhaus, 1980) and (Hall et al., 1982). Cost data from these sources were updated using the Chemical Engineering Magazine Plant Cost Index. The cost ratios used to update January 1979 and January 1982 dollars to October 1988 dollars were 1.49 and 1.14, respectively.

Utilities, raw materials, and labor costs were estimated from the equipment design and operating rate. An operating rate of 8000 hours/yr was used to calculate the direct costs of production. The total major equipment cost was multiplied by a Lang factor of 4.9 (Peters and Timmerhaus, 1980, p. 181) to estimate total capital investment. The investment and production costs were used in an investment-and-pay-out study to determine the required sales income. The required H_2 sales price was determined from the required sales income and hydrogen production rate.

3.2 Equipment Cost Methods

3.2.1 Coal Gasification

Equipment costs for the coal gasification step were estimated from data taken from a technical report by Fluor Engineers, Inc. on the design and performance of Texaco gasifiers (EPRI, 1984, Table 6-7). Total construction costs for the coal handling and preparation, oxidant feed, and gasification and particulate/ash removal steps were scaled down to the lower plant capacity using an 0.6 power relationship. The EPRI study is based on a feed of 6720 ton/day

Illinois #6 coal and the H_2 plant is based on feeding 1000 ton/day of the same coal. This yields a capacity scaling factor of 0.32. The scaled construction costs were then converted to equipment costs by dividing them by a Lang factor of 4.1 (Peters and Timmerhaus, 1980, p. 181).

3.2.2 WGS and COS-Hydrolysis Reactor Systems

Costs of the heat exchangers for the water-gas-shift reactor system were estimated from total heat-exchange area. Exchangers were assumed to be of all carbon steel construction with extended heat-transfer surfaces on the shell side. The cost of the gas-gas exchangers was assumed to be $\$11/ft^2$ of tube side area (Louks, 1988). Costs for gas-liquid exchangers were estimated from Figure 14-13, Peters & Timmerhaus, 1980.

Reactor vessel costs were estimated from total weight (Peters and Timmerhaus, 1980, Chapter 13, Table 6). Vessels were assumed to be of all carbon steel construction.

For catalyst cost estimates, see Raw Materials Costs (Section 3.3.2).

3.2.3 Heat Recovery and Steam Generation

Costs for the steam-generation plants were estimated from costs of packaged-steam-boiler plants of the same capacity (Peters and Timmerhaus, 1980, Figure B-3).

The cost of the trim cooler was estimated as above for gas-liquid exchangers.

3.2.4 U.C. Berkeley Sulfur Recovery Process

Vessel costs for the UCBSRP were estimated as above.

Heat-exchanger costs were estimated as above. For all water-cooled exchangers, the total cost was optimized with respect to cooling-water outlet temperature. The maximum cooling-water outlet temperature was assumed to be 323 K (122°F). The total cost was taken as the sum of the annual cooling water cost and an annual fixed-capital-cost charge based on the heat-exchanger cost. A pay-out period of three years (before taxes) was used to calculate the annual fixed cost charge. The annual fixed cost charge was multiplied by a Lang factor of 4.8 to estimate the annual-fixed-capital cost. For a detailed example of this calculation, see Section A.2.2, Figure A.4.

Compressor costs were based on number of compression stages and capacity (Peters and Timmerhaus, 1980, Figures 13-45 and 13-48).

Pump costs were estimated based on capacity factor [(gal/min)(psi)] (Hall et al., 1982, Figure 30).

The refrigeration system cost was estimated based on the evaporator temperature and refrigeration duty (Peters and Timmerhaus, 1980, Figure B-7)

The sulfur centrifuge cost was based on solids production rate (Hall et al., 1982, Figure 53). Material of construction: Carbon steel.

Costs for all absorber/stripper columns were based on total weight (Peters and Timmerhaus, 1980, Figures 15-24 through 15-27).

3.2.5 Adsorber System

Costs for vessels, heat exchangers and compressors for the adsorber system were estimated as above.

Valve costs were estimated based on diameter (Hall et al., 1982, Figure 54).

3.3 Direct Production Costs Methods

3.3.1 Utilities Costs Methods

Utilities costs (and credits) were estimated from consumption (and production) data taken from the equipment design. For the coal gasification step, utilities consumption was estimated from data taken from the EPRI report (EPRI, 1984, Table 5-7). A linear relationship was used to scale the costs for plant capacity. This yields a conversion factor of 0.15 which was applied to all data taken from the report.

Unit costs for utilities are given in Table 3.1.

Table 3.1

Unit Costs of Utilities

Cooling Water (m^3)	$26.00
Refrigeration (MW-hr)	11.40
Electric Power (kW-hr)	0.07
Steam @ 4.22 MPa (Mg)	11.50
Steam @ 1.15 MPa (Mg)	9.90
Steam @ 790 kPa (Mg)	8.60
Steam @ 200 kPa (Mg)	2.90

3.3.2 Raw Materials Costs Methods

Raw materials costs were estimated based on plant capacity. Catalyst costs for the WGS and COS hydrolysis reactors and Type 5A molecular sieves cost for the adsorber system were charged as raw materials over a projected three-year life.

Unit costs for raw materials are given in Table 3.2.

Table 3.2

Unit Costs of Raw Materials

Coal (Mg, delivered)	$50.00
Process Water (m^3)	0.21
Water Gas Shift Catalyst (kg)*	16.30
COS Hydrolysis Catalyst (kg)**	24.40
Type 5A Molecular Sieve (kg)***	3.46

* Bulk Density = 0.705 kg/l
** Bulk Density = 0.577 kg/l
*** Bulk Density = 0.690 kg/l

3.3.3 Maintenance and Labor Costs Methods

Maintenance and maintenance overhead costs were estimated as a percentage of the total fixed capital investment for the plant. Maintenance cost was taken as 6% of fixed capital. Maintenance overhead was assumed to be 65% of maintenance cost.

Labor cost was estimated from plant capacity and number of operating steps (Peters and Timmerhaus, 1980, pp. 195-197). The annual base labor rate was taken as $50,000/employee. The plant was estimated to contain 17 operating steps and to require 40 employee hrs/operating step/day.

Labor overhead cost was estimated as 65% of labor cost.

3.4 Cost Summaries

3.4.1 Equipment Costs Summary

Table 3.3 gives a cost summary for all major equipment for the hydrogen plant.

3.4.2 Raw Materials Costs Summary

Table 3.4 gives a summary of raw materials costs for the hydrogen plant.

Table 3.4

Raw Materials Costs

	Consumption		Annual Cost* ($million)
Coal	37,800	kg/hr	15.1
Process Water	1,100	m^3/hr	1.85
Water Gas Shift Catalyst	24.8	Mg/yr	0.405
COS Hydrolysis Catalyst	14.4	Mg/yr	0.430
Type 5A Molecular Sieve	133	Mg/yr	0.460
Total Annual* Raw Materials Cost			16.3

* Annual values based on an operating rate of 8000 hr/yr.

3.4.3 Utilities Cost Summary

Table 3.5 gives a summary of annual utilities costs for the hydrogen plant.

3.4.4 Maintenance and Labor Costs

Table 3.6 gives a summary of annual maintenance and labor costs for the hydrogen plant.

Table 3.6

Maintenance and Labor Cost Summary

	Annual Cost* ($million)
Maintenance (6% of Fixed Capital)	4.38
Maintenance Overhead (65% of Maintenance Cost)	2.85
Labor	1.90
Labor Overhead (65% of Labor Cost)	1.23
Total Annual* Maintenance and Labor Cost	10.4

* Annual values based on an operating rate of 8000 hr/yr.

Table 3.3
Major Equipment Cost Summary for Hydrogen Plant
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

	Cost ($1000)
Coal Gasification*	12,600
WGS Feed Preheater/COS Feed Cooler	3
1st-Stage WGS Reactor	93
2nd-Stage WGS Reactor	130
WGS Interstage Cooler	13
COS Hydrolysis Reactor	161
Heat Recovery/Steam Generation:	
100 psig	1,000
15 psig	151
UCBSRP Feed Trim Cooler	27
UCBSRP Equipment:	
Compressors	
First Stage CO_2 Flash	373
Second Stage CO_2 Flash	448
Light Gases Flash	30
Pumps	
Main Absorber Solvent Recycle	97
Main Absorber Side-draw to SO_2-rich Reactor	22
SO_2-rich Slurry to H_2S-rich Reactor	21
Lean Solvent to CO_2 Column	7
SO_2 Solution to SO_2-rich Reactor	7
Lean Solvent to Main Absorber	3
2nd-Stage CO_2 Flash Compressor Drain	2
Sulfur/H_2O Slurry to Melter/Decanter	2
1st-Stage CO_2 Flash Compressor Drain	1

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* For an explanation of Coal Gasification equipment, see section 3.2.1

Table 3.3 (continued)
Major Equipment Cost Summary for Hydrogen Plant
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

	Cost ($1000)
UCBSRP Equipment (continued):	
Steam Heaters	
Reboiler, Solvent Stripper	13
Reboiler, Sour Water Stripper	5
Melter, Sulfur/Water Slurry	5
Furnace/Waste Heat Boiler	7
Water Cooled Exchangers	
Intercoolers, 1st-Stage CO_2 Compressor	34
Intercoolers, 2nd-Stage CO_2 Compressor	32
Intercoolers, Light-Gases Compressor	1
Cooler, Main Absorber Side-draw	37
Cooler, SO_2 Absorber Bottoms	10
Cooler, Main Absorber Bottoms	3
Condenser, Solvent Stripper	10
Refrigeration System	
Chiller, Crystallizer Feed	75
Heat Exchangers	
Exchanger, Solvent Stripper Feed Preheat	18
Exchanger, Sulfur Slurry Preheat	5
Vessels	
Reactor, SO_2-rich	11
Reactor, H_2S-rich	15
Reflux Drum, Stripper	2
Decanter, Sulfur Melter	3
Flash Vessel, Light Gases	94
Flash Vessel, 1st-Stage CO_2	44
Flash Vessel, 2nd-Stage CO_2	29
Settler/Solvent Surge Tank	13
Absorber/Stripper Columns	
Absorber, Primary	395
Absorber, SO_2	49
Absorber, CO_2 Clean Up	111
Stripper, Solvent	37
Stripper, Sour Water	9
Centrifuge	
Sulfur Recovery Cent. (Pusher Type)	114
Total UCBSRP Equipment Cost:	2,100

Table 3.3 (continued)
Major Equipment Cost Summary for Hydrogen Plant
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

	Cost ($1000)
Adsorber System:	
Compressors	
H_2O Bed Regeneration Gas	6
CO_2 Bed Regeneration Gas	9
CO Bed Regeneration Gas	388
Water Cooled Exchangers	
Intercoolers, CO Bed Regeneration-Gas Compressor	18
H_2 Product Cooler	21
Heat Exchangers	
Regeneration Gas Heaters (3)	14
Vessels	
H_2O Removal Beds (3)	39
CO_2 Removal Beds (3)	186
CO Removal Beds (3)	691
Valves	
Assorted Large Diameter Valves	124
Total Adsorber System Equipment Cost:	1,500
Total Hydrogen Plant Equipment Cost:	**17,800**

Table 3.5
Utilities Cost Summary for Hydrogen Plant
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed

	Annual* Cost ($million)
Electric Power Consumed	
Coal Gasification	6.61
UCBSRP	2.53
Adsorber System	1.17
Total Annual* Electric Power Cost	10.3
Steam Consumed, 1150 kPa (150 psig)	
UCBSRP	0.274
Steam Produced, 4220 kPa (600 psig)	
UCBSRP	(0.333)
Steam Produced, 793 kPa (100 psig)	
Heat Recovery and Steam Generation	(12.7)
Steam Produces, 200 kPa (15 psig)	
Heat Recovery and Steam Generation	(0.584)
Cooling Water Consumed	
Coal Gasification	0.117
WGS Interstage Cooling	0.0963
UCBSRP Feed Cooling	0.0537
UCBSRP	0.104
Adsorber System	0.0453
Total Annual* Cooling Water Cost	0.416
Refrigeration Consumed	
UCBSRP	0.0146
Total Net Annual* Utilities Cost (Credit)	(2.60)

* Annual Costs based on an operating rate of 8000 hr/yr.

3.5 Investment and Pay-Out Study

The required hydrogen sales price for a three-year before-tax pay-out period was calculated from an investment-and-pay-out study. Table 3.7 shows a cost and profit sheet for the hydrogen plant where the CO_2 product has negligible value.

The investment for the plant was calculated from the equipment cost results. Fixed capital investment was estimated at 4.1 times the total equipment (major material) cost. Working capital was estimated as 80% of the total equipment cost.

Fixed costs were based on the amount of total investment. Depreciation, property taxes, and insurance were estimated at 10%, 2%, and 1% of fixed capital, respectively.

Direct costs were estimated as described above in the relevant section for each cost.

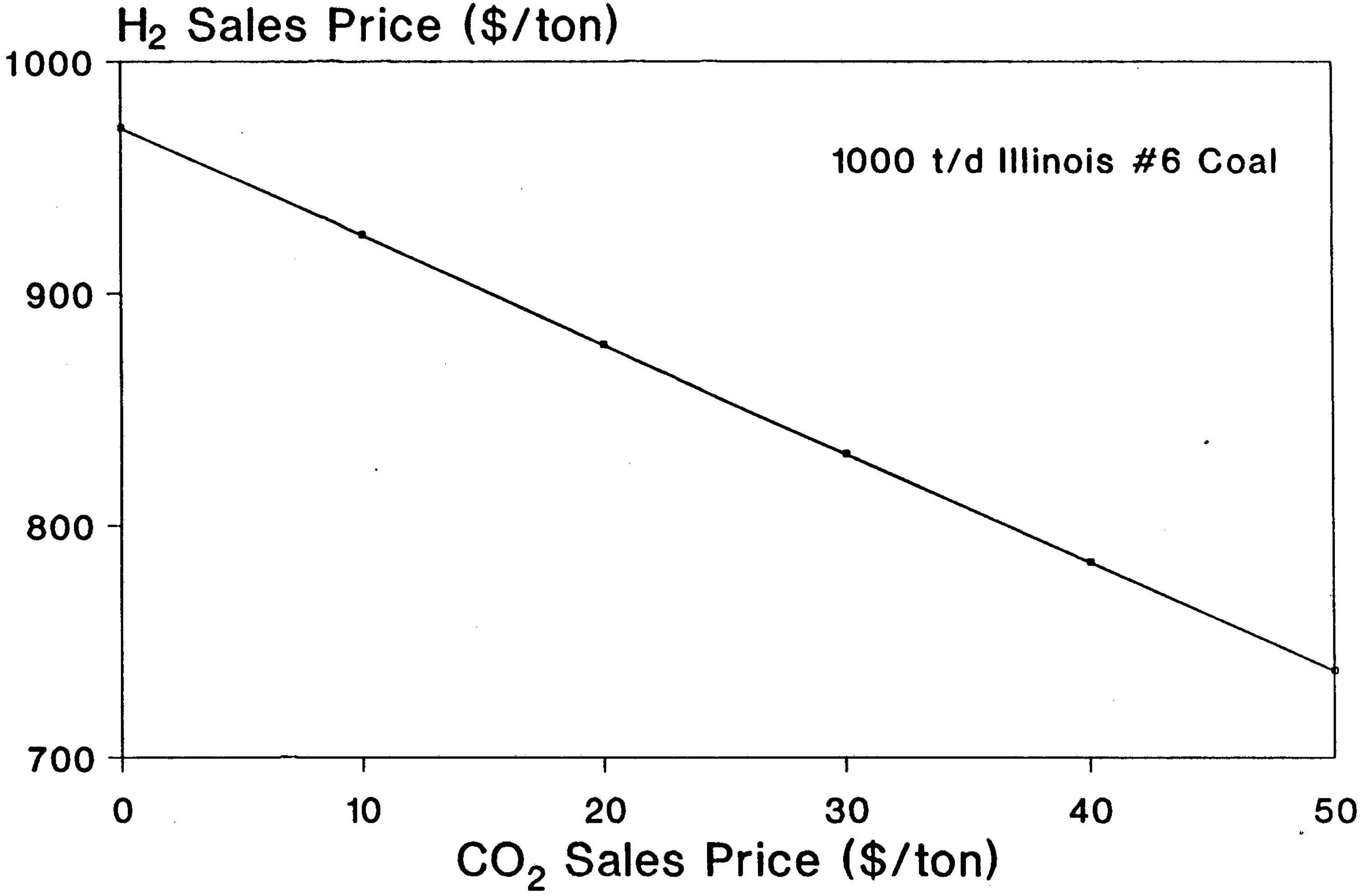
The required sales income was determined from a cash flow analysis. The cash flow was taken as sales income less total production costs. The product sales prices were determined from the total required sales income and the H_2 and CO_2 production rates.

Figure 3.1 shows a plot of the required H_2 and CO_2 sales prices. The line represents conditions that correspond to the required three-year (before tax) pay-out period. The maximum H_2 sales price corresponds to a situation where the CO_2 has no recoverable value.

Table 3.7
Cost and Profit Sheet for Hydrogen Process
Plant Capacity: 1000 ton/day Illinois #6 Coal Feed
CO_2 Value: Negligible

	$million (except as noted)	
Investment		
Total Major Materials Cost	17.8	
Fixed Capital	73.0	
Working Capital	14.2	
Total Investment	87.2	
Annual Production Costs		
Fixed Costs:		
Depreciation (10% of Fixed Capital)	7.30	
Property Taxes (2% of Fixed Capital)	1.46	
Insurance (1% of Fixed Capital)	0.73	
Total Fixed Costs:	9.49	
Direct Costs:		
Raw Materials	16.3	
Utilities	(2.6)	
Maintenance (6% of Fixed Capital)	4.38	
Maintenance Overhead (65% of Maintenance)	2.85	
Labor	1.90	
Labor Overhead (65% of Labor)	1.23	
Total Direct Costs:	24.1	
Total Annual Production Costs:	33.6	
Annual Cash Flow		
Before Tax Pay Out Period	3	yr
Required Cash Flow	29.1	
Required Net Income (before tax)	29.1	
Required Gross Sales Income	62.7	
Sales Price and Production Rate		
H_2 Production Rate	64,400	short ton/yr
H_2 Sales Price	971	$/short ton

Figure 3.1
Effect of CO_2 Sales Price on H_2 Sales Price
For a Three-Year (Before Tax) Pay-Out Period



Chapter 4 RESULTS AND CONCLUSIONS

4.1 Technical Evaluation

The results of the equipment design calculations demonstrate that the hydrogen process is technically feasible. All equipment design parameters are within acceptable design limits.

The required product purity of 95+% H_2 can easily be met with the proposed technology. The limits of attainable purity are set by the N_2 and Ar content of the syngas because these gases are not easily separable by adsorption. The Ar content of the gas is set entirely by the Ar specification in the cryogenic air-separation plant where the oxidant for the coal gasification step is produced. If the oxygen-purity specification were increased from 95% to 99.5%, the maximum hydrogen product purity would increase to 99.4%. However, the additional cost of producing high-purity oxygen is prohibitive. Order-of-magnitude design calculations for the air-separation plant indicate that the cost of the coal gasification step would increase outside acceptable limits. This would increase the required hydrogen sales price to a figure outside the range of current hydrogen values (see below).

The maximum possible product purity for the process evaluated here is set by the nitrogen content of the coal feed. Illinois #6 coal is about 1.35 weight percent nitrogen (dry, ash-free basis) (EPRI, 1984, Table 1-2). This would limit the hydrogen purity to 99.6% even if the gasifier were fed with pure oxygen (99.99+%). A more attractive method for making high-purity hydrogen (99.+%) would be to treat the product from the present process cryogenically.

4.2 Economic Evaluation

The 97.5% hydrogen produced by the process studied here must be sold for between $740 and $970/ton to generate sufficient sales revenue for the required three-year (before-tax) pay-out period. Currently, refinery grade (90+%) hydrogen is valued at between $360 and $2900 per ton, depending on purity and plant location (Sciamanna, 1989). Thus, the results of this process study indicate a potentially viable process.

The exact value of the required hydrogen sales price depends on the market for large quantities of CO_2. If the plant is constructed in an area where the high-pressure CO_2 product has recoverable value (such as in enhanced oil recovery), then the process becomes even more attractive.

4.3 Comparison with Literature Results

A previous investigation examined a similar coal-to-hydrogen process (Bartis and Marks, 1984). Their process configuration differs from the process studied here in three major areas. First, the gasifier is fed with high-purity (99.5%) oxygen. Second, the WGS reaction is carried out in a three-stage, high-temperature reactor system. Third, H_2S and CO_2 removal are accomplished with a Selexol/Claus plant and a Wellman-Lord tail gas desulfurization unit.

All of the above process differences increase the cost of the hydrogen produced by their route relative the process studied here. As discussed above, the cost of producing high-purity oxygen becomes a significant portion of the cost of the product hydrogen. The use of high-temperature in the WGS increases reactor and catalyst costs and decreases overall conversion of CO, thereby reducing hydrogen production. Finally, the Selexol/Claus and Wellman-Lord processes are more energy-and capital-intensive acid-gas treatment processes than the UCBSRP. For a comparison of the UCBSRP to conventional sulfur-recovery technology, see Lynn et al., 1987.

One would expect the above process differences to result in a hydrogen sales price that is greater than that for the process studied here. Bartis and Marks arrive at a figure of about $1500/ton (1988 dollars) for hydrogen produced by their process, about 50% higher than that obtaining by the process studied here. Another factor that contributes to this difference is their methods of estimating capital investment. In general, Bartis and Marks appear to be somewhat more conservative, using larger contingency factors and including more off-site capital investment.

4.4 Future Work

The processing steps involved in the hydrogen process proposed here are all technologies that have been demonstrated on an industrial scale, with the exception of the UCBSRP. This process should be demonstrated at least on a pilot-plant scale and if possible, on an industrial scale before further work on the hydrogen process is undertaken. Because the results of the order-of-magnitude design and cost study are favorable, further evaluation of the process is recommended. A detailed-estimate design of the process will provide more accurate cost estimates and will indicate the process' chances of success.

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APPENDIX

The Appendix to this report, a 221-page description and listing of the computer code used to simulate the flow configurations discussed above, is available upon request from:

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