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FOSSIL FUEL PROCESSING
TECHNICAL/PROFESSIONAL SERVICES

MASTER

DESIGN AND EVALUATION OF CITIES SERVICE/ROCKWELL HYDROGASIFICATION COMMERICAL PLANT

PREPARED FOR

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

DIVISION OF FOSSIL FUEL PROCESSING

UNDER CONTRACT NO.
DEAC01-78ET10159
(Formerly ET-78-C-01-3117)

AUGUST, 1980

A JOINT VENTURE OF
UOP INC. AND
SYSTEM DEVELOPMENT CORPORATION

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DESIGN AND EVALUATION OF CITIES SERVICE/ROCKWELL HYDROGASIFICATION COMMERCIAL PLANT

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Prepared for the
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Division of Fossil Fuel Processing

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ABSTRACT

Contract No. DEAC01-78ET10159 (Formerly ET-78-C-01-3117) between UOP/SDC and the United States Department of Energy (DOE) requires UOP/SDC to provide specific engineering and technical services to the DOE Division of Fossil Fuel Processing in support of the Coal Gasification Program. This report covers a preliminary conceptual design and economic evaluation of a commercial scale plant capable of converting high-sulfur bituminous caking coal to a high-Btu pipeline quality SNG. The plant, which has a rated capacity of 250 Billion Btu per day SNG, is based on Cities Service/Rockwell hydrogasification technology.

Two cases of plant design were examined to produce cost estimates accurate to ± 25% in 1979 dollars. The base case, designed for moderate production of liquids (5.8% conversion of carbon to liquid product), has a cost of SNG of \$4.43/MMBtu using the utility financing method (UFM)(1) and \$6.42/MMBtu using the discounted cash flow method (DCFM)(2) of financing. The alternate case, zero liquids production, has gas costs of \$5.00 (UFM) and \$6.96 (DCFM).

Further tests by Rockwell have indicated that 11.4% carbon conversion to liquid products (99% benzene) is possible. If the plant is scaled up to produce the same amount of SNG with this increased yield of liquid, and if the value of the benzene produced is estimated to be \$0.90 per gallon, the costs of gas for this case are \$4.38/MMBtu (UFM) and \$6.48/MMBtu (DCFM)(3). If the value of benzene is taken as \$2.00 per gallon, these costs become \$3.14/MMBtu (UFM) and \$5.23/MMBtu (DCFM).

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(1) Capital structure assumes 75% debt at 9%, 25% equity at 15%. Taxes are assumed to be 48% Federal income taxes and 15% property taxes.

(2) Capital structure assumes debt financing of land and working capital only, at 9%, equity financing of remainder at 12%. Taxes are assumed to be 48% Federal and 4% state and local income taxes, 15% property taxes.

(3) Reasons for this apparent discrepancy are analyzed in Appendix D of the text.

FOREWORD

This report describes work performed during April 1979 through August 1980 on Task Order No. 19, sponsored by the United States Department of Energy (DOE), Division of Coal Conversion, under Contract No. DEAC01-78ET10159 (Formerly Contract No. ET-78-C-01-3117). The DOE program manager is Mr. Louis Jablansky. The UOP/SDC gasification program manager is J. Cooper. The UOP/SDC task manager for this task is P.D. Agrawal.

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SECTION 1 - INTRODUCTION

Flash hydropyrolysis is rapid hydrogenation of coal achieved by bringing the reactants, coal and hydrogen, together for a very short period of time under high temperature and pressure conditions. To be commercially useful, the method selected must be capable of processing large amounts of material. It appears that all these requirements - short contact times, large mass fluxes, and high temperatures and pressures - can be met by adaptation of the aerospace technology of rocket nozzles. Significant work in this direction was originally performed by Cities Service Oil Company and Rocketdyne, which later evolved into Rockwell's Energy Systems Group. The process has been demonstrated at a very small scale (3/4 ton per hour) for a run of 45 minutes, and massive experimentation has been conducted to evaluate all the criteria involved for scale-up to commercial size equipment.

During April 1979, the U.S. Department of Energy (DOE) engaged UOP/SDC to examine the Cities Service/Rockwell (CS/R) hydrogasification process and to prepare a preliminary conceptual design of a commercial plant producing 250 billion Btu per day pipeline quality high Btu substitute natural gas (SNG) from highly caking bituminous coal. The level of effort was to be to the extent necessary to prepare an approximate (± 25%) factored cost estimate and to calculate the gas cost ($/MMBtu) for a twenty-year plant life. The gas costs were to be calculated by using both the utility financing method and the conventional DCF approach.

The Energy Systems Group of Rockwell International, in a private communication (Appendix A), furnished UOP/SDC with hydrogasification reactor material balances for two cases using Pittsburgh Seam No. 8, an Eastern Bituminous coal. The case with a moderate liquids production was selected as the BASE CASE in the UOP/SDC design effort, and the case with total hydrogasification was selected as the ZERO LIQUIDS CASE. Various reactor conditions for the two cases are defined in Table 1.1.

Table 1.1 Reactor Conditions for Case Studies (1)

	Base Case	Zero Liquids Case
Hydrogen Inlet Temperature, ^{o}F	1500	1500
Oxygen Inlet Temperature, ^{o}F	200	200
Coal Inlet Temperature, ^{o}F	200	200
Reactor Outlet Temperature, ^{o}F	1770	1900
Reactor Pressure, psig	1000	1000
Residence Time, milliseconds	2500	2000
Hydrogen Feed Rate, lb H_2/lb(MF)coal	0.319	0.366
Oxygen Feed Rate, lb O_2/lb H_2	0.157	0.224
Overall Carbon Conversion, %	56.8	62.7

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(1)Refer to Appendix A

Further tests by Rockwell have achieved carbon to liquid yields of 11.4%. Appendix C contains the initial communication from Rockwell. Appendix D gives the results obtained by scaling up the base case to produce 250 billion Btu per day SNG under the high yield conditions.

SECTION 2 - SUMMARY

2.1 PLANT SIZE AND ECONOMIC BASIS

A conceptual design has been made of a commercial plant capable of producing 250 billion Btu per day, based on Cities Service/Rockwell (CS/R) hydrogasification technology. The purpose of this design is to evaluate delivered cost of pipeline quality SNG using bituminous coal as raw material. The design includes a comprehensive "grass roots" facility containing its own utilities, hydrogen production, wastes treatment, storage, and transportation within the battery limits. Such other elements as housing, recreational facilities for employees, etc., are not included.

The economics have been evaluated in constant 1979 dollars for two different cases of financing and two different cases of process variations. The two financing modes are: (1) Utility Financing with 0.75 debt fraction, 9% interest on debt, and 15% ROE; (2) Equity Financing without tax exemptions and 12% rate of return. The process variations studied are: (1) base case with moderate quantities of liquids accompanying the product; and (2) product gas with zero liquids accompanying it. A variation based on high yield of carbon to liquid is analyzed in Appendix D.

2.2 RESULTS

Details of the studies made and their results are given in subsequent sections; the summary of those results is presented below.

2.2.1 Plant Investment

The total plant investment amounts to \$1.267 billion for the base case and \$1.268 billion for the zero liquids case. The total capital requirements(1) are \$1.379 billion and \$1.384 billion, respectively.

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(1) The values stated here do not include allowance for funds used during construction.

2.2.2 Gas Cost

The resulting gas cost for the base case, using $1.00 per MMBtu as the raw material cost, is $4.43 per MMBtu with Utility Financing and $6.42/MMBtu with discounted cash flow method. Similar costs for the zero liquid case are $5.00 and $6.96, respectively. Comparison of the two cases indicates that the case with benzene production is more attractive than the case with zero liquid production.

A series of sensitivity analyses were performed on the cost of gas by varying the coal cost, rate of return, capital requirement, coal requirement and benzene value. The results of these analyses are summarized in section 6.4.3.

A comparison of costs of the CS/R and Lurgi processes for producing SNG is given in Table 2.1. It appears that the CS/R process is at least competitive with the Lurgi within the accuracy of the estimates (±25%). When credit is taken for sale of byproduct liquids (CS/R Base Case), the cost of product SNG at $4.43/MMBtu is clearly better than that for Lurgi at $5.16/MMBtu.

2.3 AREAS FOR IMPROVEMENT

The scope of work for this economic evaluation did not allow for optimization of the CS/R hydrogasification process. The following improvements could significantly reduce the capital investment.

Reducing the hydrogen to coal ratio from 0.36 lb/lb, as used in this study, to about 0.25 would provide a reduction in the cost of the hydrogen production unit. This reduction in hydrogen consumption might also reduce the number of hydrogen production trains needed. Higher pressure (about 1200 psig as compared to present operation at 550 psig) operation of Texaco gasifier should also reduce the number of hydrogen production trains.

Replacement of the Texaco gasifier by a closely coupled, dry-char oxygasifier for hydrogen production would reduce the investment and operating costs by eliminating the char letdown and slurry feed systems. Possible use of the Shell-Koppers gasification process for this application could be investigated.

Reducing the hydrogen purity requirement would further reduce the hydrogen production unit capital investment. This modification would also result in a modest reduction of hydrogen removal unit cost.

Optimization of liquid production should be continued. For this study, the market value of raw benzene by-product is taken to be $0.90/gallon as transportation fuel. Chemical grade benzene has a current market value in excess of $1.55/gallon. The higher value, however, is considered unrealistic for this project because of uncertainties about the extent of upgrading necessary and the size of the chemical benzene market.

One other area of potential savings would be the use of a low-temperature, sulfur resistant shift catalyst, which is presently under development. The use of such a catalyst would eliminate one heating cycle prior to shift and thereby result in lower operating cost.

Table 2.1 Gas Cost Comparison for Two High Btu SNG Processes
(Capacity: 250 Billion Btu per day SNG)

	CS/R Hydrogasification Process		
	ZERO LIQUIDS CASE	BASE CASE	LURGI PROCESS(1),(2)
Total Plant Investment, $MM(2)	1,268.4	1,266.9	1,380.0
Working Capital, $MM	39.3	39.0	37.0
Total start-up Cost, $MM(3)	73.1	70.0	79.0
Allowance for funds used during construction, $MM(4)	214.1	214.0	233.0
Total Capital Requirement, $MM	1,594.9	1,590.0	1,729.0
Coal Required (ST/D)	18,573.0	17,643.0	18,291.0
Overall Thermal Efficiency (Per Cent)	57.01	63.88	60.30
Cost of Gas ($/MMBtu) (Utility Financing Method)(5)	5.00	4.43	5.16

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(1) Factored Estimates for Eastern Coal Commercial Concepts, Report FE-2240-31, Prepared by C. F. Braun & Co. under ERDA contract No. EX-76-C-01-2240, September 1978.

(2) Adjusted for second quarter 1979 dollars.

(3) Total start-up cost includes plant start-up cost, spare parts, paid-up royalties, initial charge of catalysts and chemicals, etc.

(4) For Utility Financing Method, the allowance for funds used during construction is calculated as follows: total plant investment x average spending period in years x 9%.

(5) Utility Financing Method with 0.75 debt fraction, 9% interest on debt, and 15% return on equity (ROE).

SECTION 3 - BASIC ENGINEERING DESIGN DATA

3.1 OBJECTIVE OF CONCEPTUAL COMMERCIAL PLANT DESIGN

The objective of the Commercial Plant design is to develop a conceptual plant design and to determine the cost of the gas produced by that plant.

3.2 PLANT CAPACITY

The Commercial Plant design is to have a production capacity of 250 billion Btu per day of substitute natural gas. A design objective of 330 days/yr onstream operation for gas production at 100% capacity was used. To attain this capacity, the plant is to contain multiple parallel trains in the coal handling and preparation, gasification, gas purification, hydrogen production, and, possibly, wastes treatment and byproduct recovery sections.

3.3 PRODUCT SPECIFICATIONS

3.3.1 Market Specifications

All energy products and byproducts are to meet present market specifications for the most economical product.

The product gas is to be interchangeable with present pipeline natural gas in accordance with A.G.A. Research Bulletin Number 36 entitled "Interchangeability of Other Fuel Gases with Natural Gases." It must meet the following specifications:

Delivery Pressure, psig	1000 min
Delivery Temperature, °F	140 max
Moisture Content, lb/mm SCF	7 max
Heating Value (HHV), Btu/SCF	900 min
Carbon Monoxide, V%	0.1 max
Hydrogen Sulfide, grains/100 SCF	0.25 max
Total Sulfur, grains/100 SCF	10 max

The BTX byproduct is to meet the following specifications:

Estimated Composition - 100 wt% Benzene
Potential Contaminants - H_2S, HCN, NH_3, Toluene, Xylene Napthalene, Thiophene (in trace quantities)
Fuel Value (HHV) - 17,991 Btu/lb (approximate)

The chemical by-products streams are to meet the following specifications:

Ammonia

Grade - Refrigeration or Commercial
Estimated Composition - mol%.
NH_3 - 99.5, min
H_2O - 0.5, max

Sulfur

Purity, dry basis: 99.9 wt%
Carbon Content: 400 ppm, max
Ash Content: 100 ppm, max
Color: bright yellow

3.3.2 Environmental Specifications

All energy products and byproducts are to meet present and projected future environmental specifications. The Commercial Plant design is to include pollution abatement and waste treatment facilities to assure that all emissions (airborne, solid, and liquid) comply with applicable regulations. Pollution abatement design is to emphasize water reuse and byproduct recovery.

3.4 SITE SELECTION CRITERIA

The following site selection criteria are to be used for the Commercial Plant design. The location is to be mid-continent U.S.A., which is defined as Eastern Kentucky, Ohio, Pennsylvania, and West Virginia.

- The plant site is to accommodate a "grass roots" facility.

- The site is to be an inland location with road and rail accessibility.
- Sufficient water supply for the plant needs is to be available.
- The site is to be relatively level and dry and is to have a soil load bearing capacity of 4000 pounds per square foot.
- The seismic zone of the site is to be Zone 2 or below.

3.4.1 Climatic Conditions

The site climatic conditions are defined as follows for design purposes:

Temperatures, °F	
Summer high, average	88
Summer low, average	65
Summer, extreme	104
Winter high, average	44
Winter low, average	26
Winter, extreme	-18
Design frost line, feet below surface	3
Wind direction, normal	
Summer	SW
Winter	NW
Wind velocity, miles per hour	
Summer, average	6.6
Winter, average	9.5
Peak gust	92

Rainfall, inches	
Yearly, average	41.88
One month, maximum	13.50
Twenty-four hour, maximum	6.05
Snowfall, inches	
Yearly, average	13.0
One month, maximum	20.2
Twenty-four hour, maximum	10.6
Plant elevation, feet above sea level	400
Normal atmospheric pressure, psia	14.4
Thunderstorms, mean number of days	
Yearly	46
One month	8
Worst month(s)	June, July
Season	All year
Fog, mean number of days	
Yearly	14
One month	2
Worst month(s)	Jan., Oct., Dec.
Design Temperature, °F	
Dry bulb	95
Wet bulb	76

3.5 COAL AND WATER CRITERIA

The Commercial Plant design is to be based on the following coal properties:

Rank	Bituminous
Proximate analysis, as received, wt%	
Moisture	6.00
Ash	10.60
Volatile matter	31.90
Fixed carbon	51.50
	100.00
Ultimate analysis, dry wt%	
Carbon	71.50
Hydrogen	5.02
Nitrogen	1.23
Sulfur	4.42
Ash	11.30
Oxygen	6.53
	100.00
Heating value of dry coal (HHV), Btu/lb	13,186
Heating value of coal as received (HHV), Btu/lb	12,400
Size, as received	1-1/4" x 0
Density, lb/CF	
Bulk	55
Particle	85

Hardgrove grindability index	59
Fusibility of ash in reducing atmosphere, °F	
Initial deformation	2,020
Softening temperature	2,140
Hemispherical temperature	2,260
Fluid temperature	2,360
Fusibility of ash in oxidizing atmosphere, °F	
Initial deformation	2,350
Softening temperature	2,440
Hemispherical temperature	2,480
Fluid temperature	2,510
Form of sulfur as % of total sulfur	
Pyritic	35.00
Sulfate	2.00
Organic	63.00
Total	100.00
Free swelling index	2.5 - 3.5
Ash analysis, wt%	
SiO_2	44.86
Al_2O_3	21.60
TiO_2	.92
Fe_2O_3	22.31
CaO	2.92
MgO	.70
Na_2O	.63
K_2O	1.90
P_2O_5	.46
SO_3	2.73

The Commercial Plant design is to be based on the following raw water properties:

	Avg.	Max.
Total dissolved solids, ppm	662	1449
Total hardness, ppm $CaCO_3$	140	180
Noncarbonate hardness, ppm $CaCO_3$	62	71
Calcium, dissolved, ppm	38	49
Magnesium, dissolved, ppm	96	130
Bicarbonate, ppm	137	173
Carbonate, ppm	0	19
Sulfate, total, ppm	350	570
Sodium, dissolved, ppm	27	487
Potassium, dissolved, ppm	2.4	2.8
Iron, dissolved, ppm	0.015	0.03
Iron, total, ppm	4.5	11
Fluoride, dissolved, ppm	0.25	0.4
Silica, dissolved, ppm	6.5	7
Chromium, dissolved, ppm	0.0005	0.002
Chromium, suspended, ppm	0.013	0.02
Chromium, total, ppm	0.017	0.04
Arsenic, suspended, ppm	0.002	0.003
Arsenic, total, ppm	0.003	0.005
Organic nitrogen, ppm	0.12	0.22
Phenolics, ppm	0.017	0.025
pH	6	8.5
Temperature, °F (Range)	40 - 89	
Conductivity, mho	1000	1200
Turbidity, Jackson turbidity units	---	20

3.6 PLANT DESIGN BASIS

The Commercial Plant is to be designed to meet the conditions listed below.

The only raw materials delivered to the plant are to be coal and untreated raw water. Catalysts and chemicals and fuel as required are also to be supplied.

Steam is to be generated onsite as required. Possible fuels include char, coal fines, raw coal, and fuel oil. Auxiliary fuels are to be available for emergency and start-up needs only. Oxygen of 98.5 mole percent purity is to be produced onsite as required. The co-product nitrogen is to be used as inert gas wherever practical.

On-site power generation is to be included in the design.

Coal is to be received on a five days per week and two shifts (7 hours per shift) per day basis.

Raw water storage for seven days plant supply is to be provided.

The storage and handling facilities are to meet the following requirements:

Raw coal live storage	4 days supply
Raw coal dead storage	30 days supply
Dried coal feed storage	8 hours supply
Boiler coal feed storage	16 hours supply
Benzene storage	14 days
Ammonia storage	14 days
Sulfur storage	45 days solid, 7 days liquid

Air cooling is to be utilized wherever economically practical.

3.6.1 Plant Utilities

The plant utilities are defined below.

3.6.1.1 Steam Systems

	Pressure, psig	Temperature, °F
High pressure maximum	1500	1000
(Superheated) normal	1450	900
minimum	1300	
Medium pressure maximum	680	800
(Superheated) normal	600	750
minimum	575	
Low pressure maximum	55	
(Saturated) normal	50	298
minimum	45	

3.6.1.2 Cooling Water System

	Pressure, psig	Temperature, °F
Supply	50	87
Return	35	110

3.6.1.3 Startup and Emergency Fuel Gas System

Start-up and emergency fuel gas system - 100 psig at ambient temperature.

3.6.1.4 Air Systems

Plant Air - 100 psig at ambient temperature.
Instrument Air - 60 psig at ambient temperature.

3.6.1.5 Electrical System

Nominal voltage - 161 KV, 3 phase, 60 Hz.
Maximum no-load voltage - 165 KV; minimum no-load voltage - 161 KV.
3-phase short circuit symmetrical contribution from utility system - 55 MVA.
Maximum line-to-ground short circuit contribution from utility system - 19,300A sym.
Metering required - both KW and KWH.

Utilization is as follows:

	Horsepower Range				
Service	From	To	Voltage	Phase	Hertz(Hz)
Motors	1/4	200	460	3	60
	250	4000	4000	3	60
	4500	UP	13,200	3	60
		1/2 HP - (non-process)	120	1	60
Instruments			120	1	60
Lighting Dist.			120/208	(incand. & emerg.)	
			277/480	(M/V & Fluor.)	

Standby power required for energizing lighting and instruments - 480Y/277 volt, 3 phase, 60 Hz.

3.6.2 Plant Equipment

Plant equipment designs are to be based on the guidelines given below.

3.6.2.1 Pumps

Pumps conforming to API standard 610 and AVS Standard are acceptable as determined by process requirements.

Common spare for two services is permitted.

Pump sparing is to be minimized for maximum continuous plant operation. Power failure is a valid reason for sparing critical pumps.

3.6.2.2 Compressors

The choice between centrifugal and reciprocating units is to be determined by process performance requirements.

3.6.3.3 Pressure Vessels and Boilers

Pressure vessels are to be designed per ASME Section VIII - Division I, (1977).

Field erection of vessels is to be minimized.

Boilers are to be fired by the following possible fuels: char, coal fines, and/or raw coal.

3.6.3.4 Fired Heaters

Vertical firing with horizontal furnace tube arrangement is preferred.

Fuel oil is to be used as the start-up fuel.

Extended heat transfer surface is permitted with fins 0.05" thin min. x 1" high max x 5 per inch max density.

Stack lining is required to achieve a minimum thickness of 1.5 inches LHV refractory or equivalent. Stack height is to be a minimum of 100 feet above grade as determined by draft and dispersion requirements.

3.6.3.5 Shell and Tube Heat Exchangers

The preferred straight tube length is 20 feet. This is to be 3/4" diameter with 14 BWG min for low alloy materials (5 Cr - 1/2 Mo and below) and 3/4" diameter with 16 BWG min for high alloy materials (5 Cr - 1/2 Mo and above). Cooling water thermal relief devices are to be set at 75 psig.

3.6.3.6 Air Coolers

A tube length of 40 feet is preferred.

Air coolers are to be designed for the local site conditions.

3.6.3.7 Cooling Towers

Cooling towers are to be designed for the local site conditions.

3.6.3.8 Piping

Relief valves handling non-flammable materials such as CO_2, air, etc., are to be vented to the atmosphere at a minimum of 10' above any platforms or other structures.

Relief valves handling light hydrocarbons and any other flammable materials are to be vented to a closed relief system discharging to a flare system.

Waste streams, such as storm run-off water, oily water, sanitary water, and chemical drains, are to be segregated to allow individual treatment for recycle or disposal purposes.

Minimum overhead pipe clearance is to be 12' beneath main pipe racks and 7' for personnel head room. The minimum clearance for pipe racks over roadways is to be 22'.

All piping systems are to be hydrostatically tested per ANSI B 31.3.

3.6.3.9 Civil and Structural

Erection, wet and dry operations, and hydrostatic testing are to be considered in determining load conditions.

Wind velocity used for structural design purposes is to be as determined by the site conditions. Allowances are to be made for the possibility of tornados or violent storms.

Wind pressure and its net coefficient are to be as specified in ANSI A 58.1 - 1972.

Design live loads for operating platforms are to be 100 psf; for walkways, 25 psf; and for roofs, 20 psf.

Factor of safety against overturning is to be 1.5 for both erection and operation. The buoyancy effect should also be considered.

Snow load is to be based on 20 psf for the Mid-Continent location.

Compressive strength of concrete for table tops, foundations, and walls is to be 3000 psi.

Reinforcing bars are to be per ASTM A 615-72 with a grade yield stress value of 60,000 psi.

Anchor bolts are to be based on ASTM A-307 with an allowable stress of 15,000 psi and a 1/8" corrosion allowance.

Structural steel is to be designed per ASTM Standard A-36.

3.6.3.10 Instrumentation

Basic instrument system is to be mainly electronic, except that locally mounted controllers may be pneumatic.

Field installation and instrument equipment must comply with the area's electrical classification. Both intrinsically safe barriers and explosion proof housings will be used as required.

Future installation of a computer for a data logger is required; supervisory control is contemplated.

Instrument signal wires are to be both overhead and underground, as conditions permit.

Instrument identification and symbols are to be per ISA - S5.1.

All electronic control loops are to be panel mounted.

All process charge and product streams are to be continuously integrated.

Utility flow rates are to be metered and recorded as process unit totals.

3.7 ENVIRONMENTAL CRITERIA

The Commercial Plant design is to conform to all applicable environmental and safety and health regulations. These include the following:

EPA - Water pollution, air pollution, solid waste disposal
FAA - Aircraft warning
OSHA - Safety, noise, sanitary

3.8 DESIGN AND CONSTRUCTION REQUIREMENTS

The Commercial Plant design is to conform with all applicable regulations and the latest edition of the following:

ACI - Concrete Application
AISC - Design, Fabrication, & Erection of Structural Steel for Building (1969 through October 1975)
ANSI - B31.1 (1977) - Piping and Valves Design and Selection
API - Plant Safety and Equipment Design
AREA - Manual for Railway Engineering (Current to March 1975)
ASME - Pressure Vessel and Boiler (1977)
ASTM - Materials of Construction
AWS - D 1.1-75 Structural Welding (1975)
FM - Factory Mutual Approved Guide (1976)
IEEE - National Electric Safety Code (July, 1973)
ISA - Instrument Design Code
NEC - Electrical Safety Code
TEMA - Heat Exchanger Design
UL - Electric Safety Testing Codes

SECTION 4 - COMMERCIAL PLANT CONCEPT

4.1 INTRODUCTION

In flash hydropyrolysis of coal, pulverized coal is brought into contact with hot hydrogen for a very short period of time. The contact periods are of the order of milliseconds to a few seconds (as compared to other hydrogenation processes where the reaction times are of the order of hours). Typically, flash hydropyrolysis conditions consist of temperatures of 1500°F to 2000°F, hydrogen partial pressures of 500 to 1500 psi, and residence times of 500 to 3000 milliseconds. Under these conditions, typical products formed are methane, small amounts of benzene, and traces of such other compounds as ethane, light oils, and carbon oxides. The kinetics of flash hydropyrolysis is not yet completely understood. Several theories, experimental results, and reviews (References 1-8)(1) have been advanced, and work is still continuing on these reactions.

Based on data furnished by Rockwell International, a conceptual design for a commercial hydrogasification plant to produce 250 billion Btu per day of SNG has been performed as outlined below. The detailed requirements the design had to meet were described in Section 3.

4.2 GENERAL PROCESS DESCRIPTION

The conceptual process schematic of a commercial plant for the Rockwell hydrogasification process is shown in Figure 4-1, and the various units are more completely identified in Table 4.1. There are three main input streams (coal, air, and water), a product stream (SNG), and three byproduct streams (benzene, sulfur, and ammonia). As mentioned in Section 3, the plant will have multiple parallel trains to achieve the desired capacity; the description that follows is of only one train.

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(1) These numbers refer to References given in Section 7.

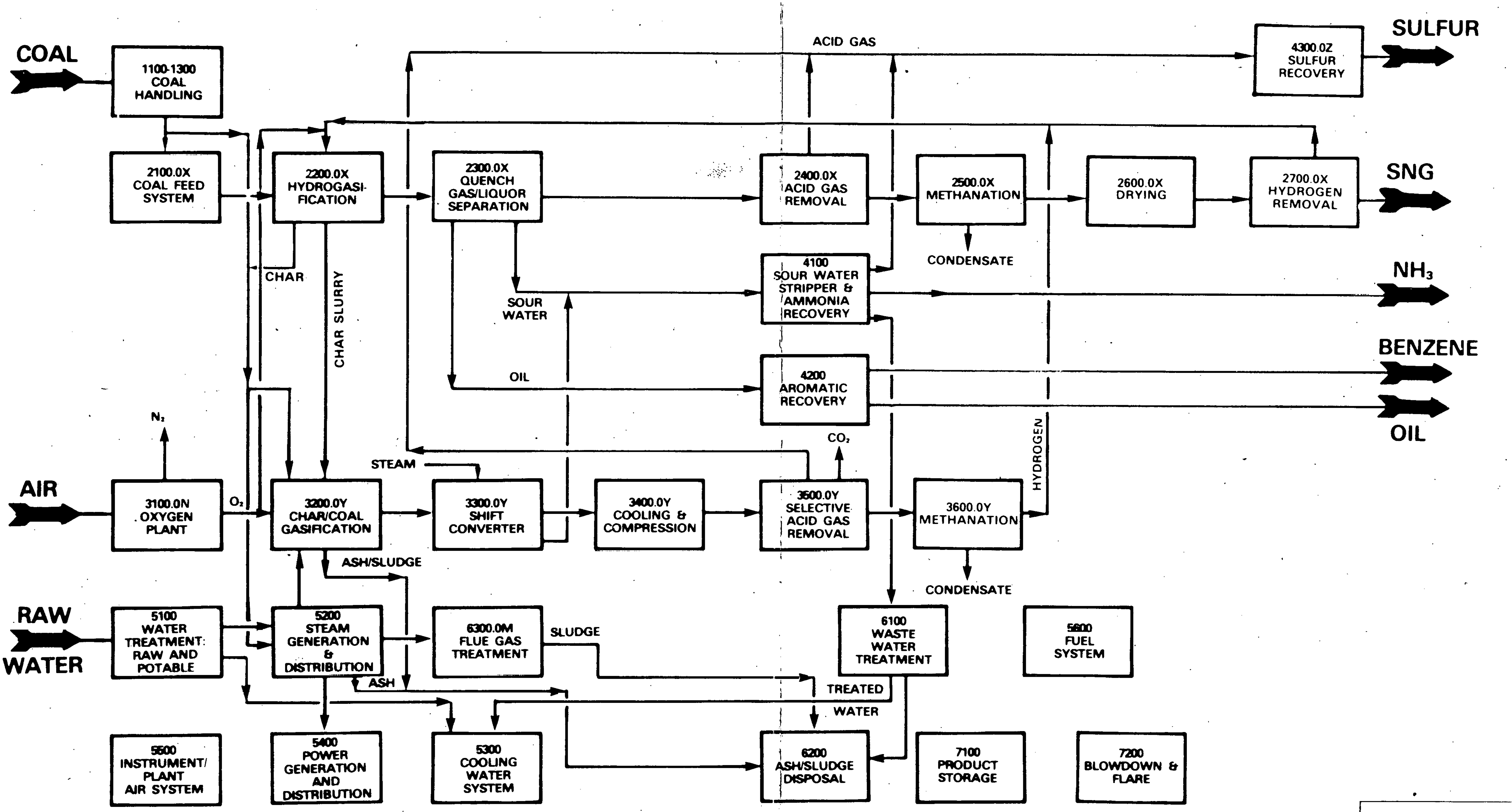

FIGURE 4-1
ROCKWELL HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

UOP/SDC
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UOP INC. AND
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CORPORATION

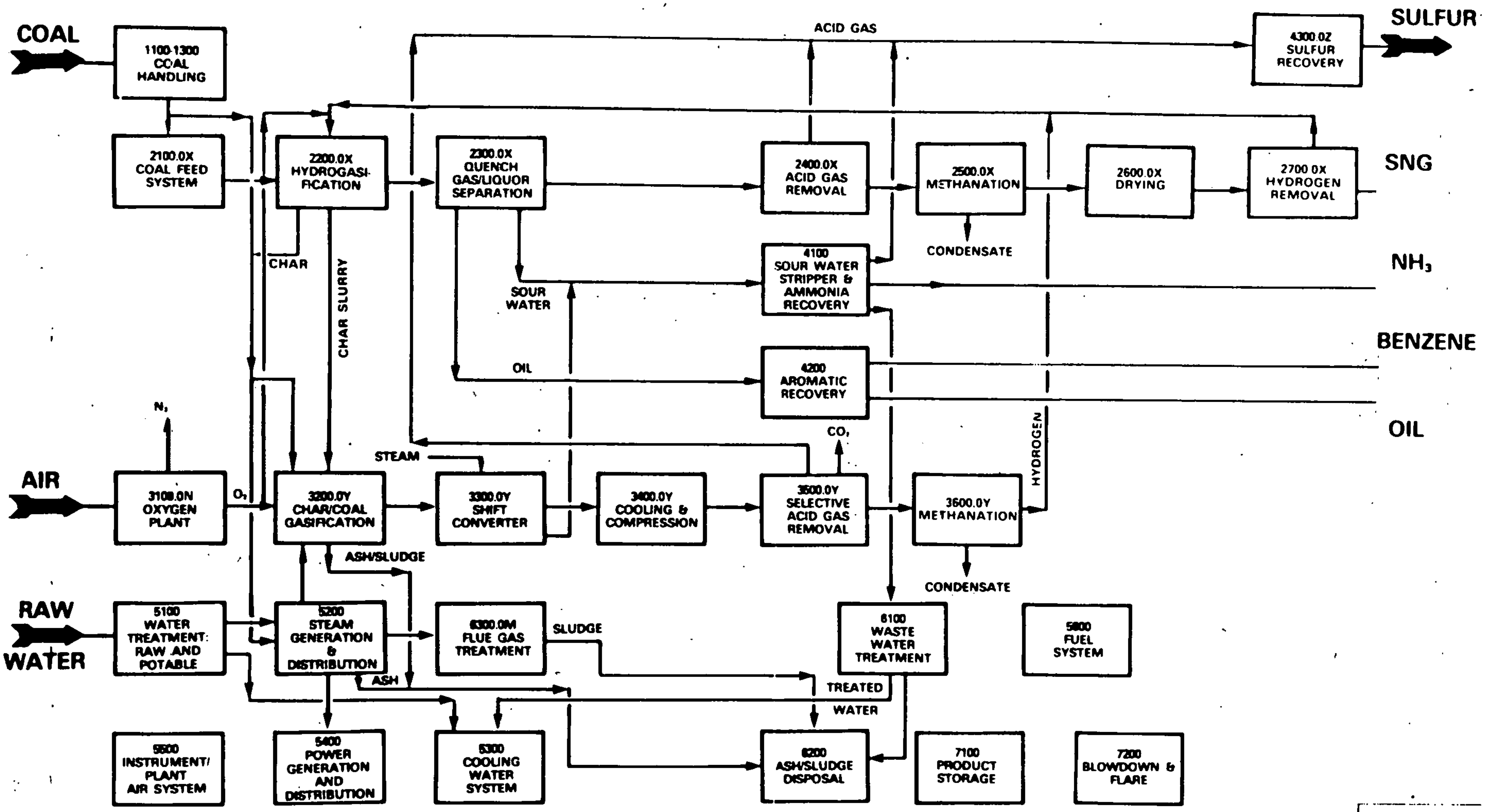

FIGURE 4-1
ROCKWELL HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

UOP SDC

Table 4.1 Names of Units of Commercial Plant 250 Billion Btu per Day SNG (Page 1 of 2)

UNIT NO(1)	UNIT NAME
	COAL HANDLING
1100	Coal Storage and Handling
1200	Coal Preparation
1300	Inter. Coal Storage and Transfer
	MAIN PROCESS TRAINS
2100.0X	Coal Feed System
2200.0X	Hydrogasification
2300.0X	Quench and Gas/Liquor Separation
2400.0X	Acid Gas Removal (Benfield)
2500.0X	Methanation
2600.0X	Drying
2700.0X	Hydrogen Removal
	HYDROGEN PRODUCTION TRAINS
3100.0N	Oxygen Plant
3200.0Y	Char/Coal Gasifier (Texaco)
3300.0Y	Shift Converter
3400.0Y	Cooling and Compression
3500.0Y	Selective Acid Gas Removal (Selexol)
3600.0Y	Methanation
	BYPRODUCTS RECOVERY
4100	Ammonia Recovery (USS Phosam)
4200	Aromatic Recovery
4300.0Z	Sulfur Recovery (Claus)
	UTILITIES
5100	Water Treatment: Raw and Potable
5200	Steam Generation and Distribution
5300	Cooling Water System
5400	Power Generation and Distribution
5500	Air System: Instrument and Plant
5600	Fuel System
5700	Sewage System

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(1) Refer to Appendix B for the logic of the unit numbering system.

Table 4.1 Names of Units of Commercial Plant 250 Billion Btu per Day SNG (Page 2 of 2)

UNIT NO	UNIT NAME
	WASTE TREATMENT
6100	Waste Water Treatment
6200	Ash/Sludge Disposal
6300.OM	Flue Gas Treatment (Dual Alkali)
7100	Product Storage
7200	Blowdown and Flare
7300	Buildings
7400	Firewater System
7500	Storm Water Treatment
7600	Loading and Unloading
7700	Site Preparation
7800	Site Finishing

The coal is transferred from storage to the coal feed system, from which it is injected into the reactor nozzles along with a hot hydrogen stream (about 2000°F). A small amount of hydrogen is burned directly with oxygen to provide the heat required to raise the temperature of the hydrogen to this figure. The length of the reactor section is designed to provide the necessary residence time at the required mass flux. At the exit of the reactor section, the solid and gaseous phases are separated in a cyclone. The solid char is sent to char-gasification for hydrogen production.

The hot gases are then quenched and the condensate phase separated into a water layer and a hydrocarbon layer. The water layer, which contains ammonia and hydrogen sulfide, is sent to sour water treatment; the hydrocarbon layer is processed in the aromatic recovery unit for BTX fractions.

The quenched gas is desulfurized in the acid gas removal system and methanated to convert traces of carbon monoxide to methane. After methanation, the gas is dried. This dried gas contains a large percent of hydrogen, which is separated and recycled to the hydrogasifier. The SNG product is then delivered into the gas pipeline.

The hydrogen required for the process is produced by gasifying the char and some coal with oxygen and steam in an entrained gasifer of the Texaco type(1). The gas from the gasifiers is treated in a shift converter to enrich the hydrogen content, then desulfurized and methanated so that the makeup gas contains only hydrogen, methane, and some inerts.

A detailed description of the main process units and the many auxiliary systems shown in Figure 4-1 is given in Section 5.

---

(1)Economics of Texaco Gasification - Combined Cycle Systems, EPRI Report No. AF-753, April 1978.

4.3 OVERALL MATERIAL BALANCE

The material balance around the hydrogasifier was generated using data transmitted by Rockwell International (Appendix A). Two cases were specified; one with no liquid production and the other with moderate liquid production.

The case with moderate liquids using Eastern Bituminous coal (Pittsburgh Seam No. 8) is considered to be the base case. Figure 4-2 shows the conceptualized process schematic with the principal material streams. These streams are identified and characterized in the material balance charts at the end of this section.

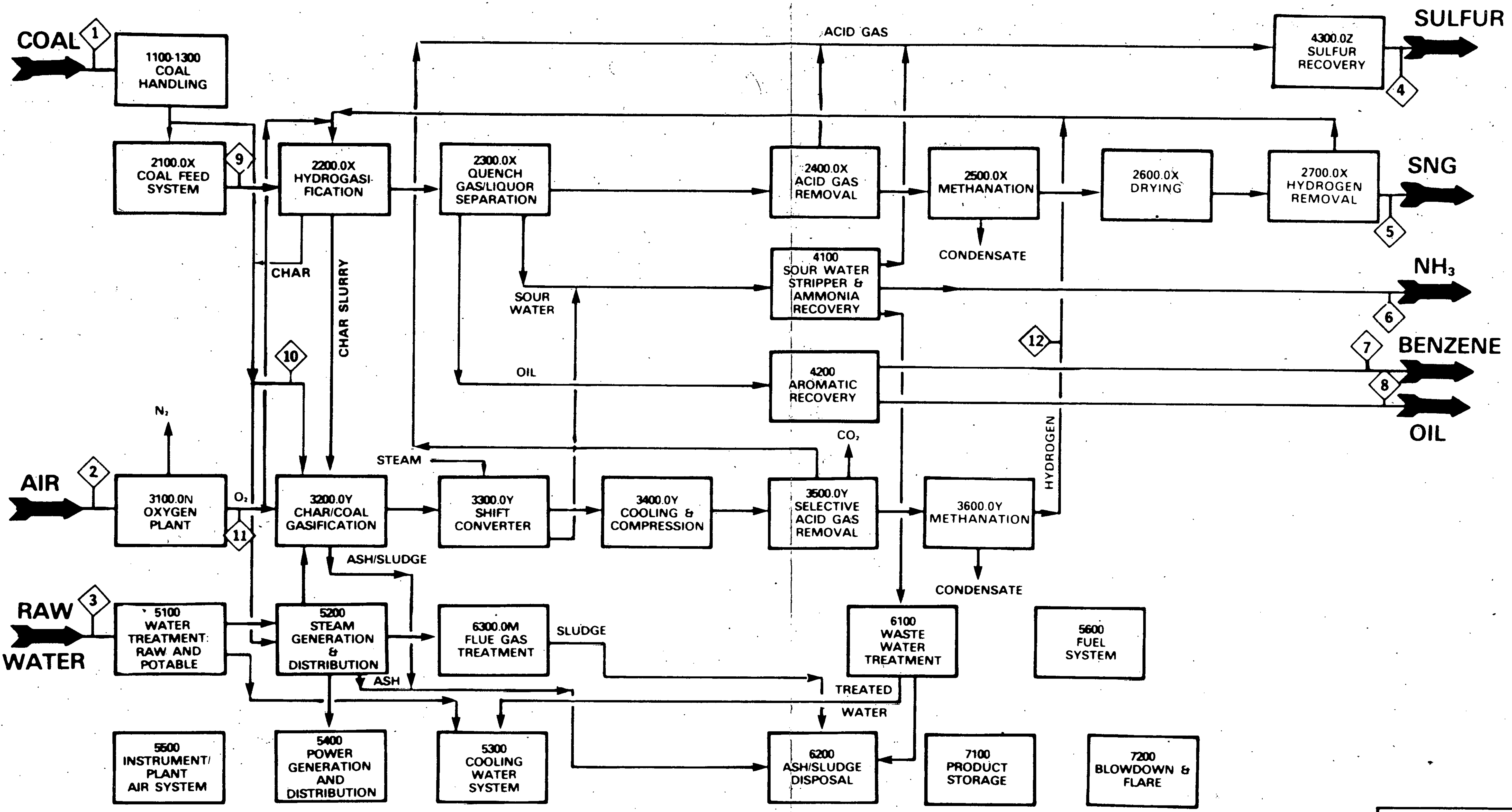

FIGURE 4-2
ROCKWELL HYDROGASIFICATION COMMERCIAL PLANT CONCEPT

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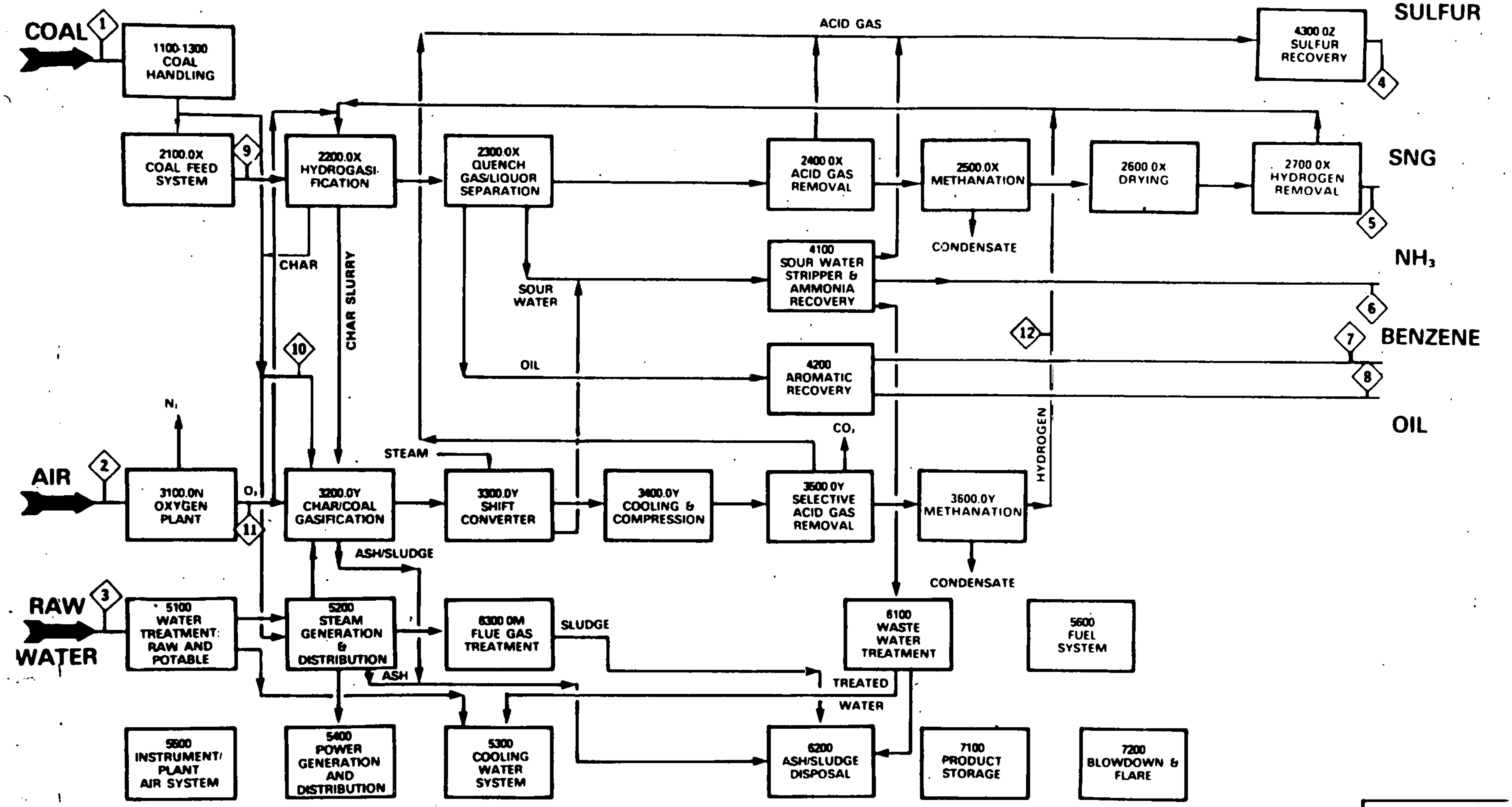

FIGURE 4-2
ROCKWELL HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

UOP SDC

4.4 OVERALL THERMAL EFFICIENCY (BASE CASE)

ENERGY INPUT	HHV	BILLION BTU/DAY
Total coal to plant	13,186 Btu/lb (MF Basis)	437.36
Total input		437.36
ENERGY OUTPUT		
SNG product		255.58
Benzene	17,991 Btu/lb(1)	16.82
Ammonia	9,086 Btu/lb(2)	2.44
Sulfur	3,992 Btu/lb(2)	4.53
Total output		279.37

$$\text{Cold gas efficiency} = \frac{255.58}{437.36} \times 100 = 58.44\%$$

$$\text{Plant Thermal Efficiency} = \frac{279.37}{437.36} \times 100 = 63.88\%$$

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(1) Measured at 60°F and 14.7 PSIA

(2) Reference: Sources and Product Economics of Chemical Products, First Edition (1973 - 1974), McGraw-Hill Publication.

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BASE CASE MATERIAL BALANCE

T.O. NO. 19
SH. NO. 1 OF 3
BY KRS
DATE 6/21/79

FOR REFERENCE SEE FIGURE 4-2

DEPARTMENT OF ENERGY
CONTRACT NO. ET-78-C-01-3117
CS/R HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

STREAM #	1		2		3		4		5	
STREAM NAME	COAL TO COAL HANDLING		AIR TO OXYGEN PLANT		WATER TO WATER TREATMENT		SULFUR TO SULFUR STORAGE		SNG PRODUCT GAS	
COMPONENT	**LB-moles/Hr**	**Lb./Hr**	**LB-moles/Hr**	**Lb./Hr**	**LB-moles/Hr**	**Lb./Hr**	**LB-moles/Hr**	**Lb./Hr**	**LB-moles/Hr**	**Lb./Hr**
Carbon		981,817								
Hydrogen		68,950							197	394
Oxygen		89,694	21,931	701,801						
Sulfur		60,770					1,479	47,334		
Nitrogen		16,800	60,415	1,691,619					30	840
Water/Moisture		87,649	1,832	32,986	392,694.4	7,068,500				
Ash		155,139								
Argon			111	4,430					7	280
Methane									27,670	442,720
TOTAL		1,460,819	84,289	2,430,836	392,694.4	7,068,500	1,479	47,334	27,904	444,234
MOLECULAR WEIGHT			28.84		18.00		32.0		15.92	
MM SCFD									253.81	
TONS/DAY	17,643 (1)		29,170				568			
GPM					14,137					
BTU/SCF									1007	

(1) INCLUDES 113 ST/D COAL TO THE DRIERS

A JOINT VENTURE OF UOP INC. AND SYSTEM DEVELOPMENT CORP.

BASE CASE MATERIAL BALANCE

T.O. NO. 19
SH. NO. 2 OF 3
BY KRS
DATE 6/21/79

FOR REFERENCE SEE FIGURE A-2

DEPARTMENT OF ENERGY
CONTRACT NO. ET-78-C-01-3117
CS/R HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

STREAM #	6		7		8		9		10	
STREAM NAME	AMMONIA TO STORAGE		BENZENE TO STORAGE		OIL TO STORAGE		COAL TO HYDROGASIFICATION		COAL TO CHAR/COAL GASIFICATION	
COMPONENT	LB-moles/Hr	Lb./Hr	LB-moles/Hr	Lb./Hr	LB-moles/Hr	Lb./Hr	LB-moles/Hr	Lb./Hr	LB-moles/Hr	Lb./Hr
Carbon								619,483		213,147
Hydrogen								43,504		14,969
Oxygen								56,593		19,472
Sulfur								38,343		13,193
Nitrogen								10,600		3,647
Water	3	54	1	18				55,303		19,028
Ash								97,886		33,680
Argon										
Methane										
Ammonia	658.6	11,196								
Benzene			499	38,945						
TOTAL	661.6	11,250	500	38,963				921,712		317,136
MOLECULAR WEIGHT	17		78							
MM SCFD										
TONS/DAY	135		467.5		NNF		11,060		3,805	

A JOINT VENTURE OF UOP INC. AND SYSTEM DEVELOPMENT CORP.

BASE CASE MATERIAL BALANCE

T.O. NO. 19
SH. NO. 3 OF 3
BY KRS
DATE 6/21/79

FOR REFERENCE SEE FIGURE 4-2

DEPARTMENT OF ENERGY
CONTRACT NO. ET-78-C-01-3117
CS/R HYDROGASIFICATION
COMMERCIAL PLANT CONCEPT

STREAM #	11		12	
STREAM NAME	OXYGEN FROM AIR SEPARATION (1)		HYDROGEN MAKE-UP (2)	
COMPONENT	LB-moles/Hr	Lb./Hr	LB-moles/Hr	Lb./Hr
Oxygen	17,352	555,276		
Hydrogen			42,780	85,560
Nitrogen	267	7,469	206	5,779
Argon	88	3,505	67	2,712
Carbon Monoxide			0.6	17
Carbon Dioxide			825	36,300
Methane			1,495.1	23,922
TOTAL	17,707	566,250	45,373.7	154,290
MOLECULAR WEIGHT	31.98		3.4	
MM SCFD			413.26	
TONS/DAY	6,795			

(1) Design Capacity of Oxygen Plant
(2) Dry Basis

SECTION 5 - PROCESS DESCRIPTION

5.1 COAL HANDLING, UNITS 1100, 1200, and 1300

Coal is received as Run of Mine coal and transferred to storage by an enclosed conveyor belt system. Large stacker reclaimers are used to handle the coal at the open storage piles. Coal is then sampled and conveyed to the primary crushers. The crushers are Flextooth type that can handle large lumps up to three inches.

The main milling operation, or secondary size reduction, is accomplished in four large wind-swept ball mills. Hot flue gas (600°F) sweeps the fines across the mill, and the heat dries the coal. About one-half of the gas is reheated and recycled; the balance is sent through a cyclone and bag house. The 200 mesh 2% moisture coal is pneumatically transferred to the storage bins in three separate systems. Each pneumatic conveying system is composed of a pulverized coal feed bin, a compressor, and a conveying duct complete with valves, abrasion resistant elbows, and diverter valves. Nitrogen from the oxygen plant is available as a transport gas.

5.2 MAIN PROCESS TRAINS

Each main processing train consists of a sequence of several units for coal feeding, hydrogasification followed by quench and cooling, and then gas treatment to separate the products from wastes and excess reactants. Three parallel trains are required for the desired capacity. From each of these trains, the products are separated and delivered, and the wastes are sent to waste treatment. Excess hydrogen is recycled to the hydrogasifier. The following is a description of the various units in each train, as shown in Figure 5.1.

5.2.1 Coal Feed System, Unit 2100.0X

The coal feed system used in this study is the dense-phase system proposed by Rockwell International. Use of the dense-phase system minimizes the amount of cold transport gas necessary to effect coal transfer.

FIGURE 5-1
ROCKWELL HYDROGASIFICATION:
MAIN PROCESS TRAIN
SCHEMATIC

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Each hydrogasifier reactor is fed by a dedicated dense-phase coal feed system comprised of a pair of pulverized coal storage bins, a pair of low-pressure charge vessels, a high-pressure lockhopper, a high-pressure coal feeder vessel, and a coal flow splitter. The low-pressure charge vessels are located beneath the coal storage bins to allow for gravity flow of coal into the charge vessels. The high-pressure lockhopper and feeder vessels are located on the same grade as the charge vessels.

The charge vessels are periodically loaded with coal from the storage bin located above them. They are then pressurized with inert gas (CO_2) to a pressure of approximately 150 psig. During a discharge period of about five minutes, the coal from the charge vessels is transferred, densephase, to the high-pressure lockhopper. A cyclone is provided on the high-pressure lockhopper to recover coal that is carried out in the gas displaced by the incoming coal charge.

The high-pressure charge vessel is pressurized with recycle hydrogen to about 1200 psig before being discharged to the reactor feeder vessel. Coal from the feeder vessel is continuously fed into the reactor through a series of flow splitter systems. About four charges per hour to the feeder system are required to maintain the required coal flow of about 140 T/hr to the hydrogasifier.

5.2.2 Hydrogasification, Unit 2200.0X

The hydrogasifier used in this study is based on Rockwell International's latest concept of a 140 T/hr commercial scale reactor.

The overall length of the reactor is estimated to be about 32 ft with an I.D. of 6 ft. Coal, hydrogen, and a small quantity of oxygen are introduced through an injection assembly.

The injector consists of six modules, each module in turn consisting of a cluster of six injector elements. Each individual injector element consists of four hot hydrogen jets impinging on a central powdered coal stream. The temperature of the hydrogen jet is raised to its desired value (2000+°F) by preheating to 1500°F in the recuperator followed by combustion with a limited amount of gaseous oxygen separately injected into each element's mixing zone.

The reactant gases and unreacted char enter a recuperator, attached directly to the bottom of the reactor vessel. The recuperator is designed to cool the char-laden gas from 1900°F to about 730°F while preheating the hydrogen stream from ambient temperature to approximately 1500°F. This unit is to be a multiple concentric tube heat exchanger, with reactor effluent flowing vertically downward inside a bundle of parallel tubes and hydrogen flowing upward in thin annuli surrounding each of the inner tubes. Basically, this is a tube and shell heat exchanger; the annuli are used to achieve high hydrogen-side heat transfer coefficients by means of high hydrogen velocity.

Unreacted char flows downward and is collected at the bottom of the gasifier. It is removed by a lockhopper and conveyed to a char quench drum, where recycle water is used as the quenching medium. The quenched char-water slurry is further cooled against cooling water in an exchanger. The pressure of this slurry is then let down in stages. A portion of the cooled and depressurized char-water slurry is sent to char/coal gasification, Unit 3200.0X, for hydrogen production.

The remaining char/coal slurry is mixed with the fines slurry from Quench and Gas/Liquor Separation, Unit 2300.0X, and solids are recovered from the slurry for use as boiler fuel. The solids recovery is accomplished by centrifuges. The water effluent from the centrifuges is recycled for char quench.

5.2.3 Quench and Gas/Liquor Separation, Unit 2300.0X

Raw gas from the hydrogasification reactor is quenched to remove entrained solids. The raw gas enters the quench tower at 1000 psig and 600°F and is contacted by water passing downward through the tower. Solids removed from the gas are collected at the bottom of the wash tower and removed as a slurry. This slurry is pumped to separate fines and water; the water is sent to Sour

Water Stripper and Ammonia Recovery, Unit 4100. Disposition of the fines was described in 5.2.2.

The overhead gas from the wash tower is cooled to approximately 100°F. The condensed oil and water are separated from the quenched gas in a separator drum. The gas is passed on to Acid Gas Removal, Unit 2400.0X, for removal of CO_2 and H_2S. A portion of the sour water is pumped back to the wash tower; the remainder is routed to Sour Water Stripper and Ammonia Recovery, Unit 4100. The oil phase is separated from the water phase and reduced in pressure. The gases released during pressure letdown are sent to Acid Gas Removal, Unit 2400.0X. The oil phase is then passed to Aromatic Recovery, Unit 4200, where oil and benzene are separated and sent to their respective storage systems. Heat is recovered from the quench process in the form of boiler feed water preheat and low-pressure steam.

5.2.4 Acid Gas Removal, Unit 2400.0X

Acid gases are removed by utilizing the Benfield Hi-Pure System. The quenched gases from Unit 2300 enter the absorber at the bottom. Hot lean potassium carbonate (K_2CO_3) solution, activated with proprietary agents, is sprayed from the top. As the quenched gases rise through the column, H_2S and CO_2 are absorbed by the solution. The traces of COS and HCN are also absorbed.

Purified gas leaves from the top of the column and is then sent to Methanation, Unit 2500.0X.

The rich K_2CO_3 solution leaves from the bottom of the absorber and is pumped to the top of the regenerator, where CO_2 and H_2S gas are stripped from the solution. The acid gases are sent to Sulfur Recovery, Unit 4300.0Z, and the regenerated absorbent is pumped back to the top of the absorber.

5.2.5 Methanation, Unit 2500.0X

The methanation process is a catalytic, fixed-bed, adiabatic, gas recycle process. A highly active nickel catalyst is used to effect the methanation reactions. Reaction temperatures are controlled by recycling a portion of cooled product gases.

This unit converts the carbon oxides in the gas from Acid Gas Removal, Unit 2400.0X, into methane. The feed to the methanation unit typically consists of carbon monoxide, hydrogen, and methane. The following main reaction occurs in the methanator:

$$CO + 3H_2 \longrightarrow CH_4 + H_2O$$

The primary methanation reactors consist of three reactors in a series-parallel arrangement. The feed gases pass through a sulfur guard bed and then split so that equal portions flow to each reactor.

Cooled methanated gas is recycled and combined with the fresh feed to each reactor for temperature control. The recycle gas acts as a heat sink to absorb the methanation heat of reaction and thus limits the temperature rise.

A cleanup methanation reactor is used to complete the methanation reactions. This reactor operates at a lower temperature than the primary methanation reactors. A portion of the gas from the third primary reactor is separated, passed through a hot recycle knockout drum, a cooler, and a cool knockout drum, and finally compressed and recycled to the first primary reactor.

The methanated gas from the clean-up reactor passes through a feed effluent exchanger, through a hot product knockout drum, and then to Product Gas Drying, Unit 2600.0X.

The methanation unit provides maximum recovery of the methanation heat of reaction by producing 1500 psig steam in waste heat boilers.

5.2.6 Drying, Unit 2600.0X

The purpose of this Unit is to dry the methanated gas from Unit 2500.0X before entering Hydrogen Removal, Unit 2700.0X.

The methanated gas is cooled to 100°F. The gas then enters a Triethylene Glycol (TEG) absorber, where it is dried to a dew point of about 35°F.

The gas enters the TEG absorber at the bottom, and TEG solution is sprayed in at the top. As the gas rises through the column, the water is absorbed by the TEG, and dry gas leaves the column from the top.

The water-laden TEG solution leaves the TEG absorber from the bottom and is regenerated by stripping with steam. The regenerated dry glycol is then recycled to the absorber. Any losses of TEG are made up by adding fresh glycol.

5.2.7 Hydrogen Removal, Unit 2700.0X

The dry product gas leaving Drying, Unit 2600.0X, contains a large quantity of hydrogen. This excess hydrogen has to be removed from the product gas before it is sent to the pipeline. The most proven method of recovering hydrogen is via cryogenic separation.

After precooling, final cleanup of traces of water, hydrogen sulfide, ammonia, carbon dioxide, and other freezable compounds is provided by molecular sieve guard beds. The gas then enters the "cold box," where the major portion of the methane is condensed in heat exchange with the effluent product streams. The uncondensed hydrogen vapor fraction is separated from the condensed liquid fraction and reheated to near ambient temperature before being recompressed and recycled to the hydrogasifiers. The methane-rich liquid stream is recovered as the SNG product stream. After pressure letdown to satisfy process refrigeration requirements, it is revaporized and reheated before being compressed to the required pipeline pressure.

5.3 HYDROGEN PRODUCTION TRAINS

A hydrogen production system is provided to supply the makeup hydrogen required for the production of 250 billion Btu/day of SNG. The system consists of three parallel oxygen plants and six parallel trains of char/coal gasifiers with associated downstream units (gas cleanup, methanation, etc.). A schematic of a process train for hydrogen production is shown in Figure 5.2.

5.3.1 Oxygen Plant, Unit 3100.0N

The oxygen required for the production of synthesis gas in the char/coal gasification is produced in three conventional air separation plants.

The design production rate of each plant is approximately 2200 T/D of oxygen with a minimum purity of 98.5%. High purity nitrogen gas (<100ppm O_2) is also produced.

Each air separation plant consists of an inlet air compressor and a cryogenic cold box, where the separation of air into oxygen and nitrogen is accomplished. The product oxygen leaves the cold box at near atmospheric pressure and is compressed to the required gasifier inlet pressure in a multistage centrifugal compressor.

5.3.2 Char/Coal Gasification, Unit 3200.0Y

A portion of char from the hydrogasifier and fresh coal is converted into raw synthesis gas (H_2 + CO) by use of the Texaco Coal Gasification Process. The Texaco gasifier is a vertical, cylindrical vessel with a carbon steel shell. The reaction section of the gasifier, the effluent gas line, and the slag separator are refractory lined.

The gasifier operates at a pressure of approximately 550 psig and temperatures in the range of 2300°F. The coal and char are charged to the gasifier as water slurry. Oxygen is combined with the coal slurry at the gasifier burners.

FIGURE 5-2
ROCKWELL HYDROGASIFICATION
HYDROGEN PRODUCTION
SCHEMATIC

UOP/SDC
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SYSTEM DEVELOPMENT
CORPORATION

The gasifier temperature is maintained above the ash fusion point to ensure free flowing molten slag. The slag, containing most of the ash present in the coal, falls into a water quench at the bottom of the gasifier.

The resultant ash slurry is withdrawn from the gasifier and sent to the slag dewatering unit.

Hot synthesis gas is withdrawn from the top of the gasifier and cooled to the required shift unit inlet gas temperature in a series of waste heat recovery boilers that produces high-pressure steam.

5.3.3 Shift Converter, Unit 3300.0Y

The purpose of this unit is to adjust the hydrogen to carbon monoxide ratio of the raw gas from Char/Coal Gasification, Unit 3200.0Y, for downstream processing in Methanation, Unit 3600.0Y. The adjustment is accomplished catalytically by the shift reaction:

$$CO + H_2O \longrightarrow CO_2 + H_2$$

The shift conversion is exothermic and takes place over a series of reaction steps. The hot, shifted gas from the final reaction step is cooled to a temperature of about 880°F in heat exchange with incoming feed gas. About 95% of CO is shifted to hydrogen in this unit.

5.3.4 Cooling and Compression, Unit 3400.0Y

Before entering the acid gas removal unit, the hot gas from the shift converter unit is cooled to near ambient temperature and compressed to about 1200 psig. Gas cooling is accomplished in a waste heat recovery boiler generating low-pressure steam followed by trim cooling. The sour water condensed during the cooling is sent to Sour Water Stripper and Ammonia Recovery, Unit 4100. The cooled gas stream is compressed, in two stages, to about 1200 psig in a centrifugal machine with intercooling. The compressed gas is transferred to Selective Acid Gas Removal, Unit 3500.0Y.

5.3.5 Selective Acid Gas Removal, Unit 3500.0Y

This unit removes carbon dioxide and hydrogen sulfide from the gas. The process uses Selexol solvent (dimethyl ether of polyethylene glycol) to remove H_2S and CO_2 from the sour gas by physical absorption.

The compressed gas from Unit 3400.0Y enters the hydrogen sulfide absorber, where H_2S is selectively removed in a regenerative process. The CO_2 absorption is suppressed to produce a sufficiently sulfur rich gas, at least 25% H_2S, to be sent to Sulfur Recovery, Unit 4300.0Z. The gas leaving the H_2S removal section passes to the CO_2 removal section, where H_2S concentration is further reduced. In the CO_2 absorber, the gas is contacted with the solvent at lower temperatures for removal of CO_2. The flashed gases from the rich solvent are recycled to minimize the methane losses. The stripping is done with nitrogen. The CO_2 goes either to the plant inert gas system or to the atmosphere. The treated gas, which contains less than 4 ppm H_2S, is passed on to Methanation, Unit 3600.0Y.

5.3.6 Methanation, Unit 3600.0Y

The feed to the methanation unit consists of carbon monoxide, hydrogen, and methane. This unit converts the carbon oxides into methane. The type of catalyst and process configuration of the unit are quite similar to those described in section 5.2.5.

The effluent gas from this unit is essentially makeup hydrogen of about 96% purity.

5.4 BYPRODUCTS RECOVERY, UNITS 4100, 4200 and 4300.0Z.

The byproducts produced by the Rockwell hydrogasification process are elemental sulfur, ammonia, and benzene.

The hydrogen sulfide-rich gases from Acid Gas Removal Units, 2400.0X and 3500.0Y, are partially burned with air to provide feed stock for Sulfur Recovery, Unit 4300.0Z. This unit uses the Claus process to produce elemental sulfur and recover heat in the form of low-pressure steam. The tail gas from these units is incinerated and sent to Flue Gas Treatment, Unit 6300.0M, to remove any oxides prior to discharge into the atmosphere.

The condensed sour water from Quench Gas/Liquor Separation, Unit 2300.0X, and Shift Converter, Unit 3300.0Y, is sent to Sour Water Stripper and Ammonia Recovery, Unit 4100. The selected process, USS Phosam, absorbs ammonia in a phosphoric acid solution. The ammonia is subsequently stripped off, condensed, and recovered. The water effluent from ammonia recovery is sent to Waste Water Treatment, Unit 6100.

Aromatics produced by the gasification reactions are condensed in the quench unit. The oil fractions are separated in Aromatic Recovery, Unit 4200. In this unit, benzene is produced as a byproduct, and aromatic oils, if any, are used as fuel.

5.5 UTILITIES, UNITS 5100, 5200, 5300, 5400, 5500, 5600, and 5700

Clarified raw water is demineralized for boiler feed water makeup in Unit 5100. This unit produces makeup boiler feed water for both high- and low-pressure boilers. The Process and Potable Water System also uses clarified water for makeup purposes. Most of the process water required throughout the plant is recycled from Waste Water Treatment, Unit 6100. Part of the clarified water is further treated, sand filtered, and chlorinated before being used for drinking and sanitary purposes.

Steam Generation and Power Generation, Units 5200 and 5400, provide utility and power generation and distribution throughout the plant. The boilers, fired by coal, coal fines, and char, generate high-pressure, superheated steam for use in the char/coal gasifiers, power generation units, and other utility systems. Low-pressure steam is generated by process heat recovery and/or by letdown through desuperheaters.

Cooling Water System, Unit 5300, is a conventional closed loop system with cooling water circulating between the process exchangers, surface condensers, and cooling towers. The makeup is clarified water. Chemicals are continuously added to prevent corrosion and scale buildup.

Plant and Instrument Air System, Unit 5500, provides service air for general utility use throughout the plant. Part of the plant air is dried by conventional techniques to serve as instrument air.

Fuel System, Unit 5600, provides the appropriate fuel for both start-up and emergency situations.

5.6 WASTE TREATMENT AND DISPOSAL, UNITS 6100, 6200, and 6300.0M

Waste Water Treatment, Unit 6100, converts the various aqueous streams into suitable recycle water. The residual water, if too contaminated for recycle purposes, is treated by biological oxidation.

Ash and Sludge Disposal, Unit 6200, collects solid waste and ash from the entire plant and disposes of them in an environmentally acceptable manner.

Flue Gas Treatment, Unit 6300.0M, handles the flue gas from Steam Generation, Unit 5200, and the incinerated tail gas from Sulfur Recovery, Unit 4300.0Z, to make them environmentally acceptable for discharge into the atmosphere. The process is a dual-alkali type using a sodium solution for the absorption step and then a lime system to convert the captured sulfur dioxide into a throwaway sludge for disposal in an appropriate landfill.

5.7 SITE FACILITIES, UNITS 7100-7800

Units 7100 and 7600 are storage and shipment facilities for the byproducts produced in the plant. Facilities are also included for bulk receipt of materials into the plant.

Blowdown and Flare, Unit 7200, is the overall relief header and flare system for the entire plant.

Buildings, Unit 7300, comprises all the buildings necessary to operate the coal gasification facility. These include administration, laboratory, warehouse, garage, maintenance, control room, switch house, fire house, and guard house.

Firewater System, Unit 7400, uses raw water directly, without any pretreatment, for firefighting and fire control.

Storm Water Treatment, Unit 7500, consists of the facilities necessary to impound storm water runoff from the plant and to discharge it in an acceptable manner.

Site Preparation, Unit 7700, comprises site clearing and grading for all process areas, dikes, ditches, ponds, roads, and railroads.

Site Finishing, Unit 7800, comprises all finishing earthwork, including landscaping. It includes any linings required for ponds and any base materials required under paved areas, roads, and railroads. It also includes final paving, such as concrete or asphalt, and final ballast as well as trackwork itself. The permanent plant fencing is also included.

SECTION 6 - ECONOMIC EVALUATION

6.1 BASIS OF EVALUATION

This section contains an economic analysis performed to establish the cost of the gas produced by the Commercial Plant described in earlier sections. A nominal production rate of 82.5 trillion Btu per year was used. The cost of gas was determined for two types of financing - utility financing and discounted cash flow private financing. The assumptions for the financing methods are shown below.

Utility Financing Method

Project Life = 20 years
Depreciation = Straight line on total capital investment (working capital and land excluded)
Federal Income Tax = 48%
Fraction Debt = 0.75
Interest on Debt = 9%
Return on Equity = 15%

DCF Method

Federal Income Tax = 48%
State and Local Tax = 4%
DCF Rate of Return on Total Capital = 12%
Depreciation = 16 years, sum-of-the-years'-digits method
Investment Tax Credit = 0
Equity = 100% (except for working capital and land)

6.2 CAPITAL REQUIREMENTS

6.2.1 Capital Cost Basis

The capital cost estimate is expressed in terms of second-quarter 1979 dollars. The overall accuracy of the capital cost estimate is ± 25%.

6.2.2 Erected Plant Cost

The erected plant cost for the Commercial Plant is summarized on a unit cost basis in Table 6.1. Erected costs were estimated using standard procedures developed through experience in the design and construction of large industrial plants. An allowance was included for the cost of such items as plant safety equipment and vehicles, office equipment, and laboratory and shop equipment. Procedures used by other reputable architect and engineer firms may vary considerably, but should lead to estimates within the accuracy of ± 25%.

6.2.3 Total Capital Requirements

The total capital requirements for base and zero liquids cases are shown in Table 6.2. The capital requirements for the zero liquids case were factored from those for the base case.

Contractor's costs include construction costs, home office engineering, and insurance. Construction costs include indirect field costs, construction tools and equipment, and construction supervision. The costs are based upon the direct field labor manhours, scope of the project, and special erection equipment required.

Table 6.1 Unit Cost Summary (Base Case)
(Page 1 of 2)

UNIT NO.	UNIT NAME	ERECTED UNIT COST, $
1100	Coal Storage and Handling	22,547,000
1200	Coal Preparation	21,842,000
1300	Inter. Coal Storage and Transfer	6,964,000
2100.0X	Coal Feed System	15,931,000
2200.0X	Hydrogasification	112,100,000
2300.0X	Quench and Gas/Liquor Separation	32,541,000
2400.0X	Acid Gas Removal	10,435,000
2500.0X	Methanation	10,677,000
2600.0X	Drying	7,950,000
2700.0X	Hydrogen Removal	58,074,000
3100.0N	Oxygen Plant	102,788,000
3200.0Y	Char/Coal Gasifier	55,413,000
3300.0Y	Shift Converter	48,682,000
3400.0Y	Cooling and Compression	17,630,000
3500.0Y	Selective Acid Gas Removal	73,666,000
3600.0Y	Methanation	7,050,000
4100	Ammonia Recovery	11,226,000
4200	Aromatic Recovery	894,000
4300.0Z	Sulfur Recovery	15,172,000

Table 6.1 Unit Cost Summary (Base Case)

(Page 2 of 2)

UNIT NO.	UNIT NAME	ERECTED UNIT COST, $
5100	Water Treatment: Raw and Potable	17,844,000
5200	Steam Generation and Distribution	106,924,000
5300	Cooling Water System	26,806,000
5400	Power Generation and Distribution	28,600,000
5500	Air System: Instrument and Plant	3,652,000
5600	Fuel System	1,045,000
5700	Sewage System	266,000
6100	Waste Water Treatment	12,368,000
6200	Ash/Sludge Disposal	29,794,000
6300.0M	Flue Gas Treatment	55,593,000
7100	Product Storage	12,833,000
7200	Blowdown and Flare	3,591,000
7300	Buildings	4,043,000
7400	Firewater System	20,204,000
7500	Storm Water Treatment	5,139,000
7600	Loading and Unloading	6,303,000
7700	Site Preparation	5,355,000
7800	Site Finishing	13,084,000
	Allowances	7,455,000
	Total Erected Plant Cost	992,481,000

Table 6.2 Capital Requirements

	$	
Plant Investment	**Base Case**	**Zero Liquids Case**
Erected Plant Cost	992,481,000	
Contractor's Costs and Fees	109,172,900	
Project Contingency	165,248,100	
Total Plant Investment	1,266,902,000	1,268,418,500
Initial Charge of Catalysts & Chemicals	16,203,800	17,579,000
Spare Parts	4,962,400	4,968,400
Paid-Up Royalties	3,250,400	3,413,000
Start-Up Costs	45,531,200	47,160,700
Total Capital Investment [DCFM]	1,336,849,800	1,341,539,600
Land Acquisition Cost	2,750,000	2,750,000
Working Capital	39,329,900	39,315,000
Total Capital Requirements [UFM](1)	1,378,929,700	1,383,604,600

---

(1) The values stated here do not include allowance for funds used during construction.

Home office engineering costs have been estimated on the basis of a single prime contractor's costs, as are the costs associated with the supervision of the subcontractors.

A project contingency was taken at 15% of the sum of erected plant cost, contractor's costs, overhead, and profit.

The initial charge of catalysts and chemicals is shown in Table 6.3.

Cost of spare parts was estimated as 0.5 percent of the cost of materials and equipment.

Paid-up royalties are shown in Table 6.4. Engineering fees for other units received from a licensor/supplier were included in the installed cost for those units.

Start-up costs were taken at 20% of the gross operating costs.

Land acquisition cost was assumed to be $5,000 per acre.

Working capital requirements are shown in Table 6.5. Requirements were taken as the sum of raw material and byproduct inventory plus 30 days gross operating costs.

Table 6.3 Initial Charge of Catalysts & Chemicals

Unit No.	Item	$	
		Base Case	Zero Liquids Case
2400.0X	Solvent	18,900	
2500.0X	Catalyst	1,358,100	
2600.0X	Glycol	42,400	
3300.0Y	Catalyst	6,765,000	
3500.0Y	Solvent	1,344,000	
3600.0Y	Catalyst	701,100	
4100	Chemicals	390,000	
4300.0Z	Catalyst	247,300	
5100,6100	Chemicals	1,560,000	
6200	Polyelectrolyte	51,000	
6300	Chemicals	3,726,000	
	TOTAL	16,203,800	17,579,000

Table 6.4 Paid-Up Royalties

Unit No.		$	
		Base Case	Zero Liquids Case
2400.0X		322,000	
2500.0X		516,000	
4100		2,412,400	
	TOTAL	3,250,400	3,413,000

Table 6.5 Working Capital Requirements

Raw Material and Byproduct Inventory	$ Base Case	$ Zero Liquids Case
Coal (35 days)	15,307,700	
Water (7 days)	57,000	
Benzene (14 days)	1,606,100	
Ammonia (14 days)	225,800	
Sulfur (52 days)	1,054,900	
Fuel Oil (14 days)	382,400	
TOTAL	18,633,900	17,878,400
Gross Operating Costs (30 days)	20,696,000	21,436,600
TOTAL WORKING CAPITAL	39,329,900	39,315,000

6.3 OPERATING COSTS

6.3.1 Operating Cost Basis

The operating cost estimates were prepared for the Commercial Plant designs based on an operating schedule of 330 days per year of operation at full capacity.

6.3.2 Operating Requirements and Unit Costs

Raw material requirements, byproduct rates, unit prices, operating labor, waste disposal, and land requirements are shown in Table 6.6. Coal, raw water, and fuel oil unit costs represent the cost as delivered to the plant. Byproduct prices are net back to the plant.

The cost of coal was set at \$1.00/MMBtu for bituminous coal feed. Coal cost was converted to \$/ton using the heating value of the coal as received.

Byproduct prices assume that there is a market available within an acceptable transportation distance. The prices for sulfur and ammonia were taken at current market prices. Because of uncertainty as to the quality and value of the byproduct raw benzene, the base case was evaluated at a benzene price of \$0.90/gallon. The predicted value of chemical grade benzene can be as high as \$1.55/gallon; however, significant expenditures in terms of equipment and hydrogen may be required to upgrade raw benzene to meet chemical grade specifications. At the same time, the market is limited enough that multiple plants producing chemical grade benzene could be expected to drive down the price in the market.

The average wage rate for operating labor was taken at \$8.20/hr. The waste disposal cost includes the cost of hauling the solid wastes to a nearby landfill site and the cost of operating the landfill. The waste disposal cost is based upon sending all non-toxic solid wastes directly to a non-hazardous landfill and treating the toxic solids to an acceptable limit before sending to landfill.

Table 6.6 Operating Requirements and Unit Costs

	Quantity		Unit Cost
Raw Materials	**Base Case**	**Zero Liquids Case**	
Bituminous Coal (as received)	17,643 ST/D	18,573 ST/D	$24.79/ST ($1.00/MMBtu)
Water	14,137 GPM	14,898 GPM	$0.40/1,000 gal
Byproducts			
Sulfur	568 ST/D	591.3 ST/D	$40/LT
Benzene	3,035 BPD	-	$ 0.90/Gallon
Ammonia	134.4 ST/D	121.5 ST/D	$120/ST
Operating Labor	75 Men/Shift	75 Men/Shift	$ 8.20/hr
Fuel Oil	(For start-up only)		$16.80/BBL
Waste Disposal	4242 ST/D	4439 ST/D	$ 1.00/ST
Land	550 Acres	550 Acres	$5,000/Acre

Solid wastes sent to the secure landfill are dewatered sludge and evaporator salt.

6.3.3 Annual Operating Costs

The annual operating costs for the Commercial Plant are shown in Table 6.7. The only raw material purchased is coal; the purchased utilities are raw water and fuel oil. The annual cost for catalyst and chemicals is summarized in Table 6.8. Operating labor is based upon 8,760 hours per year. Operating labor supervision was taken at 20% of operating labor. Administrative and general overhead was charged at 60% of operating labor and supervision. Operating supplies were taken at 30% of operating labor. A maintenance factor to cover both maintenance supplies and labor was applied to each unit's investment cost (erected cost plus contractor's charges and contingency). The factors applied to each unit are shown in Table 6.9.

Taxes and insurance were taken at 1.5% of total plant investment.

Land and working capital were assumed to be part of the capital base for UFM. For DCFM, land and working capital were assumed to be financed by debt at 9%. Purchase and resale value of the land and working capital were assumed to be equal to the value of the bonds leading to an annual cost of land and working capital of 9% of their value.

Inflation was not considered.

Table 6.7 Annual Operating Costs

	$/Year	
Operating Costs	Base Case	Zero Liquids Case
Raw Materials (Coal)	144,330,200	
Catalysts and Chemicals	6,617,000	
Utilities - Water	2,687,200	
Labor - Operating	5,387,400	
- Supervision	1,077,500	
Administrative and General Overhead	3,879,000	
Operating Supplies	1,616,200	
Maintenance Material and Labor	41,657,900	
Taxes and Insurance	19,003,500	
Waste Disposal	1,400,000	
Total Gross Operating Costs	227,655,900	235,803,300
Byproduct Credits		
Sulfur	6,694,300	6,968,900
Benzene	37,858,600	-
Ammonia	5,322,200	4,811,400
Total Byproduct Credits	49,875,100	11,780,300
Total Net Operating Costs [UFM]	177,780,800	224,023,000
Interest on Land and Working Capital	3,787,200	3,785,800
Total Annual Operating Costs [DCFM]	181,568,000	227,808,800

Table 6.8 Annual Catalyst and Chemicals Cost

Unit No.		$ Base Case	$ Zero Liquids Case
2400.0X	Solvent	9,500	
2500.0X	Catalyst	377,900	
2600.0X	Glycol	129,300	
3300.0Y	Catalyst	1,144,100	
3500.0Y	Solvent	134,000	
3600.0Y	Catalyst	222,700	
4100	Chemicals	278,800	
4300.0Z	Catalyst	123,700	
5100,6100	Chemicals	1,425,000	
6200	Chemicals	198,000	
6300	Chemicals	2,574,000	
	TOTAL ANNUAL COST	6,617,000	7,224,700

Table 6.9 Maintenance Factors

UNIT NO.	UNIT NAME	% UNIT INVESTMENT
1100	Coal Storage and Handling	6
1200	Coal Preparation	6
1300	Inter. Coal Storage and Transfer	6
2100.0X	Coal Feed System	6
2200.0X	Hydrogasification	6
2300.0X	Quench and Gas/Liquor Separation	6
2400.0X	Acid Gas Removal	3
2500.0X	Methanation	3
2600.0X	Drying	3
2700.0X	Hydrogen Removal	3
3100.0N	Oxygen Plant	3
3200.0Y	Char/Coal Gasifier	6
3300.0Y	Shift Converter	3
3400.0Y	Cooling and Compression	3
3500.0Y	Selective Acid Gas Removal	3
3600.0Y	Methanation	3
4100	Ammonia Recovery	3
4200	Aromatic Recovery	3
4300.0Z	Sulfur Recovery	3
5100	Water Treatment: Raw and Potable	1
5200	Steam Generation and Distribution	1
5300	Cooling Water System	1
5400	Power Generation and Distribution	1
5500	Air System: Instrument and Plant	1
5600	Fuel System	1
5700	Sewage System	1
6100	Waste Water Treatment	3
6200	Ash/Sludge Disposal	3
6300.0M	Flue Gas Treatment	3
7100	Product Storage	1
7200	Blowdown and Flare	1
7300	Buildings	1
7400	Firewater System	1
7500	Storm Water Treatment	3
7600	Loading and Unloading	1
7700	Site Preparation	1
7800	Site Finishing	1
	Allowances	1

6.4 ECONOMIC ANALYSIS

6.4.1 Economic Analysis Basis

The selling price of the product gas (cost of gas) was calculated by the utility financing method and by the discounted cash flow method for both the base case and the zero liquids case. Project life was taken as 25 years, plant life as 20 years. Capital was assumed to be equity capital except for land and working capital. The cash drawdown schedule during the construction period (five years) is shown in Table 6.10.

6.4.2 Cost of Gas

The derivation of the equations used to calculate the gas cost by both methods for both cases is shown in Table 6.11. The parameters used to calculate the cost of gas are also shown in Table 6.11. The cost of gas as calculated by each method for the two cases is shown in Table 6.12.

6.4.3 Sensitivity Analysis

A sensitivity analysis was performed to show the effect of the following on the cost of gas:

- Variations in coal cost
- Variations in rate of return
- Variations in total plant investment
- Variations in coal requirements
- Variations in benzene value

Results of the analysis are presented in Table 6.13. In each case, only the variable of interest was changed from its base value.

Table 6.10 Cash Drawdown Schedule

(DCF Method)

Year	$	
	Base Case	Zero Liquids Case
1	50,676,100	50,736,700
2	304,056,500	304,420,400
3	405,408,600	405,894,000
4	342,063,500	342,473,000
5	164,697,300	164,894,400
Total Plant Investment	1,266,902,000	1,268,418,500

Table 6.11 Gas Cost Equations (Page 1 of 4)

Discounted Cash Flow Method

The average product selling price is generated to produce a Net Present Value equal to zero for the project life, i.e., the discounted present value of cash outflows during construction equals the discounted present value of cash inflows during the operating phase.

Expressed in a formula

$$\left(\sum_{i=1}^{n} C_i PWF_i \right)_{\substack{\text{Construction} \\ \text{Years}}} = \left(\sum_{i=n+1}^{N} C_i PWF_i \right)_{\substack{\text{Operating} \\ \text{Years}}}$$

Where: n = period of construction
N = project life
C_i = cash flow in year i
PWF_i = present worth factor in year $i = (1 + r)^{-i}$
r = DCF rate of return on total capital

Based upon the following parameters

Equity Capital = 100% (except for working capital and land)
Project Life = 25 years
Plant Life = 20 years
Depreciation = 16 years, sum-of-the-years'-digits method
Interest on land begins in year 1

Table 6.11 Gas Cost Equations (Page 2 of 4)

The cash flows during the construction period can be expressed as:

$$\sum_{i=1}^{5} X_i\,(TCI)\,PWF_i + \sum_{i=1}^{5} (LI)\,PWF_i$$

Where: TCI = Total Capital Investment
X_i = Fraction of TCI spent in year i
LI = Interest on Land

The cash flows during the operating years can be expressed as:

$$\sum_{i=6}^{25} \left[(1 - TAXR)(AR - AOC_i - DEP_i) + DEP_i \right] PWF_i$$

Where: TAXR = Income Tax Rate
AR = Annual Sales Revenue
AOC_i = Annual Operating Cost in Year i
DEP_i = Depreciation in Year i

Equating the cash flows during the construction period to the cash flows during the operating years, substituting COG x PROG = AR, and separating terms yields:

$$COG = \frac{TCI \sum_{i=1}^{5} X_i\,PWF_i + LI \sum_{i=1}^{5} PWF_i + (1 - TAXR) \sum_{i=6}^{25} AOC_i\,PWF_i - TAXR\,(TDI) \sum_{i=6}^{25} DR_i\,PWF_i}{(1 - TAXR)\,PROG \sum_{i=6}^{25} PWF_i}$$

Where: TCI = Total Capital Investment
X_i = Fraction of TCI spent in year i
LI = Interest on Land
TAXR = Income Tax Rate
AOC_i = Operating Cost in Year i
TDI = Total Depreciable Investment
DR_i = Depreciation Rate in Year i
PROG = Production Rate of Gas

Table 6.11 Gas Cost Equations

(Page 3 of 4)

Note: Total Capital Investment Includes:

- Total Plant Investment
- Paid-Up Royalties (assumed year 5)
- Start-up Costs (assumed year 5)
- Initial Charge of Catalysts and Chemicals (assumed year 5)
- Spare Parts Purchase (assumed year 5)

Annual Operating Costs Includes:

- Start-up and Costs tax credit (assumed year 6)
- Credit for liquidation of Spare Parts Inventory (assumed year 25)
- Interest on Land and Working Capital

Total Depreciable Investment Includes:

- Interest on Land During Construction
- Total Plant Investment
- Paid-up Royalties
- Initial Charge of Catalysts and Chemicals

Utility Financing Method

Using the following parameters:

Project Life = 20 years
Depreciation = straight line on Total Capital Investment (working capital and land excluded)
Federal Income Tax Rate = 48%
Fraction Debt = 0.75
Interest on Debt = 9%
Return on Equity = 15%

Table 6.11 Gas Cost Equations

(Page 4 of 4)

$$COG^{(1)} = \frac{N + 0.12C + 0.02W}{G}$$

Where: COG = Average Gas Cost, \$/MMBtu

N = Total Net Operating Costs, \$MM/Year

C = Total Capital Requirements, \$MM (includes allowances for funds used during construction)

W = Working Capital and Land, \$MM

G = Annual Product Gas Rate, Trillion Btu/Year

---

(1) "Factored Estimates for Eastern Coal Commercial Concepts", Report FE-2240-31, prepared by C. F. Braun & Co. under Contract No. EX-76-C-01-2240, September 1978.

Table 6.12 Cost of Gas

Capital Requirement $	Base Case	Zero Liquids Case
Capital Investment	1,336,849,800	1,341,539,600
Land Acquisition Cost and Working Capital [UFM only]	42,079,900	42,065,000
Total Capital Requirements	1,378,929,700	1,383,604,600
Operating Costs, $/Year		
Net Operating Cost	177,780,800	224,023,000
Interest on Land and Working Capital [DCFM only]	3,787,200	3,785,800
Total Annual Operating Costs	181,568,000	227,808,800
Cost of Gas, $/MMBtu		
Utility Financing Method	4.43	5.00
DCF Method	6.42	6.96

Table 6.13 Sensitivity Analysis

	Cost of Gas, $/MMBtu			
	Base Case		Zero Liquids Case	
Coal Cost, $/MMBtu	UFM	DCFM	UFM	DCFM
.75	3.99	5.97	4.55	6.50
1.00	4.43	6.42	5.00	6.96
1.25	4.87	6.86	5.46	7.43
1.50	5.30	7.30	5.92	7.89
Rate of Return, %				
9	-	5.26	-	5.83
10.5	-	5.80	-	6.36
12	-	6.42	-	6.96
15	-	7.69	-	8.26
Capital Investment, $MM				
-200	3.97	5.65	4.55	6.20
Base	4.43	6.42	5.00	6.96
+200	4.88	7.18	5.46	7.73
+400	5.33	7.94	5.91	8.49
Coal Requirement, % of Base				
90	4.25	6.23	4.82	6.77
Base	4.43	6.42	5.00	6.96
110	4.60	6.60	5.19	7.16
120	4.78	6.78	5.37	7.35
Value of Liquids, $/gal				
.90	4.43	6.42	-	-
1.55	4.07	6.09	-	-
2.00	3.80	5.86	-	-

SECTION 7 - REFERENCES

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Rockwell
International

14 May 1979 In response refer to 79ESG5050

Dr. K. Sarma
UOP/SDC Joint Venture
7929 West Park Drive
McLean, VA 22101

Dear Dr. Sarma:

Here is information that we discussed on the phone last week. I will be looking forward to your call when you have reviewed this material.

Very truly yours,

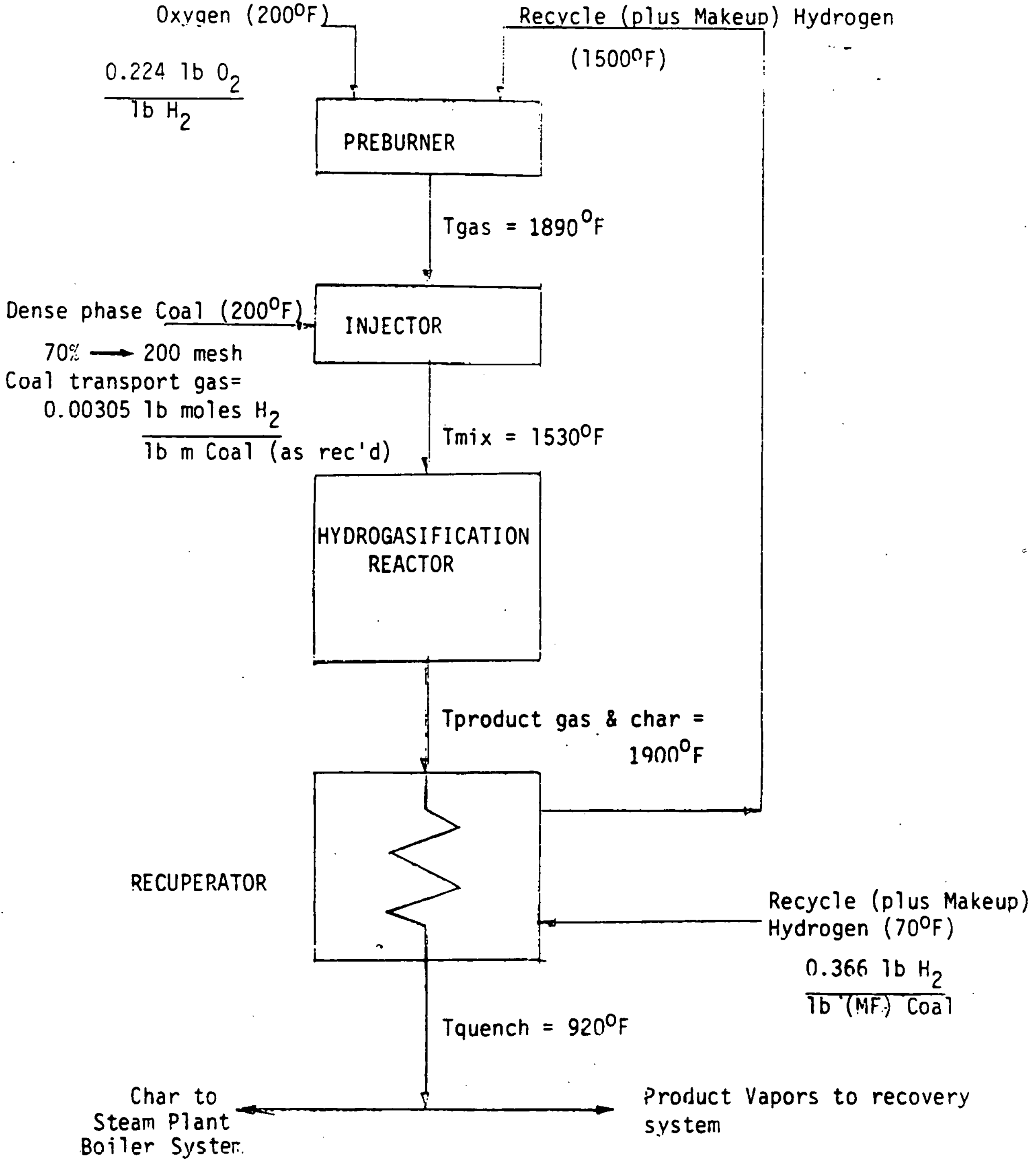
L. P. Combs

L. P. Combs
Project Engineer
Environmental & Energy Systems Division
Energy Systems Group.

3/13/79
REVISED

HYDROGASIFICATION SECTION HEAT & MATERIAL BALANCES

CASE-I: ZERO LIQUIDS PRODUCTION



3/13/79
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ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS

CASE I: ZERO LIQUIDS PRODUCTION

1. COAL CHARACTERISTICS

Type: Eastern Bituminous Coal Pittsburgh Seam No. 8

Proximate Analysis:

	As-Received	Dry
% Moisture	6.0	-
% Ash	10.6	11.28
% Volatiles	31.9	33.93
% Fixed Carbon	51.5	54.79

Ultimate Analysis:

	As-Received	Dry
% Moisture	6.0	-
% Carbon	67.21	71.50
% Hydrogen	4.72	5.02
% Nitrogen	1.15	1.23
% Sulfur	4.16	4.42
% Ash	10.62	11.30
% Oxygen	6.14	6.53

Heating Value:	As-Received	Dry
Btu/lbm	12,400	13,190

2. FEED RATES, NORMALIZED PER LB (MF) COAL:

0.366 lb H_2/lb (MF) coal (at preburner inlet)
0.224 lb O_2/lb H2 (for 1900 °F outlet reactor temperature)

Elemental Breakdown, LB Element/LB (MF) Coal

	C	H	O	S	N
(MF) Coal Feed	0.7150	0.0502	0.0653	0.0442	0.0123
Coal Moisture* (0.0204 lb/lb (MF) coal)	-	0.0023	0.0181	-	-
H_2 Feed	-	0.3660	-	-	-
H_2 Transport Gas	-	0.0062	-	-	-
O_2 Feed	-	-	0.0820	-	-
TOTALS	0.7150	0.4247	0.1654	0.0442	0.0123

*Dried to 2.0% moisture in coal pulverization/drying unit

ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS

(continued)

3. REACTOR CONDITIONS:

Hydrogen Inlet Temperature	1500°F
Oxygen Inlet Temperature	200°F
Coal Inlet Temperature	200°F
Reactor Outlet Temperature	1900°F
Reactor Outlet Quench Temperature	920°F
Reactor Pressure	1000 psig
Residence Time	2000 msec

4. ASSUMPTIONS:

Coal S $\longrightarrow H_2S$

Coal N $\longrightarrow NH_3$

$(GN_2 \longrightarrow GN_2)$

Coal O + $GO_2 \longrightarrow CO + CO_2$ + CHAR O + H_2O (diff.)

5. PRODUCT COMPOSITION:

a. <u>Overall Carbon Conversion</u>

$\bar{\eta}_{c,\ \text{overall}} = 62.7\%$

Where: $\eta_{c \rightarrow \text{Liq.}} = 0.00$

$$\left.\begin{array}{l} \eta_{c \rightarrow CH_4} = 0.572 \\ \eta_{c \rightarrow CO} = 0.049 \\ \eta_{c \rightarrow CO_2} = 0.006 \end{array}\right\} \qquad \eta_{c \rightarrow \text{Gas}} = 0.627$$

ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS

(continued)

b. Char Composition (%)

C	65.97
H	1.15
N	0.68
S	3.95
Ash	27.95
O	0.30

c. Product Gas Composition

Species	lb/lb (MF) Coal	Moles/lb (MF) Coal	Mole %
H_2	0.26526	0.13158	74.29
CH_4	0.54589	0.03405	19.23
CO	0.08172	0.00292	1.65
CO_2	0.01572	0.00036	0.20
NH_3	0.01161	0.00068	0.38
H_2S	0.03000	0.00088	0.50
H_2O	0.11945	0.00663	3.75
	1.06965	0.1771	100.00

d. Elemental Balances

(1) Ash: $\frac{0.1130 \text{ lb Ash/lb (MF) Coal}}{0.2795 \text{ lb Ash/lb Char}} = 0.4043 \frac{\text{lb Char}}{\text{lb (MF) Coal}}$

(2) Carbon:

in Char	= 0.26669 lb
in CH_4	= 0.40898
in CO	= 0.03504
in CO_2	= 0.00429
	0.7150 (100.00%)

(3) Oxygen:

in Char	= 0.00121 lb
in CO	= 0.04668
in CO_2	= 0.01143
in H_2O (diff.)	= 0.10608
	0.1654

(4) Sulfur: in Char = 0.01597 lb
in H_2S (diff.) = 0.02823
0.0442

(5) Nitrogen: in Char = 0.00275 lb
in NH_3 (diff.) = 0.00955
0.0123

(6) Hydrogen: in Char = 0.00465 lb
in H_2S = 0.00178
in NH_3 = 0.00207
in CH_4 = 0.13757
in H_2O = 0.01337
as H_2 (diff.) = 0.26526
0.4247

3/13/79
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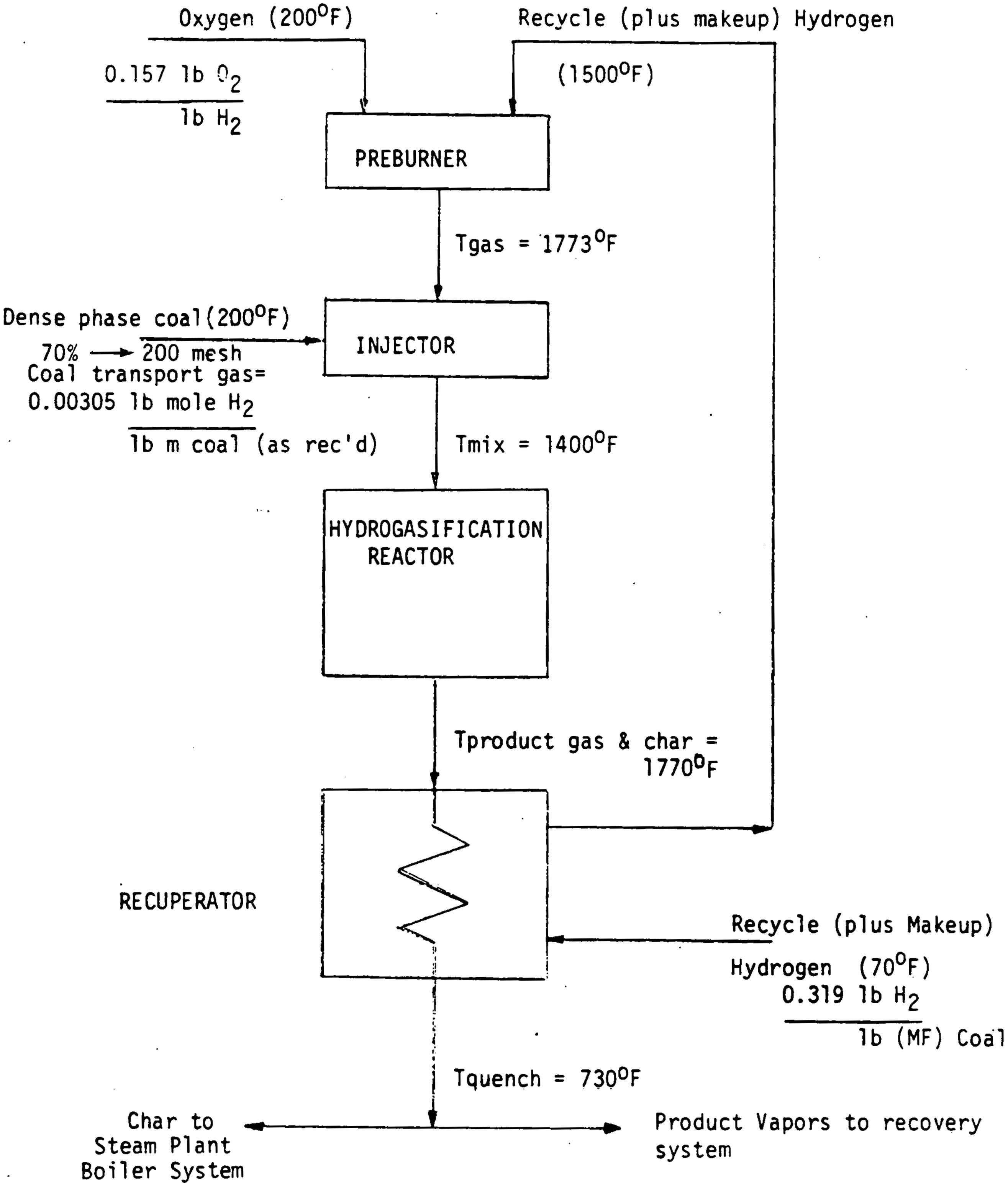
HYDROGASIFICATION SECTION HEAT & MATERIAL BALANCES

CASE-II: MODERATE LIQUIDS PRODUCTION



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ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS

CASE II: MODERATE LIQUIDS PRODUCTION

1. COAL CHARACTERISTICS

Type: Eastern Bituminous Coal Pittsburgh Seam No. 8

Proximate Analysis:

	As-Received	Dry
% Moisture	6.0	-
% Ash	10.6	11.28
% Volatiles	31.9	33.93
% Fixed Carbon	51.5	54.79

Ultimate Analysis:

% Moisture	6.0	-
% Carbon	67.21	71.50
% Hydrogen	4.72	5.02
% Nitrogen	1.15	1.23
% Sulfur	4.16	4.42
% Ash	10.62	11.30
% Oxygen (by difference)	6.14	6.53

Heating Value:	As-Received	Dry
Btu/lbm	12,400	13,190

2. FEED RATES, NORMALIZED PER LB (MF) COAL:

0.319 lb H_2/lb (MF) coal (at preburner inlet)
0.157 lb O_2/lb H2 (for 1770°F outlet reactor temperature)

Elemental Breakdown, LB Element/LB (MF) Coal

	C	H	O	S	N
(MF) Coal Feed	0.7150	0.0502	0.0653	0.0442	0.0123
Coal Moisture* (0.0204 lb/lb (MF) coal)	-	0.0023	0.0181	-	-
H_2 Feed	-	0.3190	-	-	-
H_2 Transport gas	-	0.0062	-	-	-
O_2 Feed	-	-	0.0501	-	-
TOTALS	0.7150	0.3777	0.1335	0.0442	0.0123

*Dried to 2.0% moisture in coal pulverization/drying unit

ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS
(continued)

3. REACTOR CONDITIONS:

Hydrogen Inlet Temperature	$1500^{\circ}F$
Oxygen Inlet Temperature	$200^{\circ}F$
Coal Inlet Temperature	$200^{\circ}F$
Reactor Outlet Temperature	$1770^{\circ}F$
Reactor Outlet Quench Temperature	$730^{\circ}F$
Reactor Pressure	1000 psig
Residence Time	2500 msec

4. ASSUMPTIONS:

Coal $S \longrightarrow H_2S$

Coal $N \longrightarrow NH_3$

$(GN_2 \longrightarrow GN_2)$

Coal $O + GO_2 \longrightarrow CO + CO_2 + \text{CHAR } O + H_2O$ (diff.)

5. PRODUCT COMPOSITION:

a. Overall Carbon Conversion

$\bar{\eta}_{c,\text{ overall}} = 56.8\%$

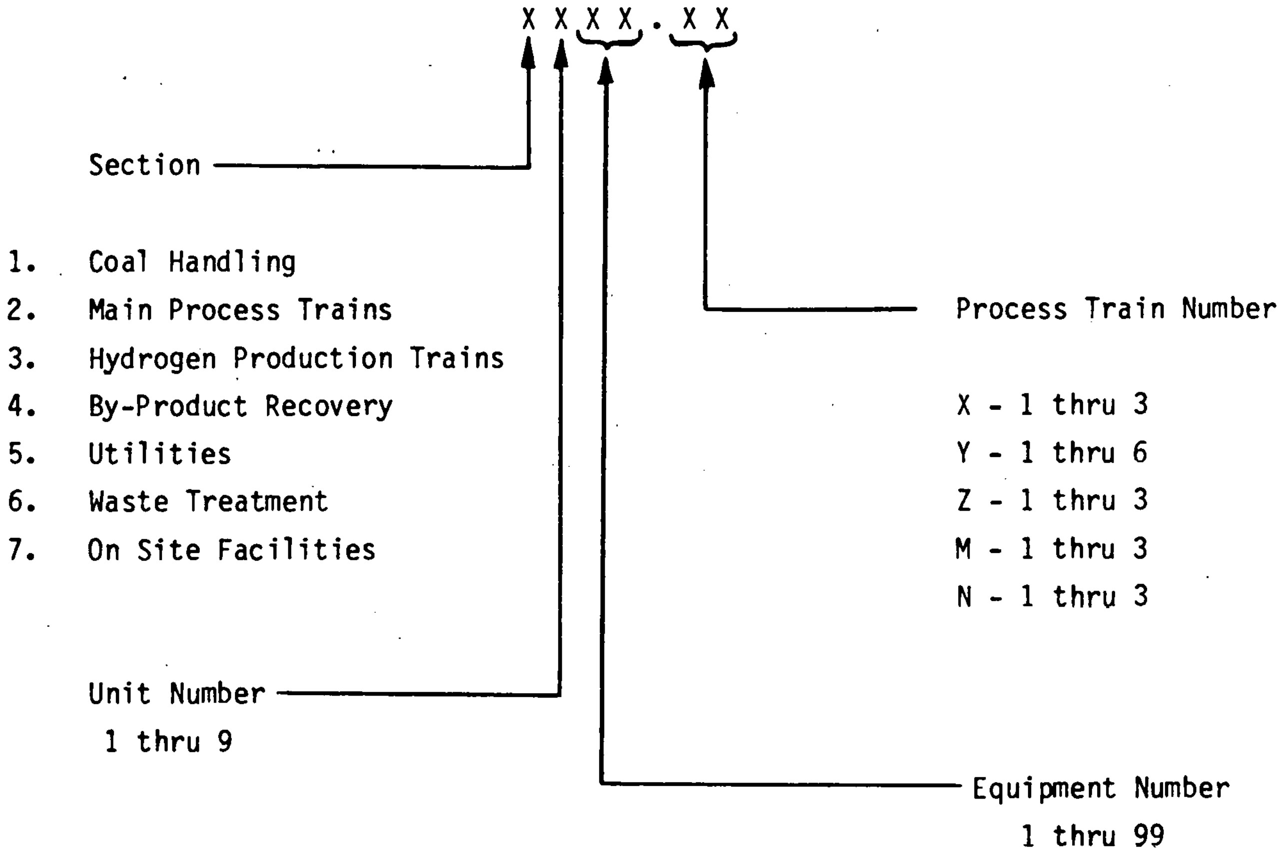
Where:

$$\left.\begin{array}{l} \eta_{c\rightarrow\text{Benzene}} = 0.058 \\ \eta_{c\rightarrow\text{Toluene}} = 0.00 \end{array}\right\} \quad \eta_{c\rightarrow\text{Liq.}} = 0.058$$

$$\left.\begin{array}{l} \eta_{c\rightarrow CH_4} = 0.474 \\ \eta_{c\rightarrow CO} = 0.032 \\ \eta_{c\rightarrow CO_2} = 0.004 \end{array}\right\} \quad \eta_{c\rightarrow\text{Gas}} = 0.510$$

APPENDIX B - COMMERCIAL PLANT UNIT NUMBERING SYSTEM

Following is a description of digitalization units and equipment of various sections of the plant:



Section

1. Coal Handling
2. Main Process Trains
3. Hydrogen Production Trains
4. By-Product Recovery
5. Utilities
6. Waste Treatment
7. On Site Facilities

Unit Number
1 thru 9

Process Train Number

X - 1 thru 3
Y - 1 thru 6
Z - 1 thru 3
M - 1 thru 3
N - 1 thru 3

Equipment Number
1 thru 99

APPENDIX C - ROCKWELL HIGH BENZENE YIELD DATA

The material in this appendix was submitted to UOP/SDC by Rockwell International. It was the basis for the discussion in Appendix D.

Energy Systems Group
8900 De Soto Avenue
Canoga Park, CA 91304
Telephone: (213) 341-1000
TWX: 910-494-1237
Telex: 181017

Rockwell
International

January 18, 1980 In reply refer to 80ESG-462

Mr. P. D. Agrawal
UOP/SDC
7929 Westpark Drive
McLean, Virginia 22102

Dear Mr. Agrawal:

The recent results obtained from Rockwell Hydrogasification Test 318-036 under Task I of the current program (ET-78-C-01-3125) appear to be very promising as a potential design point for a commercial-scale coal hydrogasification reactor system. Pertinent experimental conditions for this test have been summarized in Table A-1 of the November Monthly Report (ET-3125-14). Using Kentucky No. 9 bituminous coal, overall carbon conversion was found to be 55.0%, with carbon conversions to CH_4, C_6H_6, CO, and CO_2 being equal to 39.0%, 11.4%, 4.4%, and 0.4%, respectively. Mass balances completed to date on Test 318-036 indicate 94.5% carbon recovery, 101% hydrogen recovery, and 96.3% overall recovery.

As you know, the impact of high benzene yield on the cost of gas in a commercial-scale CS/R hydrogasification plant will be significant, and especially now in light of the continued strong market demand and high contract price for chemical-grade benzene. In your recent preliminary evaluation of the CS/R Hydrogasification Process,* the cost of SNG was reduced from \$5.05/MMBtu (zero liquids production case) to \$4.48/MMBtu (moderate benzene production case, 5.8% carbon conversion to benzene) when producing 3030 bbl/day benzene valued at \$0.90/gallon. This latter price represented the value assigned to raw benzene byproduct when used as a transportation fuel blending stock. The benzene yield in Test 318-036 (11.4% carbon conversion to benzene) is nearly twice that employed in the previous study. Furthermore, the value of chemical-grade benzene is presently \$1.65/gallon. An update of your economic analysis appears warranted to assess the impact of these new developments.

With reference to our previous discussions on the cost of benzene upgrading, I would like to submit the following new information for your consideration. There are several commercially available, low-cost processes for catalytic upgrading of benzene to high-purity (>99.9%) specifications. One such process is the DETOL® process offered by the Houdry Division of Air Products and Chemicals. A brief description of the process is presented

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*"Design and Evaluation of Rockwell Hydrogasification Commercial Plant," UOP/SDC, Contract ET-78-C-01-3117, Final Report, TR-MC-019-001, November 26, 1979

as Enclosure 1. Preliminary calculations based upon DETOL® indicate that the cost of equipment to upgrade an amount of benzene equivalent to that obtained in Test 318-036 for a commercial-scale CS/R SNG plant, nominally 6800 bbl/day, would be about $9.7 million in mid-1979 dollars. This represents about 1% of the erected commercial plant cost, and would therefore add only about $0.02 to the cost of SNG. Furthermore, the amount of hydrogen required to upgrade this quantity of benzene would be very small (approximately 0.2% of the total makeup H_2 requirement) and would have an insignificant incremental effect on the SNG price.

Enclosed for your review is a set of material and energy balances for a commercial-scale CS/R hydrogasification reactor system at high benzene yield based upon the results of Test 318-036 (denoted in Enclosure 2 as Case IV). By appropriate cost factoring from your report (TR-MC-019-001), Rockwell is currently preparing a new set of gas cost estimates for this high-yield benzene case. The objective is to estimate the effect of benzene yield, benzene price, and H_2/coal ratio on the 20-year average gas cost using the utility financing method. If your schedule permits, it would be of great benefit to the Rockwell program if you could perform similar cost-factored-type estimates.

I will be accompanying Joe Friedman and Paul Combs to Washington to visit Lou Jablansky on January 29. At that time, we could compare our estimates directly and discuss any differences.

Should you have any comments or questions, please feel free to call me at (213) 341-1000, Extension 1266. I look forward to seeing you in the near future.

Very truly yours,

D. R. Kahn

Daniel R. Kahn
Project Manager
Process Design and Economics
Fossil Energy Systems
Energy Systems Group

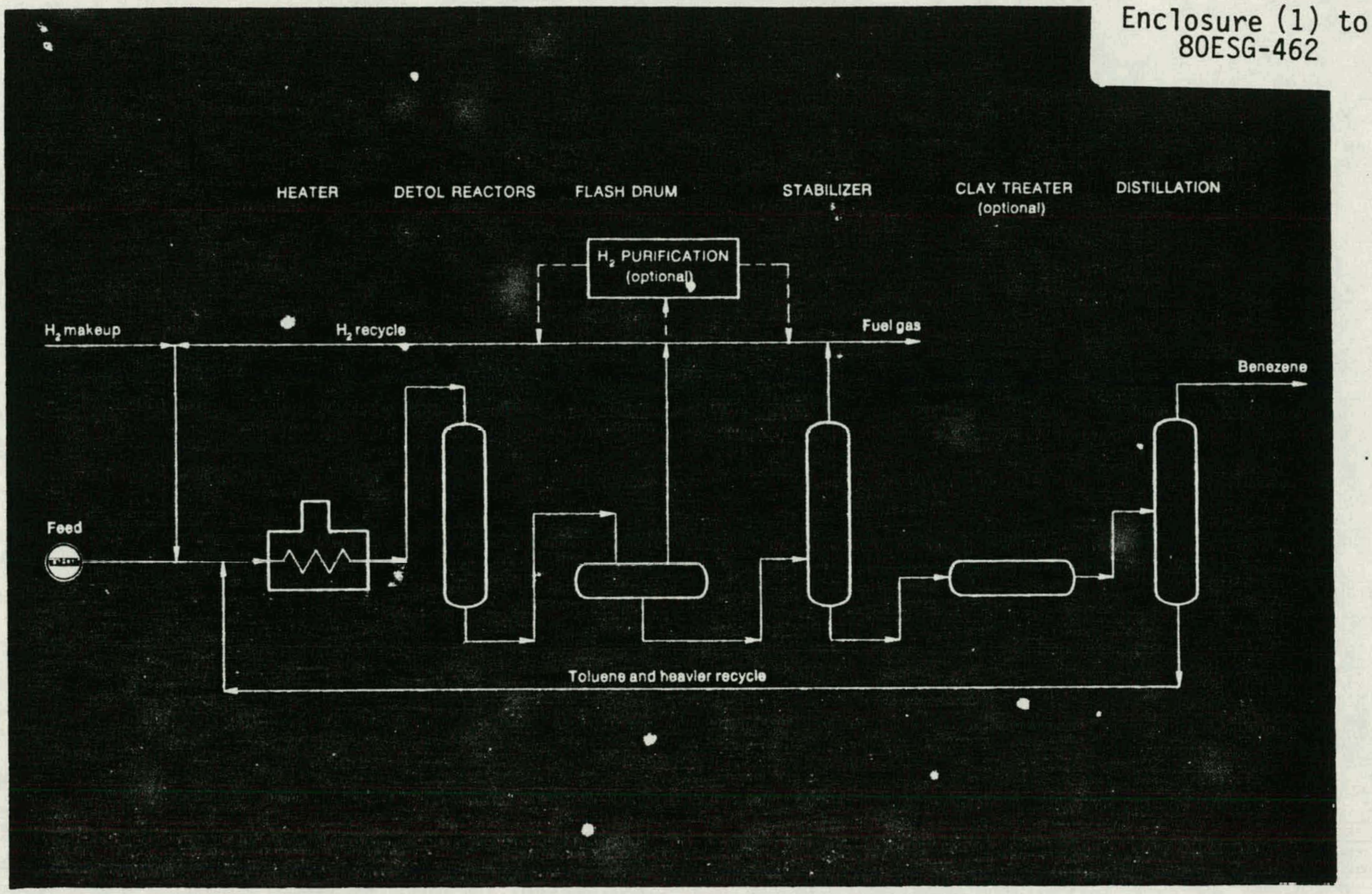
pag:5/2-3

Enclosures

cc: Department of Energy
Washington, D.C.
Mr. Lou Jablansky

Cities Service Company
Tulsa, Oklahoma
Mr. Wayne A. Fling, Jr.
Dr. Daniel P. Rimmer

Enclosure (1) to
80ESG-462



Benzene (Detol)—AIR PRODUCTS AND CHEMICALS, INC.

Application: To produce high purity benzene and heavier aromatics from toluene and/or xylenes and/or C_9 and heavier aromatics. The main product is high purity benzene which meets all normal quality tests and has a freeze point of about 5.5° C. With C_9+ aromatic feedstocks, toluene and xylenes can also be taken as product.

Description: Feed (toluene and/or xylenes and/or C_9+ aromatics), together with a hydrogen containing gaseous stream, is heated at a specified pressure to the required reaction temperature and passed over a dealkylation catalyst. Reactor effluent is cooled by heat exchange. Benzene and unconverted toluene and/or xylene and heavier aromatics are condensed, then flow to a high pressure flash drum where the major portion of materials which boil below benzene are separated as gases.

The condensed liquid consisting of benzene, toluene and/or xylene and heavier aromatics is pumped to a stabilizer. Dissolved hydrogen, hydrogen sulfide and light hydrocarbons not removed in the flash drum are stripped out. When benzene product must meet acid wash color specifications, the stabilizer bottoms are passed through a fixed bed clay treater. The clay treated aromatic liquid is then distilled in a benzene fractionator to produce the desired specification benzene.

Unconverted toluene and/or xylenes and heavier aromatics are recycled through the catalyst with the fresh feed.

Depending on the quantity and purity of available make-up hydrogen, it may be desirable to include a hydrogen concentration step to treat a portion of the vapors from the high pressure flash drum, as shown in the flow diagram. This maintains the desired hydrogen partial pressure in the system while conserving hydrogen. A cryogenic hydrogen purification unit can be used.

Yields: Benzene yield in reactor effluent is 99.0 mol % of fresh toluene or heavier aromatic charge. A typical material balance is as shown:

Component, Wt. %	DETOL Fresh Feed	Make-Up H_2 Rich Gas	Fuel Gases	Benzene Product
H_2	—	19.9	0.9	—
C_1-C_4	—	60.8	98.7	—
C_5's	—	6.9	0.4	—
C_6-C_9 NA	3.2	12.4	—	.02
Benzene	—	—	—	99.97
Toluene	47.3	—	—	.01
C_8+A	49.5	—	—	—
Total	100.0	100.0	100.0	100.00
Lb./lb. raw charge	1.000	0.199	0.441	0.758

Economics:

Investment: Varies for feedstock, but on the basis of a 100-million-gpy plant with the material balance shown above, $/bpsd) . . 1,400

Typical utility requirements, per bbl. feed

Electricity, kwh	5.8
Fuel, MM Btu	0.31*
Cooling water, gal.	450
Steam, lbs.	14.4

---

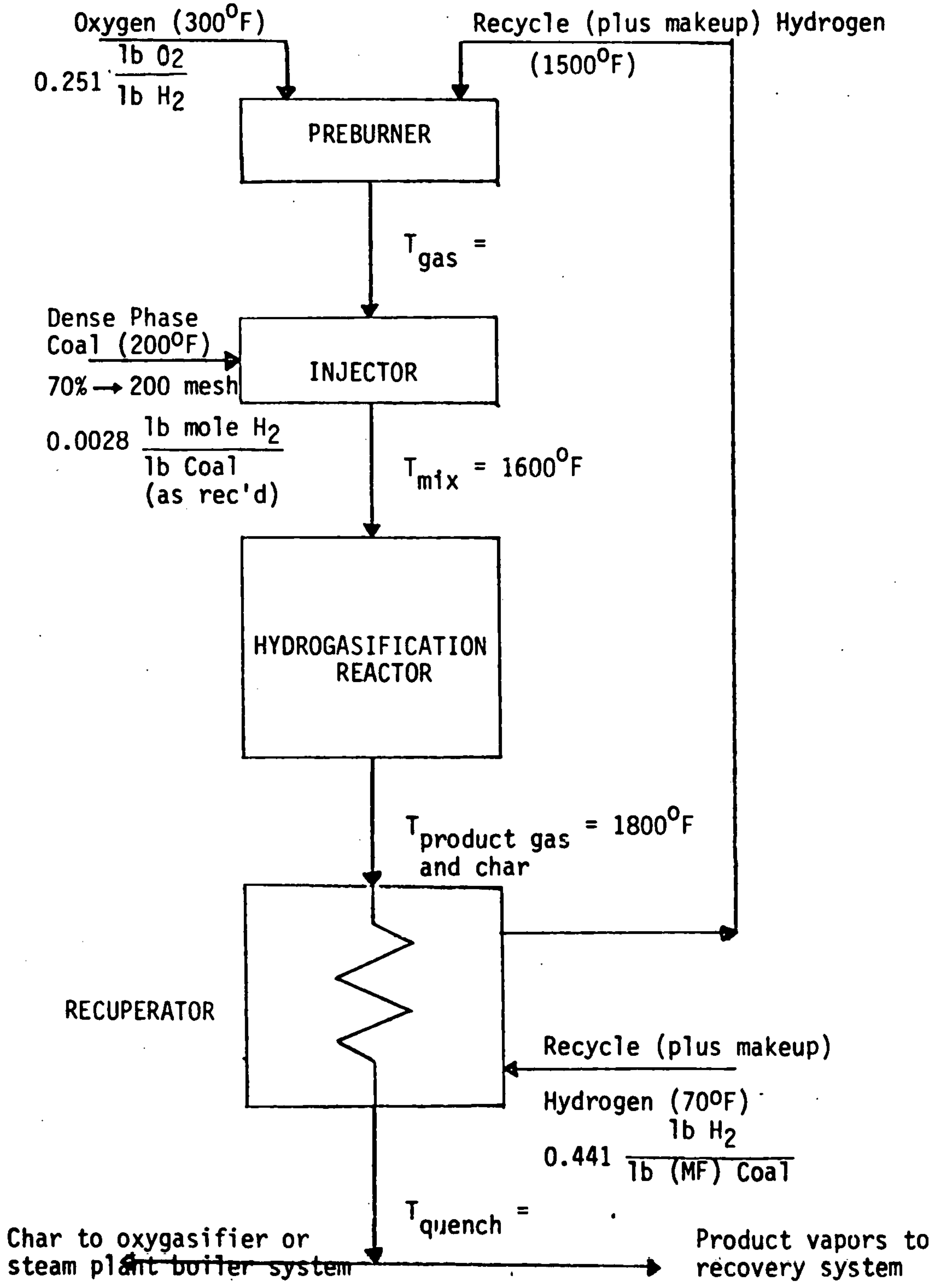
* No credit taken for vent gas streams

Commercial installations: Twelve plants with capacities ranging from about 12 million to 100 million gallons per year have been licensed.

Licensor: Houdry Division of Air Products and Chemicals, Inc.

HYDROGASIFICATION SECTION HEAT AND MATERIAL BALANCES
CASE IV: HIGH BENZENE YIELD

<u>Basis</u>: Rockwell 3/4-tph Hydrogasification Test 318-036



ROCKWELL HYDROGASIFIER OPERATING POINT ANALYSIS
CASE IV: HIGH BENZENE YIELD

1. COAL CHARACTERISTICS

Type: Kentucky No. 9

Ultimate Analysis:	As Received	Dry
% Moisture	5.4	-
% Carbon	69.54	73.51
% Hydrogen	4.80	5.07
% Nitrogen	1.25	1.32
% Sulfur	2.73	2.89
% Ash	8.28	8.75
% Oxygen (by difference)	8.00	8.46

Net Heating Value:	As-Received	Dry
Btu/lbm	12,700	13,430

2. FEED RATES, NORMALIZED PER LB (MF) COAL

0.441 lb H_2/lb (MF) coal (at preburner inlet)

0.251 lb O_2/lb H2 (for 1800°F outlet reactor temperature)

Elemental Breakdown, LB Element/LB (MF) Coal

	C	H	O	S	N
(MF) Coal Feed	0.7351	0.0507	0.0846	0.0289	0.0132
Coal Moisture* (0.0204 lb/lb (MF) coal)	-	0.0023	0.0181	-	-
H_2 Feed	-	0.4410	-	-	-
H_2 Transport Gas	-	0.0060	-	-	-
O_2 Feed	-	-	0.1107	-	-
TOTALS	0.7351	0.5000	0.2134	0.0289	0.0132

*Dried to 2.0% moisture in coal pulverization/drying unit.

3. REACTOR CONDITIONS

Hydrogen Inlet Temperature	1500°F
Oxygen Inlet Temperature	300°F
Coal Inlet Temperature	200°F
Reactor Outlet Temperature	1800°F
Reactor Outlet Quench Temperature	
Reactor Pressure	993 psia
Residence Time	

4. ASSUMPTIONS

$\text{Coal S} \longrightarrow H_2S$

$\text{Coal N} \longrightarrow NH_3$

$(GN_2 \longrightarrow GN_2)$

$\text{Coal O} + GO_2 \longrightarrow CO + CO_2 + \text{CHAR O} + H_2O\ \text{(diff)}$

5. PRODUCT COMPOSITION

a. Overall Carbon Conversion

$\eta_{c,\ \text{overall}} = 55.2\%$

Where: $\eta_{c \longrightarrow \text{Benzene}} = 0.114$

$\eta_{c \longrightarrow \text{Toluene}} = 0.00$

$\eta_{c \longrightarrow \text{liquid}} = 0.114$

$\eta_{c \longrightarrow CH_4} = 0.390$

$\eta_{c \longrightarrow CO} = 0.044$

$\eta_{c \longrightarrow CO_2} = 0.004$

$\eta_{c \longrightarrow \text{Gas}} = 0.438$

b. Char Composition

C	75.34
H	1.78
N	1.17
S	1.44
Ash	20.02
O	0.40

c. Product Gas Composition

Species	lb/lb (MF) Coal	Moles/lb (MF) Coal	Moles %
H_2	0.3664	0.18320	82.32
CH_4	0.3823	0.02389	10.74
CO	0.0754	0.00269	1.21
CO_2	0.0106	0.00024	0.11
NH_3	0.0098	0.00058	0.26
H_2S	0.0240	0.00071	0.32
C_6H_6	0.0908	0.00116	0.52
H_2O	0.1810	0.01006	4.52
	1.1403	0.22253	100.00

d. Elemental Balances

(1) Ash: $\frac{0.0875 \text{ lb Ash/lb (MF) Coal}}{0.2002 \text{ lb Ash/lb Car}} = 0.4371 \frac{\text{lb Char}}{\text{lb (MF) Coal}}$

(2) Carbon:
in Char = 0.3294 lb
in Benzene = 0.0838
in CH_4 = 0.2867
in CO = 0.0323
in CO_2 = 0.0029
0.7351 (100.00%)

(3) Oxygen:
in Char = 0.0017 lb
in CO = 0.0431
in CO_2 = 0.0077
in H_2O (diff) = 0.1609
0.2134

(4) Sulfur:
in Char = 0.0063 lb
in H_2S (diff) = 0.0226
0.0289

(5) <u>Nitrogen</u>: in Char = 0.0051 lb

in NH_3 (diff) = $\underline{0.0081}$

0.0132

(6) <u>Hydrogen</u>: in Char = 0.0078 lb

in H_2S = 0.0014

in NH_3 = 0.0017

in CH_4 = 0.0956

in C_6H_6 = 0.0070

in H_2O = 0.0201

as H_2 (diff) = $\underline{0.3664}$

0.5000

ebs:0110

APPENDIX D - ANALYSIS OF HIGH BENZENE YIELD CASE

D.1 INTRODUCTION

The cost of gas required for economic breakeven is sensitive to the quantity and value of the liquid product produced. Further testing by Rockwell International has resulted in carbon to liquid yields of 11.4% using Kentucky No. 9 bituminous coal (see letter from the Energy Systems Group, Appendix C). Pertinent experimental conditions are summarized in Table D.1. The operating requirements and thermal efficiency of a plant operated at these conditions using Pittsburgh No. 8 coal are summarized in Table D.2.

D.2 BY-PRODUCT VALUATION

Several factors influenced the value of the liquid product: its demand, its competition, its quality, and its marketing.(1)

The demand for chemical grade benzene is expected to rise from 1980 levels of about 1700 MM gal/year to 2500 MM gal/year by 1985, an increase of about 10%/year. A large portion of this growth is expected to be met by hydrodealkylation of toluene, which is also in demand as a gasoline blending stock. Demand for chemical grade benzene seems assured.

Current sources of benzene are refinery reforming, olefin processing, coal tar processing, and toluene hydrodealkylation. About two-thirds of the demand increase is expected to be met by hydrodealkylation of toluene, leading to a total toluene consumption of 850 MM gal/year by 1985. Each 250 billion Btu/day SNG plant operated at 11.4% conversion to benzene would accommodate 3.8% of 1985 demand levels (ignoring losses in upgrading). Ten such plants could thus supplant all the benzene produced by hydrodealkylation of toluene. Coal liquefaction from other sources may become commercially competitive in the same time frame as the Rockwell process, further enhancing the supply of aromatics.

---

(1) Supply and demand analyses are based on an independent study performed by Jack Dart Associates for Rockwell International.

Table D.1 Reactor Conditions for Case Studies(1)

	Base Case	Zero Liquids Case	High Benzene Yield Case
Hydrogen Inlet Temperature, °F	1500	1500	1500
Oxygen Inlet Temperature, °F	200	200	300
Coal Inlet Temperature, °F	200	200	200
Reactor Outlet Temperature, °F	1700	1900	1800
Reactor Pressure, psig	1000	1000	933
Residence Time, milliseconds	2500	2000	1775
Hydrogen Feed Rate, lb H_2/lb(MF) coal	0.319	0.366	0.441
Oxygen Feed Rate, lb O_2/lb H_2	0.157	0.224	0.251
Overall Carbon Conversion, %	56.8	62.7	55.2
Carbon Conversion to Benzene, %	5.8	-	11.4

---

(1) Refer to Appendix A and Appendix C.

Table D.2 Operating Requirements and Thermal Efficiency

	QUANTITY	HHV	BILLION BTU/DAY
ENERGY OUTPUT			
Raw Materials			
Bituminous Coal (as received)	19,778 ST/D	13,186 Btu/lb (MF Basis)	490.29
Water	15,848 GPM	-	-
Total Input			490.29
ENERGY OUTPUT			
SNG Product			250.00
Byproducts			
Sulfur	636.73 ST/D	3,992 Btu/lb	5.08
Benzene	6,800 BPD	17,991 Btu/lb	34.67
Ammonia	150.66 ST/D	9,086 Btu/lb	2.74
Total Output			295.49

Cold Gas Efficiency: $\frac{250.00}{490.29} = 51.0\%$

Plant Thermal Efficiency: $\frac{295.49}{490.29} = 60.3\%$

Commercialization of coal conversion processes has the potential of glutting the benzene market. In the short run, this will drive down the price, as did the oversupply in 1976 through 1978. The long run elasticity of demand may be such that the demand will rise, bringing the price back up.

Before benzene valuation at chemical prices is used, however, it must be shown that the liquid by-products can economically be upgraded. Initial tests report liquid products of 99% benzene. The potential contaminants (cyclopentane, cyclohexane, phenol, methylnapthalene, propylbenzene, and thiophene) may have a significant impact on the upgrading necessary. Increasing liquid yields increase the probable amounts of napthalenes and heavy paraffins.

Upgrading the benzene will probably require hydrodealkylation, napthalene removal, and benzene fractionation. The cost of these units is estimated to be between 10 and 30 million dollars. Increasing liquid yields increase the amount of impurities. Additional impurities require more severe benzene upgrading. The increased severity, in turn, requires the use of more hydrogen and thus requires that the hydrogen plant be enlarged.

Benzene is subject to deterioration, which means that an assured buyer is necessary. Even if deterioration of the benzene can be inhibited, more storage area would be necessary if the market should preclude sale of the product, or if transportation could not be arranged for whatever reason. A long term contract would insure the presence of a market but could require a sacrifice in the price obtainable.

A new benzene supplier would probably be at a disadvantage in the marketing of benzene. He might have to provide exceptional quality assurance and provide financial inducements through a lower than market price. A corporation operating one or two of these plants either would not be producing enough to gain the reputation necessary to receive top prices or would have its production committed by contract before gaining the reputation.

Utilities are expected to constitute a large fraction of the operators of these plants. They may have neither the expertise nor the interest to enter the chemical grade benzene market. Even if their plants produce large quantities of benzene, they may have little incentive to market the benzene aggressively if the by-product credit is used merely to offset operating costs in their rate setting procedures.

For all these reasons -- the impact of true commercialization of coal conversion on the supply of benzene, potential problems with the quality and value of the benzene, and possible inability and disinterest of the operators to obtain full market price -- UOP/SDC advises conservatism in the valuation of by-product credits. The base case and the high yield case both use \$0.90/gal as the base value of liquid product. This is a value appropriate for gasoline blending stock, a much larger market.

D.3 COST OF GAS CALCULATIONS

Gas cost was evaluated by prorating from the base case. The scale-up factor used is the average of those obtained using the increased use of coal and of hydrogen. Material balances were based on Pittsburgh No. 8 coal, not the Kentucky No. 9 coal used in the Rockwell test. Benzene upgrading is assumed to contribute 1% to operating costs and 0.6% to capital costs. Tables D.3 and D.4 show the results of these calculations.

With the benzene valued at \$0.90/gal, the high yield case has a cost of gas of \$4.38/MM Btu (UFM) and \$6.48/MM Btu (DCFM), versus respective values of \$4.43 and \$6.42 for the base case. As the benzene is valued more highly, the economics become much more favorable to the high yield case. For benzene at \$2.00/gal, the high yield case has COG figures of \$3.14 (UFM) and \$5.23 (DCFM), as opposed to base case values of \$3.80 and \$5.86.

It may be noted that for benzene at \$0.90/gal, the UFM and DCFM calculations give conflicting comparisons between the base and high yield cases. This apparent discrepancy is due to the different treatment of costs between UFM and

Table D.3 High Benzene Yield Economics ($\$ \times 10^6$)

(page 1 of 2)

Capital Requirement

Total Plant Investment	1,363.19
Royalties	3.64
Start Up and Preproject Expense	52.56
Initial Catalyst and Chemical Inventories	18.16
Spare Parts Inventories	5.31
Total Capital Requirement (DCFM)	1,442.86
Land (UFM)	2.75
Accumulated Interest on Construction (UFM)	230.15
Working Capital	46.73
	1,722.49

Working Capital

Coal (35 days)	18.26
Water (7 days)	.06
Benzene (14 days)	3.60
Ammonia (14 days)	.25
Sulfur (52 days)	1.18
Fuel Oil (14 days)	.43
Operating Inventory	23.78
Gross Operating Cost (30 days)	22.95
Total Working Capital	46.73

Table D.3 High Benzene Yield Economics ($ x 1000)

(page 2 of 2)

Gross Operating Costs	
Coal	161.79
Catalysts and Chemicals	7.42
Water	3.01
Labor - Operating	6.04
- Supervisory	1.21
General and Administrative Expense	4.35
Operating Supplies	1.81
Maintenance Material and Labor	44.82
Taxes and Insurance	20.45
Waste Disposal	1.57
Total Gross Operating Cost	252.47
By-Product Credits	
Sulfur	7.50
Benzene	84.82
Ammonia	5.97
Total By-Product Credit	98.29
Net Operating Costs (UFM)	154.18
Interest on Land and Working Capital (DCFM)	4.33
Net Operating Costs (DCFM)	158.51

Table D.4 Gas Cost Comparison

	Base Case		High Yield Case	
Coal Cost, $/MM Btu	UFM	DCFM	UFM	DCFM
.75	3.99	5.97	3.89	5.99
1.00 (Base)	4.43	6.42	4.38	6.48
1.25	4.87	6.86	4.87	6.98
1.50	5.30	7.30	5.36	7.47
Rate of Return, %				
9	-	5.26	-	5.25
10.5	-	5.80	-	5.83
12 (Base)	-	6.42	-	6.48
15	-	7.69	-	7.88
Capital Investment, $MM				
-200	3.97	5.65	3.92	5.72
Base	4.43	6.42	4.38	6.48
+200	4.88	7.18	4.84	7.24
+400	5.33	7.94	5.30	8.01
Coal Requirement, % of Base				
90	4.25	6.23	4.28	6.27
Base	4.43	6.42	4.48	6.48
110	4.60	6.60	4.68	6.69
120	4.78	7.79	4.88	6.90
Benzene Value, $/gal				
0.90 (Base)	4.43	6.42	4.39	6.48
1.55	4.06	6.09	3.65	5.74
2.00	3.80	5.86	3.14	5.23

DCFM. The high yield case has lower net operating costs and higher capital costs. In the UFM calculation, the lower operating cost dominates, so the cost of gas is less. In the DCFM calculations, the higher capital cost has more weight, so the cost of gas rises.

These figures are based on several assumptions and should be used with care. No consideration was given to the difference in feed coals. The amount for benzene upgrading is approximate, based on incomplete characterization of the liquid products. The high hydrogen requirement for the high yield case may be brought down in the future experiments. The cost of gas is sensitive to gross operating costs, so that a 10% change in operating costs leads to a $0.31/MM Btu change in COG - about 5%. Depending on the optimism with which the benzene market is viewed, the high yield case has a cost of gas either roughly equivalent to or significantly less than the cost of gas in the base case.