5. Engineering Research and Development
(Reporting Category C20)

Engineering research and development studies were carried out under the Catalytic Coal Gasification (CCG) Process Development Contract in conjunction with the laboratory bench-scale research and process development unit (PDU) operations. This work included both engineering and cost studies to evaluate process improvements and to guide laboratory programs; and engineering technology programs to develop fundamental process and equipment technology to support the laboratory and engineering efforts.

The engineering research and development work performed under the CCG Process Development Contract was divided into three subtasks:

- Cost Reduction and Laboratory Guidance Studies
- Systems Modeling
- Engineering Technology Studies

Engineering work on a fourth subtask, Process Definition, was not performed. Engineering studies required to provide program guidance in the areas of low gasifier fluid bed density and slower than expected methanation kinetics required additional engineering effort and precluded work on this task.

5.1 Cost Reduction and Laboratory Guidance Studies

5.1.1 CCG Commercial Plant Study Design - Offsites Revision

A Catalytic Coal Gasification Commercial Plant Study Design was prepared during the latter part of the CCG Process Predevelopment Program which was completed in January, 1978 under Contract No. E(49-18)-2369. The results of the "CCG Study Design" were documented in the Final Project Report for that contract (FE-2369-24). This was a detailed study involving substantial engineering efforts on material and energy balances, equipment specifications, and investment cost estimating.

Offsites facilities (including materials handling, utilities, and general offsites) constituted 40% of the total plant direct and indirect investment cost for the CCG Study Design. Although considerable effort was involved in specifying the offsites facilities for the Study Design, for the most part these areas were studied in less engineering depth and specified in less detail than the onsites process sections. Because the onsites and offsites design work proceeded at the same time, some inconsistencies developed between the final onsites utilities demands and the estimated demands used in specifying the utilities sections. Also, the process wastewater rate used in sizing the wastewater treating facilities was underestimated. A preliminary plant layout was used in specifying common onsite facilities and offsite piping for utilities distribution and for industrial sewers. A final look at the plant layout indicated that these requirements were probably overestimated.

In view of these factors, a revised offsites facilities definition and cost estimate was prepared during the first year of the Process Development Contract to firm up the CCG Study Design in the important offsites area. The revised Study Design served as the "base case" for screening studies to evaluate new data, process improvements, and optimum process conditions under the Process Development Contract. As a result of the offsites revision, the accuracy of these screening studies was improved.

Changes in Offsite Facilities

Most of the changes in this offsites revision were simply adjustments to equipment sizes to correct for inconsistencies between the initial and final utilities demands and plant layout requirements. However, more extensive changes were made in two sections. First, in the wastewater treating section, more detailed consideration was given to water quality and reuse options to better define treating needs and further reduce plant makeup and effluent water rates. Second, the flue gas desulfurization (FGDS) process was changed from a regenerative system using sodium carbonate to a once-through system using lime scrubbing. This change allowed integration of lime scrubbing offsites with other CCG plant offsites. For example, lime receipt for FGDS was integrated with lime receipt for onsite catalyst recovery, which uses lime as feed to $Ca(OH)_2$ digestion. Common absorbers were utilized to handle flue gas from the offsite boilers, the feed coal dryers, and the catalyst addition dryers, all of which are coal fired. In addition to these integration advantages, the technology and costs for lime (and limestone) scrubbing were better defined than for regenerative FGDS.

In general, the revised Study Design was prepared using the same approaches as the earlier Predevelopment Program Study Design. Except for the change in the FGDS process described above, the project basis was the same. The onsites process bases and material and energy balances were also unchanged. Utilities balances were updated to reflect the final onsites demands and the demands of the revised offsites facilities. Equipment lists for the revised offsites were developed by engineers specializing in offsites design. Direct equipment costs were estimated using the same techniques and cost bases used for Exxon's commercial projects. Indirect costs were estimated based on recent experience with large projects. Contingencies were included in the total investment estimate, also based on Exxon practices for actual projects.

Revised Investment

The revised investment for the CCG Study Design is presented in Table 5.1-1. (This updates Table 4.8-1 of the Predevelopment Report FE-2369-24.) The total investment is 1,530 M$ for the pioneer commercial plant feeding

Table S.1-1

CATALYTIC COAL GASIFICATION
COMMERCIAL PLANT STUDY DESIGN

INVESTMENT FOR PIONEER PLANT

Basis:
- January, 1978 Instant Plant
- Eastern Illinois Location
- 257 Billion Btu/Stream Day SNG (HHV Basis)

Plant Section	Investment Breakdown Million $	Investment Breakdown % (1)
ONSITES		
Coal Drying	27	2
Catalyst Addition	18	2
Reactor System	197	18
Product Gas Cooling and Scrubbing	86	8
Sour Water Stripping and Ammonia Recovery	20	2
Acid Gas Removal and Sulfur Recovery	161	15
Methane Recovery System	44	4
Refrigeration	31	3
Catalyst Recovery	39	3
Common Onsite Facilities	55	5
ONSITES SUBTOTAL	678	62
MATERIALS HANDLING		
Coal Handling and Storage	19	
Coke/Char Handling	5	
Chemicals Handling and Storage	20	
By-Products Storage and Shipping	3	
Waste Solids Handling and Disposal	27	
MATERIALS HANDLING SUBTOTAL	74	7
UTILITIES		
Raw Water/BFW Treating	29	
Steam Generation and Distribution	120	
Cooling Water	9	
Electric Power Distribution	23	
Miscellaneous Utilities	5	
Flue Gas Desulfurization (2)	51	
UTILITIES SUBTOTAL	237	22
GENERAL OFFSITES		
Wastewater Treating	48	
Safety and Fire Protection	13	
Site Preparation	6	
Miscellaneous Offsites	34	
GENERAL OFFSITES SUBTOTAL	101	9
TOTAL DIRECT AND INDIRECT COSTS	1,090	100
PROCESS DEVELOPMENT ALLOWANCE (25% of Onsites Direct & Indirect Costs)	169	
PROJECT CONTINGENCY (25% of Total Direct & Indirect Costs)	271	
TOTAL ERECTED COST	1,530	

Notes:

(1) Percentage breakdown of investment is based on total direct and indirect costs excluding process development allowance and project contingency.

(2) Includes desulfurization for flue gases from steam generation (coal-fired boilers) and from coal drying and catalyst addition.

Illinois No. 6 coal and producing 257 billion Btu per stream day of SNG (substitute natural gas). This is for a January, 1978 cost level at an Eastern Illinois location.

The revised Study Design investment is 110 M$ less than the investment estimated during the Predevelopment Program, a reduction of about 7%. The investment changes are broken down by plant section in Table 5.1-2, starting with the Predevelopment Program Study Design investment of 1,640 M$. The key factors which have contributed to the overall investment change are:

- Costs are substantially lower in materials handling sections (including coal drying and catalyst addition, which are grouped with the onsites). The lower investments stem in part from modest reductions in facilities requirements made as part of the offsites revisions. For example, the electrostatic precipitators used to remove fines from flue gases produced in the coal dryers and the catalyst addition dryers were deleted. Fines removal from these flue gases is now accomplished by venturi scrubbers located in the flue gas desulfurization section upstream of the lime absorbers. Also, surge coal storage silos were reduced in size. However, the major factor which lowered the estimated investment in these sections is improvements in the methods and cost bases used in cost estimating materials handling equipment, such as silos, conveyors, and associated structures and foundations. Exxon's commercial experience with materials handling equipment was quite limited when the Predevelopment Program investment estimate was prepared in late 1977, and cost estimating tools were not well developed. Experience since that date, including the Exxon Coal Liquefaction Pilot Plant now under construction, led to improved estimating approaches. Applying these new tools indicated that the cost estimates for silos and conveyors were too high in the earlier Study Design.

- Costs for common onsite facilities (piperacks, utility headers, roads, sewers, lighting, etc.) were reduced based on the final plant layout.

- Steam generation and distribution increased slightly in cost. This was due primarily to an upward revision of coal-fired boiler cost bases, also resulting from learning experience since the previous estimate was completed over a year ago. Boiler capacity is actually down 8%, due mainly to lower steam demands for lime FGDS.

- The flue gas desulfurization facilities costs are down as a result of the change from regenerative FGDS to lime scrubbing. The investment shown for FGDS is especially low because lime receipt and handling and storage. Even so, the cost for the latter section is lower because of the new cost estimating approaches for silos and conveyors.

- The investment for wastewater treating is up because of the increase in process wastewater rate and in facilities for reuse. As a result

Table 5.1-2

CCG STUDY DESIGN
SUMMARY OF INVESTMENT CHANGES

		Investment Million $
● TOTAL ERECTED COST FOR PREDEVELOPMENT PROGRAM STUDY DESIGN		1,640
● CHANGES IN TOTAL ERECTED COST		
ONSITES		
Coal Drying	(11)	
Catalyst Addition	(6)	
Common Onsite Facilities	(8)	
Other Sections	2	
MATERIALS HANDLING		
Coal Handling and Storage	(33)	
Chemicals Handling and Storage	(7)	
Otner Sections	(3)	
UTILITIES		
Steam Generation and Distribution	3	
Flue Gas Desulfurization	(16)	
Other Sections	(10)	
GENERAL OFFSITES		
Wastewater Treating	7	
Other Sections	-	
TOTAL DIRECT AND INDIRECT COSTS		(82)
PROCESS DEVELOPMENT ALLOWANCE		(6)
PROJECT CONTINGENCY		(22)
● TOTAL ERECTED COST FOR REVISED STUDY DESIGN		1,530

of more detailed study of water reuse options, the estimated average raw water makeup rate for the CCG Study Design was reduced from 7,300 gpm to 5,600 gpm.

- The percentage add-ons for process development allowance and project contingency are down in proportion to the reductions in onsites and total plant direct and indirect costs.

Thus, overall, the estimated investment for the CCG Study Design was reduced from 1,640 M$ to 1,530 M$.

Revised SNG Cost

Consistent with this revised investment, the cost of SNG produced from Illinois coal in a pioneer CCG plant was estimated to be about 6.18 $/MBtu on a 1978 basis, as shown in Table 5.1-3. (This updates Table 4.9-2 of the Predevelopment Report.) This gas cost is a required initial selling price based on 100% equity financing with a 15% current dollar DCF return. It was assumed that SNG product revenues will escalate at 6% per year and that operating costs and by-product revenues will escalate at 5% per year. On a financing basis of 70% debt/30% equity with 9% interest on debt, the initial gas cost is 4.65 $/MBtu. This cost was also based on the same DCF return on the equity and the same escalation assumptions. The complete economic basis for these gas costs was documented in the Predevelopment Report.

The revised SNG cost in the 100% equity case is 0.24 $/MBtu less than the gas cost calculated during the Predevelopment Program. The changes in the SNG cost can be summarized as follows:

	SNG Cost, $/MBtu		
SNG Cost Component	Predevelopment Study Design	Revised Study Design	Net Change
Coal	1.40	1.41	0.01
Major Chemicals	0.37	0.41	0.04
Other Operating Costs			
- Utilities	0.35	0.35	-
- Labor and Related	0.40	0.39	(0.01)
- Materials and Overheads	0.64	0.60	(0.04)
- Other	0.10	0.09	(0.01)
By-Product Revenues	(0.19)	(0.18)	0.01
Capital Charges	3.35	3.11	(0.24)
Total	6.42	6.18	(0.24)

A lower capital charge associated with the drop in investment was the main factor which contributed to the reduction in gas cost. This was partially offset by the added cost of purchasing lime (included under "major chemicals") for the lime scrubbing process used for flue gas desulfurization.

Table 5.1-3

CATALYTIC COAL GASIFICATION
COMMERCIAL PLANT STUDY DESIGN

COST OF SNG FROM PIONEER PLANT WITH 100% EQUITY FINANCING

Basis:
- January, 1978 Instant Plant, Eastern Illinois Location
- 257 Billion Btu/Stream Day SNG (HHV Basis)
- 90% Capacity Factor
- 100% Equity Financing
- 15% Current Dollar DCF Return
- Escalation Rates:
  - Operating Costs and By-product Revenues at 5%/Year
  - SNG Revenues at 6%/Year
- Total Erected Cost of 1,520 M$ (From Table 5.1-1)

SNG Cost Components	Requirements (At Full Capacity)	Unit Costs (1978)	SNG Cost Breakdown $/Million Btu (1978)
• Illinois No. 6 Coal (Cleaned)			
- To Gasifiers	14,490 ST/SD (2)	20 $/ST	1.128
- To Coal Dryer Fuel	710 ST/SD	20 $/ST	0.055
- To Offsite Boiler Fuel	2,960 ST/SD	20 $/ST	0.230
Subtotal	18,160 ST/SD		1.413
• Major Chemicals			
- KOH Solution (30 wt%)	189 ST/SD (Contained)	300 $/ST	0.221
- Lime (97% CaO) to Catalyst Recovery	1,005 ST/SD	39 $/ST	0.153
- Lime (97% CaO) to FGDS	272 ST/SD	39 $/ST	0.041
Subtotal			0.415
• Other Operating Costs			
- Purchased Electric Power	147 MW	2.5 ¢/kWh	0.343
- Raw Water	5,600 gpm	15 ¢/k gal	0.005
- Other Catalysts and Chemicals	Many Items	4.7 M$/yr	0.056
- Wages and Benefits	980 Men	21 k$/man/yr	0.244
- Salaries and Benefits	260 Men	25 k$/man/yr	0.077
- Labor Overheads and Supplies	20% of Wages, Salaries, and Benefits		0.064
- Materials and Overheads	3.3% of Total Erected Cost/Year		0.593
- Ash Disposal	8,400 ST/SD (Wet)	1 $/ST	0.033
Subtotal			1.420
• By-Product Revenues			
- Ammonia (20 wt%)	231 ST/SD (Contained)	160 $/ST	(0.144)
- Sulfur	324 LT/SD (2)	25 $/LT	(0.031)
Subtotal			(0.175)
• Capital Charges	Per above basis		3.104
TOTAL SUBSTITUTE NATURAL GAS COST (RISP) (3)			6.177
CALL			6.18

Notes:

(1) k = 10^3, M = 10^6, G = 10^9.

(2) ST/SD = short tons/stream day (i.e., one day's operation at full plant capacity). LT= long tons.

(3) Required initial selling price in first year of plant operation (1978).

Despite the 8% reduction in offsite boiler capacity mentioned earlier, the coal to boiler fuel is up about 3% in the revised Study Design. This is the reason for the small increase in coal cost shown above. The increase in boiler fuel is a reflection of a change in the approach used to estimate average requirements for all plant utilities. As described in the Predevelopment Report, the total design capacities for CCG Study Design utilities systems included: (1) normal requirements calculated from the onsite and offsite equipment lists; (2) intermittent requirements also calculated from the equipment lists; (3) allowances for estimated increases in utilities loads as facilities definition improves during project development; and (4) an additional allowance for reserve capacity in source facilities for start-up and emergency needs. (Source facilities include offsite boilers, BFW treating, cooling tower, etc.) This approach is consistent with Exxon practices for commercial projects; the allowances for items (3) and (4) are based on Exxon's experience for a broad range of commercial process plants. For the Predevelopment Program Study Design, average plant utilities requirements for operating costs were based on the calculated normal requirements plus the average intermittent requirements. For the revised CCG Study Design, the allowances for estimated increases in utilities loads during project development (item (3)) were also included in the average utilities requirements for operating costs. This is consistent with the experience showing that such increases do occur, on average, in actual projects. Adding these allowances in the revised Study Design increased operating costs only for coal fuel purchased to generate steam in the offsite boilers. Utilities savings resulting from the use of lime FGDS, more complete utilization of available steam in non-condensing steam turbine drivers, and increased reuse of wastewaters offset these additional allowances for the other utilities. Thus there was no net change in the electric power requirements (147 MW) and a substantial reduction in the raw water makeup rate (as noted earlier).

As discussed in the Predevelopment Report cited earlier, estimates of coal gasification costs can vary widely depending on the philosophy used to set the process and offsites bases, the detail of the equipment design, and the approach to the investment estimate. In addition, the method of financing, plant size, coal type, and the maturity of the technology can have significant impacts on SNG costs. The time frame for which costs are presented is also an important factor. Thus, caution must be used when comparing these economics with published estimates for other coal gasification processes. A consistent comparison of CCG with state-of-the-art gasification technology was made by Exxon Research and Engineering Company, and it concluded that significant incentive exists for development of the Catalytic Coal Gasification Process.

5.1.2 Integral Steam Reformer Heat Input Study

A key feature of the Catalytic Coal Gasification Process is the recycle of CO and H_2 to the gasifier. This forces the net products of gasification to be only CH_4 and CO_2 along with smaller amounts of H_2S and NH_3. Using this approach, the overall chemistry can be represented as follows;

$$\text{Coal} + H_2O \rightarrow CH_4 + CO_2 \qquad \Delta H \cong 0$$

Thus, coal is converted to methane in a single reaction step which is approximately thermoneutral. A small amount of heat input is required to preheat the feed coal, recycle gas, and steam to reaction temperature, to account for catalyst reactions, and to provide for gasifier heat losses.

In the Study Design developed during the CCG Predevelopment Program, this heat input was supplied by heating the steam and recycle gas in a fired heater to 1540°F. This preheat is sufficient to provide for the heat input requirements listed above. The preheat fired heater design temperature was set at 1575°F to allow for operating flexibility and control. A schematic flow plan for this system is shown in Figure 5.1-1.

During previous work, the concept of using a steam reformer for heat input was identified. In this concept, a small amount of methane is reformed to make additional CO and H_2 for feed to the gasifier. This CO and H_2 forms methane in the gasifier, thus providing both chemical and sensible heat input. The use of a reformer provided greater flexibility than the base case heat input scheme which used only sensible heat for heat input. The reformer could be either a small reformer operating in parallel with the preheat fired heater, or the reformer could replace the preheat fired heater by reforming methane already present in the recycle gas. This last alternative, called an Integral Steam Reformer, was shown by previous rough screening studies to be lower in cost than a parallel reformer but was an economic standoff with the base case utilizing a preheat fired heater.

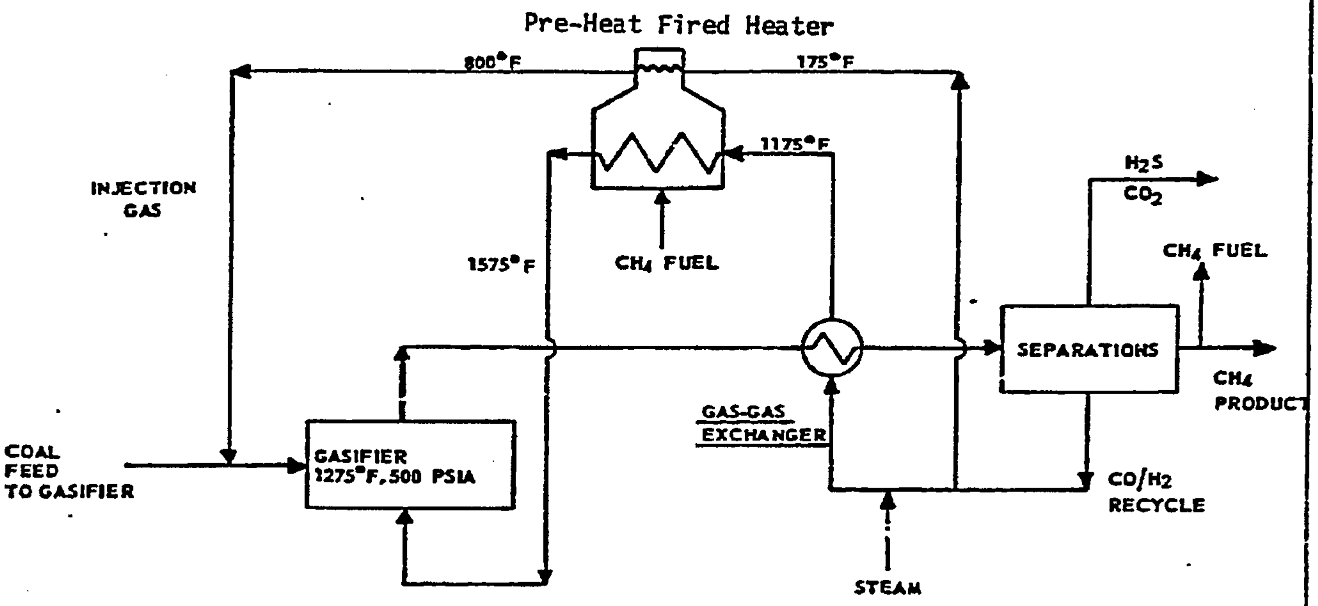
The objective of the current study was to consider the Integral Steam Reformer in greater depth using the CCG Study Design basis. A schematic flow plan for this system is also shown in Figure 5.1-1. Several screening studies were carried out to arrive at the final basis which was used for this study. Several alternative processing conditions were evaluated including a range of steam reformer coil outlet temperatures and steam conversions. The CCG reactor system material and energy balance model was modified to incorporate the steam reforming process option. Study results for reformer coil outlet temperature and steam conversion are summarized below.

- Reformer Coil Outlet Temperature - Steam reformer coil outlet temperatures (COT) from 1400°F to 1500°F were evaluated. A comparison of the cases is shown below:

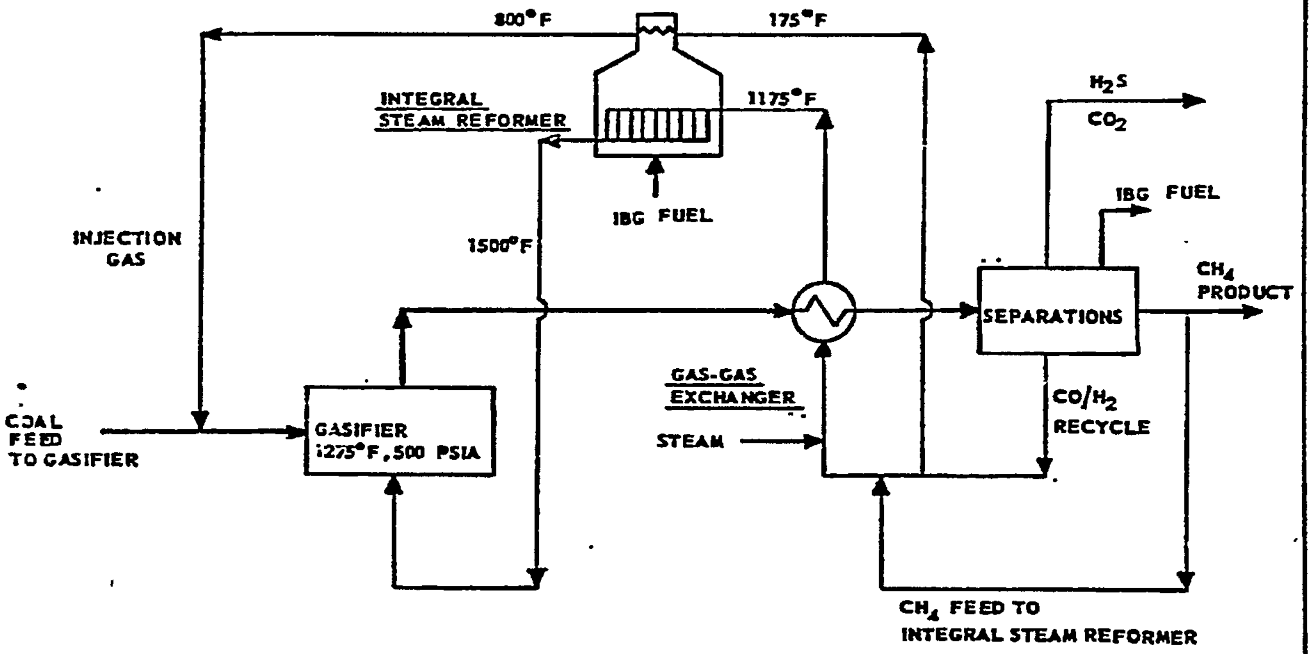
FIGURE 5.1-1

INTEGRAL STEAM REFORMING HEAT INPUT STUDIES - SIMPLIFIED SCHEMATIC FLOW PLAN

CCG STUDY DESIGN



INTEGRAL STEAM REFORMING CASE



Basis: 14,490 ST/SD Coal feed to gasifier
Gasifier operating conditions of 1275°F, 500 psia.

Coil Outlet Temperature	1400°F	1500°F
Recycle Gas Rate, lb moles/hr	66,300	53,100
Raw Gasifier Product Rate, lb moles/hr	181,600	152,800
Acid Gas Removal Feed, lb moles/hr	127,000	105,800
Overall Steam Conversion, %	39	42
Offsite Steam Required, lb moles/hr	64,400	55,700
Relative Gasifier Volume	100	95.4
Reformer Fired Heater Fuel Fired, MBtu/hr	680	630
Net Methane Product, GBtu/SD	252.1	254.8

The credits for higher temperature included reduced gas flow rates, reduced steam requirements, reduced fired heater duty, etc. The debit for the higher temperature will be a higher fired heater investment. It is believed that the credits of higher reformer outlet temperature offset the debits.

- Steam Conversion - A range of overall steam conversions from 41 to 50% was evaluated. These results are shown below:

Basis: 14,490 ST/SD Coal feed to gasifier,
Gasifier operating conditions of 1275°F, 500 psia, and
steam reformer coil outlet temperature of 1450°F.

Overall Steam Conversion, %	41	48	50
Recycle Gas Rate, lb moles/hr	59,200	53,700	51,300
Gasifier Product Rate, lb moles/hr	163,200	148,000	141,400
Acid Gas Removal Feed, lb moles/hr	113,500	109,600	108,100
Offsite Steam Required, lb moles/hr	58,600	48,400	44,000
Reformer Fired Heater Fuel Fired, MBtu/hr	650	630	620
Relative Gasifier Volume	100	130	160
Net Methane Product, GBtu/SD	253.7	254.0	254.1

The credits for higher steam conversion included reduced gas flow rates, reduced steam requirements, reduced fired heater duty, etc. The debit for the higher steam conversion will be higher gasifier investment. It is believed that the 48% steam conversion case represents the optimum balance.

The high steam reformer coil outlet temperature (1500°F) and high steam conversion (48%) process conditions were selected as the basis for evaluating additional process options. Two additional cases were evaluated. First, a lower heating value fuel was evaluated in place of methane product as the fuel for steam reforming. The stream selected was the gasifier product stream downstream of H_2S removal. This stream contained a mixture of CO, H_2, CH_4, and CO_2 and had a heating value (HHV) of about 500 Btu/SCF. The objective of using this lower heating value stream is to achieve investment and operating cost savings by reducing the feed rate to the CO_2 removal and cryogenic methane separation sections of the CCG process and by increasing the nitrogen purge from the recycle gas loop.

The second option was to use this same stream (gasifier product downstream of H_2S removal) as direct feed to steam reforming. This would be used to control gasifier heat input in place of the methane product used in the base steam reformer case. This also offers potential cost reductions in the CO_2 removal and cryogenic methane separation sections. The results of these process options studies are summarized below. All cases were run at a reformer coil outlet temperature of 1500°F and 48% steam conversion.

	Case 1	Case 2	Case 3
	Base	Lower Heating Value Fuel	Syn Gas As Reformer Feed
Fuel	CH_4	$CO/CH_4/H_2/CO_2$	$CO/CH_4/H_2/CO_2$
Reformer Heat Input Control	CH_4	CH_4	$CO/CH_4/H_2/CO_2$
Recycle Gas Rate, lb moles/hr	50,900	46,200	44,700
Raw Gasifier Product Rate, lb moles/hr	140,400	138,000	139,400
Acid Gas Removal Feed, lb moles/hr	103,800	101,400	102,300
Methane Recovery Feed, lb moles/hr	80,700	75,000	72,300
Reformer Fired Heater Duty, MBtu/Hr	620	660	660
Relative Gasifier Volume	100.0	97.0	98.6
Net Methane Product, GBtu/SD	254.7	254.6	254.7

As shown above, there is little difference in the material balances among the cases. Screening economics develped for these alternatives showed a small economic advantage (4 ¢/MBtu) for Cases 2 and 3 over Case 1. Case 2 was selected as the process basis for the Integral Steam Reformer Study. Economic advantage is gained by using product from H_2S removal as fuel. However, the use of this stream for supplemental reformer feed would result in the risk of H_2S poisoning of the reformer catalyst during process upsets. Thus product methane was used for gasifier heat input control.

In summary, the important basis items selected as a result of these screening studies are as follows: 1500°F reformer coil outlet temperature, 48% steam conversion, the use of intermediate Btu gas taken from the gasifier product gas stream after sulfur removal as fuel for the reformer, and the use of a small stream of product SNG for process control.

Two final material and energy balances were prepared: a normal balance and a design balance. The bases for the two balances are identical except that, for the design balance, the gasifier heat input requirement is increased by 40 MBtu/hr over calculated requirements to provide an allowance for control of gasifier temperature. This allowance is met by increasing the methane feed and the fuel to the integral reformer in the design case relative to the normal case. These material and energy balances differ from balances developed for the process basis screening studies because the final integral reformer design was used rather than a preliminary design. The design balance was used to develop investments for different sections of the plant by proration from the CCG Commercial Plant Study Design. The normal balance was used to define the plant operating costs. The results of these two balances are summarized below.

	Normal	Design
Coal Feed to Gasifier, ST/SD	14,490	14,490
Gasifier Temperature, °F	1,275	1,275
Raw Gasifier Product Rate, lb-moles/hr	136,600	138,100
Recycle Gas Rate, lb-moles/hr	46,200	46,500
Coil Outlet Temperature, °F	1,500	1,500
Reformer Fired Heater Duty, MBtu/hr	540	610

As shown above, the inclusion of the gasifier temperature control allowance adds about 1% to the plant gas flow rates and increases the duty of the integral reformer fired heater by about 13%. The reformer fired heater duty for the design case increases by 70 MBtu/hr compared to the normal case even though the gasifier heat input requirement was increased by only 40 MBtu/hr. In order to increase the radiant duty of the reformer by 40 MBtu/hr, it is necessary to increase the convection section duty by 30 MBtu/hr as well.

A comparison of the Integral Steam Reformer case with the CCG Study Design is shown below:

COMPARISON OF MAJOR MATERIAL AND ENERGY BALANCE EFFECTS

	CCG Study Design	Integral Steam Reformer Case
Coal Feed to Gasifier, ST/SD	14,490	
Coil Outlet Temperature (COT), °F	1,575	1,500
Normal Fired Heater Duty, MBtu/hr	485	540
Raw Gasifier Product Rate, lb-moles/hr	159,000	137,000
Recycle Gas, lb-moles/hr	57,500	46,200
Offsite Steam Demand, lb-moles/hr	60,000	46,000
Overall Steam Conversion, %	41	48
Net SNG to Sales, GBtu/SD	256.9	256.2
Relative Gasifier Volume	100	122

The offsite steam requirement is reduced by about 23% for the integral reformer because of the lower steam feed rate to the gasifier for this high steam conversion case. The reduction in recycle rate of 11,300 lb-moles/hr is a result of the removal of IBG fuel from the first stage of acid gas removal and higher steam conversion. The gasifier volume increased by 22% as a result of the higher steam conversion.

The investment for all plant facilities excluding the steam reformer was obtained by proration of individual plant sections from the CCG Study Design. The investment for the steam reformer was estimated in detail based on a study design for the fired heater. The investment for the Integral Steam Reformer Case and a comparison with the Study Design is presented in Table 5.1-4. The reactor system increased in investment by 12 M$ because of the increased gasifier volume required for higher steam conversion. The steam reformer investment is 14 M$ lower than the Study Design preheat fired heater investment because of the lower coil outlet temperature and a revised fired heater design for the different service. The reduction in the offsite steam requirement resulted in a 12 M$ reduction in steam generation facilities investment. Overall, the investment for the Integral Steam Reformer case is 4% lower than the CCG Study Design investment.

The gas cost developed for the Integral Steam Reformer case is presented in Table 5.1-5 and is summarized below and compared to the CCG Study Design.

	SNG Cost, $/MBtu	
	CCG Study Design	Integral Steam Reformer Case
Illinois No. 6 Coal	1.41	1.39
Major Chemicals	0.41	0.41
Utilities	0.35	0.34
Other Operating Costs	1.08	1.04
By-Product Revenues	(0.18)	(0.18)
Capital Charges (15% DCF)	3.11	2.99
Total SNG Cost (RISP)	6.18	5.99
Savings	Base	3.1%

The economic basis is the same as that for the CCG Study Design. Based on the same coal feed rate to the gasifier, a gas cost of 5.99 $/MBtu was obtained for the Integral Steam Reformer Study. This is a 3% reduction in the gas cost relative to the CCG Study Design. The gas cost reduction is the result of lower plant investment and a slight reduction in coal requirements. The inclusion of a reformer in place of a preheat fired heater in the CCG process increased the overall heat input flexibility and thus permits process improvements such as higher steam conversion and the use of IBG for fired heater fuel. The gas cost reduction of 3% is mainly a result of these process improvements rather than the integral reformer itself.

Table 5.1-4

INTEGRAL STEAM REFORMER HEAT INPUT STUDY
INVESTMENT FOR PIONEER PLANT

Basis:
- January, 1978 Instant Plant
- Eastern Illinois Location

Plant Section	Investment Breakdown - Million $	
	CCG Study Design	Integral Steam Reformer Case
ONSITES		
Coal Drying	27	27
Catalyst Addition	18	18
Preheat Fired Heater/Steam Reformer	51	37
Reactor System	146	158
Product Gas Cooling and Scrubbing	86	76
Sour Water Stripping and Ammonia Recovery	20	18
Acid Gas Removal and Sulfur Recovery	161	151
Methane Recovery System	44	43
Refrigeration	31	30
Catalyst Recovery	39	39
Common Onsite Facilities	55	55
ONSITES SUBTOTAL	678	652
MATERIALS HANDLING		
Coal Handling and Storage	19	19
Coke/Char Handling	5	6
Chemicals Handling and Storage	20	19
By-Products Storage and Shipping	3	3
Waste Solids Handling and Disposal	27	27
MATERIALS HANDLING SUBTOTAL	74	74
UTILITIES		
Raw Water/BFW Treating	29	27
Steam Generation and Distribution	120	108
Cooling Water	9	9
Electric Power Distribution	23	22
Miscellaneous Utilities	5	5
Flue Gas Desulfurization (1)	51	49
UTILITIES SUBTOTAL	237	220
GENERAL OFFSITES		
Wastewater Treating	48	47
Safety and Fire Protection	13	12
Site Preparation	6	6
Miscellaneous Offsites	34	34
GENERAL OFFSITES SUBTOTAL	101	99
TOTAL DIRECT AND INDIRECT COSTS	1,090	1,045
PROCESS DEVELOPMENT ALLOWANCE (25% of Onsites Direct & Indirect Costs)	169	163
PROJECT CONTINGENCY (25% of Total Direct & Indirect Costs)	271	262
TOTAL ERECTED COST	1,530	1,470

Note:

(1) Includes desulfurization for flue gases from steam generation (coal-fired boilers) and from coal drying and catalyst addition.

Table 5.1-5

INTEGRAL STEAM REFORMER HEAT INPUT STUDY

COST OF SNG FROM PIONEER PLANT WITH 100% EQUITY FINANCING

Basis:
- January, 1978 Instant Plant, Eastern Illinois Location
- 256.2 Billion Btu/Stream Day SNG (HHV Basis)
- 90% Capacity Factor
- 100% Equity Financing
- 15% Current Dollar DCF Return
- Escalation Rates:
  - Operating Costs and By-Product Revenues at 5%/Year
  - SNG Revenues at 6%/Year
- Total Erected Cost of 1,470 M$

SNG Cost Components	Requirements (At Full Capacity)	Unit Costs (1978)	SNG Costs Breakdown $/Million Btu (1978)
• Illinois No. 6 Coal (Cleaned)			
- To Gasifiers	14,490 ST/SD (2)	20 $/ST	1.131
- To Coal Dryer Fuel	710 ST/SD	20 $/ST	0.055
- To Offsite Boiler Fuel	2,620 ST/SD	20 $/ST	0.205
Subtotal	17,820 ST/SD		1.391
• Major Chemicals			
- KOH Solution (30 wt%)	189 ST/SD (Contained)	300 $/ST	0.221
- Lime (97% CaO) to Catalyst Recovery	1,005 ST/SD	39 $/ST	0.153
- Lime (97% CaO) to FGDS	247 ST/SD	39 $/ST	0.038
Subtotal			0.412
• Other Operating Costs			
- Purchased Electric Power	141 MW	2.5 ¢/kWh	0.330
- Raw Water	5,000 gpm	15 ¢/k gal	0.005
- Other Catalysts and Chemicals	Many Items	4.7 M$/yr	0.053
- Wages and Benefits	950 Men	21 k$/man/yr	0.237
- Salaries and Benefits	250 Men	25 k$/man/yr	0.074
- Labor Overheads and Supplies	20% of Wages, Salaries, and Benefits		0.062
- Materials and Overheads	3.3% of Total Erected Cost/Year		0.576
- Ash Disposal	8,300 ST/SD (Wet)	1 $/ST	0.032
Subtotal			1.369
• By-Products Revenues			
- Ammonia (20 wt%)	231 ST/SD (Contained)	160 $/ST	(0.144)
- Sulfur	324 LT/SD (2)	25 $/LT	(0.032)
Subtotal			(0.176)
• Capital Charges	Per Above Basis		2.989
TOTAL SUBSTITUTE NATURAL GAS COST (RISP) (3)			5.985
CALL			5.99

Notes:

(1) k = 10^3, M = 10^6, G = 10^9.

(2) ST/SD = short tons/stream day (i.e., one day's operation at full plant capacity). LT = long tons.

(3) RISP = required initial selling price in first year of plant operation (1978).

During the process variable studies for the Integral Reformer Study, the potential for carbon formation and laydown on the steam reforming catalyst or upstream equipment was identified as a key data need for the integral steam reformer system. Carbon laydown could result in reformer catalyst deactivation or in a severe corrosion phenomenon known as "metal dusting". This is not a serious problem for the preheat fired heater used in the CCG Study Design because the injection of small amounts of a sulfur compound into the gas stream prevented carbon laydown. This cannot be done if an integral reformer is used because the sulfur would poison the reformer catalyst. Carbon can be formed from one of the following reactions:

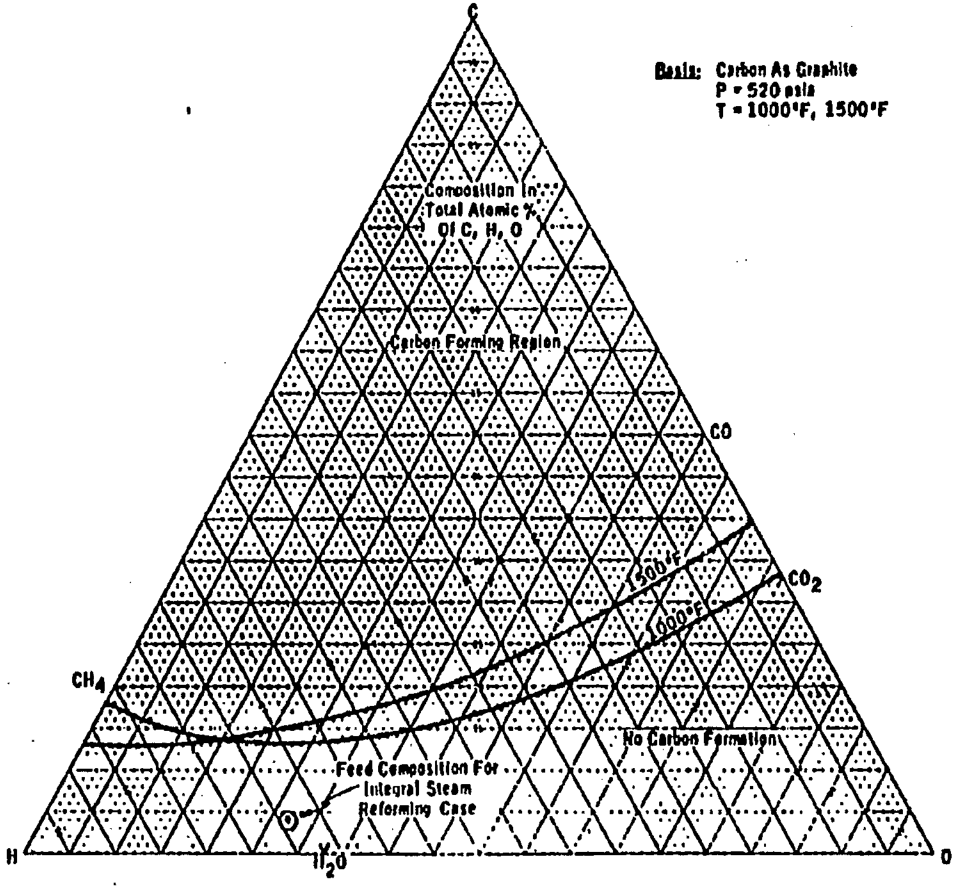
$$\begin{array}{lcl} 2CO & \rightarrow & CO_2 + C \\ CO + H_2 & \rightarrow & H_2O + C \\ CH_4 & \rightarrow & 2H_2 + C \end{array}$$

Figure 5.1-2 shows the equilibrium curves which define the carbon formation region for C-H-O atomic compositions at 1000°F and 1500°F at 520 psia. The composition of the reformer feed stream on this basis is: 4 mole % carbon, 69 mole % hydrogen, and 27 mole % oxygen. This point is shown on Figure 5.1-2 and is clearly out of the carbon formation region. Thus, with the high steam-to-carbon ratios for the integral reformer process conditions, equilibrium conditions are not favorable for carbon formation. However, the feed to the integral reformer is <u>not</u> in chemical equilibrium. Thus, it is possible that a non-equilibrium situation may exist in which carbon is laid down (for instance by the reaction $2CO \rightarrow CO_2 + C$) at a rate faster than it can be gasified away by the steam-carbon reaction ($C + H_2O \rightarrow CO + H_2$). Thus, though solid carbon cannot be present at equilibrium, it is possible that it could exist during the time the species are reacting to reach equilibrium. Thus, kinetics of the competing reactions could be important.

Data from laboratory bench-scale research on gas phase reactions indicated that carbon laydown can occur in a gas stream with compositions similar to those envisioned commercially for integral reformer feed. However, this research was directed at studies of the shift reaction, and conditions were not commercially representative for carbon laydown in terms of residence times, wall effects, etc. These factors can affect the kinetics of the competing reactions.

In the Integral Reformer Study, it was assumed that carbon laydown does not occur. The observation of carbon laydown in the laboratory was made at the same time that the process basis was set for this study. Approaches for dealing with carbon laydown were investigated. One potential method for minimizing or eliminating carbon formation upstream of or in the integral steam reformer is to shift a part of or all of the CO to CO_2. For instance, if all the CO were shifted to CO_2, carbon formation via the reaction $2CO \rightarrow CO_2 + C$ would not be possible. A material and energy balance was developed to determine the general impacts of this potential method of avoiding carbon formation. In this case, a shift reactor was added upstream of the integral reformer heat input system. The extent of the shift reaction was set so that 2% of the steam/recycle gas mixture would be CO_2. Directionally,

FIGURE 5.1-2
CARBON FORMATION EQUILIBRIUM ISOTHERMS



Basis: Carbon As Graphite
P = 520 psia
T = 1000°F, 1500°F

798-6-11-11

shifting a portion of the gas should reduce the possibility of carbon formation. The basis of 2% CO_2 in the feed to the steam reformer represented a compromise. As more gas is shifted and shift equilibrium is approached, the possibility of carbon formation from CO reversion is reduced. However, increasing the extent of the shift reaction increases the fuel requirement of the integral reformer. Because the shift reaction is exothermic and because the inlet temperature to the integral steam reformer is set at 1175°F by the outlet temperature of the gas-gas exchanger, the chemical heat released in the shift reactor must be made up in the integral steam reformer. This is illustrated in the following table:

	Reformer Without Shift	Reformer With Shift
Heat of Shift Reaction, MBtu/hr	--	-40
Reformer Fired Heater Duty, MBtu/hr	540	580

Results of the material and energy balance show a 7% increase in the reformer fuel requirement. This translates into a 0.5% reduction in the net SNG product. There were no major changes in gas rates to processing equipment. It was concluded from this work that altering the composition of the reformer feed gas stream via the shift reaction may be an economical method of preventing carbon formation. The economics of this approach will depend on the extent to which the gas must be shifted.

Two other alternatives for preventing carbon laydown have been identified. The first method is similar to the one described above. It consists of CO_2 injection into the reformer feed to alter the CO_2/CO ratio to prevent carbon laydown by the reaction $2CO \rightarrow CO_2 + C$. The second method consists of replacing the integral reformer with a small conventional steam reformer operated in parallel with a preheat fired heater. This small "supplemental" reformer would feed SNG and steam and thus carbon laydown would not be a problem. The preheat fired heater coil outlet temperature could be lowered to reduce its investment and the injection of a small amount of a sulfur compound could be used to prevent carbon laydown as in the Study Design. Work on an evaluation of supplemental steam reforming is described in the following section.

5.1.3 Supplemental Steam Reformer Heat Input Study

A study which considered the use of an integral steam reformer as a method of heat input to the CCG process gasifier was completed. In this concept, as discussed in the preceeding section, the preheat fired heater in the CCG Study Design was replaced with a reforming fired heater. Methane present in the recycle gas is reformed to make CO and H_2 which then methanate in the gasifier providing additional heat input. This permits greater heat input flexibility because additional heat input to the gasifier can be supplied by increasing the methane fed to the reformer. In the case of the preheat fired heater, additional heat could be supplied only by increasing the fired heater outlet temperature, which significantly increases fired heater investment. The Integral Reformer Study showed a 3% reduction in gas cost relative to the CCG Study Design, as described above.

The potential for carbon laydown (by the reaction $2CO \rightarrow CO_2 + C$) was identified as the major process uncertainty for the integral reformer concept. For purposes of the study, it was assumed that carbon laydown would not occur. However, bench-scale research on gas phase reactions has shown that carbon laydown can occur in a gas stream with compositions similar to those envisioned commercially for integral reformer feed.

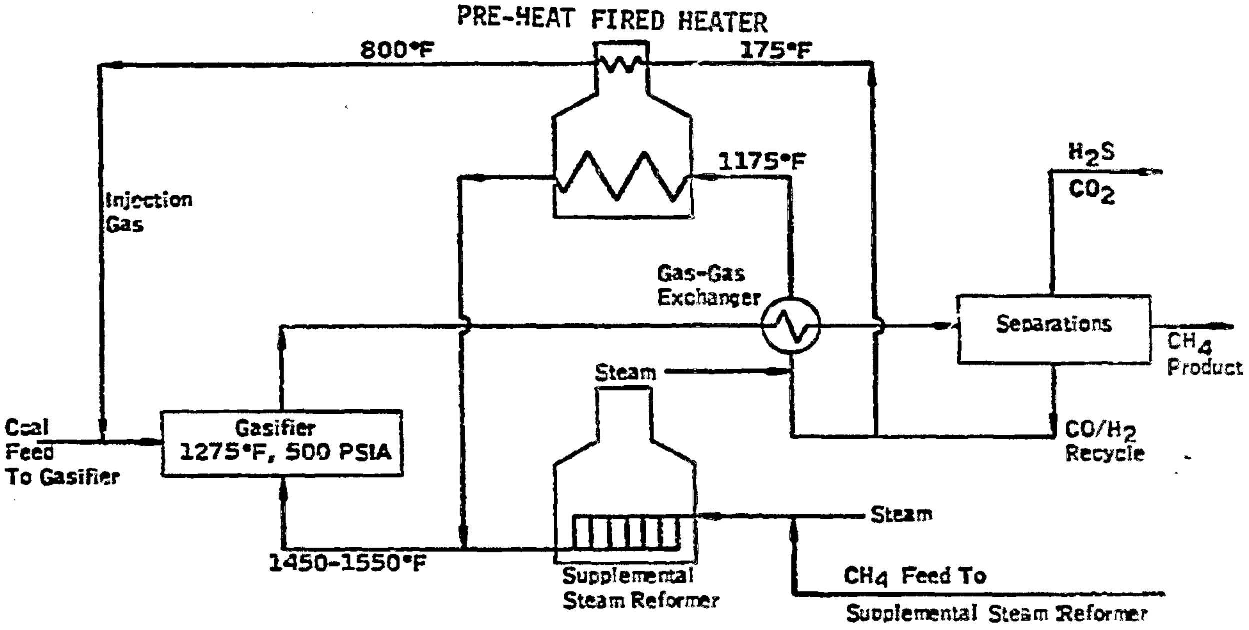
Two methods of preventing carbon formation were identified. The first consists of adding CO_2 via a shift reactor or CO_2 injection to increase the CO_2/CO ratio to prevent carbon laydown. The second method consists of operating a small conventional steam reformer in parallel with the preheat fired heater. This process concept is called supplemental steam reforming and it is shown and compared to integral steam reforming in Figure 5.1-3. The feed to the supplemental steam reformer consists of methane and steam and thus carbon laydown cannot occur by the CO reversion reaction. The preheat fired heater coil outlet temperature can be lowered to reduce its investment and carbon laydown can be prevented by the injection of a small amount of sulfur compound as in the CCG Study Design. The injection of H_2S cannot be used for the integral reformer because it would poison the reforming catalyst. The use of steam reforming for heat input increases process flexibility and permits higher steam conversions for the gasifier system.

A study evaluating the supplemental steam reforming process option was completed. The process basis for the Integral Steam Reformer Study (1500°F coil outlet temperature, gasifier effluent after sulfur removal for fuel, and 48% steam conversion) was used as a starting point for this study. The first alternative investigated was the type of fuel to be used for the preheat and steam reforming fired heaters. The options evaluated were gasifier effluent after sulfur removal, which is an intermediate Btu gas (IBG), and product SNG. Material and energy balances were prepared for cases using the different fired heater fuels. Results of these material and energy balances are summarized below.

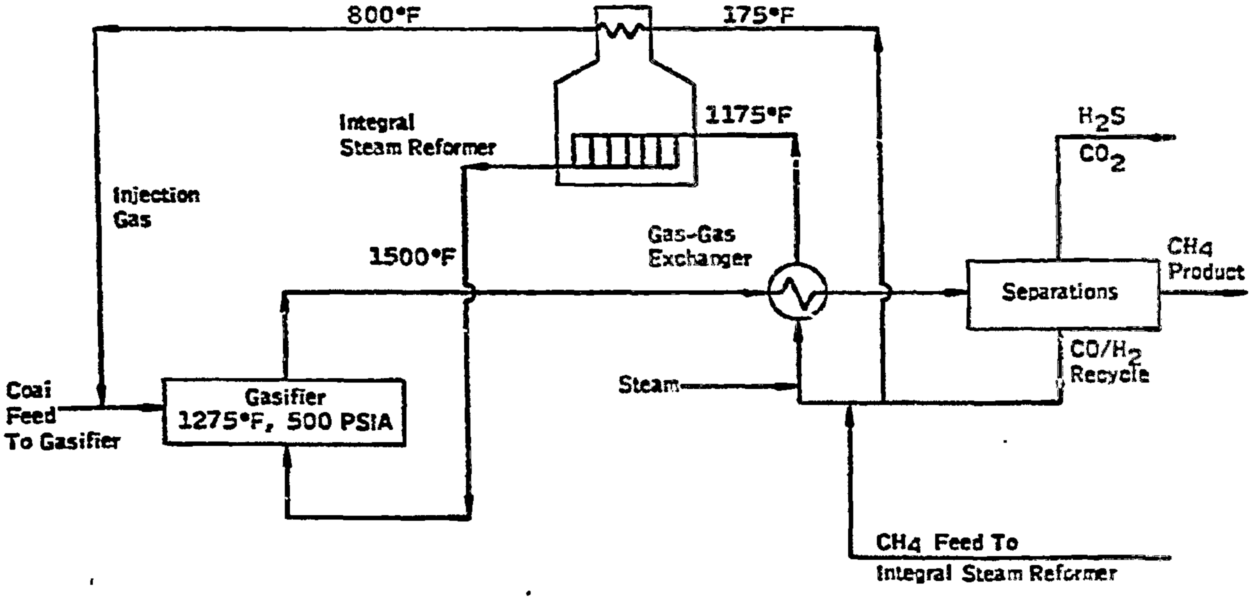
FIGURE 5.1-3

SUPPLEMENTAL STEAM REFORMING HEAT INPUT STUDIES - SIMPLIFIED SCHEMATIC FLOW PLAN

SUPPLEMENTAL STEAM REFORMING CASE



INTEGRAL STEAM REFORMING CASE



EFFECT OF FUEL TYPE

Type of Fuel for Fired Heaters	IBG Fuel	SNG Fuel
Preheat Fired Heater COT, °F	1500	
Steam Reformer COT, °F	1500	
Steam/Carbon Ratio, mole/mole	5/1	
Total Recycle Gas, lb-moles/hr	47,300	51,900
Gasifier Effluent, lb-moles/hr	140,400	143,100
Onsite Steam, lb-moles/hr	34,200	31,700
Offsite Steam, lb-moles/hr	42,100	44,400
Preheat Fired Heater Fuel, MBtu/hr	345	371
Steam Reformer Fuel, MBtu/hr	314	206
Net SNG Product, GBtu/SD	254.4	255.5

Lower gas rates were obtained for the IBG case; however, the total fired heater fuel requirement is 14% greater than the SNG case. Based on this material and energy balance study there was no clear advantage for the use of either IBG or SNG for plant fuel. SNG was chosen as the fuel for the supplemental steam reformer case based on the judgement that the higher product rate for the SNG case may provide a small advantage over the lower gas rate for the IBG case.

The effects of several process variables on supplemental steam reforming were then examined. Material and energy balances were prepared with SNG as the plant fuel. The process variables examined were preheat fired heater coil outlet temperature, steam reformer coil outlet temperature, and steam/carbon ratio in the reformer feed.

Preheat fired heater coil outlet temperatures of 1400°F to 1550°F were investigated. For these cases, the supplemental reformer was assumed to operate with a 1500°F coil outlet temperature and a feed steam/carbon ratio of 5/1. A summary of the material and energy balance results is shown below.

EFFECT OF PREHEAT FIRED HEATER COIL OUTLET TEMPERATURE

Preheat Fired Heater COT, °F	1400	1450	1500	1550
Steam Reformer COT, °F	1500			
Steam/Carbon Ratio, mole/mole	5/1			
Total Recycle Gas, lb-moles/hr	53,100	52,500	51,900	51,200
Gasifier Effluent, lb-moles/hr	146,600	144,900	143,100	141,300
Onsite Steam, lb-moles/hr	35,600	33,700	31,700	29,600
Offsite Steam, lb-moles/hr	41,300	42,800	44,400	46,000
Preheat Fired Heater Fuel, MBtu/hr	231	299	371	446
Steam Reformer Fuel, MBtu/hr	417	315	206	92
Net SNG Product, GBtu/SD	253.4	254.4	255.5	256.6

Credits for higher preheat fired heater coil outlet temperatures include lower overall plant fuel requirement, hence higher net SNG product, and lower recycle gas rates. The debits for higher preheat coil outlet temperatures are higher preheat fired heater investment and higher offsite steam requirements.

Steam reformer coil outlet temperatures of 1400°F and 1500°F were investigated with the steam/carbon ratio in the feed held constant at 5/1. For these cases, the preheat fired heater coil outlet temperature was set at 1500°F. A comparison of the material and energy balances is shown below.

EFFECT OF STEAM REFORMER COIL OUTLET TEMPERATURE

Preheat Fired Heater COT, °F	1500	
Steam Reformer COT, °F	1400	1500
Steam/Carbon Ratio, mole/mole	5/1	
Total Recycle Gas, lb-moles/hr	52,400	51,900
Gasifier Effluent, lb-moles/hr	144,500	143,100
Onsite Steam, lb-moles/hr	32,100	31,700
Offsite Steam, lb-moles/hr	44,200	44,400
Preheat Fired Heater Fuel, MBtu/hr	363	371
Steam Reformer Fuel, MBtu/hr	225	206
Net SNG Product, GBtu/SD	255.1	255.5

The credits for higher supplemental reformer coil outlet temperatures include lower recycle gas rates and slightly higher net product. Debits for higher reformer coil outlet temperature are increased investments for the reforming and preheat fired heaters which are respectively due to increased process severity and increased duty.

A range of steam/carbon ratios for the feed to the supplemental steam reformer was evaluated with the coil outlet temperature held constant at 1500°F. For these cases, the preheat fired heater coil outlet temperature was set at 1500°F. The results of the material and energy balances are shown below.

EFFECT OF STEAM/CARBON RATIO IN REFORMER FEED

Preheat Fired Heater COT, °F		1500	
Steam Reformer COT, °F		1500	
Steam/Carbon Ratio, mole/mole	3/1	5/1	7/1
Total Recycle Gas, lb-moles/hr	52,200	51,900	51,700
Gasifier Effluent, lb-moles/hr	143,900	143,100	142,800
Onsite Steam, lb-moles/hr	31,300	31,700	32,000
Offsite Steam, lb-moles/hr	44,900	44,400	44,000
Preheat Fired Heater Fuel, MBtu/hr	379	371	363
Steam Reformer Fuel, MBtu/hr	195	206	218
Net SNG Product, GBtu/SD	255.5	255.5	255.3

In general, the steam/carbon ratio in the feed to the supplemental steam reformer has small effects on the material and energy balances. For higher steam/carbon ratios the gas rates and the net SNG decrease slightly.

Based on a qualitative analysis of the above material and energy balance cases, the following process basis was chosen for the supplemental reformer case: a coil outlet temperature of 1500°F for the preheat fired heater, a coil outlet temperature of 1400°F for the steam reformer, a steam/carbon ratio in the steam reformer feed of 5/1, and SNG for the plant fuel. The basis for these choices is discussed below (except for the choice of SNG for plant fuel which was discussed previously).

A coil outlet temperature of 1500°F was chosen for the preheat fired heater because the fired heater investment starts to increase significantly as the coil outlet temperature is increased from 1500 to 1550°F. In addition, in this temperature range, it became necessary to use two radiant boxes instead of one in order to reduce the heat flux for the tubes in high temperature service. This reduces tube metal temperatures and permits the use of tube thicknesses within the range of current commercial practice. When it is necessary to use a two-box radiant section design, a step increase in fired heater investment occurs. Thus a coil outlet temperature of 1500°F was chosen to avoid the need for two boxes.

An inspection of the material balance cases for steam reformer outlet temperatures of 1400°F and 1500°F shows that gas rates are relatively unaffected by the choice of reformer temperature. Though the product SNG rate is slightly higher at a 1500°F outlet temperature, this benefit is likely outweighed by the increased investment associated with designing the reformer for 1500°F versus 1400°F. This is particularly true since the reformer would be operating with a pressure of over 500 psia. Thus a reformer coil outlet temperature of 1400°F was chosen as the basis for the study.

The material and energy balances for the steam/carbon ratio in the reformer feed cases show little change from one case to another. Since most commercial experience is with steam/carbon ratios of 5/1, this basis was selected for the supplemental reformer study.

The material and energy balance resulting from the final process basis served as the design basis for study designs of the preheat fired heater and steam reformer. These fired heater study designs were used to develop investment cost estimates for the two fired heaters. A summary for the supplemental steam reformer case is compared with the CCG Study Design in Table 5.1-6. The investment for each plant, except the fired heaters, was obtained by prorating individual sections from the CCG Study Design. The investments for the steam reformer and preheat fired heater were estimated in detail based on study designs for each.

Table 5.1-6

CATALYTIC COAL GASIFICATION SUPPLEMENTAL STEAM REFORMER STUDY INVESTMENT BREAKDOWN

Basis:
- January, 1978 Instant Plant, Eastern Illinois Location
- 14,490 ST/SD Coal to Process
- 25% Project Contingency
- 25% Process Development Allowance on Onsites

	Investment, M$	
	CCG Study Design	Supplemental Steam Reformer
Onsites		
Coal Drying/Catalyst Addition	56	56
Reactor System ex. Fired Heaters	182	204
Preheat Fired Heaters	64	23
Reformer Fired Heaters	-	19
Product Gas Cooling and Scrubbing	107	93
Sour Water Stripping/NH_3 Recovery	25	22
Acid Gas Removal/Sulfur Recovery	202	199
Methane Recovery	56	56
Refrigeration	38	40
Catalyst Recovery	49	49
Common Facilities	69	69
SUBTOTAL	848	829
Materials Handling		
Coal Handling and Storage	24	24
Coke/Char Handling	6	8
Chemicals Receipt and Storage	25	24
By-Products Storage and Shipping	4	4
Waste Solids Handling and Disposal	34	33
SUBTOTAL	93	93
Utilities		
Raw Water/BFW Treating	36	34
Steam Generation and Distribution	150	135
Flue Gas Desulfurization	64	61
Cooling Water	12	12
Electric Power Distribution	28	28
Miscellaneous Utilities	6	6
SUBTOTAL	296	276
General Offsites		
Wastewater Treating	60	58
Safety and Fire Protection	16	15
Miscellaneous Offsites	50	50
SUBTOTAL	126	123
TOTAL EX. PDA	1,363	1,321
PROCES DEVELOPMENT ALLOWANCE	169	166
TOTAL ERECTED COST	1,532	1,487
CALL	1,530	1,490

The investment for the reactor system increased by 22 M$, due to the increased gasifier volume required for the higher steam conversion case. The combined investment for the steam reformer and preheat fired heater was 22 M$ lower than the CCG Study Design preheat fired heater. This is due to the lower coil outlet temperatures for the reformer and preheat fired heater. The reduction in offsite steam requirement resulted in a 15 M$ savings for steam generation facilities. Overall, the plant investment for the supplemental steam reformer case was 3% lower than the CCG Study Design.

The gas cost for the supplemental steam reformer case is shown in Table 5.1-7. Based on the same coal feed rate, a gas cost of 6.09$/MBtu was obtained. This is about 1% less than the CCG Study Design and is the result of a lower plant investment and a lower offsite boiler coal feed rate.

Supplemental steam reforming with high steam conversion thus has the potential for a 1% gas cost advantage over the CCG Study Design. In addition to having a slight gas cost advantage, the supplemental steam reforming case has the major benefit of gasifier heat input flexibility which is not provided by the preheat fired heater. This heat input flexibility provides increased gasifier heat input by reforming more methane in the feed to the steam reformer. Thus the preheat fired heater and reformer coil outlet temperatures do not have to be increased. This heat input flexibility permits higher steam conversion, thereby reducing both offsite steam requirement and recycle gas rate.

The Supplemental Steam Reformer study was based on a steam conversion of 48% versus 41% for the Study Design. As a sensitivity to this study, a heat and material balance was developed for a supplemental steam reformer case with a steam conversion equal to that of the CCG Study Design. Investments and economics for this sensitivity resulted in a gas cost of 6.17 $/MBtu versus 6.18 $/MBtu for the CCG Study Design. The sensitivity case thus was shown to be a standoff with the CCG Study Design. This demonstrates that high steam conversion was the primary factor in the 1% gas cost advantage for the Supplemental Steam Reformer Case over the Study Design base case.

5.1.4 Two Stage Gasifier Incentive Study

In the Catalytic Coal Gasification Study Design, a simple fluidized bed gasifier with one gasification stage was used to achieve a target carbon conversion of 90%. A previous study done during the Predevelopment Phase of research investigated the use of a second gasification stage to increase overall carbon conversion to 95%. In this study, fines and char withdrawn from the first gasification stage were fed to the second gasification stage. The primary gasifier was operated the same as the gasifier in the study design and the secondary gasifier was operated in parallel at the same temperature. Steam and recycle gas from the preheat fired heater were fed in parallel to each gasification stage. This process configuration showed only a small gas cost savings of about 0.6% relative to the single stage base case.

Table 5.1-7

CATALYTIC COAL GASIFICATION
SUPPLEMENTAL STEAM REFORMER STUDY
SNG COST COMPARISON

Basis:
- January, 1978 Instant Plant, Eastern Illinois Location
- 90% Capacity Factor
- Economic Basis Consistent with CCG Study Design
- Net SNG Rates: CCG Study Design = 256.9 GBtu/SD
  Supplemental Steam Reformer = 255.2 GBtu/SD

	SNG Cost Breakdown, $/MBtu	
	CCG Study Design	Supplemental Steam Reformer
• Coal		
- To Gasifiers	1.128	1.136
- To Coal Dryer Fuel	0.055	0.056
- To Offsite Boilers	0.230	0.205
SUBTOTAL	1.413	1.397
• Major Chemicals		
- KOH (30 wt% Contained)	0.221	0.222
- Lime (97% CaO)		
+ To Catalyst Recovery	0.153	0.154
+ To FGDS	0.041	0.038
SUBTOTAL	0.415	0.414
• Other Operating Costs		
- Purchased Electric Power	0.343	0.353
- Raw Water	0.005	0.004
- Other Catalysts and Chemicals	0.056	0.052
- Wages and Benefits	0.244	0.240
- Salaries and Benefits	0.077	0.078
- Labor Overheads and Supplies	0.064	0.064
- Materials and Overheads	0.598	0.587
- Waste Solids Disposal	0.033	0.033
SUBTOTAL	1.420	1.411
• By-Product Revenues		
- Ammonia (20% Contained)	(0.144)	(0.145)
- Sulfur	(0.031)	(0.032)
SUBTOTAL	(0.175)	(0.177)
• Capital Charges	3.104	3.044
TOTAL SUBSTITUTE NATURAL GAS COST	6.177	6.089
CALL	6.18	6.09

A brief incentive study of an alternative two-stage gasification concept was completed during the first year of the development contract. The two-stage gasifier process configuration selected for this study is illustrated in Figure 5.1-4. In this scheme, coal was fed to the first stage gasifier which operated at low temperature (1225°F). The coal was fluidized and gasified by product gas from the second stage gasifier. A carbon conversion of 80% was achieved in this first stage. The char and fines from the first stage were withdrawn and fed to the second-stage gasifier. This stage was operated at a higher temperature (1325°F) to achieve high carbon conversions. Steam and recycle gas from the preheat fired heater are fed to the secondary gasifier to achieve an overall carbon conversion of 95% for the two gasifier stages.

This concept differs from the one evaluated in the predevelopment research phase in that the two gasification stages are operated in series with respect to steam and recycle gas flow. This permits operating the gasifiers at different temperatures. Reduced recycle gas rates were achieved by operating the upper stage at a lower temperature (1225°F) and high carbon conversions were obtained by operating the bottom stage at a higher temperature (1325°F).

A summary of the process basis and heat and material balance is provided in Table 5.1-8. The two-stage gasifier case was evaluated on the basis of the same coal feed rate to gasification as the CCG Study Design. Total gasifier steam required increased by 10% while the recycle gas rate decreased by 12%. Due to the lower temperature in the first-stage reactor, the preheat fired heater coil outlet temperature decreased from 1543 to 1500°F. The net SNG product rate increased to 271 GBtu/SD (up 5.6%) while the overall plant efficiency increased by 3%.

Rough screening economics were developed for this two-stage gasification scheme. As shown in Table 5.1-9, total investments are up by 5% over the base case. This is a slightly smaller percentage increase than the increase in plant SNG output (5.6% increase). The most significant investment increase is associated with the reactor system, which includes a larger first stage gasifier than the base case to compensate for the lower reactor temperature (1225°F), and for the addition of the separate second stage gasifier. Also, steam generation investments were increased due to the increased steam requirements for this case.

Process economics are presented in Table 5.1-10. The total gas cost with two-stage gasification is 2.3% less than the Study Design gas cost. Savings are achieved in coal, catalyst, and operating costs. Thus, based on these results, there appears to be a small incentive for staged gasification. However, additional research and supporting engineering studies would be required to develop a better estimate of the incentive for two-stage gasification. This study identified that additional data are required to firm up reaction kinetics at the lower gasifier temperature of 1225°F and at carbon conversions over 90%. The data base at these conditions available at the time of this study was limited since the Fluid Bed Gasifier (FBG)

FIGURE 5.1-4

SIMPLIFIED FLOW PLAN FOR TWO STAGE GASIFICATION

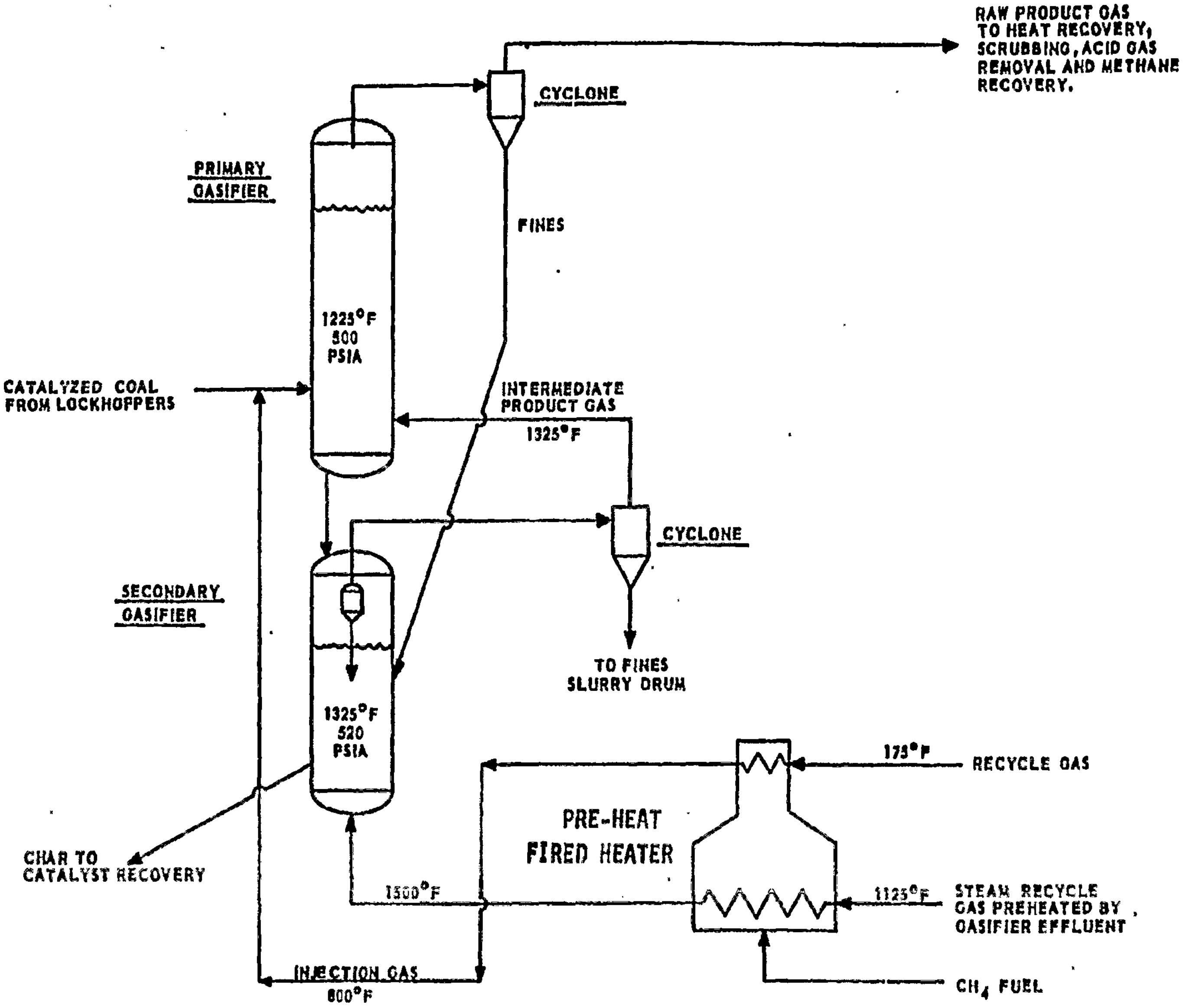


Table 5.1-8

INCENTIVE STUDY FOR TWO-STAGE GASIFICATION

Reactor System	Base Case "Primary" Gasifier Only	Two-Stage Gasification Primary and Secondary Gasifiers
Free Carbon Conversion		
Primary Gasifier	90%	80%
Overall	90%	95%
Conditions:		
Primary Gasifiers	1275°F/500 psia	1225°F/500 psia
Secondary Gasifier	-	1325°F/520 psia
Key Stream Rates:		
Coal Feed to Gasifier, ST/SD (1)	14,490	14,490
Coal to Boilers, ST/SD	2,840	3,030
Coal to Dryer Fuel, ST/SD	710	710
Total Coal, ST/SD	18,040	18,230
Total Gasifier Steam, MPH	86,000	95,000
Total Recycle Rate, MPH	57,520	50,700
Preheat Fired Heater Coil Outlet Temperature, °F	1,543	1,500
Net SNG Product Rate, GBtu/SD	257.0	271.3
Utilities Requirements:		
Electric Power, MW	147	151
Raw Water, GPM	7,300	7,300
Overall Thermal Efficiency (2)	62.6	65.7

Notes:

(1) Base case refers to CCG Study Design completed in the Predevelopment Program and documented in the Final Report FE-2369-24.

(2) Two-stage gasification evaluated on the basis of constant coal feed rate to gasification.

(3) Thermal efficiency includes purchased electric power (evaluated at a power plant heat rate of 8,950 Btu/kWh) and by-products.

Table 5.1-9

TWO STAGE GASIFICATION INCENTIVE STUDY RELATIVE INVESTMENT BREAKDOWN

Basis: Base Case Total Investment = 100

	Base Case	Two-Stage Gasification
Onsites		
Coal Drying/Catalyst Addition	4.7	4.7
Reactor System	15.2	19.0
Product Gas Cooling/Scrubbing	6.5	6.2
Sour H_2O Stripping/NH_3 Recovery	1.5	1.6
Acid Gas Removal/Sulfur Recovery	12.0	12.0
Methane Recovery	3.3	3.3
Refrigeration	2.3	2.4
Catalyst Recovery	3.0	2.9
Common Facilities	4.8	4.9
Onsites Subtotal	53.3	57.0
Offsites		
Utilities	19.8	20.5
Materials Handling	8.9	9.0
General Offsites	7.2	7.2
Offsites Subtotal	35.9	36.7
Process Development Allowance (25% of Onsite Direct & Indirect Cost)	10.8	11.4
Total Plant TEC	100.0	105.1

Table 5.1-10

TWO-STAGE GASIFICATION INCENTIVE STUDY
SUMMARY OF RELATIVE GAS COST

Basis: Base Case Total Gas Cost = 100

Gas Cost Components	Base Case	Two Stage Gasification
Coal to Gasifiers	17.6	16.6
Coal to Dryer Fuel	0.9	0.8
Coal to Offsite Boilers	3.4	3.5
Subtotal	21.9	20.9
Major Chemicals		
KOH Solution (30 wt %)	3.4	3.2
Lime (97% CaO)	2.4	2.2
Subtotal	5.8	5.4
Other Operating Costs		
Purchased Electric Power	5.3	5.2
Raw Water	0.1	0.1
Other Catalysts & Chemicals	1.1	1.0
Wages and Benefits	4.0	3.9
Salaries and Benefits	1.3	1.2
Labor Related Operating Costs	1.0	1.0
Investment Related Op. Costs	10.0	9.8
Ash Disposal	0.4	0.4
Subtotal	23.2	22.6
By-Products Credits	(2.9)	(2.9)
Capital Charges (1)	52.0	51.7
Relative Gas Cost, %/MBtu	100.0	97.7
Gas Cost Savings, %	-	2.3

Note:

(1) Capital charges based on 100% equity financing with 15% DCF return.

runs made during the predevelopment research phase were generally at temperatures of 1300°F and carbon conversions of 80-90%. Additional data were also required to allow better prediction of the rate of fines entrained from the primary gasifier and the ability of the two-stage system to retain and gasify these fines.

5.1.5 Coal Crushing Machinery for CCG

A study was carried out to determine the type(s) and performance of coal crushing/drying machinery appropriate for commercial CCG plants.

A combination of crushing and drying of the 2" x 0" washed Illinois No. 6 coal feed is expected to be the first coal preparation step in a commercial-sized coal gasification plant. A hot gas-swept mill may perform this function. This mill type was investigated with emphasis placed in two areas:

- The non-typical product size requirement
- The safety requirement in regard to pressure containment in the event of a coal dust explosion

The study investigated the two extremes of product coal size being considered for CCG:

- 99% passing 8 mesh sieve with less than 3% passing 325 mesh sieve.
- 99% passing 30 mesh sieve with approximately 17% of the finest material (that passing 325 mesh) to be separated from the main product stream for utilization elsewhere in the plant (e.g., as offsite boiler fuel). The coarser 83% of the product -- the portion going to the gasifier -- should contain less than 3% -325 mesh material.

In each alternative, the coal is reduced in water content from 16.5 wt% to 4 wt%. These two product size alternatives are non-typical in that they limit the amount of -325 mesh material to be sent to the gasifier; in most other crushing processes with these top sizes (such as pulverizing systems for boiler fuel), the production of fines is acceptable or even encouraged.

Safe mill system design involves eliminating or minimizing the effects from a possible coal dust explosion. The two most frequently considered mill system or to manufacture the mill and its associated fans, ductwork, etc. to withstand the effects of a 50 psig explosion.

Investigation of Mill Types

During the study, inquiries were made to 14 American manufacturers concerning the type(s) of equipment they manufacture for crushing/drying coal to commercial CCG requirements. These manufacturers include the makers of rod mills, cage mills, hammer mills, roller mills, and others. They were alerted to the basic CCG commercial plant crushing/drying requirements and asked to provide information about the type and size mill that they would expect to supply to such a facility. Manufacturers were also asked to express their views on the system design requirements pertaining to a coal dust explosion. Only one American design appeared to satisfy product size requirements. This proposal included an impact dryer mill with classifier and hot inert gas generator for drying and inerting.

Several European manufacturers were subsequently contacted and asked to provide information about their equipment and systems. Flow plans were received from two of these manufacturers. One of the flow plans proposed the use of an impact crusher/dryer while the other proposed using a roller mill crusher/dryer. Neither vendor expressed unreserved confidence that it could produce the product sizes desired. Both encouraged testing with small-scale test equipment. Both crusher types should be further investigated to determine their applicability to the project.

Screening quality investments for both product size alternatives were received from the American vendor and from the European impact crusher vendor. A response from the second European vendor is expected shortly. The principal differences in equipment needs for the two product size alternatives are the finer grinding system's need for an external separator and a higher horsepower mill motor.

Safety Design Requirements

To arrive at appropriate design requirements, the safety requirements in regard to pressure containment in the event of a coal dust explosion were investigated for coal crushing equipment and its associated ductwork, fans, cyclones, etc. In this effort, applicable National Fire Protection Association (NFPA) standards were reviewed, and both Exxon and outside safety experts were consulted. The investigation provided the following information:

- No NFPA standards have been written especially for coal gasification facilities.
- Those individual equipment components which are covered by NFPA standards should be designed for NFPA standards.
- Unless a reliable inerting system is available for coal crushers and the associated ductwork, fans, cyclones, etc. in the system, a 50 psig design pressure should be assumed. (A reliable system would have to provide inerting at start-up and shutdown as well as during normal operations.)

In addition, both European vendors under consideration stated that they construct all their coal mill systems with this product size to withstand a 50 psig explosion. The American vendor stated that it will build either an inerted system or one designed to withstand a 50 psig explosion.

5.1.6 Coal Feed Size Study

The objective of the coal feed size was to identify and evaluate potential commercial techniques to reduce gasifier coal top size while minimizing additional fines in the feed.

As discussed in detail elsewhere in this report, lower-than-expected gasifier fluid bed densities were observed in some PDU operations. These low densities appeared to be caused by swelling of the catalyzed coal feed during devolatilization, with subsequent production of added quantities of fines. Coal/catalyst preoxidation was evaluated as an approach to increase fluid bed density. Based on limited data from the PDU, reducing the coal feed top size may also help to increase fluid bed density. Preoxidation may be more effective in preventing swelling of smaller particles. Or, smaller particles may swell less because volatiles can more readily escape.

For purposes of this initial study, coal feed top size was set at 30 mesh, as compared to 8 mesh in the CCG Study Design. The target fines content (defined as 325 mesh minus) of the feed was set at 3 wt% or less. Some PDU operations used a 30 mesh top size feed with about 2-3 wt% less than 325 mesh. This study was carried out in conjuction with the coal crushing machinery studies described in the preceding item.

Discussions were held with three vendors to identify coal preparation systems with the potential to produce a 30 mesh top size product with with minimum fines. The vendors were requested to provide material balance, size distribution, and cost information for their systems. Based on this information, plans were to select one or more systems for further evaluation, and to develop economics to show the approximate cost impact of reducing coal feed size.

Only one of the three vendors supplied all of the requested information as of the end of the contract period. Cost information was received from a second vendor, but the information provided on material balance and size distribution was inadequate to determine if the system proposed met the necessary requirements for preparing 30 mesh top size feed. More input was requested from this second vendor. The third vendor had not yet responded to the initial request.

Preliminary analysis of the information received from the first vendor indicated that the incremental cost for reducing coal feed top size from 8 mesh to 30 mesh would be small. Producing the 30 mesh size would require an investment increase of 6 M$ for additional coal preparation facilities and would add 4 MW to the plant electric power requirements. The total product SNG cost would increase by only 0.4% relative to the CCG Study Design. This analysis assumed that the coal fines (nominally -325 mesh) separated out in preparing the 30 x 325 mesh coal feed can be utilized as offsite boiler fuel with negligible incremental cost. For the first vendor's preparation system, this coal fines stream amounted to 17% of the total feed coal, which approximately equals the offsite boiler fuel requirements in the CCG Study Design.

5.1.7 Catalyst Addition Study

Work began but was not completed on a study to identify mixing systems which are potentially suitable for adding catalyst solution to crushed and dried coal feed on a commercial scale. The objective of this engineering study was to provide engineering and laboratory guidance by defining the important process variables, technical issues, and first-pass commercial economics for candidate catalyst addition systems.

The range of process conditions at which the catalyst addition system may operate was tentatively defined. These include:

• Coal feed size	8 x 325 mesh or 30 x 325 mesh
• Coal moisture at inlet	4 wt% (wet basis)
• Catalyst solution/coal ratio	0.4-0.7 lb/lb (wet basis)
• Catalyst solution concentration	20-35 wt% K_2CO_3
• Product solids moisture	20-35 wt% (wet basis)
• Mixer residence time	1-30 min
• Mixer temperature	150-215°F

The key performance requirements identified for the coal/catalyst solution mixer include relatively uniform total catalyst loading for all particle sizes, relatively uniform distribution of catalyst within the particles, "handleable" product solids, and minimum attrition.

As is evident from the ranges shown, there is considerable uncertainty regarding the preferred values for two important process variables, solution concentration and residence time. (Variations in catalyst solution/coal ratio and product solids moisture are just reflections of the uncertainty regarding concentration.) Bench laboratory tests, and possibly tests in small pilot-scale mixing equipment, may be needed to reduce the range of uncertainty regarding the preferred conditions for effective catalyst addition.

Meetings were held and planned with mixer vendors to determine equipment types which may be suitable for the catalyst addition step, and to discuss equipment limitations. The mixer types identified for further evaluation included:

- Axial dispersion mixer with tumbling action
- Conical mixer with orbiting screw agitator
- Paddle mixer

- Ribbon mixer
- Rotary drum mixer

Further vendor discussions and analysis should be carried out to assess the suitability and performance limitations of these and other mixer types for the catalyst addition service. Two or more of these alternatives should be selected and evaluated to determine approximate relative costs.

5.1.8 Coal/Catalyst Preoxidation Studies

As described earlier in this report, some PDU operations resulted in lower-than-expected densities in the gasifier fluid bed. These low densities appeared to be interrelated with swelling of the catalyzed feed coal during devolatilization and the production of added quantities of fines. It is desirable to avoid such conditions in commercial operations for two principal reasons: first, lower bed density will reduce carbon holdup per unit volume and thus lead to larger gasifiers; and second, the added fines make will tend to lower overall carbon conversion and thus reduce the SNG yield per ton of coal fed.

Two main techniques were tentatively identified in the laboratory to increase fluid bed densities and reduce fines production: (1) operating the gasifier at a pressure below the CCG Study Design "base" pressure of 500 psia; and (2) preoxidizing the coal by exposure to air at relatively mild conditions (1 atm, 300-450°F). Laboratory work was initiated to study various combinations of pressure and preoxidation. This work was directed toward determining the relationships among gasifier pressure, degree of preoxidation, and fluid bed density, and toward defining the preferred conditions for and the material balance impacts of coal preoxidation. To provide initial guidance to these laboratory studies, a series of gasifier system material and energy balances were developed to quantify some of the potential effects of reduced pressure and of coal preoxidation on a commercial CCG plant. The results of these material and energy balance studies are presented below.

To provide further guidance to the CCG development program on the potential economic impacts of these techniques to increase fluid bed density, separate engineering screening studies were carried out to evaluate reduced pressure operation and coal/catalyst preoxidation. The latter study is described below, and the reduced pressure study is covered in a subsequent section of this report.

Initial Material and Energy Balances

The effects of coal preoxidation via air exposure on the structure and elemental analysis of the coal are not well understood. Early results did indicate that oxygen is consumed and that the amount of oxygen consumption depends on the "severity" (time and temperature) of the air exposure step. Preoxidation at "mild" conditions results in an oxygen consumption of about 2-4 wt% on dry coal, while "severe" preoxidation can result in 10-20 wt% O_2 consumption.

To provide a measure of the effects of preoxidation at different severities, commercial-scale CCG material and energy balances were developed for two assumed levels of oxygen consumption, 2 wt% and 10 wt% on dry coal. The material and energy balance results for these cases are compared to the "base" CCG Study Design in Table 5.1-11. All of the cases shown in the table were based on the same coal feed rate and gasifier conditions as the Study Design. As shown by the first three columns of the table, the most significant impact of coal oxidation on the CCG material balance is that the net SNG product rate decreases relative to the Study Design as the extent of coal oxidation increases. For "mild" preoxidation severity (2 wt% O_2 pickup), the net SNG product dropped to 253.2 GBtu/SD, or 1.4% less than the Study Design. Relatively "severe" preoxidation (10 wt% O_2 pickup) resulted in a product rate of 239.5 GBtu/SD, or 6.8% less than the Study Design. The economic debit associated with a product yield loss of nearly 7% would be quite significant. Additional debits would be incurred for the costs of facilities added to carry out the preoxidation process.

The material and energy balances indicated that other changes to the gasifier and recycle gas loop would also be required if pretreatment via air oxidation were incorporated into the commercial plant design. In all cases the steam rate to the gasifier was set to maintain the gasifier outlet gas in apparent steam-graphite equilibrium. As the extent of oxidation increases, the total gasification steam requirement decreases, which in turn decreases the steam required from the offsite coal-fired boilers. The recycle gas loop and the associated equipment would be slightly smaller relative to the Study Design. Preheat fired heater duty and coil outlet temperature both increase with oxidation extent if it is assumed that the temperature of the gasifier feed coal remains at the Study Design value of 200°F. Heat may be released in preoxidation depending on the severity and the final disposition of the oxygen consumed. This heat may be usable in a way which heats the feed somewhat above 200°F. Increasing the feed coal temperature would lower the preheat fired heater duty, coil outlet temperature, and fuel fired, and increase the net SNG product rate enough to offset some of the yield loss due to preoxidation.

The exact manner in which oxygen is consumed in preoxidation is not yet known. The first two preoxidation cases in Table 5.1-11 were based on the assumption that most of the O_2 combines with the solid coal itself, and is thus carried into the gasifier. It is possible that O_2 acts to remove hydrogen or carbon from the coal in preoxidation as H_2O or CO_2. The last two columns of the table show the impacts of these alternative assumptions on the CCG material and energy balance with 10 wt% oxygen consumption in preoxidation. The results still show substantial SNG product yield losses, ranging from 5.8-7.1% of the base product rate. Compared to the case in which the

Table 5.1-11

POTENTIAL EFFECTS OF COAL PREOXIDATION ON THE MATERIAL AND ENERGY BALANCE FOR A COMMERCIAL CCG PLANT

Basis:
- Coal Feed Rate to Preoxidation: 11,980 ST/SD (Dry)
- Gasifier Conditions: 500 psia, 1275°F
- Carbon Conversion: 90%

	CCG Study Design (Base Case)	Preoxidation Cases			
		O_2 Combines With Coal(1)		O_2 Removes H From Coal(2)	O_2 Removes C From Coal(3)
Oxygen Consumption in Preoxidation, wt% on Dry Coal	None	2	10	10	10
Temperature of Coal Feed to Gasifer, °F	200	200	200	200	200
Net SNG Product, GBtu/SD	256.9	253.2	239.5	238.7	242.0
Change in Net SNG Product, % of Base	Base	-1.4	-6.8	-7.1	-5.8
Relative Steam-Carbon Equilibrium Constant(4)	1.00 (Base)	1.00	1.00	1.00	1.00
Steam Conversion, % of Steam Fed	41.5	41.0	39.1	43.3	40.9
Steam to Coal Ratio, lb Steam/lb Dry Coal	1.58	1.57	1.53	1.64	1.47
Total Steam Requirement, lb-mole/hr	87,800	87,200	84,900	91,000	81,400
Offsite Steam Requirement, lb-mole/hr	59,200	58,400	55,400	62,900	54,000
Recycle Gas Rate, lb-mole/hr	57,600	57,400	56,800	56,800	54,300
Normal Preheat Fired Heater Coil Outlet Temp., °F	1541	1555	1597	1595	1554
Preheat Fired Heater Heat Absorbed, MBtu/hr	480	500	550	580	470

Notes:

(1) Net SNG reduction results mostly from coal oxygen pickup. Small losses of coal carbon and hydrogen as CO_2 and H_2 are also included.

(2) Net SNG reduction results mostly from removal of hydrogen as H_2O. Small losses of coal carbon and hydrogen as CO_2 and H_2 are also included.

(3) Net SNG reduction results mostly from removal of carbon as CO_2. A small loss of coal hydrogen as H_2 is also included.

(4) Steam-graphite equilibrium equals 1.00.

O_2 was assumed to combine with the coal, more steam is required if O_2 removes hydrogen from the coal, and the recycle rate is also up. The steam and recycle rates are lower and the SNG yield is higher if the O_2 removes carbon from the coal, but this was judged to be the least likely of the three possible modes of O_2 consumption.

Based on these initial material and energy balance cases, it appeared that mild preoxidation of feed coal via air exposure is a potentially low cost method of increasing gasifier fluid bed density. Material balance debits are modest for oxygen consumptions in the range of 2-4 wt% on dry coal. Severe preoxidation, with oxygen consumptions above 10 wt%, is not likely to be economically attractive.

Preoxidation Screening Study

The Coal/Catalyst Preoxidation Screening Study showed that adding fluidized beds to preoxidize the catalyzed coal feed to a commercial CCG plant may lead to a 4-8% gas cost increase over the CCG Study Design. The preoxidizers for this screening study were assumed to operate at relatively mild conditions, about 17 psia and 400°F. The facilities requirements for this system were based on the limited laboratory data available in mid-1980, so the results of this study represent only a rough, first-pass evaluation of preoxidation. However, the important process variables and technical issues for coal/catalyst preoxidation were defined as a result of this study. Thus, this screening study pointed to areas where further work should be concentrated, and provided a starting point for optimization of the preoxidation system.

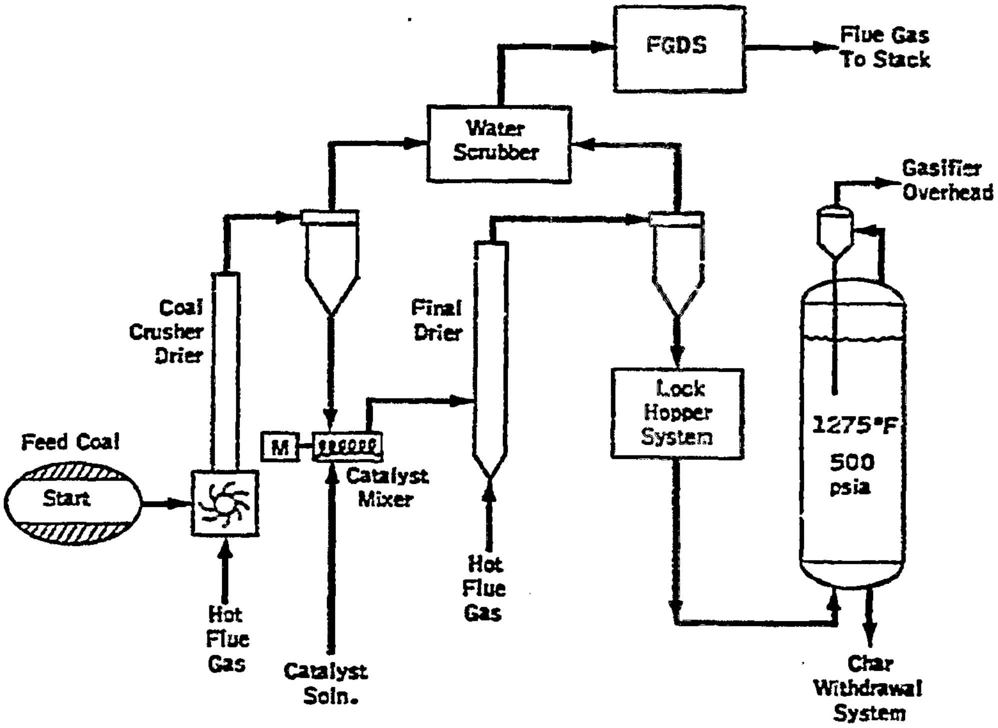
The process flowscheme developed for this study is compared with that for the CCG Study Design in Figure 5.1-5. The facilities for coal crushing/first stage drying and catalyst addition were unchanged from the CCG Study Design. In coal crushing/first stage drying, feed coal is crushed to 8 mesh top size, and simultaneously dried to 4 wt% moisture in gas-swept impact mills with entrained drying columns. The heat duty of the dryer is supplied directly by a mixture of recirculated gas and hot flue gas from a coal-fired inert gas generator (not shown). The stream of gas and evaporated moisture leaving this system is water-scrubbed to reduce the dew point and remove fines. The scrubbed gas is then fed to the boiler flue gas desulfurization (FGDS) system for SO_2 removal.

Catalyst solution is added to the dried coal in a gentle mixing step. Although the catalyst addition facilities were unchanged from the CCG Study Design, the catalyst solution basis was changed to be consistent with Case 2 of the Catalyst Recovery Screening Studies. The key impact of this basis change was an increased duty for coal/catalyst solution drying, because the catalyst solution is thus fed at 136°F, compared to 230°F for the CCG Study Design.

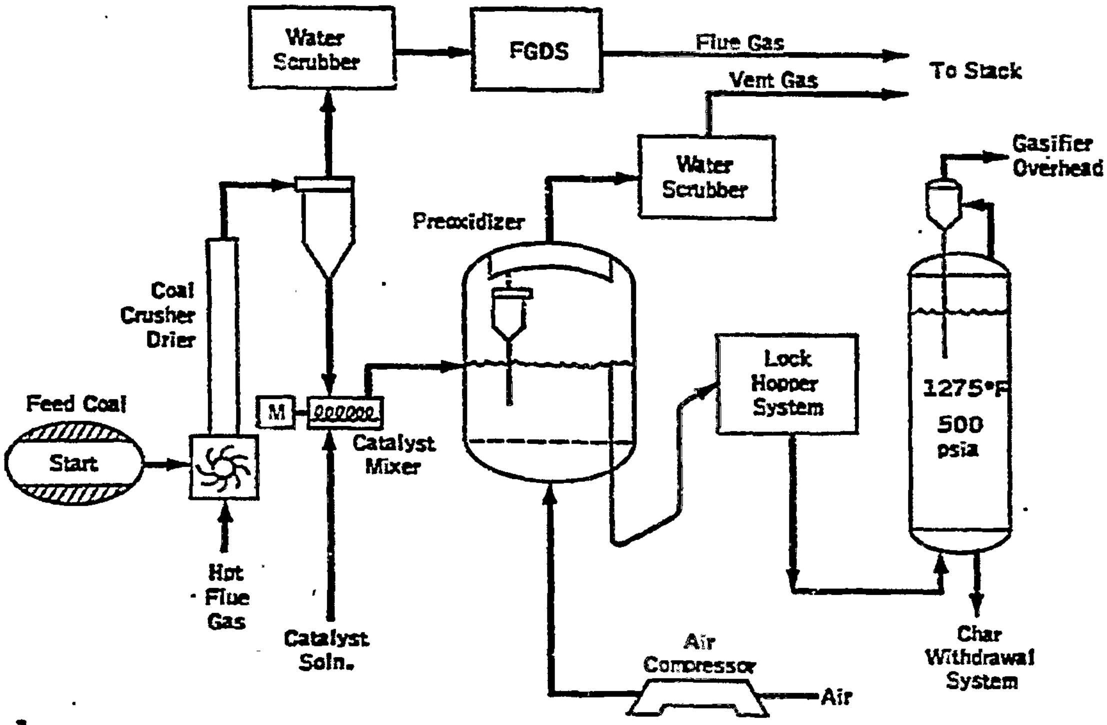
FIGURE 5.1-5

COAL/CATALYST PREOXIDATION STUDY
SIMPLIFIED SCHEMATIC FLOW PLAN

STUDY DESIGN COAL PREPARATION SYSTEM



PREOXIDATION COAL PREPARATION SYSTEM



The coal/catalyst solution mixture must be further dried before being fed to the gasifiers. In the CCG Study Design, this drying step was accomplished in an entrained dryer, where the coal/catalyst mixture was dried to 3.6 wt% moisture. The heat input method for this final drying step was the same as for the first stage dryer, and gas leaving this system was combined with first stage purge gas for water scrubbing and SO_2 removal.

In the Coal/Catalyst Preoxidation Screening Study, the final drying step was combined with the pretreatment of the coal. The coal/catalyst solution mixture is fed to a fluidized bed preoxidizer, where the exothermic oxidation provides sufficient heat to heat up and dry the coal. Since the oxidation is carried out at a relatively low temperature and without a separate, coal-fired flue gas generator, flue gas desulfurization of the preoxidizer vent gas is not necessary. However, since some fines may escape from the fluidized bed, a water scrubber is still required. Air, diluted with gas recycled from the scrubber outlet (not shown), is used to supply oxygen and to fluidize the coal/catalyst bed. The prepared coal, at 400°F, has a moisture level of 2.4 wt%.

Several process basis assumptions were made to develop this initial preoxidation screening study. The key assumptions are summarized in the following table.

PROCESS BASIS FOR COAL/CATALYST PREOXIDATION SCREENING STUDY

Item	Basis Used
Temperature, °F	400
Outlet Pressure, psig	2.5
Residence Time, hours	6
Solids Inlet Moisture, wt%	20.9
Solids Outlet Moisture, wt%	2.4
Heat Balance Method	By Heat Released In Oxidation
Treat Gas:	
- O_2 Concentration, vol%	10
- O_2 Consumed per Pass, % Treat O_2	50
- Rate, SCF/lb Dry Catalyzed Coal	17.6*
Effect of Preoxidation:	
- Oxygen Gain, wt% Dry Coal	2.5*
- Carbon Loss, wt% Dry Coal	1.5*
- Hydrogen Loss, wt% Dry Coal	0.25*
- Total O_2 Consumption, wt% Dry Coal	8.5*
Fines Loss, % Product Solids	2

---

*Calculated value

The preoxidizer temperature was set at 400°F based on bench experiments that showed an optimum pretreatment effectiveness at this temperature. The residence time was chosen to be six hours based on bench experiments. Treat rate was picked to be 10 vol % O_2 at the preoxidizer inlet with 50% O_2 consumption per pass. The total O_2 consumption required to heat balance the preoxidizer was calculated to be 8.5 wt% on dry coal. Bench preoxidation tests and subsequent solids analyses showed that, for a total O_2 consumption of 8.5 wt%, about 2.5 wt% oxygen would be gained on the solids, 1.5 wt% carbon would be lost (assumed as CO_2), and 0.25 wt% hydrogen would be lost (assumed as H_2O). Finally, fines losses were assumed to be 2% of the product solids.

An additional process step not involved with the front end facilities is necessary with coal/catalyst preoxidation. The inclusion of CO_2 treatment in catalyst recovery is required since the sulfide catalyst forms may be oxidized to sulfates during the drying/preoxidation step. These soluble, inactive salt forms could build up in the catalyst loop. CO_2 treatment removes the sulfides by converting them to carbonates and gaseous hydrogen sulfide. CO_2 treatment may also be required to precipitate silicates whether or not the feed coal is preoxidized. Silicates are also catalytically inactive. Therefore, the technical issues and cost of CO_2 treatment were not addressed in this preoxidation screening study. However, the catalyst chemistry which would result from adding this step was assumed in this study. Thus, all the catalyst entering the gasifiers was assumed to be potassium carbonate.

Table 5.1-12 is a compilation of the major impacts of adding preoxidation to the CCG Study Design in this Coal/Catalyst Preoxidation Screening Study. The facilities to carry out preoxidation include four large, low pressure preoxidizer vessels, each 50 ft in diameter by 65 ft tall (tangent-to-tangent). Three of these vessels are normally in operation, with the fourth serving as a spare. The preoxidizer fluid beds themselves are 30 feet deep. Compressors totaling over 24,000 horsepower are required to provide the air and recycle which make up the treat gas. Based on the same total coal feed rate to the plant (process feed plus fuel), the preoxidation study shows that the net product SNG will be reduced by 3% from the Study Design.

The economics for the preoxidation screening study are shown in Table 5.1-13, compared again with the CCG Study Design numbers. The additional investments for the preoxidation facilities (and adjustments to other plant equipment) add only a small incremental cost to the overall plant, an increase of less than 1%. However, the gas cost increases to 6.44 $/MBtu, 4% above the Study Design level. More than half of this gas cost increase is associated with the reduction in net SNG. The remainder is due to increased operating costs, including electric power to drive the air and recycle gas compressors.

Table 5.1-12

COAL/CATALYST PREOXIDATION SCREENING STUDY IMPACTS OF ADDING PREOXIDATION

	CCG Study Design	Preoxidation Screening Study
Preoxidation Facilities		
Preoxidizers	None(1)	Four Vessels (3N/1S) Each 50' ID x 65' T/T
Air Compression Horsepower	1,800(1)	8,100
Recycle Gas Compression Horsepower	800(1)	16,000
Impact on Rest of Plant		
Coal Requirements, T/SD		
- Process Feed	14,490	14,890
- Coal Drier Fuel	710	330
- Boiler Fuel	2,960	2,940
Total	18,160	18,160
Net SNG Product, GBtu/SD	256.9	249.7
Electric Power, MW	147	165
Preheat Fired Heater Duty, MBtu/hr	485	415

Note:

(1) As described in the text, the final drying facilities in the CCG Study Design are replaced by the preoxidation facilities in the Preoxidation Screening Study. The compression horsepowers given in the CCG Study Design column are for the air and recycle gas fans serving the final drying facilities.

Table 5.1-13

COAL/CATALYST PREOXIDATION SCREENING STUDY
SUMMARY OF INVESTMENTS AND GAS COSTS

Basis:
- January, 1978 Instant Plant, Eastern Illinois
- 100% Equity, 15% DCF Return

	CCG Study Design	Preoxidation Screening Study
Investment, Million \$(1)		
• Coal Preparation	65	105
• Gasifier System	295	270
• Gas Separations	515	505
• Catalyst Recovery	60	60
• Offsites	595	600
Total	1530	1540
% Change	Base	+0.7%
Gas Cost Breakdown, \$/Million Btu		
• Coal Cost	1.41	1.45
• Catalyst	0.42	0.43
• Utilities	0.35	0.40
• Other Operating Costs	0.90	0.94
• Capital Charges	3.10	3.22
Total	6.18	6.44
% Change	Base	+4.2%

Note:

(1) Investment includes 25% process development allowance (on onsites only) and 25% project contingency.

Two sensitivities were evaluated to show the impacts of key basis items. If the treat gas basis for preoxidation were 6 vol% O_2 and only 33% oxygen consumed per pass, the treat gas rate would go up significantly and the gas cost with coal/catalyst preoxidation would increase an additional 2% to 6% over the Study Design. Also, if in addition to this higher treat rate, the residence time of preoxidation needed to be 15 hours rather than 6 hours, the gas cost would rise to 8% higher than the Study Design.

The conclusions of this study were encouraging. Adding preoxidation of the coal/catalyst feed to increase gasifier fluid bed density was shown to have a potentially moderate cost impact on the CCG process. To minimize the cost increase for preoxidation, lower total oxygen consumption and lower treat gas rate in the preoxidation step are preferred. (At constant total oxygen consumption, the treat gas rate is lowered by increasing the treat oxygen concentration and/or consumption per pass.) As described in the following item, further engineering work on preoxidation was done to identify the relationships between the key variables and to suggest preferred preoxidation conditions for PDU runs.

In the course of the screening study, several key uncertainties and data needs were defined for the preoxidation system. These can be classified into three basic categories. General basis items include:

- Relationship between severity of preoxidation and gasifier bed density.
- Need for supplemental coal firing and resulting requirement for flue gas desulfurization.
- Preferred overall sequence.

Additional uncertainties and data needs are associated specifically with the preoxidizer fluidized bed. These include:

- Residence time and temperature requirements.
- Potential feeding problems with coal/catalyst mixture.
- Amount of fines loss.

Further uncertainties and data need are related to the coal/catalyst oxygen reactions. These items include:

- Oxygen consumption in preoxidizer and resulting SNG yield reduction. (Total oxygen consumption is the key process variable measuring the "severity" of the preoxidation step.)
- Hydrocarbon content of preoxidizer vent gas and resulting emissions control requirements, if any.

5.1.9 Preoxidation Lab Guidance Studies

The previous item describes a first-pass economic evaluation for coal/catalyst preoxidation completed in September, 1980. This screening study was done in response to early laboratory development work which showed that preoxidizing the feed to the CCG PDU resulted in higher gasifier fluid bed densities. The process basis for the first-pass study was developed from limited data, and for this reason, the system evaluated was neither well-defined nor optimized. An additional study subsequently was completed to identify probable commercial operating ranges for preoxidation process variables. In this study, constraints for individual process variables were developed based on commercial system limitations. The results of this study will help the continuing laboratory work on coal/catalyst preoxidation to focus on conditions of commercial interest, and will provide a starting point for economic optimization of the preoxidation system.

A process variables summary was developed for the preoxidation system, as shown in Table 5.1-14. This table lists the process variables for preoxidation and the apparent or actual limiting values in commercial operation. Additional limitations result from interactions among individual process variables. Defining these limitations was the focus of the study described here.

A few key process basis items used in the first-pass coal/catalyst preoxidation study were also used in this evaluation. The most important of these is the system heat balance basis, which assumes that the amount of oxygen consumed can be set so that the exothermic heat from the oxidation reactions supplies the total heat requirement of the preoxidizer. This basis would minimize commercial facilities requirements. Additional bases common to both evaluations include a preoxidation temperature of 400°F, and a moisture evaporation rate of 3,200 ST/SD. These variables are the primary factors affecting oxygen consumption requirement. The oxygen consumption requirement also depends on treat gas rate and compressor outlet temperature. However, the effects of these last two variables are relatively small, so for this evaluation the total oxygen consumption was set at 8.5 wt% dry coal based on the first-pass study heat balance. .

Using these bases and the reactor gas velocity limitations shown in Table 5.1-14, equations were developed which set treat gas rate limits as a function of preoxidizer residence time and bed height. Treat rate per unit of coal feed is in turn a function of feed oxygen concentration and oxygen consumption per pass. Criteria for the preferred commercial system were developed from these relationships and the first-pass study results. A major portion of the equipment cost for the preoxidation facilities is associated with treat rate and compression requirements. Compared to the first-pass study, this cost can be lowered by increasing the feed oxygen concentration to reduce treat rate and by reducing bed height to minimize compressor pressure rise. However, the maximum oxygen concentration is limited to about 15 mol% by potential dust explosion hazards, and the minimum bed height is set at 10 ft based on fluidization considerations.

Table 5.1-14

PROCESS VARIABLES SUMMARY
PREOXIDATION LAB GUIDANCE STUDY

Independent Variables	Approximate Commercial Limits
Coal Rate, ST/SD (As Received)	None
Inlet Solids Moisture, wt%	20 - 35 (3)
Catalyst Type	KOH and/or K_2CO_3
Particle Top Size	8 mesh - 30 mesh
Inlet O_2 Concentration, mol% O_2	0-15 (4)
Treat Rate, SCF/lb Dry Coal + Catalyst	None
Either Independent or Dependent	
Temperature, °F	300-450
Heat Input/Output, MBtu/hr (1)	None
Residence Time, hrs	None
Bed Depth, ft	10-100 (5)
Inlet/Outlet Velocity, ft/sec (2)	0.5-2.5
Bed Diameter, ft	None
Gas Atmosphere	None (6)
Dependent Variables	
Outlet Moisture, wt%	None
Total O_2 Consumed, wt% Dry Coal	None
O_2 Consumed per Pass, % Treat O_2	0-100
O_2 Consumption Rate, lb/lb Bed (Dry)/hr	?
Average O_2 Partial Pressure, psia	?
Fines Loss, wt% Product	?
Preoxidation Reaction Chemistry	?

Notes:

(1) Setting one of these variables sets the other.
(2) Setting two of these variables sets the other two.
(3) Could be reduced below 20 wt% if additional drying step is added between catalyst addition and preoxidation.
(4) Assumes use of air alone (with 21 mol% O_2) is ruled out by potential dust explosion hazard.
(5) Maximum bed depth could be limited by maximum compressor ΔP restrictions.
(6) The key variable affecting the gas atmosphere in addition to inlet O_2 concentration is inlet CO_2 concentration.

In addition to these factors, kinetic limitations must be considered. Available bench and PDU preoxidation data were used to estimate the kinetic limitations associated with decreased residence time and increased oxygen consumption per pass. Linear kinetic relationships were assumed to obtain the oxygen partial pressure and residence time requirements needed to acheive the desired oxygen consumption. Because the data base is small, the potential kinetic limitations are uncertain, and therefore, a range of possible reaction rates was estimated. The range of kinetic limitations was developed as a function of residence time and treat rate to allow a comparison with the relationship for minimum/maximum bed height. This comparison established an overall range of conditions in which the commercial preoxidizer would be likely to operate.

An example of such a comparison is shown in Figure 5.1-6. In this example, inlet treat oxygen concentration was set at 12 mol% to protect against dust explosions, and oxygen consumption per pass was set at 50% of treat oxygen. The resulting treat rate is 15 SCF/lb dry coal plus catalyst. The probable commercial operating range -- indicated by the heavy line on the graph -- is within the limits set by the minimum bed depth (10 ft), the minimum and maximum gas velocities (0.5-2.5 ft/sec), and the range of kinetic limitations. The results indicate that residence time could be as low as 2 hr and bed height as low as 10 ft depending on the actual kinetic limitations.

The large projected operating range shows the importance of the uncertainty in kinetic limitations. The estimated reaction rates range over a factor of three based on bench and PDU preoxidizer data. The probable commercial operating range can be reduced considerably when the actual rate limitations are better defined. For example, if the actual reaction rate limitation were the "mid-range" line shown on Figure 5.1-6, the allowable operating range for a commercial preoxidizer would be between a residence time of 3.2 hr with a 27-foot high bed, and a residence time of 3.8 hr with a 10-foot high bed. Although the lower bed height is preferred due to compressor pressure rise considerations, an intermediate bed height would probably be used in a commercial preoxidizer to provide flexibility for process control.

The uncertainty in kinetic limitations also prevents meaningful optimization of the system until better rate data are obtained. This is illustrated by comparing the results shown in Figure 5.1-7 with the previous example in Figure 5.1-6. The basis for this figure is identical to that for the previous figure, except that oxygen consumption per pass was increased to 75%, with a corresponding decrease in treat rate to 10 SCF/lb dry coal plus catalyst. Comparing the probable commercial operating ranges on the two figures shows that at the high reaction rate limit, a treat rate of 10 SCF/lb dry coal plus catalyst is preferred because both alternatives require the same minimum bed height. At the low reaction rate limit, however, the bed height required for the reduced treat rate alternative is higher than that required for the alternative with a treat rate of 15 SCF/lb dry coal plus catalyst. In this situation, the optimum treat rate would have to be determined based on the relative cost trade-offs associated with treat rate and compressor pressure rise.

FIGURE 5.1-6

PROBABLE COMMERCIAL OPERATING RANGE FOR PREOXIDATION

O_2 CONSUMED PER PASS = 50% TREAT O_2

BASIS:

- TEMPERATURE = 400° F
- TOTAL O_2 CONSUMED = 8.5 WT. % DRY COAL
- TREAT GAS O_2 CONCENTRATION = 12 MOL %
- TREAT RATE = 15 SCF/LB DRY COAL + CATALYST

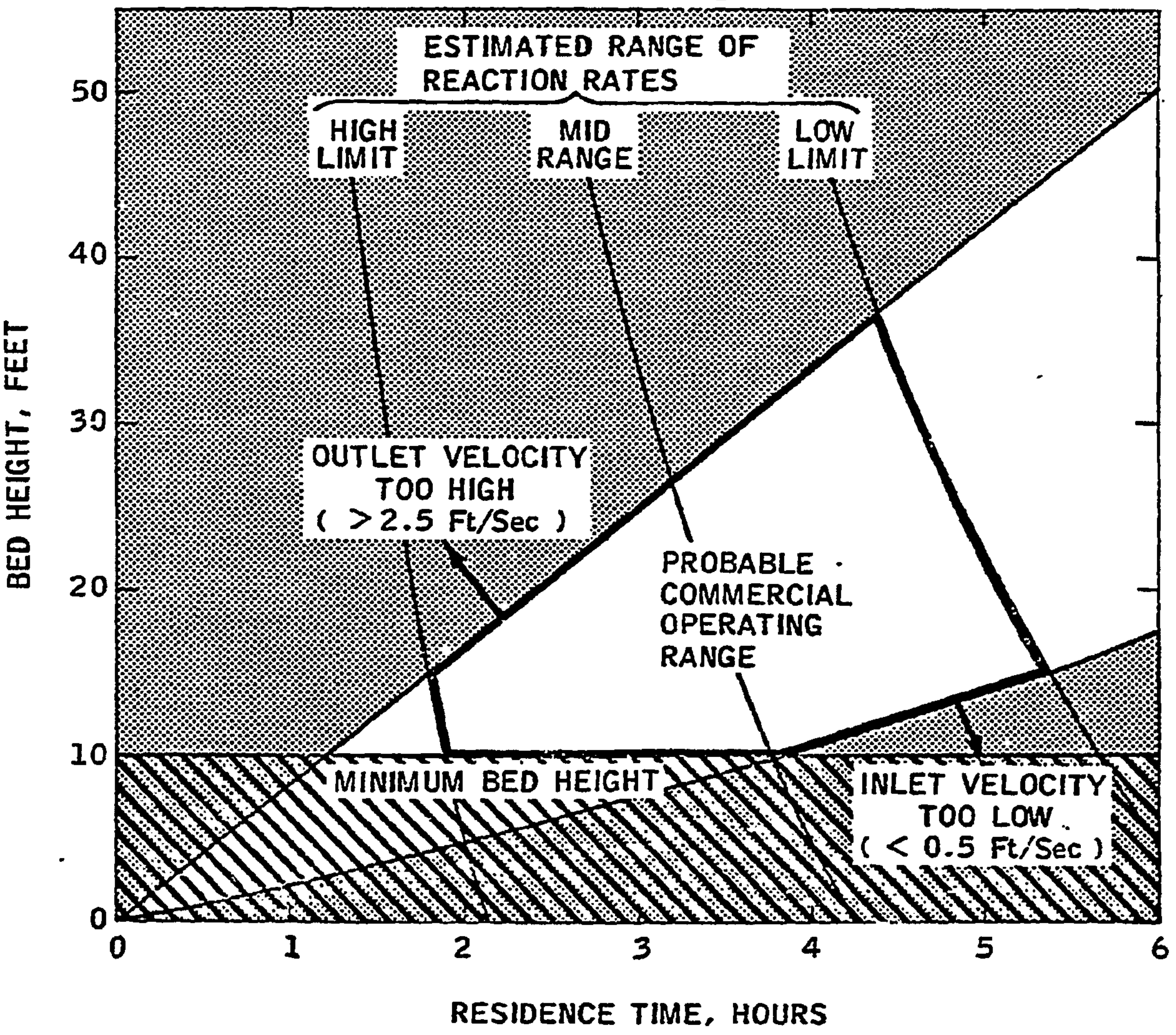


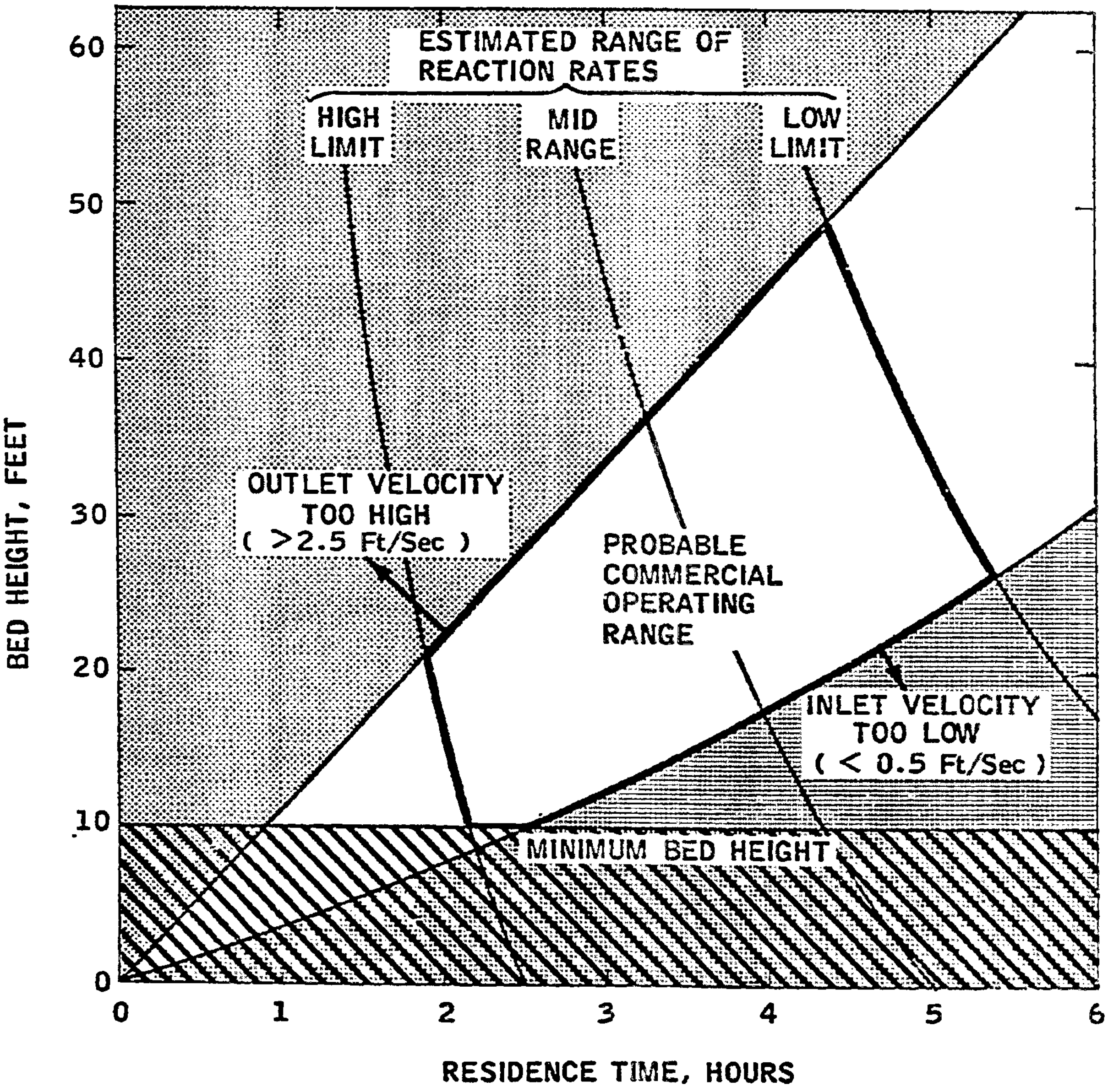
FIGURE 5.1-7

PROBABLE COMMERCIAL OPERATING RANGE FOR PREOXIDATION

O_2 CONSUMED PER PASS = 75% TREAT O_2.

BASIS:

- TEMPERATURE = 400° F
- TOTAL O_2 CONSUMED = 8.5 WT. % DRY COAL
- TREAT GAS O_2 CONCENTRATION = 12 MOL %
- TREAT RATE = 10 SCF/LB DRY COAL + CATALYST



These results show that kinetic limitations are important in developing an optimum commercial preoxidizer. Further laboratory work is needed to define these limitations. In addition, it was assumed that satisfactory gasifier coal feed is produced with a total oxygen consumption of 8.5 wt% dry coal. Limited data indicate that this is satisfactory, but further laboratory work is needed to better define the relationship between preoxidizer oxygen consumption and gasifier fluid bed density.

Based on the data available, this study showed that a preoxidizer residence time as low as 2 hours may be feasible commercially. As a result, PDU operations with a similar preoxidizer residence time are desirable. Since the kinetic limitations are not well defined, a preoxidizer with a residence time of 4 hours is recommended as a first step, with further reductions in residence time deferred until better data are available. Since PDU operations at representative treat rates and oxygen consumptions per pass are also desirable, the preoxidizer bed height should be at least 10 feet, although the broad range of 10-25 feet is of commercial interest.

5.1.10 Coal Devolatilization Impact Study

The objective of this study was to investigate the impact of uncertainties in the amount of carbon devolatilized on gasifier volume requirements and to investigate the potential risks and benefits of alternative coal feed injection points along the height of the gasifier bed.

When feed coal is injected into the fluidized bed catalytic gasifier, it is rapidly heated and devolatilized into gas phase species (such as CO, CO_2, H_2, CH_4, etc.) and hydrocarbon liquids. It is important to know the amount of feed coal devolatilized in the gasifier since this affects the amount of carbon to be gasified and influences the kinetics of the gasification reactions. The carbon-rich char remaining after devolatilization must be gasified. Sufficient residence time must be provided in the gasifier to convert the remaining carbon to gaseous products. Thus it is important to know what fraction of carbon is devolatilized versus what fraction must be gasified. The second important impact of devolatilization is the inhibiting effect of the devolatilization products on the reaction rate for gasifying the remaining carbon. Thus, it is important to know the amount of feed coal devolatilized and the composition of the devolatilization products.

Another important consideration with respect to devolatilization is the location of the point where feed coal is injected into the fluid bed. If the coal is injected near the bottom of the bed, reaction of the devolatilization products as they flow through the bed results in essentially no hydrocarbons heavier than methane in the gasifier effluent. This permits the recovery of high level heat from the gasifier overhead since fouling of heat exchangers from heavy hydrocarbons should not occur. However, it also results in the largest inhibition effect of devolatilization products on gasification rate since these products are present over almost the entire length of the bed.

If the feed coal is injected near the top of the bed, high direct methane yields from devolatilization may increase the product gas methane content above equilibrium levels. The increase would be due to insufficient residence time to reform the devolatilized methane back to equilibrium levels. The higher direct methane yield would result in lower recycle gas rates. However, there would be the risk of heavy hydrocarbons in the gasifier overhead with resultant fouling of heat exchange surfaces because of insufficient residence time to convert them to light gaseous products. In the CCG Study Design, the feed coal was injected into the bottom of the fluid bed to assure the absence of heavy hydrocarbons in the gasifier effluent.

The Coal Devolatilization Impact Study was carried out in two parts. First, the impacts of changing the amount and composition of devolatilization products and the feed point location were evaluated in a series of nine cases. These cases included three different devolatilization yields:

- Base Case - 17% Carbon Devolatilized (CCG Study Design)
- Intermediate Case - 28% Carbon Devolatilized
- Maximum Case - 36% Carbon Devolatilized

Data on the devolatilization yield for catalyzed Illinois coal at 1300°F and 500 psia in a gasification atmosphere is limited. The range of yields assumed for this study probably brackets that which would actually be obtained in a catalytic gasifier.

Three different feed points were evaluated for each devolatilization yield:

- Bottom -- 2 feet above the bottom of the bed (CCG Study Design)
- Middle -- 25-30 feet below surface of fluid bed (FBG experience)
- Top -- 5-10 feet below surface of fluid bed (high feed point incentive case).

Each of these cases was simulated using the CCG reactor model and the same gasifier coal feed as in the CCG Study Design. The model was used to determine gasifier volume and the approach to methanation equilibrium. The results of these nine cases are summarized in Table 5.1-15.

As shown in the table, with the coal feed point near the bottom of the gasifier, the predicted gasifier volume for 90% carbon conversion is reduced by 10-18% with the higher coal devolatilization yields. The approach to methanation equilibrium is unaffected for these cases as shown below:

Table 5.1-15

CATALYTIC COAL GASIFICATION
COAL DEVOLATILIZATION IMPACT STUDY

CCG GASIFIER REACTOR MODEL SIMULATION RESULTS

Devolatilization Yields	Coal Feed Point	Height of Bed Above Feed, Ft	Relative Gasifier Volume	Approach to (1) Methanation Equilibrium, °F
Base Case - 17% C Devol.	Bottom	86	100	4
"	Middle	28	88	5
"	Top	8	85	11
Intermediate Case - 28% C Devol.	Bottom	77	89 (100)	4
"	Middle	28	73 (82)	3
"	Top	9	67 (75)	-3
Maximum Case - 36% C Devol.	Bottom	70	82 (100)	4
"	Middle	28	63 (77)	0
"	Top	7	54 (66)	-31

Note:

(1) A positive value indicates a deficiency of CH_4 relative to equilibrium, while a negative value indicates an excess of CH_4 relative to equilibrium.

Devolatilization Model	Relative Gasifier Volume	Approach to Methanation Equilibrium, °F
Base	100	4
Intermediate	89	4
Maximum	82	4

Also shown in Table 5.1-15 is the effect of changes in the location of the coal feed point. With the base case devolatilization model, predicted gasifier volume can be reduced by 10-15% by moving the coal feed point up from the bottom of the gasifier bed as shown below:

Coal Feed Point	Relative Gasifier Volume	Approach to Methanation Equilibrium, °F
Bottom	100	4
Middle	88	5
Top	85	11

Feeding the gasifier in the middle of the bed can save about 12% of the gasifier volume with little effect on the approach to methanation equilibrium. The higher feed location showed little savings in volume over the middle feed case while showing a poorer approach to methanation equilbrium. The higher feed location also has a greater risk of tar production as discussed below. Operation of the FBG during the CCG Predevelopment Program with the feed 28 feet below the surface of the bed showed no tars or overhead fouling.

Additionally, it appears from the information in Table 5.1-15 that the methane content of the gasifier overhead cannot be increased above equilibrium for a system which avoids tar breakthrough in the gasifier effluent. The only case showing significant methane concentrations above equilibrium was that with very high devolatilization yield and a feed point location very near the top of the bed. It is unlikely that the devolatilization yield will be this high and it is also unlikley that the coal can be reliably fed 5-10 feet below the top of the bed without fouling of the overhead heat recovery system. For the other eight cases presented in Table 5.1-15, the methane content of the gasifier overhead is near the equilibrium amount.

In the second part of this study, the potential risks and benefits of different coal feed points were investigated. As stated previously, the potential benefit of a higher coal feed point is a gasifier volume reduction of 10-15%. The risk of heavy hydrocarbon breakthrough was quantified by running heat and material balances for a case without a high level heat recovery system. For this case, the gasifier effluent was quenched with water prior to low level heat recovery. For this case, the amount of SNG fired in the preheat fired heater doubles, and the offsite boilers increase in size by 30%. This reflects the absence of the gas-gas exchangers and high pressure waste heat boilers. These effects decrease plant thermal efficiency by about 10%. This illustrates the significant risk of tar in the gasifier overhead.

The conclusions drawn from this study are summarized below:

- The amount of feed coal devolatilization has a significant impact on gasifier volume requirements. The actual level of devolatilization for a potassium catalyzed feed coal at 1300°F and 500 psia in a gasification atmosphere is uncertain. Since the kinetic model used for the CCG Study Design was conservative (low yields), better data could reduce gasifier volume requirements.

- Fouling the high level heat recovery system by tar breakthrough would result in a serious economic debit to the process and must be avoided.

- Moving the coal feed point higher up in the fluidized bed could reduce the gasifier volume requirement by 10-15%. Tests in the PDU must be run to confirm this savings and demonstrate that no tar breakthrough occurs by raising the coal feed point.

- It appears unlikely that the methane content of the gasifier overhead can be increased above equilibrium without the risk of tar breakthrough.

5.1.11 Gasification System Screening Studies

Engineering screening studies were conducted to evaluate the economic impact of alternative gasifier operating conditions. The results of these studies provided guidance for PDU gasifier process variable studies and for selection of preferred operating conditions for the PDU demonstration run.

Impact of Reduced Gasifier Operating Pressure on the CCG Material and Energy Balance

As discussed elsewhere in this report, two main techniques had been identified in the laboratory to increase fluid bed densities and reduce fines production: (1) operating the gasifier at a lower pressure than the CCG Study Design pressure of 500 psia; and (2) preoxidizing the coal by exposure to air at relatively mild conditions. The purpose of this study was to focus on the impact of reduced pressure on the CCG system material and energy balance and thus provide laboratory guidance.

The major impacts of reduced pressure on CCG process parameters and plant facilities are shown in Table 5.1-16. A series of commercial-scale CCG material and energy balances were prepared to help quantify these impacts. These balances were prepared for gasifier operating pressures of 300 psia and 100 psia and are presented below and compared to operation at the CCG Study Design pressure of 500 psia. These cases are based on the same coal feed rate, solids properties and gasifier operating conditions as the Study Design.

IMPACT OF REDUCED PRESSURE ON CCG MATERIAL AND ENERGY BALANCE

Basis: 14,490 ST/SD Coal Feed Rate to Gasifiers
1275°F Gasifier Temperature

	CCG Study Design	Reduced Pressure Cases	
Gasifier Pressure, psia	500	300	100
Gasifier Effluent, lb-moles/hr	160,000	180,000	270,000
Recycle Gas, lb-moles/hr	60,000	80,000	170,000
CO_2 Partial Pressure, psia	72	38	8
Relative Fluidized Bed Bubble Size	1.0	1.5	3.6
Relative Gasifier Volume	1.0	1.6	3 - 7
Preheat Fired Heater COT, °F	1,540	1,500	1,420
Preheat Fired Heater Duty, MBtu/hr	480	490	560
Net SNG, GBtu/SD	257	256	253

As shown in these tables, the most significant impacts of reduced pressure are increased recycle gas rate and increased gasifier volume. These debits may be offset by the reduced cost for equipment mechanical design for the lower pressure.

The recycle gas rate was larger at lower pressure because the gasifier effluent was assumed to be in methanation equilibrium and, at lower pressure, this equilibrium results in more moles of CO and H_2 per mole of methane product. In addition, the reactor model indicated that equilibrium may not be as closely approached as pressure is reduced, however, this impact is not included in this study.

The gasifier volume was larger at lower pressure for two main reasons. First, the mass transfer rate between the emulsion and bubble phases in the fluidized bed was lower at reduced pressure because the bubbles are larger. At 500 psia and to a lesser degree at 300 psia, mass transfer was believed to have only a small impact on gasifier volume. However, at

Table 5.1-16

IMPACT OF REDUCED PRESSURE ON CCG PROCESS

Impact on Process Parameters

- Recycle Gas Rate Increases
- Bubble Size in Fluid Bed Gasifier Increases
- CO_2 Partial Pressure Is Lower
- CH_4 Produced in Gasifier Remains Constant
- Preheat Fired Heater Duty Increases
- Net CH_4 Product Decreases Slightly

Impact on Commercial Plant Facilities

- Lower Cost Mechanical Design
    - Coal Feeding from Lock Hoppers
    - Reduced Wall Thickness for Gasifier, Gas-Gas Exchanger Shell, and Preheat Fired Heater Tubes
- Increased Gasifier Volume
    - Inhibition Due to Increased Recycle Gas Rate
    - Poorer Mass Transfer
- Small to Moderate Impact on Gas Separations
    - Larger Gas Rates
    - Lower CO_2 Partial Pressure
    - Lower Feed Pressure Increases Energy Requirement for Methane Recovery
- Small Impact on Preheat Fired Heater
    - Larger Duty
    - Lower Coil Outlet Temperature

100 psia mass transfer may have a significant impact on gasifier volume; thus, the uncertainties in the bubble size and mass transfer correlations led to greater uncertainties in the reactor kinetics/contacting model predictions at 100 psia. Secondly, because of the increased recycle of CO and H_2 at lower pressure, the inhibition effect of these components on gasification rate was increased.

Reducing the gasifier pressure will result in lower cost mechanical designs, directionally offsetting the debits due to increased recycle gas rate and gasifier volume. Design and operation of the lock hoppers, the lock hopper pressurization system, and the preheat fired heaters will be simpler at reduced pressure. The preheat fired heaters will have both reduced design coil outlet temperatures and reduced design pressure. Based on these initial cases, it appeared that reducing the gasifier pressure to 300 psia was potentially a low cost method of increasing gasifier fluid bed densities. The increases in gas flow rates and gasifier volume for a gasifier operating at 300 psia are moderate and would be directionally offset in many sections of the plant by reductions in design pressure. However, because of the excessive increases in gas flow rates and gasifier volume, operating a gasifier at 100 psia was not likely to be economically attractive.

An engineering screening study to evaluate gasifier operation at 300 psia is described later in this report.

Impact of Alternative Gasifier Operating Conditions on the CCG Material and Energy Balance

A study of the impact of gasifier operating conditions on the CCG material and energy balance has been completed. The following process variables were investigated: catalyst loading, gasifier temperature, gasifier feed steam rate, carbon conversion, and gasifier pressure. The study of gasifier pressure is covered in the preceding section.

The operating conditions for the CCG Study Design were used as the base case for this study. These conditions include a gasifier temperature of 1275°F, pressure of 500 psia, catalyst loading of 15 wt% K_2CO_3 equivalent, 90% carbon conversion and a steam rate based on graphite equilibrium at the gasifier effluent. Since the coal char is more active than graphite, setting the feed steam rate in this manner ensures a reasonably consistent gasification driving force in the fluid bed. For the Study Design this resulted in a steam-to-dry-coal weight ratio of 1.58. The present study was also based on the Study Design coal feed rate of 14,490 ST/SD. The impact of changes in operating conditions was investigated by changing one variable at a time while keeping the others constant.

The interim version of the reactor kinetics/contacting model was used to predict the gasifier volume for these studies. The results are preliminary since many of the cases in this study explore the impact of process variables where the current data base was limited.

The impacts of changes in gasifier operating conditions on gas flow rates, preheat fired heater temperature, and gasifier volume are described below.

The first gasifier process variable investigated was catalyst loading. Since the Study Design was based on a loading of 15 wt% K_2CO_3 equivalent, material and energy balances were developed for loadings of 10 and 20 wt% and are shown below.

IMPACT OF CATALYST LOADING

Item	Base Case	Sensitivities	
Catalyst Loading, wt% K_2CO_3	15%	10%	20%
Preheat Fired Heater Temperature, °F	1540	1500	1580
Gasifier Volume	1.0	1.2	1.0
Catalyst Recycle Rate	1.0	0.7	1.3

With lower catalyst loading of 10 wt%, the preheat temperature is reduced because of the lower sensible heat required to preheat the prepared coal feed to reaction temperature. The gasifier volume increases by 20% but the amount of catalyst which must be recovered and recycled was only 70% of that in the base case. Opposite effects were observed for the case with higher catalyst loading of 20 wt% except that the gasifier volume is not reduced as would be anticipated. This was due to saturation of the active catalyst sites. However, this phenomenon was not well understood and was the subject of later laboratory work.

The next gasifier operating variable investigated was operating temperature. Results are shown below.

IMPACT OF GASIFIER TEMPERATURE

Item	Base Case	Sensitivities			
Gasifier Temperature, °F	1275	1200	1250	1300	1350
Preheat Fired Heater, Temperature, °F	1540	1410	1500	1570	1620
Gasifier Feed Steam Rate	1.00	1.14	1.05	1.00	0.98
Total Recycle Gas Rate	1.00	0.88	0.96	1.12	1.37
Gasifier Volume	1.0	1.5	1.1	0.9	0.8

With lower gasifier temperature, the preheat fired heater temperature drops more than the gasifier temperature because of the lower sensible heat required to preheat the prepared coal feed. The gasifier steam rate was based on apparent steam-graphite equilibrium which required more steam at lower temperatures. The recycle rate was reduced at lower temperatures because the gasifier effluent was in methanation equilibrium and, at lower temperature, this equilibrium results in less moles of CO and H_2 per mole of methane. The reactor model predicted a 50% increase in gasifier volume at 1200°F. However, this was based on preliminary estimates of the gasification reaction activation energy. The temperature dependence of the gasification reaction rate was updated later in the laboratory program.

The impacts of changing the gasifier feed steam rate are shown below.

IMPACT OF GASIFIER FEED STEAM RATE

Item	Base Case	Sensitivities		
Gasifier Feed Steam Rate	1.00	1.40	0.80	0.75
Total Recycle Gas Rate	1.00	1.41	0.82	0.77
Preheat Fired Heater Temperature, °F	1540	1460	1610	1640
Gasifier Volume	1.0	0.8	1.5	2.0

Near the base case conditions, the change in recycle gas rate was nearly proportional to the change in the gasifier feed steam rate. As both the steam and recycle gas rates increased, there was more gas to carry sensible heat into the gasifiers. The sensible heat in the steam plus recycle gas above the gasifier temperature was used in effect to preheat the feed coal and to make up for heat losses and endothermic reactions between catalyst and ash. Thus, the preheat fired heater temperature was reduced. Gasifier volume increased as steam rate was reduced. The large change in gasifier volume (from 1.5 to 2.0) caused by a change in the feed steam rate from 80% to 75% of the base level shows the impact of approaching the equilibrium steam requirement.

Carbon conversion was the last process variable studied. The results are shown below.

IMPACT OF CARBON CONVERSION

Item	Base Case	Sensitivities			
Carbon Conversion, %	90%	80%	85%	95%	98%
Gasifier Feed Steam Rate	1.00	0.89	0.94	1.05	1.08
Net SNG	1.00	0.90	0.95	1.05	1.08
Gasifier Volume	1.0	0.8	0.9	1.5	2.9

The change in steam requirement and net SNG product was proportional to the change in carbon conversion. For example, to increase carbon conversion by 5%, the steam requirement must be increased by 5% and the net SNG is thus increased by 5%. The gasifier volume increase was not proportional to carbon conversion since a 5% increase in carbon conversion from 90% to 95%

approximately doubles the catalyst to carbon ratio of the char in the gasifier bed and results in a smaller holdup of carbon per unit of volume. This in turn led to significantly larger gasifier volume requirements. As mentioned in the discussion of the catalyst loading sensitivity cases, the impact of the catalyst to carbon ratio was the subject of later laboratory work.

5.1.12 Gasifier Pressure Screening Study

As discussed elsewhere in this report, one technique identified in the laboratory to increase fluid bed density and reduce fines production is operating the gasifier at a lower pressure than the CCG Study Design pressure of 500 psia. The results of preliminary studies to investigate the impacts of reduced pressure on the CCG material and energy balance are reported in the preceding section of this report. It was concluded that reducing the gasifier pressure to 300 psia is potentially a low cost method of increasing gasifier fluid bed density. In order to provide laboratory guidance for the selection of operating pressure for the PDU demonstration run, a more detailed study of the impact of reduced gasifier operating pressure was conducted.

As the first step in this study, a commercial-scale CCG material and energy balance was prepared for a gasifier operating pressure of 300 psia. The key process parameters associated with this balance are compared with operation at 500 psia in Table 5.1-17. This case was based on the same coal feed rate, solid properties, and gasifier operating conditions (except for pressure) as the Study Design. As shown in the table, the major process impacts of reduced pressure are increased gas rates and increased gasifier volume.

The recycle gas rate in this case is higher because the gasifier effluent is approximately in methanation equilibrium and, at reduced pressure, this equilibrium results in more moles of CO and H_2 per mole of methane formed (which is constant). Also, the reactor kinetics/contacting model shows that equilibrium will not be as closely approached as pressure is reduced. The approach to methanation equilibrium in the reduced pressure case is 10°F, rather than the 5°F used in the Study Design. This larger approach to equilibrium is another factor contributing to increased recycle gas rate.

There are two main reasons for the increased gasifier volume at 300 psia. First, due to the increased recycle of CO and H_2, the inhibition effect of these components on the gasification rate is increased. Secondly, the mass transfer between the emulsion and bubble phases in the fluid bed is lower at reduced pressure because the bubbles are larger. As stated above, the impact of gasifier operating pressure on solids properties is not reflected.

Table 5.1-17

IMPACT OF LOWER CCG GASIFIER PRESSURE

KEY PROCESS PARAMETERS

	CCG Study Design	Reduced Pressure Screening Study
Gasifier Operating Conditions:		
Pressure, psia	500	300
Temperature, °F	1275	1275
Coal to Gasifiers, ST/SD	14,500	14,500
Steam to Gasifiers, lb-moles/hr	87,600	87,600
Relative Steam/Graphite Equilibrium	1.00	1.07
Approach to Methanation Equilibrium, °F	5	10
Gasifier Superficial Velocity, ft/sec	1.1	1.1
Key Gas Rates:		
Gasifier Effluent, lb-moles/hr	159,000	182,000
Total Recycle Gas, lb-moles/hr	57,500	80,600
Bed Density, lb/ft^3		
Bulk (Fluffed)	24	24
Fluidized	15.8	16.8
Bed Dimensions:		
Height, ft	97	83
Diameter, ft	22	30
Relative Gasifier Volume	1.00	1.59
Preheat Fired Heater COT:		
Normal, °F	1541	1497
Design, °F	1575	1523

Another major impact of reduced pressure is lower cost mechanical designs for equipment. Design and operation of the lock hoppers, the lock hopper pressurization system, and the preheat fired heaters is simpler at reduced pressure. The preheat fired heater has both lower coil outlet temperature and pressure. However, for the gasifiers and other gas handling systems, the savings for lower design pressure are offset by larger gasifier volume and larger gas flow rates.

In the gasifier area, new equipment specifications were developed based on the commercial-scale CCG material and energy balance for a gasifier operating pressure of 300 psia. As a result of the lower gasifier operating pressure, the number of moles of gas in the recycle stream, and therefore the gasifier effluent, is increased. Combined with the lower pressure, this approximately doubles the volumetric flow rate of gas. Therefore, because the gasifiers were designed for the same superficial velocity as was used in the CCG Study Design, the gasifier diameter was increased from 22 feet to 30 feet. The tangent-to-tangent height of the gasifier was decreased to 113 ft to provide the residence time estimated by the reactor model to achieve 90% carbon conversion. The changes in design pressure and vessel diameter result in gasifier walls 16% thinner than those specified for the Study Design. The combination of larger gasifier diameter, shorter gasifier height and thinner gasifier walls results in approximaely 11% more metal required for the fabrication of the gasifier vessels. The cyclone design is similar to that used in the Study Design except that since the gas volumetric flow rate has doubled, two parallel trains of two cyclones in series are used. The char withdrawal system and the coal feed system designs are much the same as the Study Design except they are designed for a lower pressure.

In the Gasifier Pressure Screening Study, the pressure of the feed to acid gas removal is 250 psia, versus 450 psia in the Study Design. Because of this difference (and the correspondingly lower CO partial pressure), a brief optimization study was performed to choose the best processing sequence. The scheme which requires the minimum power input incorporates the following items:

- A compressor on the feed to acid gas removal to compress the stream from 250 psia to 450 psia.
- Heavy glycol acid gas removal operating at 450 psia.
- The CO stripper methane recovery scheme designed by Air Products (as described in Section 5.1.16).
- A horsepower requirement of 137,000 for methane recovery (excluding acid gas removal).

Investments and economics for the CO stripping scheme were developed for the Study Design from Air Products' final report to the DOE. Costs for the reduced pressure case were developed to provide a consistent basis to assess the impact of the lower pressure on this section of the CCG plant.

Low-level heat integration is also affected by operating the gasifier at 300 psia. In the Study Design with a 500 psia gasifier, generation of 65 psig steam was the major method of low-level heat recovery. This was possible since the temperature of the product gas downstream of the venturi scrubber was sufficiently high to generate 65 psig steam. With the gasifier operating at 300 psia, the temperature of the product gas leaving the venturi scrubber is too low for the 65 psig steam generation. Several options were considered to utilize this low-level heat from the gasifier product gas.

The option for low-level heat recovery which was chosen includes supplying heat to the H_2S/NH_3 stripper reboilers by direct process heating and generating the amount of 40 psig steam required for all available users. This method of low-level heat recovery involves efficient utilization of low-level heat and savings in steam generation facilities, but the heat transfer area for the stripper reboilers increases. This, however, is offset by higher temperature approaches for the 40 psig steam generation system. The major debit for this method of heat recovery is an increase in the heat rejected to the atmosphere.

The design of the preheat fired heaters is much simpler for this case compared to the CCG Study Design. Due to the higher recycle gas rate which results from lower pressure operation, the coil outlet temperature (COT) of the heaters is about 50°F lower. The combination of lower pressure and lower COT allows increased heat transfer rates in the heaters resulting in fewer tubes and smaller heaters. This resulted in a significant investment savings.

The size of the gas-gas exchangers has been increased to reflect the increased gas flow rates and duty and poorer heat transfer for the lower pressure operations. The area has increased about 50% which increases the shell diameter about 20%. This increase in size appears to present no mechanical problems.

In order to provide a consistent 500 psia case for comparison with the low pressure case, the CCG Study Design was adjusted to include improved gas separations and catalyst recovery via water wash with filters since these features are included in the 300 psia case.

The investments for the adjusted (500 psia) Study Design and the low pressure (300 psia) screening study are compared in Table 5.1-18. Major equipment items impacted by the reduced gasifier operating pressure were redesigned and cost estimated in detail. The remaining sections were cost estimated by prorating costs from the Study Design. In the onsites, the reactor system investment for the 300 psia case was 36 M$ lower than the

Table 5.1-18

CATALYTIC COAL GASIFICATION GASIFIER PRESSURE SCREENING STUDY INVESTMENT COMPARISON

Basis:
- January, 1978 Instant Plant, Eastern Illinois Location
- 14,490 ST/SD Coal to Process
- 25% Project Contingency
- 25% Process Development Allowance on Onsites
- Same Solids Properties in Both Cases

	Investment, M$	
	Adjusted CCG Study Design at 500 psia(1)	Gasifier Pressure Study at 300 psia
Onsites		
Coal Drying/Catalyst Addition	57	57
Reactor System	265	229
Product Gas Cooling and Scrubbing	102	98
Sour Water Stripping/NH_3 Recovery	21	29
Acid Gas Removal/Sulfur Recovery	143	173
Methane Recovery/Refrigeration	77	81
Catalyst Recovery	94	94
Common Facilities	70	70
SUBTOTAL	828	830
Materials Handling		
Coal/Coke Handling	30	32
Chemicals Receipt and Storage	7	7
By-Product Storage and Shipping	4	4
Waste Solids Handling and Disposal	26	26
SUBTOTAL	67	69
Utilities		
Raw Water/BFW Treating	35	34
Steam Generation and Distribution	146	152
Flue Gas Desulfurization	70	71
Cooling Water	11	13
Electric Power Distribution	29	32
Miscellaneous Utilities	6	7
SUBTOTAL	297	309
General Offsites		
Wastewater Treating	61	61
Safety and Fire Protection	16	16
Miscellaneous Offsites	51	52
SUBTOTAL	128	129
TOTAL EX. PDA	1,321	1,337
PROCESS DEVELOPMENT ALLOWANCE	166	166
TOTAL ERECTED COST	1,487	1,503

Note:

(1) CCG Study Design adjusted for improved gas separations and for catalyst recovery via water-wash with solid-liquid separations using rotary drum filters.

Study Design. The reason for this is the lower cost mechanical design for the reduced pressure. The acid gas removal investment increased by 30 M$. This is due to larger equipment required to handle the increased volume of gas, and additional investment for the acid gas feed compressors. The investment for steam generation facilities increased by 4% because of a higher offsite steam requirement. Overall, the total plant investment increased by 1% for the low pressure case.

The gas costs at the different pressure levels are compared in Table 5.1-19. The economic basis is consistent with that used in the Study Design. A gas cost of 6.29 $/MBtu was obtained for the low pressure case which is about 2% higher than the Study Design. Lower net product rate and higher investment were the reasons for the increase in the gas cost.

This study shows that with the gasifier operating at 300 psia, the investment will increase 1% and the gas cost will increase 2% over a comparable 500 psia case. The effect of pressure on solids properties was not included in these cases.

5.1.13 Gasifier Methanation Study

PDU operations have indicated slower methanation kinetics than were predicted by the kinetic model used for the CCG Study Design. The effects of slower methanation kinetics (as measured by an approach to methanation equilibrium much greater than the 5°F calculated for the Study Design) are increases in the gasifier effluent rate, the syngas recycle rate, and either the gasifier steam requirement or the gasifier volume.

To measure the economic impact of a larger-than-expected approach to methanation equilibrium for the purpose of laboratory guidance, commercial-scale CCG material and energy balances were developed for two assumed approaches to methanation equilibrium, 30°F and 70°F. These approaches reflect the approximate range of early PDU operations.

The primary debit due to the slower methanation kinetics is an increase in the gasifier effluent rate. This can be partially compensated for by increasing the gasifier volume and thereby increasing the steam conversion (as measured by the multiple of the steam-graphite "equilibrium" constant at the outlet).

Material and energy balance results for a 30°F approach case and a 70°F approach case are compared in Table 5.1-20 with the CCG Study Design. Both of the cases shown in the table are based on the same coal feed rate and the same gasifier conditions. In the Study Design, as well as the 30°F case, the gasifier exit gas composition reflects "steam-graphite equilibrium". The 70°F case reflects 1.3 times "steam-graphite equilibrium".