Transfer Line Operation

Solids must travel up the inclined transfer line to return to the reactor from the dipleg. Gas must be fed into the transfer line to keep the particles moving in order that they will flow back into the reactor. Gas was supplied to the transfer line at various rates and the behavior of the solids in the inclined tube was observed.

Gas superficial velocities below about 0.20 ft/sec in the transfer line resulted in stagnant solids along the entire length of the line. As the superficial gas velocity was increased, solids activity increased along the top of the transfer line while solids in the bottom of the line remained stationary. Solids in the top half of the 60° section of the line began to slug at a superficial gas velocity of about 0.3 ft/sec. Slugs broke up at the angle between the 60° and 45° sections and solids in the 45° section were motionless. Gas velocities of about 1-2 ft/sec. were required to eliminate zones of stagnant solids along the bottom of the transfer line. At these gas velocities, the solids slugged up the line and then flowed back down the bottom of the line. Generally, the solids activity in the 60° part of the transfer line was greater than that in the 45° part of the line.

Intersection Block Studies

Subsequent experiments on the cold model were designed to determine how to control dipleg and transfer line fluidization simultaneously by varying purge gas rates and locations. The purge gas can enter the system at any of five locations in the intersection block. A diagram of the intersection block with the purge locations numbered 1 through 5 is shown in Figure 3.3-7. Based on the experiments described above, most of the gas entering the fines return system at the intersection block should travel up the transfer line. High gas flow rates are required in the sloping line to eliminate zones of stagnant solids. Purge gas flow traveling up the vertical dipleg should be kept to a low value to avoid interference with cyclone performance but should be enough to keep the solids in the dipleg fluidized.

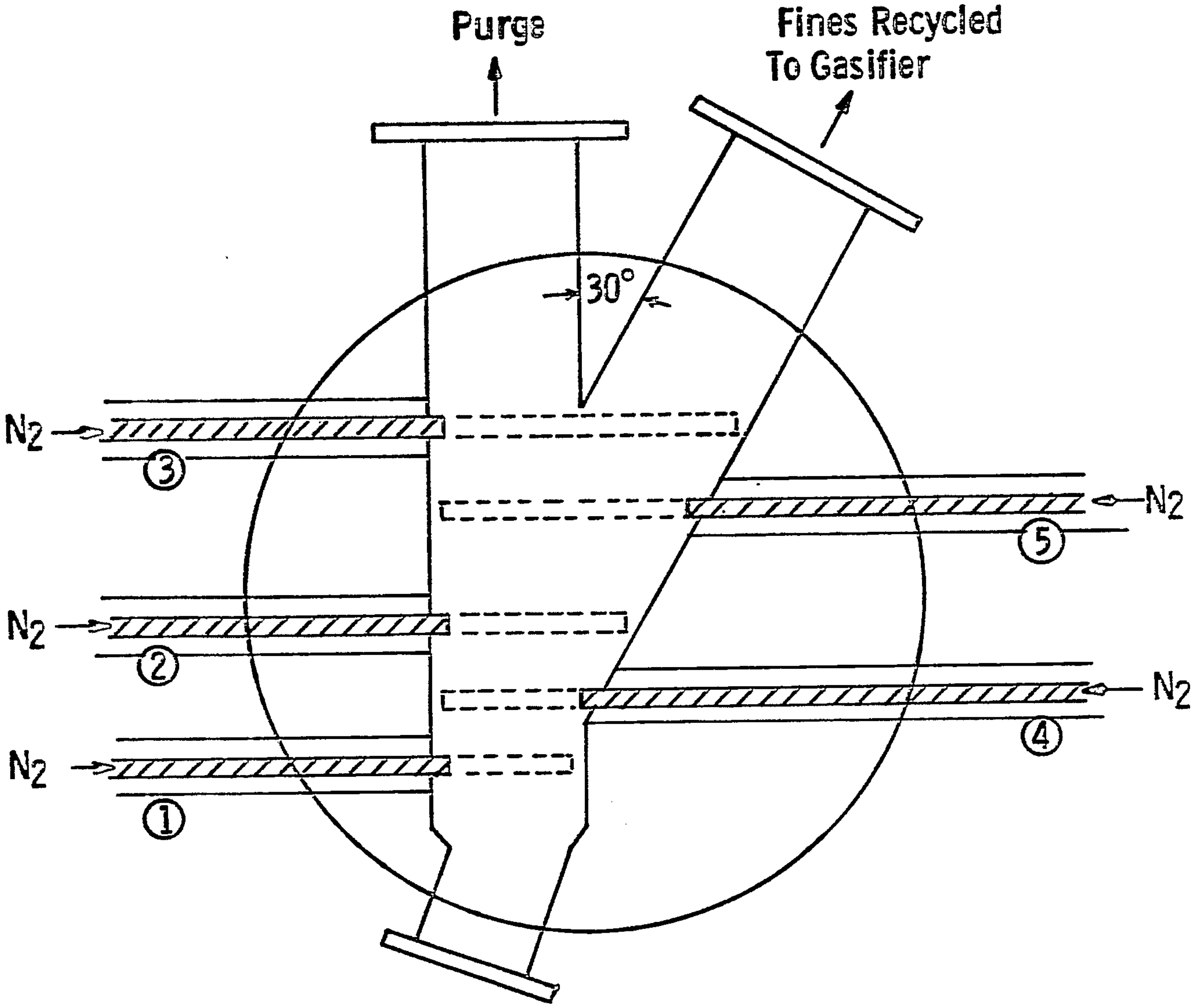
Each of the intersection block purges is equipped with a sliding tube that can be moved into the intersection block as indicated in Figure 3.3-7. Sliding the tube into the intersection block to different positions results in different gas flow patterns.

Purge location #3 gave the best control of flow up either the dipleg or the transfer line but not to both simultanecusly. When the tube was extended beyond the entrance to the dipleg, most of the gas went into the tranfer line and there was little solids motion in the dipleg. When the tube was retracted to the wall (as shown in Figure 3.3-7), most of the purge gas flowed up the dipleg. Purge location #2 produced gas flow patterns similar to location #3 but control was not as good. Most of the purge gas flowed up the transfer line in the most extended tube position, but there was intermittent slugging in the dipleg which did not occur when purge location #3 was used. Purges #1 and #4 supplied purge gas only to the vertical dipleg at all tube extensions.

FIGURE 3.3-7

DIPLEG INTERSECTION BLOCK

Cold Model Version



Purge #5 gave little control of flow up the transfer line. Most of the purge gas flowed up the dipleg when the tube was extended to greater than 1/3 of the maximum extension into the intersection block.

These results indicate that purge location is important in controlling fluidization of the fines return system. A purge directly into the base of the transfer line is required to supply high gas flow rates to the transfer line while allowing negligible amounts of gas into the dipleg. Required flow to the dipleg can be supplied from other purge locations in the intersection block.

On the basis of the above work, the PDU intersection block has been modified to provide purge locations which should control flow of purge gas to the dipleg and intersection block.

4. Advanced Study of the Exxon Catalytic Coal Gasification Process (Reporting Category C04)

4.1 Kinetics of Gasification and Devolatilization

The conversion of coal to gaseous products via Exxon's catalytic gasification process can be envisioned as a two-step process. First, the coal undergoes rapid devolatilization to yield coal char and numerous volatile products. The resulting char is then gasified with steam and recycle gas to produce a mixture of methane, hydrogen, and carbon oxides. Additional amounts of these products are also produced from the devolatilization products as they pass through the bed of char. The purpose of this work is to better characterize the reaction rates and yield structures for the devolatilization and char gasification steps. The results of this investigation can then be combined with appropriate mass transfer correlations to predict reaction rates and conversions in fluid bed gasifiers and help define optimum process conditions.

The kinetics of char gasification have previously been investigated during the predevelopment phase of catalytic gasification research. The majority of the kinetic data was obtained using a fixed bed reactor at 1300°F and catalyst loadings of 10 and 20% (wt.) potassium carbonate on dry Illinois coal. The coal was devolatilized under an inert atmosphere before loading in the fixed bed reactor. Some data was also obtained at 1200°F.

Engineering sensitivity studies using the limited temperature data have indicated an economic incentive for lowering the gasifier temperature below 1300°F. Additional kinetic data at various temperatures on steady state char is necessary before a confident optimization of the gasifier conditions can be made.

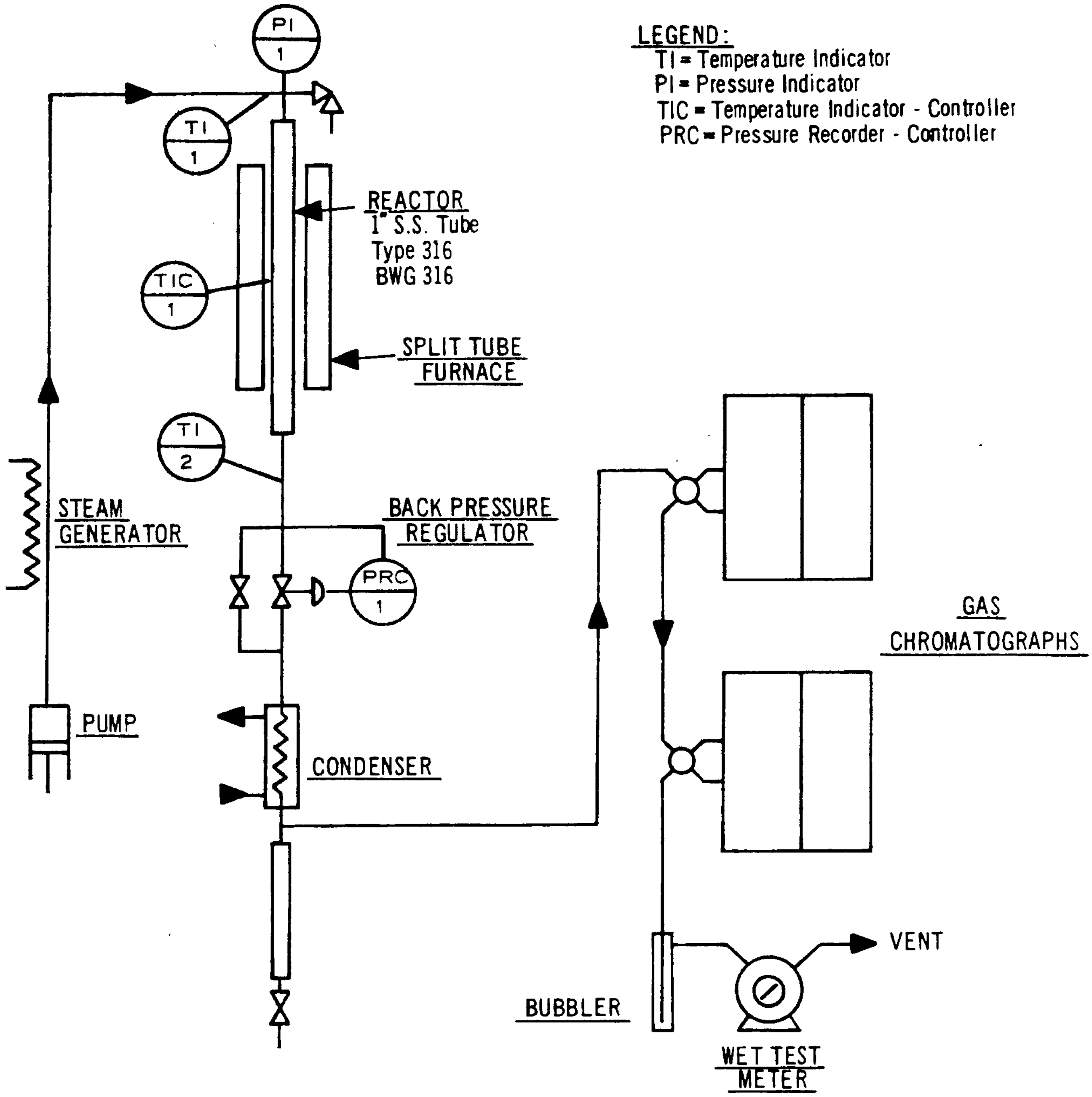
In view of this need, a laboratory program was designed to expand the kinetic data base for steam gasification of Illinois char. Feed for these studies is Illinois char produced at various levels of carbon conversion by the Fluid Bed Gasification Unit (FBG) under steady state conditions rather than the devolatilized coal used previously. The process variable studies will include:

- Effects of variations in potassium/carbon ratio in the steady state char.
- Variations in temperature and pressure around the base conditions of 1300°F and 500 psig, respectively.

A fixed bed unit was recommissioned for use in this program. A simplified flow diagram of this unit is shown in Figure 4.1-1. The unit consists of a high pressure water pump, steam generator, fixed bed reactor, unreacted steam condenser, gas chromatographs, and dry gas flow measurement system.

FIGURE 4.1-1

SIMPLIFIED FLOW DIAGRAM OF BENCH SCALE GASIFICATION UNIT



Numerous instrumentation problems were identified and corrected. These problems included a leaking gas chromatograph sampling valve system as well as several faulty temperature and pressure indicators.

A series of shakedown runs was then made at 1300°F and 500 psig using Illinois No. 6 char with a catalyst loading of 20% (wt.) potassium carbonate on dry coal. The purpose of these runs was to check the operability of the unit before initiating the temperature study. During the data workup for these runs, a problem with the gas analyses was discovered. The sum of the unnormalized compositions of the individual product gases was significantly less than 100%.

Two possible causes of this low total were:

(1) incorrect calibration gas analysis, and

(2) nonlinear response of the gas chromatograph with respect to gas composition.

Samples of product gas were collected during subsequent runs and analyzed on a mass spectrometer as well as on several other gas chromatographs on site. A comparison of the results from the on-line gas chromatograph with those from the other systems indicated a nonlinearity in the on-line analysis with respect to hydrogen concentration. This nonlinearity was confirmed through the analysis of gas samples of known hydrogen composition on the on-line unit.

Although the incorporation of a nonlinear hydrogen response factor into the data workup procedure resulted in unnormalized product gas analyses totaling essentially 100%, the final results indicated a much lower gasification rate than that obtained during the predevelopment phase of catalytic gasification research. As a result of these observations, the entire gas chromatograph system was again checked for gas leaks. Several leaks were found throughout the gas chromatograph sampling system as well as a malfunctioning thermal conductivity detector. The entire gas chromatograph sampling and detection system was then rebuilt. A new thermal conductivity detector as well as new automatic switching valves were installed in the unit. New chromatographic columns were also installed in accordance with the gas chromatograph manufacturer's specifications. The stability of the gas chromatograph's response, unfortunately, was not significantly increased following the replacement of the items mentioned above. In addition, various efforts to service the unit by the manufacturer were not successful.

In view of the recurring problems with the on-line gas chromatograph as well as the lack of success by the manufacturer in servicing the instrument, a new gas chromatograph system was purchased for the fixed bed unit. The experimental program using the high pressure fixed bed unit was postponed until the delivery and installation of the new chromatograph.

An atmospheric pressure mini-fluid bed gasification unit was subsequently recommissioned for use in the gasification kinetic program. A schematic of this unit is shown in Figure 4.1-2. The reactor portion of the unit consists of a 1/4" I.D. quartz U-tube inside a hot steel block. Water is fed to the U-tube using a small syringe pump and is vaporized in the reactor. Ceramic beads are placed in the inlet leg of the U-tube to enhance the vaporization process and help disperse the flow. The exit gases from the reactor flow into an oxidizer where all carbon species are converted to carbon dioxide. After condensing any unreacted steam, the gas stream is bubbled through a sodium hydroxide solution where the amount of total carbon converted is automatically monitored using the change in conductivity of the solution. Initial studies will be made using Illinois No. 6 char produced by the FBG earlier this year.

Feed to the mini-fluid bed unit consists of steam and/or hydrogen. Hydrogen is used to simulate the presence of synthesis gas (75% hydrogen) in the feed to a commercial gasifier. Feed flow compositions to the unit are being chosen to match either (a) the conditions under which the FBG was operated during the predevelopment program of gasification research, or (b) the conditions specified in the predevelopment commercial study design. These conditions are shown below.

Gasification Reactor Conditions

	FBG Conditions	Study Design Conditions
$\frac{\text{Moles Steam Fed/hr}}{\text{Moles Carbon in reactor}}$	0.53	1.34
$\frac{\text{Moles Syn Gas Fed/hr}}{\text{Moles Steam Fed/hr}}$	1.54	0.49

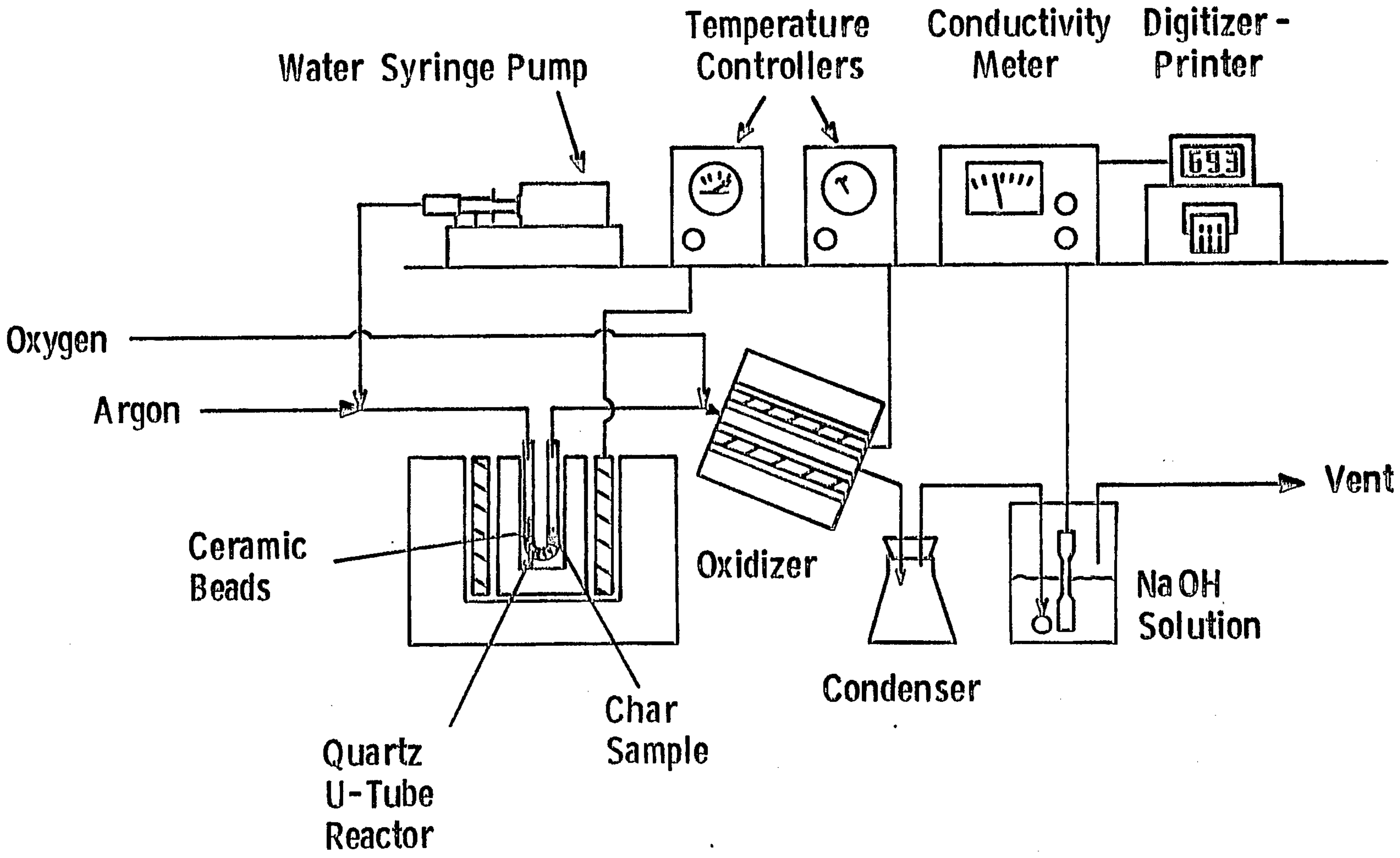
For comparison, runs will also be made using steam only as feed.

Initial kinetic studies are being made using steady-state Illinois No. 6 chars at different levels of carbon conversion produced earlier this year by the FBG. The available chars are listed below along with their degree of carbon conversion and catalyst loading.

Sample No.	Percent Carbon Conversion	Catalyst Loading, K/C Molar Ratio
A	83	0.169
B	76	0.118
C	74	0.122
D	76	0.148
E	84	0.233

FIGURE 4.1-2

SCHEMATIC OF MINI-FLUID BED REACTOR UNIT



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The kinetic behavior of these chars is being investigated as a function of their potassium to carbon molar ratio.

Numerous runs have been made in the mini-fluid bed gasifier at both FBG and Study Design conditions. During the course of the experimental program, a gas leak was discovered in the hydrogen feed line to the unit. This leak caused the H_2/H_2O feed ratio to be lower than the target conditions. The affected runs were repeated once the leak was eliminated. Subsequent data workup of the runs revealed much scatter in the observed gasification rate for duplicate runs. These results were believed to be caused by a lack of fluidization of the reactor bed. The reactor was then inspected at typical operating conditions and indeed, the reactor bed was not fluidized. In addition, gas channeling was observed in the bed. To alleviate this problem, the reactor feed system was modified. Argon, an inert gas, was added to the feed stream in sufficient amount to produce a fluidized bed. This modification should lead to better reproducibility in the data. The experimental investigation of the FBG chars is continuing using the new reactor configuration.

4.2 Catalyst/Char Equilibrium Studies

Bench scale studies are in progress to determine the effects of variable pH and potassium ion concentration on the amount of catalyst remaining on the char. This information is needed for the design of a multiple stage char washing process to recover potassium from the char. The equilibrium concentration of potassium on digested char, undigested char, and fines will be determined as a function of potassium concentration in solutions of constant pH and as a function of the pH of solutions of constant potassium concentration. Data will be obtained at room temperature and at the solution boiling temperature. This fundamental information will be used in both the PDU and the commercial CCG catalyst recovery system process definition.

Preliminary experiments on the effect of agitation on equilibration and on particle breakdown have been completed. Methods of agitation considered were 1) magnetic stirrer, 2) rotating flask, 3) wrist-action shaker, and 4) no agitation.

Figure 4.2-1 shows the effects of the four methods on the particle size distribution of digested FBG bottom char. Both the magnetic stirrer and the wrist-action shaker cause particle breakdown. The rotating flask method did not decrease the particle sizes.

Table 4.2-1 shows the effect of agitation on the potassium absorbed on digested char in contact with solutions containing the same potassium concentration at the same pH. The data indicates that agitation is necessary and that the rotating flask method does not provide sufficient agitation.

FIGURE 4.2-1

DIGESTED CHAR BREAKS DOWN UNDER EFFICIENT AGITATION

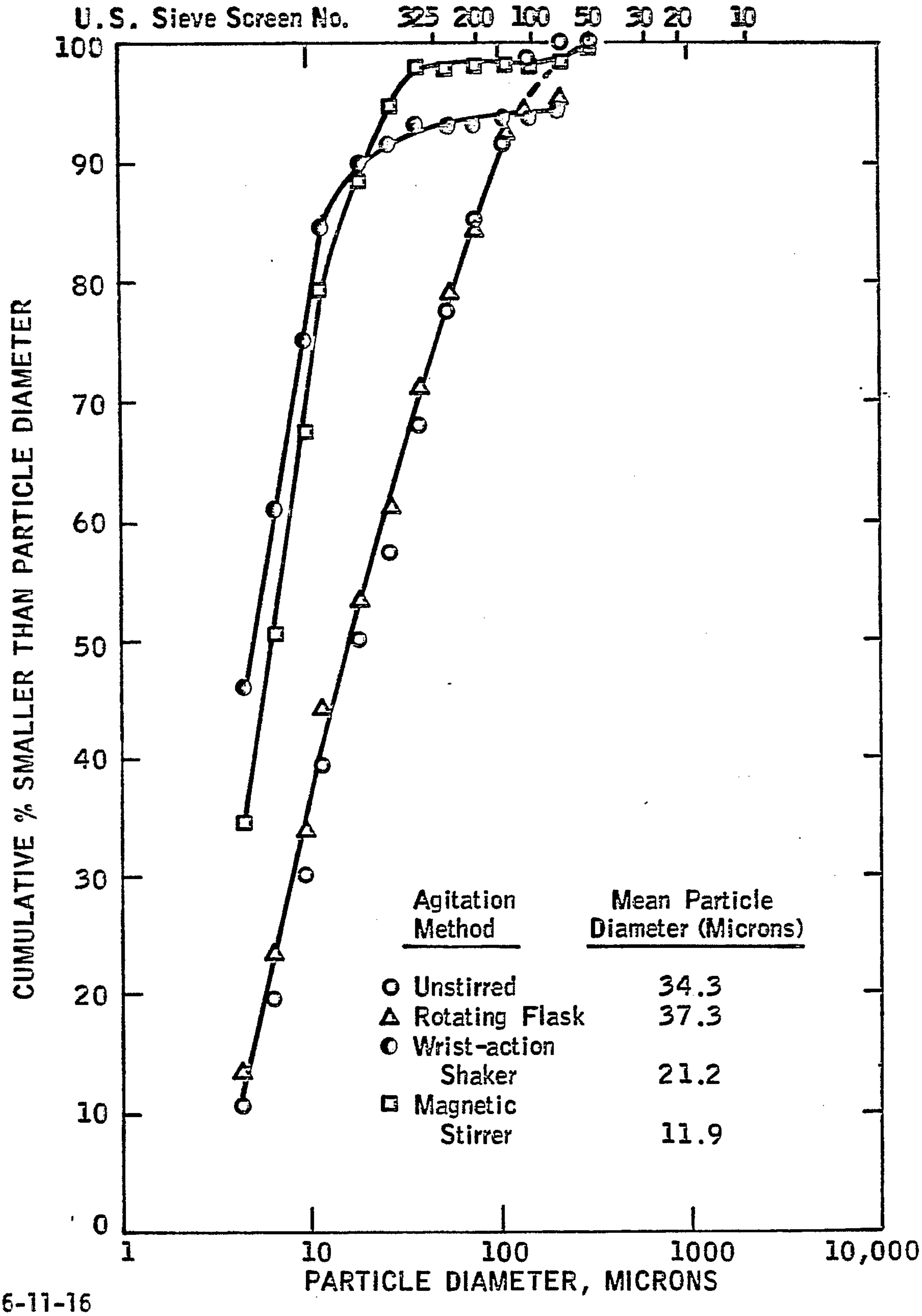

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Table 4.2-1

Effect of Agitation on Potassium Absorption

- Digested FBG Bottom Char
- Ambient Temperature
- $[K^+] = 1.0M$ (pH = 13.0)

Agitation Method	% (wt.) K^+ Absorbed on Char
None	0.09
Rotating Flask	0.10
Wrist-action Shaker	2.08

As a result, all ambient temperature equilibrations are being performed using the wrist-action shaker since K^+ absorbtion rather than particle breakdown is considered to be of primary importance in these experiments. This method was chosen over the magnetic stirrer because the shaker can handle a larger number of samples simultaneously. Since gasifier fines are also to be studied, the extent of particle breakdown for this material using the wrist-action shaker was then determined. Figure 4.2-2 shows that the particle size distribution of this material is not changed with agitation by this method.

4.3 Effect of Catalyst Impregnation on Char Properties

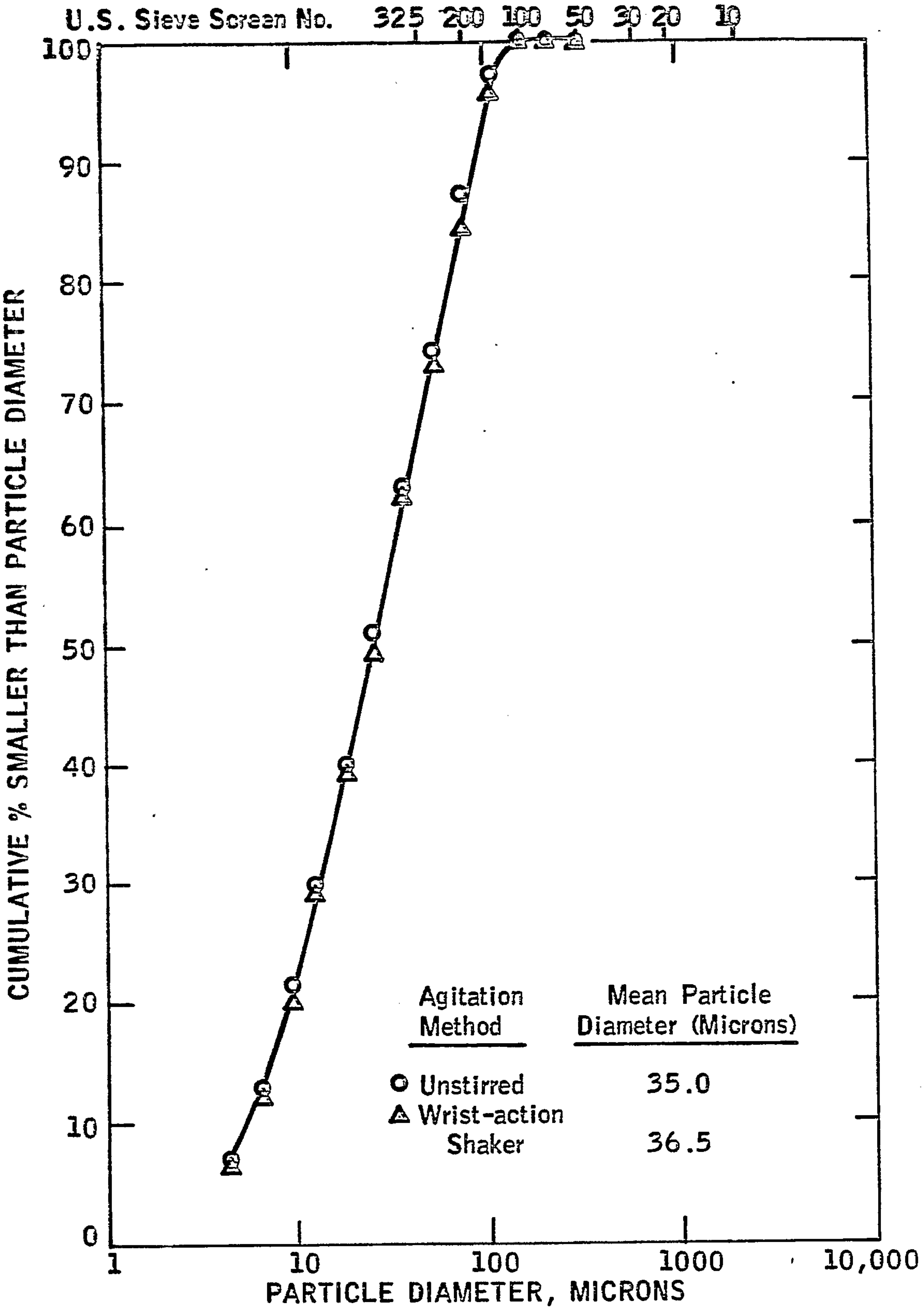
The FBG had been operated successfully during the predevelopment contract on a feedstock of potassium carbonate (K_2CO_3) catalyzed Illinois No. 6 coal. During the last quarter of 1978, operation with a new carload of Illinois No. 6 coal and with potassium hydroxide (KOH) as the catalyst was accompanied by some initial operability problems. Operations were improved by removing the large (+16 mesh) particles from the feed coal.

Bench scale studies were initiated to address the effect of variables in catalyst impregnation on both agglomeration and the bulk density of devolatilized coal (char).

The particle size distributions of the coals used in the predevelopment work and in recent work (1978) are shown in Tables 4.3-1 and 4.3-2. K_2CO_3 catalyzed coal used in predevelopment operations did not contain as many large particles (+20 mesh) as that currently used. The +20 mesh particles account for 4.7% of the weight of the predevelopment feed coal and 28.1% of the recent feed coal. For both coals the catalyst loading of these large particles is low versus the smaller size fractions as shown by the potassium analyses in Tables 4.3-1 and 4.3.2. Since the catalyst inhibits swelling and agglomeration during devolatilization, the low catalyst loading on the large +20 mesh particles was thought to account for the poor operability of the FBG when feeding a coal with a relatively large fraction of such particles.

FIGURE 4.2-2

GASIFIER FINES DO NOT BREAK DOWN WITH SHAKING



Effect of Coal Particle Size

Samples of both the 1977 and 1978 feed coals and the large particles (+20 mesh) only from the 1978 feed were charred in the laboratory at 1300°F and atmospheric pressure in nitrogen. The results are pictured in Figure 4.3-1. The 1977 feed did not agglomerate. The 1978 feed did form some agglomerate with the agglomerates containing most of the large particles initially present. The sample containing only +20 mesh particles agglomerated severely.

Table 4.3-1

Sieve Analysis of Predevelopment (1977) FBG Feed Coal

- Illinois No. 6 coal
- 15% K_2CO_3 treated
- Sampled 6/12/77

Mesh Size	% (wt.) of Sample	% K_2O H_2O Soluble	% K_2O Acid Soluble
+20	4.7	3.90	7.36
-20 + 60	59.3	5.41	7.96
-60 + 100	21.1	6.51	9.13
-100 + 200	11.4	7.08	9.86
-200 + 325	2.0	11.24	13.08
-325 + 400	0.5	11.83	15.48
-400	1.0	14.65	18.47

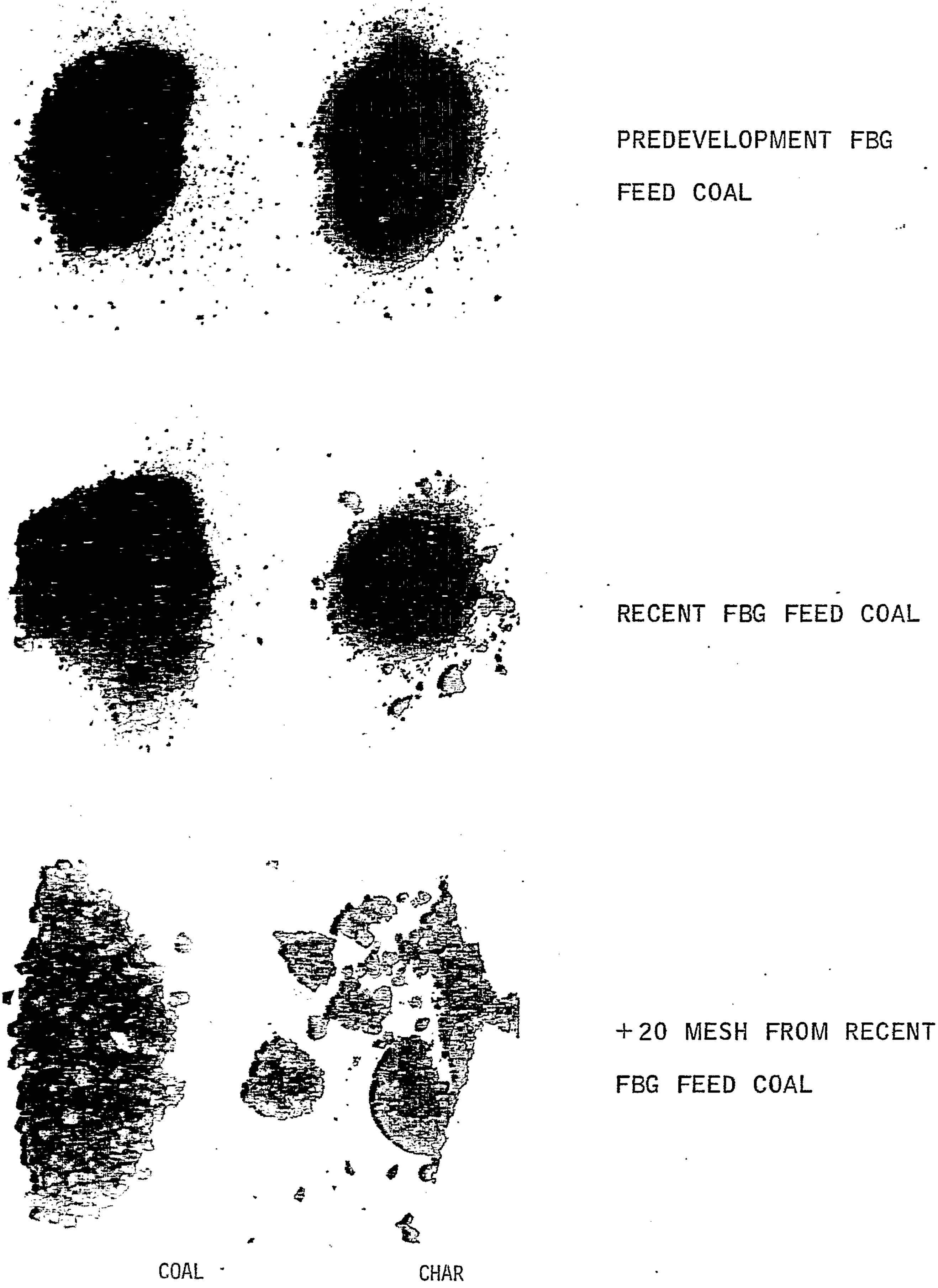
Table 4.3-2

Sieve Analysis of 1978 FBG Feed Coal

- Illinois No. 6 Coal
- 15% KOH treated
- Sampled 11/29/78

Mesh Size	% (wt.) of Sample	% K_2O H_2O Soluble	% K_2O Acid Soluble
+20	28.1	5.58	9.98
-20 + 60	52.6	8.25	11.49
-60 + 100	14.8	8.83	12.91
-100 + 200	2.7	5.8	11.41
-200 + 325	1.3	10.40	13.75
-325 + 400	0.4	14.85	17.40
-400	0.1	--	--

FIGURE 4.3-1
AGGLOMERATION TESTS



The data in Tables 4.3-1 and 4.3-2 show that the large (+20 mesh) particles in the 1978 FBG feed coal had a lower catalyst loading than the remainder of the feed. Laboratory chars prepared from these larger particles showed a high degree of agglomeration (Figure 4.3-1). The study described below was performed to address the question of whether or not the low catalyst loading was the cause of agglomeration of the large particles during devolatilization.

A sample of uncatalyzed FBG feedstock was divided into sieve fractions. Portions of the individual fractions were then treated with either KOH or K_2CO_3 catalyst. The laboratory procedure for catalyst impregnation simulated that used in the Catalyst Addition Unit (CAU) of the FBG. In this procedure, the coal was mixed with a 30% (wt.) catalyst solution in the appropriate quantity to result in a final catalyst loading on the coal equivalent to 15% (wt) K_2CO_3. Analysis of the sieve fractions treated in this manner showed that each fraction had the same catalyst loading.

The mixture was then dried under nitrogen and the treated coal samples were charred in a laboratory muffle furnace. The chars were examined for agglomeration and their loose bulk densities measured. The results are shown in Tables 4.3-3 and 4.3-4 below.

Table 4.3-3

KOH Catalyzed FBG Feedstock

- Illinois No. 6 Coal
- 12% KOH treated

Sieve Cut	Loose Bulk Density of Muffle Furnace Char (g/cc)	Agglomeration
+20	.51	No
-20 + 50	.52	No
-50 + 100	.56	No
-100	.52	No

Table 4.2-4

K_2CO_3 Catalyzed FBG Feedstock

- Illinois coal
- 15% K_2CO_3 catalyzed

Sieve Cut	Loose Bulk Density of Muffle Furnace Char (g/cc)	Agglomeration
+20	.58	No
-20 + 50	.53	No
-50 + 100	.55	No
-100	.55	No

The lack of agglomeration, particularly for the +20 mesh particles, suggests that uniform catalyst impregnation would allow this sieve size to be included in the reactor feed. In addition, the observed loose bulk densities have virtually the same value for chars from coal of all particle sizes and for equivalent loadings of both KOH and K_2CO_3 catalysts.

It would be desirable to be able to use larger size particles in the gasifier feed than the -16 + 100 mesh range that is currently used. The analytical data reported above (Tables 4.3-1 and 4.3-2) shows that the large (+20 mesh) particles in the FBG feed coals had a lower catalyst loading than the remainder of the feed. Laboratory chars prepared from these particles showed a high degree of agglomeration. Further bench scale studies (Tables 4.3-3 and 4.3-4) then showed that when particles of this size contained the desired catalyst loading, agglomeration was no longer observed. This was done by impregnating individual sieve cuts of raw coal separately. Therefore, it should be possible to include larger size particles in the gasifier feed if a method of uniform catalyst impregnation is obtained.

Char Bulk Density

The observed value of the bulk density of the devolatilized coal (0.51-0.58 g/cc) is higher than densities of char from the fluidized bed pilot plant reactor (0.2-0.4 g/cc) which suggests that muffle furnace char may not be directly comparable to reactor char.

Scanning electron microscope analysis showed that all of these chars consisted of particles which remained angular and irregular in shape, indicating that they did not go through a plastic state during devolatilization. FBG bottom chars consist of rounded, enlarged particles that have melted and resolidified.

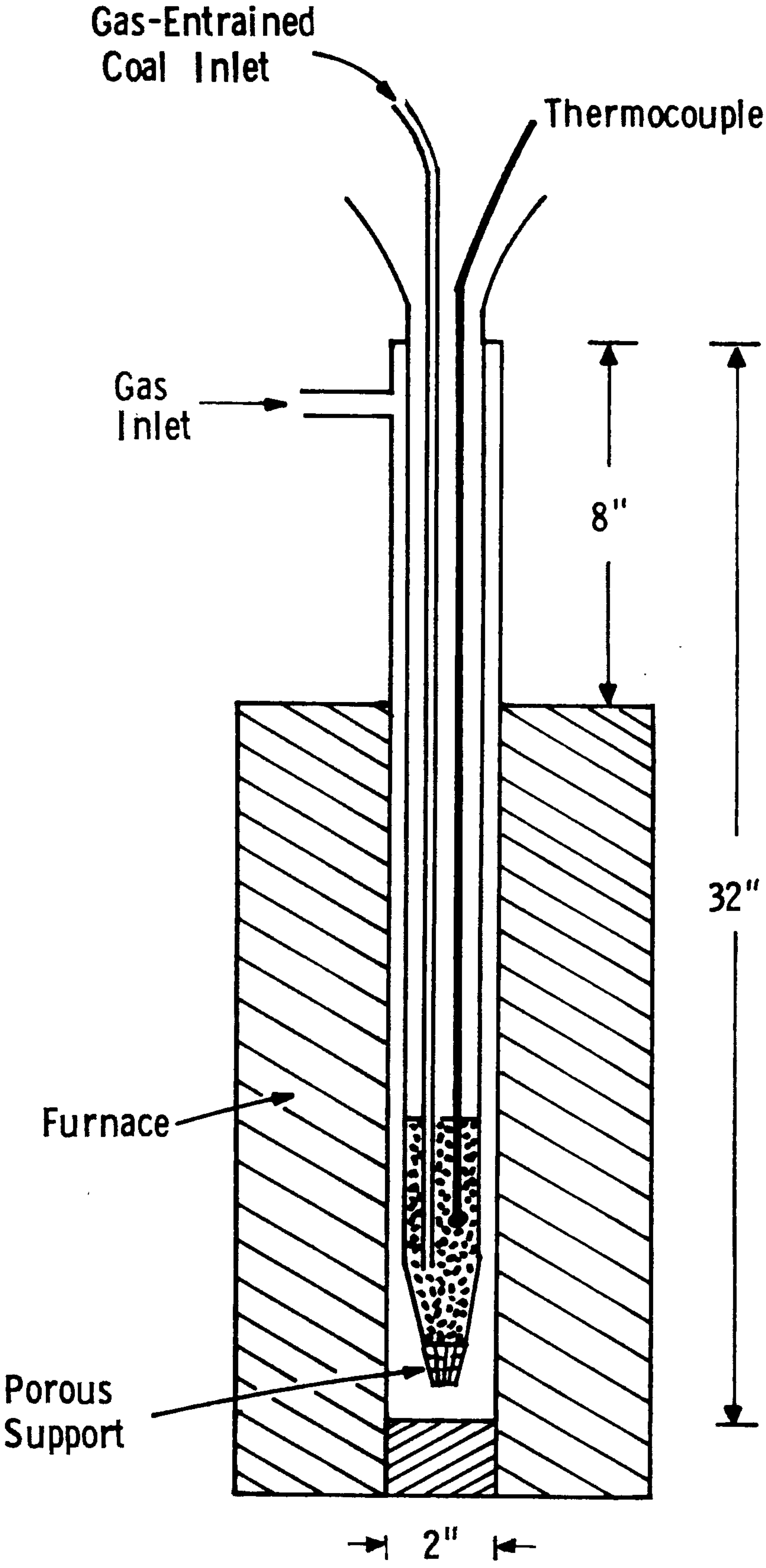
Therefore, work is in progress to obtain a devolatilization process which is a reproducible test of the characteristics of the coal sample devolatilized. A procedure which closely simulates pilot unit devolatilization is considered desirable.

An existing small fluidized bed reactor is being modified for this purpose. The unit is designed to simulate coal addition to a hot, fluidized bed gasifier in all respects except pressure conditions. Figure 4.3-2 illustrates the unit. The reactor system is constructed of quartz while the coal addition system is stainless steel. The bed is supported by a porous screen and is fluidized by gas which is preheated in the outer section of the vessel. The coal addition tube is adjustable to allow entrance of the coal sample at variable positions within or above the bed. A movable thermocouple is used to measure bed temperature at any desired position.

Preliminary experiments have shown that fine (100 - 200 or - 200 mesh) char cannot be used as a bed material because it would not properly fluidize. Therefore, 100 - 200 mesh sand has been chosen for the bed material for the reactor due to its fluidizing properties. A fine cut of bed material is required in order to separate the bed from the product char. Future work will study the effect of catalyst impregnation variables or char bulk density with the goal of learning how to make high density char.

FIGURE 4.3-2

BENCH SCALE FLUIDIZED BED UNIT



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5. Engineering Research and Development (Reporting Category C20)

Engineering research and development studies are being 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 includes both engineering and cost studies to evaluate process improvements and to guide the continuing laboratory programs, and engineering technology programs to develop fundamental process and equipment technology to support the laboratory and engineering efforts. The overall objective of the engineering work is to define the conceptual commercial CCG process at the end of the contract period.

The engineering research and development work under the CCG Process Development Contract is divided into four major subtasks:

Cost Reduction and Laboratory Guidance Studies
Systems Modeling
Process Definition
Engineering Technology Studies

During the period covered by this report, the engineering efforts focused on the first, second, and fourth sub-tasks. Work on the Process Definition is not scheduled until July, 1980.

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" are 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 to firm up the CCG Study Design in this important area. The revised Study Design will serve as the "base case" for screening studies to evaluate new data, process improvements, and optimum process conditions under the present Process Development Contract. As a result of the offsites revision, the accuracy of such screening studies will be 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 are better defined today 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 is the same. The onsites process bases and material and energy balances are 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 Illinois No. 6 coal and producing 257 billion Btu per stream day of SNG

TABLE 5.1-1

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 $	% (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.

(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, has led to improved estimating approaches. Applying these new tools shows 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.) are reduced based on the final plant layout.

- Steam generation and distribution has slightly increased in cost. This is 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 is shared with the onsites catalyst recovery system. The investment for the shared lime facilities is included under chemicals handling and storage. Even so, the cost for the latter section is lower because of the new cost estimating approaches for silos and conveyors.

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)	
Other 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

- The investment for wastewater treating is up because of the increase in process wastewater rate and in facilities for reuse. As a result of more detailed study of water reuse options, the estimated average raw water makeup rate for the CCG Study Design has been 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 is 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 is now 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 is also based on the same DCF return on the equity and the same escalation assumptions. The complete economic basis for these gas costs is 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)

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 1,530 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		0.598
- 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).

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

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 startup 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 has 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 have offset these additional allowances for the other utilities. Thus there has been 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 has been made by Exxon Research and Engineering Company, and it has been concluded that significant incentive exists for development of the Catalytic Coal Gasification Process.

5.1.2 Coal Crushing Machinery for CCG

A study is underway to determine the type(s) and performance of coal crushing equipment appropriate for commercial catalytic coal gasification plants. Initially, effort has been directed toward determining design pressure requirements.

To arrive at appropriate design requirements, the safety requirements in regard to pressure containment in the event of a coal dust explosion are being investigated for coal crushing equipment and its associated ductwork, fans, cyclones, etc. In this effort, applicable National Fire Protection Association (NFPA) standards have been reviewed. This review and associated discussions with NFPA contacts and an outside coal handling safety consultant have 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 associated ductwork, fans, cyclones, etc. in the system, a 50 psig design pressure should be assumed initially. (A reliable system would have to provide inerting at start-up and shutdown as well as during normal operations).

Work on this study will continue with vendor and consultant contacts with the intent of selecting the appropriate type(s) of machinery for coal crushing at a CCG facility. At the same time, the issue of design pressure requirements will be reviewed with these contacts for their additional input.

5.1.3 Evaporation of Catalyst Solutions

A laboratory guidance study has been made to estimate the economic impact of evaporating dilute catalyst solutions from catalyst recovery to concentrations which are suitable for direct addition to the gasifier feed coal. These estimates of evaporation costs will be used to help assess technical and economic tradeoffs in the catalyst recovery section. As recovered solution concentration is reduced below the level in the CCG Study Design, fewer washing stages are required to achieve the same overall recovery. Also, the solid-liquid separations are easier in dilute solutions, due to lower viscosities, and in the case of separations based on gravitational forces (e.g., settlers, centrifuges), due to larger particle-solution density differences. The potential cost savings for dilute solutions must be weighed against the added costs to concentrate the recovered solution to the same level used in the Study Design.

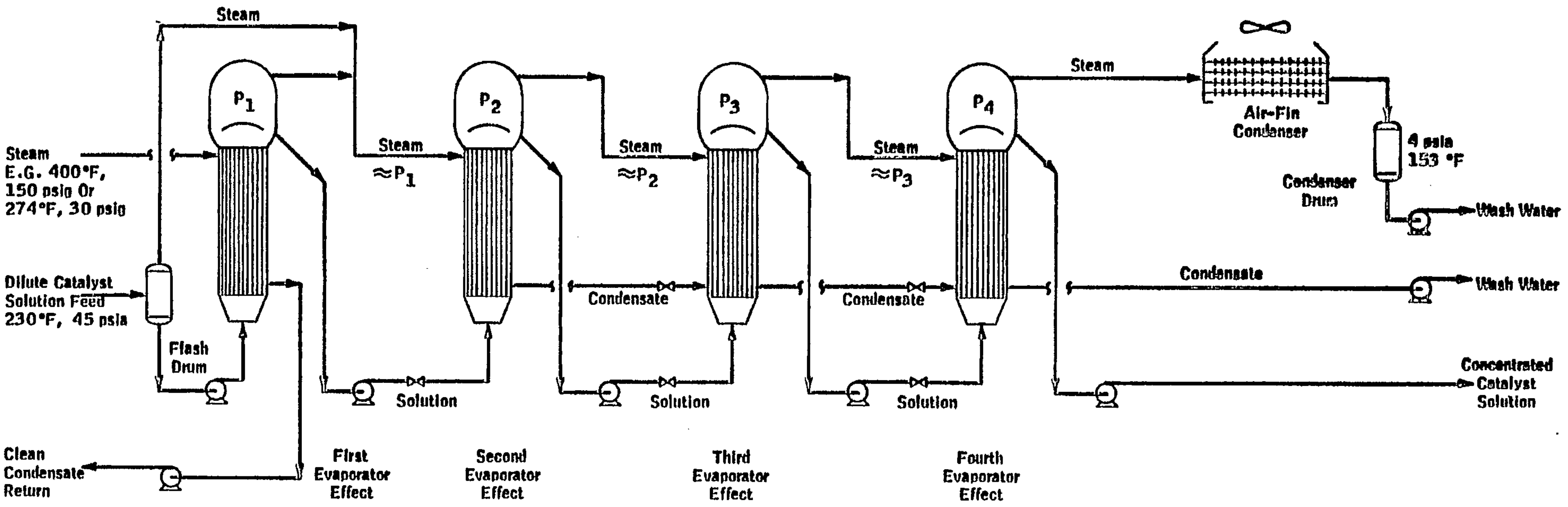
In order to estimate the costs for evaporation, a series of screening studies were carried out. Figure 5.1-1 shows the general process flowsheet for these screening studies. It includes a conventional, multiple-effect evaporator for concentrating the catalyst solution and an air-fin condenser for recovering the evaporated water for recycle to catalyst recovery. The multiple-effect evaporator uses process steam in the first effect to concentrate the catalyst solution. Vapor raised in the first effect is condensed in the second effect to further concentrate the remaining solution. The vapor from the second effect is then condensed in the third effect, and so on. The vapor from the last effect is condensed in the air-fin condenser. To operate the evaporator in this manner, the solution pressure in each effect is maintained lower than the pressure in the preceding effect. The pressure in the last effect was set at 4.5 psia. This pressure is typical of multiple-effect evaporators and was selected because it gave the lowest combined evaporator-condenser area for representative cases.

The process basis for the current studies was set based on the CCG Study Design. The catalyst feed rate to the evaporator is the same as the catalyst rate from catalyst recovery in the Study Design (equivalent to 122.8 klb/hr of KOH). Two catalyst solution concentrations, 5 and 10% (wt.) were considered as feeds to the evaporator system. The concentrated product from the evaporator is a 32.2% (wt.) KOH catalyst solution, which is the same concentration as the recovered catalyst solution fed directly to the catalyst addition/entrained drying system in the Study Design. Steam to concentrate the solution in the evaporator is potentially available from two sources. Low pressure steam (e.g., 10-30 psig) can be produced from onsite waste heat, and higher pressure steam (e.g., 150 psig) can be produced by letting down high pressure steam from offsite boilers across non-condensing steam turbine drivers.

To estimate the economic impact of concentrating the dilute catalyst solutions, heat and material balances were made for each catalyst solution feed (5 and 10% (wt.) KOH) with each steam source and with a variable number of effects in the evaporator. Based on these balances, both onsite and offsite equipment was sized and utility demands were determined. The number of parallel evaporation trains was set to maintain individual evaporator area below 32,000 ft^2 (the approximate maximum commercial size today). The incremental investment and operating costs were estimated based on comparable equipment and operatring costs for the CCG Study Design. The incremental impact on the gas cost was then estimated using the CCG Study Design economic basis (100% equity financing, 15% DCF return on investment, January 1978 cost level, East Illinois location). By minimizing these incremental gas costs, the approximate optimum number of effects for each feed concentration at each steam pressure were selected. Table 5.1-4 summarizes these optimum cases. The range of incremental gas costs shown in the table reflects the sensitivity of the gas cost to uncertainties in the evaporator costs and the inclusion of a 25% process development allowance.

Figure 5.1 - 1

FORWARD FEEDING MULTIPLE-EFFECT EVAPORATOR



Note: (1) Pressures Are Cascaded So That $P_1>P_2>P_3>P_4$ = 4.5 psia

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TABLE 5.1 - 4

INCREMENTAL GAS COST FOR CONCENTRATING DILUTE CATALYST SOLUTIONS BY EVAPORATION

Process Basis

• Catalyst Feed:	122.8 k lb/hr KOH (dry basis)
• Feed Concentration:	5 wt% KOH or 10 wt% KOH
• Product Concentration:	32.2 wt% KOH
• Available Steam:	Offsite boiler steam at 150 psig and/or onsite waste heat steam at 10-30 psig

Economic Basis

- CCG Study Design producing 257 GBtu/SD SNG
- 100% equity financing/15% DCF return

	5% KOH Feed		10% KOH Feed	
Evaporator Steam Basis	Evaporator Effects @ Steam Pressure, Psig	Incremental Gas Cost, $/MBtu SNG	Evaporator Effects @ Steam Pressure, Psig	Incremental Gas Cost, $/MBtu SNG
• All Offsite Boiler Steam	5 @ 150	0.37-0.47	5 @ 150	0.17-0.22
• "Unlimited" Waste Heat Steam	2 @ 30	0.25-0.33	2 @ 30	0.11-0.14
• "Limited" Waste Heat Steam (Limit set by 1977 CCG Study Design)	4 @ 30 3 @ 10 5 @ 150	0.32-0.46	4 @ 30	0.12-0.19

A comparision of the results for the high-pressure (offsite boiler) steam and unlimited low-pressure steam cases shows that for both feed concentrations, the impact on gas cost is minimized by utilizing the onsite waste heat to raise the required low-pressure steam. However, evaluation of the Study Design heat balance indicates that there is not sufficient waste heat available to raise the low-pressure steam required to operate the evaporator at the optimum conditions. With this constraint, either more effects must be added to the evaporator to make it more thermally efficient or high-pressure steam must be used to fill the deficit. If more effects are added to the evaporator, less steam is required, but the incremental gas cost will increase due to high investment charges. If only a few effects are added, the incremental gas cost increases above the optimum, but is still less than that for all high-pressure steam. The last line in Table 5.1-4 summarizes the rough optimum cases using the low-pressure steam estimated to be available based on the CCG Study Design heat balance.

In the case of 5% KOH feed with limited steam, all available 30 psig steam is used in a four-effect evaporator to concentrate about 40% of the total feed. Additionally, the low-level waste heat which remains after raising the 30 psig steam is used to raise 10 psig steam. The 10 psig steam is used in a three-effect evaporator to concentrate about 30% of the feed. The remaining feed (30%) is concentrated in a five-effect evaporator with high-pressure steam. (The incremental gas cost of using all 10 psig steam is greater than the incremental gas cost of using a combination of 10 psig and 30 psig steam.) In the case of 10% (wt.) KOH feed, the solution can be evaporated to 32.2% (wt.) entirely with 30 psig steam in a four-effect evaporator.

The impacts of evaporating dilute catalyst solutions on the overall CCG process efficiency and gas cost are much less if the solution from catalyst recovery is 10% (wt.) KOH rather than 5% (wt.). For 10% (wt.) KOH solution, no supplemental offsite steam is required, and thus the impact on process efficiency is slight. The 10% (wt.) KOH case also shows a clear economic incentive over the 5% (wt.) case. The incremental gas cost for concentrating the 10% (wt.) solution to 32.2% (wt.) is 0.12-0.19 $/MBtu, only 2-3% of the CCG Study Design gas cost of 6.18 $/MBtu. However, evaporating more dilute solutions could have a significantly greater cost impact. The incremental gas cost for concentrating the 5% (wt.) solution is 0.32-0.46 $/MBtu. As discussed above, the use of dilute catalyst solutions will reduce the number of stages required for catalyst recovery. Studies will be conducted later in the program to find the optimum balance between evaporation costs and catalyst recovery costs.

5.1.4 Catalyst Recovery System Screening Studies

A series of engineering screening studies have begun to evaluate the economic impacts of alternative processing approaches and solid-liquid separation devices for catalyst recovery. The results of these studies will be used in selecting the most attractive alternatives for more detailed laboratory and engineering study later in the current program. These screening studies will assess the process and economic impacts of countercurrent water-washing of the char to recover the catalyst both with and without an initial calcium hydroxide digestion step. Filters, settlers, centrifuges, and hydroclones will be considered to carry out the solid-liquid separations between washing stages.

Work thus far has centered on establishing a representative process basis for the studies. Particular attention has been given to the catalyst reactions and material balance around the catalyst recycle loop and to the anticipated particle size distributions for the solids. The catalyst reactions are important in comparing the cases without digestion with those utilizing digestion. The particle size distributions are important in comparing cases utilizing different solid-liquid separation techniques.

The first case to be considered is countercurrent water-wash with digestion, using filters for the solid-liquid separations to produce a moderately concentrated catalyst solution (about 17% (wt.)). The feed rates of spent gasifier char and potassium catalyst to catalyst recovery are the same as in the CCG Study Design. The char feed consists of 68% coarse char withdrawn from the bottom of the gasifier and 32% fines collected in external cyclones.

In this first screening study, the char feed is slurried with semi-rich catalyst solution from the first water-wash stage and is digested at 300°F and 70 psia with a residence time of one hour. Here, lime is added to give a calcium/potassium ratio of 0.7 mole/mole. About 90% of the total potassium fed is solublized during digestion. The slurry from digestion is filtered to remove all of the solids. This clarified solution contains about 17% (wt.) potassium salts. The solids in the filter cake are sent to the countercurrent water-wash to recover the remaining solubilized catalyst.

In the countercurrent water-wash, the digested solids are repeatedly washed in slurry mixing vessels and filtered to recover 95% of the solubilized catalyst. Each countercurrent water-wash stage operates at atmospheric pressure and near the boiling point of the catalyst solution. The filters used between each washing stage remove 99% of the solids from the catalyst solution. The filter cake from each stage contains 70% moisture and 30% solids.

Future work on this first catalyst recovery screening study includes making a material balance for digestion and water-wash to determine the number of washing stages required to recover 95% of the soluble catalyst at the desired concentration. The Catalyst Recovery Material Balance Model described later in this report will be used to facilitate making the material balance. Equipment sizes and specification lists will be prepared based on the material balance, and the investment and operating costs for catalyst recovery with this basis will be estimated. These costs will be compared to those predicted for alternative processing approaches and other solid-liquid separation devices to select the most attractive alternatives for further study later in the program.

5.1.5 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 furnace 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.

A brief incentive study of an alternative two-stage gasification concept has been completed. The two-stage gasifier process configuration selected for this study is illustrated in Figure 5.1-2. In this scheme, coal is fed to the first stage gasifier which operates at low temperature (1225°F). The coal is fluidized and gasified by product gas from the second stage gasifier. A carbon conversion of 80% is achieved in this first stage. The char and fines from the first stage are withdrawn and fed to the second-stage gasifier. This operates at a higher temperature (1325°F) to achieve high carbon conversions. Steam and recycle gas from the preheat furnace are fed to the secondary gasifier to achieve an overall carbon conversion of 95% for the two gasifier stages.

This concept differs from that 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 are achieved by operating the upper stage at a lower temperature (1225°F) and high carbon conversions are 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 5.1-5. 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 furnace 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 5.1-6, 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 a larger first stage gasifier volume required for the lower reactor temperature (1225°F) than the base case and for the addition of the separate second stage gasifier. Also, steam generation investments are increased due to the increased steam requirements for this case.

FIGURE 5.1-2

SIMPLIFIED FLOW PLAN FOR TWO STAGE GASIFICATION

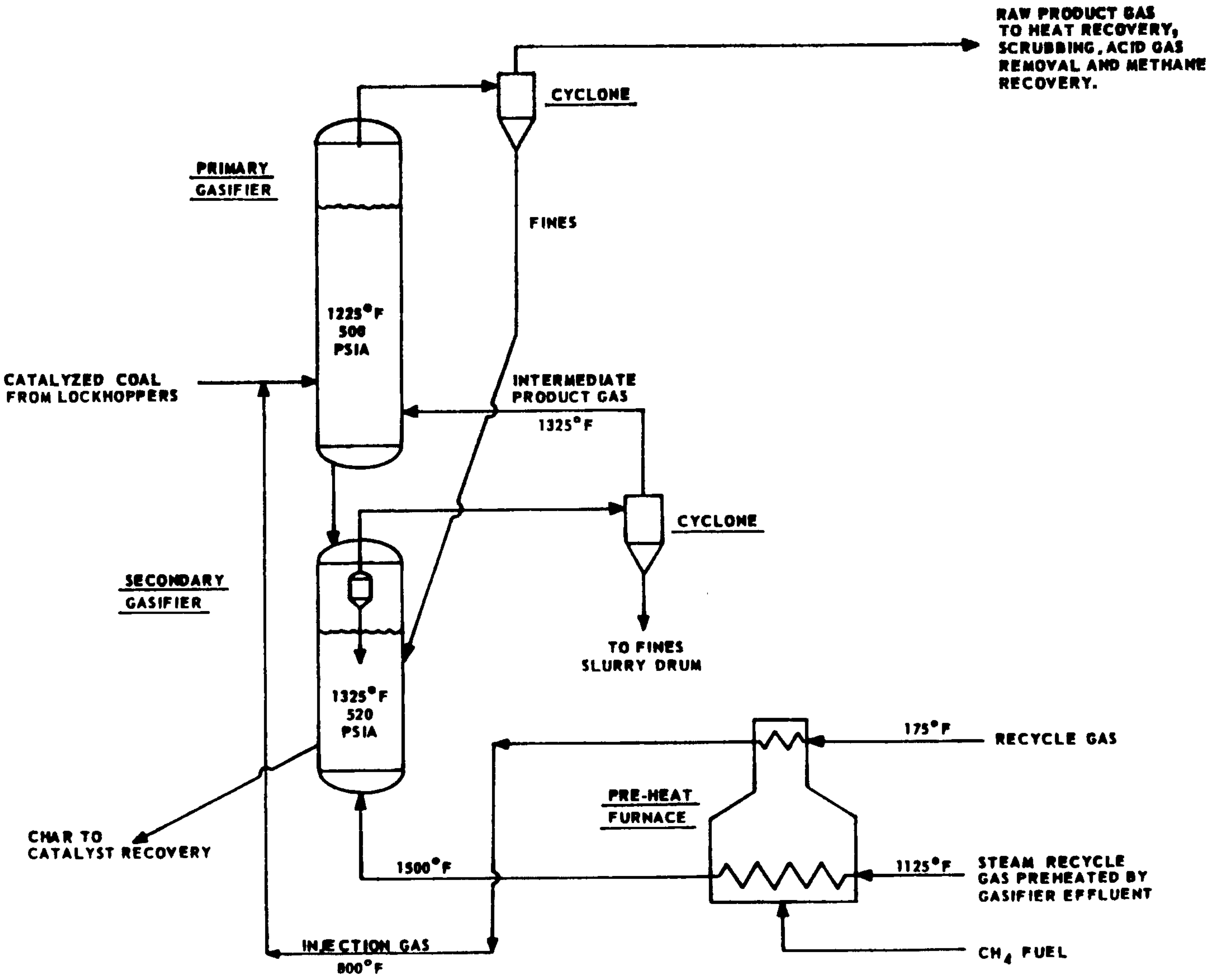

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Table 5.1-5

INCENTIVE STUDY FOR TWO-STAGE GASIFICATION

Reactor System	Base Case(1) "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 (2)	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 Furnace 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 (3)	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 5.1-6

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
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

Process economics are presented in Table 5.1-7. 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. Additional data are required to firm up reaction kinetics at the lower gasifier temperature of 1225°F and at carbon conversions over 90%. The current data base at these conditions is limited since the Fluid Bed Gasifier (FBG) runs made during the predevelopment research phase were generally at temperatures of 1300°F and carbon conversions of 80-90%. Additional data are 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 the fines. Data on lower gasification temperatures, higher carbon conversions and fines generation will be obtained as part of the current Process Development Program. This data can then be used for a more definitive estimate of the incentive for a two-stage gasification system.

5.1.6 CCG Char Properties

Data on solids properties for the catalytic gasifier are needed as input information for Activity A of Subtask 4.4, Catalytic Gasifier Solids Balance Model. Such data is also needed as input information for the CCG Gasifier Reactor Model. A brief study to summarize solids properties data from Fluid Bed Gasifier (FBG) operations during the predevelopment research phase has been completed. This data will be used to start work on the Gasifier Solids Balance Model since solids properties data from the PDU are not yet available.

Composition and physical property data has been summarized for the feed coal, overhead fines, mid char and bottoms withdrawal char. Estimates have been made of solids composition, and physical properties such as particle size distribution and density. This information will enable scoping studies and development of calculational procedures leading to the development of a Catalytic Gasifier Solids Balance Model. However, when data is available from the 1 T/D Process Development Unit, this will be used for definitive development of the Solids Balance Model and for input to the gasifier kinetics-contacting model.

5.1.7 Integral Steam Reformer Heat Input Study

A key feature of the Exxon 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:

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

Table 5.1-7

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.

Thus, coal is converted to methane in a single reaction step which is approximately thermally neutral. 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 1977 CCG Study Design, this heat input was supplied by heating the steam and recycle gas in a furnace to 1540°F. This preheat is sufficient to provide for the heat input requirements listed above. The preheat furnace 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 5.1-3.

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 provides greater flexibility than the base case heat input scheme which uses only sensible heat for heat input. The reformer could be either a small reformer operating in parallel with the preheat furnace, or the reformer could replace the preheat furnace 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 furnace.

A study was initiated during February to consider the Integral Steam Reformer in greater depth. A schematic flow plan for this system is also shown in Figure 5.1-3. Several alternative processing conditions have been 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. Initial 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 have been evaluated. A comparison of the cases is shown below:

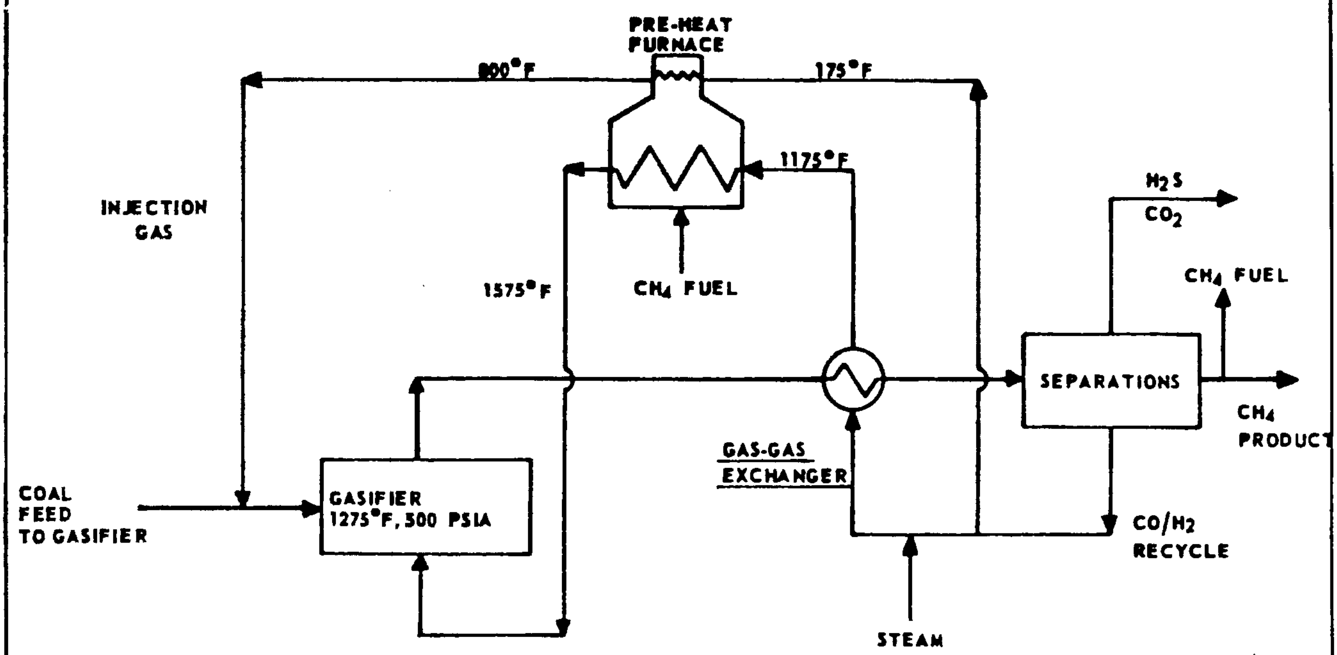
Basis: 14,490 ST/SD Coal feed to gasifier
Gasifier operating conditions of 1275°F, 500 psia.

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 Furnace Fuel Fired, MBtu/hr	680	630
Net Methane Product, GBtu/SD	252.1	254.8

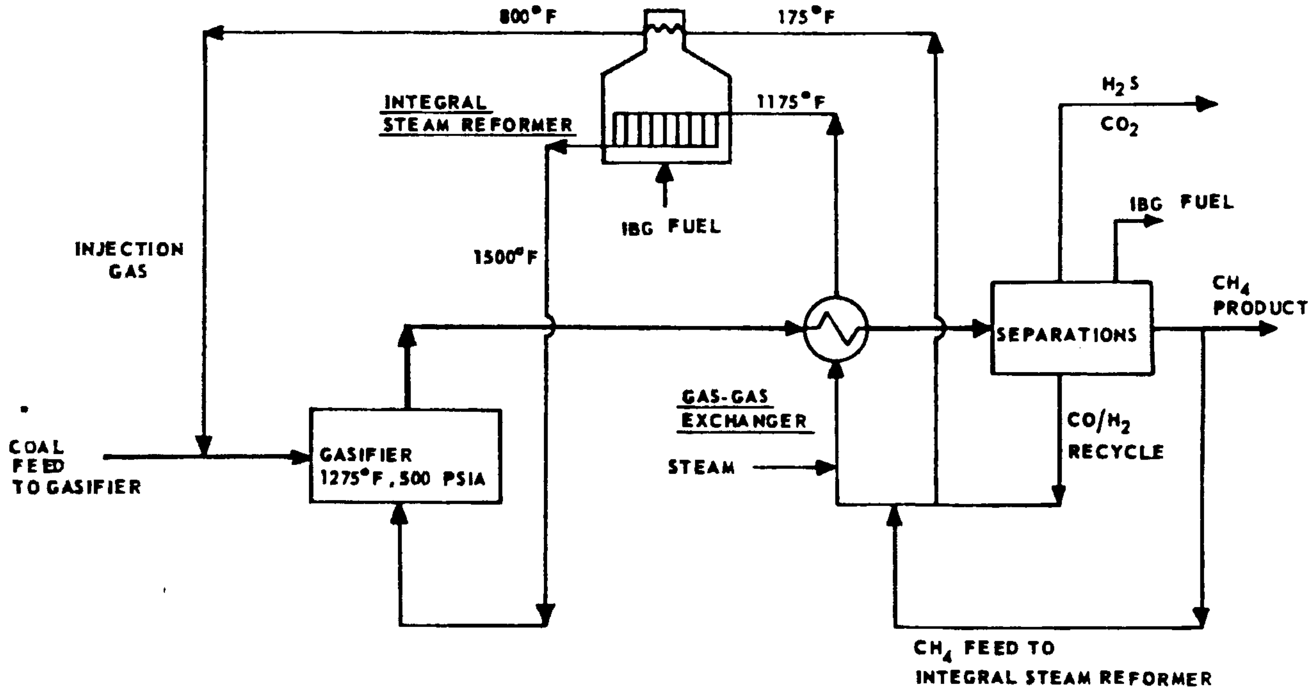
FIGURE 5.1-3

INTEGRAL STEAM REFORMING HEAT INPUT STUDIES - SIMPLIFIED SCHEMATIC FLOW PLAN

CCG STUDY DESIGN



INTEGRAL STEAM REFORMING CASE



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The credits for higher temperature include reduced gas flow rates, reduced steam requirements, reduced furnace duty, etc. The debit for the higher temperature will be a higher furnace 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	47	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 Furnace 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 include reduced gas flow rates, reduced steam requirements, reduced furnace duty, etc. The debit for the higher steam conversion will be higher gasifier investment. It is believed that the 47% steam conversion case represents the optimum balance.

The high steam reformer coil outlet temperature (1500°F) and high steam conversion (47%) 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 Base	Case 2 Lower Heating Value Fuel	Case 3 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 Furnace 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 will be used for gasifier heat input control.

During the process variable studies described above, the potential for carbon formation and laydown on the steam reforming catalyst or upstream equipment has been 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 furnace used in the CCG Study Design because the injection of small amounts of a sulfur compound into the gas stream can prevent 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:

$$2CO \rightarrow CO_2 + C$$

$$CO + H_2 \rightarrow H_2O + C$$

$$CH_4 \rightarrow 2H_2 + C$$

Figure 5.1-4 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: carbon 4 mole %, hydrogen 69 mole %, and oxygen 27 mole %. This point is shown on Figure 5.1-4 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 <u>not</u> favorable for carbon formation. However, the feed to the integral reformer is not in chemical equilibrium. Thus, it is possible that a nonequilibrium 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, $C + H_2O \rightarrow CO_2 + H_2$. 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.

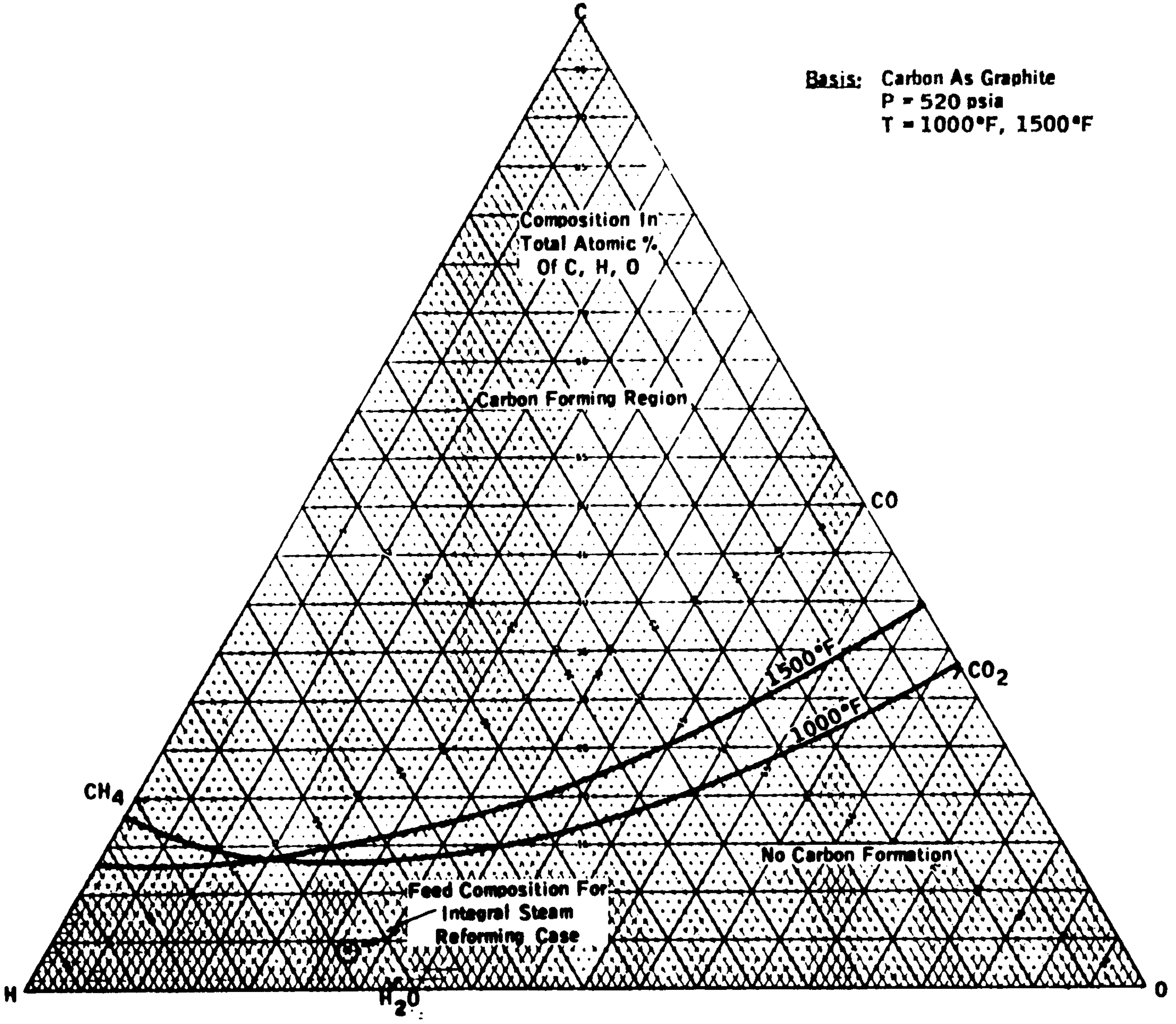
Recent data from bench-scale research on Gas Phase Reactions (see Section 1.3 of this report) have shown that carbon laydown can occur in a gas stream with compositions similar to those envisioned commercially for integral reformer feed. However, this research was directed at studies of the shift reaction, 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. More representative experiments directed at the issue of carbon laydown are planned as part of the Engineering Technology Study under Activity I, Preheat Furnace Tube Selection. These experiments will address the issue of carbon formation and, if necessary, explore ways to avoid it. One potential way which has been identified to avoid carbon laydown is to alter the gas composition by increasing the CO_2/CO ratio.

The process basis for the Integral Steam Reformer Heat Input Study is now complete. The design of the steam reformer furnace has been initiated. The furnace will then be cost estimated and utilities and operating costs will be developed. Investments for other plant sections will be prorated from the CCG Study Design and overall economics for Integral Steam Reforming will be developed. This study is expected to be completed during the third quarter of 1979.

5.1.8 Cryogenic Acid Gas Removal Incentive Study

An engineering screening study has been completed which evaluated the economic incentives for using a cryogenic fractionation scheme for acid gas removal in the Exxon Catalytic Coal Gasification Process. This study included the definition of the process flow scheme, detailed material and energy balances, design of the required equipment, and development of investment, operating costs and economics for this process concept.

FIGURE 5.1-4
CARBON FORMATION EQUILIBRIUM ISOTHERMS



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Previous work done under the CCG Predevelopment Contract led to the conclusion that carbon dioxide (CO_2) freeze-out would occur in some part of the acid gas fractionation system over the entire range of possible tower operating conditions. For the current study, it was assumed that the freeze-out problem could be handled in a simple manner within the system. Further work to determine the actual effect of CO_2 freeze-out would be necessary to determine the actual technical feasibility of the proposed scheme.

A simplified block flow diagram of the Cryogenic Acid Gas Removal (AGR) Scheme is presented in Figure 5.1-5. The scheme incorporates two new distillation towers. In the first tower, the Acid Gas Fractionator (AGF), CO_2 and H_2S are separated from an overhead H_2, CO, and CH_4 stream. The overhead stream is then fed to cryogenic Methane Recovery. The bottoms CO_2 and H_2S stream from the Acid Gas Fractionator is fed to the second tower, the Acid Gas Splitter (AGS), where the overhead is essentially pure CO_2 and the bottoms is an 80/20 mixture of CO_2/H_2S. This bottoms stream is then sent to sulfur recovery. A flow plan showing process operating conditions and major equipment is presented in Figure 5.1-6.

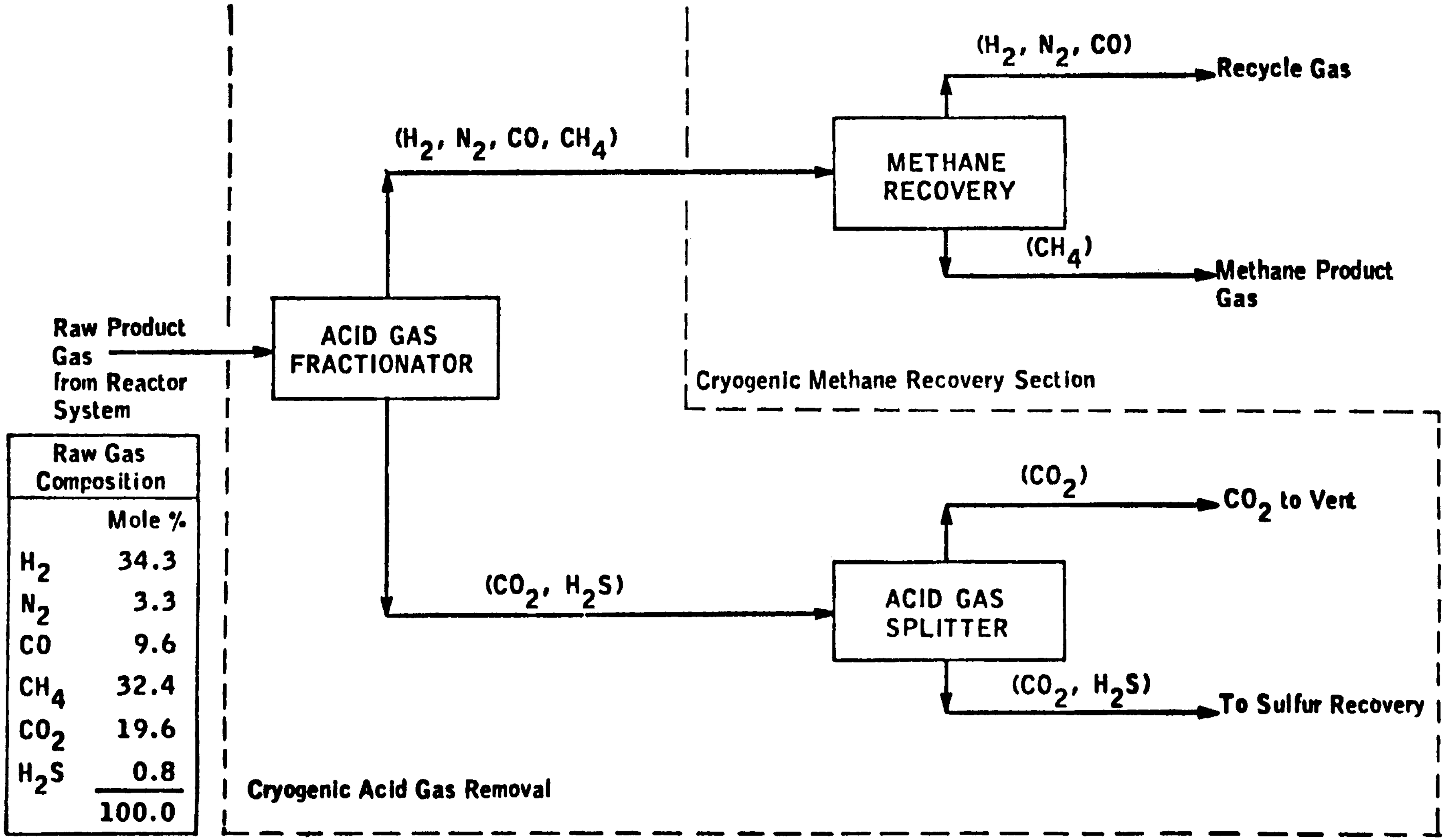
During the study, various process conditions, flow schemes, and heat integration/refrigeration options were investigated. The alternatives were compared on the basis of minimizing total system horsepower requirements. This is believed to be the major investment and operating cost parameter in cryogenic systems. The design bases for the three towers involved in the study are described below.

In the Acid Gas Fractionator, an overhead CO_2 concentration of 150 vppm was specified to eliminate the need for molecular sieve adsorption for CO_2 removal upstream of methane recovery. The AGF bottoms specification was set to limit methane losses to 0.1% of the methane fed to the tower. This low level of methane losses is relatively easily achieved and compares to methane losses of about 1% for the heavy glycol solvent absorption system used in the CCG Study Design. The reduced methane losses result in a higher product SNG rate for the cryogenic acid gas removal case compared to the Study Design. Alternative AGF operating pressures were evaluated. High pressure is desirable to increase tower operating temperatures which might minimize the impact of CO_2 freeze-out. Pressures of 1000 psia and 850 psia were evaluated and the lower pressure level provided about a 7% savings in feed/product compression and refrigeration power requirements. AGF feed temperatures between -60°F and -140°F were evaluated and the minimum power requirements were obtained at a feed temperature of about -115°F. This produced a 17% savings versus a feed temperature of -60°F.

The Acid Gas Splitter (AGS) separates a CO_2 overhead product from an 80% CO_2/20% H_2S bottoms product. After energy and refrigeration recovery, the CO_2 stream is vented to the atmosphere. An overhead H_2S concentration of 10 vppm in the CO_2 vent stream was specified, consistent with the Study Design. The H_2S containing bottoms product is fed to a Claus Plant for sulfur recovery. The AGS operating conditions selected enable use of a heat pump loop with propylene refrigerant for both the condenser and reboiler duties. The specification of a lower CO_2 level

FIGURE 5.1-5

CRYOGENIC ACID GAS REMOVAL FLOW SCHEME



Raw Gas Composition	Mole %
H_2	34.3
N_2	3.3
CO	9.6
CH_4	32.4
CO_2	19.6
H_2S	0.8
	100.0

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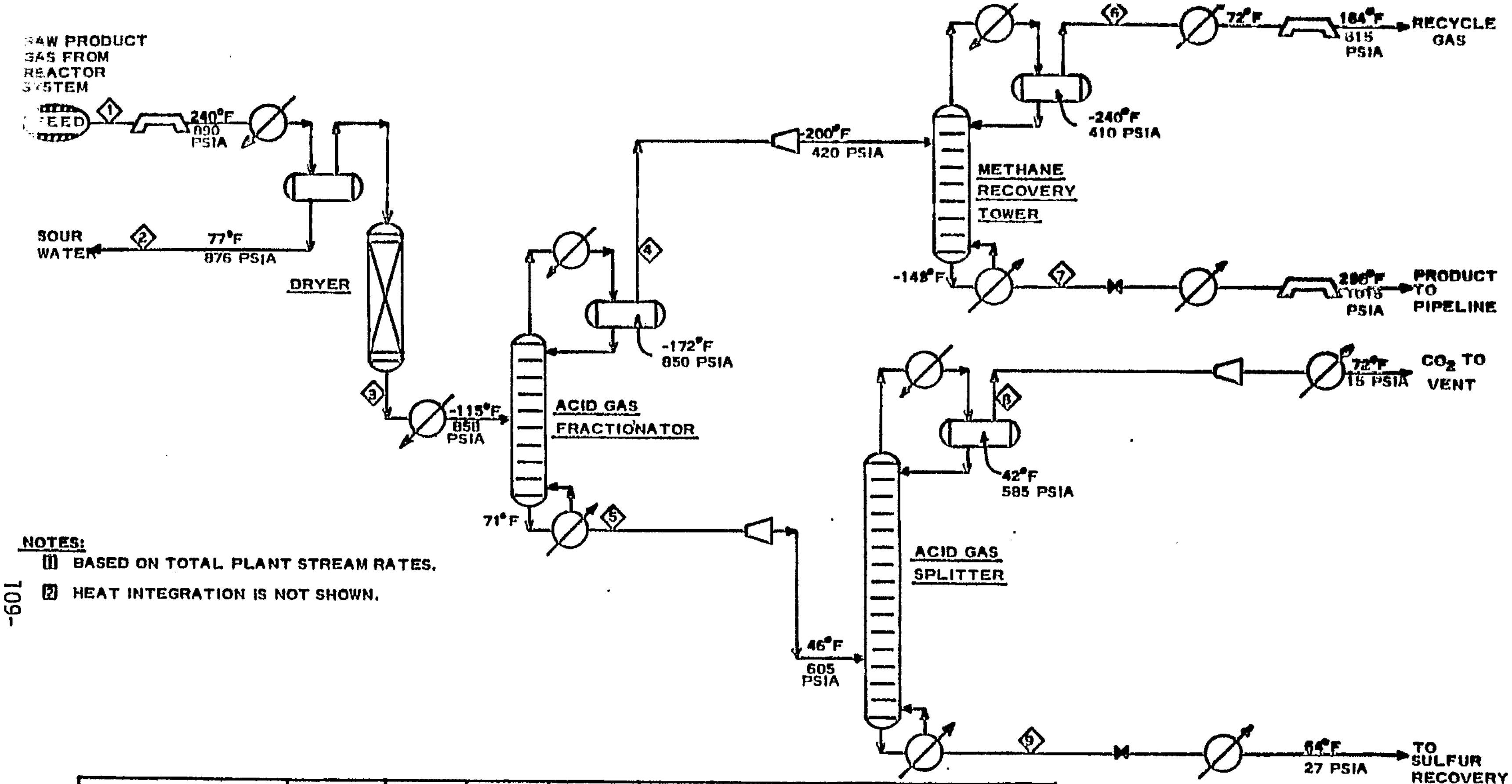

NOTES:
[1] BASED ON TOTAL PLANT STREAM RATES.
[2] HEAT INTEGRATION IS NOT SHOWN.

STREAM NUMBER	①	②	③	④	⑤	⑥	⑦	⑧	⑨
PRESSURE (PSIA)	450	876	866	850	865	410	420	585	606
TEMPERATURE (°F)	100	77	77	-172	72	-240	-143	43	53
FLOWRATES, MPH(1)									
CO	10510		10510	10510		10480	30		
CO_2	21633		21633	13	21620		13	18106	3514
H_2	37671		37671	37671		37671			
H_2O	233	175							
CH_4	35657		35657	35635	22	5750	29885	22	
C_2H_6	5		5		5			4	1
H_2S	878		878		878				878
COS	14		14		14				14
N_2	3585		3585	3585		3585			
TOTAL	110,186	175	109,953	87414	22539	57486	29920	18132	4407

Figure 5.1-6
SIMPLIFIED FLOW PLAN (2)
CRYOGENIC ACID GAS REMOVAL
AND METHANE RECOVERY

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in the AGS bottoms would require additional stages and/or reboiler duty and would raise the bottoms temperature. This would significantly increase power requirements in the propylene heat pump loop. Cost savings in the Claus plant would be unlikely to offset these debits.

In the Methane Recovery Tower (MRT), a CO/H_2 overhead stream is separated from the CH_4 bottoms product. The tower specifications are consistent with the Study Design (0.1% CO in product methane, 10% CH_4 in the recycle gas). The MRT feed from the AGF overhead is cooled and flashed to 420 psia (the same as in the Study Design). Tower feed temperatures from -198°F to -240°F were evaluated, and -200°F was chosen as the basis. At this condition, expanding the bottoms product provides the entire MRT condenser and feed cooling duty. This stream is also used to help cool the AGF feed.

An effort was made during the study to optimize the heat integration/refrigeration scheme for the process. The final scheme, as shown in Figure 5.1-7, consists of the following:

- An external three-level cascade refrigeration system utilizing methane, ethylene and propylene refrigerants provides both the Acid Gas Fractionator condenser duty (-172°F process temperature) and a portion of the feed cooling duty.

- A single heat pump loop of propylene refrigerant accomplishes both the condenser and reboiler duty for the Acid Gas Splitter.

- The overhead stream from the Methane Recovery Tower (MRT) is used to subcool the methane bottoms product. This bottoms stream is then adiabatically expanded to provide the refrigeration requirements for the condenser (-240°F process temperature) and feed cooling of the MRT.

- The remainder of the Acid Gas Fractionator feed cooling is accomplished by feed/effluent heat exchange with the methane product, recycle gas, and CO_2 vent gas.

The utility requirements developed for this system are presented below:

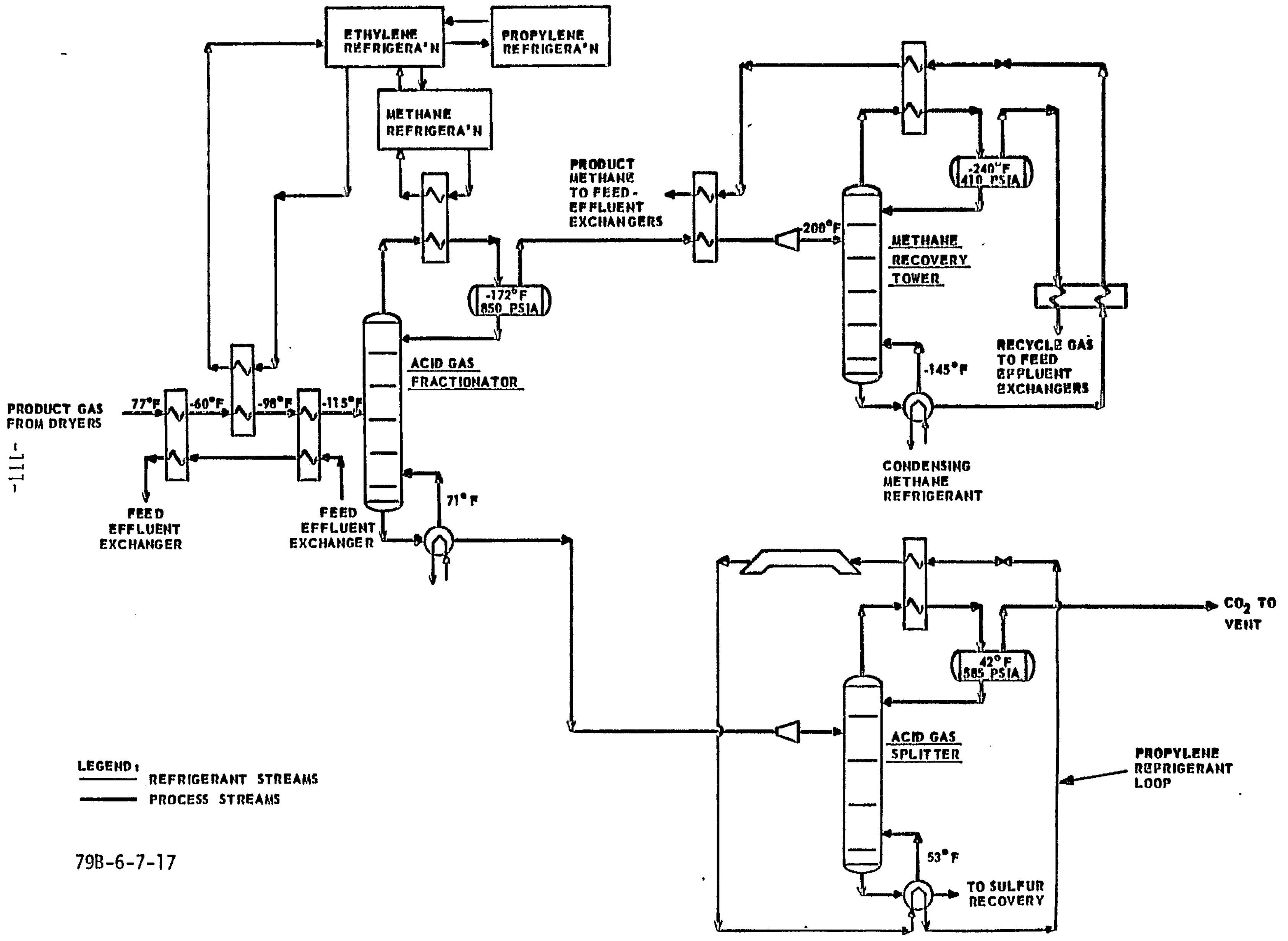
Utility Requirements

	CCG Study Design	Cryogenic Acid Gas Case
Brake Horsepower	194,000	267,000(1)
AGR Steam (65 psig), klb/hr	415	-
Total Cooling Water, kgpm	79	59

Note: (1) Includes 21,000 HP credit for expanders.

FIGURE 5.1-7

CRYOGENIC ACID GAS REMOVAL REFRIGERATION AND HEAT INTEGRATION FLOW SCHEME



The total brake horsepower requirement for the new system is 38% greater than for the CCG Study Design. Steam requirements for the Acid Gas Removal Section have been completely eliminated in the new scheme, and total plant cooling water requirements have been reduced 25%.

A breakdown of the investment for the Cryogenic Acid Gas Removal Case compared to the Study Design is presented in Table 5.1-8. The investment for the cryogenic acid gas removal section is 59 M$ lower than the Study Design investment for heavy glycol acid gas removal. Investment savings in sulfur recovery, methane recovery and other onsites are balanced by increased investment for refrigeration. The offsite investment in water and steam systems is reduced by 10 M$ because of reduced steam requirements. This is somewhat offset by a 5 M$ investment increase for electric power distribution because of the larger power requirement. Overall, the investment for the cryogenic acid gas removal case is reduced by 100 M$ compared to the Study Design.

A breakdown of the gas cost for the Cryogenic Acid Gas Removal Case is presented in Table 5.1-9. A summary of the gas cost for the new case as compared to the Study Design is shown below:

Gas Cost Summary

	CCG Study Design	Cryo. Acid Gas
Coal Feed to Gasifier	14,490 ST/SD	14,490 ST/SD
Net SNG Product	257 GBtu/SD	261 GBtu/SD
Plant Investment	1,530 M$	1,430 M$
SNG Cost Components	---------Gas Cost,	$/MBtu---------
Illinois No. 6 Coal	1.41	1.37
Major Chemicals	0.41	0.40
Utilities	0.35	0.51
Other Operating Costs	1.08	1.01
By-Product Revenues	(0.18)	(0.17)
Capital Charges (15% DCF Return)	3.11	2.86
Total SNG Gas Cost (RISP)	6.18	5.98
Savings		3.2%

The total gas cost with cryogenic acid gas removal is 3.2% less than the Study Design gas cost. The debit caused by increased power requirements is more than offset by savings from increased net SNG product and lower capital charges associated with the net reduced investment. However, recent studies by Air Products and Chemicals, Inc., under contract to DOE, have concluded that the selective (two-stage) heavy glycol solvent absorption process specified for the CCG Study Design can be optimized for use with the CCG process. Their results indicate that the gas cost for the optimized system can be reduced by about 1-2% versus the configuration used in the CCG

TABLE 5.1-8

CATALYTIC COAL GASIFICATION CRYOGENIC ACID GAS REMOVAL STUDY

INVESTMENTS

Basis: • Same Coal Feed to Gasifier (14,490 ST/SD)
as CCG Study Design

Plant Section	Study Design Base Case (M$)	Cryo. Acid Gas Case (M$)	Change (M$)
Onsites			
Acid Gas Removal	140	81	(59)
Sulfur Recovery	22	19	(3)
Methane Recovery	44	41	(3)
Refrigeration	31	38	7
Other Onsites	442	439	(3)
Onsites Subtotal	679	618	(61)
Offsites			
Water Systems	38	35	(3)
Steam Systems	171	164	(7)
Electric Power Distribution	23	28	5
Other Offsites	179	179	-
Offsites Subtotal	411	406	(5)
Total Direct and Indirect Costs	1,090	1,024	(66)
Process Development Allowance	169	153	(16)
Project Contingency	271	253	(18)
TOTAL ERECTED COST	1,530	1,430	(100)

TABLE 5.1 - 9

GAS COST SUMMARY
CRYOGENIC ACID GAS REMOVAL INCENTIVE STUDY

Basis:
- **January, 1978 Instant Plant, Eastern Illinois Location**
- **261 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**
- **Total Erected Cost of 1430 M$**

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	1.111
- To Coal Dryer Fuel	705 ST/SD	20$/ST	0.054
- To Offsites Boiler Fuel	2,660 ST/SD	20$/ST	0.205
Subtotal	17,855 ST/SD		1.370
• Major Chemicals			
- KOH Solution (30 wt%)	189 ST/SD (Contained)	300$/ST	0.217
- Lime (97% CaO)			
+ To Catalyst Recovery	1,005 ST/SD	39$/ST	0.151
+ To Flue Gas Desulfurization	249 ST/SD	39$/ST	0.037
Subtotal			0.405
• Other Operating Costs			
- Purchased Electric Power	219 MW	2.5 ¢/kWh	0.504
- Raw Water	5,400 gpm	15¢/kGal	0.004
- Other Catalysts and Chemicals	Many Items	5.4 M$/yr	0.065
- Wages and Benefits	935 Men	21 k$/man/yr	0.228
- Salaries and Benefits	250 Men	25 k$/man/yr	0.072
- Labor Overheads and Supplies	20% of Wages, Salaries and Benefits		0.060
- Materials and Overheads	3.3% of Total Erected Cost/Year		0.551
- Waste Solids Disposal	8,391 ST/SD	1$/ST	0.032
Subtotal			1.516
• By-Product Revenues			
- Ammonia (20 wt%)	231 ST/SD (Contained)	160 $/ST	(0.142)
- Sulfur	324 LT/SD (2)	25 $/LT	(0.030)
Subtotal			(0.172)
• Capital Charges			2.858
TOTAL SUBSTITUTE NATURAL GAS COST (RISP) (3)			5.977
CALL			5.98

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.

Study Design. Thus the actual incentive for cryogenic acid gas removal as defined in this study is a gas cost savings of only 1-2%. This incentive is small relative to the likely problems in handling CO_2 freeze-out. Optimization of the cryogenic acid gas removal system could reduce its cost but would make it more difficult to deal with CO_2 freeze-out. Thus, there is little incentive for research on the cryogenic acid gas removal system as defined by this study.

5.1.9 Incentive Study for Removing Methane from Recycle Gas

A brief screening study was carried out to determine whether there is an incentive for reducing the methane content of the gas stream recycled to the catalytic gasifier. In the CCG Study Design the recycle gas contained 10 mole % methane. This was thought to be the lowest methane content in the recycle gas that could be practically achieved with a cascade refrigeration system consisting of propylene, ethylene, and methane loops. Lower methane content would require lower temperatures and the addition of a nitrogen refrigerant loop to the cascade.

The effect of removing methane from the recycle gas was simulated using a material and energy balance program for catalytic coal gasification. The process basis and conditions were identical to the CCG Study Design except for the removal of all the methane from the recycle gas stream. The design changes required in the cryogenic methane recovery system were not evaluated at this time. The key differences between the "no methane in recycle gas" case and the CCG Study Design are listed in Table 5.1-10 and summarized below:

- Total recycle gas rate reduced by 17%.
- Raw gasifier effluent gas rate reduced by 8%.
- Feed to methane recovery tower reduced by 11%.
- Preheat furnace fuel fired down by 6%.
- Overall net methane product increased by 0.2%.
- Offsite steam requirement reduced by 6.8%.
- Feed to acid gas removal reduced by 9%.
- Gasifier volume reduced by 4%.

Although the preheat furnace duty requirement to heat balance the gasifier was lower in the "no methane in recycle gas" case, the furnace coil outlet temperature was calculated to be 32°F higher. This is due to the steam/recycle gas rate being about 10% lower than in the Study Design.

TABLE 5.1-10

SUMMARY OF SCREENING STUDY FOR REMOVAL OF CH_4 IN CCG RECYCLE GAS

Study Design Base Case - 10% CH_4 in Recycle Gas

Incentive Study - 0% CH_4 in Recycle Gas

	Base Case (1)	No CH_4 in Recycle Gas	% Change
Gasifier Temperature, °F	1,275	1,275	-
Coal Feed to Gasifier, ST/SD	14,490	14,490	-
Plant Rates and Operating Conditions			
Net CH_4 Product, lb moles/hr	27,973	28,015	+ 0.2
Total Recycle Gas, lb moles/hr	57,200	47,500	-17
Gasifier Steam/Recycle Gas, lb moles/hr	131,000	117,200	-11
Raw Gasifier Product, lb moles/hr	164,800	151,000	- 8
Acid Gas Removal Feed, lb moles/hr	110,400	100,400	- 9
Methane Recovery Feed, lb moles/hr	87,100	77,200	-11
Normal Preheat Furnace COT, °F	1,543	1,575	+32°F
Preheat Furnace Fuel Fired, MBtu/hr	530	500	- 6
Steam Consumption, lb moles/hr(2)	38,900	37,500	- 4
Steam Conversion, %	41	42	+ 2
Overall Net CH_4 Product, GBtu/SD	257.0	257.4	+ 0.2
Steam Generated Offsite, lb moles/hr	59,300	55,300	- 7
Relative Gasifier Volume	100	96	- 4

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

(2) Steam consumption = steam in preheat furnace inlet + water with coal + cooling steam - steam in reactor effluent.

In the methane recovery section of the plant, more refrigeration would be required to reduce the methane content of the recycle gas stream. This would require greater investment and operating cost in that section.

Overall, it was concluded that there are incentives for reducing the methane content of the recycle gas stream. More detailed studies, including the impact of higher methane recovery section refrigeration requirements, will be made at a later time.

5.2 Systems Modeling

Systems modeling work is being carried out as part of the CCG Process Development Program to develop material and energy balance tools which will reduce the engineering effort required to do screening studies and process definition studies. A material balance model for the catalyst recovery system was completed in March, 1979. Work is continuing on the development of a material and energy balance model for the CCG reactor system.

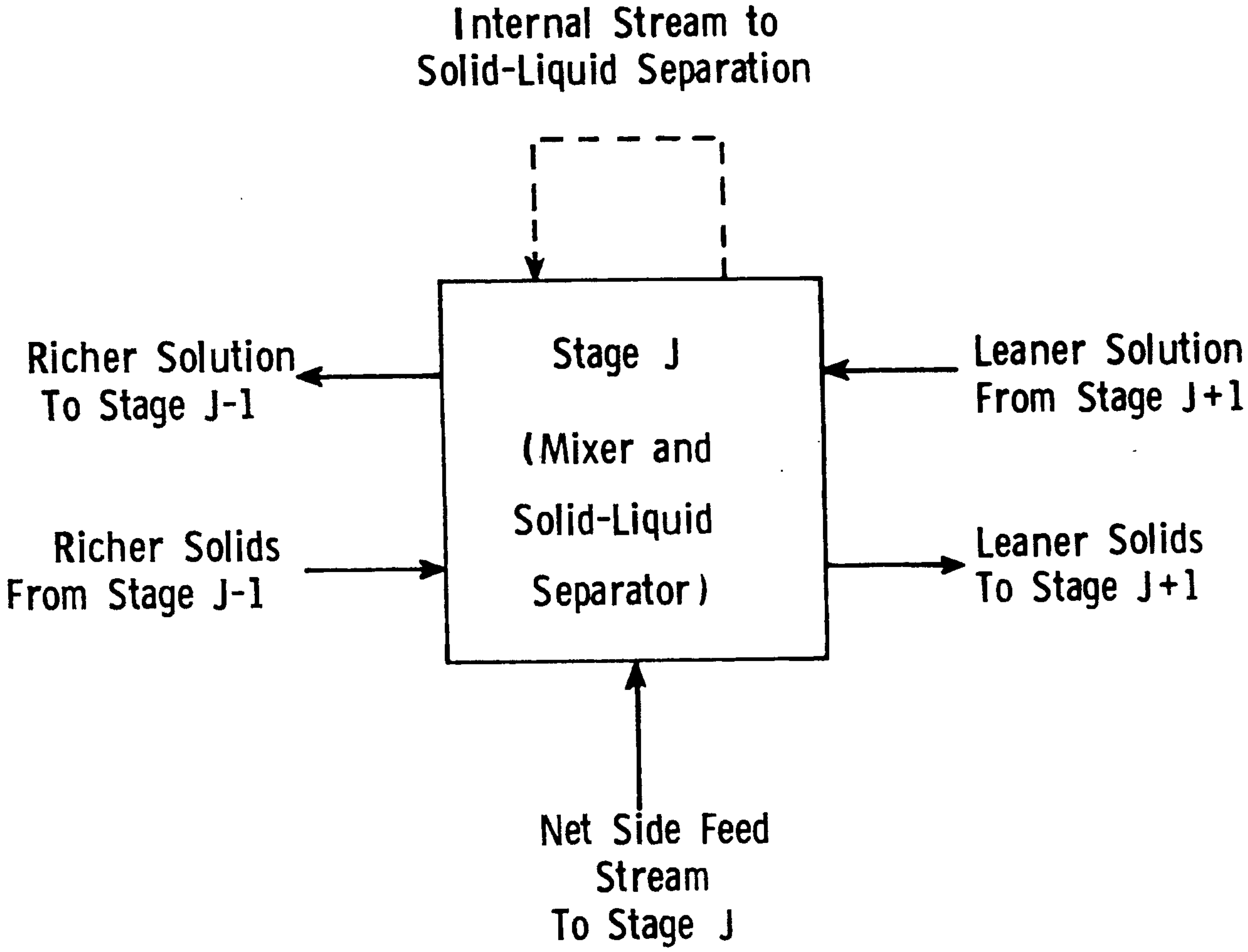
5.2.1 Catalyst Recovery Material Balance Model

Catalyst recovery as incorporated in the CCG Commercial Plant Study Design involves "digestion" of gasifier char and fines with $Ca(OH)_2$ to solubilize most of the catalytic potassium salts, followed by multi-stage countercurrent leaching with water to remove the soluble catalyst from the gasifier and calcium solids. Material balances for this system have required extensive stage-by-stage hand calculations, as well as some simplifying assumptions. The new catalyst recovery material balance model has been developed to perform rigorous stage-by-stage calculations taking into account the solid-liquid separation efficiencies for individual stages. This computer model will be used shortly in catalyst recovery system screening studies to evaluate alternative processing approaches and solid-liquid separation techniques.

Figure 5.2-1 represents one stage in the countercurrent leaching sequence. Each stage involves mixing of solids from a richer (more concentrated) stage with solution from a leaner (less concentrated) stage, followed by solid-liquid separation to produce a richer solution stream and a leaner solids stream. The catalyst recovery model is capable of handling these four streams as well as an internal stream representing the feed to the solid/liquid separation device and a net side feed stream. The latter stream would be used to represent any special feeds or products that may be involved. One example is $Ca(OH)_2$ digestion, where calcium solids are added and water is consumed in chemical reactions. Provision is also made within the model to reflect adsorption of soluble potassium salts on the solids.

Figure 5.2-1

CATALYST RECOVERY MATERIAL BALANCE MODEL: STAGE CONFIGURATION AND STREAMS



The model is capable of calculating any one of the following three parameters, with the remaining two specified by the user:

- Overall catalyst recovery
- Recovered "rich" solution concentration
- Number of washing (leaching) stages.

Varying rich solution concentration is equivalent to varying wash water rate. Other required inputs are the rich solids feed to the first (richest) stage as well as the solid-liquid separation performances and side feed streams for all stages.

The material balance routines in the model were validated by duplicating the catalyst recovery material balance for the CCG Study Design. The material balances for soluble catalyst salts, water, and insoluble solids all closed to within ± 0.01%. Numerous test cases were run to validate various material balance convergence and output options. After minor modifications to improve the convergence methods, all cases converged satisfactorily. Computer costs per run were very low. The model is now available for use in engineering and laboratory studies of the catalyst recovery system.

5.2.2 CCG Reactor System Material and Energy Balance Model

A second systems modeling effort began in December, 1978, to develop updated material and energy balance tools for the CCG reactor system. The catalytic gasification reactors and the associated recycle gas loop and preheat furnaces are key parts of the commercial process flowsheet. Five of the eight process blocks in the CCG Commercial Plant Study Design are involved in the reactor system modeling effort. These include the Reactor, the Product Gas Cooling and Scrubbing, the Acid Gas Removal, the Methane Recovery, and the Refrigeration sections. These sections carry out the gasification step and the cleanup and separation of the raw gasifier product gases.

A "first pass" reactor system material and energy balance model was used in preparing the CCG Commercial Plant Study Design. Although this model is accurate and proved satisfactory for use in the Study Design effort, the gasifier material balance routine is not specifically intended for coal gasification and the energy balance calculations are complex and cumbersome. In applying this first-pass model, extensive hand calculations are necessary to set up the material balance and to develop solids enthalpy terms for the overall energy balance. Improved reactor system material and energy balance techniques and computational tools are desirable to allow the laboratory guidance and process definition studies planned under the current program to be carried out efficiently and consistently.

The updated CCG reactor system model will be incorporated within the framework provided by Exxon's proprietary process network simulation program, known as "COPE". Three main blocks and a fourth optional block are being programmed to model the gasifier itself:

- The first block models the CCG gasifier solids material and energy balance. This block feeds coal and catalyst and produces "reacting coal" (the portion of the solids feed which is gasified) and spent solids (residual char, ash, and catalyst). Solids stream enthalpies, including the effects of catalyst-coal reactions, are also calculated.

- The second block feeds the "reacting coal" and the various gaseous feed streams and produces an effluent gas at specified shift and methanation equilibria.

- The third block carries out the overall gasifier energy balance. The model has the flexibility to energy-balance other related reactor systems, such as steam reformers.

- The fourth block incorporates the gasifier kinetics/contacting model as updated during the CCG Predevelopment Program. This optional feature allows calculation of the gasifier bed size along with the material and energy balance.

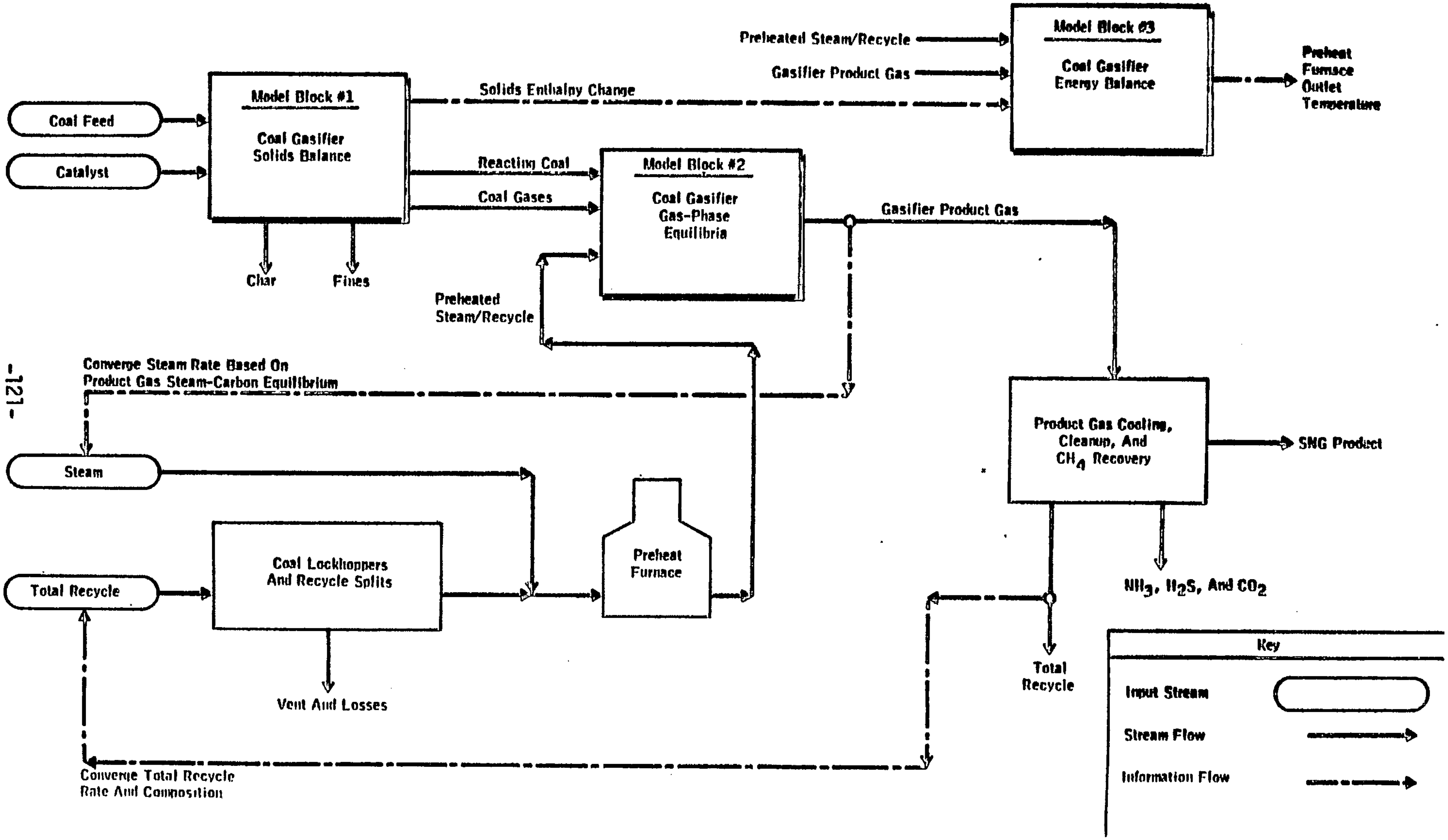
The gasifier model was broken down into these four independent functional blocks to facilitate modeling of flowsheets or gasifier configurations different from the base case in future lab guidance and process improvement studies.

In order to simulate the material and energy balance for a CCG reactor system, the model blocks are incorporated in a COPE process network. The network used to model the reactor system for the CCG Commercial Plant Study Design is illustrated in simplified form in Figure 5.2-2. The network joins together the three required blocks, models the material balances for the product gas cleanup and separations steps downstream of the gasifier, and converges the overall material balance and gasifier/preheat furnace energy balance.

The calculations are relatively complex. Two nested loops are used to converge upon the overall material balance. The inner loop determines the steam rate to the gasifier based on product gas steam-carbon equilibrium (or gasifier steam conversion). Within this inner loop, the gasifier material balance is calculated by model blocks one and two. The principal feeds are coal, catalyst and preheated steam/recycle, and the principal products are char, fines and gasifier product gas. The outer loop converges the recycle (synthesis gas) stream rate and composition, using a series of COPE operations. After the material balance is converged, the gasifier energy balance is closed by model block three. The gas-phase feed and product streams are fed to model block three directly. The impacts of solids on the gasifier energy balance are accounted for by using a solids enthalpy change transferred from model block one. Model block three calculates the steam/recycle preheat furnace outlet temperature required to maintain the desired gasifier operating temperature. An option to reflect shift reaction in the preheated steam/recycle stream has been included in this block. Under this option, the

FIGURE 5.2-2

FLOW DIAGRAM FOR COMPUTER SIMULATION OF CCG COMMERCIAL PLANT STUDY DESIGN



computer routine will converge upon the required preheat temperature assuming a specified percentage (0-100%) of the shift reaction which would occur if the stream were in full equilibrium.

The overall modeling effort was about two-thirds complete at the end of the reporting period. The equilibria and energy balance blocks--blocks two and three--were completed, and were validated using the commercial base case (the Predevelopment Program CCG Study Design) and other selected cases. The gasifier solids balance block has also been completed and validated, with the exception of subroutines to model catalyst-coal reactions. The material and energy balance bases for catalyst-coal reactions are being developed, and programming of these reactions will begin shortly. Other work still remaining includes the programming of the fourth block containing the gasifier model, and the final validation and documentation of the overall model.

Initial validation runs for the overall model have shown considerable savings in computer charges. For example, a run using the new tools to model a commercial gasifier with an integral steam reformer for heat input cost 50% less than the same case modeled using the old methods. In addition, the energy balance model block saves considerable engineering effort by eliminating development of a complex network of computer operations to perform heat balance calculations for each different CCG case.

5.3 Engineering Technology Studies

As part of the CCG Process Development Program, a coordinated set of engineering technology programs is being conducted to develop fundamental process and equipment technology to support the overall laboratory and engineering process development effort. As of June, 1979, work was underway on five of these programs, as described below. Additional programs will be initiated later in 1979.

5.3.1 Evaluation of Construction Materials for Catalytic Gasification

The overall objective of this engineering technology program is to assembly a data base on materials performance for those plant sections which have materials considerations unique to catalytic gasification. A five-part in-situ materials testing/ corrosion monitoring program has been devised for the PDU to identify problem areas and to assemble a data base for selecting materials for CCG process equipment. The program consists of corrosion racks, corrosion probes, nondestructive testing inspection, component examination, and stream sampling. In a separate effort, materials screening tests in alkali-containing gasifier environments have been instituted cooperatively with the Bureau of Mines. These separately-funded bench-scale tests are to be conducted at the Bureau of Mines Tuscaloosa Metallurgy Research Center.

Construction materials for the CCG Commercial Plant Study Design were specified conservatively, based heavily on limited materials data from earlier work on thermal gasification processes. Accordingly, materials test and development work are required for conditions specific to the CCG process. These include equipment items in the gasification, raw gas heat exchange, wet scrubbing, sour water, char handling, and catalyst recovery systems. Potential materials problems identified in these areas are high temperature sulfidation, chloride and caustic stress corrosion cracking, sour water corrosion, and erosion in solids/gas and liquid/slurry services.

Materials Evaluation Program for the PDU

The major objective of the PDU materials evaluation program is to assemble a data base for designing full-scale commercial equipment, with emphasis on hostile process environments. Specific objectives are listed below:

(1) Determine corrosion/erosion behavior of selected metals in the PDU via corrosion racks, corrosion probes, and non-destructive testing (NDT) inspection. Also evaluate chemical and erosion resistance of refractory specimens in gasifier.

(2) Evaluate chloride and/or caustic induced stress corrosion cracking by means of U-bend specimens in char digester.

(3) Relate process conditions to corrosion phenomena by chemical analyses of stream samples.

(4) Determine corrosion/failure mechanisms from analysis of failed equipment components. In addition, perform systematic metallurgical examination of critical working components to assess in-service deterioration.

During the reporting period, efforts have focused on defining and initiating a program to meet these objectives. An extensive program for materials evaluation in the PDU has been developed. This program consists of five interrelated elements:

- Corrosion racks
- Corrosion probes
- NDT inspection
- Component examination
- Stream sampling

These five program elements are discussed in more detail in the following paragraphs.

Corrosion racks are devices on which small metal specimens (coupons) are assembled and secured for in-situ exposure inside operating equipment. Their purpose is to yield time-averaged corrosion rates based on weight loss measurements. Also, coupons are useful for predicting severity of pitting, and identifying corrosion mechanism. Table 5.3-1 itemizes the location and test materials for the eight corrosion racks provided for the PDU. Note that one of the three racks installed in the gasifier is fitted with specimens consisting of castable refractory. The racks were designed, fabricated and assembled by the ER&E Corrosion Laboratory at Florham Park, New Jersey, which is responsible for pre- and post-exposure evaluations of specimens. All of the racks are mounted on blind flanges (nozzles) or pipe plugs (couplings). They are at site and will be installed after the PDU shakedown period. A second set of corrosion racks will be fabricated during the second half of 1979.

Electric resistance corrosion probes, the type to be employed at the PDU, measure corrosion rate as a function of increasing electrical resistance of a corroding wire element. Through their quick response characteristics, they can flag large fluctuations in corrosion rate which would remain undetected from time-averaged weight loss measurements obtained from coupons. The two probes to be installed in the PDU are described in Table 5.3-1. They are of the non-retractable type, which is considered appropriate for pilot plant applications where fairly frequent shutdowns provide ample opportunity for probe removal. The probes have been purchased and will be installed after the unit is lined out.

Nondestructive testing (NDT), also called nondestructive examination (NDE), is a useful inspection technique for measuring wall thickness of equipment. Ultrasonic thickness testing (UT), the technique being employed at the PDU, may be performed during operation, within the temperature limitations of the transducer. The NDT program set up for the PDU is outlined in Table 5.3-2. All baseline UT measurements have been completed except for the gasifier shell and for the char digester. The latter has not yet been fabricated.

The fourth element of the PDU materials evaluation program is component examination. Failure analysis of equipment components is an important adjunct to coupon, probe, and NDT generated data for assessing materials performance in catalytic gasification applications. In addition, it is highly instructive to examine destructively critical equipment components which are still in working order after extended service exposure. Accordingly, a two-part program has been set up for the PDU, which provides for selected components to be examined in the ER&E Metallurgical Laboratory at Florham Park. The first part involves routine failure analysis of components to determine the cause and mode of failure. In the second part, similar types of examinations will be performed on intact working components from the following potential problem areas:

- Lock hopper valves
- Char slurry drum letdown valves

TABLE 5.3-1

CATALYTIC COAL GASIFICATION PDU CORROSION RACKS AND PROBES

Test Site	Equipment Location	Location	Type of Device	Specimen Type	Test Materials[1]
1	Gasifier	Dense phase	Rack	Refractory cylinders	Kaiser Lo-Erode[2]
2	Gasifier	Dense phase	Rack	Metal cylinders	HK-40, 304 SS, 309 SS
3	Gasifier	Dilute phase	Rack	Metal discs	HK-40, 310 SS, 304 SS, 309 SS, 304 SS Alonized
4	Sour water accumulator	Liquid	Rack	Metal cylinders	CS, 304 SS, 316 SS, Carpenter 20Cb3, Ti, Monel
5	Sour water accumulator	Liquid	Probe[3]	Wire element	CS
6	Sour water stripper	Packing	Rack	Metal cylinders	304 SS, 316 SS, CS
7	Sour water stripper	Packing	Rack	Metal cylinders	Carpenter 20Cb3, Monel, Ti
8	Char slurry drum	Liquid	Rack	Metal cylinders	CS, 316 SS, Inconel 625
9	Char digester	Liquid	Rack	Metal U-bends	CS, 316 SS, Monel, Inconel 600, Allegheny Ludlum 29-4
10	Char digester	Liquid	Probe[3]	Wire element	CS

Notes: (1) Abbreviations:
CS - carbon steel
304 SS - Type 304 stainless steel (18 Cr-8 Ni)
309 SS - Type 309 stainless steel (25 Cr-12 Ni)
310 SS - Type 310 stainless steel (25 Cr-20 Ni)
316 SS - Type 316 stainless steel (18 Cr-8 Ni-2 Mo)
HK-40 - Cast 25 Cr-20 Ni-0.4 C alloy

(2) Kaiser Lo-Erode specimens, with and without 304 SS fiber reinforcement

(3) Non-retractable electric resistance probe

Table 5.3-2

Catalytic Coal Gasification PDU NDT Inspection Program

Equipment Item	Inspection Points	Frequency
Gasifier	Opposite cyclone inlet, plus 4-6 selected spots	3 mo interval
Gasifier O/H line to cyclone	Every 3 feet and at elbows	3 mo interval
Cyclone	4-6 selected spots, including inlet area	Each turnaround
Cyclone dipleg	Every 2 feet of last 6 feet at gasifier inlet	Each turnaround
Cyclone line to filter	Every 20 feet	Each turnaround
Scrubber	Bottom 1 foot	3 mo interval
Gasifier line to char pot	Every 4 feet	Each turnaround
Char pot	Bottom head and lower shell, plus 4-6 selected spots	3 mo interval
Char digester	Body head and shell	Each turnaround

- Gasifier overhead line
- Recycle gas preheater coil

Initial component examinations are expected to be carried out during the second half of 1979.

Interpretation of corrosion data and inspection results necessitates information on the aggressive stream constituents present in the environment. Accordingly, stream sampling has also been incorporated into the materials evaluation program. The requested analyses are tabulated in Table 5.3-3.

CGU Failure Analyses

Two failure analyses have already been performed on cracked 316SS and 310SS piping removed from ER&E's small Continuous Gasification Unit (CGU). Lessons learned from these analyses are pertinent to CCG equipment design and operation, and were factored into the PDU materials testing program. For this reason, these results are reported here.

The failed 316SS tubing section was part of the CGU char withdrawal system, used for transferring char from the reactor to a char pot. Normal operating temperature is about 800°F; however, overheating in excess of 1000°F had been reported. The sectioned tubing revealed four cracks in the form of mixed mode stress corrosion cracking (i.e., a combination of intergranular and transgranular crack paths). Chlorides were detected in trace amounts in one crack, whereas sizeable quantities of potassium were found in all four cracks. Based both on the presence of potassium and the crack morphology, the failure is attributed to hydroxyl ion induced stress corrosion cracking. More familiarly known as caustic embrittlement, it can produce either pure intergranular or mixed mode cracking.

Chloride stress corrosion cracking, originally suspected as the cause of failure, was held unlikely because it characteristically propagates in a highly branched transgranular fashion. Also ruled out was polythionic acid stress corrosion cracking which cracks stainless steels in a purely intergranular mode. It was recommended that the tubing be replaced in Incoloy 825. This material has improved resistance to all forms of stress corrosion cracking, and moreover possesses good high temperature strength and sulfidation resistance.

The failed 310SS (25 Cr-20 Ni) tubing section was located between the CGU reactant mix point and a blowdown pot used intermittently to clear plugs in the feed line. The normal process environment is a mixture of catalyzed coal, synthesis gas and steam at 500 psig and 1300°F. Two ball valves suspended directly from the tubing may have imposed considerable bending stresses. The failure was in the form of transgranular cracking suggestive of chloride stress corrosion, but no evidence of chloride was detected. Significantly, as with the above described char piping failure,

TABLE 5.3-3

CATALYTIC COAL GASIFICATION PDU STREAM SAMPLING AND ANALYSES

Location/Service	Type of Sample	Required Analyses	Sampling Frequency
Gasifier overhead	Gas(1)	Chemical composition	Monthly
Sour water accumulator	Liquid	pH, Cl^-, CN^-, NH_3, H_2S, phenol	Monthly
Filter pot	Solid	Chemical analysis	Quarterly
DEA regenerator overhead	Gas	CO_2, H_2S, NH_3	Monthly
Char pot	Slurry	Liquid - pH, Cl^-, CN^-, NH_3, H_2S Solid - chemical analysis	Monthly
Char digester	Slurry	Chemical analysis	Quarterly
Char for disposal	Solid(2)	Chemical analysis	Quarterly
Recycle gas	Gas	Chemical composition	Monthly

Notes: (1) Gas composition calculated from liquid samples taken at scrubber and sour water accumulator.

(2) Sample taken at catalyst recovery area.

appreciable amounts of potassium were found inside the crack. However, unlike the char piping crack, there was no intergranular propagation. In view of these conflicting pieces of evidence, the cause of failure remains somewhat speculative. All in all, a stronger case can be made for potassium hydroxide as the more likely crack-inducing substance. This conclusion is based on the observation that the cracks were not as extensively branched as classic transgranular chloride stress corrosion cracks. Incoloy 825 was recommended as a replacement material. As with the char piping failure, the basis for this recommendation is the better resistance of Incoloy 825 to all forms of stress corrosion cracking as compared to 300 series stainless steels.

Materials Screening Tests at Tuscaloosa Metallurgy Research Center

As a result of a joint DOE/BM/ER&E meeting in March, 1979, a materials test program geared to the CCG process will be conducted at the Bureau of Mines Tuscaloosa Metallurgy Research Center in University, Alabama. Funding for this program will be through modification of the active Interagency Agreement EX-76-A-01-2219 between DOE and the Bureau of Mines. These tests are to be conducted in test apparatus already built and used for similar experiments studying materials for thermal gasification processes.

The objective of the test program is to screen candidate metals and refractories in simulated CCG environments. Specifically, the intent is to evaluate the effect of potassium hydroxide (gasification catalyst) in accelerating attack on construction materials, and to elucidate the nature of such attack. Close attention will be given to complex liquid phases composed of alkalis and metal sulfides. Such aggressive slags have not been encountered in CCG laboratory units, but are nevertheless possible from thermodynamic considerations. The detrimental effect of alkali contamination on refractories was demonstrated at Tuscaloosa in a series of 1978 test runs simulating thermal gasification environments at 980°C (1800°F).

The test conditions and parameters proposed in the work statement are summarized in Table 5.3-4. Standard post-exposure evaluation techniques (weight and dimension changes) will be supplemented by selective chemical analyses, X-ray diffraction and electron microscopy, all to be performed by Tuscaloosa. The projected starting date is July, 1979.

5.3.2 Vapor-Liquid Equilibria in Sour Water/Catalyst Systems

This program's objective is to develop a vapor-liquid equilibrium (VLE) model applicable to the design of the sour water systems in the CCG Process. The systems for which such a model would be used include the wet scrubbers and condensate drums for the gasifier product gas, as well as the sour water stripping facilities.

TABLE 5.3-4

CONDITIONS/PARAMETERS FOR MATERIALS SCREENING TESTS (BUREAU OF MINES, TUSCALOOSA METALLURGY RESEARCH CENTER)

Temperature Pressure Flow rate Number of runs Run length	1350° F (730°C) 500 psig 2 SCFH 2 100 hours
Gas Composition, mole%	H_2 21.5 H_2O 31.9 CO 6.0 CO_2 14.1 CH_4 21.8 N_2 2.1 NH_3 1.4 H_2S 1.2
Alkali contamination of gas atmosphere	Run 1 - Crucibles of molten KOH placed in gasifier Run 2 - Same as Run 1 plus KOH solution pumped to gasifier in amount of 50 ppm KOH (mole basis) per mole of gas
Alkali contamination of test specimens	I - None II - Soaked in KOH solution III - Dipped in KOH melt IV - Contacted with KOH impregnated coal (Illinois #6)
Metal specimens	304 SS 310 SS 446 SS (or E-Brite) Incoloy 800 Incoloy 800 Alonized
Refractory specimens (dense)	50% alumina castable 95% alumina castable 50% alumina brick

A detailed review of the anticipated sour water streams was conducted to identify the compositions, temperatures, and pressures of interest. Subsequently, a literature search was conducted to identify the available experimental data on the volatility of ammonia, carbon dioxide, and hydrogen sulfide in aqueous solutions, including solutions containing catalytic potassium compounds. Preliminary screening of the quaternary data (ammonia-carbon dioxide-hydrogen sulfide-water) has shown that they are of poor quality above 140°F. Accurate high-temperature quaternary data must therefore be obtained. Additional data on the volatility of ammonia, carbon dioxide, and hydrogen sulfide in aqueous solutions containing potassium compounds are also needed.

An experimental program to obtain these data has been formulated. The program (shown below) consists of twelve runs on aqueous mixtures containing ammonia, carbon dioxide, hydrogen sulfide, and potassium hydroxide.

Experimental Vapor-Liquid Equilibrium Measurements

	Liquid-Phase Mole Fractions					
Run Number	NH3	H2S	CO2	KOH	Water	Temp., °C
1	0.23	0.04	-	-	0.73	120
2	0.056	0.006	-	-	0.938	140
3	0.036	0.004	0.032	-	0.928	50
4	0.027	0.004	0.004	-	0.965	130
5	0.076	0.013	0.003	-	0.908	130
6	0.046	0.010	0.004	-	0.94	170
7 and 8	-	0.015	0.015	0.03	0.94	130 and 190
9 and 10	0.01	-	0.03	0.03	0.93	130 and 190
11 and 12	0.01	0.03	-	0.03	0.93	130 and 190

Note: All chemicals should be at least 99% pure.

An acceptable cost quotation was received from a vendor for these measurements. A subcontract to perform this work was prepared and the consent of the DOE contracting officer was obtained. The subcontract should be executed shortly by the vendor and Exxon Research and Engineering Company. Work in the near future will involve monitoring this experimental program.

5.3.3 Physical and Thermodynamic Properties of Catalyst Recovery Solutions

The objective of this program is to collect the physical and thermodynamic properties needed to design the processing equipment in the catalyst recovery system. A review of this system has identified the important properties as: viscosity, density, enthalpy, and boiling point for aqueous solutions containing up to about 30 weight percent dissolved potassium compounds. Temperatures of interest range from 60 to 300°F. Potassium hydroxide and potassium carbonate are the potassium compounds of primary interest.

A literature search for properties of aqueous solutions containing potassium hydroxide or potassium carbonate has been completed. Pertinent articles are still being collected and evaluated. Preliminary results indicate that the data base for potassium hydroxide-water mixtures is adequate for all properties of interest. For potassium carbonate-water mixtures, experimental data may not extend much above 200°F. Methods have to be developed to extend the available data to the higher temperatures of interest and to solutions containing several potassium compounds.

A book by H. S. Harned and B. B. Owen ("The Physical Chemistry of Electrolyte Solutions," ACS Monograph Series #137, Third Edition, Reinhold Publishing Corporation, New York, 1958) has been found to provide useful methods for predicting properties of aqueous solutions containing several dissolved electrolytes. Their method for predicting densities of multi-component solutions gave errors of less than 1% when tested against data on the potassium hydroxide-potassium carbonate-water system. Future work will involve testing Harned and Owen's methods for predicting other properties of multi-component solutions.

5.3.4 Environmental Control: Water and Solids Effluents

The objective of this program is to generate the data needed for a quantitative assessment of the environmental impact of the CCG Process. The main focus of this program will be to characterize wastewaters, spent solids, and solids slurries produced in the CCG PDU. Once the effluent characteristics are known, potential treatment alternatives will be identified.

This engineering technology program began in January, 1979. The potential solid and liquid waste streams were identified using process flow charts. As a followup, a trip was made to become familiar with the PDU and to insure that all sampling port locations are accessible. It appears that there will be a need for four liquid sampling locations and for two or three solids sampling locations. A list of analyses to be run on the liquid and solid wastes and on the solids leachates has been set up along with a short guide to sampling methods and preservation techniques for gasification wastewaters. Each of the samples will be tested extensively to determine what contaminants will be present and, of those, which might present effluent quality problems in a commercial plant.

Two samples of CCG solids slurries, containing digested and undigested chars from bench-scale catalyst recovery experiments, were obtained for study. The samples had previously been washed with hot water. The samples were leached by the EPA method, and the leachate was submitted for detailed analyses. The following contaminants will be determined: alkalinity, ammonia nitrogen, Kieldahl nitrogen, nitrate nitrogen, Cl^-, F^-, CN^-, free CN^-, SCN^-, $S^=$, $SO_4^=$, $SO_3^=$, and phenol. Preliminary testing indicates that leachate from the digested sample contained 7-8 times the amount of Total Organic Carbon (TOC) and Chemical Oxygen Demand (COD) found in the undigested char leachate.

The full testing program will begin when the PDU is through its initial shakedown phase.

5.3.5 Environmental Control: Atmospheric Emissions

This second environmental control program is directed toward identification of potential atmospheric emissions sources and, where possible, the quantification of these emissions through testing in the PDU. An assessment will then be made of the air quality impact of a commercial CCG plant, and control alternatives will be identified for potential problem sources.

An inventory of atmospheric emissions sources in a commercial-scale CCG plant has been initiated. The major potential sources are expected to be the coal handling facilities, waste solids handling, and the CO_2 vent stream from acid gas removal. Emission streams from the PDU have been examined to identify those which might be representative of a commercial plant. Three streams have been selected for field sampling during the PDU operation; these include the coal dryer vent, the lock hopper surge bin vent, and the catalyst recovery waste disposal stream. Emission estimates for other potential sources in the commercial plant will be based on emission factors from the literature or on the experience of other operating plants with similar facilities.

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