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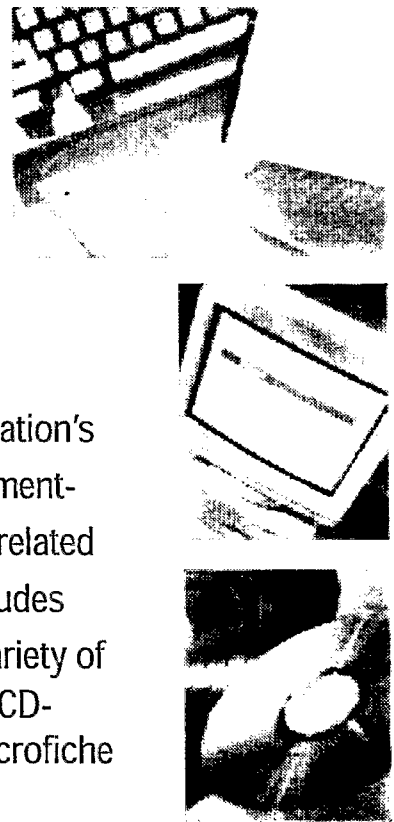
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OPTIMIZATION OF COAL GASIFICATION PROCESSES

Research and Development Report No. 66

Interim Report No. 2

Prepared for

OFFICE OF COAL RESEARCH
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16. Abstracts

This report is designed to assist in the development of processes for making pipeline-quality gas from coal through mathematical optimization techniques. The report is a summary and a supplement to the comprehensive OCR R&D Report No. 66, Volumes I and II, Interim Report No. 1 published on the project, in April 1972. The appendix contains the process descriptions and optimization study results on three alternative processes after the Interim Report was submitted for publication.

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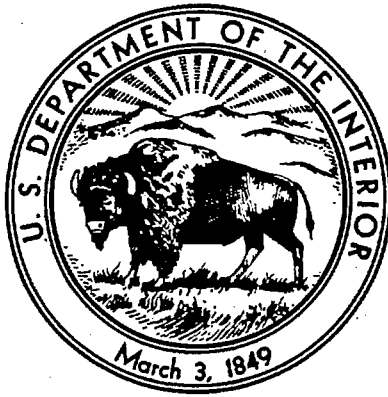OPTIMIZATION OF COAL GASIFICATION PROCESSES

by

Department of Chemical Engineering
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Prepared for
Office of Coal Research
U. S. Department of the Interior
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As the Nation's principal conservation agency, the Department of the Interior has basic responsibilities for mineral, water, fish, wildlife, land, park, and recreational resources. Indian and Territorial affairs are other major concerns of America's "Department of Natural Resources."

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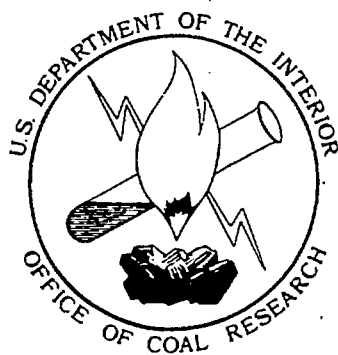
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1.0 INTRODUCTION

Much has been published recently about the impending shortage of clean energy in the United States. Certainly the growth and economic healthiness of a nation rests with its ability to hold and efficiently utilize an adequate supply of potential energy reserves. A shortage in energy supply not only causes immediate inconvenience, but it also dampens the prospects for industrial growth and long-range economic prosperity. The unused reserves of natural gas and oil in the United States have shown signs of eventual depletion and already some large customers have been notified that their natural gas supply might be limited in the future.

Although coal represents roughly 95% of the fossil fuel reserves in the United States, [13], it is the raw material source for less than 25% of the energy now being consumed, [20]. Coal, as a solid, is inefficient to handle, to transport and to use in the final energy consumption stage. Coal is also accompanied by the two publicly acclaimed major sources of environmental pollution - sulfur and ash. Thus, a major research and development effort is needed to provide an economical method or methods to convert the most abundant fossil fuel - coal - into a pollutant-free and more useable form - either as a liquid or as a gas.

Since coal gasification technology is such a broad subject while time and financial resources are limited, the studies on the potential coal gasification methods must be concentrated on those processes which present the most attractive commercial possibilities. The developments of each of these processes have not reached the same level to permit their respective advantages and disadvantages to be easily compared. The recently developed techniques of mathematical optimization are readily adaptable to this type of situation. These techniques involve mathematically simulating the processes under study and then projecting those simulated design and operating characteristics to specific optimum criteria - lowest manufacturing cost, lowest capital equipment cost, best thermal or carbon efficiency, etc. Only by projecting each process to its optimum operating and design conditions, can one realistically compare one process with another.

At West Virginia University this optimization study was conducted under the sponsorship of the Office of Coal Research, to compare the possible alternative coal gasification processes, some of which have been proposed or are now being developed by either the Office of Coal Research contractors or by the U. S. Bureau of Mines. This report is a summary and a supplement to the comprehensive O.C.R. Interim Report recently published on the project [35]. In the Appendix of this report are the process descriptions and optimization study results on three alternative processes studied after the Interim Report was submitted for publication.

2.0 THE OPTIMIZATION PRINCIPLES AND DESIGN ASSUMPTIONS
USED IN THIS STUDY

If time and money were limitless, each proposed process could
be explored in detail and the final evaluations and decisions reserved
until all the research and development work is finished with all
design questions answered. Unfortunately, this ideal situation never
exists for R&D money will always be in short supply and the desired
product is wanted immediately, not in the distant and uncertain future.
To effectively utilize limited time and financial resources, a systematic
method of attacking such complex problems as that of designing an in-
tegrated pipeline-gas manufacturing plant is required. In recent years
a methodology of system analysis through simulation and optimization
based on system models has become a key element in the programing, planning
and budgeting of major governmental and industrial projects. This method
can be directly applied to the study of the proposed gas-from-coal production
processes.

2.1 Review of General Optimization Theory and Procedures

It is not the purpose here to thoroughly define and explain all
aspects of the numerous optimization techniques. The interested reader
should refer to several recently published texts on this broad subject [2], [8]
and to the subject review given in the Interim Report. [35] The general
purpose of optimization is to mathematically simulate the process under
study, with its numerous independent and dependent variables. The processes
are then optimized to find the set of optimum independent variables which
will yield the best or optimum value of a selected objective function,
such as the lowest gas manufacturing cost, the lowest capital investment,
the highest efficiency of the carbon or the energy utilization, etc.

The procedure steps in applying the optimization methods are;

(a) Define the specific objective of the study.
(b) Establish the operating or design criteria limitations.
(c) Determine the constraints and process boundaries.
(d) Develop any potential alternates to the basic process
     which offer a possibility of improving the objective function
     value.
(e) Formulate the models for the process and its alternates.
(f) Simulate the process performance.
(g) Evaluate and rank the alternates according to their effect
     on the overall objective.
(h) Analyze the sensitivity of the various independent variables,
     review the assumptions and develop new alternatives.
(i) Optimize the models and select the "best" of the alternatives.

More comprehensive discussion and a broader explanation of each of the steps listed above are presented in the Interim Report.   [35]

In order to make a fair comparison among the different processes and different operating conditions, it is required to establish a set of well-defined criterion which will be used consistently for the evaluation of all the processes. Depending on the nature of processes or the problems many different kinds of objectives might be selected. These functions are separated into two broad types, economical and technical. The economical functions are related to the process costs or to the profit relationships.

In the general study of the coal gasification processes, it was easily recognized that the total cost of producing the product gas was greatly influenced by the purchase cost of the raw coal. Thus, a decrease in the amount of coal required to produce a specific amount of product gas (aimed at the maximum carbon efficiency) would likely result in the lowest gas production price. Also, since the major loss of carbon is directly related to the heat energy lost in the various reaction systems, the maximizing of the thermal efficiency of the system should lead closely to the minimum gas manufacturing cost as well. The thermal efficiency is defined as the heat of combustion of the product gas (Btu per production unit) divided by the heat of combustion of raw coal entering the overall process system (Btu per production unit). The amount of coal considered is not only the coal fed directly to the gasification system, but also includes the coal used in steam and electricity generation. In this manner the primary objective function, that of computing the lowest cost for the gas can be approximated by optimizing the process models with respect to the easier-to-manipulate secondary objective function, that of maximizing the thermal efficiency.

After selecting and defining the specific objective function, the next step is to select the strategies and techniques to be used in reaching the maximum or minimum point of that function. In this study, a simplification strategy was used to prepare the mathematical relationships and then one of several optimization techniques were used to optimize first the several subsystems and then the overall plant. Simplification involves the initial recognition and discarding of the independent variables which are found to have an insignificant effect on the outcome of the optimization results. After simplification, only those independent variables which are judged as having the greatest effect on the process operation, are then used in the mathematical optimization manipulation.

The "Complex Method of Optimization" was developed by Box [3] and is a constrained version of the "Simplex Method" developed by Nelder and Mead. [23] It was successfully applied to the optimization of a gas-liquid absorber-stripper system by Umeda [29] and was later modified by Umeda and Ichikawa [30] to be more effective in solving optimal design problems. While it does not converge as rapidly as does some of the other direct

search techniques, the "Complex Method" does not require derivatives of the objective function and it can be programmed easily in a computer calculation routine.

The application of the "Complex Method" is discussed by Beveridge and Schechter [2] and in greater detail by Paviani [24]. This method involves a direct search for the optimized node or region in the space regime formed by the independent variables and bounded by the contraint relationships. Each set of feasible variable values, constituting one point or "vertex" in the variable space, is mathematically combined to obtain a single value of the objective function. Following a systematic progression of manipulations of this "simplex" of vertices; comparison of objective function values, rejection of the "worst" vertex point and choosing of a new vertex by "reflection", "expansion", "contraction", and "halving"; the simplex will roll about the variable space directed toward the optimization point about which the simplex will finally contract. The specific steps involved in this optimization technique are detailed by Paviani [24] and by Umeda [29], [30].

Since the "Complex Method" is a numerical search technique, there is no guarantee that the method will locate the true optimization point if the objective function has more than one optimization peak; however, if several sets of calculations starting at varied points in the space of variables converge to the same vertex, then a reasonable assurance of global optimum is obtained.

The individual subsystems were each optimized using the minimum capital requirement cost as the objective function. Both dynamic programming and maximum principles were applied for the optimization of subsystems. The overall plant thermal efficiency was maximized to recognize the optimum values of the significant design and operating variables. These optimum values were used to design the equipment and compute the capital equipment costs.

Finally, based on the Office of Coal Research accounting procedure, the unit cost of the gas product was determined and sensitivity tests were performed to determine the effects of changes in certain independent variables on the final gas price.

2.2 Assumed Ground Rules for Comparing Coal Gasification Alternatives

The problem of optimizing coal gasification processes would be overwhelming unless simplifying assumptions were established before the overall problem is attacked. In this study several potential coal gasification alternatives are first considered, each of them consisting of several process units, such as gasification, hydrogasification, devolatilization, shift conversion, gas purification, methanation, sulfur recovery,

oxygen production, etc. The details of the alternatives considered will be discussed in Section 3.0. The most promising candidates were then selected and the optimization of these processes were conducted. Although there is a common objective function for all the processes, the system variables are not the same for all the processes. In order to make a fair comparison among the alternates, it is necessary to establish a set of uniform ground rules and assumptions before the actual calculations can be started.

(1) Since common system variables do not exist among all the potential coal gasification processes, whenever the economics of the processes are compared, each process should always be operating at its optimum conditions.

(2) The design base for the coal gasification plant will be 250 x 10^9 Btu/day, and the heating value of the product pipeline gas will be within the range of 900 to 920 Btu per standard cubic feet.

(3) Two ranks of coal will be used for this study; bituminous and lignite. The coal analyses are shown in Table 1.

(4) The cost of the bituminous coal was varied from $2 to $8 per short ton and the cost of lignite was varied from $1.50 to $4.50 per short ton. Sensitivity studies later determined the effect of changes in the raw coal price on the final product gas cost.

(5) The Office of Coal Research accounting procedure is used for estimating the product gas manufacturing cost. The financial factors used in the calculation are;

Debt-Equity Structure	–	65%
Gross Return Rate	–	7%
Federal Income Tax	–	50%
Interest on Debt	–	5%

The effects of changing the "Debt-Equity Ratio", the "Debt Interest Rate" and the "Gross Return Rate" were studied in a sensitivity analysis after the major optimization calculations were completed.

(6) The entire gasification plant to be designed will be self sustaining. In other words, the facilities required for power generation, steam generation, oxygen production, water treatment, cooling towers, etc., will be included in the overall design of the complete coal gasification system.

(7) No char is to be sold as a marketable by-product from the gasification plant; however, the char produced in the gasifier might be used for on-site steam and power generation.

(8) No credit is given for marketing the by-product elemental

sulfur produced in the gas purification subsystems, because the sulfur market is predicted to decrease in the near future. However, it is assumed that enough sulfur can be sold to pay for the operating expenses of the sulfur recovery units.

(9)   The efficiency of converting coal to steam, based on the enthalpy of the steam produced divided by the heat of combustion of the coal used, is assumed to be 75%. The efficiency of generating electricity, based on the Btu equivalent of the electrical energy generated divided by the heat of combustion of the coal used, is assumed to be 35%. Sensitivities of these assumptions are tested by varying the boiler efficiency from 75% to 90% and varying the power generation efficiency from 35% to 40%.

The design criteria stipulations and other assumptions used in simulating and optimizing the coal gasification processes are detailed in the comprehensive Interim Report. [35]

TABLE 1

COMPOSITIONS OF THE PREPARED COALS USED IN THIS STUDY

	BITUMINOUS	LIGNITE
ULTIMATE ANALYSIS (Weight Per Cent)		
Carbon	71.20%	64.80%
Hydrogen	5.14%	4.17%
Oxygen	6.03%	21.22%
Nitrogen	1.23%	0.95%
Sulfur	4.19%	0.68%
Ash	12.21%	8.18%
PROXIMATE ANALYSIS (Weight Per Cent)		
Moisture	1.3%	4.3%
Volatile Matter	34.6%	39.3%
Fixed Carbon	52.0%	48.6%
Ash	12.1%	7.8%
HEAT OF COMBUSTION (Btu/Pound)	13,063	10,091

3.0 ALTERNATIVE COAL GASIFICATION FLOW SCHEMES

3.1 Process Subsystems

For convenience in the process simulation calculations, the processes were separated into several individual subsystems. In this study, the coal gasification plant was sub-divided into five general units.

Coal Preparation and Pretreatment

This subsystem involves the receiving and cleaning of the raw coal. The refuse rejected during coal preparation is assumed to be 36% in the case of bituminous coal and 43% in the case of lignite. An additional 7.6% of the coal is separated as undersized fines. These fines might be used along with gasifier char to feed the steam or electricity generating .plant.. The coal is then crushed and pulverized to the desired particle size. The energy required for coal preparation is estimated as being the equivalent of the heat of combustion of 5% of the coal entering the gasification unit.
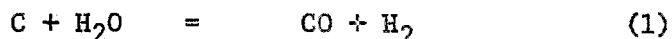
If the coal used as feed material is of a rank or grade which would cake and/or agglomerate in the gasifier, a pretreatment step is necessary. The pretreatment of coal involves the partial volatilization and oxidation of the coal particle surface with steam and oxygen, a reaction which results in a loss of a significant amount of potentially valuable volatile matter in the coal. Lignite which does not agglomerate requires no pretreatment before the gasification step. Certain gasifier reactor designs, such as the entrained reactor and the free fall reactor, also eliminate the need to pretreat bituminous coal.

Coal Gasification

The purpose of gasification is to convert the solid coal into gases that can be converted later into a pipeline-quality gas having a heating value of more than 900 Btu per standard cubic foot.

In simulating the gasifier reaction system, a minimum number of reactions are assumed to occur;

The Steam-Carbon Reaction:

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

The Water-Gas Shift Reaction:

$$CO + H_2O = CO_2 + H_2 \qquad (2)$$

The Hydrogasification Reaction:

$$C + 2H_2 = CH_4 \qquad (3)$$
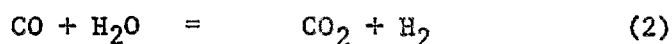
Thermodynamically, Reaction (1) is highly endothermic while Reactions (2) and (3) are exothermic. Kinetically, Reaction (1) is favorable at temperatures above 1700°F and Reaction (3) is favorable at high hydrogen partial pressures and at temperatures around 1350°F.

If the heat required in Reaction (1) is provided by direct coal oxidation, the combustion reactions would be;

$$C + 1/2\ O_2 \quad = \quad CO \qquad\qquad (4)$$

$$CO + 1/2\ O_2 \quad = \quad CO_2 \qquad\qquad (5)$$

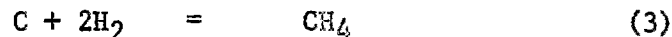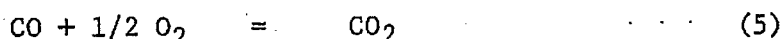Although the direct heating method is more thermally efficient than are the several indirect heating techniques, the presence of CO_2 in the gasifier effluent will require larger and more expensive purification systems.

Indirect heating techniques involve heat carriers such as pebbles, molten salts, dolomite solids, or molten slag. Also heat can be added by electrical heating systems or from nuclear reactors.

Five general types of gasifier reactor designs were considered, each having its individual advantages and disadvantages. The moving bed reactor can be arranged so that certain designated portions of the reactor can be designed to favor specific reactions; however, the feed material must be a noncaking or **pretreated** coal to prevent agglomeration and/or bridging. The solid residue can be withdrawn as a dry ash, in which case the temperature must be held below the ash-softening temperature of the coal, or as a molten slag, in which the reaction temperature can be as high as 2300-2500°F. A fluidized bed offers excellent temperature uniformity and heat transfer characteristics; however, all caking coals must be pretreated and the reaction temperature is limited by the ash-softening properties. Also, because of the vigorous mixing of the solids and the formation of bubbles in the fluidized bed, a complete conversion of the coal cannot be obtained. On the other hand, both the free-fall and the entrained types of gasifier designs provide enough space between the coal particle to minimize the agglomeration or bridging problems, thereby allowing raw coal to be fed directly into the reactor without a pretreatment step; however, these two designs require extremely large vessel sizes to provide the needed particle residence time.

The gasification reactors can be classified into three types depending on the principal reactions taking place in them. In the "gasifier", coal or char is reacted with steam to produce a synthesis gas of H_2 and CO using the path of Reactions (1) and (2). It is assumed in this study that the water-gas shift reaction, Reaction (2), reaches thermodynamic equilibrium. Although reported research data indicate that the gasifier contains a small amount of methane, for calculation simplicity in this

study it was assumed that no methane was formed. When the required heat is provided by direct means, Reactions (4) and (5) must also be considered. It is assumed that there will be no free oxygen existing in the gasifier effluent gas. The synthesis gas produced can be directly used as a reducing medium for further gasification or it may be catalytically shifted to yield additional hydrogen.

In a "hydrogasifier", the coal or char is reacted with a stream of hydrogen-rich gas, such as synthesis gas or hydrogen produced by the other reactions, to form methane by Reaction (3). For ease of calculation, it was assumed that only the carbon-hydrogen reaction, Reaction (3), will take place in this reactor and that the reaction temperature will be 1650°F. The reactivity of the particular coal or char will have a significant effect on the product gas quality and the reactor design. It has been experimentally determined that the equilibrium constant for the coal-hydrogen reaction exceeds many times the equilibrium constant for the graphite-hydrogen reaction, [10],[21],[36].

The "devolatilization" reactor is used to vaporize the volatile hydrocarbons from the coal particle, the volatile matter comprising more than 35% of the coal weight. Because the complete mechanism of coal devolatilization has not reached full understanding, in light of experimental evidence it was assumed that 35% of the oxygen coming into the reactor with the coal becomes CO and the remaining 65% becomes H_2O. [35] In this study, the devolatilization unit was stipulated to operate at 1350°F. Proper design of the devolatilization reactor permits the feeding of raw coal into the reaction system, with the evolved volatile matter being added to the product gas stream instead of being wasted as would be case of a separate pretreatment step.

The effluent gas from the gasification units contains solid dust particles, tar and soot which must be removed by cyclone separators, electrostatic precipitators or wet scrubbers from the gas stream before the gas can be further processed. Solid particles from the dust collection system which still contain a certain amount of unreacted carbon can be sent back to the gasifier for further gasification.

Shift Conversion

Hydrogen-rich gas required for the hydrogasification can be supplied by various means, the most convenient method being to shift the synthesis gas composition to increase the hydrogen content. Also, the gas from the gasifier often has to be further methanated to increase the heating value and, before the methanation step, the $H_2:CO$ ratio of the gas must be adjusted to about 3 to 1. Thus, the shift conversion operation can serve two roles in the integrated gas production plant.

The main reaction taking place in the shift converter is:

$$CO + H_2O = CO_2 + H_2 \qquad (2)$$
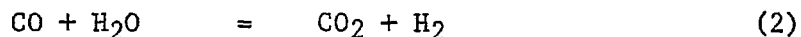
This reaction is mildly exothermic and the quantity of heat removed from the reactor will depend on the CO content of the entering gas stream.

The effluent gas from the gasifier is cleaned of dust and tar and is then cooled to a temperature around 800°F by a waste heat recovery system. The cooled gas is then mixed with a specific amount of steam before entering the shift converter. The added steam not only supplies the water required for shift conversion but also plays a role as a diluent to depress the deposition of the carbon. Catalysts used for shift conversion are iron-chromium oxide compounds.

Gas Purification

The purification of the gas coming from the gasifiers and shift converters is an essential part of the pipeline gas production, not only from the pollution point of view, but it also helps achieve the high caloric value gas required for pipeline gas quality. Carbon dioxide adds nothing to the heating value of the final gas and dilutes the concentration of the H_2 and CO in the stream entering the catalytic methanator. The methanation catalysts, usually containing nickel compounds, are extremely sensitive to any contaminating sulfur species.

In order to economically remove CO_2 and H_2S from the gas stream, a combination of three methods will be used. Gas coming from the shift converter is passed through a hot potassium carbonate process, then through a monoethanolamine process and, finally, an activated carbon tower. The MEA solution is preferred over the carbonate solution for removal of hydrogen sulfide; however, because of its lower heat requirement and better operating flexibility, the hot potassium carbonate process is more economical for the removal of CO_2. Heat and energy recovery units such as turbines, etc., aid in increasing the operation efficiency of this system. The CO_2 and H_2S removed by the first two processes are sent to sulfur recovery plants, where, depending on the concentration of H_2S, the sulfur in the elemental form is recovered either by the Claus Process followed by a Stretford Process, or by a Stretford Process alone. The gas purifier effluent contains less than 1.5% (volume) of CO_2 and less than 0.1 grain of H_2S per 1000 standard cubic feet.

Methanation

The last step of coal gasification is that of methanation. Almost all the coal gasification processes require additional units for the con-

version of excess carbon monoxide and hydrogen into methane to achieve a
high heating value of pipeline gas quality. The degree of methanation varies
considerably, depending on the type of process used in the gasification.

Methanation can be described as follows:

$$CO + 3H_2 \quad = \quad CH_4 + H_2O$$
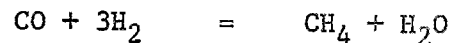
This is a highly exothermic reaction and the method of removing
heat from the reacting gas is the major problem in economic operation of
methanators.

Based on the type of heat removal the methanation can be classified
as the following schemes:

    a)   the heat extraction scheme
    b)   the cold quench scheme
    c)   the recycle scheme
    d)   the cold quench-recycle scheme

The heat extraction scheme can be used for gas streams with low
and intermediate CO concentrations, the cold-quench scheme is used for
intermediate CO concentration, whereas the cold-quench-recycle scheme and
the recycle scheme are used for high CO concentrations in the feed
stream. The CO concentration of the product is less than 0.2%.

The methanator can be a fixed bed or a tube-wall reactor. The
catalysts used for methanation are nickel or ruthenium types which
easily are poisoned by sulfur compounds.

3.2 Alternative Subsystem Arrangements

The process subsystems described in Section 3.1 can be now combined
to form many different arrangements. Among those possible system arrangements,
five typical alternates were selected here for further evaluation, with
two or more modifications made for each alternate. The alternates are
illustrated in Figures 1 through 5 and are summarized in Table 2. Some
of the alternates described below are similar to specific coal gasification
schemes now being developed by certain organizations in the United States
and abroad, such as the "Modified Lurgi Process" (Lurgi), "Synthane Process"
(U. S. Bureau of Mines), "HYGAS - Oxygen Process" (Institute of Gas Technology),
"BIGAS Process" (Bituminous Coal Research, Inc.), "Synthane Process"
(U. S. Bureau of Mines), "HYGAS-Electrothermal Process" (Institute of Gas
Technology), and the "CO_2 Acceptor Process" (Consolidation Coal Company).
These processes are roughly related to Alternates I-1, I-2, II-2, II-3,
III-2, IV and V, respectively, although large discrepancies may exist
between the alternates and the respective process scheme under current
development.
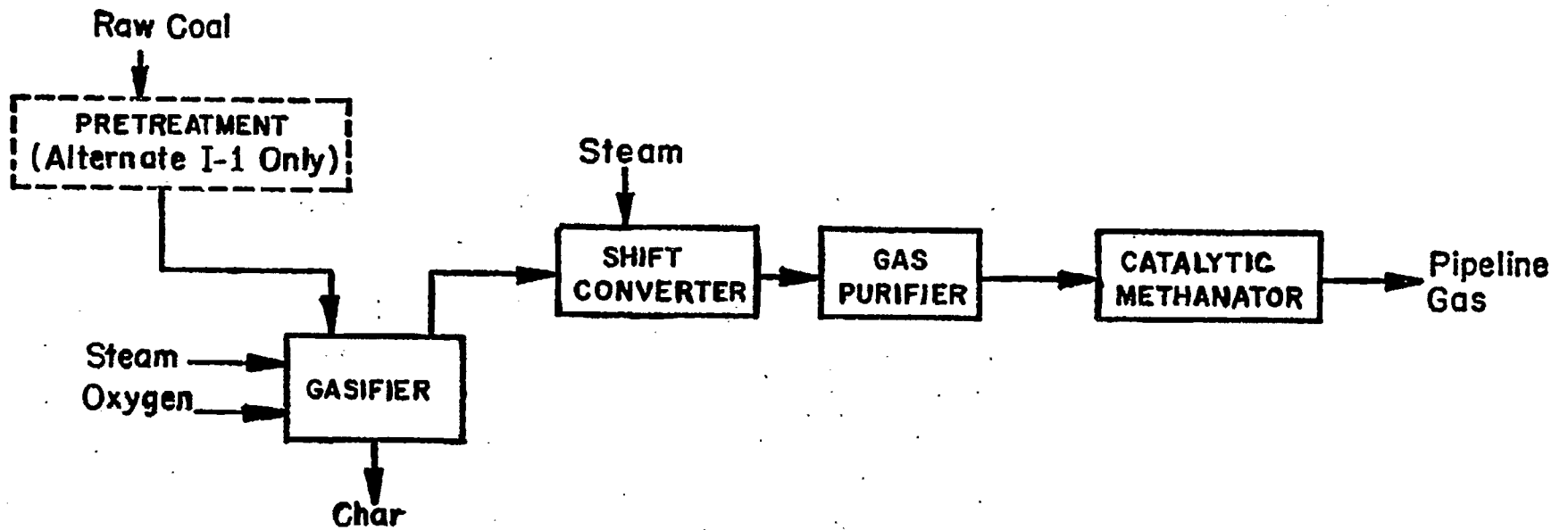
Figure 1. Flow Scheme for Alternate I

Figure 2. Flow Scheme for Alternate II
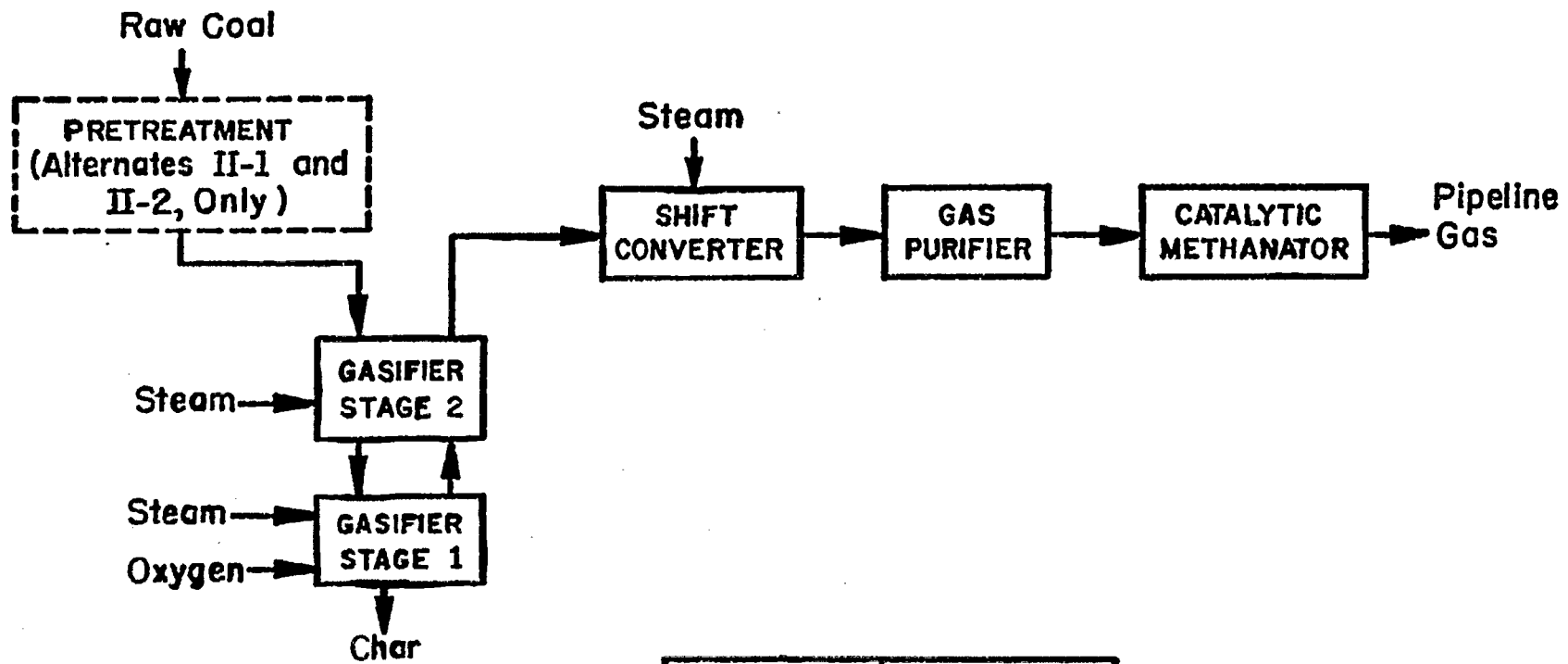
	STAGE 1	STAGE 2
Alternate II-1:	Slagging	Fluidized
Alternate II-2:	Fluidized	Fluidized
Alternate II-3:	Slagging	Entrained
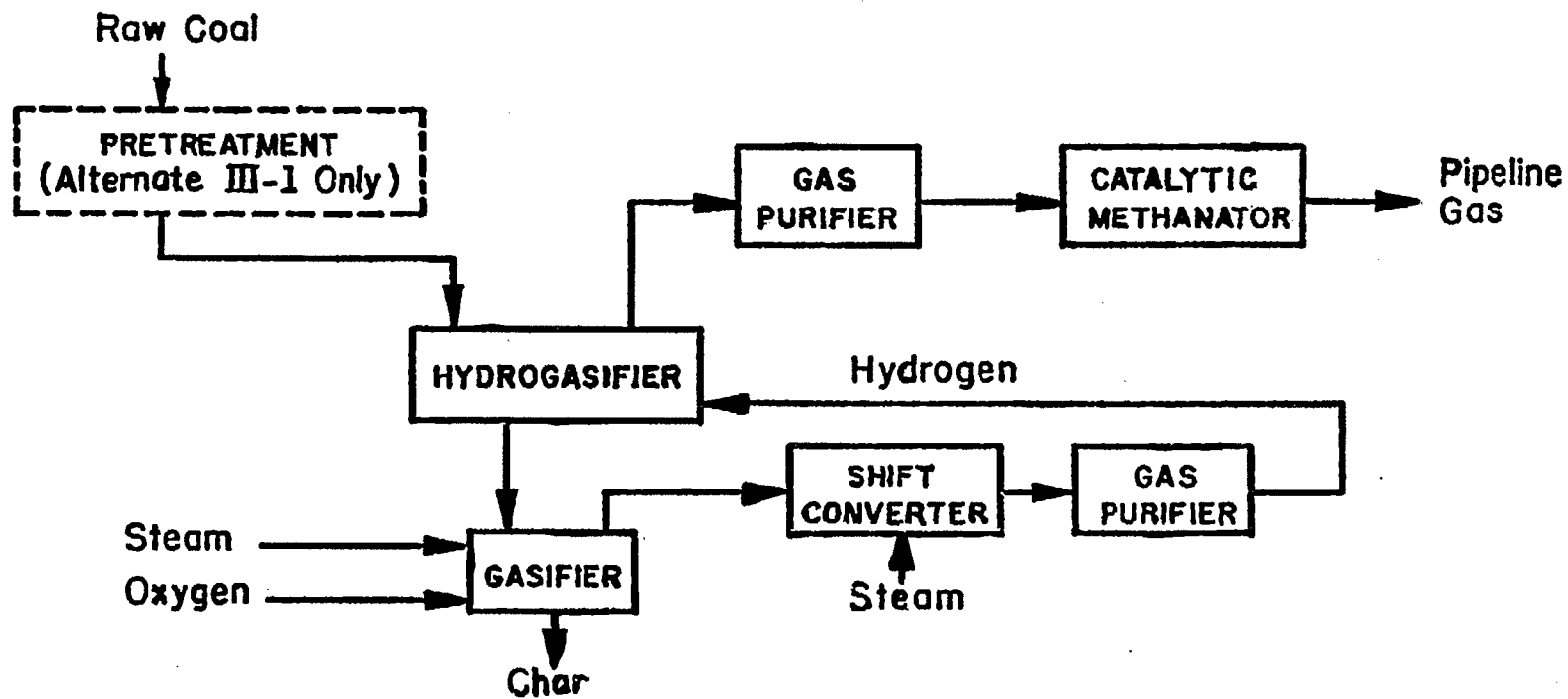
Alternate III-1:	Fluid Bed Hydrogasifier
Alternate III-2:	2-Stage Hydrogasifier (a) Dilute Phase Top Section (b) Fluidized Bottom Section

Figure 3. Flow Scheme for Alternate III
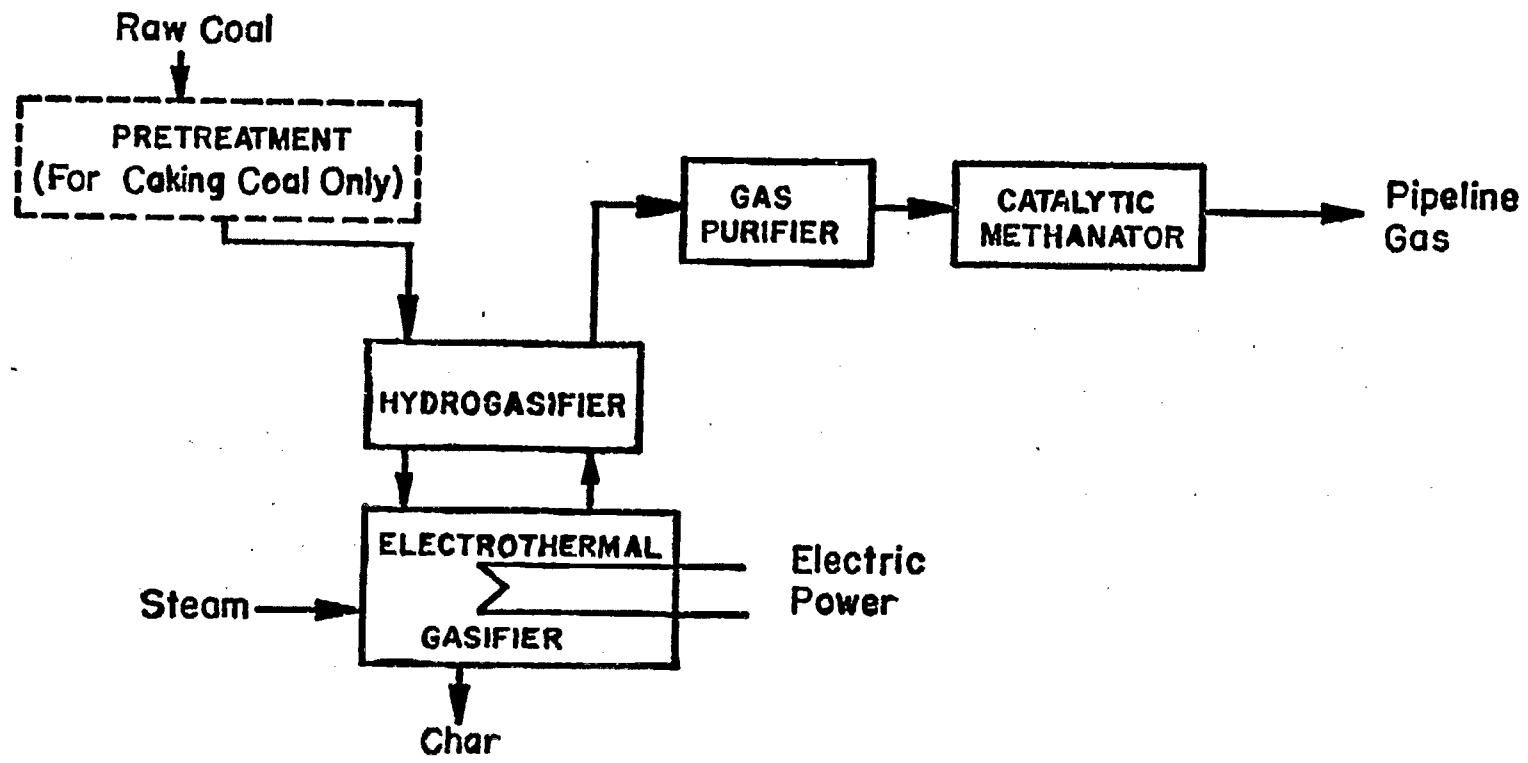
Figure 4. Flow Scheme for Alternate IV
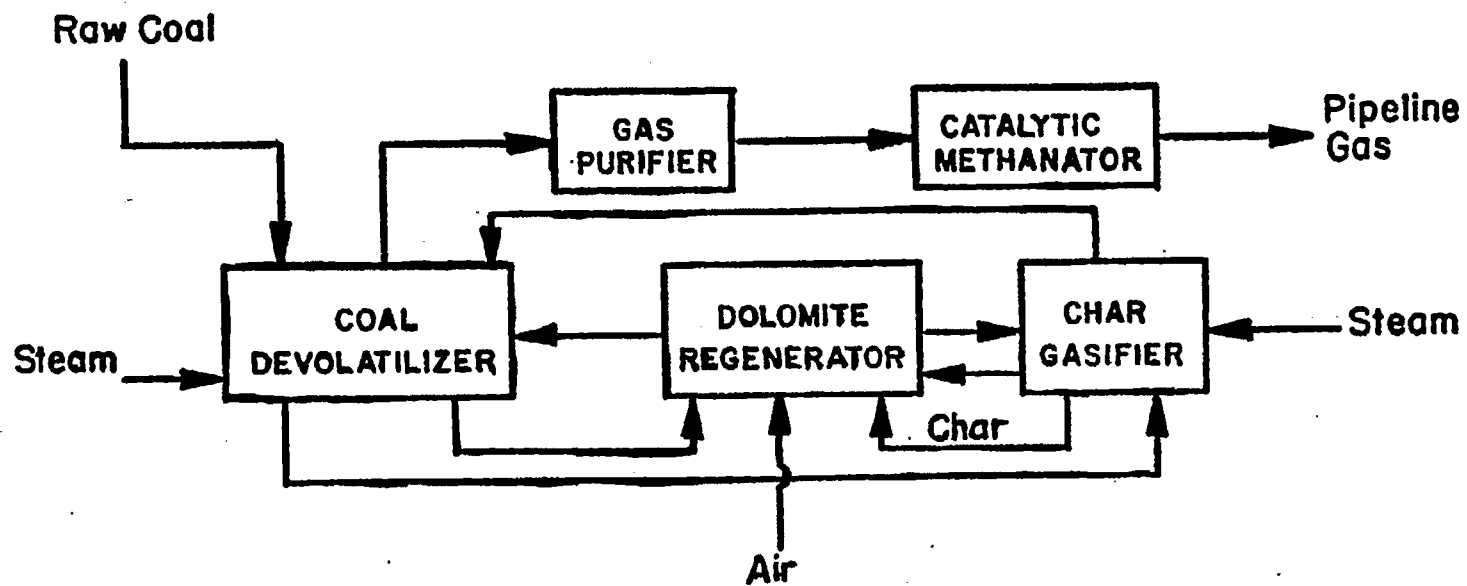
Figure 5. Flow Scheme for Alternate V

TABLE 2 - SUMMARY OF ALTERNATIVE COAL GASIFICATION PROCESSES

| PROCESS ALTERNATE | COAL TYPE | | GASIFICATION SUB-SYSTEM | | | | PURIFICATION SYSTEM | | METHANATION |
| | | | TYPE OF REACTOR | | | Heat Supply | | | |
	Rank	Pretreat	Devolatilization	Primary	Secondary		CO_2-H_2S Removal	Sulfur Recovery	
I-1	B	Yes	-	F	-	D	P-M-A	ST	CQR
I-2	B	No	FF	F	F	D	P-M-A	ST	CQR
II-1	B	Yes	-	F	S	D	P-M-A	ST	CQR
II-2	B	Yes	-	F	F	D	P-M-A	ST	CQR
II-3	B	No	-	E	S	D	P-M-A	ST	CQR
III-1	B	Yes	-	F	F	D	(1) P, (2) M-A	CL-ST	CQ
III-2	B	No	FF	F	F	D	(1) P, (2) M-A	CL-ST	CQ
IV-B *	B	Yes	F	F	ET	ID	P-M-A	ST	CQR
IV-L **	L	No	F	F	ET	ID	P-M-A	ST	CQR
V-B *	B	No	F	-	F	ID	P-M-A	ST	CQR
V-L **	L	No	F	-	F	ID	P-M-A	ST	CQR

COAL RANK

B-Bituminous
L-Lignite

* Feed is Bituminous Coal
** Feed is Lignite

REACTOR TYPE

E-Entrained Bed
ET-Electrothermal Bed
F-Fluidized Bed
FF-Free Fall Reactor
S-Slag Bed

HEAT SUPPLY

D-Direct
ID-Indirect

GAS PURIFICATION

A-Activated Carbon Tower
M-Monoethanolamine Process
P-Hot Potassium Carbonate Process

METHANATION

CQR - Cold Quench Recycle Scheme
CQ - Cold Quench Scheme

SULFUR RECOVERY

CL-Claus Process
ST-Stretford Process

Alternate I

This alternate is illustrated in Figure 1 and is further classified into two sub-alternates, depending on the gasifier designs.

(a) Alternate I-1: Raw coal obtained from the coal mine is prepared and pretreated before it is charged to a fluidized bed gasifier. Coal particles are fluidized and gasified with steam and oxygen in the gasifier. The effluent gas which contains mainly CO and H_2 is catalytically shifted in a shift converter. After CO_2 and H_2S are removed in a purification system, the gas is catalytically methanated to pipeline gas quality.

(b) Alternate I-2: Prepared coal is directly charged into a fluidized gasifier without any pretreatment. The gasifier consists of three different zones. The devolatilization zone, where the coal particles are mixed with hot steam and a small amount of oxygen, is located at the upper part of the reactor. The dense-phase fluidized bed, where the devolatilization approaches completion and the non-catalytic methanation takes place, is located at an expended mid-section of the gasifier. The hot dilute fluidized bed, where oxygen and steam react with coal to produce synthesis gas, is located at the contracted bottom part of the gasifier. The product gas leaves the gasifier at a point between the dense phase and the dilute phase fluidized zones and the residual char is withdrawn from the bottom of the gasifier. The effluent gas passes through the same shift conversion, purification and methanation units as in Alternate I-1.

Alternate II

Depending on the type of gasifier selected, this Alternate, illustrated in Figure 2, has been divided into three sub-alternates.

(a) Alternate II-1: Two gasifiers connected in series are used for this alternate. The first stage, located at the bottom is a slagging zone and the second stage, located at the top, is a fluidized bed. Pretreated coal particles are injected with steam near the bottom of the second stage where they contact with the synthesis-gas produced in the first stage and are devolatilized and partially methanated in the second stage. The residual char passes downward through a standpipe to the first stage where it is gasified with oxygen and steam to form synthesis gas. The ash formed in the first stage is withdrawn from the reactor as slag through a lock-hopper system. The gas product from the second stage is passed through the shift conversion, gas purification and methanation systems to form pipeline gas.

(b) Alternate II-2: This sub-alternate is operated on the same principle as Alternate II-1 except both stages are fluidized beds. Because a fluidized bed is used for the first stage, the gasifier cannot be operated at temperatures higher than the ash-softening temperature of coal unless some mechanical device is used to destroy or retard the agglomeration tendency of the coal particle.

(c) Alternate II-3: The first stage of this alternate is a slagging zone and the second or upper stage is an entrained bed. The entrained bed operation allows the coal particles, without any pretreatment, to be directly fed into the reactor. The partially gasified particles in the second stage are entrained by the synthesis-gas rising from the first stage and separated from the gas stream in a cyclone separator. Solid particles collected in the separator are introduced to the first stage where they react with oxygen and steam to form the synthesis gas. The gas product goes through the conversion procedure as in Alternate II-1 to reach pipeline gas quality.

Alternate III

This Alternate is illustrated in Figure 3. Depending on the structure of the gasifier system, this Alternate is further classified into two sub-alternates.

(a) Alternate III-1: Pretreated coal particles are fed to a fluidized bed hydrogasifier where they are contacted with a hydrogen-rich gas stream. The residual char goes to another fluidized bed gasifier where it is reacted with steam and oxygen to form synthesis gas. The synthesis gas is shifted completely in a converter and returned as the hydrogen-rich gas to the hydrogasifier. The effluent gas of the hydro-gasifier is purified and methanated to form the pipeline gas.

(b) Alternate III-2: This alternate involves a direct hydro-gasification of raw coal in a unique two-stage reactor. Raw coal is charged from the top of a free-fall stage where it contacts with a hot gas mixture of H_2 and CH_4 rising from the bottom stage. In this region the coal is devolatilized and rendered non-caking, and the volatile hydrocarbons produced are converted to form methane. The char from the top stage flows down into the second stage where it is partially hydrogenated with fresh hydrogen to produce the hydrogen-methane gas used in the top stage. The residual char passes through the same steps as in Alternate III-1 to form hydrogen which is used for the hydrogasification of coal. The effluent gas of the top stage of gasifier is purified and methanated to form pipeline gas.

Alternate IV

This process (Figure 4) consists of a two-stage hydrogasifier and an electrothermal fluidized bed synthesis-gas generator. Before entering the hydrogasifier, the prepared and pretreated coal is mixed with light oil to form a slurry which is pumped into a fluidized bed at the top section of the gas-ifier. The light oil is evaporated in the drying section. The dried coal par-ticles fall into the first stage of the hydrogasifier where devolatilization and

a non-catalytic partial methanation occurs in the presence of hydrogen-rich gas. The residual char from the first stage gasifier falls into the second stage where partial gasification occurs by reaction with steam in the hydrogen-rich gas system. Part of the char produced from the second stage gasifier goes to an electrically heated, fluidized synthesis-gas generator. This char is gasified with steam, with the heat supplied through electrodes positioned within the fluidized bed. Since the required electricity must be generated by the burning of fresh coal, coal fines, residue char or product gas, a substantial energy loss is associated with the converting of the combustion heat into electricity. However, the using of indirect electrical heat greatly decreases the amount of carbon dioxide generated, thereby substantially reducing the size of the later gas purification subsystem. The technology of designing and constructing electrodes, suitable for use in this reactor system, has not been perfected and is still under active development. The generated synthesis-gas is directly introduced to the bottom of the hydrogasifier. The effluent gas of the hydrogasifier is purified and methanated to form pipeline gas. This process can be run by using either bituminous coal or lignite. Pretreatment is not required when the lignite is used for gasification because of its non-caking property.

Alternate V

As shown in Figure 5, the crushed coal is fed to a devolatilizer where it reacts with hydrogen-rich gas from the gasifier. The residual char is transferred to the gasifier where the carbon reacts with steam. Calcined dolomite acts as a heat carrier and moves through the devolatilizer and the gasifier. The heat provided by the dolomite includes the sensible heat as well as the heat produced in the following exothermic reaction:

$$CaO + CO \rightleftharpoons CaCO_3$$
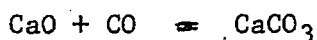
The mixture of dolomite and residual char from the gasifier is transferred by a pneumatic conveyer system to the regenerator where the char is burned with air to supply the heat needed to heat and recalcinate the dolomite solids. The gaseous product of the devolatilizer is purified and methanated to form pipeline gas.

4.0 COMPARISON OF COAL GASIFICATION ALTERNATE PROCESSES

4.1 Utilization Efficiencies

The thermal efficiency is defined in Section 2.1 as the combustion heat in the product gas divided by the combustion heat quantity contained in the raw coal fed to the total plant. By maximizing this efficiency value, the coal gasification processes have been optimized based on the simplification strategy and the "Complex Method of Optimization" discussed in Section 2.1. The results of this series of optimizations are shown in Table 3. Also listed in Table 3 are the carbon efficiencies for the different alternative processes; the "carbon efficiency" being defined as the pound-moles of carbon present in the product gas divided by the pound-moles of carbon fed to the overall plant. The carbon entering in the raw coal has three major final destinations; to the product gas stream (mainly in the form of methane), to the auxiliary utility plants (electrical power, steam and oxygen) and to the formation of non-useable by-products (char, CO_2 and non-recoverable matter evolved in the pretreatment step). The distribution of the entering carbon among these ultimate destinations are shown in Table 4.

As seen in Table 3, the thermal efficiencies and carbon efficiencies are directly related; i.e., a high thermal efficiency usually indicates a high carbon efficiency. Of the alternative processes considered in this study, Alternate III-2 utilizes its energy best with a 77.8% thermal efficiency and a carbon efficiency of 43.5%. The worst or lowest set of efficiencies is associated with Alternate I-1, which had a thermal efficiency of 46.4% and a carbon efficiency of 26.8%.

A major reason why some alternates have significantly greater thermal and carbon efficiencies than do other alternate systems can be attributed to the direct feeding of raw coal to the gasifiers, thereby eliminating the coal pretreatment step. As discussed in Section 3.1, the pretreatment step causes the loss of a considerable amount of reactive carbon as well as valuable hydrogen, resulting in an increase of approximately 10% in the total coal required to form the fixed amount of product gas, as can be seen in Table 4. Unfortunately, mechanical and design problems associated with the feeding of raw caking coal directly into the gasifier may adversely affect the possibility of achieving these predicted higher thermal efficiencies. These problems will be discussed in a later section of this report.

Another factor significantly affecting the efficiency values is the design decision to either form most of the methane in the gasification stage, (the "hydrogasification" reaction -- Reaction (3)), and use the final methanation subsystem as just a polishing step, or to form synthesis gas (CO and H_2) in the gasification stage and leave a large proportion of the methane to be formed in the final catalytic methanation units. The optimization study results favor the methane formation in the gasification subsystem. The difference between these alternate designs lies in feeding

TABLE 3

THERMAL AND CARBON EFFICIENCIES FOR DIFFERENT ALTERNATIVE PROCESSES

	EFFICIENCIES	
ALTERNATES	THERMAL	CARBON
I-1	46.4%	26.8%
I-2	64.1%	36.8%
II-1	56.2%	32.3%
II-2	53.0%	29.5%
II-3	68.1%	38.8%
III-1	61.4%	35.5%
III-2	77.8%	43.5%
IV-Bituminous	49.8%	28.5%
IV-Lignite	66.2%	31.5%
V-Bituminous	66.8%	37.8%
V-Lignite	67.8%	35.1%

TABLE 4 CARBON UTILIZATION IN INTEGRATED PIPELINE GAS PLANT

ALTERNATE	TOTAL AMOUNT OF CARBON REQUIRED IN THE PROCESS lb-mole/hr	AMOUNT OF CARBON IN PRODUCT GAS		AMOUNT OF CARBON USED IN UTILITY PLANTS				AMOUNT OF CARBON REJECTED AS NON-USEABLE BY-PRODUCT	
				STEAM PLANT		ELECTRICAL PLANT INCLUDING OXYGEN			
		lb-mole/hr	%	lb-mole/hr	%	lb-mole/hr	%	lb-mole/hr	%
I-1	100,670	27,540	27.3	11,970	11.9	5,830	5.8	55,300	55.0
I-2	72,890	27,360	37.5	2,260	3.1	4,420	6.1	38,850	53.3
II-1	83,630	27,860	33.3	1,210	1.4	6,590	7.9	47,970	57.4
II-2	88,120	27,240	30.9	2,520	2.9	5,700	6.4	52,660	59.8
II-3	68,570	27,380	39.9	5,480	8.0	4,520	6.6	31,190	45.5
III-1	76,060	27,300	35.9	1,500	2.0	3,300	4.3	43,960	57.8
III-2	60,050	26,200	43.6	3,170	5.3	3,020	5.0	27,660	46.1
IV- B *	93,530	27,240	29.1	13,850	14.8	24,050	25.7	28,390	30.4
IV- L **	89,680	27,100	30.2	18,395	20.5	21,750	24.2	24,450	25.1
V-.B *	69,950	27,210	38.9	--	--	--	--	42,740	61.1
V-.L **	75,519	26,960	35.7	--	--	--	--	58,810	64.3

*   Feed is bituminous coal
** Feed is lignite

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the raw coal into a more thermally regulated hydrogenating atmosphere
where the volatile compounds are converted directly to methane, or
in feeding the raw coal into the severe pyrolytic atmosphere of the
synthesis gas generator where all the hydrocarbons are decomposed
almost entirely to CO and H_2, compounds which must be later reacted
again in the catalytic methanation system. Henry and Louks [15] discussed
the merits of various subsystem arrangements with regard to improvements
in overall plant efficiency and corresponding lower gas manufacturing
costs.

This reasoning can be used to explain the better overall
thermal efficiency (better by 9.7%) of Alternate III-2 as compared
with Alternate II-3. In Alternate III-2, 94% of the methane was
formed in the hydrogasifier compared with only 60% of the methane of
Alternate II-3 being formed in the gasification section. Using
pretreated coal, Alternate III-1 produced 93% of the methane in the
hydrogasifier and Alternate II-1 produced 78% in the gasification
subsystem, which explains the 5.2% difference in overall plant thermal
efficiencies between these two alternates.

Carbon dioxide is formed by either the carbon-oxygen reactions
for the purpose of directly supplying heat, Reactions (4) and (5),
or by the water-gas shift reactions, Reaction (2), used to regulate
the CO to H_2 ratio of the product gas stream. The amounts of CO_2
removed in Alternates I, II and III are approximately 35 to 47
mole per cent of the total carbon required in the process. Since,
in Alternate IV, electricity indirectly supplies the required
heat, the amount of CO_2 formed is only 20% of the total carbon required.
However, in Alternate IV, the high percentage of carbon used in the
electrical generating plant offsets the possibility of achieving an
overall high plant efficiency.

The design of the gasifier will affect the amount of unreacted
carbon discharged as residue char. In Alternates II-1 and II-3, the
slagging bed reactors will discharge a residue char with a carbon
content near to zero per cent. However, fluidized bed reactors are
specified in most of the other alternate designs because of the ability
to operate the reactor at uniform temperatures. However, the amount
of carbon remaining in the residue char from this type of reactor
is approximately 6 to 28 percent of the total carbon required in the
process. This char can be either discarded as a non-useable by-product
waste or utilized as a fuel to generate steam or electrical energy.
Studies have demonstrated that chars with 60% or greater carbon content are
useable as a fuel source and those chars were so used. The utilization of
all the char, regardless of the carbon content, will mean a thermal
efficiency increase of from 1.4% to 7.4% (average 4.6%) and a carbon efficiency
increase of from 1.0% to 5.7% (average 3.1%) over the cases where the char
would be rejected as useless waste.

4.2 Capital Equipment Costs

It should be clearly stated that the capital costs presented in this
section and the manufacturing cost values given in the following section
are relative values and were computed for comparative purposes

TABLE 5 BARE EQUIPMENT COST

ALTERNATE SECTION	BARE EQUIPMENT COST, MILLIONS OF DOLLARS										
	I-1	I-2	II-1	II-2	II-3	III-1	III-2	IV-B **	IV-L ***	V-B **	V-L ***
PREPARATION AND STORAGE	11.800	14.616	9.400	10.620	14.513	10.630	12.600	11.200	24.063	15.000	10.980
PRETREATMENT	6.180	--	5.650	6.220	--	6.500	--	6.625	--	--	--
GASIFICATION	3.685	4.500	10.205	12.837	4.126	14.367	15.000	33.952	33.952	32.557	32.557
SHIFT CONVERSION	4.013	2.683	3.368	3.675	3.338	3.986	3.975	--	--	--	--
GAS PURIFICATION 1	19.000	14.386	12.840	15.816	15.816	7.712	7.000	10.560	12.000	16.790	21.900
GAS PURIFICATION 2	--	--	--	--	--	4.800	4.800	--	--	--	--
METHANATION	3.757	1.691	3.305	2.220	3.030	0.360	0.450	1.635	1.290	2.250	2.700
OXYGEN PLANT	32.219	29.048	31.939	26.373	30.325	24.623	23.100	--	--	1.330*	1.330*
ELECTRIC POWER PLANT	23.025	16.747	18.838	15.373	17.437	14.065	11.440	42.603	38.556	4.962	4.270
SULFUR RECOVERY PLANT	7.500	6.210	5.300	6.500	6.200	7.660	6.950	4.400	4.850	4.010	1.140
OFFSITE FACILITIES	19.000	19.000	19.000	19.000	19.000	19.000	19.000	19.000	19.000	19.000	19.000
SUBTOTAL BARE COST	130.179	108.881	119.845	118.634	113.785	113.703	104.315	129.975	133.711	95.899	93.877

* Cost of product gas compressor   *** Feed is lignite

** Feed is bituminous coal

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REPORT PREPARED BY		COAL TYPE	BARE EQUIPMENT COSTS, MILLIONS OF DOLLARS							
			LURGI	"CO2 ACCEPTOR" [4], [7] [22]	"BI-GAS" [1], [9] [14]	"HYGAS" ELECTRO-THERMAL [17][18][25][28]	"HYGAS" STEAM-OXYGEN [16]	"HYGAS" STEAM-IRON [16]	"SYNTHANE" [12],[21],[33]	"KELLOGG" [15],[19],[27]
ESSO (1972) [26]		Bituminous	216.2	-	200.0	226.2	189.8	177.3	161.0	-
ESSO (1972) [26]		"Western"	192.8	148.4	200.0	226.2	189.8	177.3	161.0	-
I.G.T.	(1967) [28]	Bituminous	-	69.0	120.7	-	124.7	87.8	-	114.3 (a) 90.3 (b)
I.G.T.	(1964) [17]	Lignite	-	-	-	-	36.0 (c) 40.5 (d)	-	-	-
I.G.T.	(1967) [18]	Bituminous	-	-	-	76.9 (e) 92.3 (f)	-	-	-	-
U.S. BUREAU of MINES	(1964) [34]	Lignite	-	36.6	-	-	54.2	-	-	-
U.S. BUREAU of MINES	(1970) [31]	Bituminous	194.6 (g) (i) 142.4 (h) (i)	-	-	-	-	-	-	-
U.S. BUREAU of MINES	(1969) [32]	Bituminous	-	-	-	-	-	-	166.5 (i)	-
AIR PRODUCTS [1] (1970)		Bituminous	-	-	139.6	-	-	-	-	-
CONSOLIDATION COAL COMPANY [4] (1969)		Lignite	-	78.2	-	-	-	-	-	-

(a) With Power By-Product
(b) Without Power By-Product
(c) I.G.T. Flowsheet

(d) Bureau of Mines Flowsheet
(e) Gasification With Synthesis Gas
(f) Gasification With Hydrogen

(g) 8.7% CH_4 Yield From Gasifier
(h) 15.6% CH_4 Yield from Gasifier
(i) Includes Mining Facilities

only. They are not to be considered as estimations of the absolute
cost of manufacturing a pipeline-quality gas using these processes
because of the many economic variations stemming from plant locations,
raw coal composition differences, inflation of equipment and operating
costs, tax structure differences, etc.

Based on the solutions obtained from the optimization of the
thermal efficiencies of the overall coal gasification alternates,
the capital costs of the different alternate processes were estimated. The
total plant investments were estimated by optimizing the various sub-
systems with regard to the minimum capital investments, the optimiza-
tion procedure being done on each individual stage of the process,
such as a fixed bed catalytic shift converter, the gas purification
units, the methanation units, etc. [35]

The equipment capital costs for the alternates, as shown in
Table 5, range from $94 million for Alternate V-L* to $134 million
for Alternate IV-L.**An examination of the costs of those processes
directly using oxygen reveals that the oxygen plant represents the most
expensive capital equipment item, followed by the electrical power plant
cost. The costs of the coal preparation plant, the gasification
units and the gas purification systems are also significant items. In
this study an amount of $19 million was allocated to each process to
cover the cost of offsite facilities such as the steam generation plant,
the water treatment system, the cooling towers, stacks, auxiliary buildings,
land acquisition, etc.

As stated before, the costs given here are to be used only to
compare the various alternative processes; however, the values are in
the range of capital cost estimations found by other investigators,
as shown in Table 6.

4.3 Gas Manufacturing Costs

Using the capital investments for the alternative processes as
given in the last section, and assuming a raw bituminous coal cost of
from $2 to $8 per ton or a lignite cost of either $1.50, $3, or $4.50
per ton, the manufacturing costs of the pipeline-quality gas produced
by the different processes were calculated using the Office of Coal Research
accounting procedure, the gas price averaged over a 20-year lifetime of the
plant. The results of these calculations are presented in Table 7. For
the processes using bituminous coal as the raw material, the gas price for
Alternate III-2 is the lowest, followed by Alternate I-2 and II-3. For
the lignite-fed plants, Alternate V produces a cheaper gas than does Alternate
IV. The relationship between the thermal efficiency and the final gas
price can be seen by comparing the results given in Table 3 with those in
Table 7. This direct relationship justifies the decision to optimize the
thermal efficiency of the overall processes as the objective function followed
by the subsystem optimization of minimum capital costs, instead of directly
optimizing the cost of gas production.

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*   Alternate V fed with lignite
** Alternate IV fed with lignite

TABLE 7

TWENTY-YEAR AVERAGE GAS PRICE

	BITUMINOUS COAL PRICE			
$/TON	2	4	6	8
¢/MILLION BTU	11.9	23.8	35.7	47.6
ALTERNATE	GAS PRICE, ¢/MILLION BTU			
I-1	61.11	87.91	114.71	141.51
I-2	48.59	68.75	88.91	109.07
II-1	51.62	71.76	91.90	112.04
II-2	53.42	75.67	97.92	120.17
II-3	49.80	69.64	89.48	109.32
III-1	50.41	71.49	92.57	113.65
III-2	44.76	62.73	80.70	98.67
IV-BITUMINOUS	59.24	85.29	111.34	137.39
V-BITUMINOUS	49.26	70.69	92.12	113.55

	LIGNITE PRICE		
$/TON	1.50	3.00	4.50
¢/MILLION BTU	14.9	29.8	44.7
ALTERNATE	GAS PRICE, ¢/MILLION BTU		
IV-LIGNITE	60.53	87.13	113.75
V-LIGNITE	53.31	79.15	105.00

TABLE 8 - A SURVEY OF ESTIMATED GAS PRICES FROM PROCESSES PROPOSED FOR DEVELOPMENT

REPORT PREPARED BY		COAL TYPE	COAL COST	TWENTY-YEAR AVERAGE GAS PRICE - CENTS/MILLION Btu			"HYGAS"				
				LURGI	"CO₂ ACCEPTOR" [4],[7] [22]	"BI-GAS" [1],[9],[14]	ELECTROTHERMAL [17], [18] [25], [28]	STEAM-OXYGEN [16]	STEAM-IRON [16]	"SYNTHANE" [12], [21] [33]	"KELLOGG" [5], [19] [27]
ESSO (1972) [26]		Bituminous	30¢ (a)	127.1	-	121.9	124.2	113.1	113.2	114.4	-
		"Western"	15¢ (a)	94.0	80.5	98.0	97.9	87.5	83.9	88.6	-
I.G.T.	(1967) [28]	Bituminous	16.1¢ (a)	-	47.7	58.4	-	57.8	50.2	-	56.1 (d) 58.5 (e)
	(1964) [17]	Lignite	$1.25 (b)	-	-	-	-	50.6 (f) 45.7 (g)	-	-	-
	(1967) [18]	Bituminous	16.1¢ (a)	-	-	-	51.1 (h) 59.3 (i)	-	-	-	-
U.S. BUREAU OF MINES	(1964) [34]	Lignite	$1.25 (b)	-	40.0 (1)	-	-	45.0 (1)	-	-	-
	(1970) [31]	Bituminous	(c)	55.6 (j)(1) 43.5 (k)(1)	-	-	-	-	-	-	-
	(1969) [32]	Bituminous	(c)	-	-	-	-	-	-	43.1 (1)	-
AIR PRODUCTS (1970) [1]		Bituminous	$2.00 (b) $2.50 (b) $3.00 (b)	-	-	58.7 68.9 69.3	-	-	-	-	-
CONSOLIDATION COAL (1969) COMPANY [4]		Lignite	8.0¢ (a) 9.5¢ (a) 11.0¢ (a)	-	38.1 40.6 43.1	-	-	-	-	-	-

(a) Coal Cost Per Million Btu
(b) Coal Cost Per Short Ton
(c) Includes Cost of Mining
(d) With Power By-Product
(e) Without Power By-Product
(f) I.G.T. Flowsheet

(g) Bureau of Mines Flowsheet
(h) Gasification With Synthesis Gas
(i) Gasification With Hydrogen
(j) 8.7% CH₄ Yield From Gasifier
(k) 15.6% CH₄ Yield From Gasifier
(1) Gas Price Is Cents Per 1000 SCF

The gas manufacturing costs computed in this study fall within the ranges of estimated costs given by other investigators, the values being given in Table 8.

4.4 Sensitivity of Certain Process Variables

After the search for the optimized plant designs has been completed, it is desirable to examine the effect of changes in the several parameters used in the study. The examination will insure, first of all, that the computed values are truly optimal and whether the parameters chosen are reliable and controllable factors.

The sensitivity of each of the many parameters can be used to determine the factors and steps of the process that significantly affect the price of the gas produced. These factors and steps can then be further investigated in more detail to provide better approaches to the overall coal-to-gas conversion scheme.

In this study, the sensitivity of six parameters were investigated, three of these being cost and operating variables of the particular process and the rest being general cost accounting values. It was found that all the sensitivity relationships are linear and therefore additive.

The effects on the final gas production price caused by (a) changes in the purchase cost of the raw coal, (b) variations in the bare capital investment cost, and (c) changes in the stream factor (the number of working days per year) can be related by Equation (8);

$$\Delta C = (C - C_b) = f_P (P - P_b) + f_B (B - B_b) + f_S (S - S_b) \quad (8)$$

where; ΔC = Difference in final product gas price - ¢/Million Btu

C = Final Product Gas Price - ¢/Million Btu

C_b = Base Gas Price - ¢/Million Btu (The values computed in this study are listed in Table 9)

P = Actual Raw Coal Purchase Price - $/Short Ton

P_b = Base Raw Coal Purchase Price (The values used in this study were $4/Ton for bituminous and $3.00/Ton for lignite.)

B = Actual Bare Capital Equipment Cost - Millions of Dollars

B_b = Base Capital Equipment Cost - Millions of Dollars (The values computed in this study are listed in Table 9.)

S = Actual Stream Factor - Operating Days/Year

TABLE 9 - GAS PRICE ADJUSTMENT COEFFICIENTS OF COST PARAMETERS AND STREAM FACTORS

ALTERNATE	BASE GAS PRICE: C_b (¢/Million Btu)	TOTAL BARE EQUIPMENT COST: B_b (Millions of Dollars)	GAS PRICE ADJUSTMENT COEFFICIENTS					
			RAW COAL COST: f_p (¢/Million Btu) per ($/Ton)	EQUIPMENT COST: f_B (¢/Million Btu) per (Million $)	STREAM FACTOR: f_S (¢/Million Btu) per (Days/Year)	DEBT: f_D (¢/Million Btu) per (Unit %)	INTEREST: f_I (¢/Million Btu) per (Unit %)	GROSS RETURN RATE: f_R (¢/Million Btu) per (Unit %)
I-1	87.91	130.179	13.40	0.235	-0.1101	-0.048	-0.42	1.88
I-2	68.75	108.881	10.08	0.235	-0.0863	-0.040	-0.34	1.57
II-1	71.76	119.845	10.07	0.235	-0.1011	-0.044	-0.38	1.70
II-2	75.67	118.634	11.13	0.235	-0.1008	-0.044	-0.37	1.71
II-3	69.64	113.785	9.92	0.235	-0.1038	-0.042	-0.36	1.62
III-1	71.49	113.703	10.54	0.235	-0.0967	-0.042	-0.37	1.64
III-2	62.73	104.315	8.99	0.235	-0.0890	-0.038	-0.33	1.49
IV-B*	85.29	129.975	13.03	0.235	-0.1104	-0.048	-0.43	1.87
IV-L**	83.95	133.711	16.68	0.235	-0.1124	-0.049	-0.43	1.50
V-B*	70.69	95.899	10.72	0.235	-0.0830	-0.036	-0.31	1.40
V-L**	75.34	93.877	15.96	0.235	-0.0905	-0.035	-0.31	1.10

* Feed is bituminous coal
** Feed is lignite

S_b = Base Stream Factor (The value used in this study
was a stream factor of 0.95 or 348 operating
days per year)

f_P = Gas Price Adjustment Coefficient For Raw Coal
Price Changes (¢/Million Btu)/($/Short Ton)

f_B = Gas Price Adjustment Coefficients For Capital
Equipment Cost Changes (¢/Million Btu)/($ Million)

f_S = Gas Price Adjustment Coefficients For Stream
Factor Changes (¢/Million Btu)/(Operating Days/Year)

The values for f_P, f_B and f_S are listed in Table 9 for each of the
alternate coal gasification processes.

A direct comparison of the sensitivity of these variables with each
other is not easy because each has a different base; however, using the
averaged values for the gas prices, total equipment costs and the respective
adjustment coefficients, as given in Table 9, a 10% (or 40¢/ton) increase
in the raw coal cost will cause the gas price to increase by 4.6¢/million
Btu, while a 10% change in total capital investment would cause only a
2.7¢/million Btu rise, and a 10% decrease in the number of plant operating
days per year would increase the gas price by 3.4¢/million Btu.

The sensitivities of certain cost accounting rates were also
studied since changes in their base values would certainly be reflected
in the final product gas price. The "Debt Rate" is that portion of the
total capital investment which is considered as debt (65% in this study),
the remainder (35%) being equity. The debt is retired on a straight-line
depreciation over a 20-year period. The "Interest Rate" in this study
was set at 5%, probably rather low according to the current market values.
The "Gross Return-On-Rate Base" is the total fixed investment (which
depreciates over the 20-year period) plus the fixed working capital which
is defined as one month's inventory of raw materials (including raw coal)
plus the accounts receivable for one month. The "Gross Return Rate" is
considered to be the interest on the debt plus the net income available
for dividends and is assumed in this study to be 7% of the "Gross Return-
On-Rate Base".

Since the rate of change of the 20-year averaged gas is linear with
respect to these terms, the sensitivities can be considered additive.

$$\Delta C = (C - C_b) = f_D (D - D_b) + f_I (I - I_b) + f_R (R - R_b) \qquad (9)$$

where; D = Actual Debt Ratio,%

D_b = Base Debt Ratio (Assumed in this study to be
65%).

I = Actual Interest Rate, %

I_b - Base Interest Rate (Assumed in this study to be 5%)

R = Actual "Gross Return Rate",%

R_b = Base "Gross Return Rate" (Assumed in this study to be 7%).

f_D = Gas Price Adjustment Coefficient for Changes in the Debt Ratio (¢/Million Btu)/(Unit%)

f_I = Gas Price Adjustment Coefficient for Changes in the Interest Rate (¢/Million Btu)/(Unit%)

f_R = Gas Price Adjustment Coefficient for Changes in the "Gross Return Rate" (¢/Million Btu)/(Unit%).

The values of f_D, f_I and f_R for each of the coal gasification plant alternative processes are listed in Table 9. A quick comparison of the coefficients indicates that the gas price would be most sensitive to changes in the value of the "Gross Return Rate", while corresponding changes in the interest rate and in the debt ratio would affect the gas price to much smaller amounts.

       Boiler efficiency and power generation efficiency were assumed to be 75% and 35%, respectively, in this study. In view of the recent developments in technology producing more efficient boiler designs for large operation units and better power cycles through various combinations of power generation systems, the overall thermal efficiencies for the gasification plant would certainly improve. The processes which require larger amounts of steam and/or electrical power will be affected more directly by these efficiency improvements. For example, Alternative IV requires a large amount of electrical power to indirectly heat the synthesis gas generator. The effects on the overall thermal efficiencies of certain selected alternates by increasing the steam generation efficiency and the electrical power generation efficiency are shown below.

Boiler Efficiency	75%	90%	
Power Generation Efficiency	35%	40%	
	Thermal Efficiencies		
Alternate I-2	64.1%	64.9%	
Alternate II-2	53.0%	53.7%	
Alternate II-3	68.1%	69.6%	
Alternate III-1	61.4%	62.0%	
Alternate III-2	77.8%	79.0%	
Alternate IV-Bituminous	49.8%	51.6%	54.5%*

* Boiler Efficiency of 90%, Power Generation Efficiency of 50%

5.0 DISCUSSION AND CONCLUSIONS

5.1 Relationship Between Gas Price and Process Efficiency

The price of gas is significantly affected by the cost and utilization efficiency of a coal fed to the integrated gas plant. It is shown by comparing the values given in Tables 3 and 7 that the gas price and the thermal efficiency are directly related and that roughly 30 to 60% of the gas price can be associated with that of the raw coal, depending on the cost.

5.2 Sensitivity of the Cost of Coal and Lignite

The changes of gas price with different costs of coal are indicated by the values in Table 9. Gas prices from the gasification processes feeding lignite are lower than those feeding bituminous coal. However, a more detailed study should be made comparing the gasification characteristics of different ranks of coal and lignite.

5.3 Equipment Cost

In gasification processes, the combined cost of the oxygen production plant and the associated power generation plant accounts for roughly 40% of the total equipment cost. The equipment costs for the gasification reactor units and the gas purification systems represent the next most expensive items among the capital equipment costs.

5.4 Pretreatment of Raw Coal

Pretreatment of coal to prevent agglomeration in the gasifier results in approximately a 6 to 19 percent weight loss of the coal, losing not only reactive carbon but also valuable hydrogen. Research efforts directed toward the development of gasification systems utilizing raw coal or a less severe pretreatment of the coal as well as an effective recovery of the volatile waste in the pretreatment step would be desirable.

For example, if a noncaking bituminous coal of the same composition as given in Table 1 were used as the feed to the processes requiring pretreated coal, the process efficiencies would be improved as shown below.

	Coal Feed With Pretreatment		Coal Feed Without Pretreatment	
	Thermal Efficiency	Carbon Efficiency	Thermal Efficiency	Carbon Efficiency
Alternate I-1	46.4%	26.8%	55.5%	30.4%
Alternate II-1	56.2%	32.3%	68.5%	36.9%
Alternate II-2	53.0%	29.5%	64.5%	33.7%
Alternate III-1	61.4%	35.5%	75.2%	40.8%
Alternate IV-Bituminous	49.8%	28.51%	58.6%	31.8%

If the coal must be pretreated, the degree of pretreatment must be just enough to reduce the agglomerating properties of the coal particle to an acceptable level. As much as possible of the valuable volatile matter should be retained with the coal being fed to the gasification reactors. It has been suggested that in order to reduce the loss of the desirable volatile hydrocarbons, the temperature of pretreatment should be low and the time of heating of the coal particle should be short. These conditions can be approached by a flash volatilization of small coal particles. [15]

5.5 High Pressure Solid Feeding

A problem common to every coal gasification process is the uniform feeding of coal particles into high-pressure reactors. The feeder must be able to feed pulverized coal into the gasification reactor operating at high pressure and high temperatures and be capable of steady controllable operation. The technical aspects of feeding coal to provide a uniform distribution of the coal particles into a large diameter gasifier without causing agglomeration has not been fully developed, nor have the problems associated with removing solid matter such as ash or char from high pressure and high temperature reactors been completely solved. As shown in the sensitivity study results concerned with the stream factor (the days of operation per year) of the gasification plant), the gas prices are quite sensitive to the downtime of the unit. This means that the shutdown of the plant due to mechanical failures will significantly affect the averaged gas manufacturing cost. In order to maintain a smooth operation of the gasification plant, much work is needed to devise reliable coal feeders for high pressure and high temperature gasifiers.

5.6 Effect of Pressure of Gasifier Operation

In this study, the gasification reaction systems (with the exception of Alternate V) were assumed to operate at approximately 1000 psi pressure so that the product gas could be tied directly with high pressure pipeline distribution systems. In addition, the kinetics of hydrogasification reaction is much more favorable at higher pressures. High pressure will likely reduce the equipment size and eliminate the final stage of gas compression, but the needed increase in vessel and piping wall thickness, etc., may counteract the savings. A rough study made on the effect of the operating pressure for potential cost savings indicated that reaction system pressures high enough to match pipeline pressure are likely to provide the optimum system.

5.7 Methane Formation by Devolatilization, Hydrogasification and Methanation

The main routes for methane formation in an integrated coal gas-ification process are: (a) devolatilization of the coal, (b) hydrogenolysis of the coal (the carbon-hydrogen reaction, Reaction (3)), and (c) the catalytic methanation of hydrogen and carbon monoxide. Thermodynamically, the production of methane by direct coal-hydrogen reactions utilizing devolatilization and hydrogenolysis is more efficient than the carbon monoxide-hydrogen reaction (the methanation reaction, Reaction (6)).

The amount of gas produced by the devolatilization depends mainly on the type of coal fed and the arrangement of the devolatilizer chamber. In Alternates I-2, II-3 and III-2, raw coal without any pretreatment is charged directly into the gasifier. This permits the volatile matter of the coal to be fully utilized as potential product. As indicated in Table 3, the thermal efficiencies of the processes using a raw coal feed are higher than those with a pretreated coal feed.

The hydrogenolysis of coal (the carbon-hydrogen reaction) is affected by the activity of the char produced from devolatilization. There is evidence that the free energy of formation of fresh-formed carbon can be 2,600 calories/gram-mole more than that of graphite. [16] It has been postulated [10], [36], [37], [38] that the primary solid phase product of the initial breakdown of coal by the devolatilization is a highly active species or intermediate. This intermediate is then involved in two com-peting reactions; namely, the polymerization among the active intermediates themselves to form inactive char and the carbon-hydrogen reaction to form methane. Once the inactive char is formed, it is relatively inert to reaction with hydrogen. To depress the polymerization of the active intermediate, good contact of freshly formed char with the hydrogen-rich gas stream is necessary.

Catalytic methanation of CO and H_2 is a comparatively inefficient method to produce methane from coal. However, due to the specification that the product pipeline gas would have a CO content lower than 0.2% the methanation is a necessary step in an integrated coal gasification process. It appears that, from the optimum efficiency point of view, the final methanation step should be used only to convert the final traces of the CO in the product and that as much as possible of the methane should be generated in the gasification subsystem. Producing a major portion of the methane in the catalytic methanation stage would tend to lower the overall efficiency of the gasification process.

5.8 Extraction of Char from the Gasifier

In a self-sustaining coal gasification plant, the facilities for generating steam, electrical power and oxygen must be included in the design.
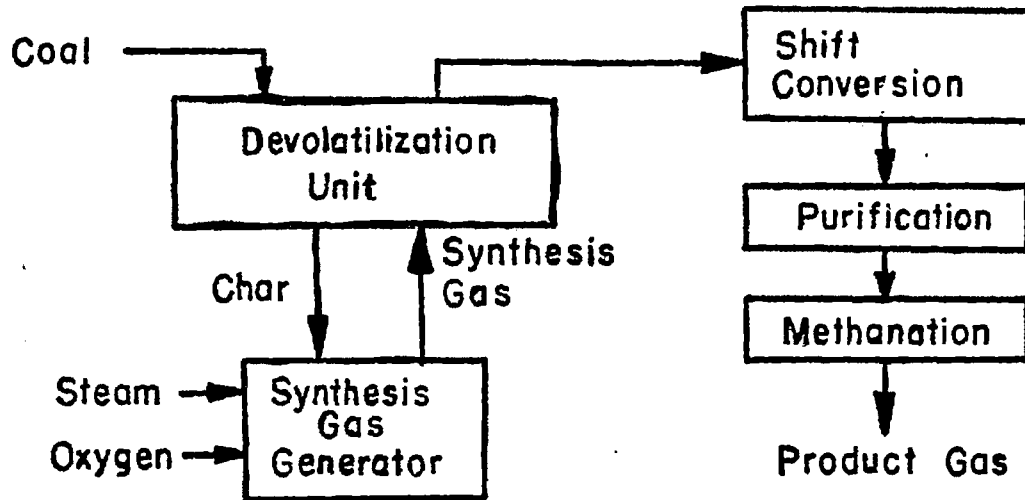
It would be desirable to use the by-product char from the gasifier as fuel to these units to combat at least the following two problems; (a) the problem of disposing of this by-product which has a rather low carbon content but is still combustible, and (b) the problem of the SO_2 pollution-controls required if raw coal were to be burned in the steam and power generation unit.

Char can be discharged from the high-temperature carbon-steam-oxygen gasifier as a completely-reacted residue or a partially-reacted char can be removed from the gasification system between the hydrogasifier and the synthesis gas generator. The hydrogenated char has a much higher carbon content than does the residue char. For a gas manufacturing plant with a fixed final product capacity, using hydrogenated char would increase the amount of fresh raw coal charged to the overall system. This would also mean that the desired gases; CH_4, H_2, and CO; could be more efficiently produced by utilizing the increased amount of volatile matter in the fresh coal supply. However, the increase in fresh raw coal charged to the gasifier would also mean an increase in the oxygen contained in the raw coal, with the oxygen eventually forming CO, CO_2 and H_2O. Since the CO content in the final pipeline gas product is specified to be lower than 0.2%, the increase of the CO content in the devolatilizer effluent will be directly related to a larger final methanation unit and to a lower overall utilization efficiency. Because at the optimum conditions the amount of hydrogenated char removed from the gasification phase is not enough to generate the total amount of steam and electricity required, the additional fuel for utility purposes must be provided by a certain amount of raw coal. The steam and electricity required for the process might be produced by an arrangement similar to the low-Btu fuel gas production scheme followed by combined cycle power generation to be an efficient and pollution-free method of producing steam and electricity.

5.9 Shift Conversion

In the coal gasification processes the shift conversion is used to either produce hydrogen or to adjust the composition ratio of H_2 to CO to the desired value for subsequent methanation. An interesting study has been made comparing the efficiencies of two positions of the shift conversion unit in the process system, as pictured in Figure 6. In the gasification by synthesis gas method, the CO and H_2 mixture formed in the high temperature secondary gasifier is fed directly back into the de-volatilizer. The resulting effluent from the devolatilizer must be shifted to the proper composition for the final methanation step. In the hydrogen gasification scheme, the gas from the synthesis gas generator is shifted to a hydrogen-rich composition and purified to remove the carbon dioxide before being injected into the hydrogasification unit. The effluent from the hydrogasifier has a composition suitable for direct catalytic methanation without further shifting. An optimization study made on these two flow schemes and the intermediate schemes indicates that the hydrogasification
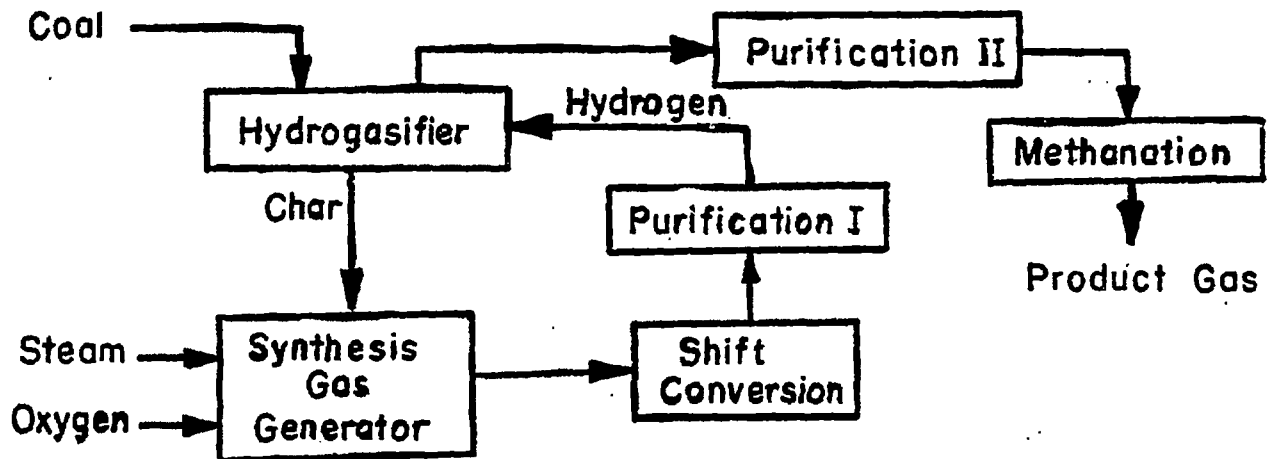
Figure 6. Alternate Positions for the Shift Conversion
Unit in the Plant Flowsheet

method is more thermally efficient than is gasification by synthesis gas. This conclusion can be explained by the following two reasons: (a) The contact of the hydrogen-rich gas with the coal will enhance both the hydrogenolysis of the volatile matter and the carbon-hydrogen reaction in the hydrogasification phase, both methane-forming reactions having a comparably higher thermal efficiency than do the reactions in the methanator unit. (b) The amount of steam required to shift the synthesis gas, estimated by Reaction (2), depends very heavily on the amount of carbon monoxide present in the inlet gas stream to the shift converter. In the case of the synthesis gas gasification, considerably more steam could be required to shift the gas composition since a larger proportion of the product carbon follows the carbon monoxide route to become methane than in the hydrogasification scheme. A larger utilization of steam means a corresponding decrease in the thermal efficiency of the overall gasification process.

5.10 Sulfur Recovery

To prevent environmental pollution, the H_2S removed from the product gas stream in the gas purification unit is treated by the Claus Process and/or the Stretford Process to convert the H_2S to elemental sulfur, the most inert sulfur state with respect to potential pollution. Because of the predicted oversupply of sulfur in the near future, no credit for selling this potential by-product is assumed in the projected gas price. It is assumed in this study, however, that enough of the sulfur will be sold to pay for the operating expenses of the sulfur recovery plant. Thus, the cost of equipment for the sulfur recovery plant, but not the operating expenses of that plant nor the cost of storing the solid sulfur, is considered in the gas price calculation. Since properly stored elemental sulfur represents minimum harm to the environment, the solid sulfur can be stockpiled if there is no immediate market for its disposal.

5.11 Catalytic Methanation

The catalytic methanation of a gas stream having relatively low concentrations of CO (in the 3% CO or less range) has been practiced in fixed bed reactors for many years. However, the coal-to-gas conversion processes proposed in this study require the catalytic methanation of a gas stream having as much as 15-20% CO, a concentration range which has not as yet been treated in a large-scale methanation system.

The catalytic methanation reaction, Reaction (6), is highly exothermic and heat transfer problems when directly treating large CO concentrations rules out the use of the fixed bed reactor unless a large gas recycle scheme is used to effectively dilute the CO concentration contacting the catalyst. Large recycle flows through the reactor are technically possible, but the capital cost and operating expenses will amount to a significantly large sum. Also, in a recycle stream there tends to be a build-up of trace compounds whose long term effect on the catalyst useful life is not now known. A better reaction system with regard to improved heat transfer characteristics is needed and a fluidized bed reactor seems to be a logical candidate, but most of the catalysts developed to date have poor abrasion properties which renders them unsuitable for use in a fluid bed. A number of alternate

methanation processes are being developed under the sponsorship of the U. S. Office of Coal Research to treat high concentrations of CO in the gas stream. The U. S. Bureau of Mines is developing a methanation reactor in which Raney nickel catalyst is spray-coated onto tube walls, the gas passing through and contacting the catalyst on either the inside or outside of the tubes while a heat-transfer medium contacts the other side. The search must continue for rugged catalysts and improved reaction chambers to treat these higher CO concentrations.

5.12 Limitations of this Study

The major assumption made in this study which cannot be proven without actual operating experience is whether the proposed system is mechanically operable. In this area we claim no expertise and must rely on the assurances of the various agencies developing the processes that the recognized and/or hidden difficulties are all solvable and none will cause enough of a problem to drastically alter the process. Some of the problems associated with these processes have been discussed, but actual operation and experience will be required to validate the assumption that the problems can be resolved.

Not only the initial mechanical operation of the proposed systems, but also the reliability of most of the processes to operate continuously for long periods of time remains untested. The "stream factor" adjustment coefficients given in Table 9 indicate that the 20-year average cost of the manufactured high-Btu gas will increase about 1.3% for every ten days the plant stands idle. This cost debit value does not include the high cost of any non-routine maintenance or system revision caused by unreliable equipment or processes. It is likely that, since the plant capital costs and the gas manufacturing costs of the various alternates do not vary by more than 18% from the averaged cost for all the alternates, the comparative reliability of the processes, more than the simple comparison of the thermal efficiencies, will carry a substantial weight in deciding which process alternative is best.

Another factor not explicitly considered in this study is the effect on the overall plant cost of large concentrations of undesirable trace compounds in the waste streams, either as gaseous wastes or liquid wastes. Treatment to prevent the discharge of such a toxicant may substantially increase the size and cost of the required treatment facilities.

5.13 Effect of the Plant on the Surroundings

Although this study was confined to the technical aspects of the coal-to-gas conversion processes, mention must be made of the impact that such a plant will have on the local environment where it is located. One plant producing 250 million cubic feet per day of pipeline gas would require at least 21,600 tons/day of coal (7.5 million tons per year),

which is 25% more coal than is produced in the largest coal mine in the United States. Associated with this enormous mining operation will be the control problems of acidic mine drainage pollution, preparation plant pollution problems and refuse disposal. The gasification plant will consume more than 2.8 million gallons per day of non-recoverable process water and 21.0 million gallons per day of make-up water to the cooling water system (6% blowdown). In many Appalachian regions this represents a significant portion of the available high-quality surface water. Beside the product gas, the plant will reject over 450 tons of elemental sulfur and almost 2000 tons of char or ash each day, in addition to emitting 13,900 tons of carbon dioxide to the atmosphere through its stacks.

Aside from the known wasted by-products, there are potential trace pollutants from the process which can turn out to be enormous production headaches after the plant has been started up. Of considerable concern will be water contaminants such as ammonia, phenol and thiocyanates, air pollutants such as COS, mercaptans, CS_2, thiophenes, NO_x compounds, aromatics and others, and finally the sulfur, mercury and arsenic contents of the discarded solid char, ash and tars.

Increasing public awareness and concern for the environment will demand the maximum safeguards against process upsets and potentially offending wast disposal methods. Because of the huge size of these proposed plant ventures and the havoc that an improperly designed facility can impose on a locality, all aspects of the technical design must be studied with regard to maximum control over all air, water and waste disposal pollution treatment methods.

LITERATURE CITED

[1]   Air Products and Chemicals, Inc., "Engineering Study and Technical
        Evaluation of B.C.R. 'Two-Stage Superpressure Gasification
        Process'", APCI Project No. 00-0-1234, Report prepared for
        the Office of Coal Research, O.C.R. Contract No. 14-32-0001-
        1204, September 1970.

[2]   Beveridge, G.S.G.,and R.S. Schechter, Optimization Theory and
        Practice, McGraw-Hill, New York, 1970.

[3]   Box, M.J., "A New Method of Constrained Optimization and a Com-
        parison With Other Methods", Computer Journal, Vol. 8, No. 1,
        1965, pp. 42-52.

[4]   Clancey, J.T., U.D. Marwig and D.R. Lindahl, "Pipeline Gas From
        Lignite Gasification - Current Commercial Economics", R & D
        Report No. 16, Interim Report No. 4, Office of Coal Research,
        U. S. Department of the Interior, May 9, 1969.

[5]   Cover, A.E., W.G. Schreiner and G.T. Skaperdas, "The Kellogg Coal
        Gasification Process", Paper presented before the 162nd National
        Meeting, American Chemical Society, Division of Fuel Chemistry,
        Washington, D.C., September 13-17, 1971; Preprints of meeting,
        Vol. 15, No. 3, pp. 1-11.

[6]   Curran, G.P., J.T. Clancey, D.A. Scarpiello, C.E. Fink and E. Gorin,
        "Carbon Dioxide Acceptor Process", Chemical Engineering Progress,
        Vol. 62, No. 2, February 1966, pp. 80-86

[7]   Curran, G.P., C.E. Fink and E. Gorin, "CO_2 Acceptor Gasification
        Process: Studies of Acceptor Properties", Fuel Gasification,
        Advances In Chemistry Series No. 69, American Chemical Society,
        Washington, D. C., 1967, pp. 141-165.

[8]   Denn, M.M., Optimization by Variational Methods, McGraw-Hill, New
        York, 1969.

[9]   Farnsworth, J.F.,and R.A. Glenn, "Status and Design Characteristics
        of the BCR/OCR BI-GAS Process", Paper presented before the 162nd
        National Meeting, American Chemical Society, Washington, D.C.
        September 13-17, 1971; Preprints of meeting, Vol. 15, No. 3,
        pp. 12-31.

[10]   Feldmann, H.F., W.H.Simons, J.A. Mima and R.W. Hiteshue, "Reaction
        Model for Bituminous Coal Hydrogasification in a Dilute Phase",
        Paper presented before the 160th National Meeting, American
        Chemical Society, Division of Petroleum Chemistry, Chicago, Illinois
        September 13-18, 1970.

[11]   Feldmann, H. F., P.M. Yavorsky, C.Y. Wen, and W.H. Simons, "Supplemental
         Pipeline Gas from Coal by the Hydrane Process", Paper presented
         at the 71st National Meeting, American Institute of Chemical
         Engineers, February 20-23, 1972, Dallas, Texas.

[12]   Forney, A.J. ,and W.P. Haynes, "The Synthane Coal-To-Gas Process:
         A Progress Report", Paper presented before the 162nd National
         Meeting, American Chemical Society, Division of Fuel Chemistry,
         Washington, D.C., September 13-17, 1971; Preprints of meeting,
         Vol. 15, No. 3, pp. 32-39.

[13]   Gambs, G.C.,and A.A. Rauth, "The Energy Crisis", Chemical Engineering,
         May 31, 1971, pp. 56-68.

[14]   Glenn, R.A., E.E. Donath and R.J. Grace, "Gasification of Coal Under
         Conditions Simulating Stage 2 of the BCR Two-Stage Super-
         Pressure Gasifier", Fuel Gasification, Advances in Chemistry
         Series No. 69, American Chemical Society, Washington, D.C.,
         1967, pp. 81-103.

[15]   Henry, J.P., Jr.,and B.M. Louks, "An Economic Study of Pipeline Gas
         Production from Coal", Chemical Technology, April 1971,
         pp. 238-247.

[16]   Hottel, H.C.,and J.B. Howard, New Energy Technology: Some Facts
         and Assessments, the MIT Press, Cambridge, Massachusetts, 1971.

[17]   Institute of Gas Technology, "Addendum - Proposal for Development
         of an Economic Process for Production of Pipeline Gas from
         Lignite", submitted to the Office of Coal Research, U.S.
         Department of the Interior, February 1964, 31 pages.

[18]   Knabel, S.J.,and C.L. Tsaros, "Process Design and Cost Estimate
         for a 258 Billion BTU/Day Pipeline Gas Plant - Hydrogasification
         Using Synthesis Gas Generated by Electrothermal Gasification
         of Spent Char", Office of Coal Research Contract No. 14-01-
         0001-381, Institute of Gas Technology, November 1967, 31 pages.

[19]   Lefrancois, P.A., K.M. Barclay and G.T. Skaperdas, "Bench-Scale
         Studies of the Kellogg Coal Gasification Process", Fuel
         Gasification, Advances In Chemistry Series No. 69, American
         Chemical Society, Washington, D.C., 1967, pp. 64-80.

[20]   Mills, G.A., "Gas From Coal - Fuel of the Future", Environmental
         Science and Technology, Vol. 5, No. 12, December 1971, pp.
         1178-1183.

[21]   Mills, G.A., "Progress in Coal Gasification, U.S. Bureau of Mines",
         Paper presented at the Third American Gas Association Synthetic
         Pipeline Gas Symposium, Chicago Illinois, September 17-18, 1970.

[22]   Mosher, D.R., U.D. Marwig and J.A. Phinney, "Basic Features of the
         CO_2 Acceptor Gasification Process", Paper presented before
         the 162nd National Meeting, American Chemical Society,
         Division of Fuel Chemistry, Washington, D.C., September 13-17,
         1971; Preprints of Meeting, Vol. 15, No. 3, pp. 40-51 .

[23]   Nelder, J.A.,and R. Mead, "A Simplex Method for Function Minimization";
        Computer Journal, Vol. 7, 1964, pp. 308-313.

[24]   Paviani, D.A., "A New Method for the Solution of the General
        Non-Linear Programming", Unpublished Ph.D. Dissertation,
        The University of Texas at Austin, 1969, pp. 42-47.

[25]   Sheldrick, M.G., "Coal Gasification Warms Up", Chemical Engineering,
        July 12, 1971, pp. 59-61.

[26]   Siegel, H.M., T. Kalina and H.A. Marshall, "Compilation of Gas
        Costs for Various Coal Gasification Processes", Paper reviewed
        by the Federal Power Commission – National Gas Survey, Synthetic
        Gas – Coal Task Force, Washington, D.C., Meeting, February 17-
        18, 1972.

[27]   Skaperdas, G.T., "Commercial Potential for the Kellogg Coal Gasification
        Process", R & D Report No. 38, Office of Coal Research, U.S.
        Department of the Interior, September 1967, 150 pages.

[28]   Tsaros, C.L., "Comparison of Economics of Processes for Making
        Pipeline Gas from Coal", Special Report, Office of Coal
        Research Contract No. 14-01-0001-331, Institute of Gas Tech-
        nology August 1967, 11 pages.

[29]   Umeda, T., "Optimal Design of an Absorber-Stripper System: Applica-
        tion of the Complex Method", Industrial and Engineering Chem-
        istry, Process Design and Development, Vol. 8, No. 3, July 1969,
        pp. 308-317.

[30]   Umeda, T.,and A. Ichikawa, "A Modified Complex Method for Optimiza-
        tion", Industrial and Engineering Chemistry, Process Design
        and Development, Vol. 10, No. 2, April 1971, pp. 229-236.

[31]   U.S. Bureau of Mines, "An Economic Evaluation of a Lurgi Gasification
        System (Including Mining and Coal Pretreatment) To Produce
        High-Btu Gas from Bituminous Coal, (250-Million-SCFD-High-
        Btu-Gas Plant)", Report No. 70-21-A and Workbook, Process
        Evaluation Group, Morgantown Research Center, U.S. Bureau of
        Mines, October 1970.

[32]   U.S. Bureau of Mines, "An Economic Evaluation of Fluidized Gasifica-
        tion at 40 Atmospheres Followed by Shift Conversion, Purification
        and Single-Stage Hot-Gas Recycle Methanation (Integrated Plant
        Including Mine)", Report No. 68-8 (Revised), Process Evaluation
        Group, Morgantown Research Center, U.S. Bureau of Mines, June
        5, 1969.

[33]   U.S. Bureau of Mines, "Status of the Synthane Coal-To-Gas Process",
        Pittsburgh Energy Research Center, U.S. Bureau of Mines,
        November 1971, 32 pages.

[34]   U.S. Bureau of Mines, "The Utilization of Lignite as a Source of
        Synthetic Pipeline Gas – An Economic Analysis", Process Evaluation
        Morgantown Research Center, U.S. Bureau of Mines, January 29,
        1964.

[35] ·Wen, C.Y., "Optimization of Coal Gasification Processes", R & D
      Report No. 66, Interim Report No. 1, Office of Coal Research,
      1972, Two Volumes.

[36] Wen, C.Y.,and J. Huebler, "Kinetic Study of Coal Char Hydrogas-
      ification: Rapid Initial Reaction", Industrial and Engineering
      Chemistry, Process Design and Development, Vol. 4, No. 2,
      April 1965, pp. 142-147

[37] Wen, C.Y.,and J. Huebler, "Kinetic Study of Coal Char Hydrogas-
      ification: Second-Phase Reaction", Industrial and Engineering
      Chemistry, Process Design and Development, Vol. 4, No. 2,
      April 1965, pp. 147-154.

[38] Zahradnik, R.L.,and R.A. Glenn, "The Direct Methanation of Coal",
      Paper presented before the 158th National Meeting of the
      American Chemical Society, Division of Fuel Chemistry,
      September 7-12, 1969, New York, New York.

<u>A P P E N D I X</u>

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A-1 INTRODUCTION

The Office of Coal Research Interim Report, "Optimization of Coal Gasification Processes" [35], was submitted for publication on September 15, 1971. In that report the study results of five alternative coal gasification processes were described. Since this time, three other process subalternates were simulated and optimized, and the computation results are presented here.

Alternate I-2 and Alternate III-2, described in this Appendix, are very similar to the previously described Alternate I (hereafter called Alternate I-1) and Alternate III (hereafter called Alternate III-1), respectively, except that in each case unique design arrangements of the gasification sections allow the feeding of raw coal directly into the gasification vessels, thus eliminating the pretreatment steps. In the Interim Report, the Alternate V process was examined only with respect to the gasification of lignite. Its use in converting bituminous coal to pipeline quality gas is examined here.

It must be clearly stated that the capital cost and gas manufacturing cost values presented here are relative values to be used for comparative purposes only. They are not to be considered as true estimations of the absolute cost of the gas because many influencing factors such as plant location, raw coal composition differences, the removal of trace components in the waste water stream, etc., were not considered.

A-2 ALTERNATE I-2

A-2.1 Process Description

The key difference between this process and Alternate I-1 is that the pretreatment of caking coals is performed in the same vessel as the gasification reactions. Thus, the thermally inefficient external pretreatment step is avoided and all the hydrocarbon precursors of methane contained in the raw coal are retained in the product gas stream. The gasifier vessel consists of three different zones; the devolatilization zone at the top, the dense-phase fluidized bed zone in the middle and the dilute-phase fluidized bed zone at the bottom. A diagram of the gasification subsystem is shown in Figure A-1 and a flowsheet for the overall process is shown in Figure A-2.

Prepared coal is directly charged to the devolatilization zone located at the upper part of the gasifier where the coal particles are immediately partially oxidized by steam and a minimum amount of oxygen to retard their agglomerating properties. The principal gases formed during the devolatilization phase are methane, carbon monoxide, and hydrogen. These gases enter the gasification zone to become part of the product gas stream, adding to the overall methane production of the system.

The dense-phase fluidized bed zone is located at the expanded midsection of the gasifier vessel. Coal particles dropping from the top chamber are fluidized by a stream of hot synthesis gas moving upward from the bottom chamber which allows the devolatilization reactions and the hydrogen-carbon reaction to be completed in this zone. Experimental data indicate that more than half of the ultimate product methane is formed in the top two zones. [21]

The dilute-phase fluidized bed zone located in the contracted bottom section of the gasification vessel is a synthesis gas producer. The synthesis gas is formed by reacting the char from the dense-phase fluidized bed with oxygen and steam. The temperature of the dilute-phase fluidized bed is around $1900^{\circ}F$. The hot synthesis gas (a mixture of H_2 and CO) flows upward into the middle chamber of the gasifier to be used as the fluidizing medium as well as the hydrogen source for the carbon-hydrogen reaction. Char residue is withdrawn as ash from the bottom of the gasifier, and the product gas stream leaves the vessel at a location between the top two zones.

The gasifier effluent passes through a water-gas shift converter to adjust the H_2/CO molar ratio to about 3:1 for the final methanation step. Before the gas stream from the shift converter is methanated, the CO_2 and H_2S are removed and the sulfur converted to the elemental form. The methanation reaction can be performed in several types of reaction systems such as the newly developed hot gas recycle system or the tube-wall reactor. However, depending on the CO concentration of the gas being methanated, it is believed that a suitable methanation scheme can be selected from the arrangements discussed in Chapter VII of the Interim Report. [35]

A-2.2 Results of the Overall Plant Optimization

Following the procedures described in the Interim Report [35], this
process was mathematically simulated and optimized using the overall plant
thermal efficiency maximization and the subsystem capital investment minimization
as the objective functions. At the optimum operating conditions based on
these optimization calculations, the material balances throughout the process
were computed, with the resultant quantities shown in Figure A-2 and the
compositions of the various gas streams listed in Table A-1.

Based on these flow-quantity values, the various process subsystems were
designed and the total bare equipment cost computed. Using the standardized
Office of Coal Research accounting procedure, the total capital investment was
calculated as $131,510,000, with the investment summary listed in Table A-2.
The annual operating expense breakdown is given in Table A-3, resulting in
an estimated 20-year averaged gas price of 68.75¢ per million Btu.

The process was then studied to determine the sensitivity of the gas
manufacturing price to changes in selected parameters. The gas price was
found to be significantly affected by variations in the purchase price of the
raw coal as shown in Figure A-3, the gas price changing 10.08¢/million Btu for
each $1/ton change in the raw coal purchase cost. The sensitivities of the
gas manufacturing price to changes in certain cost accounting rates are
illustrated in Figure A-4.
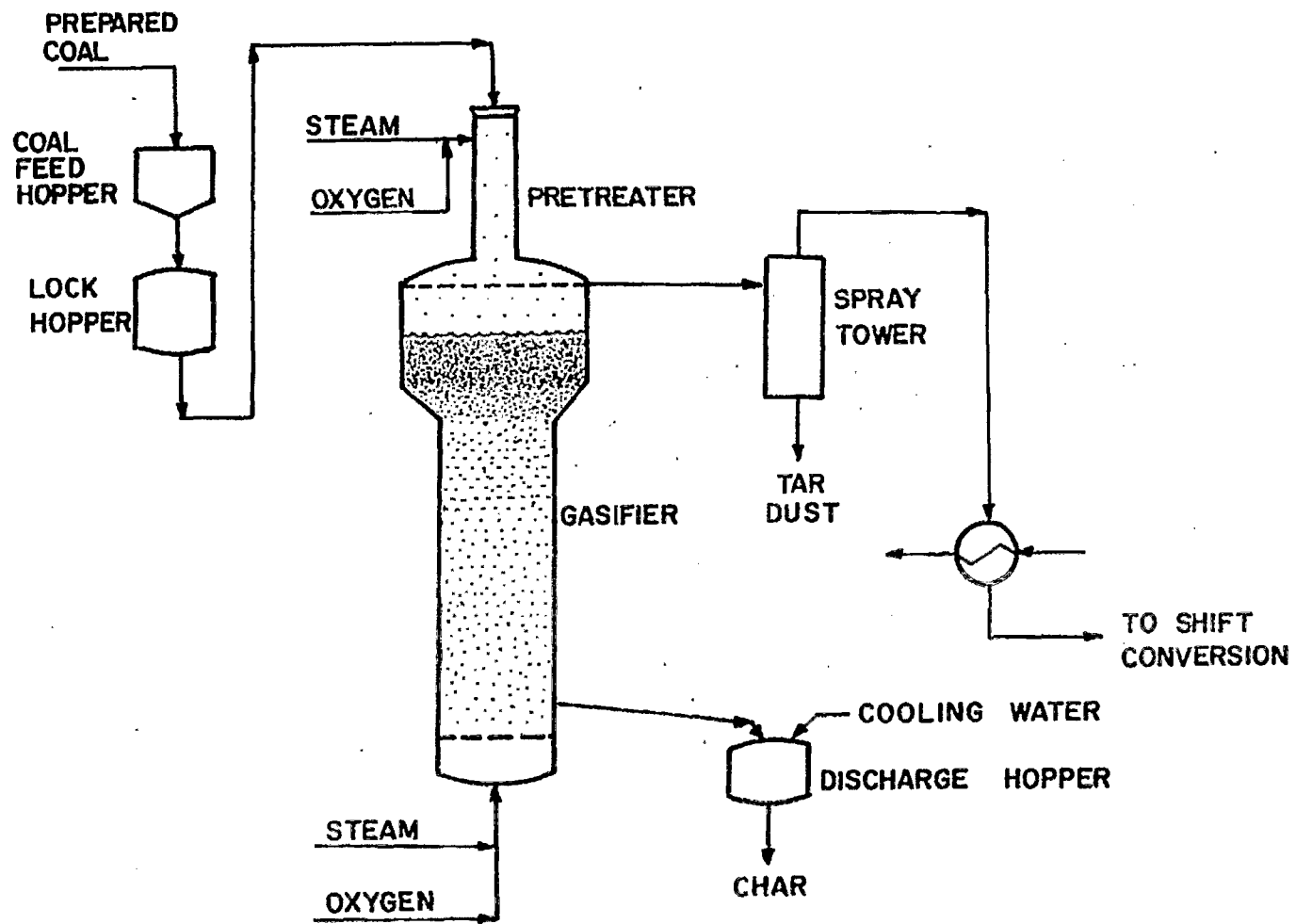
FIGURE A-1 GASIFICATION PHASE OF ALTERNATE I-2
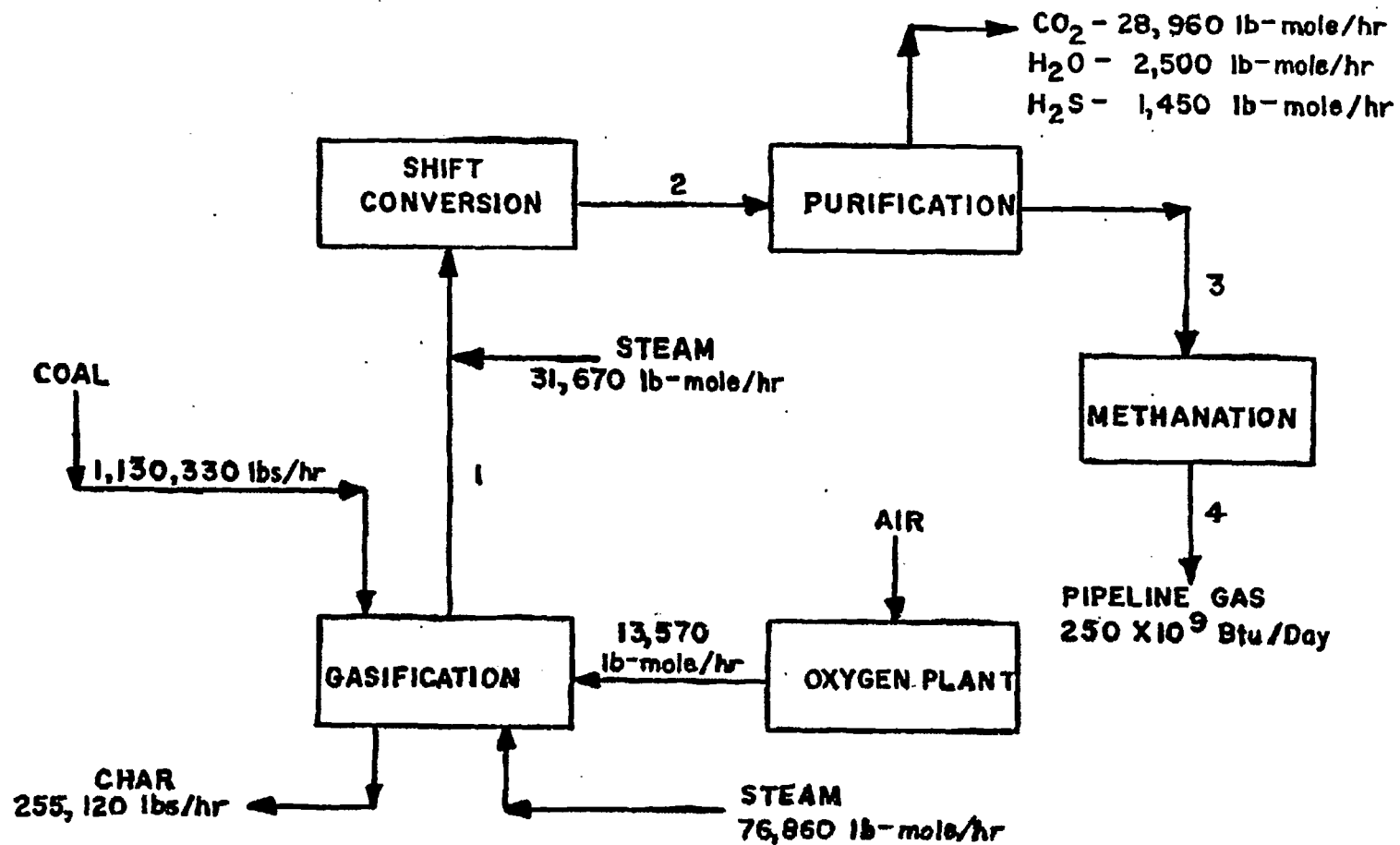
FIGURE A-2   FLOW DIAGRAM OF OVERALL GASIFICATION PLANT FOR ALTERNATE I-2

Table A-1   Gas Composition (Mole%) and Total Flow Rate
of Alternate I-2.

Stream No.*	1	2	3	4
CO_2	18.41	33.51	0.96	1.82
CO	11.66	9.38	15.72	0.12
CH_4	14.33	20.64	32.97	91.68
H_2O	37.51	3.00	0.25	0.46
H_2	16.56	30.81	49.22	4.26
H_2S	1.15	1.66	--	---
N_2	0.38	0.56	0.88	1.66
Flow Rate lb-mole/hr	126,780	88,000	55,090	29,220

*See Figure A-2 for stream number location

Table A-2

INVESTMENT SUMMARY FOR ALTERNATE I-2

	Bare Cost, $
Preparation and Storage	$ 14,616,000
Pretreatment	—
Gasification	4,500,000
Shift Conversion	2,683,000
Gas Purification	14,386,000
Methanation	1,691,000
Oxygen Production Plant	29,048,000
Electric Power Plant	16,747,000 ·
Sulfur Recovery Plant	6,210,000
Offsite Facilities	19,000,000
Subtotal, Bare Cost	$108,881,000
Contractor's Overhead and Profit	8,416,000
Interest During Construction	5,865,000
Total Fixed Investment	$123,162,000

Working Capital

30-Days Coal Inventory @ $4/Ton	$3,058,000	
30-Days Other Direct Material Inventory	62,000	
Accounts Receivable	5,228,000	
Total Working Capital	$8,348,000	8,348,000
Total Capital Investment		$131,510,000

Table A-3

ANNUAL OPERATING EXPENSE AND REVENUE
REQUIREMENT FOR ALTERNATE I-2

	$/Year
Raw Material (@ $4/Ton)	$ 34,861,000
Other Direct Materials	706,000
Direct Operating Labor	986,000
Maintenance	3,266,000
Supplies	490,000
Supervision	99,000
Payroll Overhead	108,000
General Overhead	2,420,000
Depreciation	6,158,000
Local Taxes and Insurance	3,695,000
Contingencies	1,056,000
Byproduct Credit	(1,350,000)
Operating Expense	$52,495,000
Gross Return, 20-Year Average	4,680,000
Federal Income Tax, 20-Year Average	2,429,000
Total Revenue Requirement	$59,604,000
20-Year Average Price of Gas, ¢/Million Btu	68.75¢
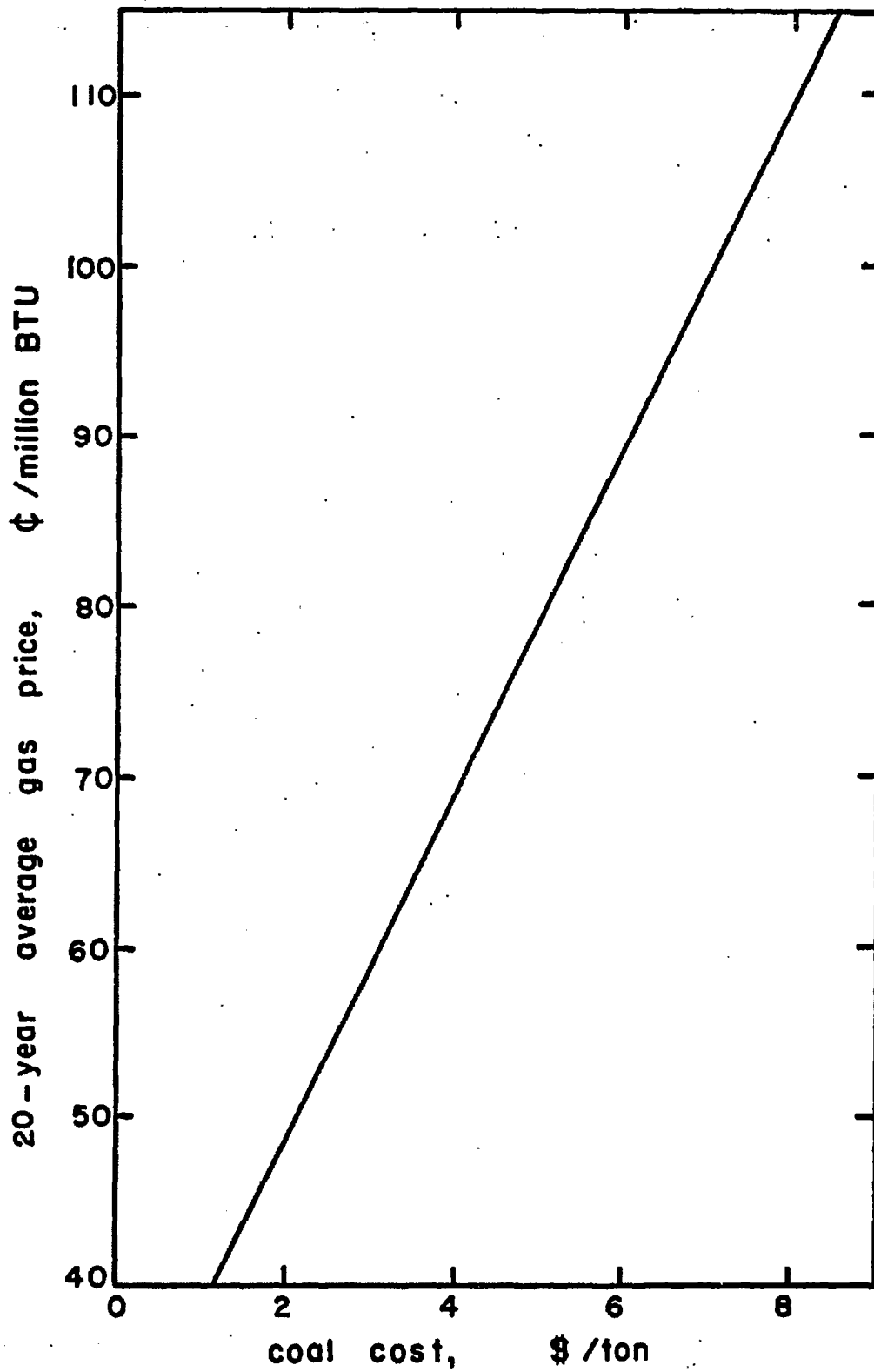
FIGURE A-3   PRICE OF GAS FROM ALTERNATE 1-2 AS FUNCTION
OF THE PURCHASE COST OF THE RAW COAL
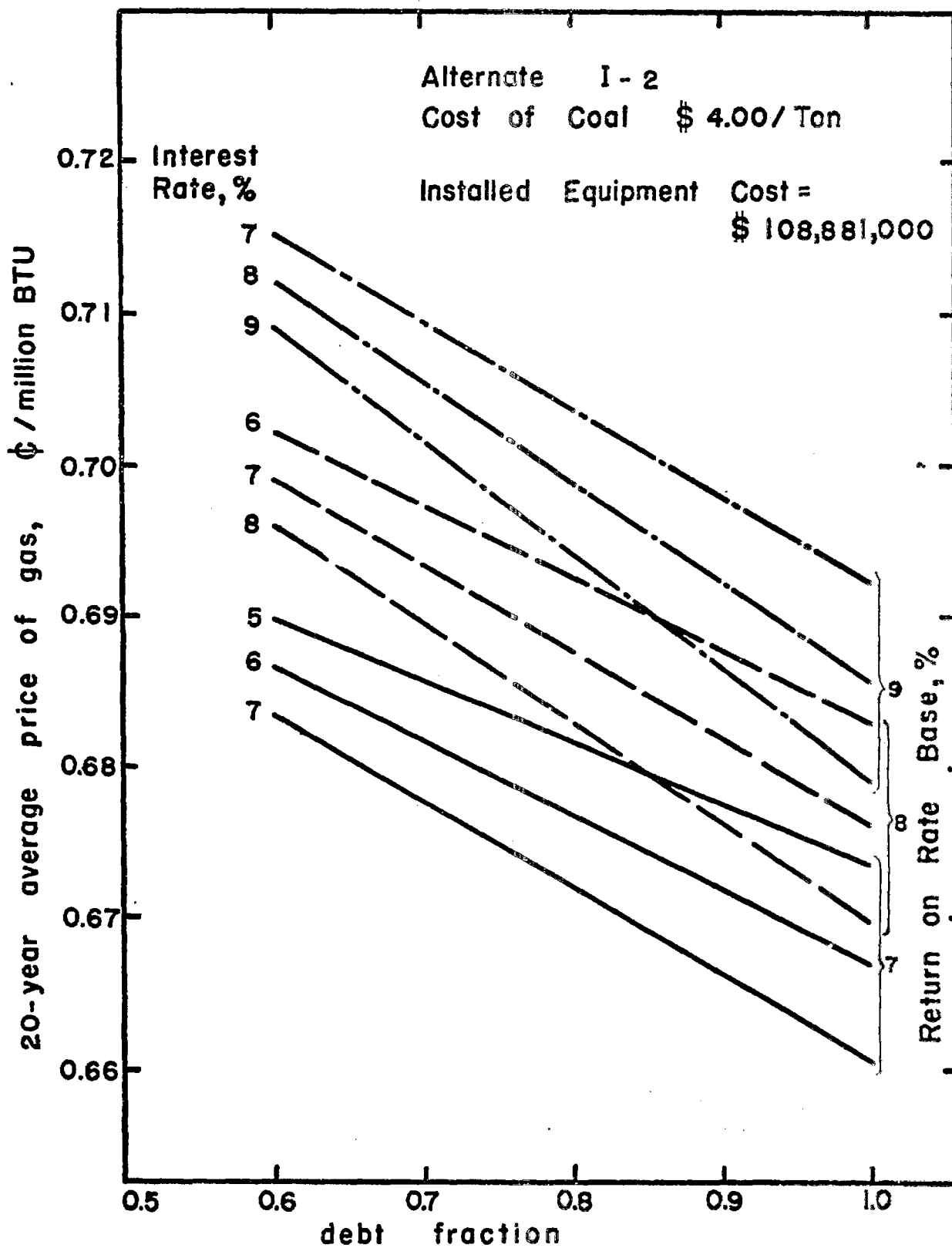
FIGURE A-4   EFFECT OF VARYING FINANCIAL FACTORS ON THE PRICE
OF PIPELINE GAS – ALTERNATE I-2

A-3 ALTERNATE III-2

A-3.1 Process Description

A schematic diagram of the gasification phase of this process is shown
in Figure A-5 and a flow scheme of the entire process is illustrated in
Figure A-6. This alternate involves a direct hydrogasification of the raw
coal in a unique two-stage reactor. Raw coal is charged to the upper stage,
named the dilute-phase devolatilizer section, where it is contacted with
a hot gas mixture of H_2 and CH_4 rising from the bottom stage. In this region
the coal is devolatilized and becomes a non-caking char. The gases produced
in the devolatilization reactions, consisting mainly of CH_4, H_2 and CO,
are mixed with the gas coming from the bottom stage to form the gasifier
effluent stream. The non-caking char produced in the devolatilizer falls
into the bottom stage, named the fluidized bed hydrogasifier section, where
partial gasification occurs in the presence of almost pure hydrogen. The
carbon-hydrogen reaction is considered as the principal reaction taking
place in this reaction zone. The residue char from this hydrogasifier vessel
is transported to a separate steam-oxygen gasifier where a synthesis gas of
CO and H_2 is produced. This gas mixture is further shifted and purified
producing the nearly pure hydrogen stream that is injected into the hydro-
gasifier.

The effluent gas leaving the hydrogasification vessel passes through
a second purification system where the H_2S and CO_2 are removed and then into
a final methanation step to convert the final traces of CO to CH_4.

A-3.2 Results of the Overall Plant Optimization

Following the procedures described in the Interim Report [35], this
process was mathematically simulated and optimized using the overall plant
thermal efficiency maximization and the subsystem capital investment
minimization as the objective functions. At the optimum operating conditions,
based on these optimization calculations, the material balances throughout the
process were computed, with the resultant quantities shown in Figure A-6
and the composition of the various gas streams listed in Table A-4.

Based on these flow-quantity values, the various process subsystems
were designed and the total bare equipment cost was computed. Using the
standardized Office of Coal Research accounting procedure, the total capital
investment was calculated as $125,412,000, with the investment summary listed
in Table A-5. The annual operating expense breakdown is given in Table A-6,
resulting in an estimated 20-year averaged gas price of 62.73¢ per million Btu.

The process was then studied to determine the sensitivity of the gas manufacturing price to changes in selected parameters. The gas price was found to be significantly affected by variations in the purchase price of the raw coal as shown in Figure A-7, the gas price changing 8.99¢/million Btu for each $1/ton change in the raw coal purchase cost. The sensitivities of the gas manufacturing price to changes in certain cost accounting rates are illustrated in Figure A-8.
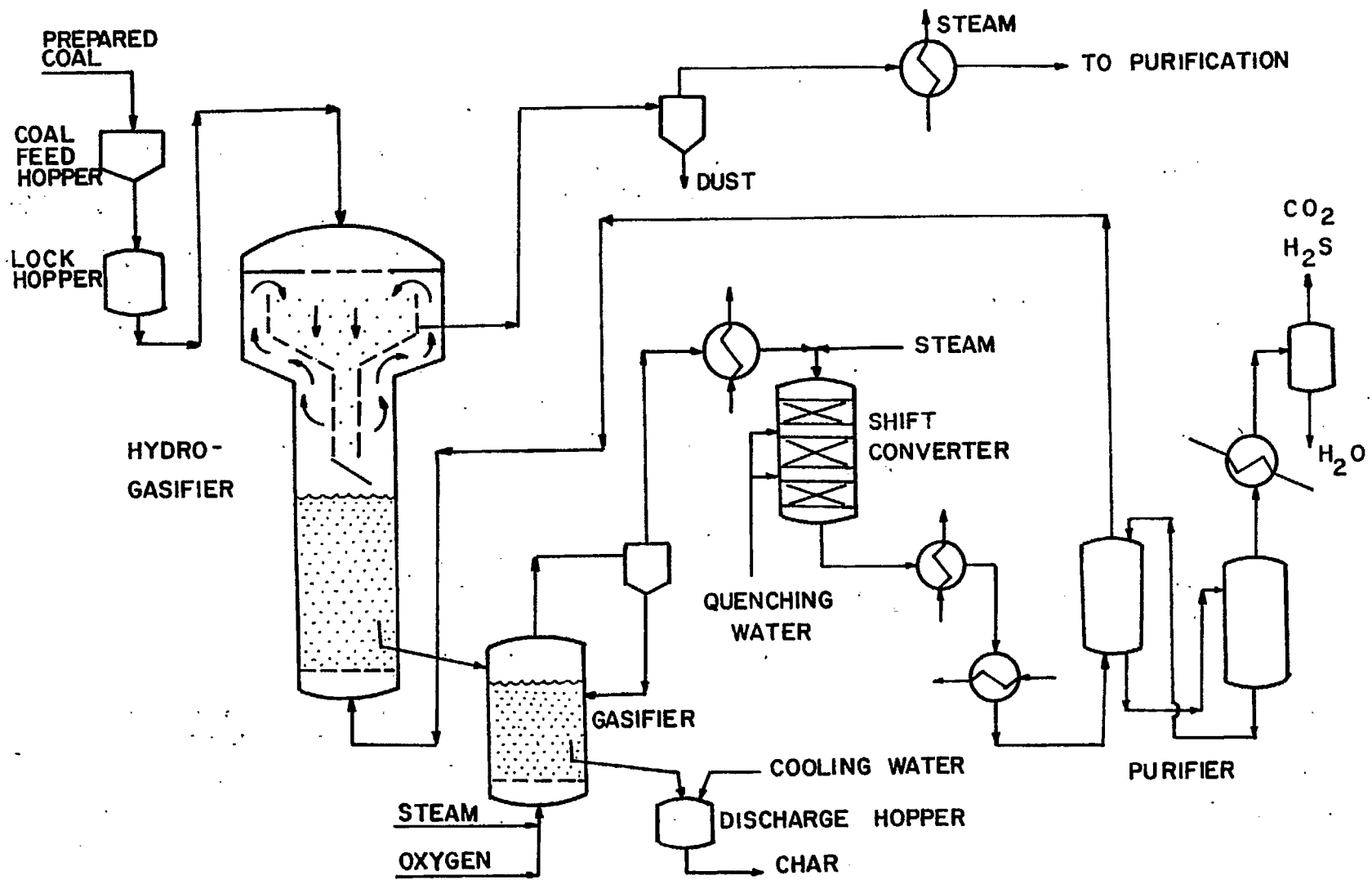
Figure A-5   Gasification Phase of Alternate III-2

CO_2 — 460 lb-mole/hr
H_2O — 3,660 lb-mole/hr
H_2S — 1,184 lb-mole/hr

COAL

918,850 lbs/hr

PURIFICATION

6

METHANATION

7

PIPELINE GAS
250 x 10^9 Btu/Day

5

DILUTE PHASE REACTOR

4

CO_2 — 25,800 lb-mole/hr
H_2O — 1,970 lb-mole/hr

HYDRO-GASIFICATION

3

PURIFICATION

2

SHIFT CONVERSION

AIR

OXYGEN PLANT

9,270 lb-mole/hr

GASIFICATION

1

STEAM
20,220 lb-mole/hr

STEAM
72,920 lb-mole/hr

CHAR
127,472 lbs/hr
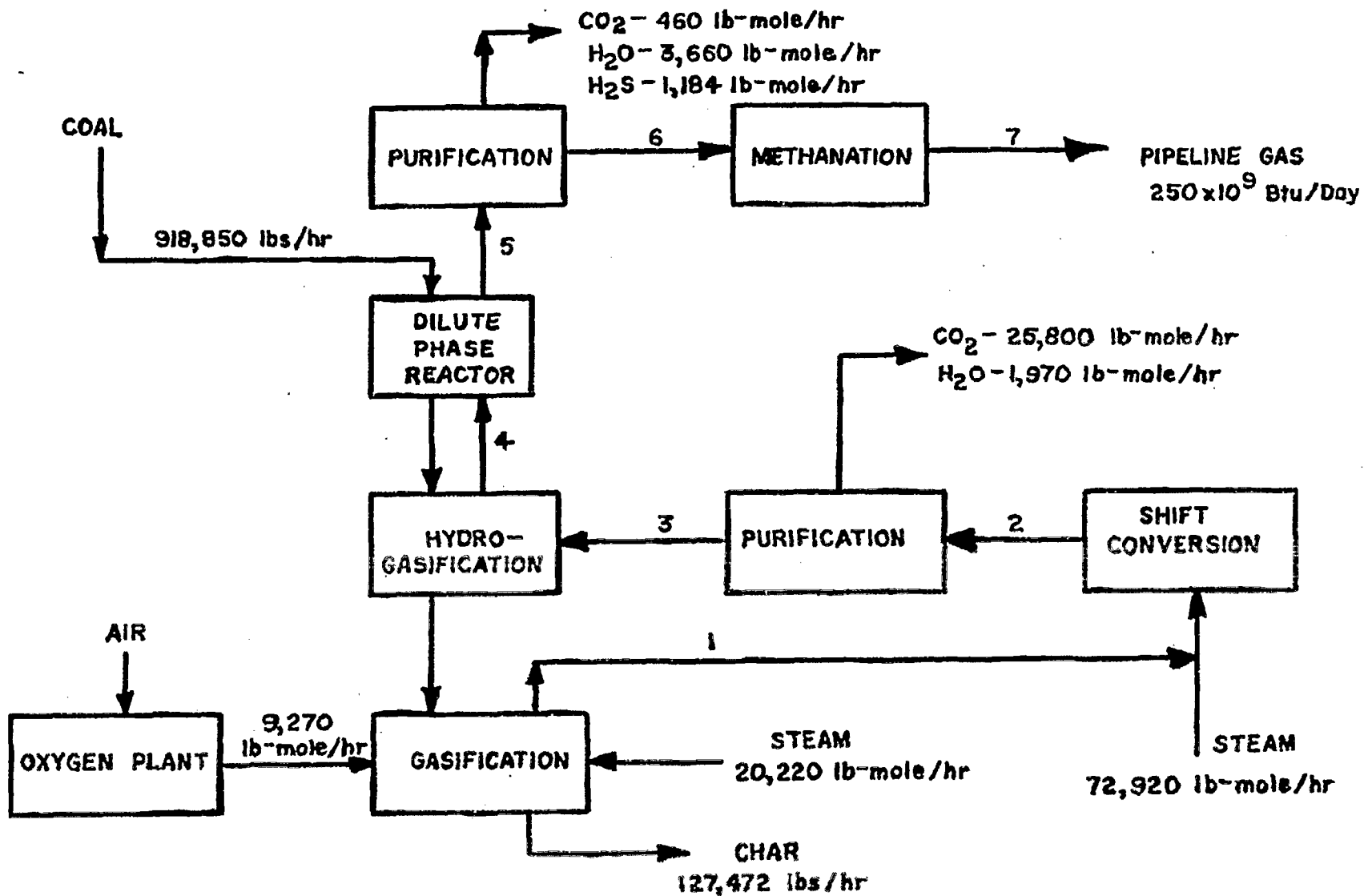
FIGURE A-6   FLOW DIAGRAM OF OVERALL GASIFICATION PLANT FOR ALTERNATE III-2

Table A-4 Gas Compositions (Mole %) and Total Flow Rate of Alternate III-2

Stream No.*	1	2	3	4	5	6	7
CO_2	9.21	38.88	1.16	1.71	1.16	--	--
CO	49.69	1.79	3.05	4.15	3.77	4.35	0.12
CH_4	--	--	--	47.59	62.10	71.68	87.35
H_2O	10.90	3.00	0.15	0.37	9.71	0.58	0.06
H_2	30.20	56.33	95.64	46.18	19.29	22.27	11.15
H_2S	--	--	--	--	2.98	--	--
N_2	--	--	--	--	0.99	1.12	1.32
Flow Rate lb-mole/hr	47,680	67,520	39,770	26,960	39,730	34,420	29,862

*See Figure A-6 for stream number location

Table A-5

INVESTMENT SUMMARY FOR ALTERNATE III-2

	Bare Cost, $
Preparation and Storage	$ 12,600,000
Pretreatment	—
Gasification	15,000,000
Shift Conversion	3,975,000
Gas Purification	11,800,000
Methanation	450,000
Oxygen Production Plant	23,100,000
Electric Power Plant	11,440,000
Sulfur Recovery Plant	6,950,000
Offsite Facilities	19,000,000
Subtotal, Bare Cost	$104,315,000
Contractor's Overhead and Profit	8,063,000
Interest During Construction	5,619,000
Total Fixed Investment	$117,997,000

Working Capital

30-Days Coal Inventory @ $4/Ton	$2,623,000	
30-Days Other Direct Material Inventory	21,000	
Accounts Receivable	4,771,000	
Total Working Capital	$7,415,000	7,415,000
Total Capital Investment		$125,412,000

Table A-6

ANNUAL OPERATING EXPENSE AND REVENUE
REQUIREMENT FOR ALTERNATE III-2

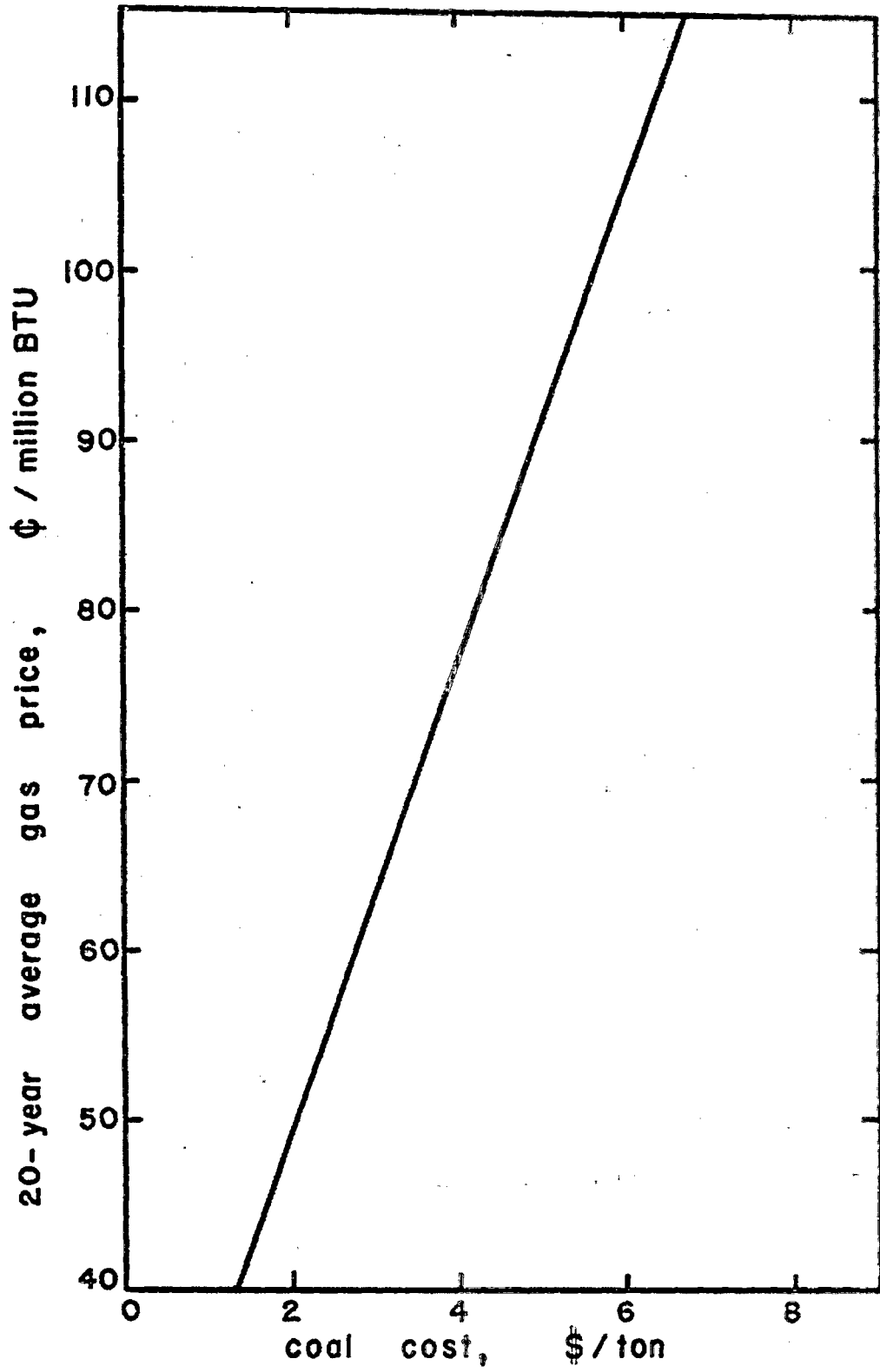|	$/Year
Raw Material (@ $4/Ton)	$29,908,000
Other Direct Materials	234,000
Direct Operating Labor	986,000
Maintenance	3,129,000
Supplies	469,000
Supervision	99,000
Payroll Overhead	108,000
General Overhead	2,342,000
Depreciation	5,900,000
Local Taxes and Insurance	3,540,000
Contingencies	934,000
Byproduct Credit	-
Operating Expense	$47,649,000
Gross Return, 20-Year Average	4,442,000
Federal Income Tax, 20-Year Average	2,296,000
Total Revenue Requirement	$54,387,000
20-Year Average Price of Gas, ¢/Million Btu	62.73¢
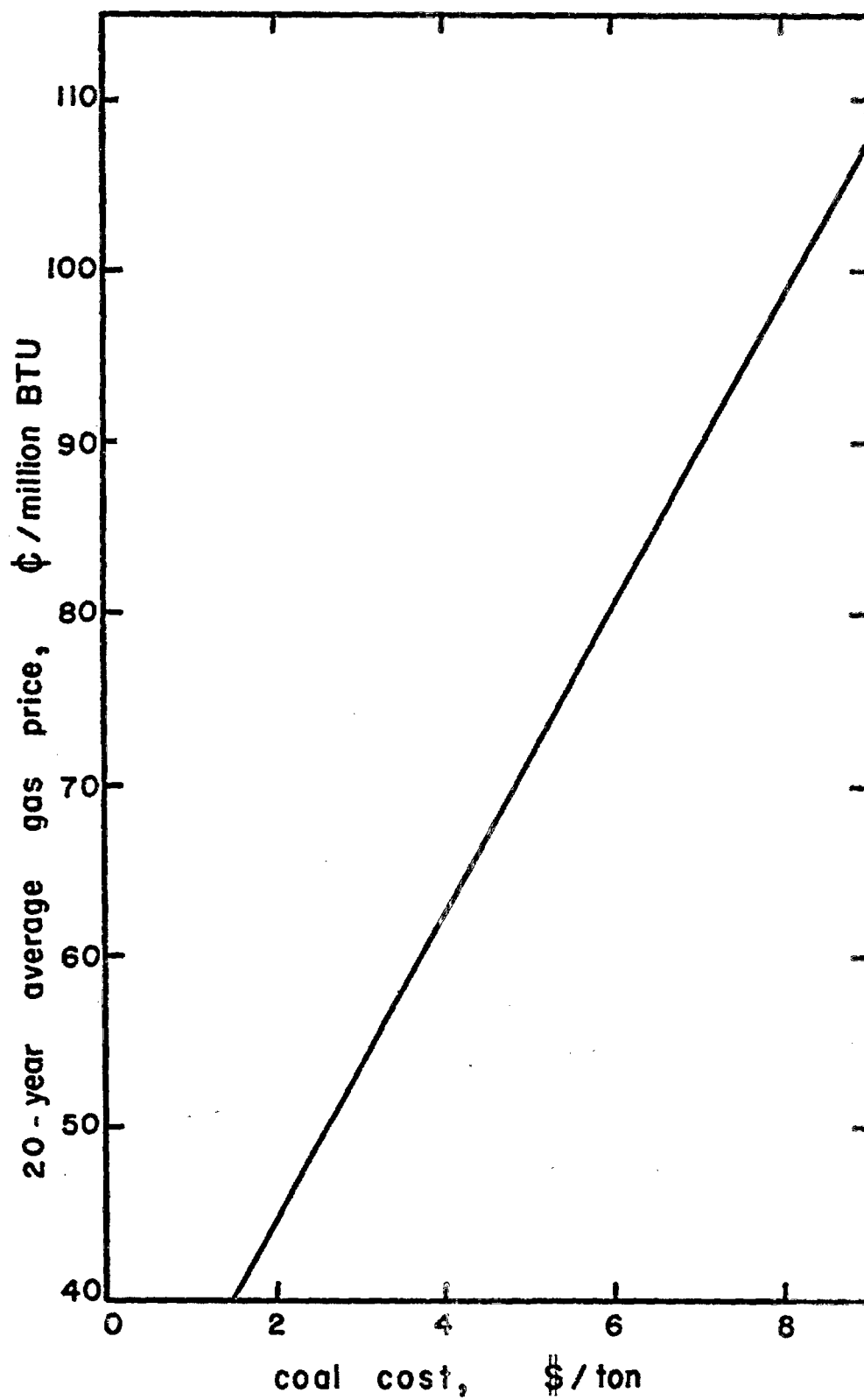
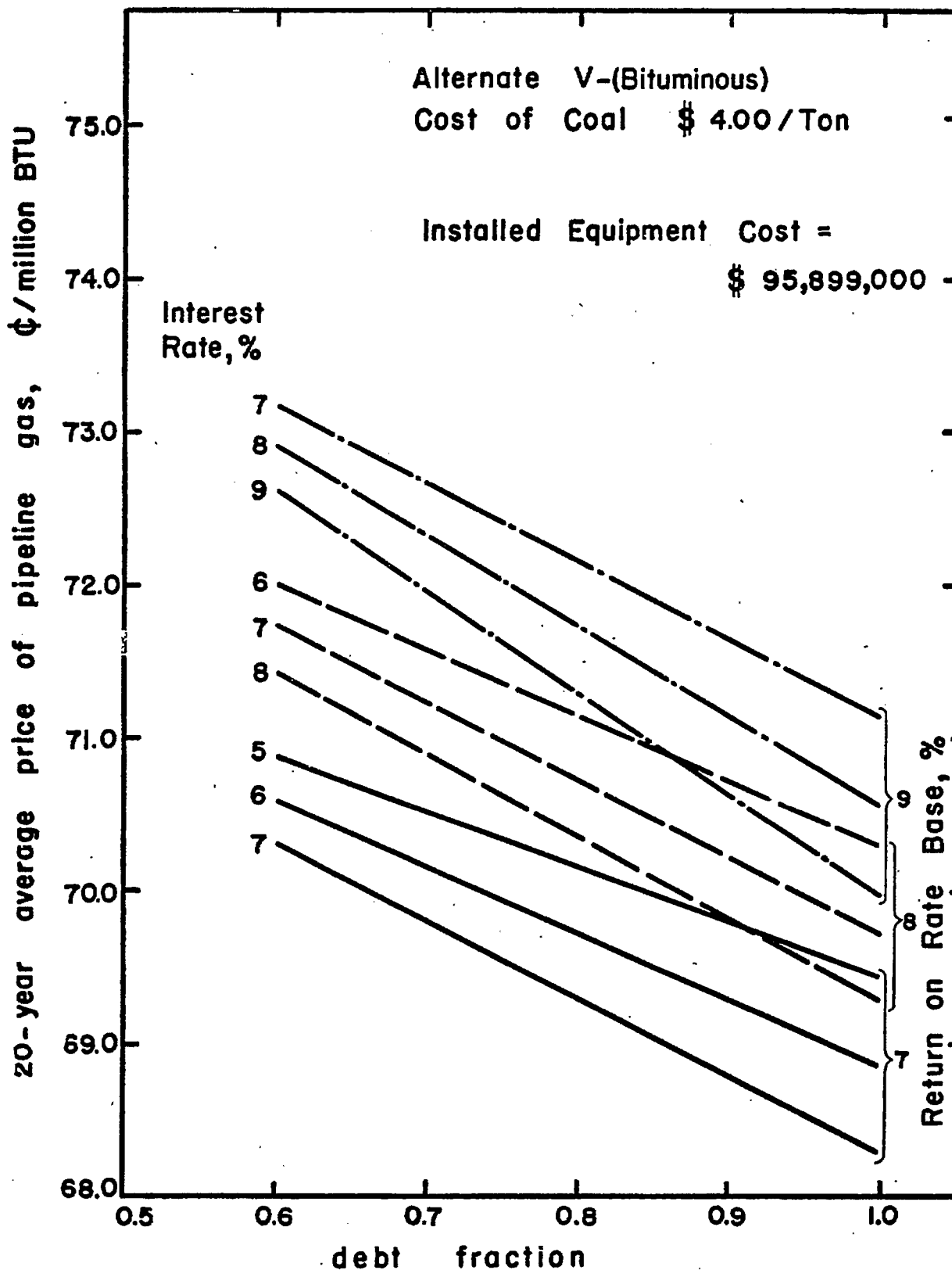FIGURE A-7   PRICE OF GAS FROM ALTERNATE III-2 AS
FUNCTION OF THE COST OF COAL
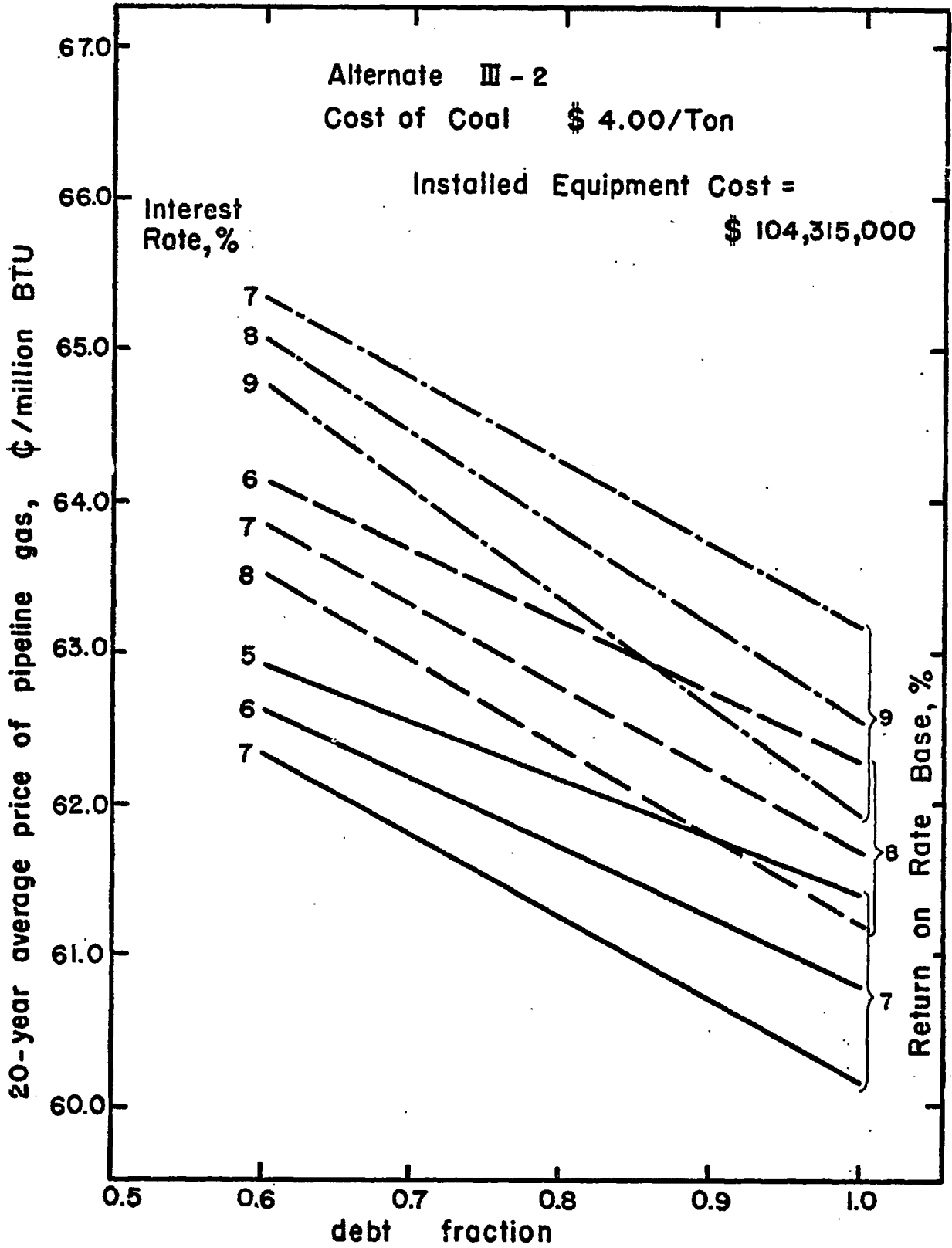
FIGURE A-8 EFFECT OF VARYING FINANCIAL FACTORS ON THE
PRICE OF PIPELINE GAS - ALTERNATE III-2

A-4 ALTERNATE V-(BITUMINOUS)

A-4.1 Process Description

The process scheme of Alternate V was described in the Interim Report [35] for the processing of lignite and no changes in the design are assumed necessary if the feed were bituminous coal. The operating pressure is assumed to be about 300 psig and the gasification vessels are indirectly heated by the transfer of heated dolomite solids which act as both a heat transfer medium and as a CO_2 acceptor. The dolomite is calcined and heated in a separate regenerator fired by the residue char from the gasifier and with fresh coal. A detailed description of this process was given in the Interim Report [35].

The gasification scheme is illustrated in Figure A-9 and the overall process pictured in Figure A-10.

A-4.2 Results of the Overall Plant Optimization

Following the procedures described in the Interim Report [35], this process was mathematically simulated and optimized using the overall plant thermal efficiency maximization and the subsystem capital investment minimization as the objective functions. At the optimum operating conditions, based on these optimization calculations, the material balance throughout the process were computed, with the resultant quantities shown in Figure A-10 and the composition of the various gas streams listed in Table A-7.

Based on these flow-quantity values, the various process subsystems were designed and the total bare equipment cost was computed. Using the standardized Office of Coal Research accounting procedure, the total capital investment was calculated as $117,223,000, with the investment summary listed in Table A-8. The annual operating expense breakdown is given in Table A-9, resulting in an estimated 20-year averaged gas price of 70.69¢ per million Btu.

The process was then studied to determine the sensitivity of the gas manufacturing price to changes in selected parameters. The gas price was found to be significantly affected by variations in the purchase price of the raw coal as shown in Figure A-11, the gas price changing 10.72¢/ million Btu for each $1/ton change in the raw coal purchase cost. The sensitivities of the gas manufacturing price to changes in certain cost accounting rates are illustrated in Figure A-12.
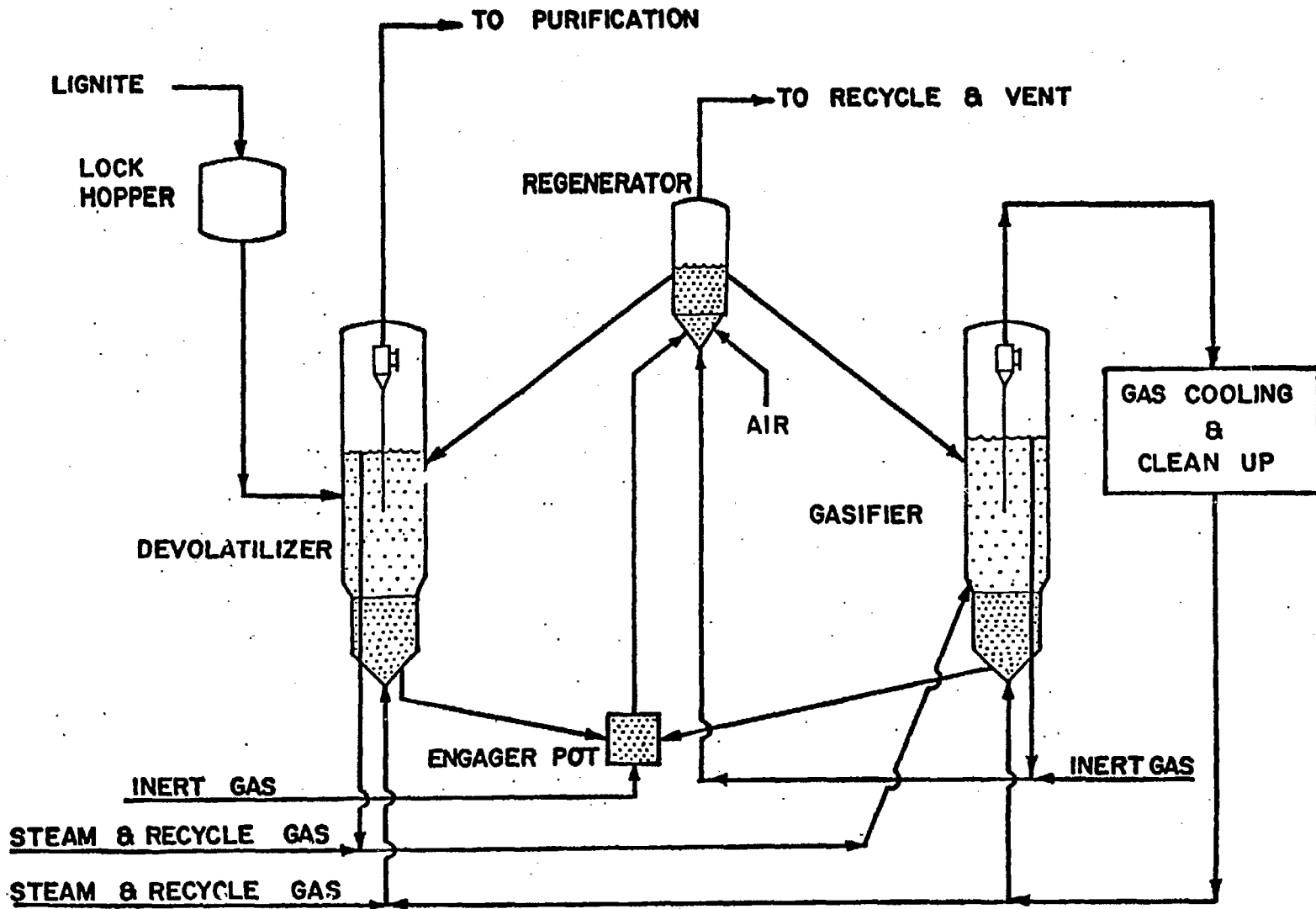
Figure A-9   Gasification Phase of Alternate V
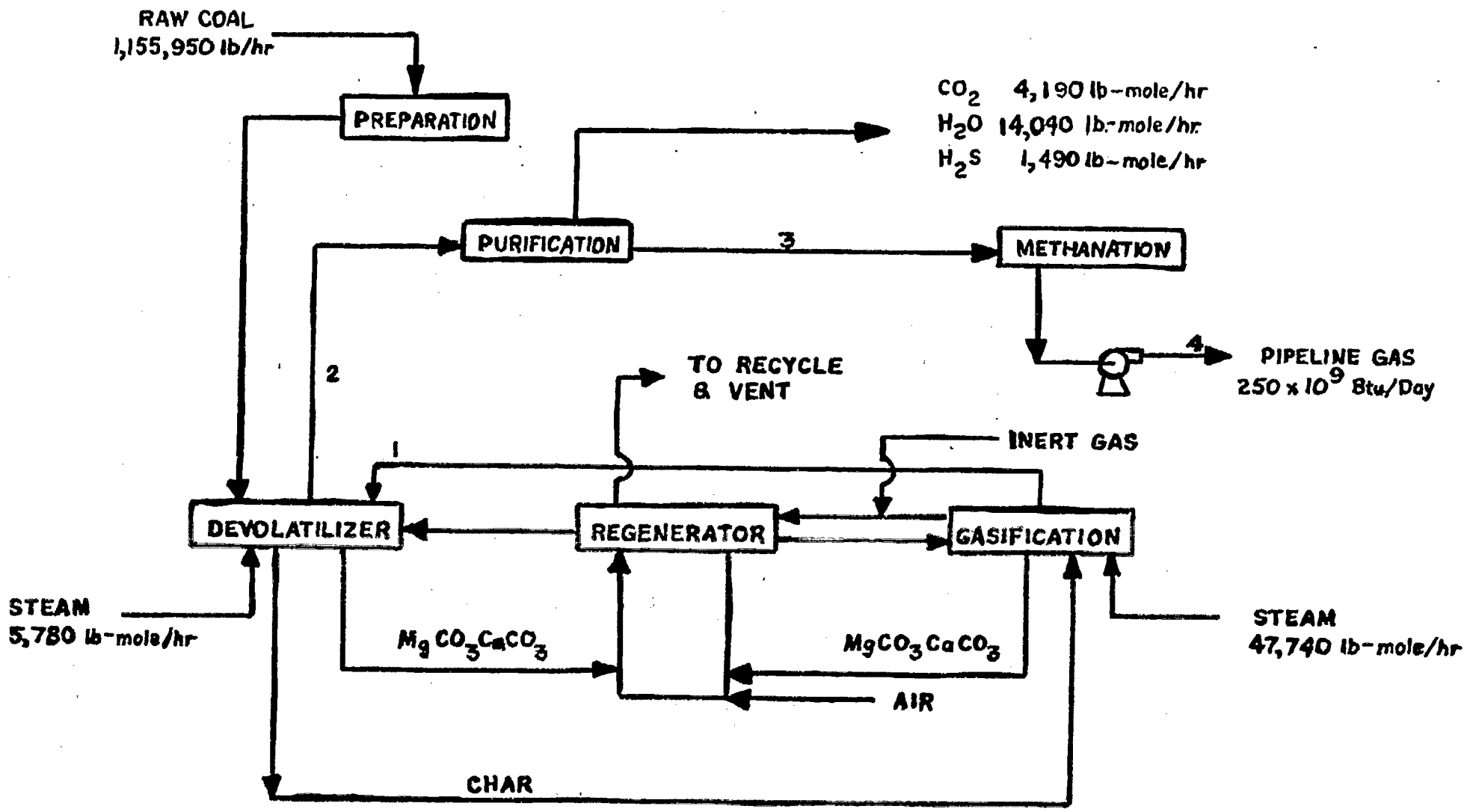
FIGURE A-10 COAL GASIFICATION PROCESS ALTERNATE V-(BITUMINOUS)

Table A-7   Gas Composition (Mole %) and Total Flow Rate
of Alternate V-Bituminous

Stream No.*	1	2	3	4
CO_2	5.27	5.72	1.03	2.25
CO	10.95	13.21	17.21	0.14
CH_4	–	18.07	23.54	89.16
H_2O	29.82	18.84	3.00	0.10
H_2	53.96	41.80	54.45	6.63
H_2S	–	1.76	–	–
N_2	–	0.60	0.77	1.72
Flow Rate lb-mole/hr	56,990	84,890	65,170	29,730

*See Figure A-10 for stream number location

Table A-8

INVESTMENT SUMMARY FOR ALTERNATE V-(BITUMINOUS)

	Bare Cost, $
Preparation and Storage	$ 15,000,000
Pretreatment	—
Gasification	32,557,000
Shift Conversion	—
Gas Purification	16,790,000
Methanation	2,250,000
Product Compressor	1,330,000
Electric Power Plant	4,962,000
Sulfur Recovery	4,010,000
Offsite Facilities	19,000,000
Subtotal, Bare Cost	$ 95,899,000
Contractor's Overhead and Profit	7,412,000
Interest During Construction	5,166,000
Total Fixed Investment	$108,477,000

Working Capital

30-Days Coal Inventory @ $4/Ton	$3,127,000	
30-Days Other Direct Material Inventory	243,000	
Accounts Receivable	5,376,000	
Total Working Capital	$8,746,000	8,746,000
Total Capital Investment		$117,223,000

FIGURE A-11   PRICE OF GAS FROM ALTERNATE V-BITUMINOUS
AS A FUNCTION OF THE COST OF COAL

FIGURE A-12   EFFECT OF VARYING FINANCIAL FACTORS ON THE PRICE OF PIPELINE
GAS – ALTERNATE V – BITUMINOUS

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