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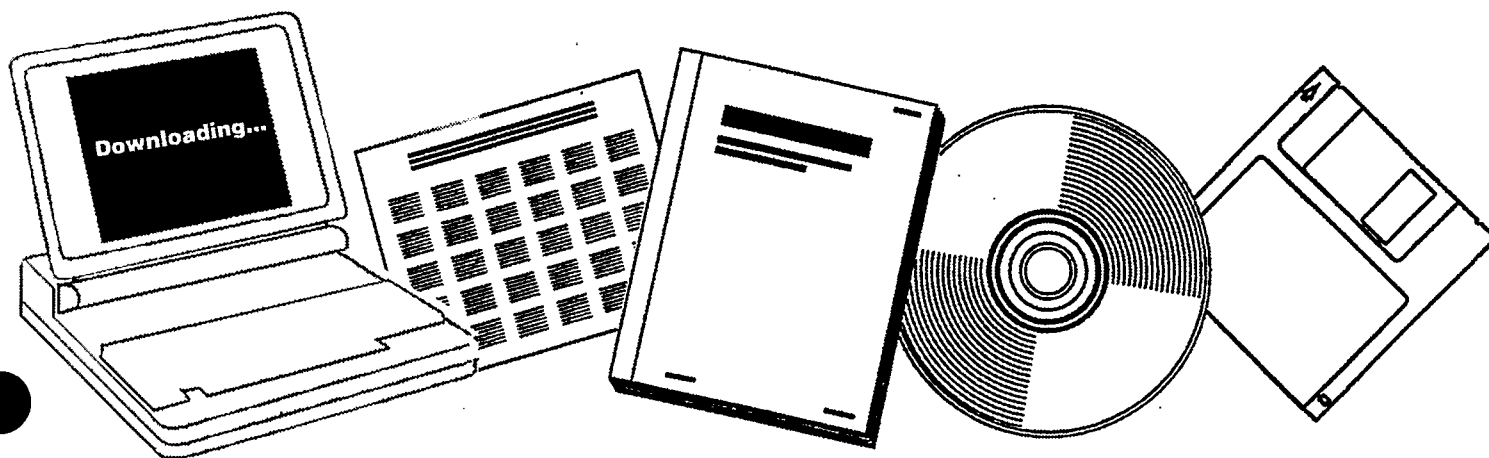
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**OPTIMIZATION OF COAL GASIFICATION
PROCESSES. VOLUME 1. CHAPTERS I THROUGH
VII**

WEST VIRGINIA UNIV., MORGANTOWN. DEPT.
OF CHEMICAL ENGINEERING

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OPTIMIZATION OF COAL GASIFICATION PROCESSES

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RESEARCH AND DEVELOPMENT REPORT NO. 66
Interim Report No. 1
Contract No. 14-01-0001-497

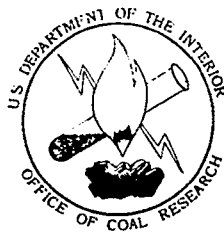
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SUMMARY

This project has the objective of assisting the Office of Coal Research to determine those processes which hold more promise for potential economical development for the commercial production of a high-heating-value pipeline gas.

Since the time and financial resources are limited, the studies are concentrated only on the processes which present the most attractive commercial possibilities. The mathematical optimization techniques along with the methodology of system analysis have been developed for use in optimizing various types of proposed processes and indicating the most advantageous among the available choices.

In using optimization techniques, a generalized economic standard method of comparison is established. Representative types of problems of fundamental importance to the coal gasification processes are defined and identified. Information relating to the coal gasification available in the literature and from the OCR contractors and other pertinent sources has been collected and classified. The various steps involved in a specified process are studied and the contribution of those steps to the economics of the whole process has been evaluated. This study identifies those steps having a significant effect so that a more precise and detailed evaluation can be made of those problem areas which are critical to the success of the alternative processes under consideration. This study also identifies all steps having negligible effect on the cost of the entire process so that such steps may be eliminated from further consideration. The study has indicated areas of

serious deficiency in the technical knowledge which are necessary for the successful application of proposed coal gasification scheme.

Depending on the types and nature of the problems considered, an effective and efficient optimization technique is then selected and tested for the various processes. If the existing techniques are inadequate, new techniques are developed. Computer programs are designed to determine the optimum operating conditions for the critical steps and paths of the various processes, optimal design of various systems, and policies of supply and types of coal considered.

This information is compiled in this study and the results interpreted in practical terms specifying the characteristics of coal used, the capital and operating costs of the plants as a whole, and of sections of such plants, including the necessary benefit/cost relationships. Thus, the most attractive processes or alternatives are recommended, and those areas of coal gasification technology are identified where further research and development are likely to produce beneficial results.

Although a number of coal gasification schemes to manufacture pipeline gas have been proposed and are under different stages of investigation, any of these schemes can be represented by the five separate phases of operation; namely, coal preparation and pretreatment, coal gasification, shift conversion, gas purification, and methanation. Depending on the individual scheme, some phases of operation may dominate others in terms of its size and cost.

This report deals with each of the five phases, presenting the pertinent technical information, examining the constraints and alternate processes, and formulating models for computer simulation and optimization.

Each of the subsystems optimized is then integrated to arrive at an overall evaluation of the various gasification processes. The following conclusions and recommendations are made:

1. The gas price is most significantly affected by the amount and cost of coal or lignite required for the integrated plant. Depending on the cost of coal or lignite, approximately 40 to 60% of the gas price is attributable to the cost of coal.
2. Pretreatment of coal to prevent agglomeration in the gasifiers would result in approximately 6 to 19% weight losses of coal. Since the cost of coal is by far the largest cost item, every effort should be made in the effective utilization of coal. Any means by which raw coal or char with the least pretreatment can be fed to the gasification reactor will reduce the gas price considerably. This points to the urgent need for the development of a raw coal feeding system, or the development of the technology of recovering the volatile matters lost in the pretreatment.
3. Table S-1 compares the gas price (without by-product credit), carbon utilization, thermal efficiency, total fixed investment, and operating expenses for each alternate process studied. It is seen that the gas price is lower for the process (Alternate II-3) which is assumed to be capable of feeding raw coal to the gasification reactor. The highest gas price, shown by alternate I, is due to the inefficient use of carbon and hydrogen in coal by reacting coal with oxygen during the initial period and by extensive water-gas shift reaction and methanation required later in the process.
Since the gas prices are affected by many factors such as cost of coal, accounting procedure adopted, etc., which are subject to change depending on the economic climate, they should be considered as the estimated relative prices and only be used for comparison among the various alternatives studied.
4. Although most of the processes considered are operated at approximately 1000 psig in order to produce methane at the pipeline pressure, effects of pressure on gasification systems should be investigated. Since most of the gasification reactions are favored when the pressure is increased, high pressure operation should reduce the reactor size and improve the gas purification efficiency. The equipment costs for these two phases of operation are a significant part of the total equipment cost. The advantage of a higher pressure operation, however, is offset by the requirement of thicker reactor walls, resulting in higher reactor costs. The operation at pressures lower than 1000 psig will require compression cost to bring it to the pipeline gas condition.
5. From the thermodynamic point of view, for the production of methane, direct hydrogen coal reactions utilizing devolatilization and hydrogenolysis are more efficient than the carbon monoxide-hydrogen reaction (methanation reaction). Therefore, if the

TABLE S-1

OPERATING EXPENSE, FIXED INVESTMENT, THERMAL EFFICIENCY,
CARBON UTILIZATION, AND GAS PRICE FOR DIFFERENT PROCESSES

Alternate Process		Total Fixed Investment MM \$	Operating Expense MM \$/year	Overall Plant Thermal Efficiency ⁽¹⁾ percent	Carbon Utilization ⁽²⁾ percent	Gas Price ⁽³⁾ ¢/MM Btu
Bituminous Coal	I	138.0	66.4	45.6	28.7	85.9
	II-1	127.1	53.4	62.2	37.9	70.0
	II-2	124.4	56.6	53.8	34.2	73.6
	II-3*	117.9	51.6	63.2	38.4	67.4
	III	129.5	54.6	55.6	33.7	71.7
	IV-1	141.8	64.7	48.1	29.1	84.2
Lignite	IV-2*	146.2	45.8	57.1	32.2	62.2
	V*	92.7	32.5	59.2	31.2	43.3

(1) Overall Plant Thermal Efficiency = $\frac{\text{Btu of product gas leaving plant}}{\text{Btu of raw coal fed to plant}}$

(2) Carbon Utilization = $\frac{\text{lb-mole of carbon in product gas}}{\text{lb-mole of carbon fed to the plant}}$

(3) 20-year average gas price based on Bituminous Coal at \$4.0/ton and Lignite at \$1.5/ton

* Raw coal (or Lignite) is fed to the gasifier for these processes, while for others coal must be pretreated prior to gasification.

water-gas shift reaction is needed in the process, the shift reaction should be carried out, if possible, before the coal gasification reaction so as to maximize the hydrogen-coal reaction in the gasifier, and minimize the methanation reaction needed to achieve pipeline quality.

6. In gasification processes requiring oxygen, the cost of the oxygen plant and the associated power generation plant is the largest portion of the total equipment cost; occupying roughly 40% of the total.
7. The equipment cost either for the gasification phase or for the gas purification phase seem to be the second largest item among the total equipment costs, depending on the alternate considered.
8. Gas prices with lignite feeds shown in Table S-1 are lower than that with bituminous coal feeds. However, more detailed study based on different ranks of coal and lignite should be made in order to draw a definite conclusion.
9. In view of the large exothermic heat of reaction produced in the methanation reactor, it is desirable to operate the methanator in a state of fluidization for rapid heat removal. Catalysts rugged enough to sustain attrition in fluidized beds and less sensitive to sulfur poisoning should be developed.
10. The technology of the solids feeding and removal systems to and from a high temperature and pressure gasifier has not been fully developed. Additional efforts are needed to devise operational and more economical solid feeders which can provide uniform distribution of coal in a large diameter gasifier without agglomeration.

The results presented above are an engineering estimate based on a number of simplifying assumptions and thus are subject to certain variations. Particularly, in view of the future development of new technology, some of the engineering problems which hinder an otherwise sound process may be solved, and could alter the economic picture of the process. However, it is believed that a measure of effectiveness of a number of coal gasification processes in relation to their costs has been established which will be useful in economic evaluation of future potential for the commercialization of the various alternates considered.

Chapter 1. INTRODUCTION

INTRODUCTION

West Virginia University, under contract to the Office of Coal Research, has been engaged in the study of Optimization of Coal Gasification Processes to determine those processes which hold more promise for potential economical development for the commercial production of a high-calorie-value pipeline gas.

Since coal gasification technology is so widely varied while time and financial resources are limited, the studies must be concentrated on the process or processes which present the most attractive commercial possibilities. Mathematical optimization techniques along with methodology of system analysis have been developed for use in optimizing various types of proposed processes and indicating the most advantageous among available choices.

The methodology of system analysis through simulation and optimization based on system models has in recent years become a key element in the programming, planning and budgeting of major governmental and industrial projects. Pipeline gas production from gasification of coal appears to require a comprehensive, long-range program which would include not only a more sophisticated energy conversion and product recovery technology than had hitherto been available, but also the integration of air and water pollution control, with land use planning and transportation system development.

In using optimization technique, a generalized economic standard method of comparison is established. Representative types of problems of fundamental importance to coal gasification processes

are defined and identified. Information which relates to coal gasification available in the literature and from OCR contractors and other pertinent sources has been collected and classified. The various steps involving a specified process are studied and the contribution of that step to the economics of the process has been evaluated. The study identifies those steps having significant economic effect so that a more precise evaluation can be made of those problem areas which are most critical to the success or failure of the alternative or alternatives under consideration. This study also identifies all steps having negligible effect on the cost of the entire process so that such steps may be eliminated from further consideration. The study has indicated an area of serious deficiency in technical knowledge and information which are necessary for the successful application of the coal gasification schemes proposed.

Based upon the data and information collected and screened, necessary process and performance equations in terms of their restraining variables are determined or developed so that representative optimal solutions can be provided. Depending on the types and nature of the problems considered, an effective and efficient optimization technique is then selected and tested for the various processes. If existing techniques are inadequate, new techniques have been developed. Aside from the optimization techniques already developed at West Virginia University, emphasis has been made on the use of dynamic

optimization methods including dynamic programming, linear programming, geometric programming and the maximum principle.

Whenever possible, the problems identified are treated from both deterministic and stochastic points of view. Computer programs are designed to determine the optimum operating conditions for the critical steps and paths of the various processes, optimal design of various systems, and policies of supply and types of coal considered.

This information is compiled in this report and the results interpreted in practical terms specifying characteristics of coal used, capital and operating costs of the plants as a whole, and of sections of such plants, including the necessary benefit/cost relationships. Thus, the most attractive alternatives or processes are recommended and those areas of coal gasification technology most likely to produce beneficial results through future experimental research and development are identified.

1. Classification of Coal Gasification Systems

The various gasification processes may be classified into the following phases:

- (a) Coal Preparation and Pretreatment Phase
- (b) Coal Gasification Phase
- (c) Shift Conversion Phase
- (d) Gas Purification Phase
- (e) Methanation Phase

A general flow diagram of the coal gasification processes is presented in Figure 1-1. Although a number of coal gasification

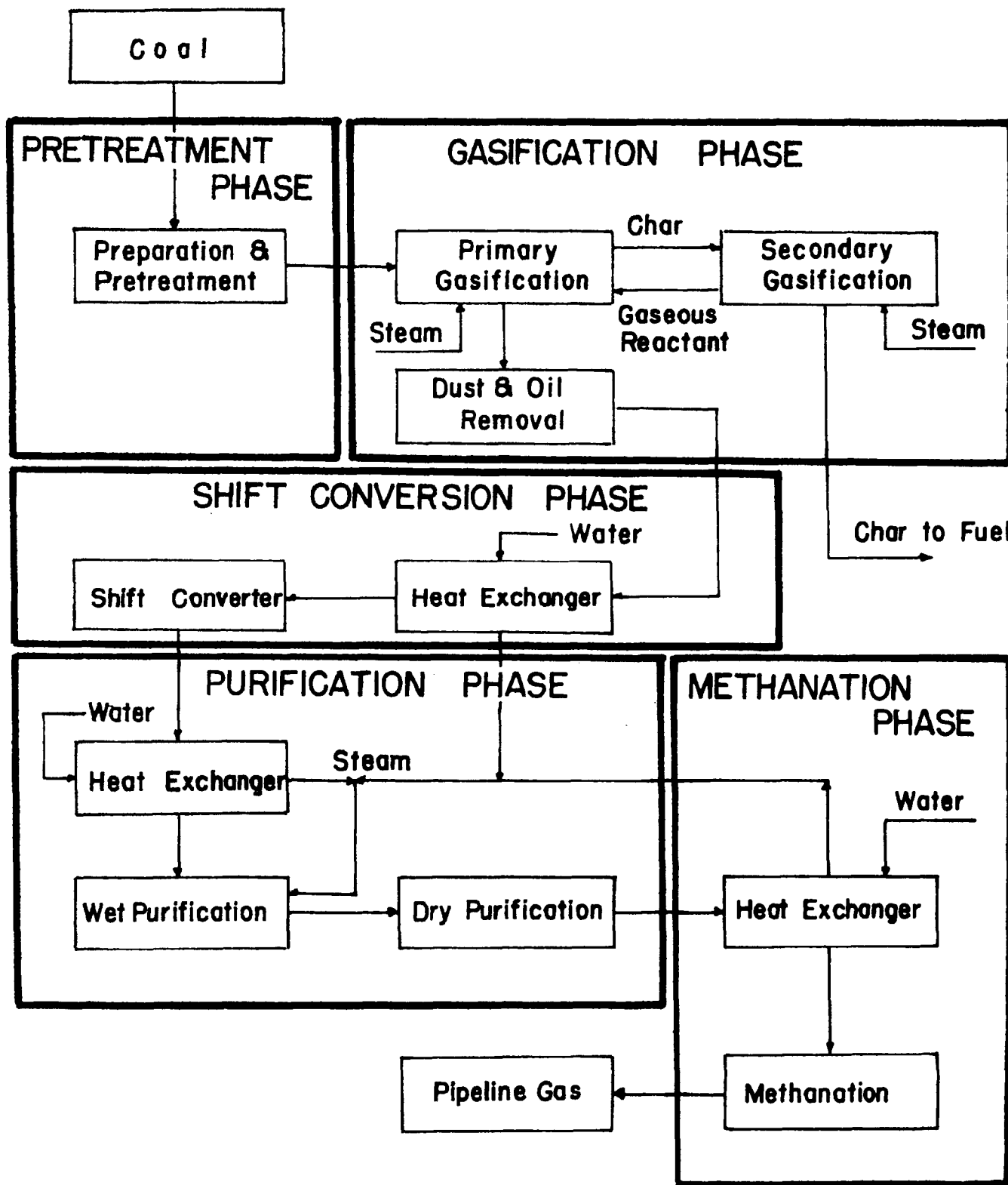


Figure I-1 General Flow Diagram of Coal Gasification Processes

processes to manufacture pipeline gas have been proposed and are under investigation either on a pilot plant scale or on a bench scale, it is believed that practically any of these schemes can be represented by the five phases shown in the diagram. Depending on the type of each individual process, naturally some phases may dominate others in terms of its size and cost, and will differ in detail; these five phases all involve similar process steps which are the essential and major subsystems of an overall pipeline gas plant from coal gasification.

This report will deal with each of the five phases presenting the pertinent technical information, examining the constraints and alternate processes, and formulating models for computer simulation and optimization. Each of the subsystems optimized is then integrated to arrive at an overall evaluation of the various gasification processes from which conclusions and specific recommendations regarding future research and development will be made. To achieve this goal, a methodology of systems analysis and optimization as described below is followed. (2)

2. Methodology of Systems Analysis and Optimization

A logic diagram illustrating the strategy of methodology to perform systems analysis and optimization is shown in Figure I-2. This methodology is applied to selected problems of coal gasification processes.

There are a number of alternative ways to gasify coal which are confronted with many problems of different magnitudes and scopes. Often the resources or

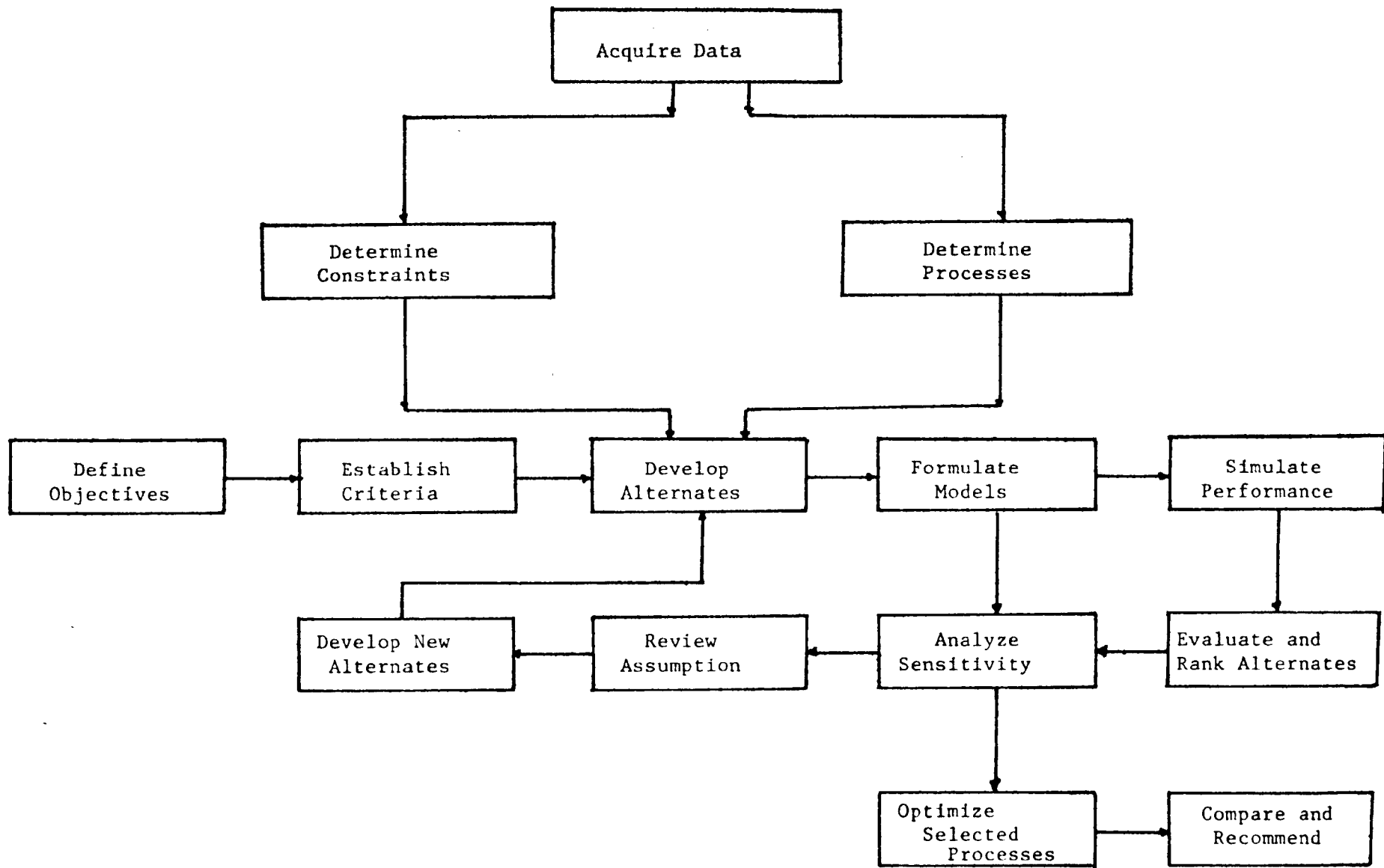


Figure I-2. Block Diagram of Methodology of System Analysis

facilities are not adequate for performing each activity in the most effective way. Thus, the problem is one of combining activities and resources in such a way as to maximize overall effectiveness. The success of a systems analysis and an engineering campaign depends critically on the quality and variety of the specific problems.

i. Define objectives

The objectives of this contract are to establish a generalized standard method of comparison through mathematical optimization techniques which can be utilized in evaluating coal gasification processes and future change in such programs and to select the process or processes presenting the most commercial attractiveness.

ii. Establish criteria

The systems analysis methodology requires that a set of criterial indices be developed so that alternative problem solutions can be compared. The important point is that all alternatives are tested against the same set of criteria so that the objective evaluation of the relative merit of each process is possible. In this light a set of economic indices has been proposed and presented in Chapter II.

iii. Determine constraints and processes

It is necessary to examine all the constraints and identify whether or not some of these constraints will vary with time and operating conditions. Since a number of the processes to be suggested or proposed have not yet commercially been tested, there will be a cloud of uncertainty surrounding the data upon which the

system design rests. These uncertainties must be defined as constraints so that either;

(a) the process components are purposely designed to be more durable, more flexible, and of greater capacity than is demanded on the basis of the best information available in order to protect the system from unknown effects, or

(b) recommendations will be made to conduct additional research when uncertainty surrounds a critical feature of a novel system thereby putting less capital investment in jeopardy. Although the data which are unavailable or uncertain may be estimated with sufficient accuracy by generalized correlation and prediction method, the reasons for the lack of accurate data should be known. Therefore, the leeway allowed in the definition of a satisfactory solution, must be specified.

iv. Develop alternates

The alternatives shown in the various chapters on each of the phases represent a sample from a larger number of alternatives that should be proposed before it is possible to have a proper base upon which to begin the engineering of a process. It is clear that these initial concepts can only be plausible, and that only after a considerable investment in engineering effort can the true nature of the alternatives become apparent. The defective alternatives must be eliminated early so that this investment will not be wasted on schemes that cannot possibly be shaped into a practical system. Herein lies a most critical aspect of process engineering.

On the one hand, we cannot afford the investment in time and talent to go into engineering detail to properly assess the plausibility of all the alternative methods of solving a given problem. But, on the other hand, we cannot properly limit attention to one or a few of the alternatives without having first made a detailed assessment of all known alternatives. There is the great risk of eliminating the optimal concept along with the majority of concepts which are not even plausible. The systems approach makes use of the computer simulation to reduce drastically the chance of committing this error. However, it is impossible to carry each alternative through to a complete design to make a detailed comparison among the alternatives. The design of a single system may be an enormous task even with the aid of a computer, and this effort cannot be wasted on alternatives which are defective and cannot be shaped into practical systems. Therefore, alternatives must be prescreened to eliminate those which have lower potential. Included among the questions that can be asked during the preliminary screening are:

- (a) Is the concept consistent with fundamental laws of physics?
- (b) Can the concept be shown to be inferior to one of the other alternatives suggested by a paired comparison?
- (c) Can the concept be shown to be equivalent or inferior to a known inferior processing concept?
- (d) Can the concept be shown to require too much technical or economic extrapolation from existing technology, thus involving too high a risk?

(e) Is the concept unsafe?

(f) Does the concept suggest a better alternative?

These are just a few of the methods that can be used to screen the inferior alternatives. In fact, the creation and preliminary screening of alternatives often occur simultaneously.

v. Formulate models

The synthesis and evaluation of the effectiveness of alternatives discussed require the development of a group of descriptive and/or predictive mathematical models. Since most of the data available for formulation of a model are from a small scale unit, not only is it necessary that the performance characteristics of the unit must be represented realistically, but also to distinguish between physical effects and chemical effects so that the extrapolation needed in scale-up from a laboratory unit can be safely made. The model formulated must represent the flow behavior, the reaction mechanism and the heat and mass transfer phenomena of the real system close enough to yield realistic performance character of the actual unit. However, a model can never represent a complete picture of the reality. In fact a simple model may be quite adequate in most instances and only occasionally a much more refined and elaborate model is necessary. A good model however, must recognize its own inadequacies so that it can serve as a mean to develop a more complete model if it becomes necessary. Hence, in formulating a model, it is imperative that we differentiate the major factors that are significantly important from the minor factors

that may be safely neglected. The economic information such as equipment cost, operating cost, etc., must also be formulated along with the performance model so that the comparison based on the total economic picture can be made later.

vi. Simulate Performance

In order to make certain that the models developed are indeed realistic, a computer simulation of the system performance under a given set of conditions is carried out. For example, the results of simulation such as effluent gas distribution, temperature profiles, pressure drops, diameter and height of the reactor bed, etc., can be compared with the actual laboratory experimental results if the information is available. Together with material balance and heat balance the above results can be checked to see if any of the simplifying assumptions and correlations used in formulation of the model are unreasonable.

If the results of simulation deviate drastically from experimental performance, the assumption, simplification, parameters of models and even the model itself must be reexamined and a more realistic model reconstructed. Finally, system stability should be checked by small perturbation of the input conditions such as concentration, flow rates, temperatures, etc., to see if the mathematical model adopted can be used for optimization.

vii. Evaluate and rank alternatives

The models developed above are designed to facilitate the evaluation of alternative processes in terms of effectiveness criteria

and costs. The alternatives may be ranked according to the preliminary evaluation based on level of risks. An approximate analysis of the alternatives seeking to detect weaknesses which are dominant is all that is necessary at this stage. However, as attention is focused on the more plausible alternatives, precision is required and simple principles of screening are too coarse for the task. It is necessary to define the economic environment in which the process is to function and establish a criterion which, when used during process design, will lead to the economically optimal process.

viii. Analyze sensitivity, review assumptions and develop new alternatives

In general, sensitivity analysis is a quantitative investigation on the effect of variation of a variable on its related variables by mathematical methods. The purpose of sensitivity analysis can be divided into two areas. First, in order to confirm that a coal gasification process selected as a result of a system analysis is, in fact, the optimal alternative, it is necessary to determine whether the models employed to assess the effectiveness and cost of the alternatives are highly sensitive to variations in the input parameters or assumptions on which they are based. The choice of the alternative selected would be open to serious questions if a significant reordering of alternatives can result from a relatively minor change in some input parameter. If the system's performance is found to be sensitive to variation in parameters, some methods of reducing sensitivity of the model have to be developed. Second, it is important to identify which of the

various steps or parameters involved have a significant economic effect on the entire process and which of these may be of secondary importance from an overall economical venture.

Rather sophisticated methods of sensitivity analysis have been developed by Chang and Wen [1,3]. In general elements of sensitivity need not compromise the validity of the system's analysis, provided that they are recognized as such and evaluated. In the same sense, an assessment of the sensitivity of the analysis to the initial assumptions on which it is predicted may indicate that relaxation or modification of these assumptions will result in a significant alteration of the ranking of alternative plans. A sensitivity analysis and review of the initial assumption is therefore an essential part of the final evaluation of an array of coal gasification alternative processes. Only through such an approach may we be certain that the specific processing alternatives, whether newly created at this stage or those that have been analyzed and evaluated, have the quality for the practical solution of the coal gasification problems.

ix Optimize and select processes

Since all possible alternative processes have been roughly evaluated and ranked, only those selected processes are now optimized. The results are then compared for economical feasibility as well as for determination of the "best" process. In optimization, a certain function of several variables of the system, called objective function, is to be maximized or minimized with some constraints imposed on the

variables. The objective function in coal gasification processes will be the operating and capital costs of the system. In economic analysis, cost factors of operating costs and capital costs are evaluated and put together with system variables to form cost equations which are then used to formulate an objective function. The optimizer has several variables under his control, which are called the decision variables. The decision variables in the coal gasification processes could be the temperature, pressure, flow rates, and many others which must be determined within the allowed constraints so as to maximize the objective function.

Many of the systems are stagewise in structure, whereas others are continuous. A stagewise process generally can be described by a system of different equations; a continuous process is, on the other hand, described by a system of differential equations. Because of the inherent restriction on human decisions and their execution, many continuous processes are actually carried out stage by stage. Furthermore, a continuous process usually can be approximated by the stagewise process. The task of optimization is to find the value of decision variables at each stage so that the objective function of multistage process is maximized. Based on the objective function and the performance equations resulting from mathematical model of the system, one can select a most effective and efficient technique to optimize the process. Fortunately, there are a number of search techniques available. These include direct search, dynamic programming, linear programming, geometric programming, maximum principle, variational methods and others.

Finally, sensitivity analysis of the optimal policy should be performed. The optimum solutions are obtained based on specific values of parameters and therefore will change with the variation in system parameters. These parameters may be kinetic constants, heat and mass transfer coefficient, cost factors, among others. It is obvious that the optimal performance of a system depends on how close the true values of the system's parameters correspond to those used in obtaining optimal solutions. Unfortunately, a system's parameters encountered in the coal gasification processes are known to be only approximate since the pilot plant scale studies have not been completed. In addition, system parameters such as utility cost, fuel cost, etc. may vary from the specific values depending on the location, time and market demand. In other words, the problem of parameter variation or uncertainty is often present in the process optimization considered. Therefore, in order to obtain a meaningful optimal design with parameter variation, the already developed mathematical methods for solution of this type of problem as shown by Chang and Wen [1,3] will be used.

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Chapter II. COST INFORMATION

COST INFORMATION

1. Equipment Cost1.1 Cost of Catalyst Supporting Trays, E_s

$$i \text{ Mild steel tray: } E_s = 0.195 N I_f (D + 5)^{3.13} \quad (\text{II-1})$$

$$ii \text{ Chrome-type tray: } E_s = 0.216 N I_f (D + 5)^{3.13} \quad (\text{II-2})$$

where N is the number of trays required

I_f is the cost factor

D is the diameter of reactor, ft.

1.2 Compressor Cost, E_{cp}

The cost of gas compressor is governed by the brake horse power which is a function of flow rate, temperature, and pressure of the gas. The following equation is used to estimate the brake horse power [6].

$$B_H = \frac{0.0643 T_s q_p}{520 E \eta} \left[\left(\frac{P_d}{P_s} \right)^\gamma - 1 \right] \quad (\text{II-3})$$

where B_H is the brake horse power, h.p.

T_s is the temperature at suction, °R

q_p is the volume of gas compressed, S.C.F./min.

E is the mechanical efficiency, 80~85%

η is $(K-1)/K$

K is C_p/C_v , ratio of specific heats

P_d, P_s are the pressures at discharge and at suction, respectively, atm.

$$\text{Hence, } i \text{ Reciprocating compressor: } E_{cp} = 698 (B_H)^{0.81} \quad (\text{II-4})$$

$$ii \text{ Centrifugal compressor: } E_{cp} = 378 (B_H)^{0.852} \quad (\text{II-5})$$

1.3 Control Valve Cost

The cost of a control valve varies widely depending on the size and the manufacturer. On the average, \$8,000 per valve for a large single reactor, and \$4,000 for the small reactors in parallel are used in the estimation.

1.4 Fin Tube Cost, E_F

In the heat extraction system, heat generated in the reactor must be removed internally. The fin tubes may be used effectively for this purpose by embedding them into the catalyst. The cost of fin tubes is obtained from the bare tube heat transfer area A_b , as [7]:

$$E_F = C_y I_f [350(A_b/60)^{0.882}] \quad (\text{II-6})$$

where C_y is the cost year index.

1.5 Heat Exchanger Cost, E_H

The cost of a heat exchanger is computed based on the required heat transfer area, A_o [7]:

$$E_H = C_y I_f [850(A_o/50)^{0.562}] \quad (\text{II-7})$$

1.6 Motor Cost, E_M

The motor cost is expressed in terms of required horse power as:

$$E_M = 46 H^{0.955} \quad (\text{II-8})$$

where H is horse power.

1.7 Pump Cost, E_p

Pumps are required to deliver the coolant water. The pump cost is calculated from [2,6]; for steel-made centrifugal pump,

$$B_p = q \rho_w \Delta h / (246,800 E) \quad (\text{II-9})$$

$$\text{and } E_p = 684 (B_p)^{0.467} \quad (\text{II-10})$$

where q is the volumetric flow rate of water, gal./min.

ρ_w is the density of water coolant, lb./cu.ft.

Δh is the hydraulic head, ft.

B_p is the brake horse power, h.p.

1.8 Reactor Shell Cost, E_R

The estimated cost of high pressure reactor outshell is based on the weight of an empty reactor. The thickness of the reactor wall, T_h is calculated from [1]:

$$T_h = PR / (SE' - 0.6p) \quad (\text{II-11})$$

where P is the design pressure, psig

R is the inside radius of the cylinder, in.

S is the maximum allowable stress value, psig

E' is the efficiency of longitudinal joints in cylindrical shells.

In addition, 1/4-inch thickness is added for corrosion allowance.

The weight of the reactor W_R which includes top and bottom blank is then computed by

$$W_R = \frac{\pi}{4} \rho_m \left[\left(D + \frac{T_h}{4} \right)^2 - D^2 \right] L + \frac{F_d^2 T_h}{6} \quad (\text{II-12})$$

Therefore, the cost of the reactor becomes

$$E_R = C_R I_f W_R \quad (\text{II-13})$$

where

L is the reactor height, ft.

ρ_m is the density of the material, lb/cu.ft.

F_d is the flat blank diameter of top and bottom domes, ft.

C_R is dollars per pound of the material used for the reactor shell

1.9 Turbine Cost

The cost of hydraulic turbine is approximately the same as that of centrifugal pump. When the stainless steel is used the cost is about 1.8 times that of ordinary steel.

2. Cost of Direct Material and Utility

2.1 Catalyst Cost, E_C

The cost of the Harshaw catalyst used in methanation processes is [4]

$$E_C = 2.5 W_C \quad (\text{II-14})$$

and the cost of water-gas shift catalyst of Girdler is [3]

$$E_C = 20 V_C \quad (\text{II-15})$$

where W_C , V_C are the amount of catalyst expressed in pounds and in cubic feet, respectively.

2.2 Cost of Packings, E_A

The packings such as rings and saddles are used in the gas purification towers and in the cold-quenching water-gas shift reactors. The cost of packings is estimated by

$$E_A = 5.0 V_p \quad (\text{II-16})$$

where V_p is the volume of packings in cu.ft.

2.3 Cooling Water Cost

Treated water: \$0.12 per thousand gallon

Spent water: \$0.05 per thousand gallon

2.4 Cost of Iron Oxide

The cost of iron oxide used in gas purification processes is estimated at \$0.05 per pound.

2.5 Cost of K_2CO_3

\$3.50 per hundred pound is used

2.6 Cost of Monoethanol Amine Solution [5]

2.5N solution of monoethanol amine is estimated at \$0.35 per gallon.

2.7 Electricity Cost

An approximated value of 11 mil per kw-hr is used.

2.8 Steam Cost

Although the cost of steam depends largely upon the process and manufacturer, \$0.60 per thousand pound is employed as the conservative value for the high pressure (1000 psig) steam. However, a more precise value of steam cost may be obtained in terms of the rate of steam required as shown in Figure II-1 [9].

3. Raw Material Cost

3.1 Coal Cost

The cost of coal is one of the most important factors affecting the price of pipeline gas. However, it changes depending on the types of coal and the locations of the mine. The present study is based on the following price at the minemouth:

Bituminous coal: varies from \$2.0/ton to \$8.0/ton.

Lignite coal: varies from \$1.0/ton to \$5.0/ton.

Anthracite coal: \$10.0/ton

4. Calculation of Revenue Requirement

In order to optimize the process, formulation of objective function is necessary. The objective function is developed based on the annual

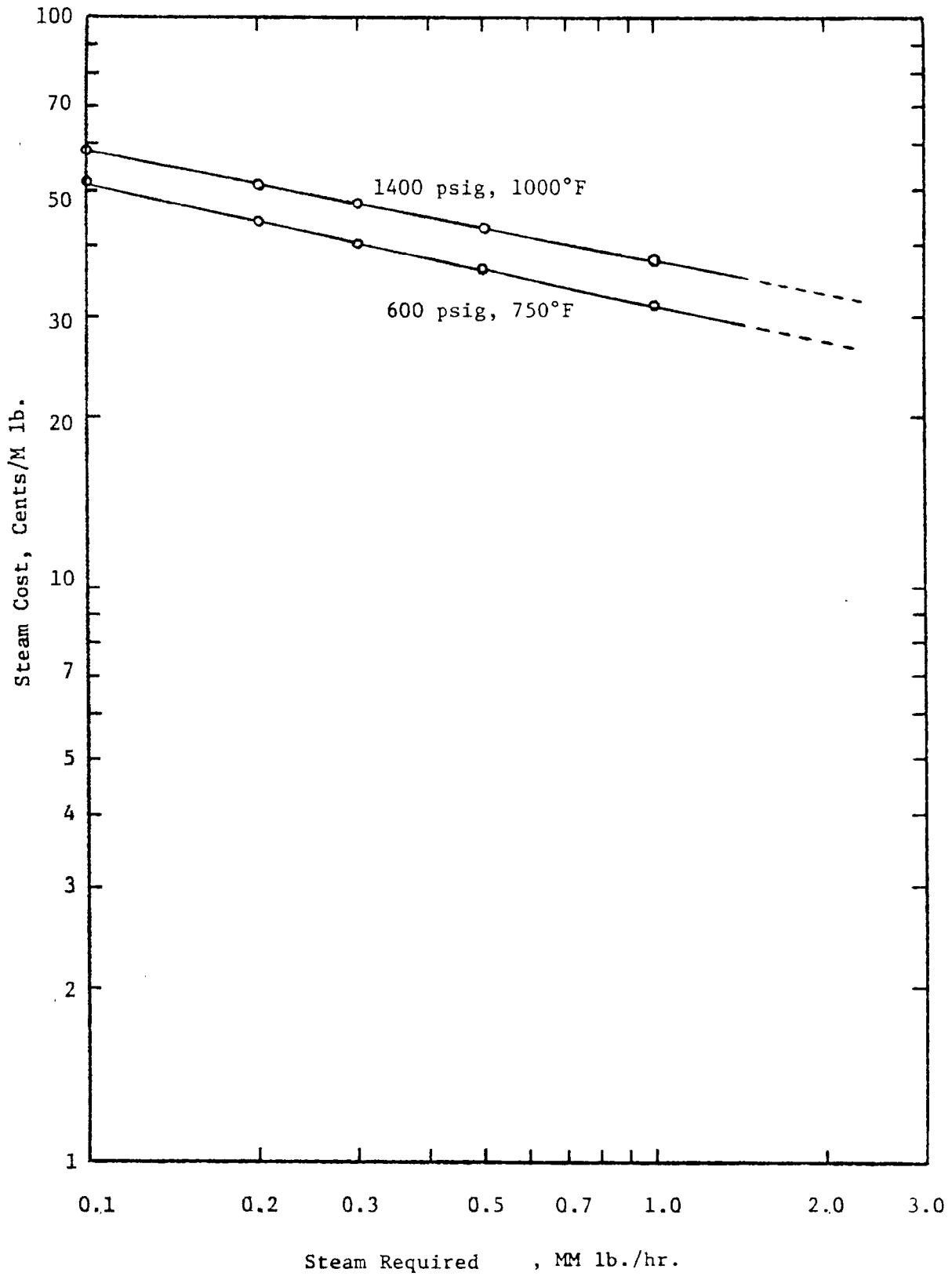


Figure II-1 Steam Cost in Terms of Rate of Steam Required

cost. The accounting procedure is based on a modified version of "Utility Gas Production General Accounting Procedure" proposed by the American Gas Association and adopted by the Office of Coal Research. The procedure estimates the annual revenue requirement under the following conditions [8]:

Debt-equity structure	65% debt (1/20th retired annually)
Return-on-rate base	7%
Federal income tax rate	48%
Interest on debt	5%
Depreciation, 20 year straight line	5%
State and local taxes and insurance	3%

The revenue requirement is composed of three factors: operating costs; return-on-rate base; and federal income taxes. The actual calculation is executed using the computer program which is available from the Office of Coal Research. Appendix B.1 shows the computer program.

Notation

A_b	bare tube heat transfer area, [sq.ft.]
A_o	heat transfer area, [sq.ft.]
E_A	cost of packings, [\$]
E_C	catalyst cost, [\$]
E_{CP}	compressor cost, [\$]
E_F	fin tube cost, [\$]
E_H	heat exchanger cost, [\$]

E_M	motor cost, [\$]
E_P	pump cost, [\$]
E_R	reactor shell cost, [\$]
E_S	cost of catalyst supporting trays, [\$]
T_h	thickness of the reactor wall [in.]
W_R	weight of the reactor shell, [lb.]

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- [2] Chilton, C., "Cost Engineering in the Process Industries," McGraw-Hill, New York, p. 50, 1960.
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Chapter III. COAL PREPARATION AND PRETREATMENT

COAL PREPARATION AND PRETREATMENT

This section deals with the crude preparation, and/or pretreatment of coal for gasification. Since preparation and/or pretreatment of coal are required for gasification processes regardless of the alternate schemes selected, this study presents the costs of this phase based on the tonnage of coal used per day. The cost of coal preparation and/or pretreatment will be included in the computation of the price of coal in Chapter VIII for each of the specific alternates selected.

1. Crude Preparation of Coal

Crude preparation of coal (both bituminous and lignite) is shown schematically in Figure III-1. Coal received from the mine is introduced to the breaker which reduces the size of the raw coal from 10 inches to 1 1/2 inches while removing approximately 20 percent refuse. Then coal is either sent to an intermediate storage, or to the heavy duty washer where an additional 20 percent refuse is removed.

The economic analysis of the crude preparation of bituminous coal is shown in Table III-2. For different coal feed rates, other than that specified in the Table, a 0.6 power scale-up factor was applied.

2. Preparation of Coal

- 2.1 Preparation of Bituminous Coal

The general preparation process is shown schematically in Figure III-2. The broken clean coal is sent to a crusher and the boilers. The crusher pulverizes the coal and the coal is then sent to a dryer. The

Table III-1 Composition of Bituminous Coal

Approximate Analysis wt.%	Prepared Coal	Dried Coal	Pretreated Char
Moisture	5.12	1.3	0.30
Volatile Matter	33.26	34.6	27.47
Fixed Carbon	49.99	52.0	59.77
Ash	11.63	12.1	12.46
Ultimate Analysis wt.%			
Carbon		71.20	71.40
Hydrogen		5.14	3.82
Oxygen		6.03	6.85
Nitrogen		1.23	1.41
Sulfur		4.19	4.02
Ash		12.21	12.50

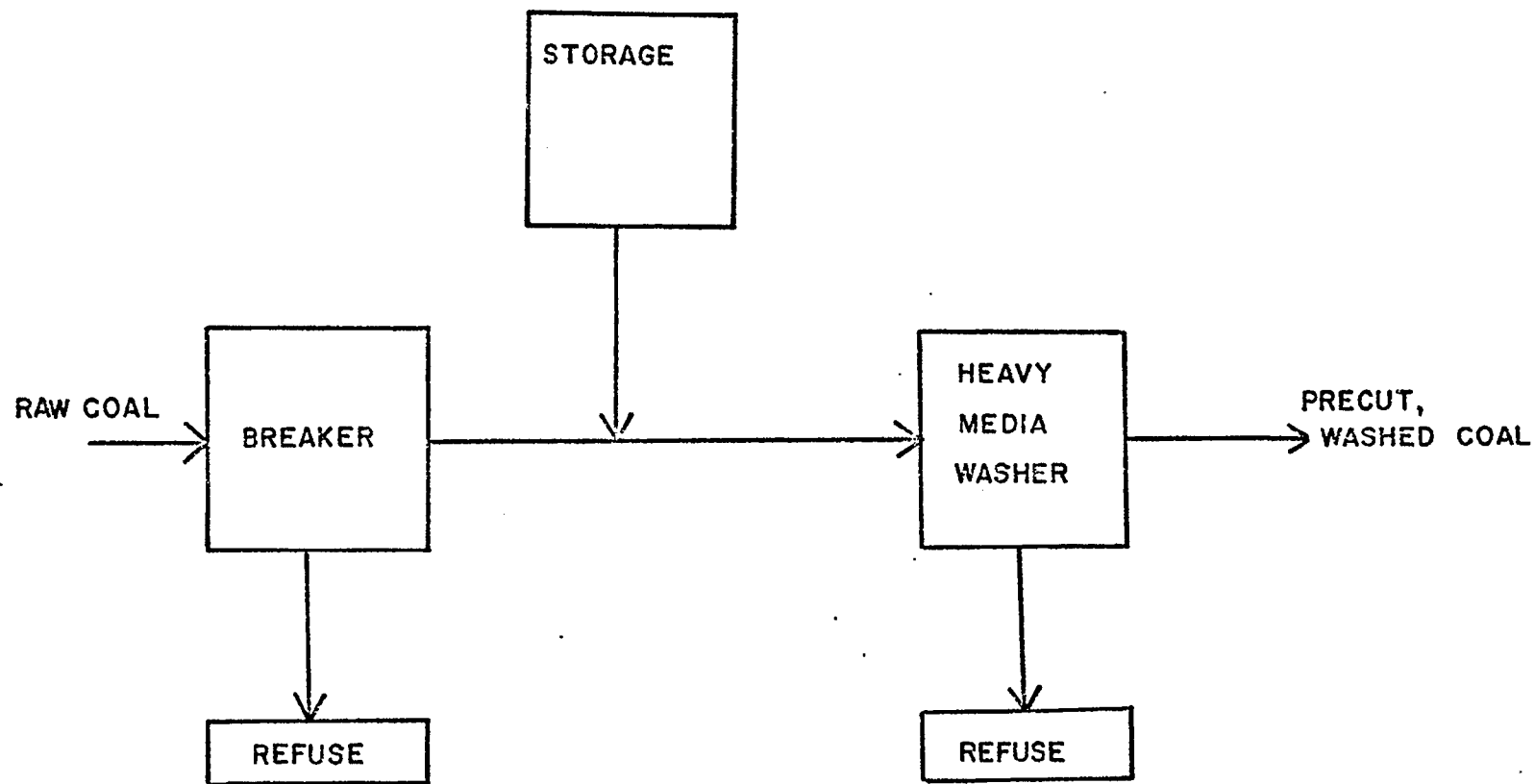


Figure III-1. Schematic Flow Design for Crude Preparation of Coal

Table III-2 Economic Analysis of Crude Preparation Process

Base: 13,700 tons/day of dry prepared coal.

<u>Item</u>	<u>M Tons/Day</u>	<u>Installed Equipment Cost, MMS</u>	<u>%</u>
Breaker	28.8	2.46	26.9
(Refuse)	(5.8)		
Conveying To and From Washing Plant	23.0	.665	7.2
Heavy Media Washing Plant	23.0	6.03	65.9
(Refuse)	(4.6)	_____	_____
		9.155	100.0

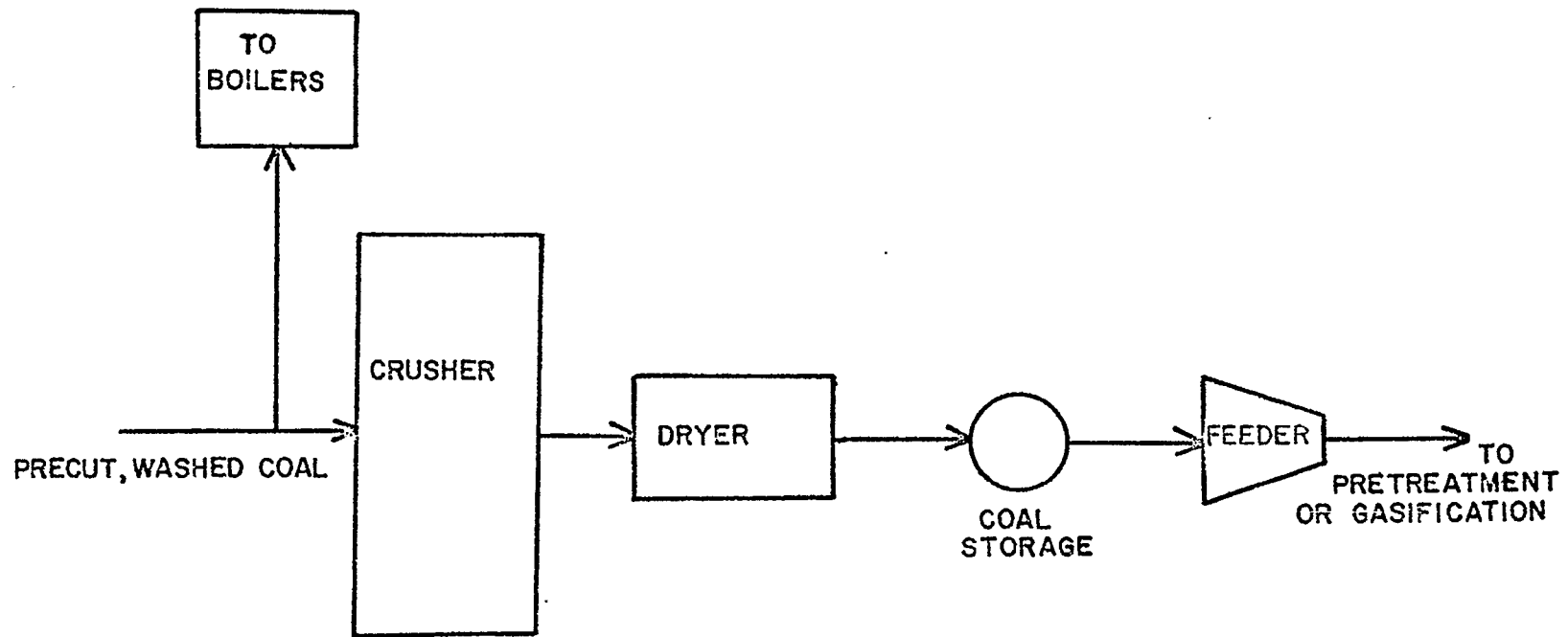


Figure III-2. General Process of Preparing Bituminous Coal

dried pulverized coal is then sent to storage.

Figure III-3 shows more details of the process. Coal is transported to the receiving hoppers from the heavy media washer and then transferred to the primary screens by collecting conveyers. The fines (minus 3/16 inch) and the oversize (plus 1 1/2 inch) are separated from the mainstream of coal by the primary screens. The oversize is reduced by roll crushers to the correct size of coal. The secondary screens receive the coal from the crushers and remove the fines. Fines from the primary and secondary screens are sent to the power plant.

The middle fraction of the primary screens is transported to the transfer house along with the oversize from the secondary screens where the coal can either be stockpiled or sent to a coal storage silo. The coal is then fed into a dryer.

2.2 Preparation of Lignite

The preparation of lignite is shown schematically in Figure III-4. Lignite undergoes a similar crude preparation process as does bituminous coal. The lignite from the washer is dumped into a receiving storage bin. Lignite is sent to a hammer mill (not shown in Figure III-4) where it is ground to minus 1/4 inch. Then it is conveyed to a lignite dryer. The lignite is fed to the dryer column by a screw conveyer where it is heated to 500°F by hot gases. Substantially all of the moisture and some of the oxygen in the lignite are driven off at this temperature. Part of the dried lignite is sent to the furnace to be burned in excess air to produce the hot gases which dry the lignite. Cyclone separators separate the dried lignite from the gases. The remainder of the lignite

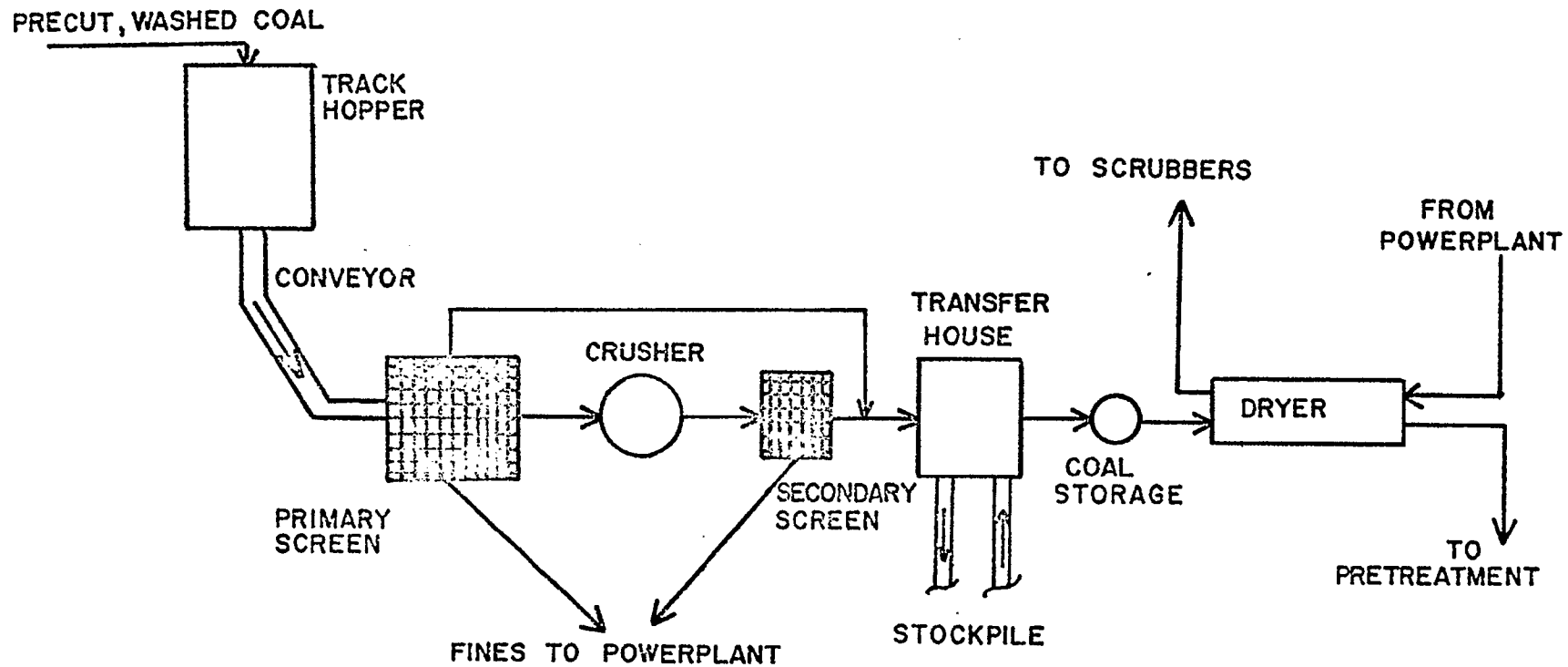


Figure III-3. Detailed Schematic of Preparation Process for Bituminous Coal

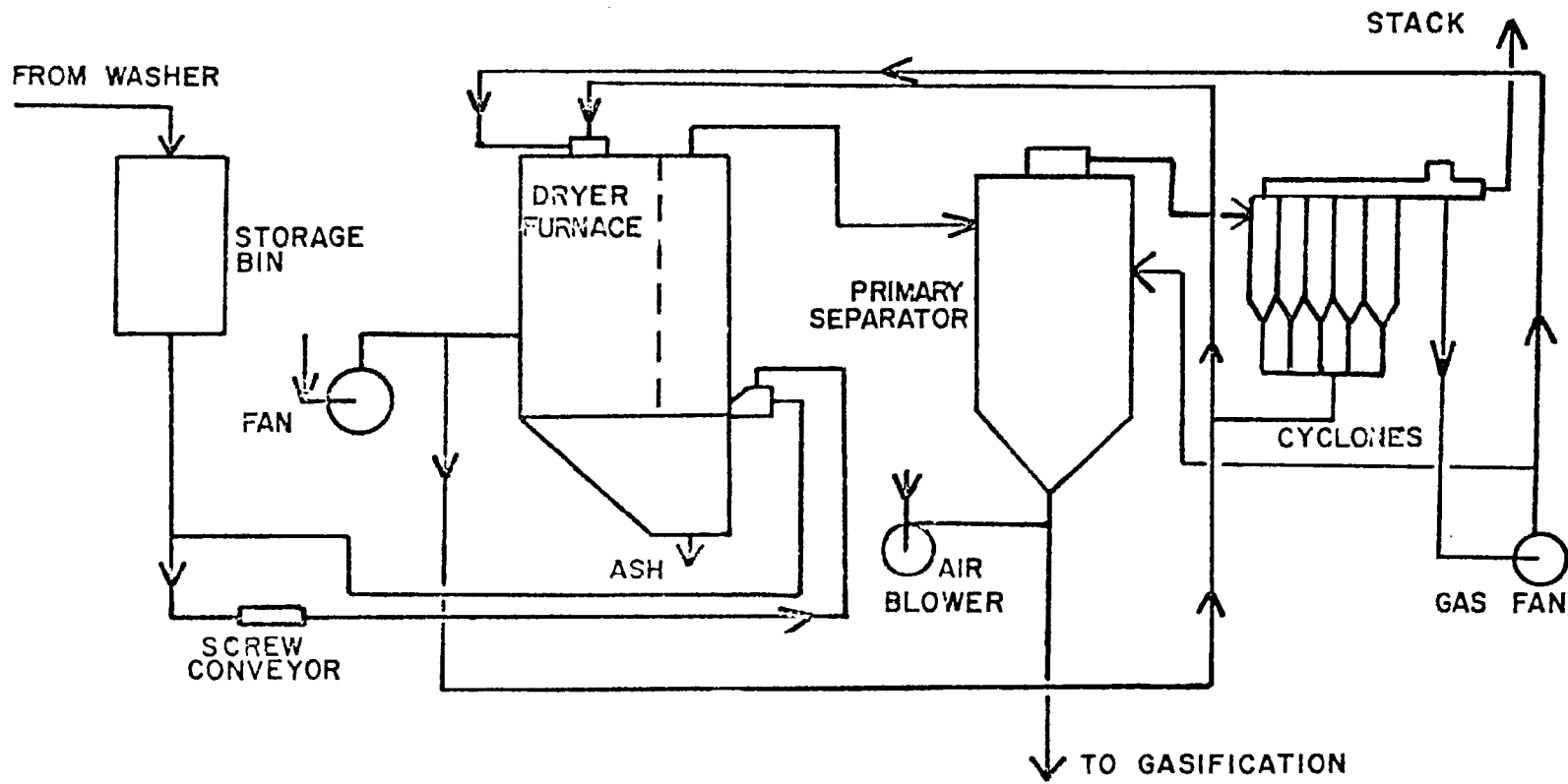


Figure III-4. Schematic Flow Diagram of Preparation of Lignite

is fed through a lock hopper and a pressure feeder system into the gasification unit.

3. Pretreatment

Volatile matter comprises about 35 weight percent in an average sample of bituminous coal. Pretreatment must be minimized to preserve as much volatile matter as possible. Since pretreatment is an oxidation reaction, the extent of oxidation is related to the extent of the pretreatment. Minimum pretreatment which allows production of a non-caking coal retains about 26 percent volatile matter in the pretreated char.

There are essentially three types of pretreaters -- fixed bed, free-fall, and fluidized bed.

In the fixed bed pretreater, coal is charred by treatment with oxygen and steam. The temperature is about 800°F and the pressure is approximately 325 psig. The units are assumed to be pressurized by the steam-oxygen mixture. The steam content is 99 volume percent with oxygen comprising the remaining 1.0 volume percent. The oxygen-coal ratio is about 2.7 SCF/lb coal. The steam-oxygen flow rate is about 29.5 MM SCFH, and varies with the amount of coal to be pretreated.

In the free-fall pretreater, the temperature is 1100°F and the pressure is 300 psig. Coal is dropped through a countercurrent flow of steam containing 5~12 volume percent oxygen. The oxygen-coal ratio varies about 2.4 SCF/lb coal. The residence time is only approximately 2 seconds.

Coal does not reach the temperature needed for decaking in a two second residence time when the preheating or reaction temperature is too low. If the oxygen is insufficient or the reaction temperature is too low, the coal agglomerates and plugs the treater.

Oxygen mixed with steam or inert gases such as nitrogen, carbon dioxide, etc., is used to treat caking coal in the fluidized bed pretreater. The temperature range is approximately 700°F to 775°F. The lower temperature corresponds to the plastic temperature of a certain coal. Below this temperature, pretreated coal would not be free flowing in the gasifier. Localized combustion begins near 775°F, causing runaway temperatures because of the inability of the bed to dissipate the heat.

Minimum pretreatment for a free flowing coal requires an oxygen-coal ratio of greater than 1.0 SCF/lb of coal fed. Increasing the oxygen consumption would produce more and more devolatilized coal, which is contrary to the purpose of minimum pretreatment.

The amount of oxygen which has reacted rather than the oxygen concentration, governs the extent of pretreatment. Oxygen concentration is about 10 volume percent. However, faulty gas distribution leads to localized combustion if the oxygen concentration is high.

Residence time in a continuous fluidized bed reactor must be long enough to minimize the effect of the untreated feed short circuiting into the product. Free-flowing coal can be produced with coal residence times ranging from 70 to 120 minutes, corresponding to oxygen-coal ratios of 1.2 to 2.4 SCF/lb coal.

4. Feeding Apparatus

The major coal feeding methods which have been investigated are lock hopper feed, slurry feed, and piston feed.

4.1 Lock Hopper Feed

This system is technically feasible at the present time. However, valve erosion, due to high differential pressures which would be encountered, would present a maintenance problem in a full scale plant such that the economic feasibility of this system is questionable. Periodic compression and decompression required for the lock hopper are other disadvantages of this system.

4.2 Slurry Feed

The slurry feed system offers the only continuous feed possibility of the three methods investigated. However, a satisfactory method of separating the carrier fluid from the coal has not yet been developed. Therefore, the slurry system does not appear to be free from technical problems at the present time.

4.3 Piston Feed

Many of the maintenance problems associated with the lock hopper system are also present in the piston feed system. However, the piston feeder was considered as the feeding system in this study because it has a potential for further development and is a convenient system for economic evaluation. Pneumatic conveyers transport pulverized coal from a low pressure storage vessel to a hopper which is pressurized by a piston. The coal then is passed to a high pressure surge vessel for feeding into the gasifier.

5. Summary

A summary of the various stages of the preparation and pretreatment process is shown in Table III-3 for both bituminous coal and lignite.

Figure III-5 represents the relationship between the installed equipment cost of the preparation (including the crude preparation process, and/or the drying processes) and the flow rate of raw coal used.

Figure III-6 shows the installed equipment cost of the pretreatment process as a function of the flow rate of prepared bituminous coal. (Lignite generally does not require pretreatment.)

Figure III-7 shows the relationship between the raw coal input rate and the prepared coal (wet) output rate of the preparation process.

Figure III-8 shows the relationship between the prepared coal (wet) input and the pretreated char output rate of the pretreatment process.

Figure III-9 represents the reduction in the required prepared coal (dry) if this coal bypassed the pretreaters and was sent directly to the gasifiers as a function of the weight percent of dry coal lost in pretreatment for various char (or coal) feed rates into the gasifier.

As is evident from Figures III-8 and III-9, pretreatment of coal significantly influences the amount of coal required for gasification. In order to prevent agglomeration in the gasifier, pretreatment is required for most of the bituminous coal investigated. However, Figure III-9 clearly indicates that any means by which char with less

Table III-3 Summary of Preparation and Pretreatment Costs

Bituminous Coal

Pretreated Coal Fed Into Gasifier, M Tons/Day	Crude Preparation Installed Equipment Cost, MM\$	Preparation Installed Equipment Cost, MM\$	Pretreatment Installed Equipment Cost (Including Dryer) MM\$	Total Cost MM\$
13.7	9.16	1.70	6.46	17.32
15.0	9.69	1.80	6.84	18.33
20.0	11.49	2.13	8.13	21.75

Lignite

Prepared Lignite Fed Into Gasifier M Tons/Day	Crude Preparation Installed Equipment Cost, MM\$	Preparation Installed Equipment Cost, MM\$	Drying and Feeding Installed Equipment Cost, MM\$	Total Cost MM\$
15.0	12.33	2.05	6.01	20.39
20.0	13.13	2.14	7.07	22.34

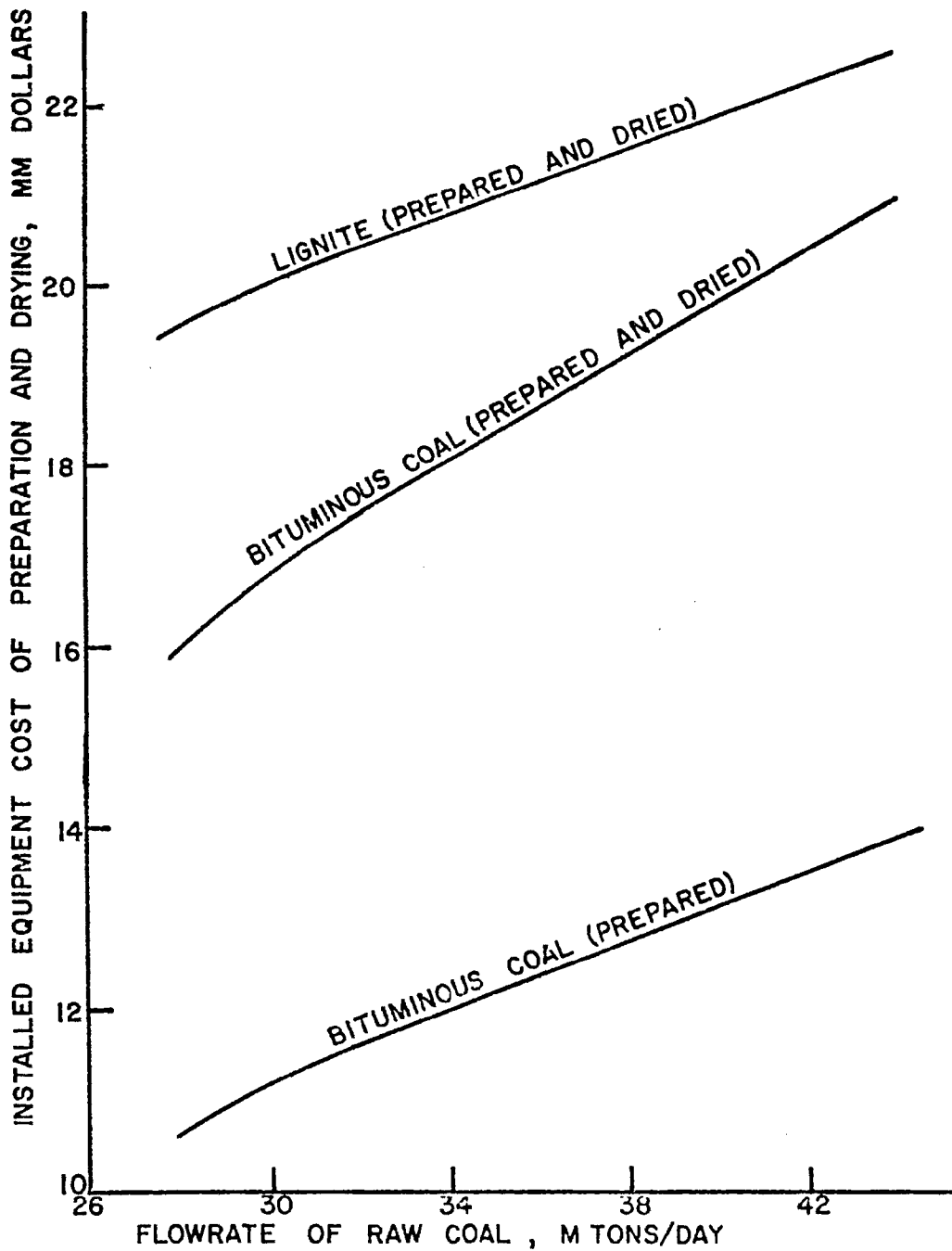


Figure III-5. Effect of Raw Coal Input Rate on Installed Equipment Cost of Preparation and Drying

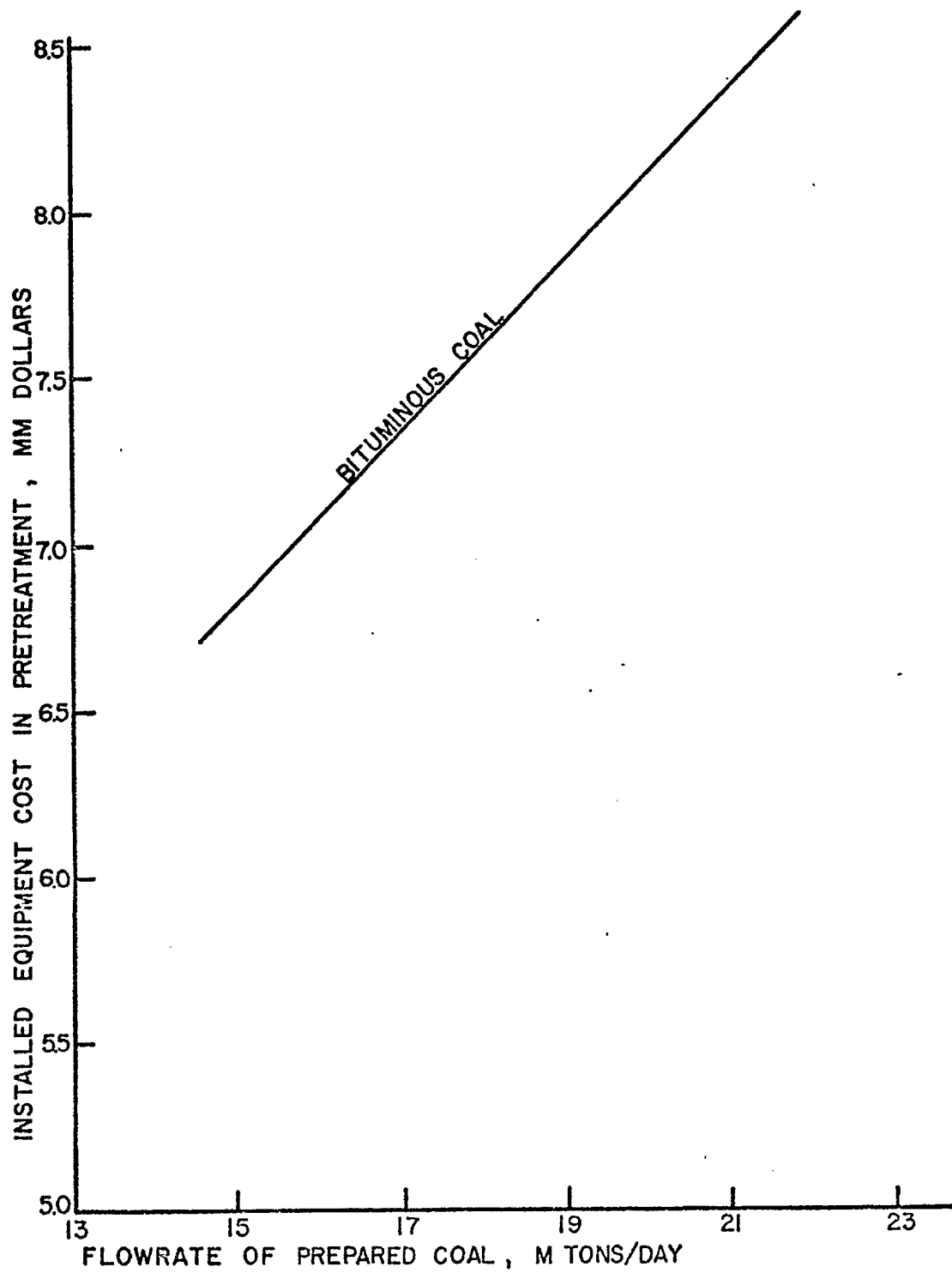


Figure III-6. Installed Equipment Cost of Pretreatment as a Function of Prepared Coal Flow Rate.

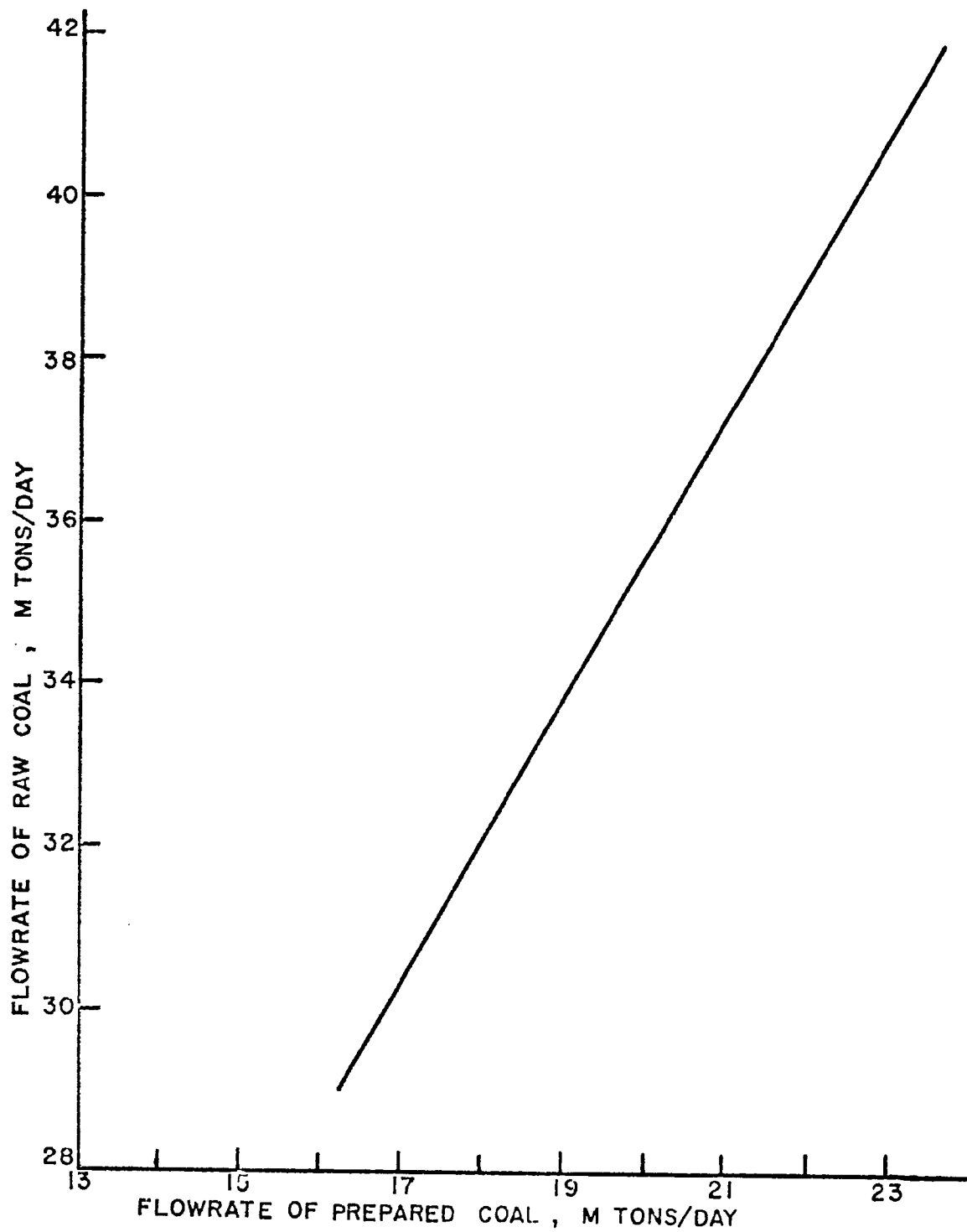


Figure III-7. Raw Coal Input Rate Required as a Function of (Wet) Prepared Coal Output Rate

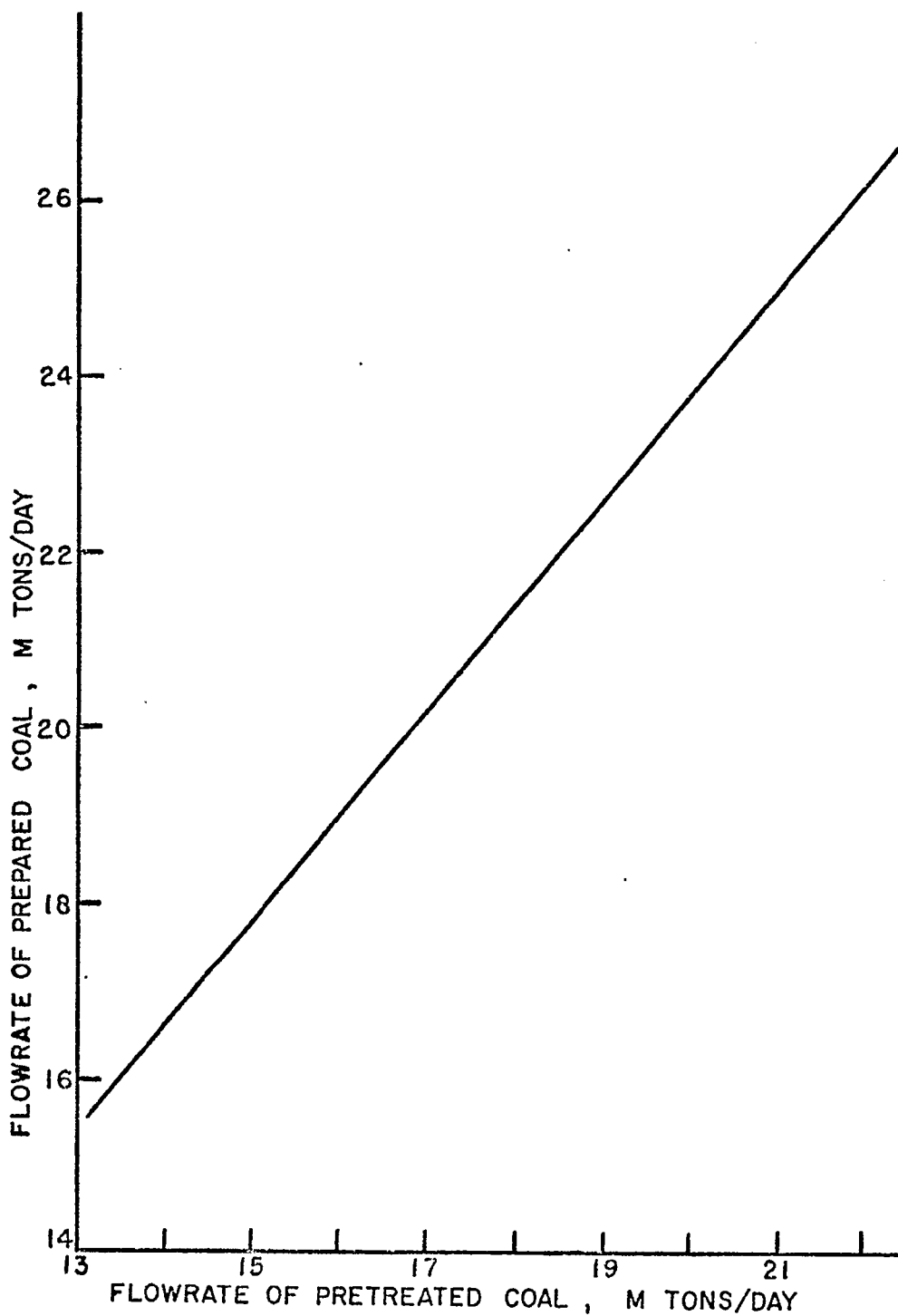


Figure III-8. (Wet) Prepared Coal Input Rate Required as a Function of Pretreated Char Output Rate

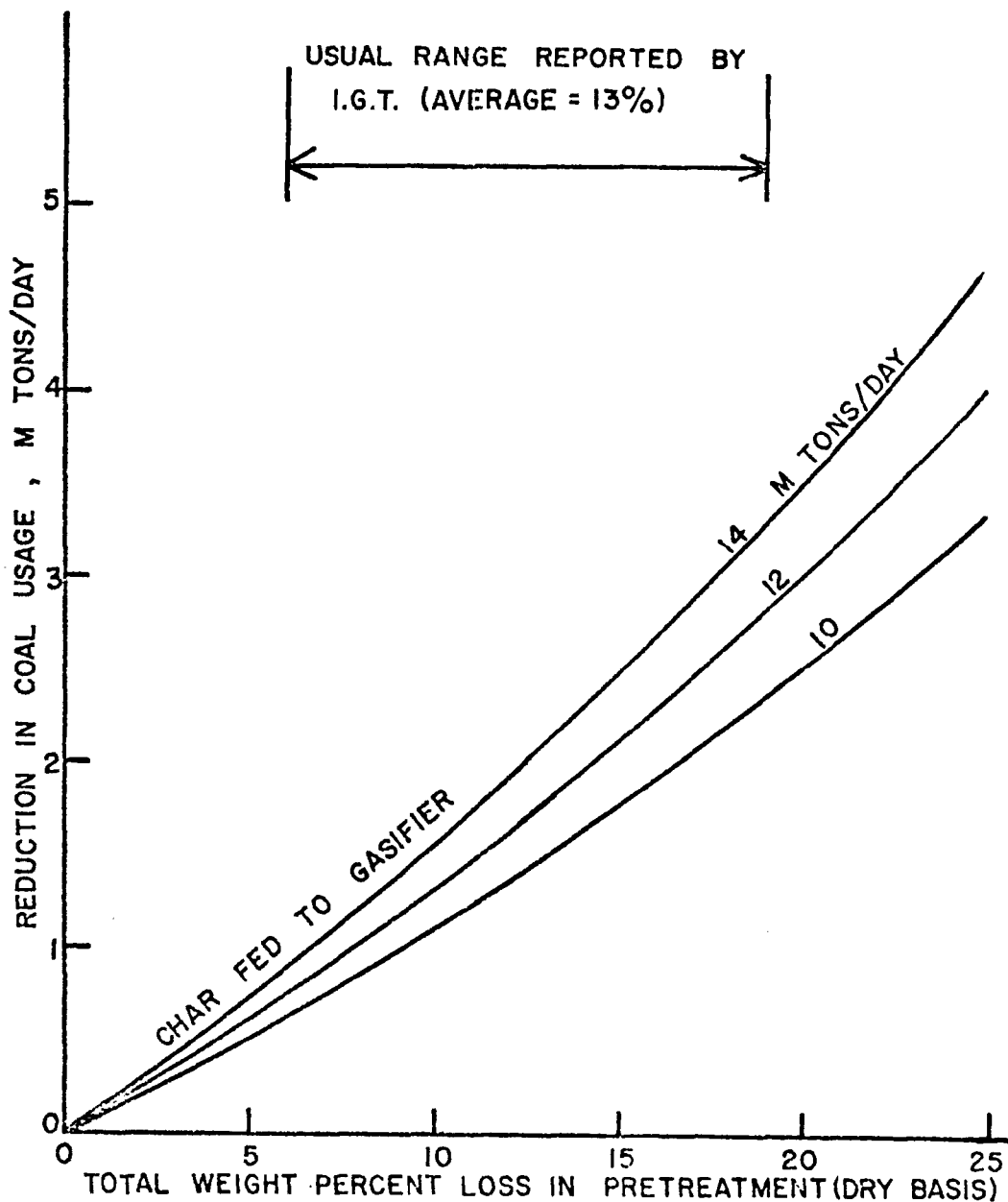


Figure III-9. Reduction of Coal Usage (If Nonpretreated Coal Were Fed to the Gasifier as a Function of Pretreatment Weight Loss and Gasifier Feed Rate)

pretreatment can be fed to the gasifier will reduce the overall cost of gasification considerably. If, for example, prepared, but untreated, coal could be fed directly to the gasifiers, approximately 1500 to 2000 tons per day of coal can be saved in comparison to feeding pretreated char (based on the average of 13% loss in weight by pretreatment).

However, there are a number of possibilities of recovering the volatile matter lost in the pretreatment. Effluent from pretreatment may be recovered in the form of liquid or gas fuel, which can be injected into the gasifier. At present, the technology of recovery has not fully developed to justify economic evaluation of this phase of operation. On the other hand, in order to feed raw coal to the gasifier without causing agglomeration of coal particles, a feeder system which can distribute coal particles uniformly into the reactor is needed. The technology of the feeder system has not been fully developed either.

Figure III-10 represents utilities requirements as functions of raw coal used.

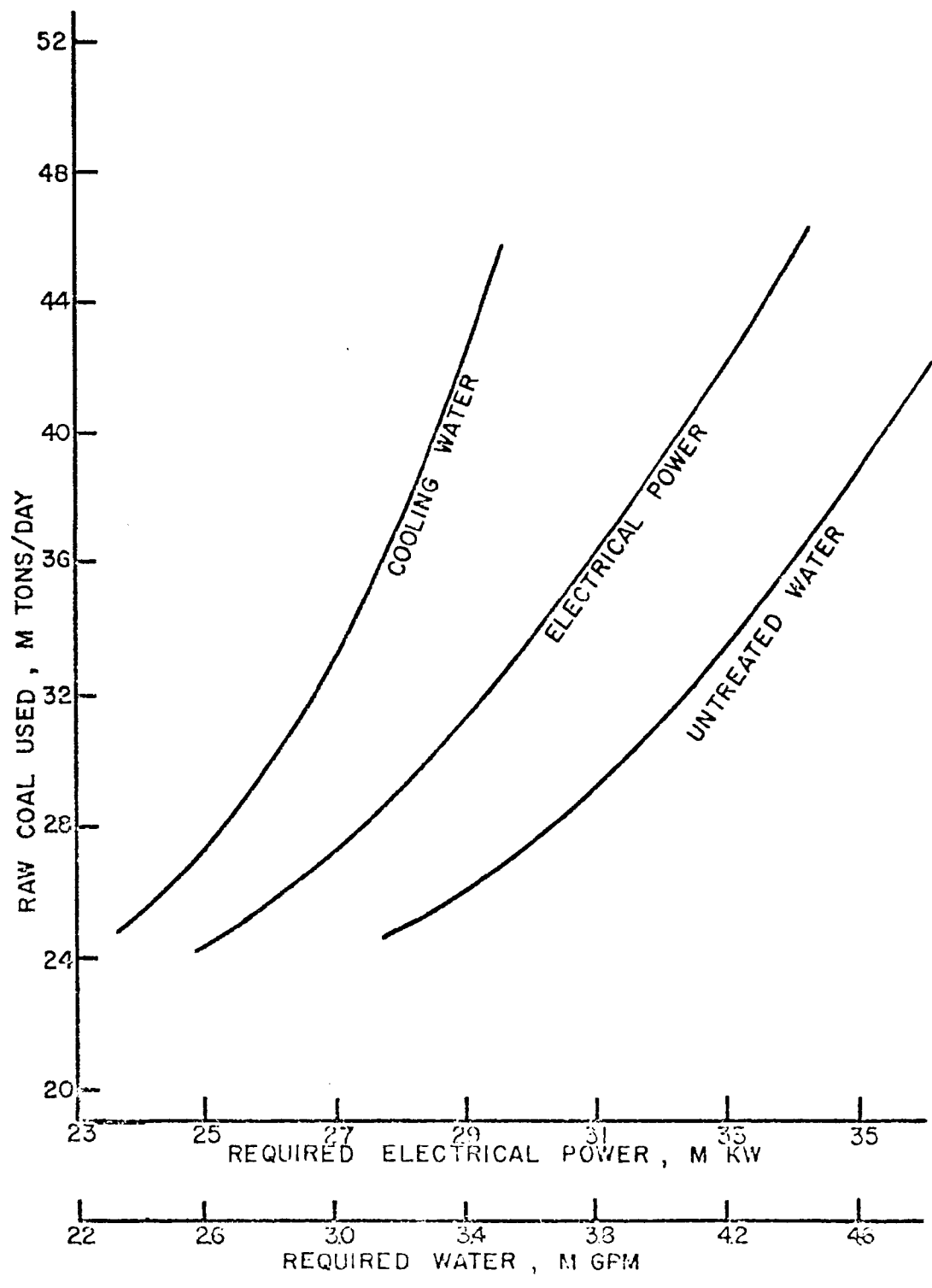


Figure III-10. Utilities Requirement as a function of Raw Coal Used

Literature

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Chapter IV. GASIFICATION



GASIFICATION

The main purpose of the gasification is to convert the highly carbon containing solid coal into gases which either with or without further treatments, will produce pipeline gas having heating value of more than 900 BTU/SCF. Besides the specified heating value it is expected that the pipeline gas so produced will be compatible with natural gas. In other words, the pipeline gas produced from coal must be composed predominantly of methane. Natural gas, for domestic or industrial use, usually contains more than 90% methane.

Methane can be obtained simply by pyrolysis of coal. Coal, in addition to carbon, contains some volatile hydrogen, which when heated to a certain temperature in absence of air or oxygen can combine with carbon to form methane. Gasification of coal by pyrolysis alone is not an economical method because large portions of carbon as char are rejected as a by product of pyrolysis. The pyrolysis of coal is usually coupled with other methods of gasification.

Another method of producing methane is by the hydrogasification process. It is also termed as hydrogenation, hydrogenolysis or hydrocarbonization. By this method methane is produced directly from the reaction of carbon and hydrogen. The ultimate analysis shows that the atomic ratio of carbon to hydrogen in coal is about 1 to 0.8 for Bituminous coal and 1 to 0.7 for Lignite, compared to the ratio of 1 to 4 in methane. It is evident that an external hydrogen supply is necessary for converting coal or residual char from the coal pyrolysis into a gas rich in methane. There are many processes by

which hydrogen may be produced. The methods for hydrogen production will be discussed later in this chapter.

Methane can also be obtained from the synthesis gas-methanation process. This is a dual-step process, making synthesis gas (H_2 - CO mixture) and catalytically upgrading it to methane. In the synthesis gas production the carbon-steam, water gas shift and carbon-oxygen reactions take place simultaneously. The first reaction is endothermic whereas the second and third reactions are exothermic. The overall heat balance of gasification shows that heat is required for the successful production of synthesis gas from coal. Heat can be supplied externally by electricity or from a nuclear reactor. It can also be supplied internally by burning a part of the coal with oxygen or air.

Because of the difference in volatile matter content, moisture content, and caking characteristics of coal, the mode of the gasification varies depending on the coal used for gasification. A number of alternate methods have been formulated for coal gasification processes. The schematic diagrams of these methods are presented in the following section. A brief discussion of each alternate method will be given. The most favorable methods, likely to become commercially feasible, will be chosen for further study. The energy balance, computer simulation of gasifier performance, and cost estimation of these processes will be made.

1. Alternative Coal Gasification Processes

Production of high BTU pipeline gas from coal gasification can be classified into the following three basic methods:

Pyrolysis

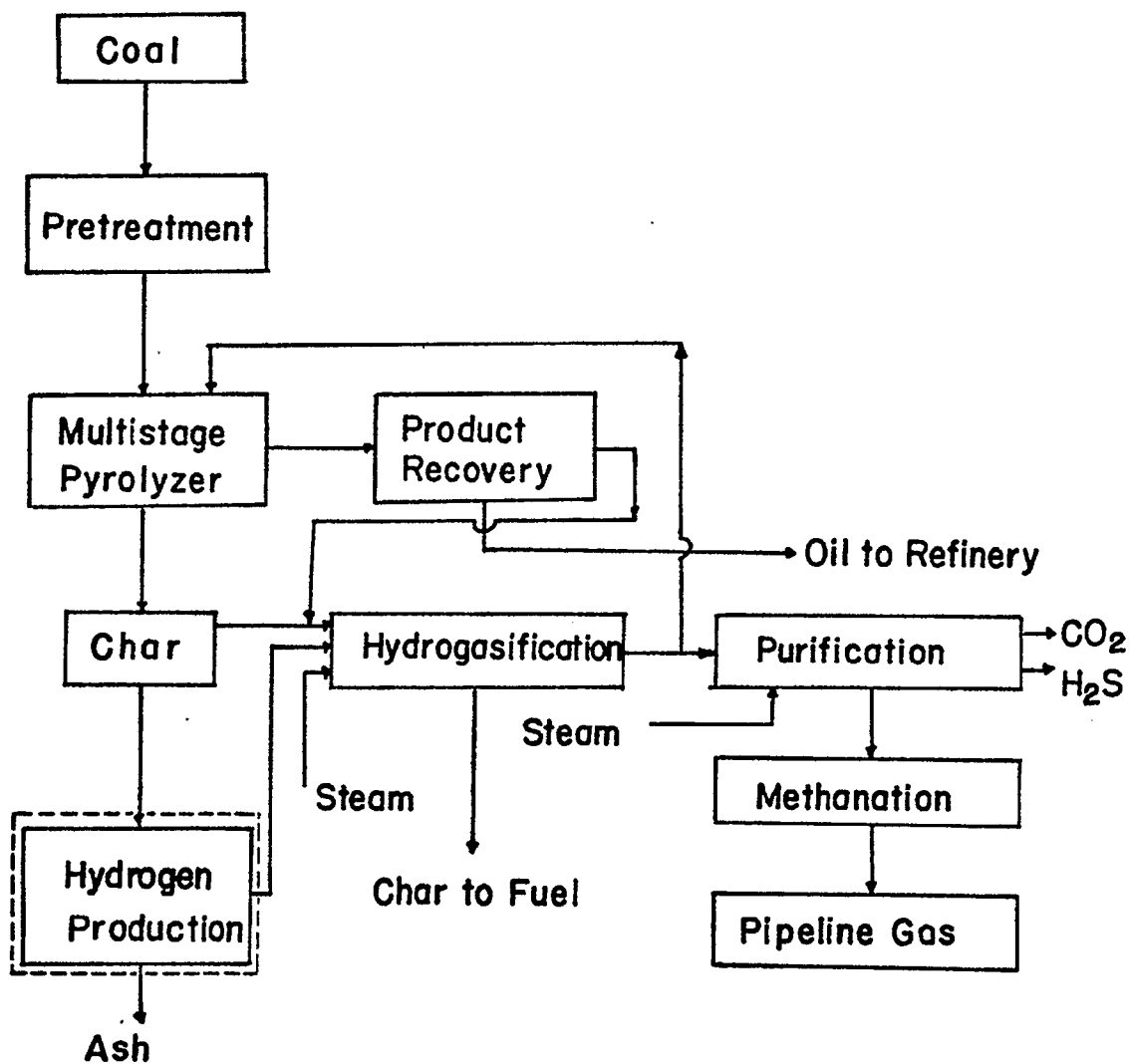
Hydrogasification

Synthesis gas methanation

In order to economically utilize coal to produce pipeline gas one or more of the above methods are usually used together. For example, char, a by-product of pyrolysis, can be used to produce hydrogen which will be used as a raw material in hydrogasification. A diagram for the processes of coal gasification is presented in Figure IV-1. From this diagram a number of alternative pipeline gas production schemes can be traced out, and the details are discussed in the following.

1.1 Pyrolysis of coal followed by hydrogasification and methanation

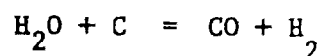
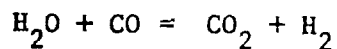
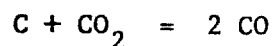
A schematic diagram of this process is shown in Figure IV-2. Coal after pretreatment is put into a multistage pyrolyzer where a part of the hot effluent gas from the hydrogasifier is introduced. The condensable gas in the gas products is separated from the main stream as crude oil in a product recovery. Methane and other non-condensable gases are transferred to the hydrogasifier. After pyrolysis, coal becomes char which contains mainly the relatively less active carbon. A part of this char is introduced to the hydrogasifier, whereas the remainder is used for hydrogen production. Char reacts with steam and hydrogen to form more methane in the hydrogasifier. A part of the effluent gas from the hydrogasifier is recycled back to the pyrolyzer for heating. The remainder of the gas is sent to purification and methanation. The residual char from the hydrogasifier can be used as fuel in a power plant. Hydrogen used for hydrogasification can be produced by the following methods:



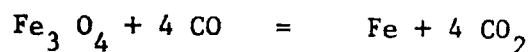
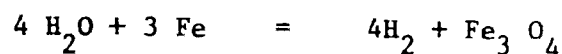
Note: The block enclosed by the dotted line represents the various alternative processes discussed in Section 1.1, i,ii,iii,iv,v.

Figure IV-2 Flow Diagram for Processes With Pyrolysis of Coal Followed by Hydrogasification and Methanation

- i. Hydrogen can be produced by char gasification followed by catalytic water gas shift conversion and purification. The reactions involved in this process are:



- ii. Hydrogen can be produced by passing steam through a hot iron bed where iron-steam reaction takes place. Iron oxide, a by-product of the reaction, is reduced back to iron by producer gas produced from char. The reactions involved in this process are:



Hydrogen production and iron oxide reduction can be done in two separate fluidized beds.

- iii. Hydrogen can be produced by high pressure water electrolysis. Water is made conductive by addition of caustic potash and is dissociated into hydrogen and oxygen at 420 psig by the application of D.C. current. Hydrogen so produced is then compressed to gasification pressure.

- iv. Hydrogen can be produced by the carbon steam reaction:

- (a) Hydrogen is produced from an electrothermal gasification system, which includes catalytic water gas shift conversion and purification.

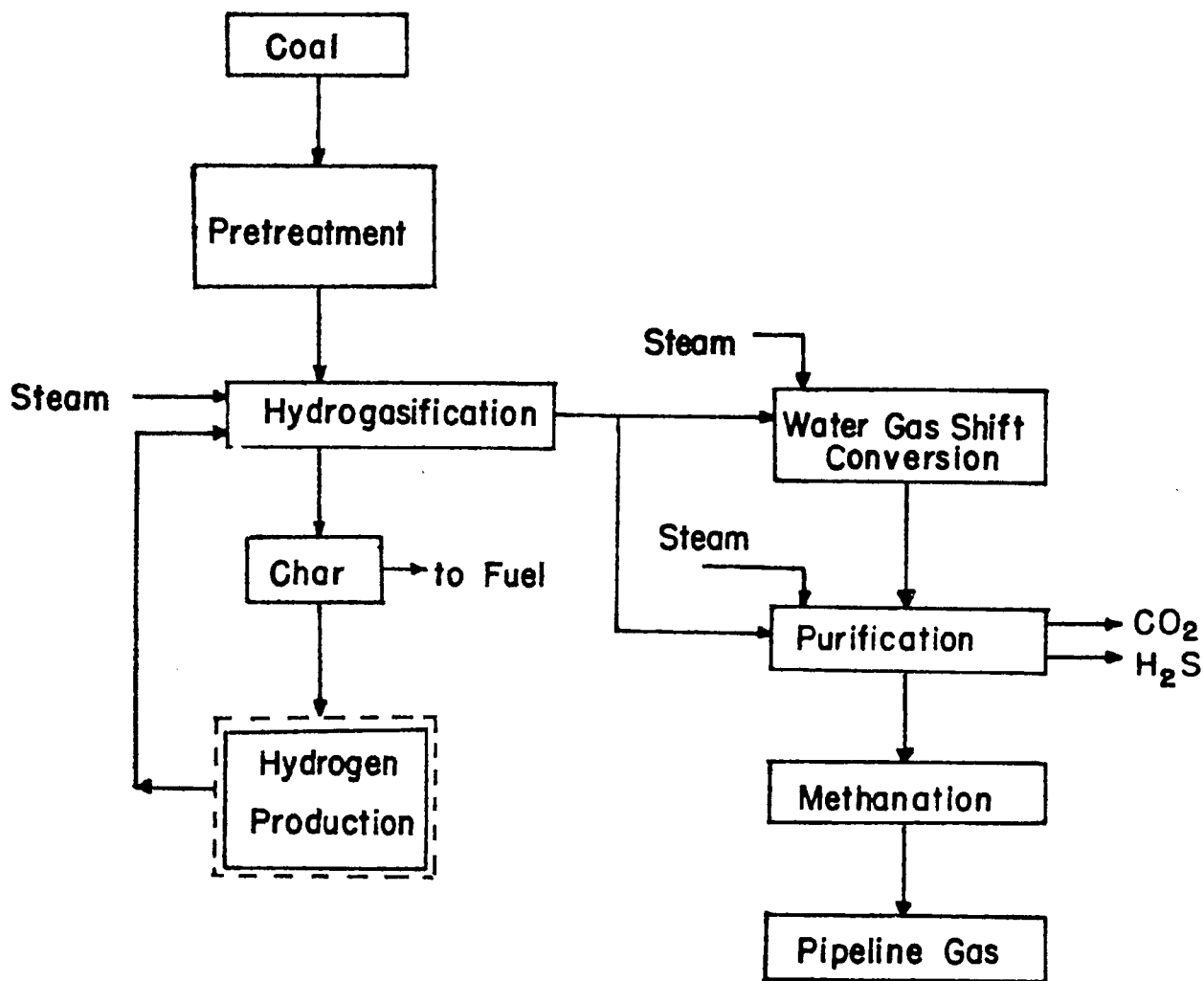
- (b) Synthesis gas can be produced from an electrothermal gasification system. The gasification product is a hydrogen rich gas mixture. (IGT Lignite hydrogasification)
- (c) Hydrogen can be produced by the carbon-steam reaction in a gasifier with the following heat carrier systems: CO₂ acceptor and molten ash methods, Kellogg molten salt method, and slag method (Rummel Double Shaft).
- (d) Hydrogen can be produced by the carbon-steam reaction with heat supplied directly by a nuclear reactor or indirectly through a heat transfer medium.
- v. Hydrogen can be produced by catalytic reformation by reacting a part of the product methane with steam. This is followed by catalytic water gas shift with excess steam and removal of CO₂. The reactions are:



Any one of the above hydrogen production methods can be coupled with the main gasification system to form an alternate method.

1.2 Coal hydrogasification followed by upgrading methanation

The pretreated coal is introduced to a gasifier, where it is reacted with hydrogen or hydrogen rich gas and steam. A schematic diagram of the process is shown in Figure IV-3. Hydrogen can be obtained from any one of the hydrogen production methods discussed



Note: The block enclosed by the dotted line represents the various alternative processes discussed in Section 1.1,i,ii,iii,iv,v.

Figure IV- 3 Flow Diagram for Processes With Coal Hydrogasification Followed by Upgrading Methanation

in the preceding section. The effluent gas of the hydrogasifier is further treated by catalytic water gas shift, purification and methanation steps to form pipeline gas. The above series of treatments is called upgrading methanation.

Hydrogasification processes vary depending on how hydrogen for hydrogasification is produced. I.G.T. hydrogasification produces hydrogen for hydrogasification from electrothermal gasification of spent char. If Lignite is gasified by synthesis gas produced from electro-thermal gasification of spent char, it will be referred to as the I.G.T. Lignite Hydrogasification.

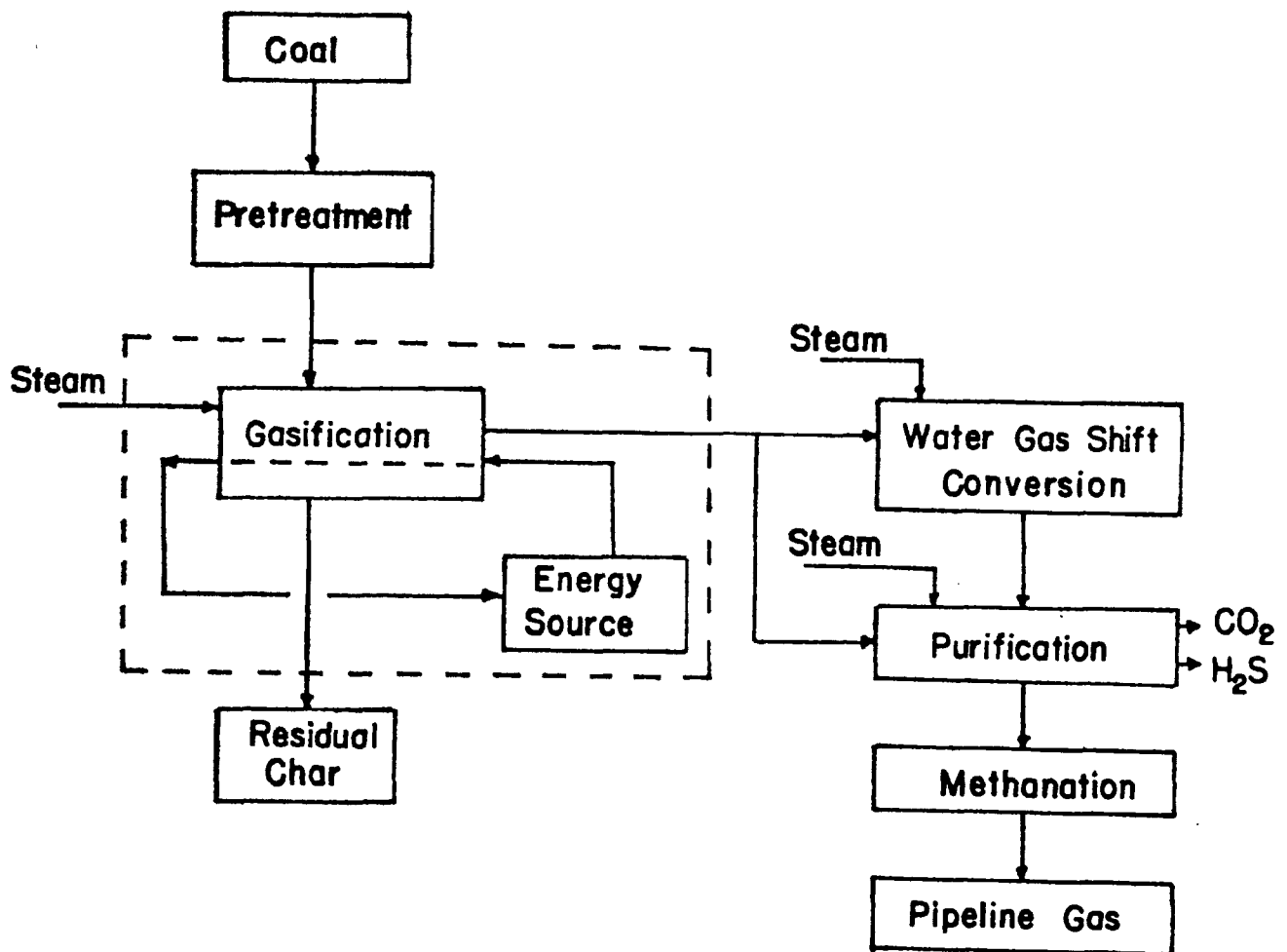
1.3 Coal gasification with steam followed by upgrading methanation

Coal can be gasified directly by steam if a proper energy supply for the reaction is provided. A schematic diagram of the process is shown in Figure IV-4. Pretreated coal is reacted with steam in a gasifier where heat is supplied externally. The effluent gas so produced mainly contains CO, H₂, and CH₄ having a low heating value. To achieve the specified heating value of 900 BTU/SCF the crude gas is further treated by upgrading methanation.

Alternate methods for coal gasification with steam followed by upgrading methanation are discussed below.

- i. External heat is supplied to the gasifier through a heat carrier system.

(a) Heat carried by pebbles: Pebbles are heated by burning char with air and then introduced to the gasifier. Heat is transferred from the hot pebbles to coal particles. Coal is gasified with steam and the effluent gas is further treated by upgrading



Note: Blocks enclosed by the dotted line represents various alternative processes discussed in Section 1.3.

Figure IV-4 Flow Diagram for Processes With Coal Gasification Using Steam Followed by Upgrading Methanation

methanation. The relatively low temperature pebbles with a certain amount of carbon deposited on the surface are returned to the heat carrier regenerator where they are burned and sent back to the gasifier. The Mayland Pebble - Bed Gasifier is a typical example of this process. Since this gasifier is normally operated at atmospheric pressure a product compressor is needed at the end of upgrading methanation.

(b) Heat carried by molten salts: This process is proposed by M. K. Kellogg Company. Molten sodium carbonate is used as a heat carrier as well as a catalyst for the endothermic carbon-steam and the exothermic carbon-oxygen reactions needed for coal gasification. Gasification occurs in the molten sodium carbonate by introducing steam containing finely divided coal at the bottom of the reactor. By continuously circulating molten salt containing carbon from gasifier to the combustor, combustion of the carbon by air injected at the bottom of the combustor produces heat which is transferred to molten salt. The reheated melt is circulated back to gasifier continuously. Occasionally some make-up salt is put into the system for continuous operation.

(c) Heat carried by dolomite: This process is called the CO_2 Acceptor Gasification Process and has been developed by the Consolidation Coal Company. Dolomite is used as a heat carrier and is circulated between the gasifier and the heat carrier regenerator. The fresh and hot CaO-Ca(OH)_2 mixture, a product obtained by heating dolomite, is contacted with steam containing finely divided coal particles in a gasifier. Utilizing the heat carried in by the heat

carrier, coal is gasified with steam. CO_2 , a by-product of the gasification, is reacted with CaO to form CaCO_3 . CaCO_3 with some coal particles is continuously withdrawn from the bottom of the gasifier and sent back to the heat carrier regeneration system for reheating.

The molar ratio of CO to H_2 in the effluent gas of the gasifier at approximately 1600°F and 330 psia is controlled at about 1/3. Thus, the catalytic water gas shift conversion can be eliminated from the upgrading methanation. Because of the low pressure operation of the gasifier a product gas compressor is needed at the end of methanation. One advantage of using dolomite as a heat carrier is that CaO in the gasifier can also react with H_2S to form CaS , reducing a substantial amount of sulfur content in the effluent gas.

(d) Heat carried by slag: In this process air and coal are injected tangentially in one shaft, and steam and coal are injected into another shaft. Vertical partitions slightly submerged in slag bath separate the two shafts so that products of combustion and synthesis gas leave in separate streams. The heat required for gasification is supplied by heat generated in the combustion shaft and transferred by the rotating slag bath to the gasification shaft. Rummel Double-Shaft Gasifier is a typical example of the process in which the gasifier is of entrained bed type and is operated under atmospheric pressure. To produce pipeline gas by using Rummel Double-Shaft Gasifier a product compressor is needed to attain specified pressure of that gas.

ii. External heat is supplied to the gasifier through an electric heating system.

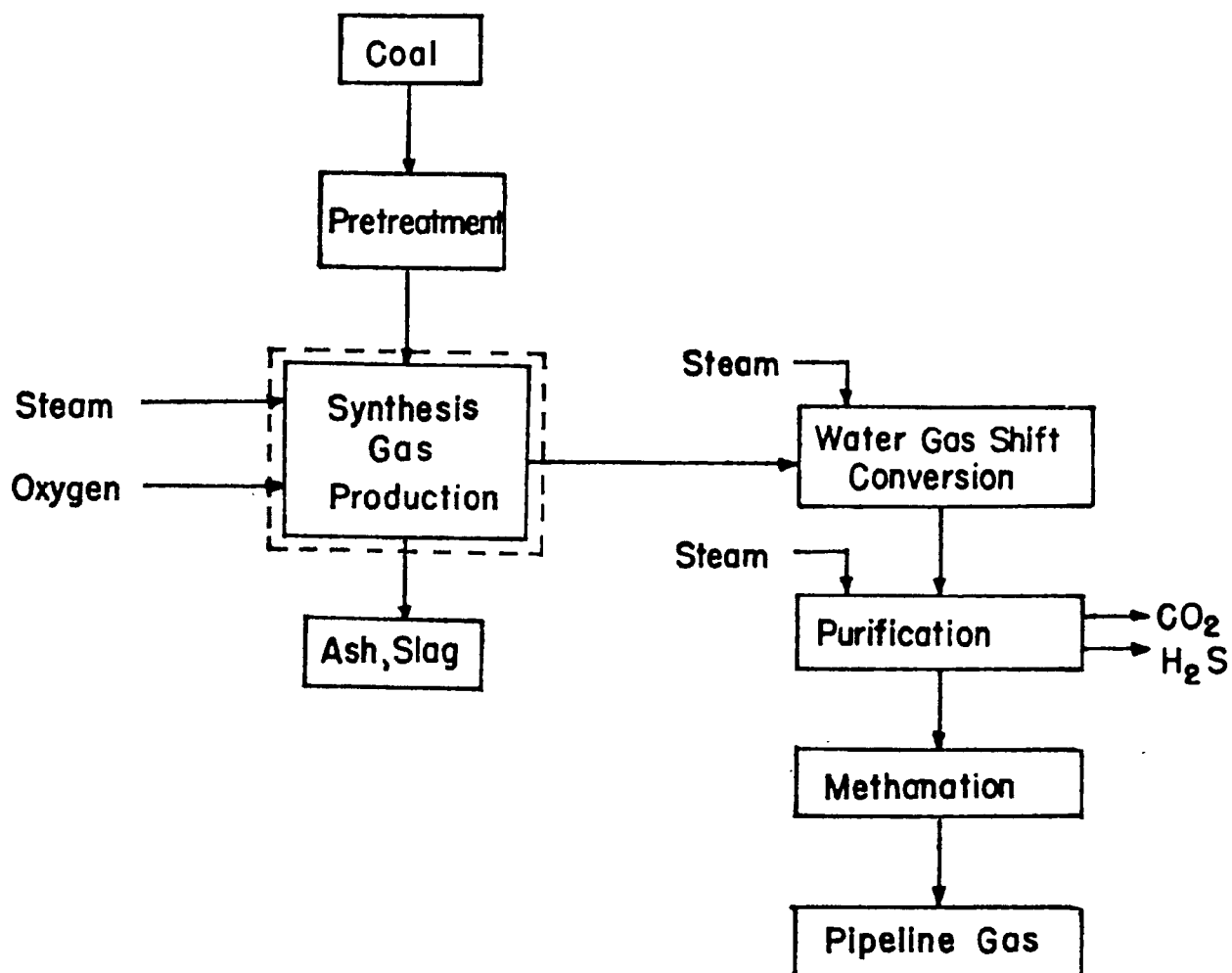
Heat generated by passing electric current through a fixed or a fluidized bed of coal is directly used for gasification. Therefore the thermal efficiency of the gasifier in this case is higher than in other types. Jenson Electric Gasifier, the U.S. Bureau of Mines Electric Gasifier, and the Electro-Fluidized Bed of Iowa State University belong to this class of gasifier. The former two gasifiers are operated at atmospheric pressure requiring a product compressor for each.

- iii. Heat required for gasification is supplied by a nuclear reactor.

This scheme has been intensively studied by the Atomic Energy Commission and the U.S. Bureau of Mines. Two methods have been considered. One is the direct-cycle method in which the process stream passes through and reacts in a nuclear reactor. The other is the process-stream-preheating method in which one or more of the streams are heated in the nuclear reactor, and the gasification takes place in a separate vessel. However, these systems produce too much radioactivity in the product which cannot be used for fuel or other purposes. An alternate method of using an indirect heating system, with helium as the heating medium, has also been proposed.

1.4 Synthesis gas production followed by upgrading methanation.

A schematic diagram of this process is shown in Figure IV-5. Pretreated coal is introduced into a gasifier where it is reacted with steam and oxygen or air to form synthesis gas. When air is used the gasifier should be operated cyclically. The synthesis gas



Note: The block enclosed by the dotted line represents various alternative processes listed in Table IV-1.

Figure IV-5 Flow Diagram for Processes With Synthesis Gas Production Followed by Upgrading Methanation

is then subjected to upgrading methanation to form pipeline gas. Many processes have been proposed for synthesis gas production. They are summarized in Table IV-1. In some cases where the gasifier is operated under atmospheric pressure a product gas compressor is required in the system. Only Lurgi Gasifier will be briefly discussed.

In the fixed bed pressure Lurgi dry ash gasification, the pretreated coal is charged from the top of the gasifier through lock hoppers. Steam and oxygen are introduced from the bottom of the reactor. Temperature is high at the bottom and low at the top of the bed. Ash produced from gasification is continuously withdrawn from the bottom of the reactor through a specially designed rotating grates. Only the nonagglomerating coal can be used in this kind of gasifier. The relatively low oxygen requirements make this process attractive despite relatively low throughputs and high steam requirements that are required to condition the ash properly for removal from the grates.

In "Pressure Slagging Gasifier" the restriction of using the nonagglomerating coal is eliminated. The ash produced from gasification is continuously removed in a melt form from the bottom of the reactor through a slag tap. In some cases, fluxing material such as limestone is added to improve the fluidity of the slag in the gasifier. In this type of process the gasifier can be operated at a temperature higher than ash fusion temperature. This means that more oxygen can be introduced into the gasifier, and more

Table IV-1-a Summary of Synthesis Gas Producers [3]
(Using Steam and Oxygen)

USING STEAM AND OXYGEN

<u>NAME</u>	<u>OPERATING PRESSURE</u>	<u>ASH OR SLAG</u>
UGI Converted	A	Ash
Thyssen Galoczy	A	Slag
Kerpely	A	Ash
Leuna Slagging	A	Slag
BASF-Leuna Slagging	A	Slag
Wellman-Galusha	A	Ash
Bamag-Winkler Atmospheric	10 psig	Ash
Koppers-Totzek	A	Slag
B & W-DuPont	A	Slag
Rummel Single-Shaft	A	Slag
Lurgi Dry-Ash*	450 psig	Ash
BASF-Flesch Demag	A	Ash
Panindco	A	Ash
USBM Vortex	A	Ash
Inland Steel	A	Ash
Gas Council-Lurgi	450 psig	Slag
BCURA-Lurgi Slagging	450 psig	Slag

A - atmospheric

E = elevated

* To be discussed

Table IV-1-a (Continued)

<u>NAME</u>	<u>OPERATING PRESSURE</u>	<u>ASH OR SLAG</u>
USBM-Lurgi Slagging	450 psig	Slag
Hydrocarbon Research	450 psig	Ash
Texaco	450 psig	Ash
USBM Morgantown	E	Slag
Bianchi	E	Ash
I.G.T. Cyclonizer	E	Slag
Nichalo-Hereshoff Furnace	A	Ash
Cameron and Jones	A	Ash
Multi-Stage Conveyor	E	Ash
Fixed-Bed Super Pressure	1050 psig	Ash
Fluidized-Bed Super Pressure	1050 psig	Ash
Two-Stage Super-Pressure* Entrained	1050 psig	Slag
Mayland Pebble-Bed	-	Ash
Koppers-Totzek Pressurized	450 psig	Slag
Rummel Single-Shaft Pressurized	450	Slag
Rummel Modified Single Shaft Pressurized	450	Slag
Gas Council Fluidized-Bed	E	Ash
Catalytic Steam Methanation		Slag

Table IV-1-b Summary of Synthesis Gas Producers[3]
(Using Air)Using Air

Gas Integrate	A	Ash
Pintsch Hillebrand	E	
ICI Moving Burden	A	Ash
Heller Process	A	
USBM Annular Retort	A	Ash
Maccormac-Rummel Double-Shaft		
Standard Oil Fluidized Bed	A	Ash

energy can be supplied from the combustion of coal to enhance the carbon steam reaction. Thus, the throughputs of the gasifier are substantially increased.

1.5 Gasification of Coal by Synthesis Gas Followed by Upgrading Methanation.

The pretreated coal is introduced into a gasifier (primary gasifier), where it is reacted with up-coming hot synthesis gas. The coal is partially reacted in the gasifier. The unreacted coal char is collected by a cyclon separator and introduced into a synthesis gas producer (secondary gasifier). The coal char is then gasified by oxygen and steam to form synthesis gas. The effluent gas from the primary gasifier passes through shift conversion, purification, and methanation steps, and finally becomes pipeline gas. The schematic flow diagram is shown in Fig. IV-6. B.C.R. Two-Stage Super-Pressure gasification developed by Bituminous Coal Research, Inc. is an example of this type of gasification system. It can be described as follows:

The gasifier, operating at 1115 psia, is of entrained type and is separated into two reaction stages. The lower part of the gasifier is called stage 1, and the upper part, stage 2. Steam and oxygen are introduced to the bottom part of stage 1, where they react with down-flowing hot char from stage 2. Temperature in this section of the reactor is about 3000°F. Ash produced from gasification is withdrawn from the bottom of the reactor in a melt form. Coal and steam are introduced at stage 2. Fresh coal entering the gasifier is immediately contacted with up-coming hot gas from stage 1, and devolatilization takes place rapidly. The remaining less active

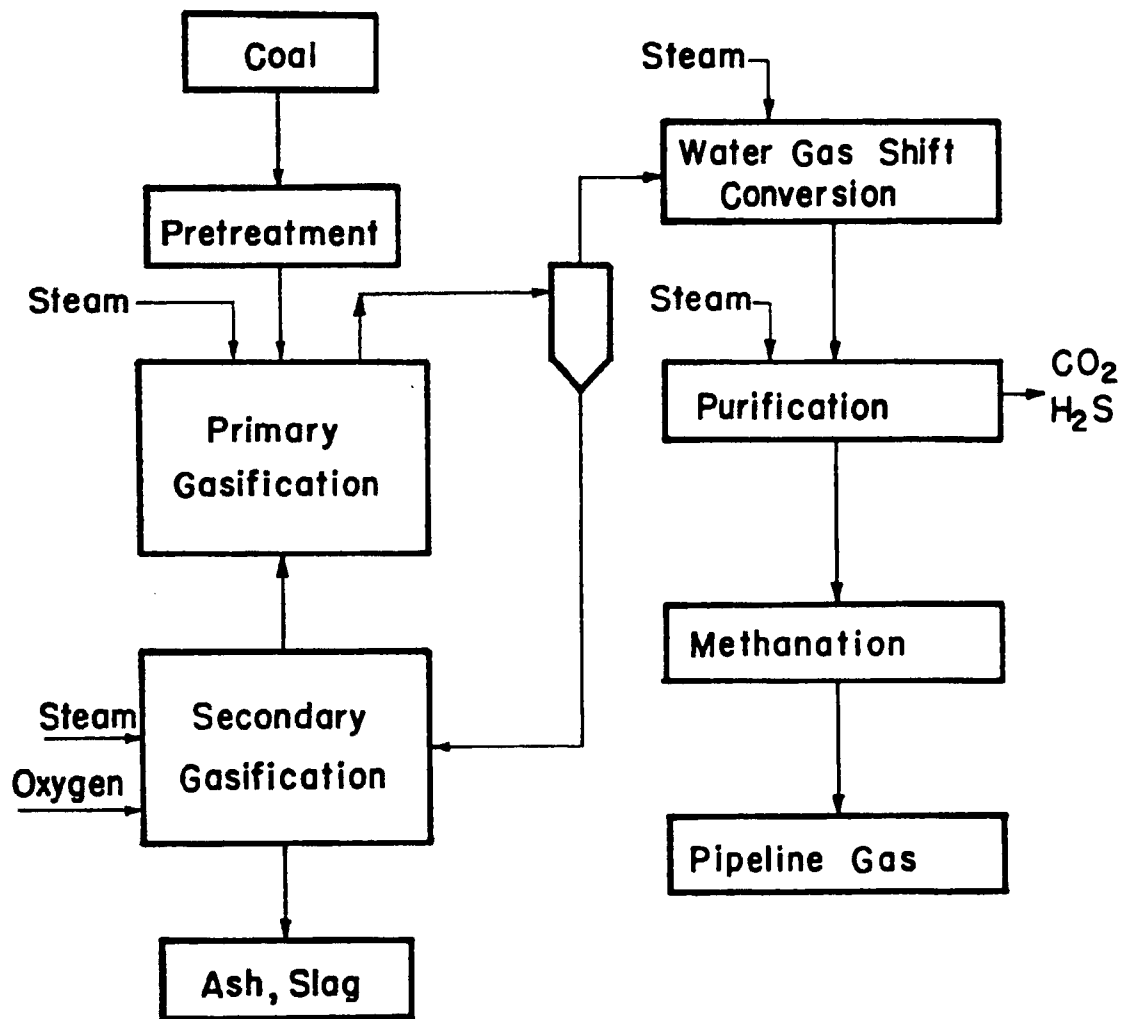


Figure IV-6 Flow Diagram for Processes with Gasification of Coal by Synthesis Gas Followed by Upgrading Methanation.

carbon is then reacted with steam-hydrogen mixture to form more methane during the time coal stays in the gasifier. The temperature of stage 2 is kept at 1700°F. The effluent gas from the gasifier is then sent to the upgrading methanation process for further treatment.

2. Material and Energy Balances

2.1 Introduction

The various alternates of gasification processes are summarized and discussed in the previous section. As the next step, we will compare these processes and select the most promising economic process for future development. For this purpose, it is necessary to analyze first the overall material and energy balances of the gasifier and then simulate and optimize the gasifier by using a suitable reactor model.

The purpose of this section is to provide a description of the overall energy and material balances for the gasifiers for both primary and secondary gasification. This may be used to evaluate the effect of process alternates and to suggest the promising operating conditions.

2.2 Basic Equations

The material and energy balance calculations are carried out based on Fig. IV-7. The basis of the computation is 1 lb-mol of feed stock (coal). As shown in Fig. IV-7, the feed stock and the gaseous medium are introduced into the reactor, where M_C , M_H , M_O , M_S , M_{ash} , and M_W are carbon, hydrogen, oxygen, sulfur, ash, and water content in the unit amount of feed stock, respectively, and M_{O_2} , M_{CO_2} , M_{N_2} , M_{H_2} , M_{H_2O} , M_{CH_4} , and M_{CO} are mol-volume composition of the gaseous medium fed into the reactor. H_{pf} , H_{pg} , and H_{ps} represent the heat quantity preheated of the feed stock, inlet gas excluding water vapor and the inlet steam, respectively.

and A is the mole fraction of CH_4 in the pipeline gas, which must be at least 0.86 and 0.92 for gas with heating value of 900 BTU/SCF and 950 BTU/SCF, respectively.

iii. Shift conversion unit.

Before the gas mixture from the hydrogasifier is introduced into a shift converter, the temperature of the gas is brought to 770°F by passing it through a waste heat recovery system. The cooled gas is then mixed with a suitable amount of steam at 545°F. The outlet gas temperature of the converter is fixed at 880°F. When the concentration of water vapor in the inlet stream is high, there is no need to add steam to the unit. The outlet gas temperature is then determined by the amount of CO being shifted. The equations governing this unit are as follows:

$$m_{\text{CO}_2} = M_{\text{CO}_2} + \eta_{\text{CO}} \cdot M_{\text{CO}}$$

$$m_{\text{CO}} = M_{\text{CO}} (1 - \eta_{\text{CO}})$$

$$m_{\text{CH}_4} = M_{\text{CH}_4}$$

$$m_{\text{H}_2\text{O}} = M_{\text{H}_2\text{O}} - \eta_{\text{CO}} \cdot M_{\text{CO}}$$

$$m_{\text{H}_2} = M_{\text{H}_2} + \eta_{\text{CO}} \cdot M_{\text{CO}}$$

i.v. Purification unit.

The CO_2 concentration in the outlet gas of this unit is fixed at 1% (mole). The effluent gas from the purifier is saturated with water vapor at the outlet gas temperature of the unit, i.e., 250°F.

The material balances for the unit are:

$$m_{\text{CO}_2} = \frac{1}{99} (m_{\text{CO}} + m_{\text{CH}_4} + m_{\text{H}_2\text{O}} + m_{\text{H}_2})$$

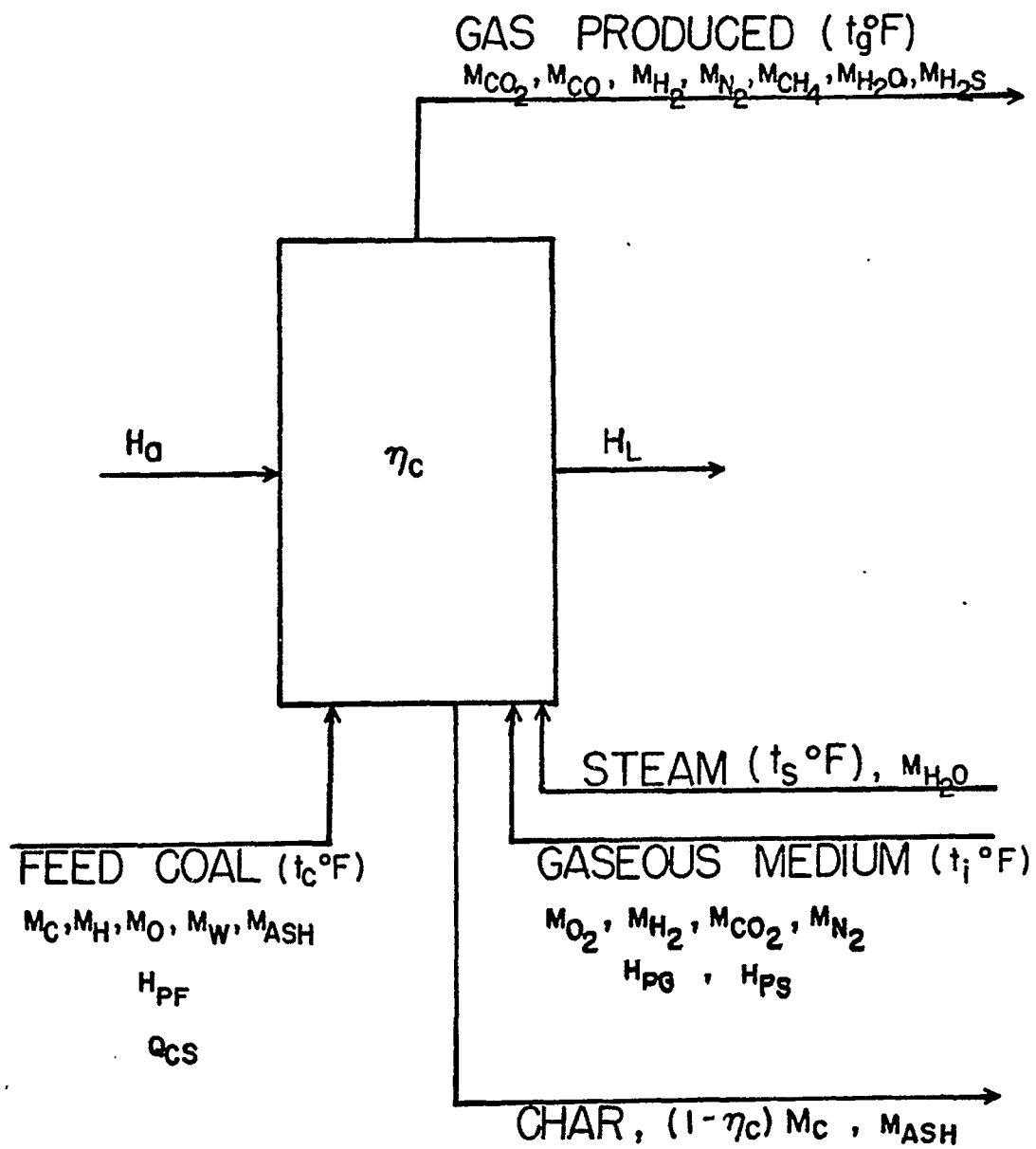


Figure IV-7 Schematic of Gasifier Material and Energy Balance Calculation

In almost all experimental work, heat is added by means of an electric heater; and in some special processes, such as the CO₂-acceptor process, a heat carrier is used. The heat to be added is designated H_a, while heat loss is expressed by H_l. η_C is the conversion of carbon; (1-η_C) M_C, therefore, represents the moles of carbon at the outlet per mole of coal fed. The composition of exit gas is given by m_{CO₂}, m_{H₂}, m_{CO}, m_{N₂}, m_{CH₄}, and m_{H₂O} in terms of moles per mole of coal fed.

From these definitions, the material balances for carbon, oxygen, nitrogen, and sulfur are given by [17]:

$$\eta_C M_C + M_{CO_2} + M_{CH_4} + M_{CO} = m_{CO} + m_{CH_4} + m_{CO_2} \quad (IV-1)$$

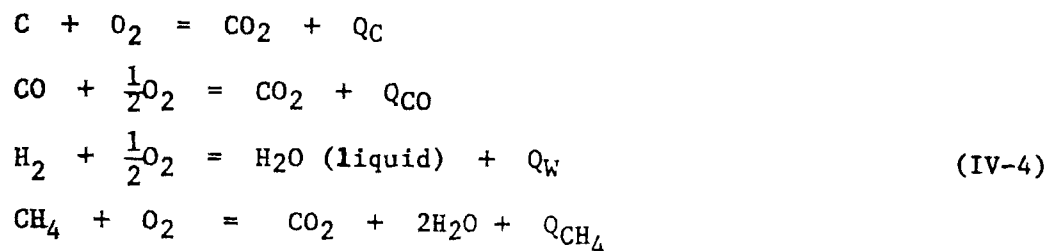
$$M_O + \frac{1}{2}(M_W + M_{H_2O}) + \frac{1}{2}M_{CO} + M_{CO_2} = m_{CO_2} + \frac{1}{2}m_{CO} + \frac{1}{2}m_{H_2O} \quad (IV-2)$$

$$M_H + M_W + M_{H_2O} + M_{H_2} + 2M_{CH_4} = m_{H_2} + m_{H_2O} + 2m_{CH_4} + m_{H_2S} \quad (IV-3)$$

$$M_{N_2} + M_N = m_{N_2}$$

$$M_S = m_{H_2S}$$

Next, let us consider the enthalpy balance of the gasifier. Enthalpies of the various gases are shown in Table IV-2. Q and q denote heat of combustion and formation, respectively, and both quantities are related by the following equations:





$$Q_{CH_4} = Q_C + 2Q_w - q_{CH_4} \quad (IV-6)$$

When the heat of the formation of coal is defined by q_{CS} , the enthalpy balance around the reactor is given by

$$\begin{aligned} & (2M_O + M_w) H_w + H_{pf} - q_{CS} \text{ [enthalpy of feed stock]} \\ & + M_{CO_2} \cdot H_{CO_2} + M_{CO} \cdot H_{CO} + M_{CH_4} \cdot H_{CH_4} \quad \text{[enthalpy of} \\ & + [M_{CO_2} \cdot \bar{C}_{p,CO_2} + M_{CO} \cdot \bar{C}_{p,CO} + M_{H_2} \cdot \bar{C}_{p,H_2} \quad \text{inlet gas]} \\ & + M_{N_2} \cdot \bar{C}_{p,N_2} + M_{CH_4} \cdot \bar{C}_{p,CH_4}] (t_i - t_o) \\ & + M_{H_2O} [H_{H_2O} + \bar{C}_{p,H_2O} (t_s - t_o)] \text{ [enthalpy of steam} \\ & \quad \text{introduced]} \\ & + H_a \quad \text{[Heat input]} \\ & = m_{CO_2} \cdot H_{CO_2} + m_{CO} \cdot H_{CO} + m_{CH_4} \cdot H_{CH_4} \quad \text{[enthalpy of} \\ & + [m_{CO_2} \cdot \bar{C}_{p,CO_2} + m_{CO} \cdot \bar{C}_{p,CO} + m_{H_2} \cdot \bar{C}_{p,H_2} \quad \text{produced gas]} \\ & + m_{N_2} \cdot \bar{C}_{p,N_2} + m_{CH_4} \cdot \bar{C}_{p,CH_4}] (t_g - t_o) \\ & + m_{H_2O} [H_{H_2O} + \bar{C}_{p,H_2O} (t_g - t_o)] \text{ [enthalpy of unreacted} \\ & \quad \text{steam]} \\ & + H_\ell \quad \text{[Heat loss]} \quad (IV-7) \end{aligned}$$

Where t_o is the reference temperature. The enthalpies of exit gas and inlet gas based on dry conditions are assumed to be represented by

$$H_{pg} = [M_{CO_2} \cdot \bar{C}_{p,CO_2} + M_{CO} \cdot \bar{C}_{p,CO} + M_{H_2} \cdot \bar{C}_{p,H_2} + M_{N_2} \cdot \bar{C}_{p,N_2} + M_{CH_4} \cdot \bar{C}_{p,CH_4}] (t_i - t_o) \quad (IV-8)$$

$$H_{eg} = [m_{CO_2} \cdot \bar{C}_{p,CO_2} + m_{CO} \cdot \bar{C}_{p,CO} + m_{H_2} \cdot \bar{C}_{p,H_2} + m_{N_2} \cdot \bar{C}_{p,N_2} + m_{CH_4} \cdot \bar{C}_{p,CH_4}] (t_g - t_o) \quad (IV-9)$$

Enthalpy of ash and char is considered in the heat loss term H_ℓ .

Defining the latent heat of vaporization of water by v_w , the following equation is obtained from Table IV-2.

Table IV-2 Heats of combustion and enthalpies [17]

Material	State	Heat of Combustion BTU/lb-mol	Enthalpy at 77°F BTU/lb-mol
C	solid	$Q_C = 169,700$	$H_C = 0$
O ₂	gas	--	$H_{O_2} = 0$
H ₂	gas	$Q_w = 123,000$	$H_{H_2} = 0$
N ₂	gas	--	$H_{N_2} = 0$
CO ₂	gas	--	$H_{CO_2} = -Q_C$
H ₂ O	liquid	--	$H_w = -Q_w$
H ₂ O	gas	--	$H_{H_2O} = -(Q_w - v_w)$
CO	gas	$Q_{CO} = 121,900$	$H_{CO} = -(Q_C - Q_{CO})$
CH ₄	gas	$Q_{CH_4} = 383,000$	

$v_w =$ Latent heat of water, 18,950 BTU/lb-mol

$$H_{H_2O} = -Q_w + v_w = H_w + v_w \quad (IV-10)$$

Substitution of Eqs. (IV-8) to (IV-10) into Eq. (IV-7) gives

$$\begin{aligned} & (2M_O + M_w + M_{H_2O} - m_{H_2O}) H_w + (M_{CO_2} - m_{CO_2}) H_{CO_2} \\ & + H_{pf} + H_{pg} + H_{ps} + H_a - q_{cs} \\ = & (m_{CO} - M_{CO}) H_{CO} + (m_{CH_4} - M_{CH_4}) H_{CH_4} + H_{eg} \\ & + H_{es} + H_l \end{aligned} \quad (IV-11)$$

where

$$\begin{aligned} H_{ps} &= M_{H_2O} [v_w + \bar{c}_{p,H_2O} (t_s - t_o)] \\ H_{es} &= m_{H_2O} [v_w + \bar{c}_{p,H_2O} (t_g - t_o)] \end{aligned} \quad (IV-12)$$

Then from Equation (IV-1)

$$M_{CO_2} - m_{CO_2} = -\eta_C M_C + (m_{CO} - M_{CO}) + (m_{CH_4} - M_{CH_4}) \quad (IV-13)$$

from Equation (IV-3)

$$\begin{aligned} M_w + M_{H_2O} - m_{H_2O} &= m_{H_2} - M_{H_2} - M_H + \\ & 2(m_{CH_4} - M_{CH_4}) \end{aligned} \quad (IV-14)$$

from Table IV-2 and Equation (IV-6)

$$H_{CH_4} = -q_{CH_4} = Q_{CH_4} - Q_C - 2Q_w \quad (IV-15)$$

The gross caloric value of unit amount of coal is expressed by

$$Q_g = M_C Q_C + (M_H - 2M_O) Q_w - q_{cs} \quad (IV-16)$$

Rearrangement after substituting Eqs. (IV-13) to (IV-16) into

Eq. (IV-11) gives the final equation:

$$\begin{aligned} & (m_{CH_4} - M_{CH_4}) Q_{CH_4} + (m_{CO} - M_{CO}) Q_{CO} + (m_{H_2} - M_{H_2}) Q_w \\ = & Q_q [(\alpha + \beta + \omega) - (\gamma + \delta)] \end{aligned} \quad (IV-17)$$

$$\text{where } \alpha = 1 - \frac{(1 - \eta_C) M_C Q_C}{Q_g}$$

$$\beta = \frac{H_{pf} + H_{pg} + H_{ps}}{Q_g}$$

$$\begin{aligned}
 \omega &= \frac{H_a}{Q_g} \\
 \gamma &= \frac{H_{eg} + H_{es}}{Q_g} \\
 \delta &= \frac{H_l}{Q_g}
 \end{aligned}
 \tag{IV-18}$$

Let η_G be gasification efficiency, defined by

$$\eta_G = \frac{(m_{CH_4} - M_{CH_4}) + (m_{CO} - M_{CO}) + (m_{H_2} - M_{H_2})}{Q_g}$$

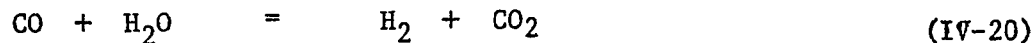
Thus, eq. (IV-17) becomes a dimensionless equation.

$$\eta_G = (\alpha + \beta + \omega) - (\gamma + \delta)
 \tag{IV-19}$$

Here

- α represents the ratio of the heat generated by conversion of carbon, η_C , to that for 100% conversion.
- β represents the ratio of the total enthalpy, referring to the reference temperature (t_0) of all feeds (solids and gases) per lb. coal, to the gross calorific value of 1 lb. coal.
- ω represents heat added per lb-coal fed divided by the calorific value of lb coal.
- γ represents the ratio of the total enthalpy, referring to the reference temperature (t_0) of all products (solids and gases) per lb coal to the calorific value of 1 lb coal.
- δ represents heat loss per lb coal fed divided by calorific value of lb coal.

If the assumption is made that the water-gas-shift reaction



is at equilibrium in the reactor:

$$K = \frac{m_{\text{H}_2} \cdot m_{\text{CO}_2}}{m_{\text{CO}} \cdot m_{\text{H}_2\text{O}}} \quad (\text{IV-21})$$

Then the product gas composition and its flow rate can be calculated from Eqs. (IV-1) to (IV-3) and (IV-21) if the reactor temperature T , conversion factor η_C , weight fractions of C, H, O, in feed coal, and one of the exit gases are specified. Several representative results calculated are shown in Figs. IV-8 through IV-10. Fig. IV-9 shows the result at $T = 1700^\circ\text{F}$, $C = 1.0$ and 0.1% CH_4 in the exit gas. By using this figure, the concentrations of CO and H_2 in the exit gas are obtained for each value of M_{O_2} and $M_{\text{H}_2\text{O}}$. When M_{O_2} is fixed, there is a value of $M_{\text{H}_2\text{O}}$ at which the hydrogen concentration becomes maximum. However, when $M_{\text{H}_2\text{O}}$ is fixed, the CO concentration decreases monotonously as M_{O_2} is increased. (The concentration shown in Fig. IV-9 is the equilibrium concentration with methane.)

By combining Eqs. (IV-1), (IV-2), and (IV-3) we obtain

$$(m_{\text{CO}} - M_{\text{CO}}) + m_{\text{H}_2} = 2\eta_C M_C - 2M'_{\text{O}_2} + M'_{\text{H}_2} - 4(m_{\text{CH}_4} - M_{\text{CH}_4}) \quad (\text{IV-22})$$

where

$$\begin{aligned} M'_{\text{O}_2} &= M_{\text{O}_2} + M_{\text{O}} \\ M'_{\text{H}_2} &= M_{\text{H}_2} + M_{\text{H}} \end{aligned} \quad (\text{IV-23})$$

If the heat is supplied by reaction of coal with oxygen or hydrogen without recycle gas, we have

$$M_{\text{CH}_4} = M_{\text{CO}} = M_{\text{CO}_2} = 0$$

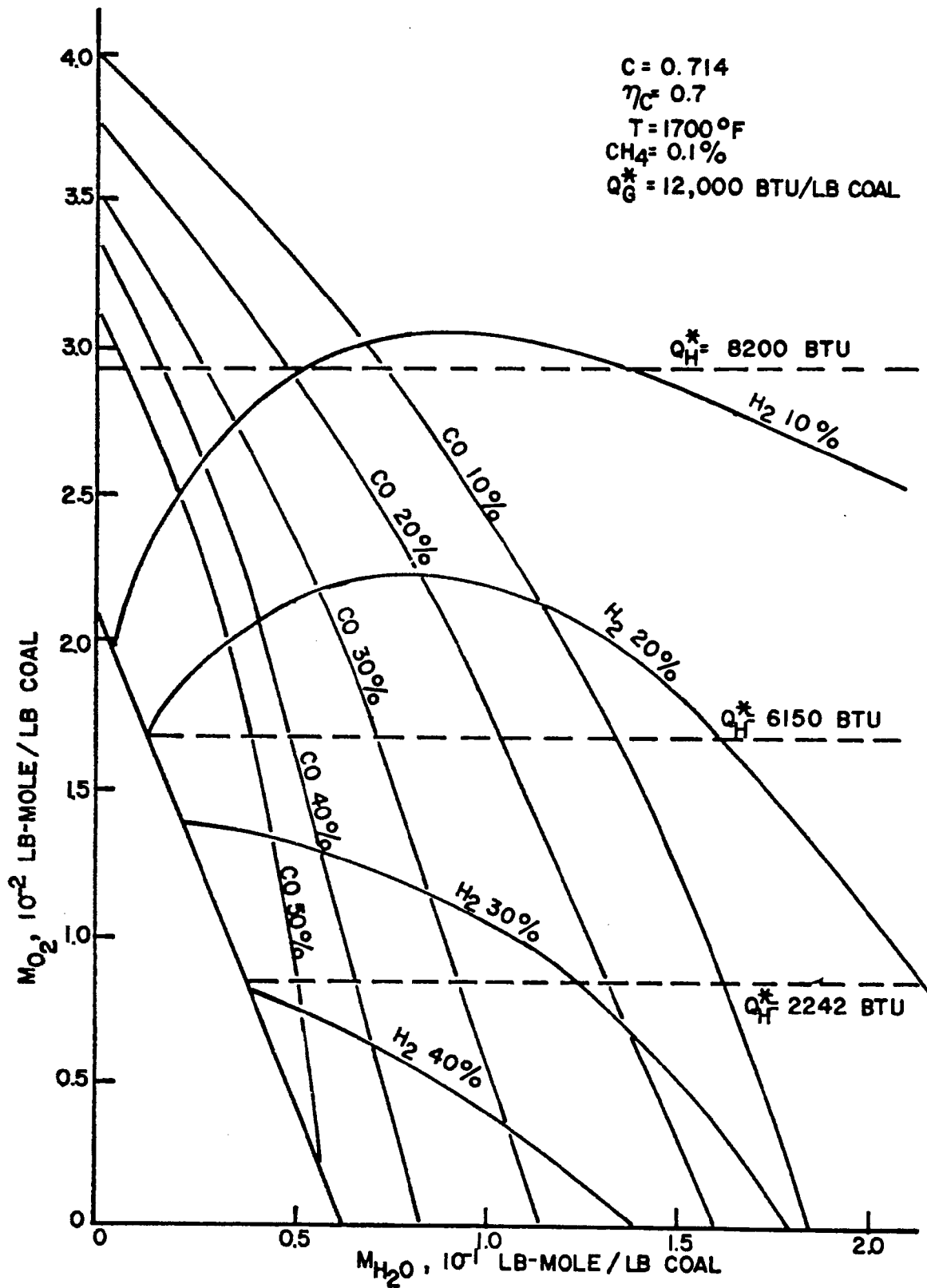


Figure IV-8 Effect of Flow Rates of Steam and Oxygen on Product Gas Compositions and Heating Values

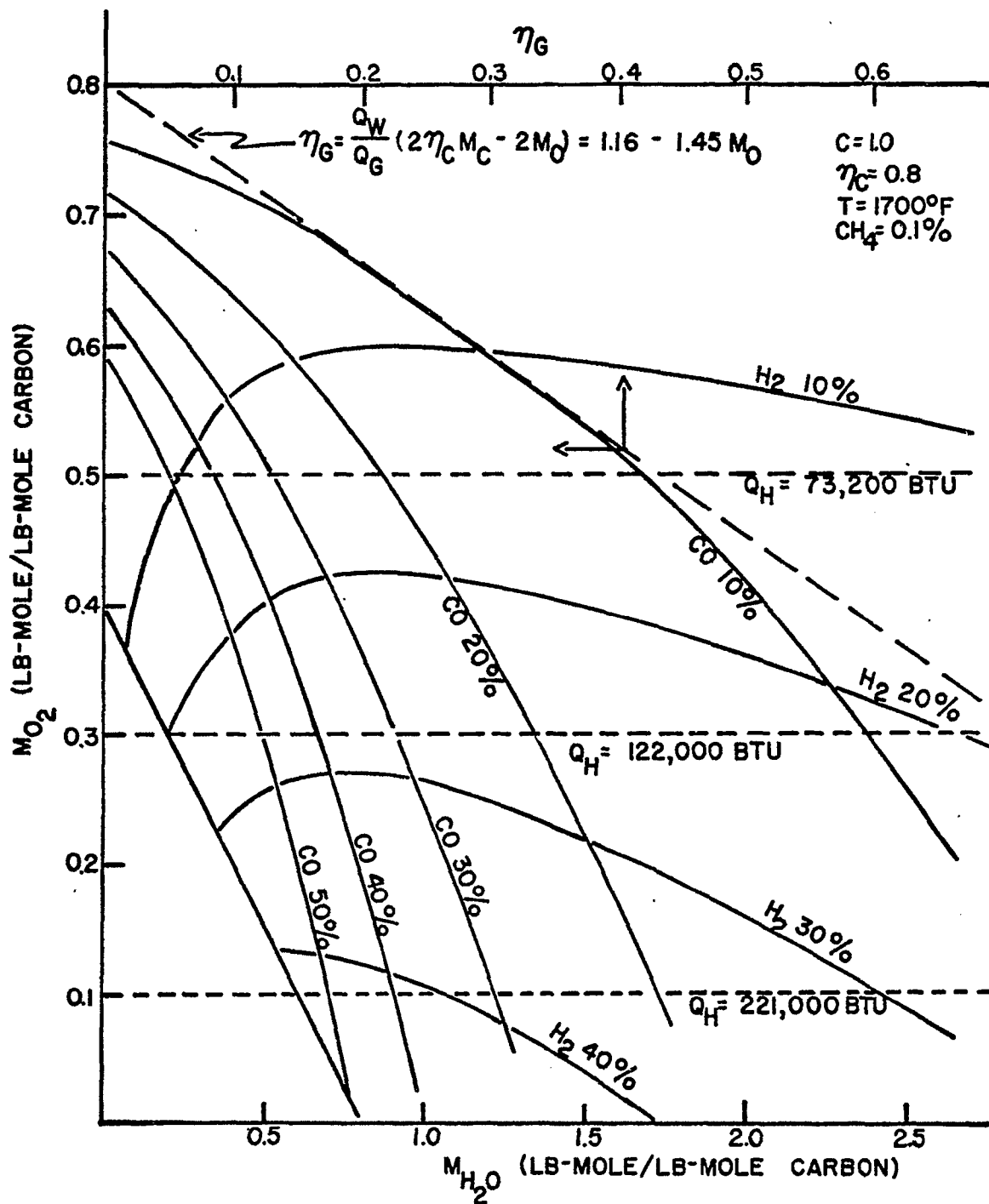


Figure IV-9 Effect of Carbon Conversion on Gasification Efficiency, Product Gas Compositions, and Heating Values.

$$M_{H_2} = 0 \quad \text{or} \quad M_{O_2} = 0$$

Hence, Eq. (IV-22) becomes

$$m_{CO} + m_{H_2} = 2\eta_C M_C - 2M_{O_2}' + M_{H_2}' - 4m_{CH_4} \quad (IV-24)$$

Eq.(IV-24) shows that the yield of CO and H₂ depends only on oxygen or hydrogen supplied.

Let us define the heating value of exit gases as:

$$Q_H = m_{CH_4} Q_{CH_4} + m_{CO} Q_{CO} + m_{H_2} Q_w \quad (IV-25)$$

Because the heat of combustion of CO ($Q_{CO} = 121,900$ BTU/lb-mol) is almost equal to that of H₂ ($Q_w = 123,000$ BTU/lb-mol), Eq. (IV-25) may be rewritten as:

$$Q_H \cong (m_{H_2} + m_{CO}) Q_w + m_{CH_4} Q_{CH_4} \quad (IV-26)$$

Substitute Eq. (IV-24) into Eq. (IV-26),

$$Q_H \cong [(2\eta_C M_C - 2M_{O_2}') + M_{H_2}'] Q_w + m_{CH_4} (Q_{CH_4} - 4Q_w) \quad (IV-27)$$

When the methane content in the exit gas is low, the term $m_{CH_4} (Q_{CH_4} - 4Q_w)$ in Eq. (IV-27) can be neglected. Thus,

$$Q_H = (2\eta_C M_C - 2M_{O_2}' + M_{H_2}') Q_w \quad (IV-28)$$

The heating value of product gas depends only upon M_{O_2}' or M_{H_2}' being introduced into the gasifier.

Comparing Eq. (IV-17) with Eq. (IV-25) eliminating M_{CO} and M_{CH_4} , we then get

$$Q_H = \eta_G Q_g + Q_w M_{H_2}' \quad (IV-29)$$

The relations of Eqs. (IV-28) and (IV-29) are shown in Fig. IV-10.

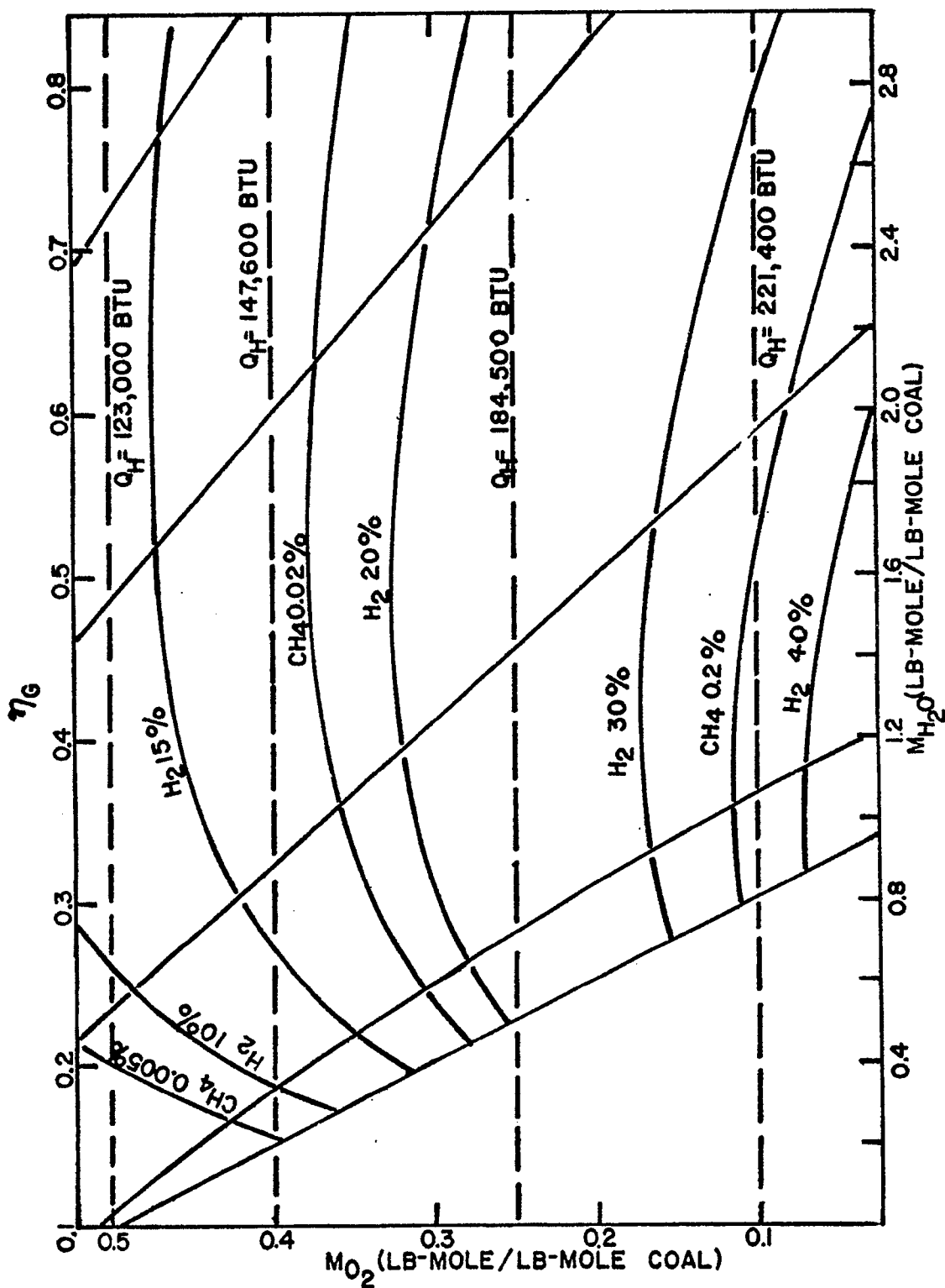


Figure IV-10 Effect of Flow Rates of Steam and Oxygen on Gasification Efficiency and Product Gas Compositions and Heating Values.

When oxygen is used, the amount necessary to sustain the temperature can be calculated from Equations (IV-28) and (IV-29) by letting M_{H_2} equal zero.

$$M_{O_2}' = - \frac{\eta_G Q_g}{2Q_w} + \eta_C M_C + M_H$$

$$M_{O_2} = \eta_C M_C - \frac{\eta_G Q_g}{2Q_w} + M_H + M_O \quad (IV-30)$$

If gasifier efficiency is assigned, then M_{O_2} can be calculated from this equation.

When the heating medium is hydrogen as in hydrogasification, the amount of hydrogen required is given by Eq. (IV-28) by letting $M_{O_2} = 0$.

$$\therefore M_{H_2} = \frac{Q_H}{Q_w} - 2\eta_C M_C - M_H \quad (IV-31)$$

For convenience in calculation, the basis can be converted from 1 lb-mole to 1 lb of coal fed as follows. By using the average molecular weight \bar{M} and the weight fraction of carbon in coal

$$M_C = \frac{c\bar{M}}{12} ; \quad M_H = \frac{h\bar{M}}{2} ; \quad M_O = \frac{x\bar{M}}{32}$$

$$Q_g = Q_g^* \bar{M} ; \quad M_{O_2} = M_{O_2}^* \bar{M} ; \quad M_{H_2} = M_{H_2}^* \bar{M}$$

Superscript * refers to one lb of coal fed while c, h, and x represent the weight fraction of C, H, O, in coal. Then Equations (IV-29) to (IV-31) can be rewritten as:

$$Q_H^* = \eta_G Q_g^* + Q_w M_{H_2}^* \quad (IV-32)$$

$$M_{O_2}^* = \eta_C \frac{c}{12} - \frac{\eta_G Q_g^*}{2Q_w} + \frac{h}{2} + \frac{x}{32} \quad (IV-33)$$

$$M_{H_2}^* = \frac{Q_H^*}{Q_w} - \eta_C \frac{c}{6} - \frac{h}{2} \quad (IV-34)$$

2.3 Analysis of Performance Data

In the previous section, the equations are developed in order to estimate the amount of gas produced, and the required amount of oxygen and hydrogen. The performance data reported for several types of gasifiers can be analyzed and compared with each other by using these equations. The results are shown in Table IV-4 and Table IV-5.

By using these data and results, the gasifier for various processes may be optimized by means of a suitable model.

Table IV-4 Coal and Gas Analyses of Reported Performance Data [20]

		Winkle	Leuna	Lurgi	Koppers Injection	
		Generator	Slagging	Gasifier	Brown Coal	Bituminous Coal
Coal Analysis %	C	63.7	86.8	71.22	56.2	80.5
	H	2.2	--	5.27	4.71	4.27
	O	--	--	4.02	--	1.46
	N	5.5	--	16.10	20.58	1.19
	S	--	--	3.39	0.33	1.88
	Moisture	--	9.1	--	13.00	1.95
	Ash	28.6	1.8	--	5.18	8.75
Gas Analysis %	CH ₄	0.8	0	20.6	0	0
	CO	29.6	61.4	18.3	35	42
	H ₂	43.8	31.0	52.2	45	42
	CO ₂	23.1	6.8	6.8	19	15
	N ₂	1.5	6.8	1.2	1	1
	H ₂ S	1.2	0	0.9	small	small

Table IV-5 Analysis of Reported Performance Data [20]

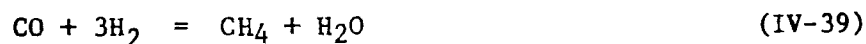
Process		Winkle Generator	Leuna Slagging	Lurgi Gasifier	Koppers Injection	
					Brown Coal	Bituminous Coal
Q_g^*	BTU	10361	12275	12130	9560	14350
C		0.637	0.868	0.7122	0.562	0.805
η_C		0.577	0.996	0.647	0.95	0.94
O ₂		4.84	9.19	2.48	6.52	10.7
Steam Introduced, lb		0.902	0.705	1.58	0.97	1.57
Steam Unreacted, lb		0.062	0.015	0.314	0.33	0.52
Gas Produced (dry)	ft ³	20.61	37.97	23.06	31.64	42.37
H ₂	ft ³	9.03	11.77	8.23	14.2	17.8
CO	ft ³	6.10	23.32	2.97	11.0	17.8
CH ₄	ft ³	0.16	--	3.44	--	--
t _s	°F	300	572	850	2192	2192
t _g	°F	1650	750	572	1650	2192
Calculated Value	α	0.633	0.996	0.707	0.952	0.952
	β	0.101	0.081	0.187	0.109	0.112
	γ	0.083	0.032	0.199	0.119	0.176
	δ	0.137	0.073	0.085	0.053	0.064
	ω	--	--	--	--	--
	η_G	0.514	0.972	0.617	0.843	0.788

3. Effective Utilization of Coal in the Integrated Pipeline Gas Producing Plant

3.1 Introduction

In the previous section material and energy balances around different gasification processes were presented. In this section, not only the gasifiers, but also other parts of the entire gasification system, are included in order to provide a logical way of assessing effectiveness of utilization of coal in an integrated gas production plant.

A number of reactions are involved in the conversion of coal into gases. Main reactions are the devolatilization, the carbon-steam reaction, the water-gas shift reaction, the carbon hydrogen reaction and the methanation reaction.



where C^* is carbon in char.

Besides these main reactions, coal is also needed to provide the heat and the steam required for the gasification. As is evident from the stoichometric relations shown above, the key to the economic production of pipeline gas from coal is the effective generation of hydrogen needed for the formation of methane.

Hydrogen can be generated either together with or separately

from the main gasification reactions. Regardless of the scheme adopted, the reactions involving the generation of hydrogen are highly endothermic requiring supplies of heat either by reactions having large exothermic heats of reaction (such as carbon combustion with oxygen) or through heat transfer media (such as in the electrothermal gasification process). Methods of hydrogen production have been briefly discussed in Section 1.1.

Both reactions in Eqs. (IV-38) and (IV-39) are highly exothermic reactions. The carbon-hydrogen reaction can be carried out at temperatures above 1300°F. Thus the heat generated from this reaction may be directly used for carbon-steam reaction in Eq. (IV-36), which is a highly endothermic reaction and must be reacted at a high temperature (above 1700°F). On the other hand, the catalytic methanation reaction must be carried out at temperatures between 500°F to 850°F. The heat generated from this reaction may be used for the production of steam needed in other parts of the integrated gasification plant. Heat required for the gasification may be supplied by burning a portion of coal with pure oxygen in the gasifier. It can also be supplied by burning coal in a separate reactor and subsequent transfer of the heat into the gasifier through a proper medium.

Therefore, it is clear that carbon in coal must play a dual role in the gasification system. In other words, it has to provide, not only the hydrogen required to form methane, but also the heat required to produce hydrogen. In addition, process steam and electric power must also be generated through the use of coal for a self-sustaining plant. Thus, it is highly desirable to identify the

process schemes that would make the most effective use of carbon in coal for the integrated pipeline gas producing plant.

As was already discussed in the previous section, differences in the various schemes proposed for coal gasification processes come mainly from the attempt to provide the efficient usage of carbon and hydrogen in gasifiers.

Since different types of coal are to be used for the gasification, and considering the different localities where gasification plants may be built, it would be complicated, if not impossible, to take into consideration all the factors involved that affect the price of pipeline gas produced. Simplified methods based on material balance, heat balance, and thermodynamics, together with primary kinetic information, have been used by various investigators for the evaluation of different schemes. Different bases for comparison have been employed. Some are based on the quantity of heat added to the gasifier and unit cost of heat [11]. Others are based on the percentage of carbon in methane/percentage of carbon in coal [2]. Another method used is "thermal efficiency", which is defined as the BTU of pipeline gas produced divided by the BTU of total coal fed. Different bases imply different emphases placed on the effectiveness of the process; the former on the means of supplying heat, and the latter on the uses of carbon in a gasifier. However, it seems more realistic to consider the efficiency based on the integrated gasification system including the energy and material requirement of the total plant.

Thus, in this study, the process efficiency is based on coal required to generate gaseous components necessary for methane production and the equivalent amount of coal needed to supply energy for the total system.

In other words, the total coal requirement is defined as:

$$\begin{aligned} \text{Total Coal} &= \text{Coal for Gasification} + \text{Coal for Steam Generation} \\ &+ \text{Coal for Oxygen Production.} \end{aligned}$$

Here coal for gasification includes that used for primary and secondary gasification. Coal for steam generation includes that used for producing steam required in a gasification system minus the equivalent amount of coal needed to generate steam from the gasifier heat removing devices. The equivalent amount of coal needed for oxygen production is calculated from the energy required for oxygen production in an air liquefaction plant.

Although this study is primarily based on the thermodynamic point of view, the result of this study will show the selection of effective schemes for a gasification system. Also the results will provide the ranges of design and operating variables needed in a more detailed and complete optimization study of gasification systems planned in the later sections.

3.2 Assumption and Derivations of Equation

Although there are a number of alternate coal gasification processes as shown in the previous sections, we can classify them into a few essential units, namely, gasification unit,

shift conversion unit, purification unit and methanation unit. Mathematical equations governing the performance of these units are derived based on a number of simplifying assumptions. They are briefly discussed below:

i. Gasification unit. (The secondary gasification unit.)

In this unit, char or coal is gasified with steam and oxygen. The product gas that emerges out of the unit, which may be called synthesis gas, consists mainly of carbon monoxide and hydrogen. In some cases, as in the electrothermal gasification process, instead of using oxygen as a gasification medium, electrothermal energy is used for supplying the heat required in the gasifier. Assumptions made and equations derived for this unit are basically the same as those presented in Section 2.2. They are briefly summarized as follows:

a. The solid fuel gasified in this unit is char which is obtained from other coal gasification unit(s), e.g., hydrogasification unit. In a few special cases, when char produced from the system is not enough for the gasification, additional coal may be provided as a supplement for this unit.

b. Oxygen and steam are the only gaseous feeds employed in the unit.

c. No free oxygen exists in the effluent gas of this unit.

d. The water-gas shift reaction reaches equilibrium as the gaseous product emerges from the unit.

e. No methane is produced in this unit.

f. Gasifier is operated adiabatically or at a rate of heat loss equivalent to 2% of the heating value of coal.

Based on the above assumptions, material and energy balances can be written as:

Carbon balance:

$$\eta_C \cdot M_C = m_{CO_2} + m_{CO}$$

Oxygen balance:

$$\frac{1}{2}(M_W + M_{H_2O}) + M_{O_2} = m_{CO_2} + \frac{1}{2}(m_{CO} + m_{H_2O})$$

Hydrogen balance:

$$M_H + M_{\text{steam}} = m_{H_2} + m_{H_2O}$$

Energy balance:

enthalpy of feed char + enthalpy of inlet gas =
enthalpy of gaseous product + enthalpy of solid product
(ash).

Equilibrium relation:

$$K_{P_{WGS}} = \frac{(P_{CO_2}) (P_{H_2})}{(P_{CO}) (P_{H_2O})} = \frac{m_{CO_2} \cdot m_{H_2}}{m_{CO} \cdot m_{H_2O}}$$

ii. Hydrogasification unit. (The primary gasification unit)

In this unit, coal is gasified by a gaseous medium containing mainly CO and H₂. In some cases, the hydrogen concentration in the gaseous medium can be very high. Since coal is gasified in a hydrogen rich gas, a large amount of methane is produced due to the carbon-hydrogen reaction and pyrolysis of coal. Hydrogen, participating in the reaction, comes from two sources; a portion of which is originally present in coal and the remainder which

is generated by the carbon-steam reaction and the water-gas shift conversion. Assumptions made for the calculation of this unit are:

a. The water-gas shift reaction reaches equilibrium at the outlet of the hydrogasifier.

b. Since coal-hydrogen-methane equilibrium is known to exceed the graphite-hydrogen-methane equilibrium, calculations of exit composition are based on the carbon-hydrogen-methane equilibrium constant which is multiplied by a factor called approach factor ranging from 1 to 8. Approach factors then serve to represent kinetic parameters of the carbon-hydrogen reaction. Detailed discussion of the kinetic rate of this reaction will be presented in a later section.

c. When the composition of the effluent gas from the hydrogasifier is just right for direct methanation without shift conversion, the carbon conversion in this unit must be limited so that the heating value of at least 900 BTU/SCF in the resultant pipeline gas is reached.

d. The hydrogasifier is adiabatically operated or at a rate of heat loss equivalent to 2% of the heating value of coal.

Based on these assumptions, the material and energy balances of the unit can be written as:

Carbon balance:

$$n_C M_C + M_{CO_2} + M_{CO} = m_{CO} + m_{CO_2} + m_{CH_4}$$

Oxygen balance:

$$M_O + \frac{1}{2}(M_W + M_{CO} + M_{H_2O} + M_{steam}) + M_{CO_2} = m_{CO_2} + \frac{1}{2}(m_{CO} + m_{H_2O})$$

Hydrogen balance:

$$M_H + M_W + M_{H_2O} + M_{H_2} + M_{steam} = 2m_{CH_4} + m_{H_2O} + m_{H_2}$$

Energy balance:

Enthalpy of feed coal and enthalpy of inlet gas + enthalpy of steam added = enthalpy of char as solid product + enthalpy of gaseous outlet.

Equilibrium relations:

Water-gas shift equilibrium:

$$K_{P_{WGS}} = \frac{P_{CO_2} \cdot P_{H_2}}{P_{CO} \cdot P_{H_2O}} = \frac{(m_{CO_2})(m_{H_2})}{(m_{CO})(m_{H_2O})}$$

Carbon-Hydrogen-Methane Equilibrium

$$a \cdot K_{P_{CH_4}} = \frac{P_{CH_4}}{(P_{H_2})^2} = \frac{\sum m_i \cdot m_{CH_4}}{P_T (m_{H_2})^2}$$

When the effluent gas from the hydrogasifier is purified and methanated without the shift conversion, the following constraint, which can be back calculated from the composition of pipeline gas, must be imposed on the hydrogasifier.

$$A = \frac{(m_{CH_4} + m_{CO} \cdot \eta_{CO}) (P_T - P_{H_2O})}{[m_{CO_2}(1 - \xi) + m_{CO}(1 - 3 \cdot \eta_{CO}) + m_{CH_4} + m_{H_2}] P_T}$$

where η_{CO} is the conversion of CO in the methanator,

ξ is the fraction of CO₂ removed in the gas purifier,

$$m_{CO} = M_{CO}$$

$$m_{CH_4} = M_{CH_4}$$

$$m_{H_2O} = \frac{P}{P_T - P} (m_{CO_2} + m_{CO} + m_{CH_4} + m_{H_2})$$

$$m_{H_2} = M_{H_2}$$

v. Methanation unit.

The effluent gas from the purifier is methanated to produce more methane. The methanation is carried out to the extent that the CO concentration in the pipeline gas must be less than 0.2%. The product gas is cooled to a temperature of 100°F, and during the process of cooling, excess water is removed from the gas stream. The material balances of this unit are shown as follows:

$$m_{CO_2} = M_{CO_2}$$

$$m_{CO} = M_{CO}(1 - \eta_{CO})$$

$$m_{H_2O} = M_{H_2O} + M_{CO} \cdot \eta_{CO}$$

$$m_{CH_4} = M_{CH_4} + M_{CO} \cdot \eta_{CO}$$

$$m_H = M_H - 3\eta_{CO} \cdot M_{CO}$$

The following assumptions are also made for the calculation of the amount of coal used in other units:

a. Steam required for gasification and shift conversion is supplied from a steam generation unit where water is heated by burning the excess char and coal if needed.

b. As will be shown in Chapter VI of this report, the amount of low pressure steam required for the purification unit is roughly equal to the steam generated from waste heat recovery systems of shift conversion and methanation units.

c. Oxygen used for the gasification is produced from the liquefaction of air. The energy required for liquefaction is converted to an equivalent amount of coal to produce the needed power for liquefaction [15]. By this method, different gasification processes can be compared based on the same standard; namely the quantity of coal required for an integrated and self-sustaining pipeline gas production plant.

3.3 Description of Considered Alternate Gasification Schemes.

A number of conceptual gasification schemes can be formulated by combining the various basic units discussed in the last section. In this section, only a few of the possible alternate schemes are examined in evaluating the effectiveness of the utilization of coal.

i. Alternate I

The flow diagram of Alternate I is shown in Fig. IV-5. In this system coal is gasified by oxygen and steam in a gasifier. The gas emerged from the gasifier undergoes shift conversion, purification, and methanation to form pipeline gas.

ii. Alternate II

The flow diagram of this system is shown in Fig. IV-6.

This system is equivalent to the BCR Two Stage Super-Pressure Gasification Process (Bigas Process)

iii. Alternate III

Alternate III is shown in Figure IV-3. Here the hydrogen is produced by the method described in Section 1.1i. The carbon conversion in the hydrogasifier must be controlled so that the effluent gas upon shifting, purification, and methanation has the specified heating value needed for the pipeline gas.

iv. Alternate IV

Alternate IV is shown in Figure IV-3. Electrothermal gasifier is used to generate reducing gases for subsequent hydrogasification. Heat required for the endothermic steam-carbon reaction is supplied by electrical energy rather than from the carbon-oxygen reaction. The effluent gas from the gasifier is fed to the purifier and the methanator to produce pipeline gas.

v. Alternate V

The flow diagram of this alternate is shown in Figure IV-4. Heat required in the gasifier and the devolatilizer is supplied by hot calcined dolomite from the heat carrier regenerator. This process is called the CO₂ Acceptor Gasification Process mentioned in Section 1.3.1. Because of the lack of accurate information on the thermodynamic and kinetic data, this process has not been studied in detail.

3.4 Results and Discussion

The five alternates mentioned in the previous section are simulated in a computer based on different ranks of coal as feed material. For the purpose of the evaluation of the effective utilization of coal, only the results obtained from one

type of coal will be discussed in detail. However, the results of calculation for other types of coal will be listed in the later section. The composition of the coal used for the detailed analysis of alternate schemes is as follows: [13]

Ultimate Coal Analysis, wt%

C	71.20
H	5.14
O	6.03
N	1.23
S	4.19
ash	<u>12.21</u>
	100.00%

Proximate Coal Analysis

Moisture	1.3
Volatile Matter	34.6
Fixed Carbon	52.0
Ash	<u>12.1</u>
	100.0%

Caloric Value: 13063 BTU/lb

i. Alternate I

This scheme is the simplest of the various alternates tested. The results of simulation for this scheme are shown in Figure IV-11. In this scheme, methane is produced mainly by the catalytic methanation of CO and H₂. The effects of steam to coal ratio and reactor temperature are discussed below:

a. Effect of steam to coal ratio

The effect of steam to coal ratio on the efficiency of gasification for various reactor temperatures is shown in Figure IV-11. It is seen that the total raw coal requirement is at a minimum for steam to coal ratio between 0.6 and 0.9, depending on the reactor temperature. Since the gasifier is operated isothermally, a high steam to coal ratio would demand more heat to raise the steam temperature to that of the reactor. The increased energy requirement can only be met by burning more coal with more oxygen. On the other hand, if the steam to coal ratio is reduced, more H₂ and CO would be produced from carbon-steam reaction due to the decreased carbon-oxygen reaction. However, a greater amount of steam will be required later in the water-gas shift converter to shift CO to H₂ in order to manufacture the pipeline gas of specified heating value. Thus, at a lower steam to coal ratio, more coal would be needed in the steam plant to generate more steam for the shift converter. This explains the existence of minimum total coal requirements in Figure IV-11.

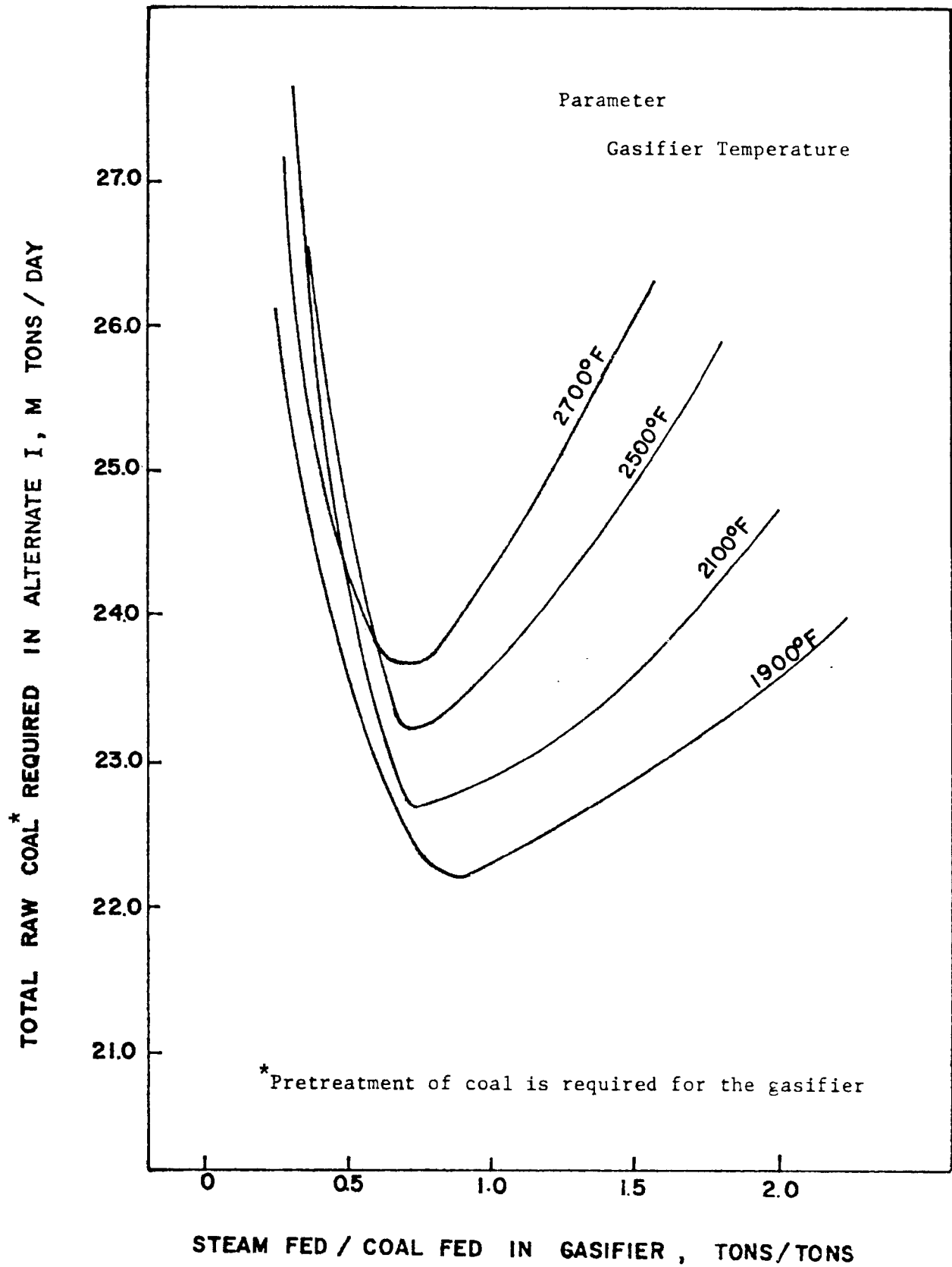


Figure IV-11 Effect of steam flow rate on Efficiency of Gasification for Alternate I (Capacity 250×10^9 BTU/DAY of Pipeline Gas with Heating Value 900 - 920 BTU/SCF)

b. Effect of reactor temperature

Figure IV-11 shows the effect of the reactor temperature on the efficiency of coal utilization for Alternate I. At a fixed steam to coal ratio, the total amount of coal required increases with an increase in reactor temperature. In order to operate an isothermal gasifier at a high temperature, more oxygen is required for carbon-oxygen reaction to sustain the reactor temperature and the carbon-steam reaction. This reduces the coal utilization efficiency.

ii. Alternate II

The results of the computer simulation for this alternate are shown in Figs. IV-12 to IV-16 and Figs. IV-16A to C. The process description of the gasification phase for Alternates II-1, II-2, and II-3 are given in Figs. IV-34, IV-36, and IV-38, respectively.

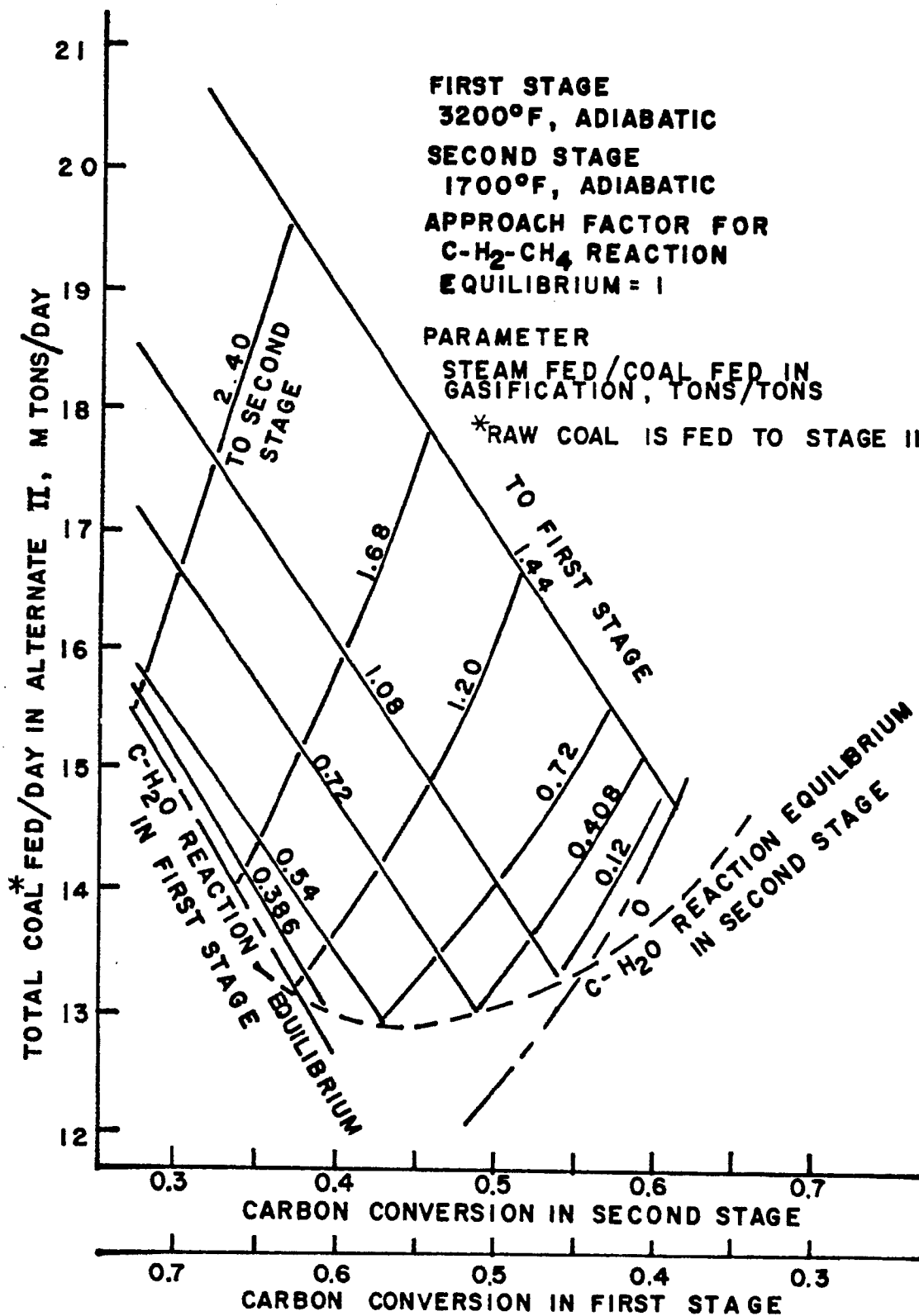


Figure IV-12 Effect of Carbon Conversion on Efficiency of Gasification Process of Alternate II (capacity 250×10^9 BTU/Day of Pipeline Gas with Heating Value, 900 BTU/SCF)

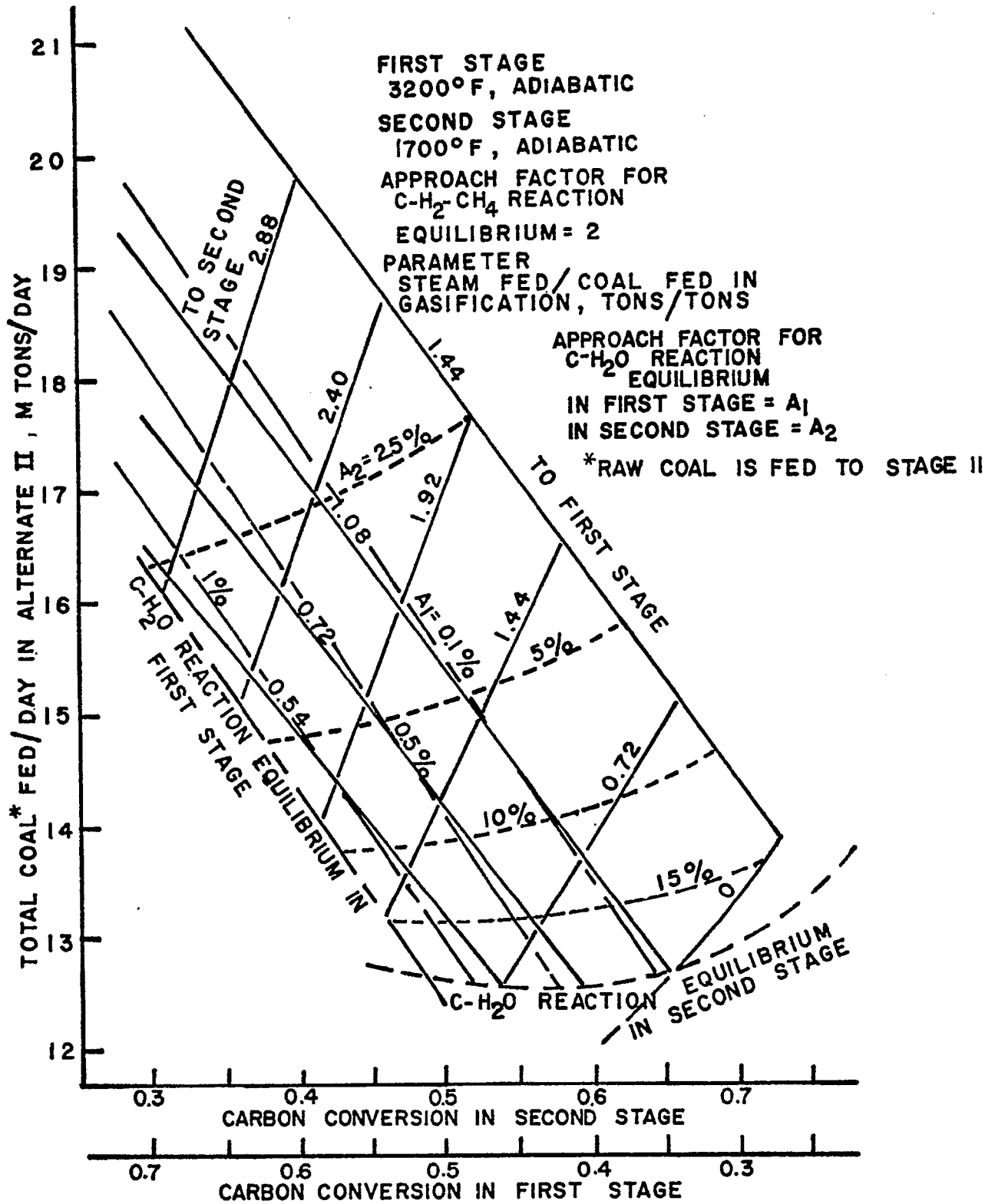


Figure IV-13 Effect of Approach Factor for C-H₂-CH₄ Equilibrium on Efficiency of Gasification Process of Alternate II (capacity 250X10⁹ BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

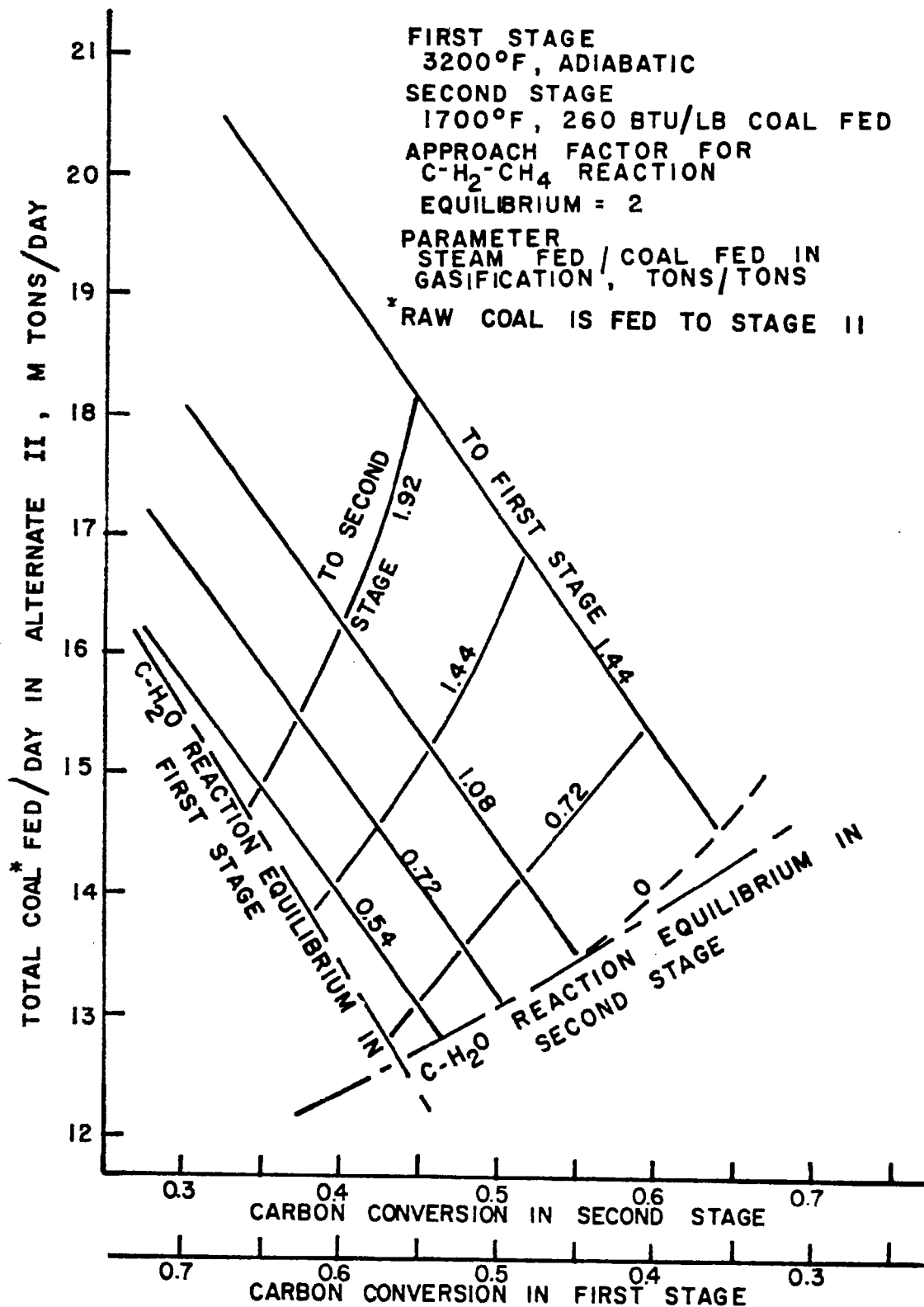


Figure IV-14 Effect of Heat Removal from the Second Stage on Efficiency of Gasification for Alternate II (capacity 250×10^9 BTU/Day of Pipeline Gas with Heating Value, 900 BTU/SCF)

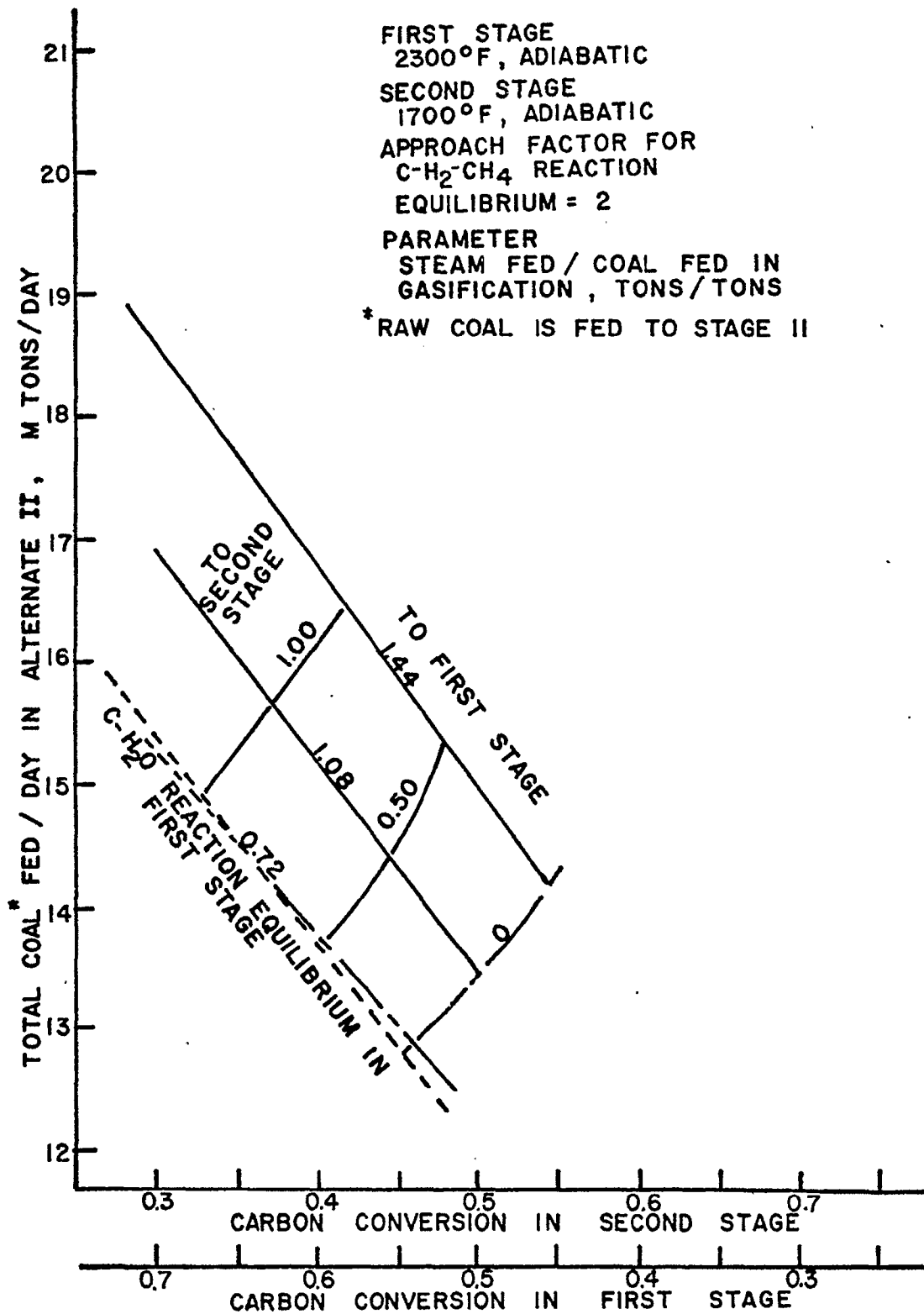


Figure IV-15 Effect of Operating Temperature in the First Stage on Efficiency of Gasification for Alternate II (capacity 250×10^9 BTU/Day of Pipeline Gas with heating value 900 BTU/SCF)

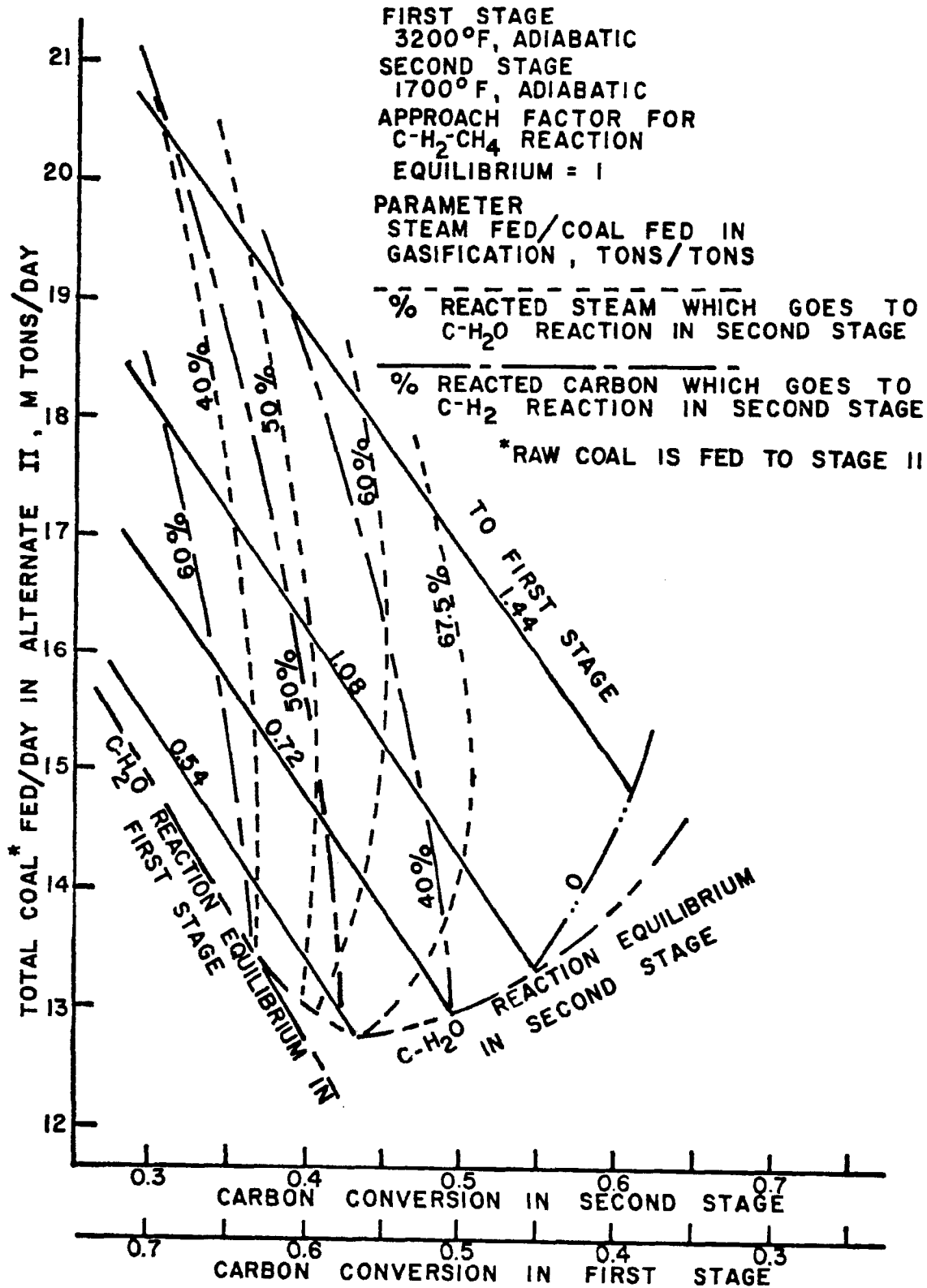


Figure IV-16 Effect of Conversions of Carbon and Steam in the Second Stage on Efficiency of Gasification for Alternate II (capacity 250X10⁹ BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

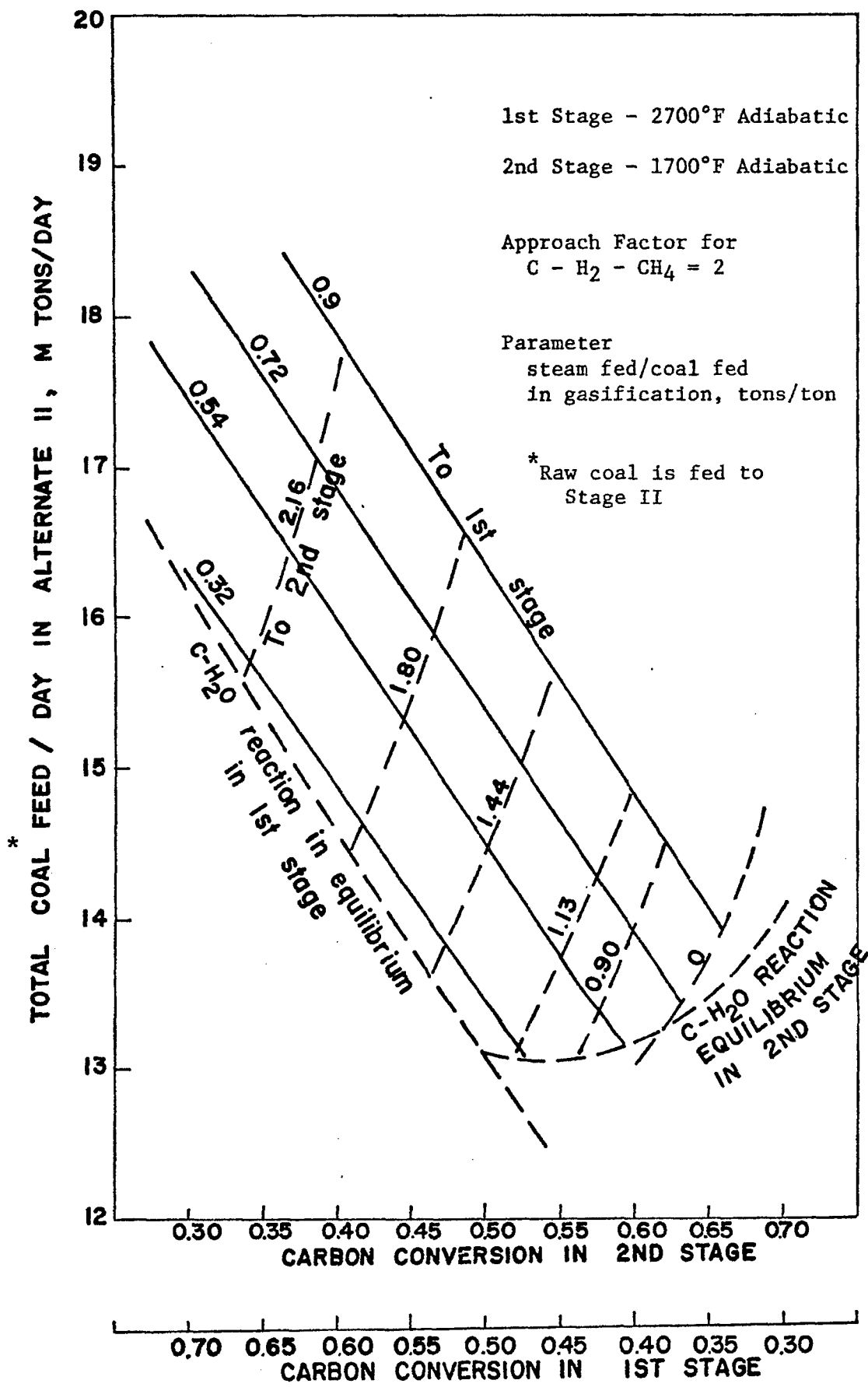


Figure IV-16A Effect of Operating Temperature In the First Stage On Efficiency of Gasification for Alternate II (Capacity 250×10^9 BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

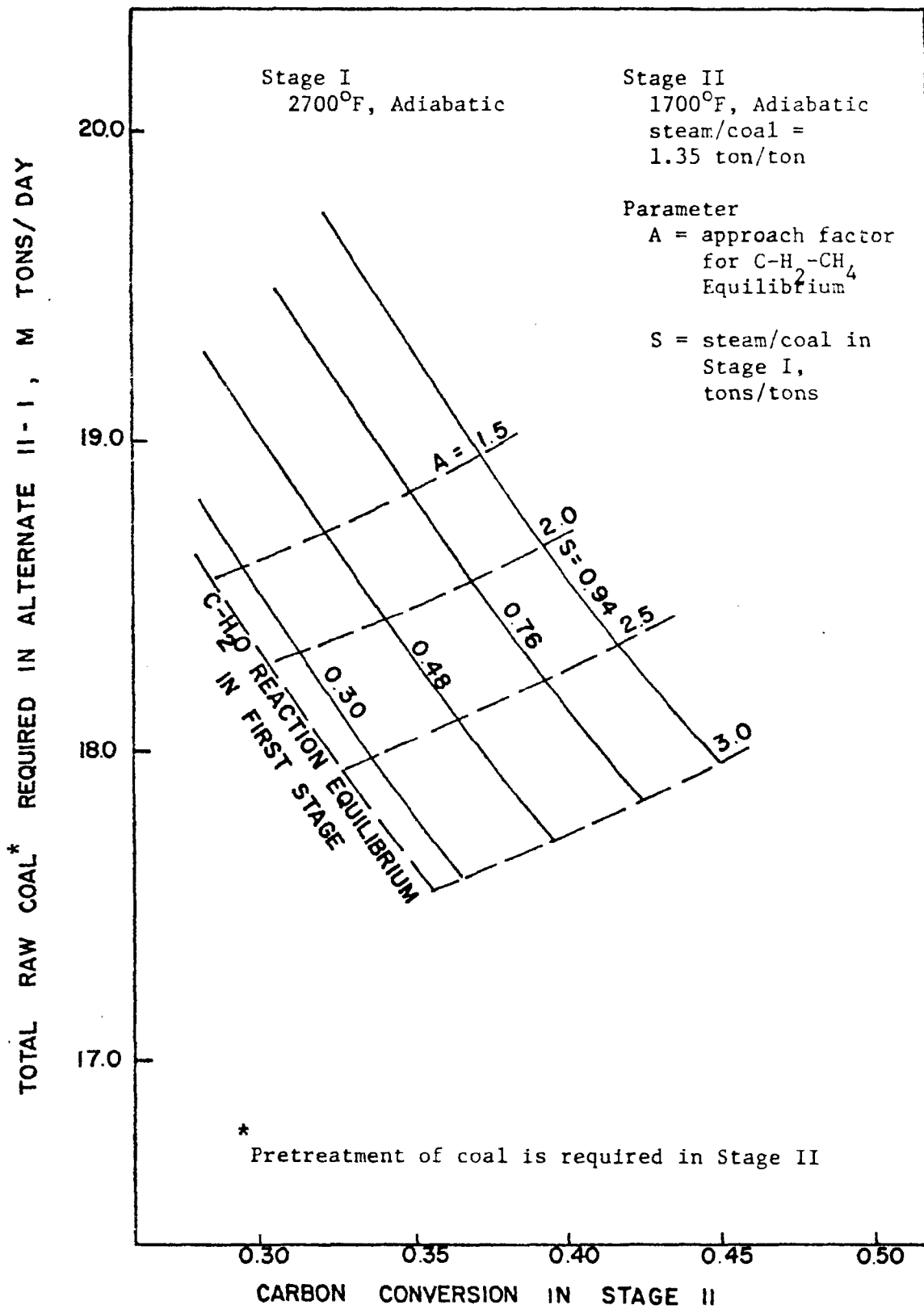


Figure IV-16B

Effect of steam flow rate on Efficiency of Gasification for Alternate II-1 (Capacity 250×10^9 BTU/DAY of Pipeline Gas with Heating Value 900 - 920 BTU/SCF)

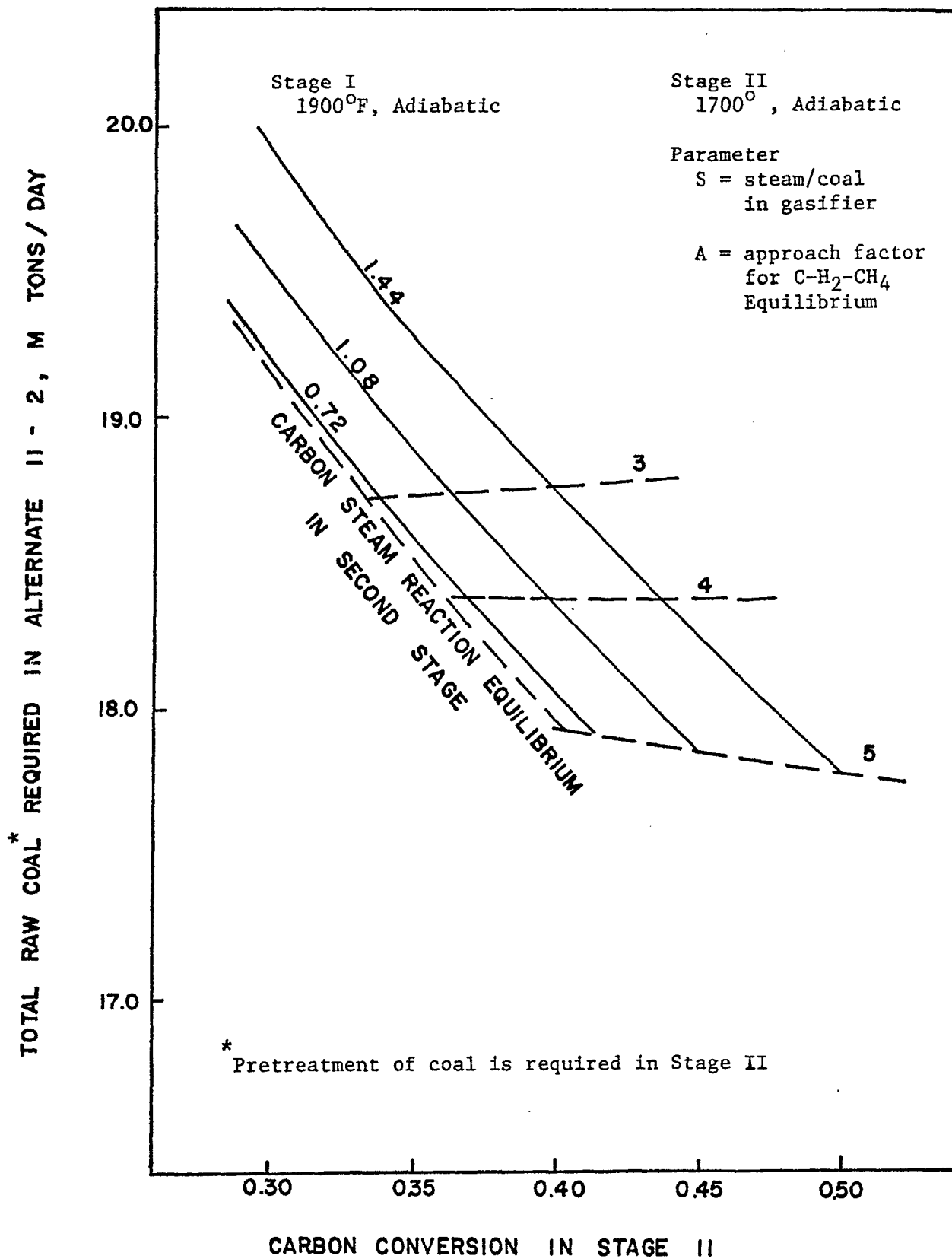


Figure IV-16C Effect of steam flow rate on Efficiency of Gasification for Alternate II-2 (Capacity 250×10^6 BTU/DAY of Pipeline Gas with Heating Value 900 - 920 BTU/SCF)

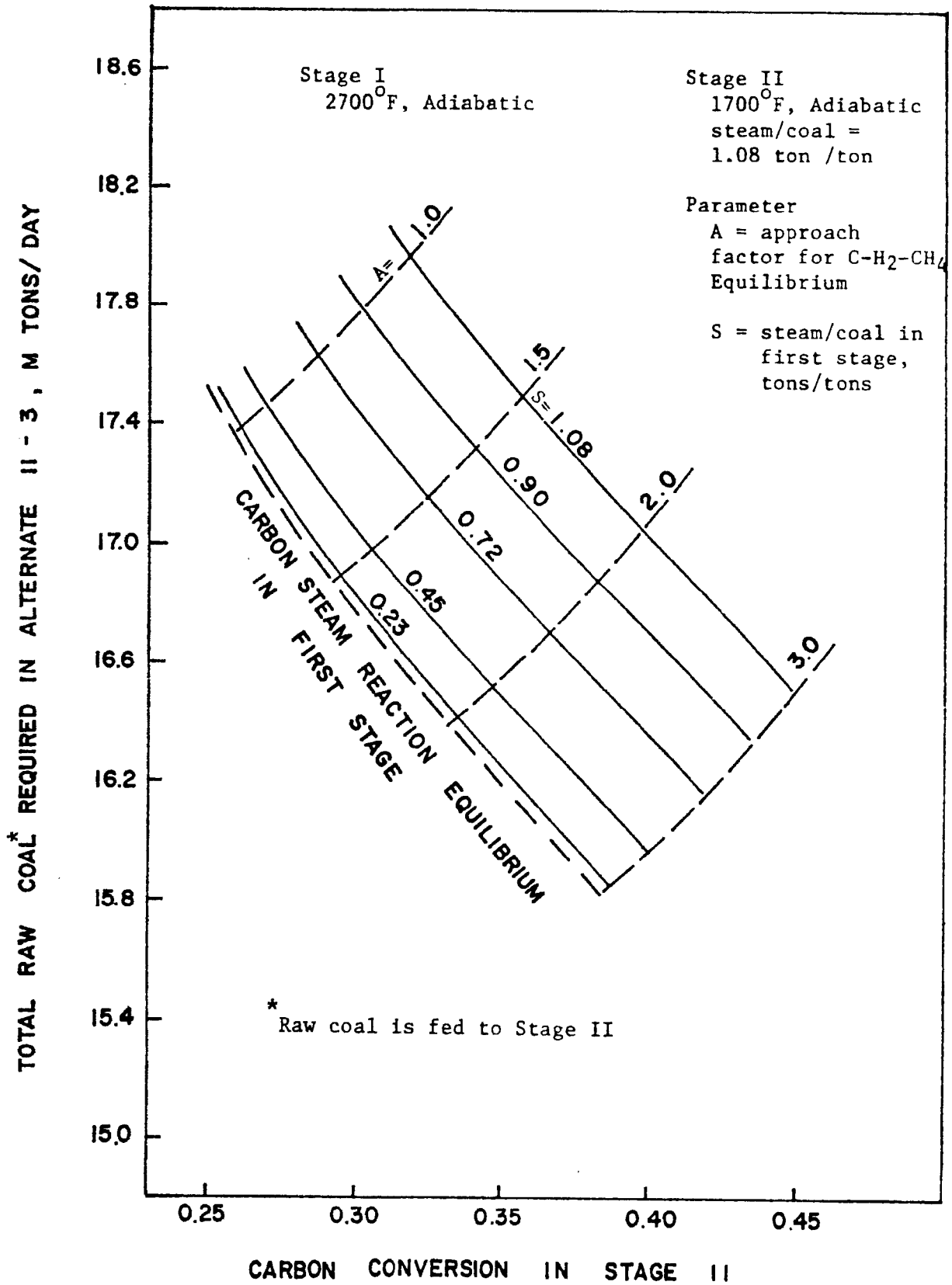


Figure IV-16D Effect of steam flow rate in Stage I on Efficiency of Gasification for Alternate II-3 (Capacity 250 X 10⁶ BTU/DAY of Pipeline Gas with Heating Value 900 - 920 BTU/SCF)

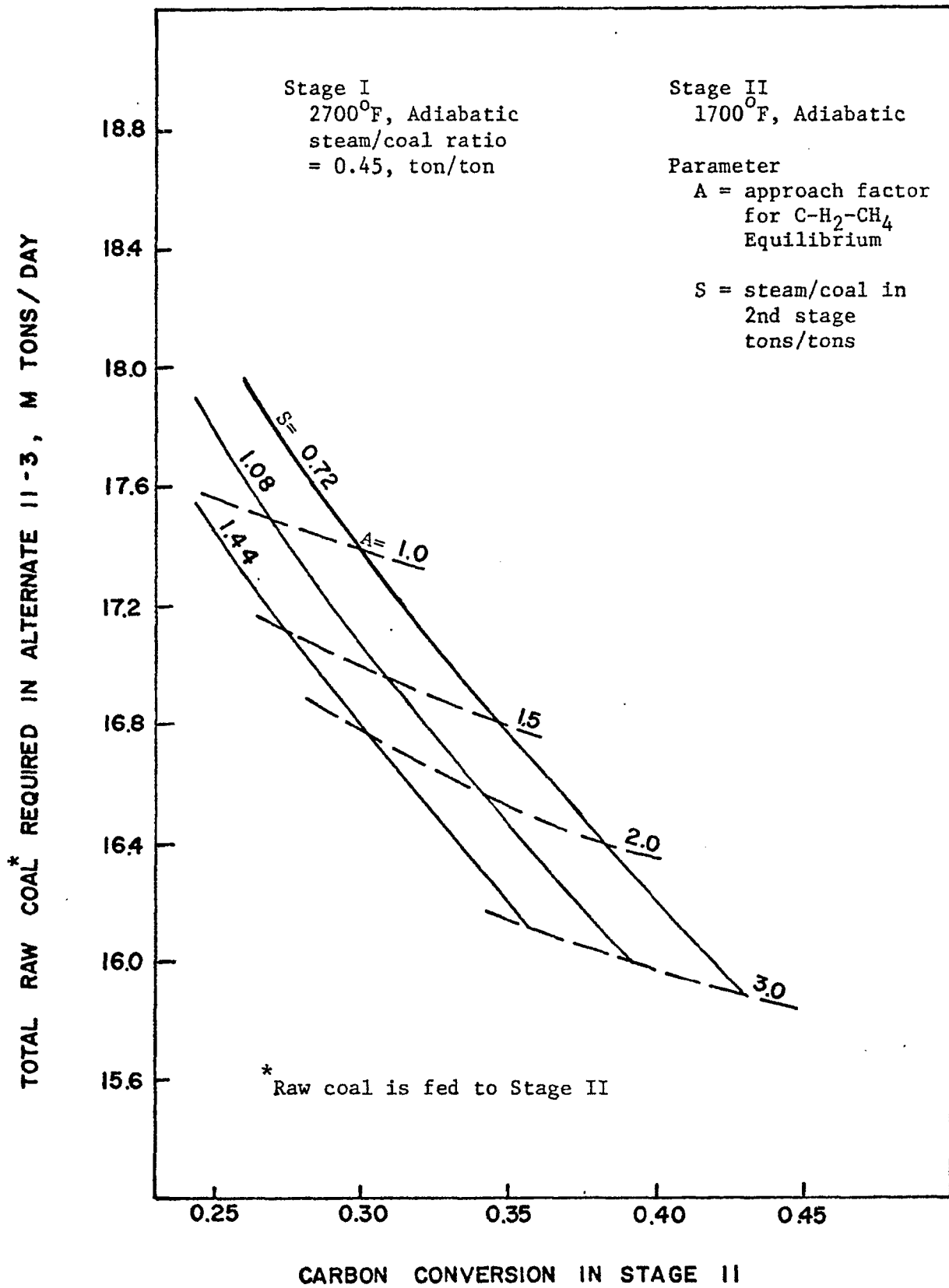


Figure IV-16E Effect of steam flow rate in Stage II on Efficiency of Gasification for Alternate II-3 (Capacity 250×10^9 BTU/DAY of Pipeline Gas with Heating Value 900 - 920 BTU/SCF)

The total amount of coal required per day is governed by the operating parameters such as operating temperatures, steam to coal ratio in both stages, and approach factors for the carbon-hydrogen-methane equilibrium. The carbon-steam equilibrium in both stages has an effect on the efficiency of the process. Various approach factors of the above equilibrium are shown in Fig. IV-13.

a. Effects of steam to coal ratio.

The effects of steam to coal ratio in both stages are shown in Fig. IV-12. At a given second stage carbon conversion, the coal utilization is seen to become better as the ratio of steam to coal is decreased approaching the low limit bounded by the carbon steam reaction equilibrium. The reason for this trend can be explained as in Section 3.4.i.a.

b. Effect of reactor temperature

Comparing Figs. IV-13 and IV-15 the effect of first stage operating temperature on effectiveness of coal utilization is readily apparent. At the same carbon conversion and steam to coal ratio, low operating temperatures give a better coal utilization than high temperatures, as discussed in Section 3.4.i.b.

Figs. IV-13 and IV-15 indicate that operation of the gasifier at a higher temperature requires somewhat less amount of coal per day than that at a lower temperature.

c. Carbon conversion.

The reactions in second stage are postulated as given in Equations (IV-35), (IV-37), and (IV-38).

Carbon-hydrogen reaction, Eq. (IV-38), is a highly exothermic reaction. This reaction can provide heat required for the endothermic carbon-steam reaction, Eq. (IV-36). Fig. IV-16 shows the percentage of reacted carbon which goes to carbon-hydrogen reaction, and the percent of reacted steam which goes to carbon-steam reaction. As indicated in Fig. IV-16, at low conversion, more than 50% of reacted carbon goes to the carbon-hydrogen reaction. In the second stage, in order to maintain the reactor at a predetermined temperature, a large amount of steam is required to absorb the heat generated. As can be expected, coal utilization is less effective at a low conversion than at a high conversion in the second stage. The required steam in the second stage decreases when carbon conversion is increased, approaching the carbon steam reaction equilibrium.

d. Approach factor for carbon-hydrogen-methane equilibrium

The effect of the approach factor on coal utilization is shown in Figs. IV-16B, C, D, and E. Apparently, a higher approach factor gives a better coal utilization at a fixed carbon conversion. It has been reported [26,27] that coal-hydrogen-methane equilibrium for coal-hydrogen system exceeds the graphite-hydrogen-methane equilibrium with the approach factor ranging from 1 to 8. However, for coal-hydrogen-steam system [2,9] the approach factors are usually less than 4.

iii. Alternate III

The result for this alternate scheme is shown in Figs. IV-17 to IV-20, and Figs. IV-21 and 21A. In all figures except Fig. IV-21A, there are three boundaries to limit the operation of this scheme. In regions to the left of the dotted line, the gas product

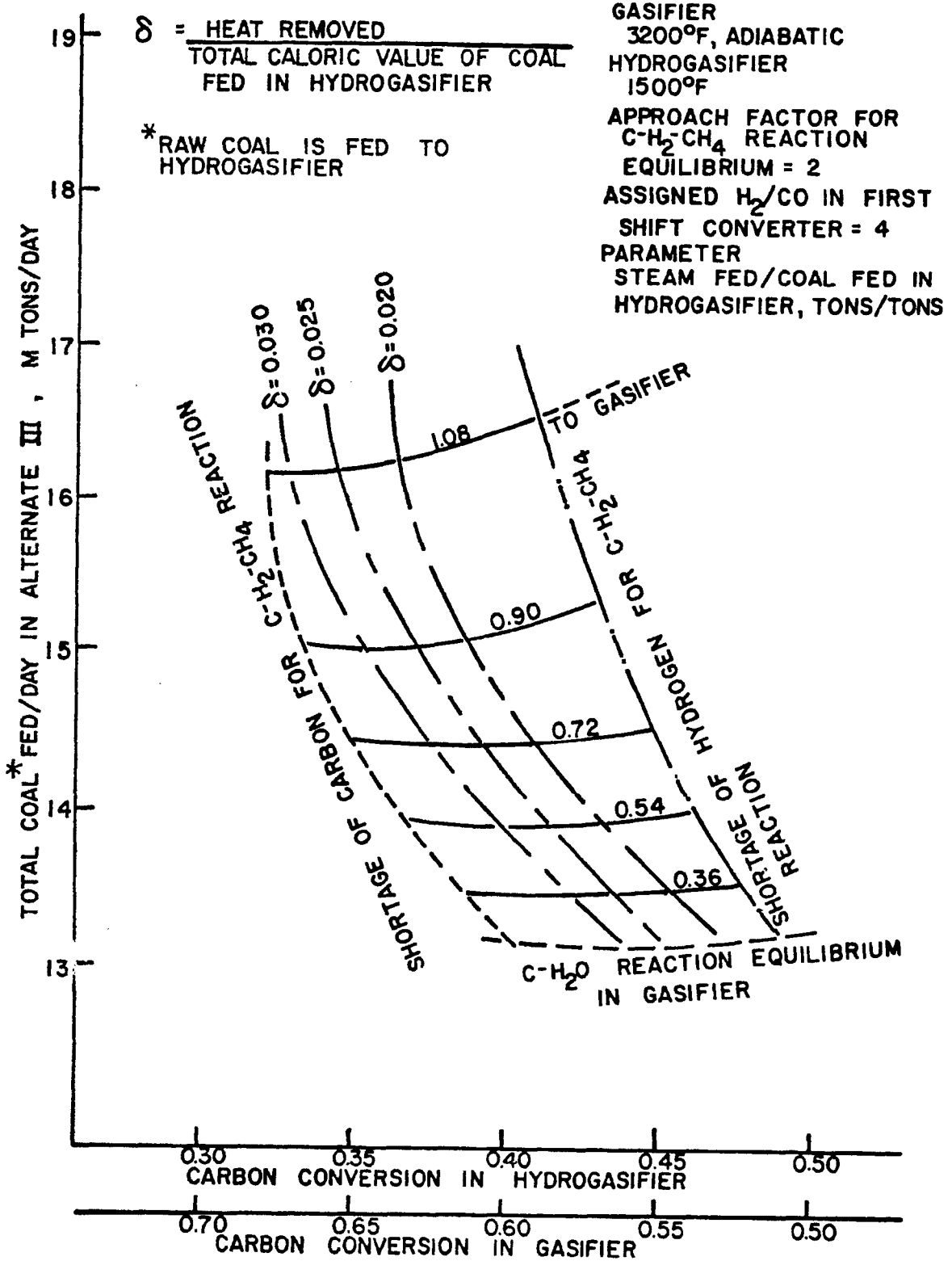


Figure IV-17 Effect of Carbon Concersion on Efficiency of Gasification for Alternate III (capacity 250X10⁹ BTU/Day of Pipeline Gas with heat value 900 BTU/SCF)

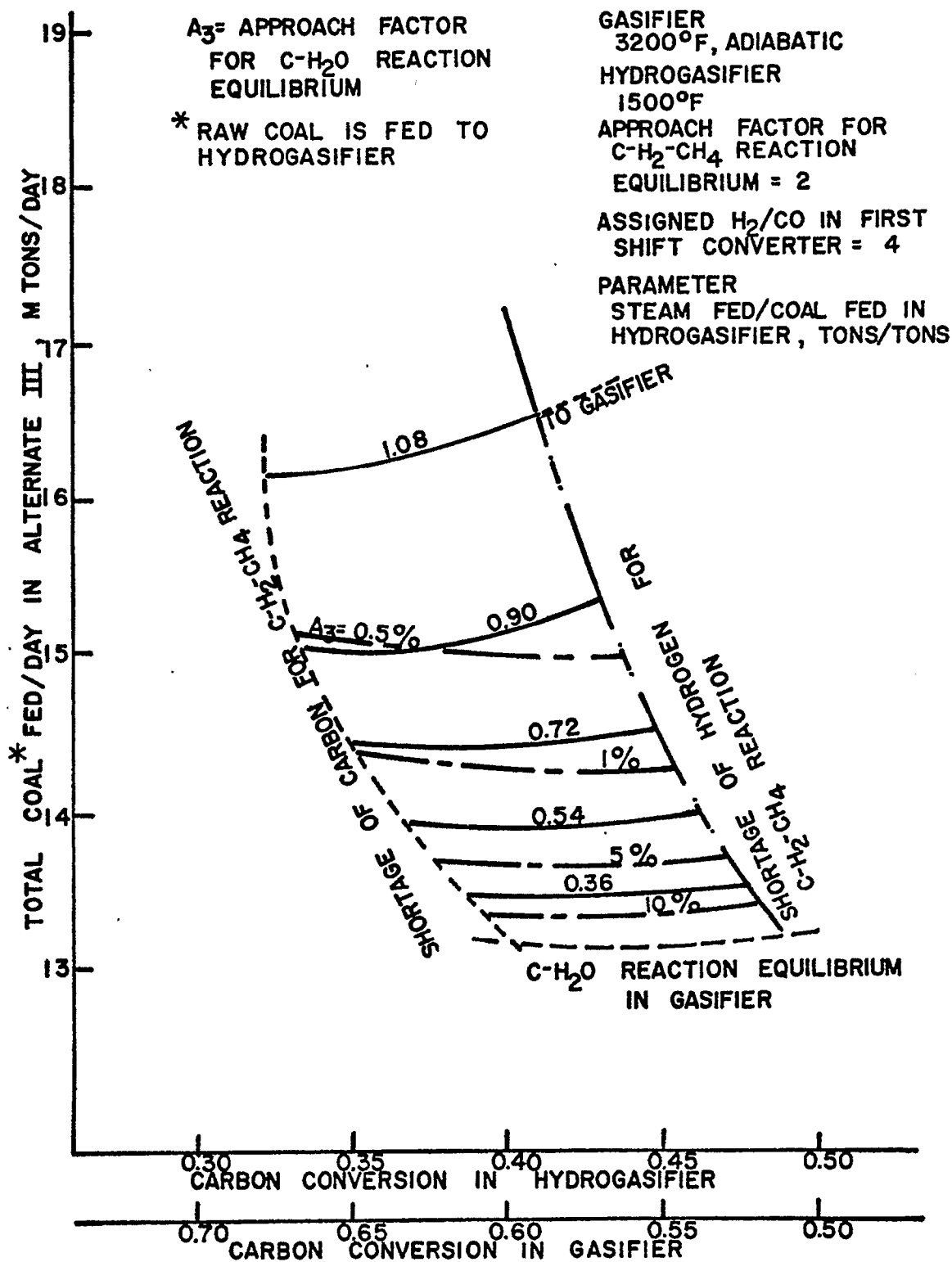


Figure IV-18 Effect of Approach Factor for C-H₂O Reaction Equilibrium on Efficiency of Gasification for Alternate III (capacity 250X10⁹ BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

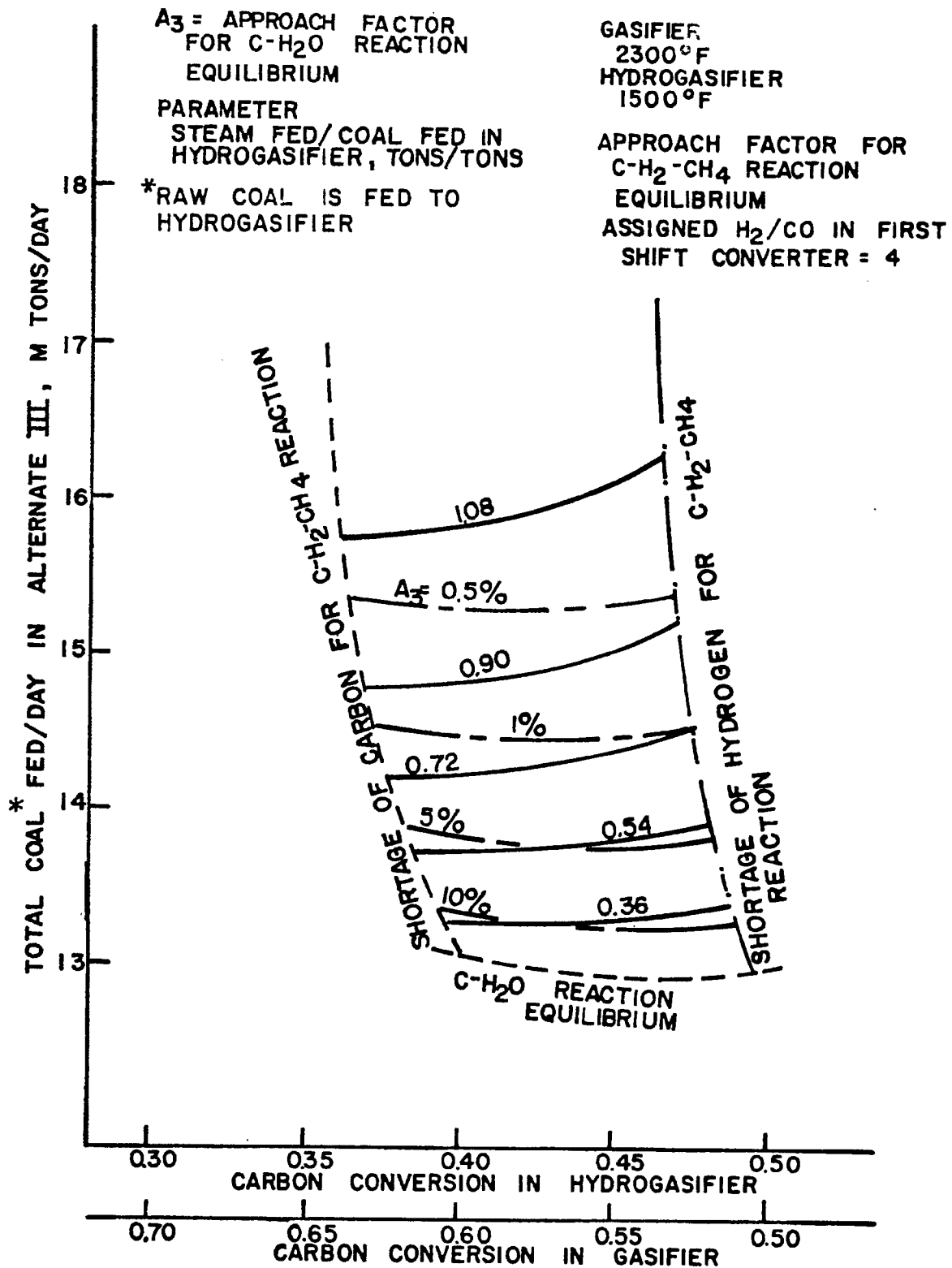


Figure IV-19 Effect of Reactor Temperature on Efficiency of Gasification for Alternate III (capacity 250X10⁹ BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

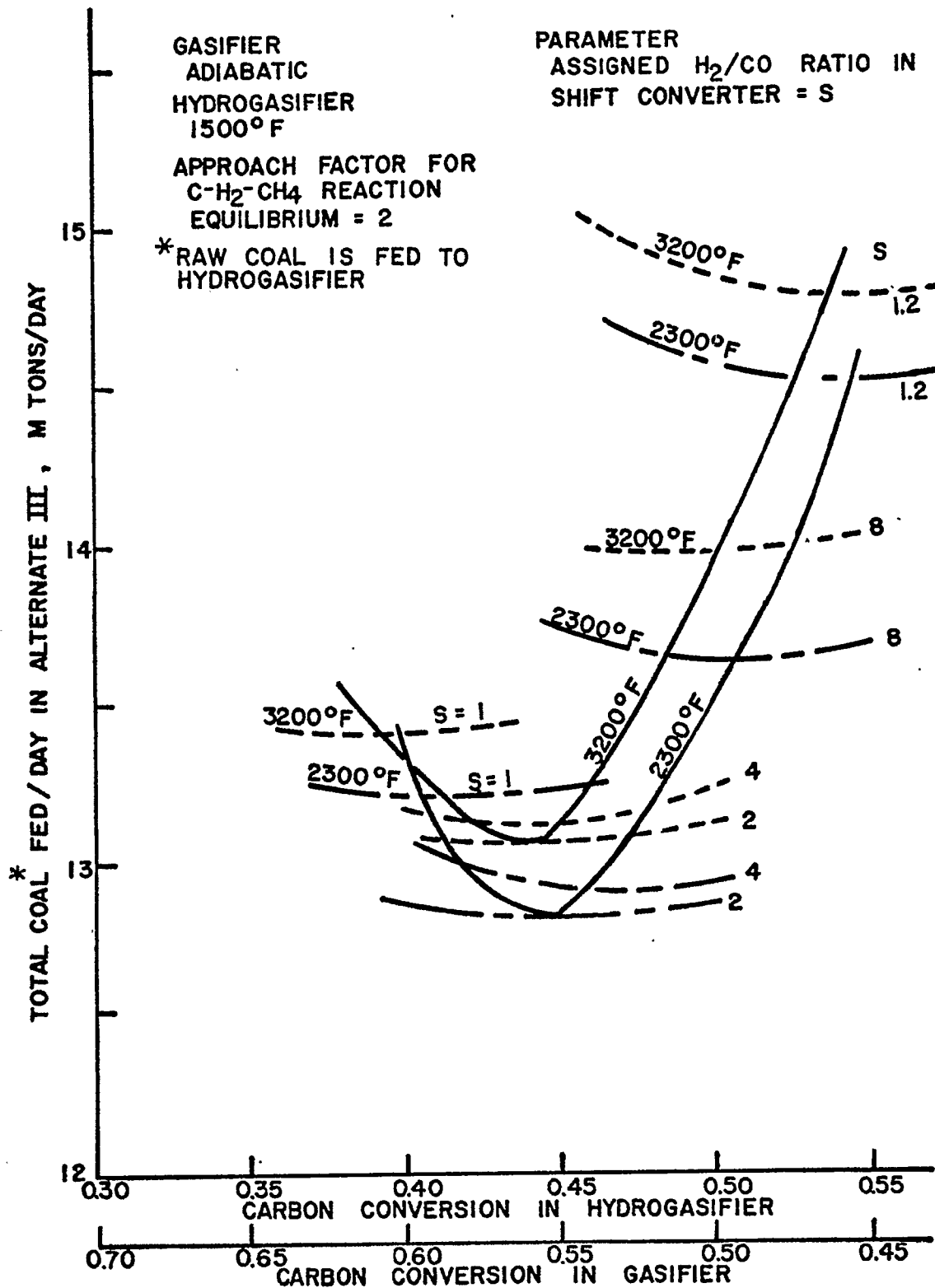


Figure IV-20 Effect of Reactor Temperature and Shift Ratio on Efficiency of Gasification for Alternate III (capacity 250X10⁹ BTU/Day of Pipeling Gas with Heating Value 900 BTU/SCF)

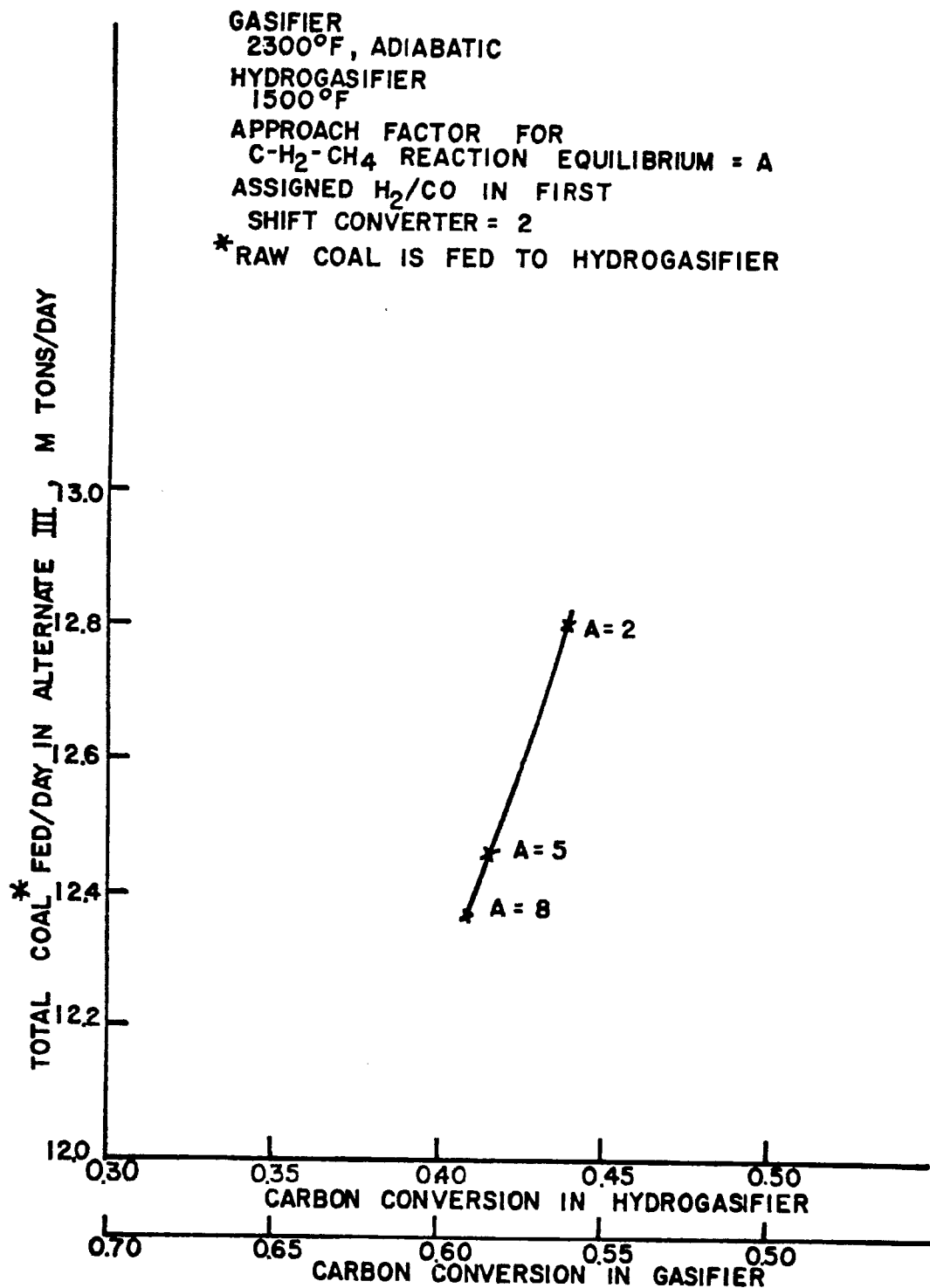


Figure IV-21 Effect of Approach Factor for C-H₂-CH₄ Equilibrium on Efficiency of Gasification for Alternate III (capacity 250X10⁹ BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)

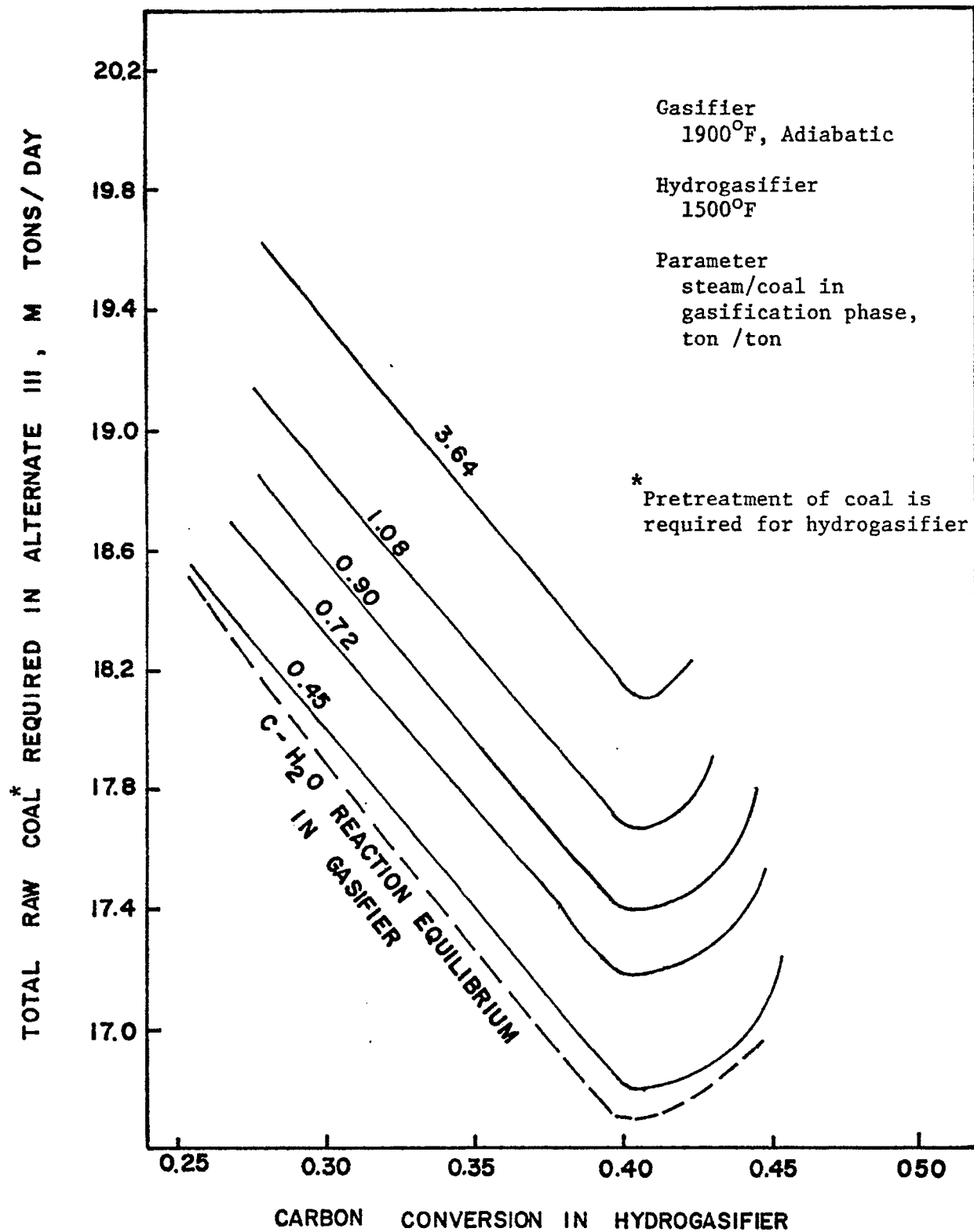


Figure IV-21A

Effect of steam flow rate on Efficiency of Gasification
for Alternate III (Capacity 250×10^9 BTU/DAY of Pipeline
Gas with Heating Value 900 - 920 BTU/SCF)

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does not have enough methane to reach the required 900 BTU/SCF. This is because less carbon and excess hydrogen from the first shift converter are available. In the region to the right of the dotted line, there is not enough hydrogen to sustain an approach factor of 2 for the carbon-hydrogen-methane equilibrium.

Between the two lines, as shown by Fig. IV-17, if less steam in the gasifier is used, coal utilization can be expected to improve until it is hindered by the carbon steam reaction equilibrium. The best coal utilization of this scheme seems to be obtained at approximately 45% of carbon conversion in the hydrogasifier, and a H_2 to CO ratio of 4 in the first shift converter, with an approach factor of 2 for the carbon-hydrogen-methane equilibrium.

Fig. IV-20 shows the lines of approximate minimum points for various H_2 to CO ratios in the first shift converter, and for operating temperatures 2300°F and 3200°F in the gasifier. When the H_2 to CO ratio equals approximately 2, the lowest amount of total coal required is obtained. This is because at this ratio the amount of steam required for the first and second shift converters is at a minimum. It is also indicated in Figure IV-20 that low operating temperatures provide better coal utilization.

The approach factor for the carbon-hydrogen-methane equilibrium may reach as high as 8 depending on the rank of coal to be used for gasification. Thus, large approach factors are used in this study for the purpose of testing the sensitivity of this factor. Fig. IV-21 shows the effect of this factor on the

minimum amount of total coal required at the gasifier operating temperature of 1500°F and a shifting ratio, i.e., H₂ to CO of 2 in the first shift converter.

iv. Alternate IV

The effect of carbon conversion on gasification efficiency is shown in Figure IV-22. High carbon conversion in hydrogasifier gives a better coal utilization since more methane is produced by the carbon-hydrogen reaction. In this figure, total carbon conversion in both gasifiers, the hydrogasifier and the electrothermal gasifier, is varied from 65 to 80%. The residual carbon in the char produced from electrothermal gasifier is used to supplement the fuel requirement in the steam generation plant and the power plant.

3.5 Effectiveness of Coal Utilization for Different Ranks of Coal

Physical properties of various ranks of coal are listed in Table IV-6. The results of computer simulation are shown in Fig. IV-23. As expected, coal utilization efficiency of Alternate III, using lignite, is lower than any other rank of coal being tested. This is because lignite contains lower carbon and available hydrogen. Here, available hydrogen is defined as the amount of hydrogen which is not combined with oxygen present in coal. Owing to the low hydrogen and high oxygen content, subbituminous coal has a lower utilization efficiency than that of bituminous coal.

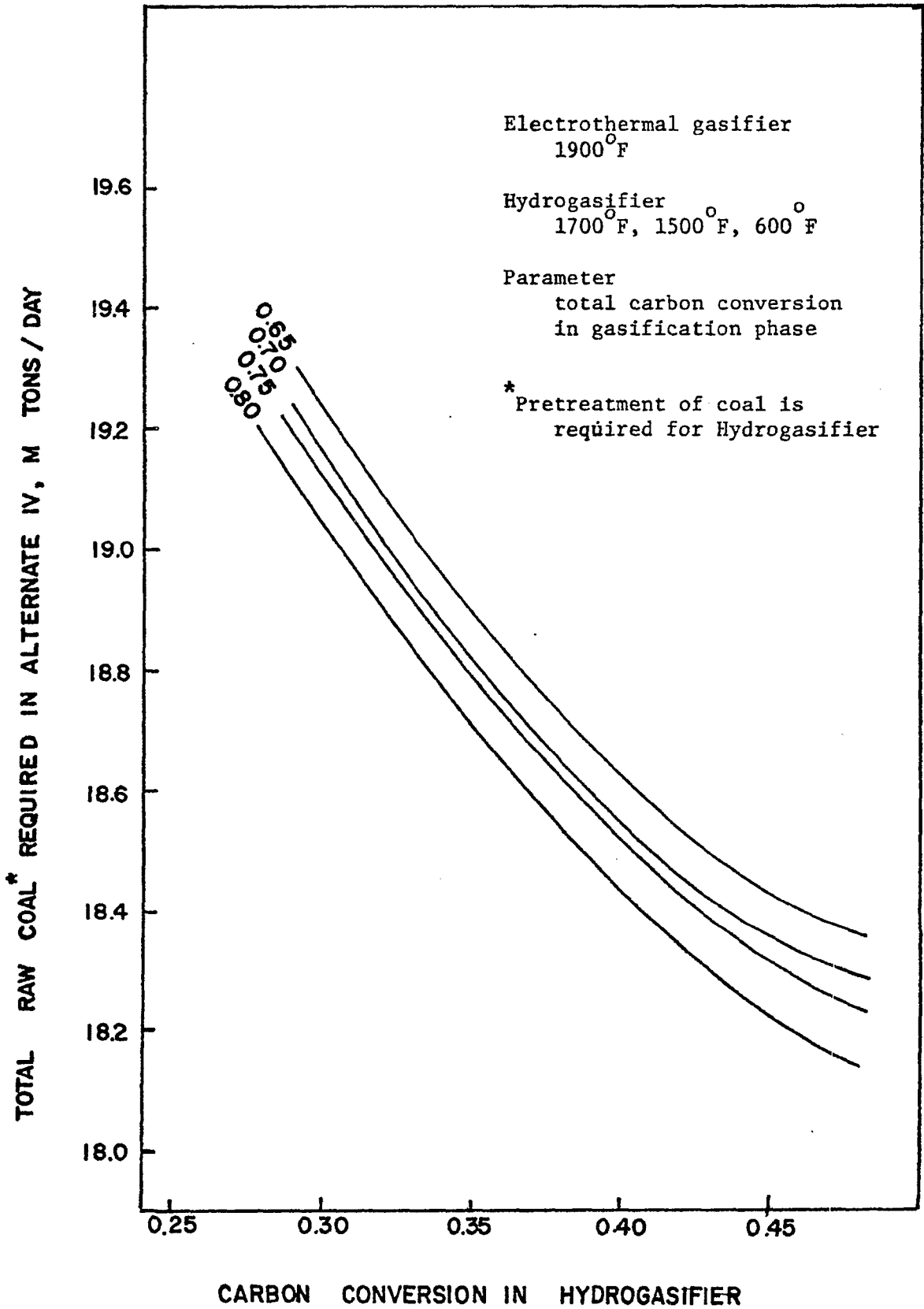


Figure IV-22 Effect of carbon conversion on Efficiency of Gasification for Alternate IV (Capacity 250×10^9 BTU/DAY of Pipeline Gas with Heating Value 900 ~ 920 BTU/SCF)

Table IV-6 Typical Physical Properties of Various Types of Coal [13]

Coal Type	Proximate Analysis, Wt%				Ultimate Analysis, Wt%						Caloric Value BTU/lb coal
	Moisture	Volatile Matter	Fixed Carbon	Ash	C	H	O	N	S	Ash	
Lignite (Montana)	4.3	39.3	48.6	7.8	64.8	4.17	21.22	0.95	0.68	8.18	10091
Subbituminous (Colorada)	3.7	35.2	56.5	4.6	75.10	2.56	15.90	1.33	0.38	4.73	10918
Bituminous (Oitts,HVA)	3.9	32.6	48.8	14.7	67.9	4.91	6.38	1.18	4.33	15.30	12114
Bituminous (Pitts, Ireland Mine)	1.3	34.6	52.0	12.1	71.2	5.14	6.03	1.23	4.19	12.1	13063

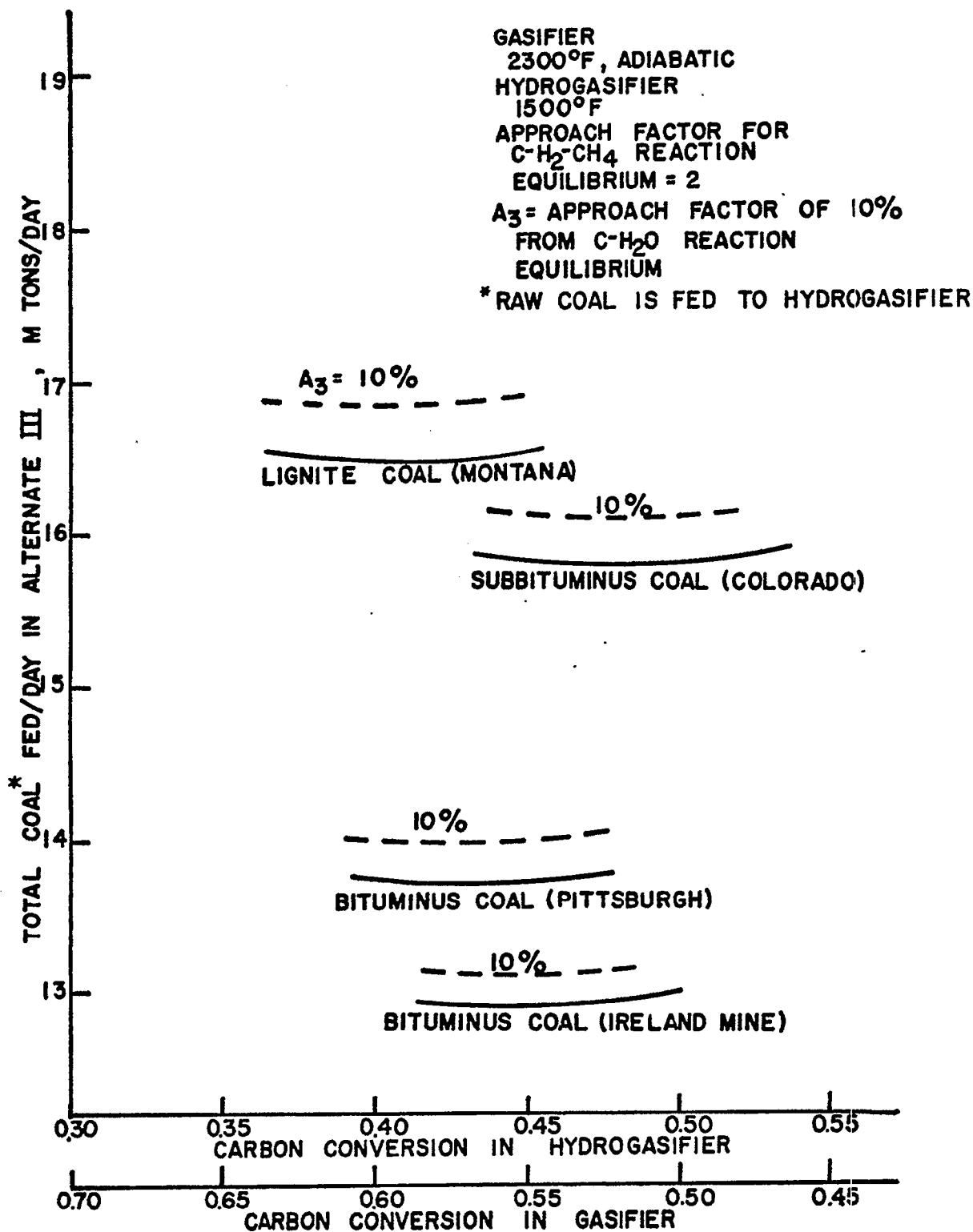


Figure IV-23 Effect of Different Ranks of Coal on Efficiency of Gasification for Alternate III (capacity 250×10^9 BTU/Day of Pipeline Gas with Heating Value 900 BTU/SCF)