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COMPUTER MODELING OF THE MERC FIXED BED GASIFIER

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Prepared By

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For The

United States Department of Energy
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COMPUTER MODELING OF MORGANTOWN ENERGY RESEARCH CENTER'S FIXED BED GASIFIER

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1. INTRODUCTION

This report describes the modeling of a fixed bed stirred gasifier operated by the Morgantown Energy Research Center (MERC) of the United States Department of Energy at Morgantown, West Virginia. This work was conducted in part under a MERC project entitled: "Advanced Gasification Concepts--Engineering Assessment". One objective of this project was to increase the fundamental understanding of existing gasification processes with mathematical modeling, and thereby assist the Department of Energy in its overall project planning.

Models are used for scale-up and optimization purposes and also for extrapolation beyond the normal operating conditions. However, very often, due to the complexity of the real system and the mathematical limitations, certain simplifying assumptions are made. Therefore, before using any model, its assumptions and hence its limitations should be examined and clearly understood. In this report, the theory and the development of the model are described in Sections 2 and 3. Results and conclusions are presented in Sections 4 and 5. Background information about the MERC's gasifier is provided in the following section.

1.1 MERC COAL GASIFIER

The recent energy crisis has given a great impetus to research efforts, especially in the field of coal gasification. Coal can be gasified to produce either pipeline quality gas (900-1000 BTU/SCF) or low/medium BTU gas (100-400 BTU/SCF). Low BTU gas, is obtained by

gasifying coal with a mixture of air and steam. Although not suitable for long distance transportation, low BTU gas has a great potential when used near the source of production. This is especially true with regard to power generation. Various gasifiers which are currently available or being developed for the production of low or medium BTU gas can be broadly classified into three categories depending on the type of coal bed used.[3,4,16] They are:

(1) Fixed bed gasifiers
(2) Fluidized bed gasifiers
(3) Entrained bed gasifiers

In fixed bed gasifiers, coal is charged from the top of the gasifier through lock-hoppers, while air and steam are introduced from the bottom of the reactor. Because of this countercurrent flow, the sensible heat of the ash is recovered by the cold incoming gas stream, and at the top of the bed, the sensible heat of the gas is utilized to heat the coal feed. Generally, high conversion of coal is obtained in the fixed bed gasifiers because of the long residence time. Fines of coal, which tend to block the passage of gas through the bed, cannot be used in fixed bed gasifiers. Caking coals also cannot be gasified without pretreatment or without the use of the stirrer to break up the agglomerated particles.

Entrained bed gasifiers use very small particles and can gasify caking coals. Some of the coal particles are blown out of the gasifier and carried in the gas stream. The residence time of solids is very short. The flow of solid and gas can be either upward or downward.

Solids are in motion continuously in the fluidized bed. Gas

flow rates are less than that used in the entrained bed so as to prevent the excessive elutriation. The fluidized bed provides excellent heat exchange and hence can be operated at lower temperatures. However, caking coals cannot be gasified because of agglomeration.

Fixed bed coal gasifiers commercially available today include the Lurgi, the Wellman-Galusha and the Woodall-Duckham. MERC (previously of the U.S. Bureau of Mines) constructed and began testing a fixed bed gas producer pilot plant in 1968. The main objective of this pilot plant was to demonstrate that highly agglomerating coals could be gasified at high pressures if stirring is provided in the bed where coal becomes plastic and fuses upon completion of devolatilization. Results obtained from these tests have been published in various reports.[8,9,12,13,14,17,18] In this section, Lurgi and Wellman-Galusha gasifiers, along with one being developed by the General Electric Company are described and compared with the MERC gasifier.

1.1.1 Description of the gasifier

MERC's high pressure gasification system is shown in Figure 1. The gasifier used is similar to other commercial fixed bed producers except for its smaller diameter (3.5 feet ID) and its provision for stirring deeply within the fuel bed. A schematic diagram of the gasifier is shown in Figure 2. Air mixed with superheated steam is introduced below the grate at 400-450°F (475-500°K) and flows upward through the descending fuel. A stepped grate of 9.6 square

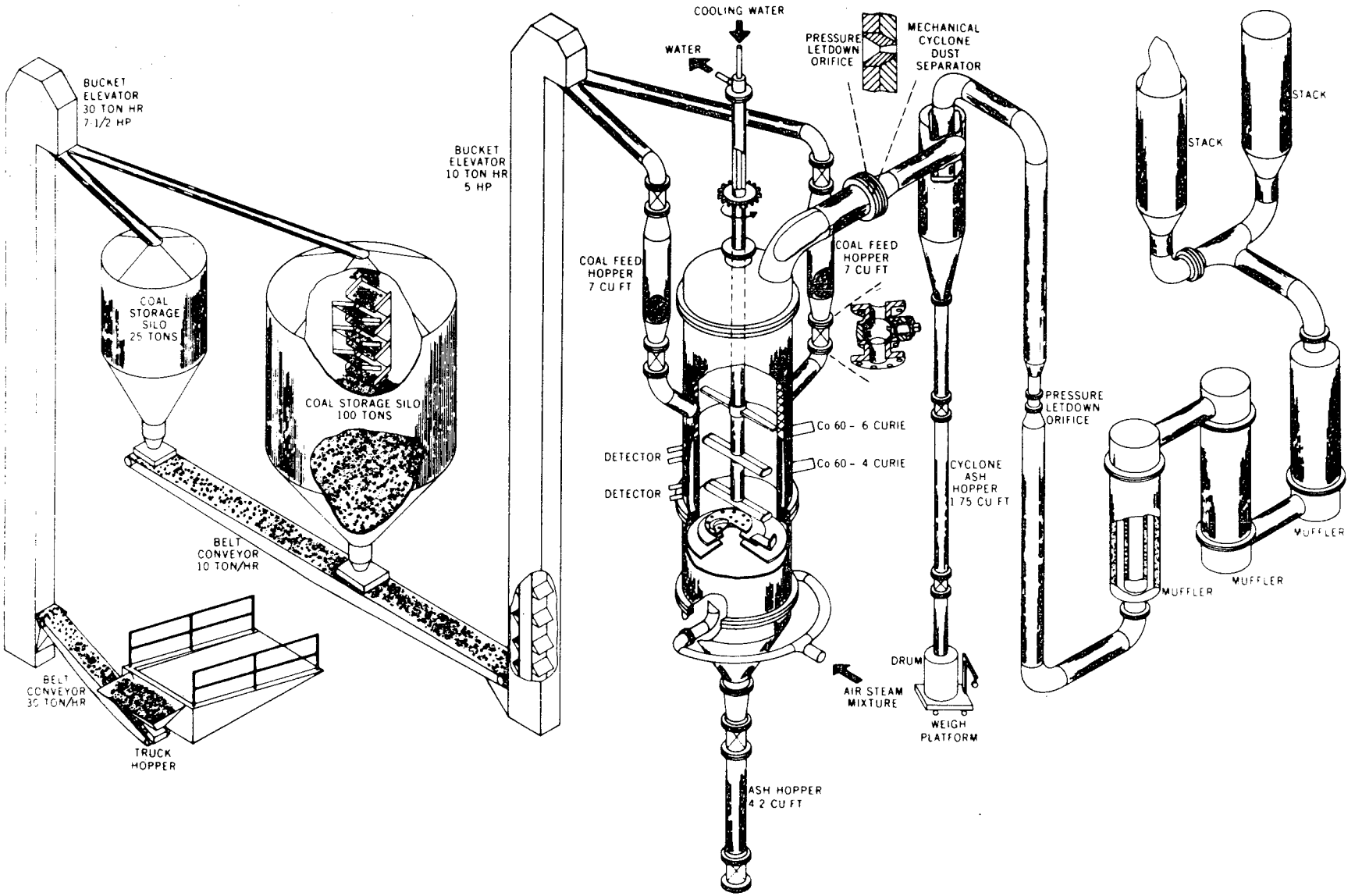


FIGURE 1 - MERC STIRRED-BED GASIFICATION SYSTEM

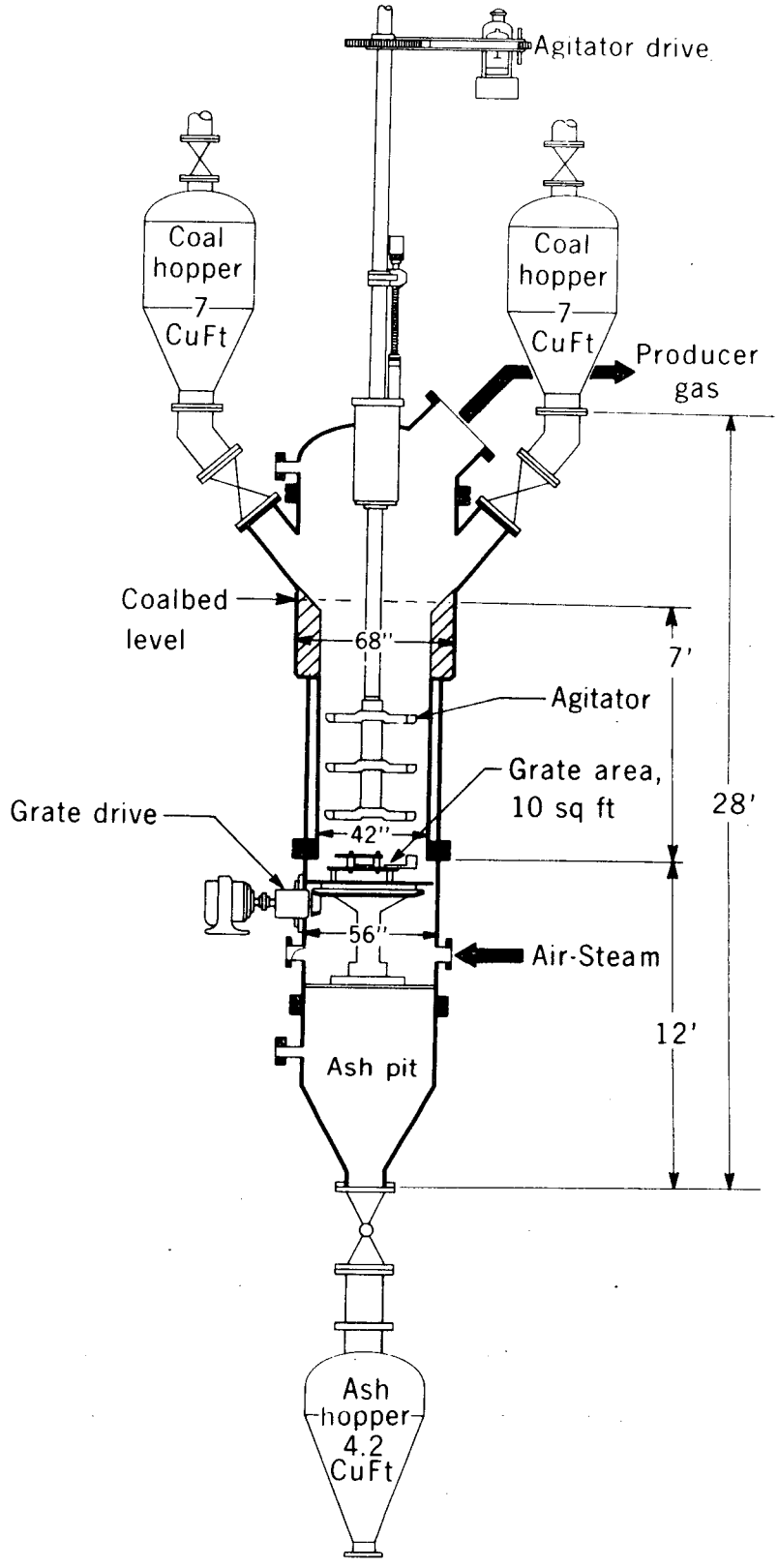


FIGURE 2 - EQUIPMENT LOCATION AND DIMENSIONS, FIXED-BED GASIFIER

feet (0.9 m^2) area supports the fuel which can either rotate continuously at a slow rate or operate on a time basis with a manual on-off control adjusted to match ash production. The frequency of ash discharge is governed by the grate temperature which is maintained below 700°F (650°K). Ash is removed through a lock hopper, then weighed and sampled for analysis. Producer gas exits through an offtake in the top cover. Pressure in the gasifier is developed by resistance to gas flow through the offtake line which contains fixed diameter orifices. Some of the dust in the gas is removed by a cyclone separator, then discharged through a lock hopper and subsequently weighed and sampled. A small gas flow is diverted from the main stream, cooled and cleaned of dust, tar and water before it is analyzed for CO, CO_2, H_2, N_2, O_2, CH_4 and H_2S.

The stirrer rotates at one-half revolution per minute while also moving vertically to about two feet. Continuous stirring of the bed maintains a dense fuel bed providing better contact between gas and solids, which yields a product gas of higher quality and composition. The stirrer arrangement is shown in Figure 3. Nuclear density gauges indicate conditions inside the pressure vessel by detecting bed levels and voids as shown in Figure 4.

The walls of the vessel are maintained at low temperature by cooling water passing through the water jacket. Thirteen inch thick refractory is used in the upper portion of the bed. The details are shown in Figure 2.

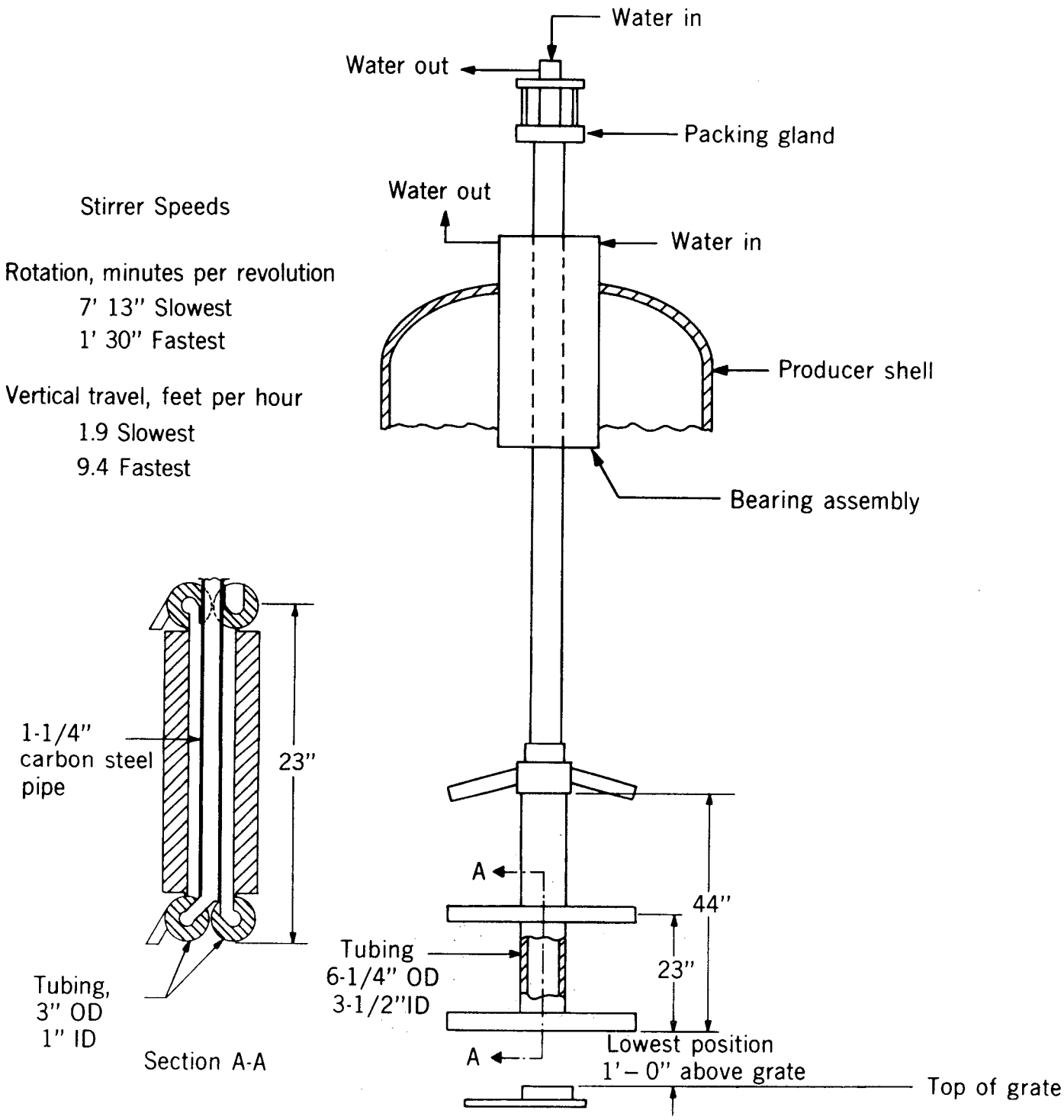


FIGURE 3 - STIRRER ARRANGEMENT

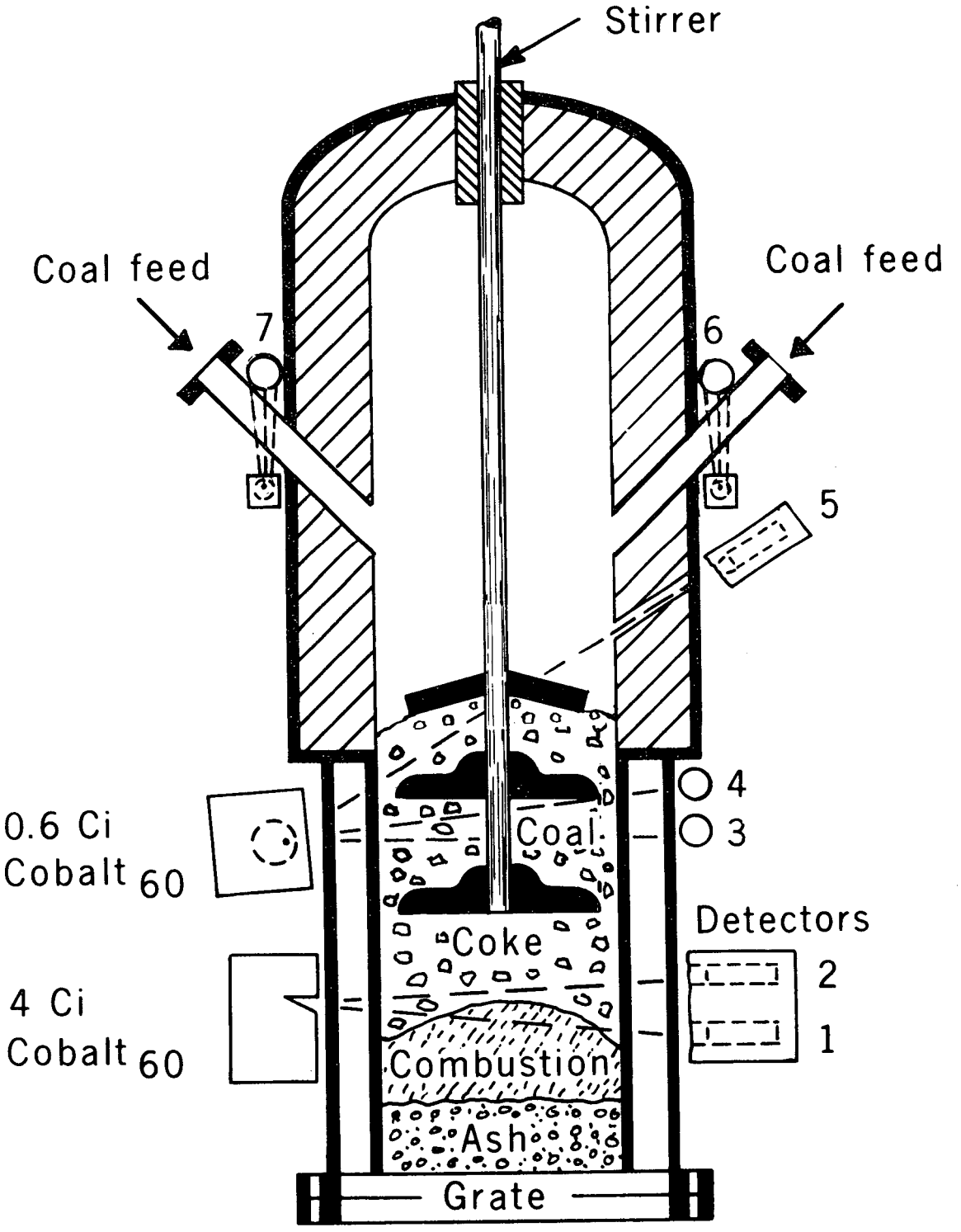


FIGURE 4 - NUCLEAR DENSITY GAGES APPLIED TO GAS PRODUCER

1.2 MEASUREMENT OF DATA

A data period commences when steady conditions are attained as shown by a constant coal rate over several hours. Samples collected during a data period include dust, tar, and water entrained in the gas, cyclone dust and ash. Dust, tar, and water content of the product gas are calculated based upon the weights collected from a sample of measured volume (about 25 scfh) taken over a timed interval. Direct measurement of gas production is impossible due to metering devices becoming inoperative as the result of rapid clogging of tar and dust. Gas production is calculated by obtaining a preliminary value from a mass balance in which gas output is taken as the difference between the input (coal, air and steam) and the output (bottom ash, tar and water). Gas composition is determined by an on-line chromatograph which analyzes a gas sample for CO, CO_2, H_2, N_2, and CH_4 every seven minutes and then prints the data. Composite samples are collected by continuous sampling and are analyzed on a laboratory chromatograph which gives the contents of H_2S, C_2H_6 and O_2 and other components. Final compositions are adjusted to an air free basis and an average value is calculated for a data period using all analyses recorded. The gas sampling system is presented in Figure 5. Further details about MERC's pilot plant can be found in the references listed at the end of this report.

1.3 COMPARISON OF MERC GASIFIER WITH OTHER FIXED BED GASIFIERS

In the following section, other currently available fixed bed gasifiers, namely Lurgi, Wellman-Galusha and GEGAS-D are described briefly. Performance of these gasifiers is compared with that of

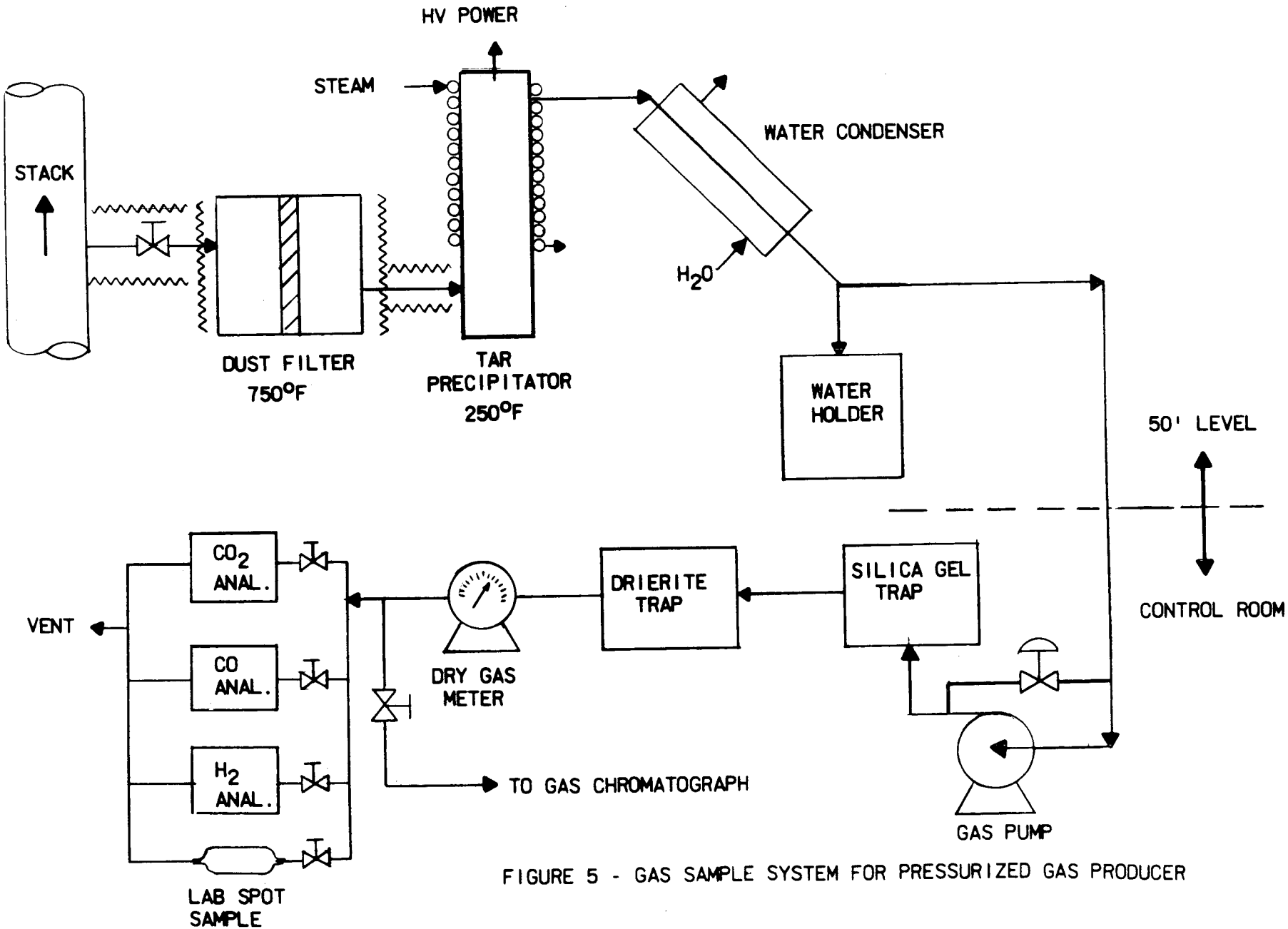


FIGURE 5 - GAS SAMPLE SYSTEM FOR PRESSURIZED GAS PRODUCER

the MERC's gasifier.

1.3.1 Lurgi Gasifier

The Lurgi gasifier is a cylindrical vessel with a diameter of 12-13' in which coal flows downward by gravity and steam and oxygen stream flows upward as shown in Figure 6. Lurgi gasifiers, which use non-caking coals only, have been widely used in South Africa and Europe. Recently, tests were carried out successfully at Westfield, Scotland to gasify various American coals in the Lurgi gasifier. A mechanical stirrer was used during these tests to prevent the agglomeration of caking coals[6].

1.3.2 Wellman-Galusha Gasifier

The Wellman-Galusha gasifier shown schematically in Figure 7 is a self-contained unit and does not require a steam plant. Air passing through the water jacket becomes saturated with water, thus supplying the steam required for gasification. Mild caking coals can also be gasified in the producer using a stirrer. Wellman-Galusha producers have been built in sizes ranging from 1.5 feet in diameter to 10 ft.[15] The gasifying capacity varies from 7.5 to 99 lbs/ft^2-hr.

1.3.3 General Electric Pressure Gasifier

The General Electric Company is presently operating a fixed bed producer known as GEGAS-D gasifier. This gasifier is a vessel with a diameter of 3 feet and is equipped with a stirrer as shown in Figure 8. It was recently operated at 225 psig with a coal feed

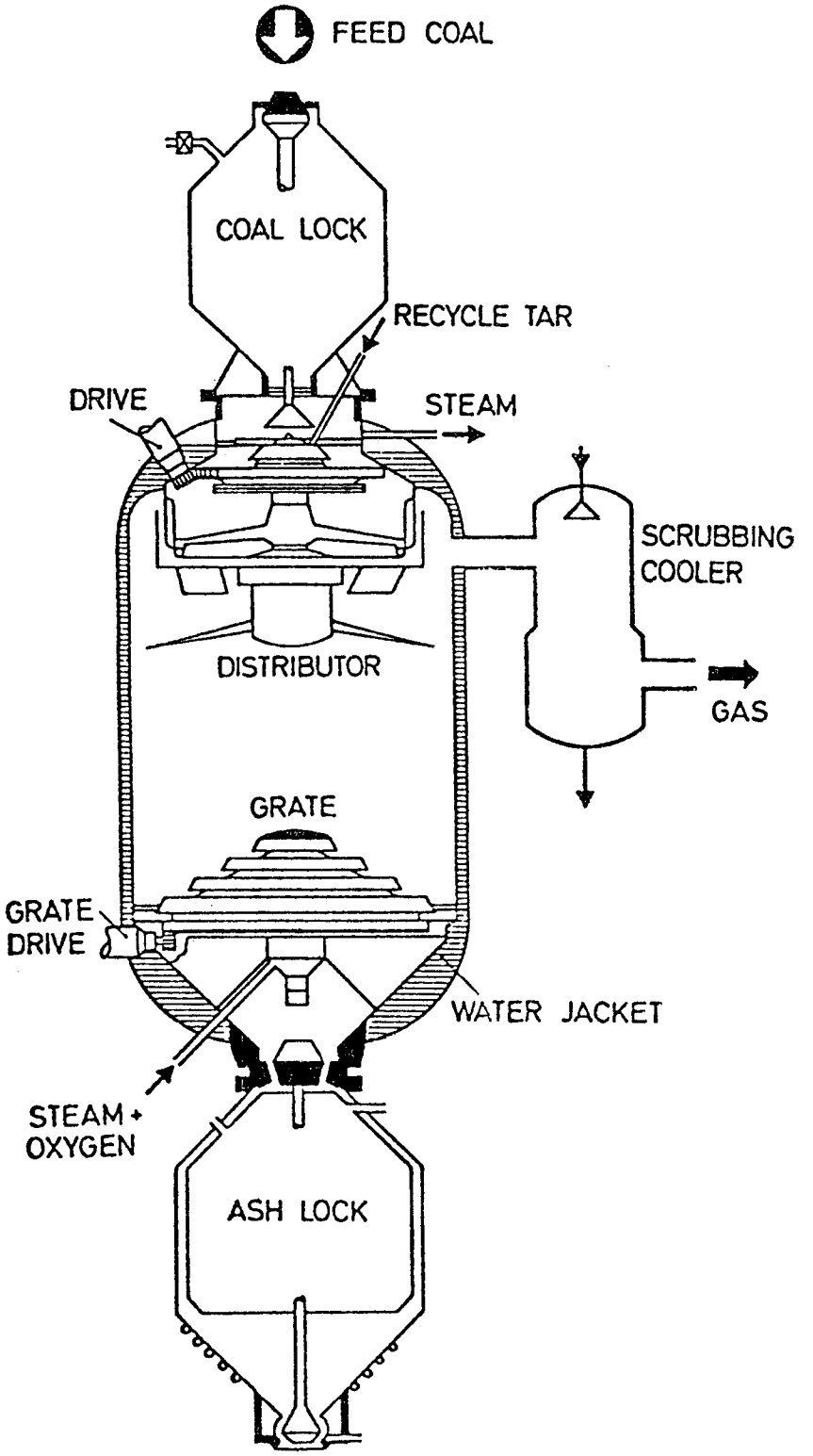


Figure 6 Lurgi pressure gasifier

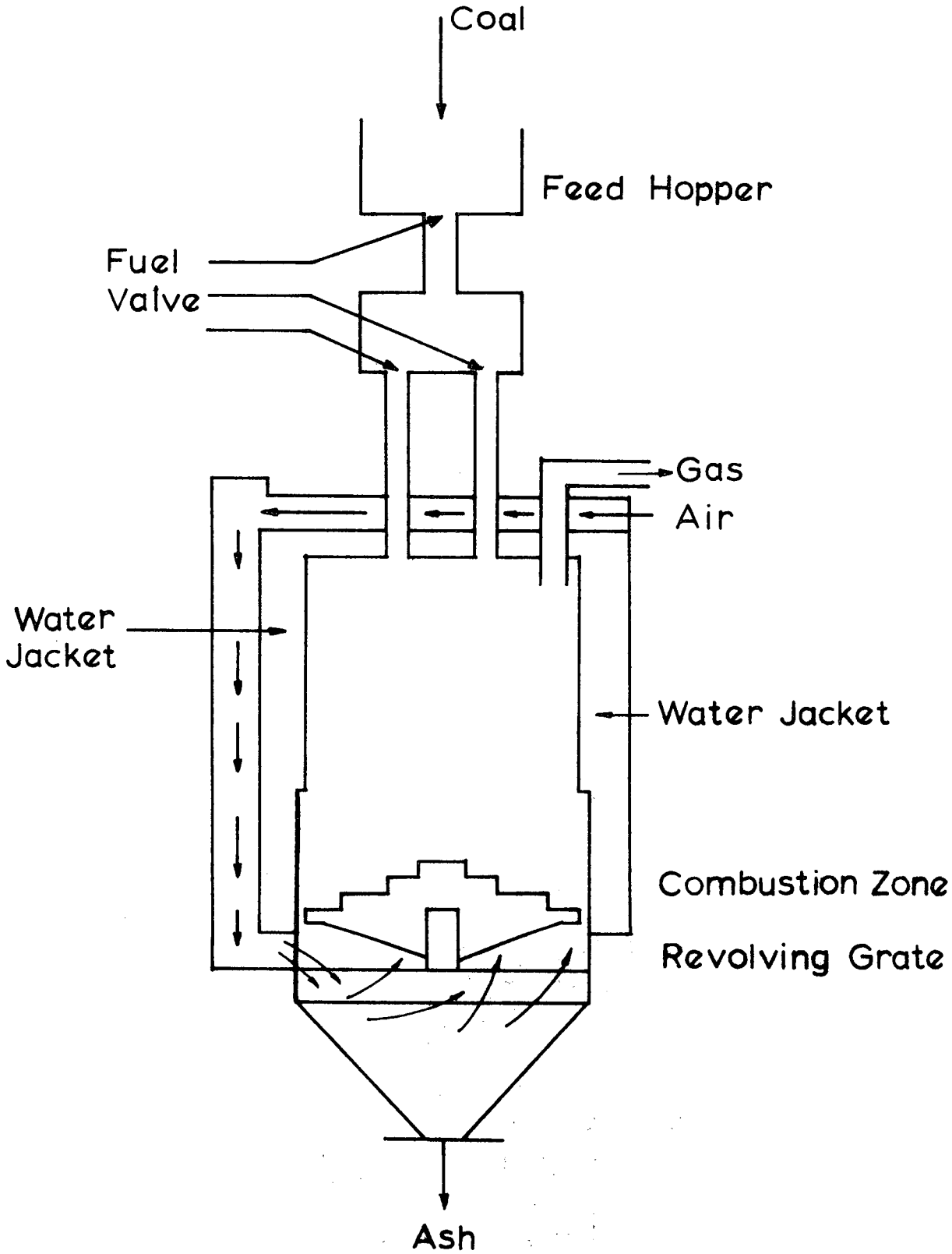


Figure 7 Wellman-Galusha gasifier

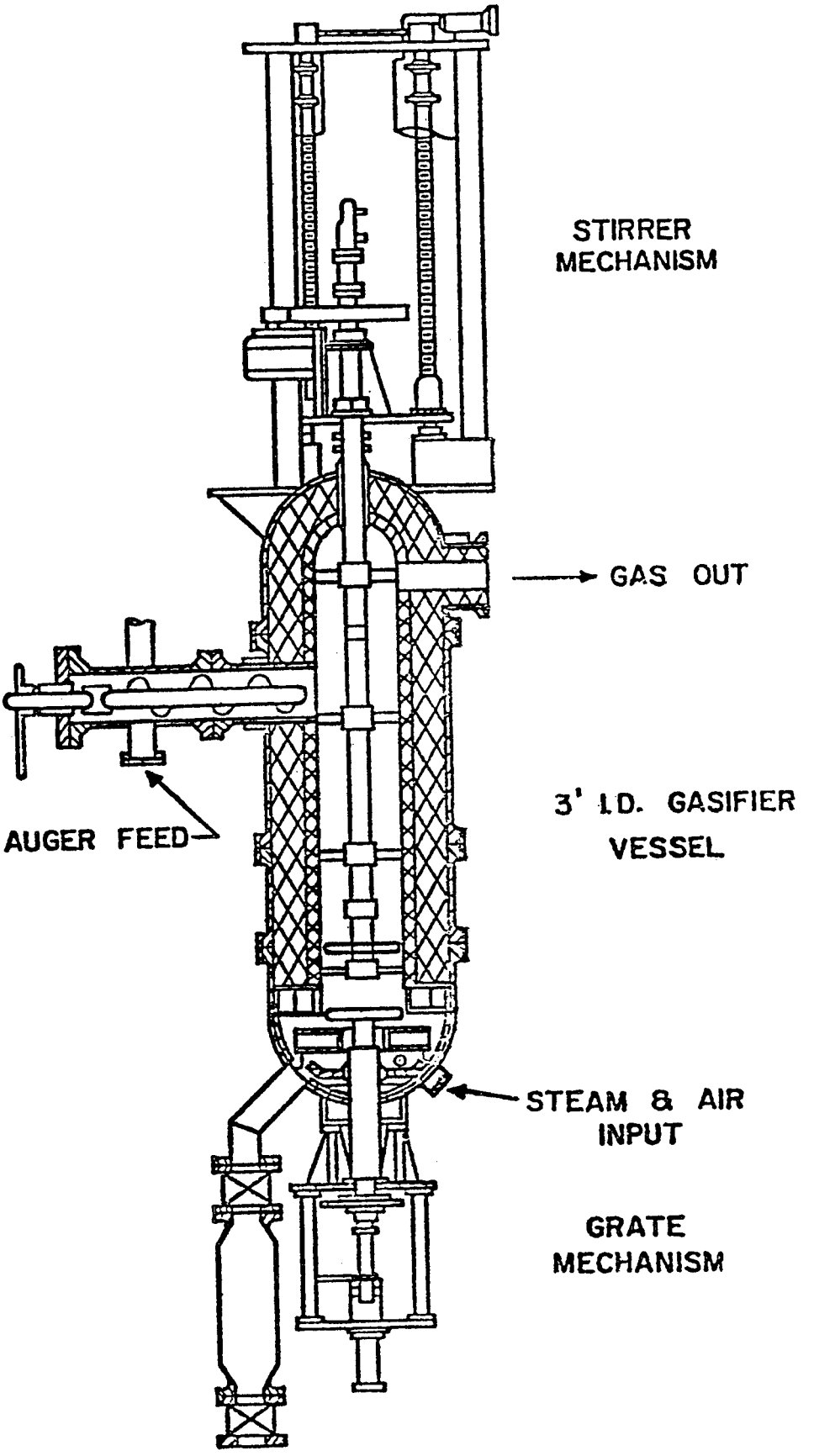


Figure 8 General Electric GEGAS-D gasifier

rate of 1000 lb/hr. The gasifier is well insulated to operate at low air to coal and steam to coal ratios. General Electric is also developing a proprietary extrusion process to feed coal directly into the gasifier at high pressures. Tar is used as a binding material for coal fines. The final product obtained has a heating value of about 160 BTU/SCF.

1.3.4 Comparison

In Table 1, characteristics of the various gasifiers are listed for relative comparison. As previously stated, Lurgi gasifiers have been used commercially for non-caking coals only, but recently tests were performed at Westfield[6] to gasify American coals with steam and oxygen. Wellman-Galusha gasifiers are well suited for industries with samll fuel requirements, such as space heating, steam generation, et., because of the small gasifying capacity. Wellman-Galusha gasifiers are operated at atmospheric pressure, requiring the compression of the product gas if the product gas is to be used for power generation.

The General Electric Company's GEGAS-D gasifier is essentially the same as MERC's gasifier except for the difference in the coal feeding system. Results of the tests performed so far show that the GEGAS-D gasifier's air requirement seems lower and thermal efficiency seems higher compared to the MERC gasifier. The main reason is the small heat loss in the GEGAS-D gasifier due to the heavy insulation of the gasifier. Heat loss in MERC's pilot gasifier is about 10-13% of the total heat input as compared to 3-4% loss in the GEGAS-D

TABLE 1

PERFORMANCE CHARACTERISTICS OF MOVING BED GASIFIERS

Gasifier	Lurgi[6,25]		Wellman-Galusha[15]		GEGAS-D[26]	MERC[13,14,17,18]
Diameter, ft	12	10(O.D)		10	3	3.5
Height, ft	N.A.	N.A.		9	N.A.	6.5
Gasifying capacity, lb/hr ft^2		100-400		7.5-99	200.	100-200
Pressure, psig	300-450	350.		atmospheric	200-300	15-225
Type of coal		Pittsburgh #8		Anthracite	Pittsburgh #8	Arkwright Bituminous
Coal composition						
C	57.12	74.46	N.A.	73.66	67.42	75.92
H	3.93	5.1		2.25	4.98	5.70
O	8.27	4.36		6.93	7.39	4.92
N	0.83	1.43		0.66	1.35	1.38
S	4.45	2.30		0.56	3.82	2.71
Ash	13.3	7.50		9.55	15.02	8.25
Moisture	12.1	4.75		6.4	2.53	1.12
Air/coal, lb/lb		—	3.4	—	2.63	2.5-3.67
Oxygen/coal lb/lb	—	0.61	—	0.77	—	—
Steam lb/lb		3.10	0.4	1.4	0.45	0.5-0.74
Gas Composition						
CO	14.54	17.9	26.	40.0	25.8	16.-23.
CO_2	16.22	30.8	4.5	16.5	6.7	7.-12.
N_2	42.85	2.4	52.0	1.5	49.2	48.-55.
H_2	22.36	38.8	13.0	41.0	17.0	13.-17.
CH_4	3.88	8.4	3.0	0.9	3.2	2.- 3.5
C_2H_6	—	0.7	—	—	—	0.3
C_2H_4	—	0.3	—	—	—	—
H_2S	—	0.7	0.5	—	—	0.3-0.6
O_2	—	—	—	—	—	0.1
H.V. of Gas BTU/SCF	158.	283.		270.	160.	100.-180.
Steam Decomposition %		21.1	N.A.	N.A.	54	30-70%
Thermal Efficiency	N.A.	77.0			74	65 -75%
Heat Loss; (% of heating value of coal)					≈ 4	10 -17%

gasifier[26]. However, if the MERC's gasifier is scaled-up to the commercial size, this heat loss will be expected to reduce considerably. Further test results from the GEGAS-D gasifier will have to be examined prior to making any quantitative comparison.

The model developed for MERC's gasifier in this report can be used, with minor modifications, to predict the performances of the Lurgi and GEGAS-D gasifiers.

2. THEORY

2.1 REACTIONS IN A FIXED BED GASIFIER:

In a fixed bed gasifier, air (or oxygen) and steam are introduced below the grate and travel upward in the dirction opposite to that of the coal flow. Sensible heat of ash is used to preheat the air (or oxygen) and the steam feeds. Coal moving downward is successively dried, devolatilized, gasified and burned as the temperature increases in the gasifier. The gasifier can be divided roughly into three main zones:

(1) Combustion Zone

(2) Gasification Zone

(3) Devolatilization and Drying Zone

In the combustion zone, directly above the ash zone, the following reactions take place:

$$C^* + 1/2\ O_2 \rightarrow CO$$

$$C^* + O_2 \rightarrow CO_2$$

$$CO + 1/2\ O_2 \rightarrow CO_2$$

$$H_2 + 1/2\ O_2 \rightarrow H_2O$$

C* in above reactions refers to carbon present in char rather than in its pure form.

The combustion zone is relatively narrow and part of the heat generated is absorbed by the endothermic reactions.

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

$$C^* + CO_2 \rightarrow 2\ CO$$

The combustion gas flows upward into the gasification zone where further endothermic reations occur along with the water - gas shift reaction.

$$CO + H_2O \rightleftarrows CO_2 + H_2$$

Depending upon the hydrogren pressure, methane is produced by the hydrogasification reaction.

$$C^* + 2H_2 \rightarrow CH_4$$

The gases then flow upward into the devolatilization zone near the top of the bed where coal is devolatilized. Tar, higher hydrocarbons, CO, CO_2, CH_4 and H_2 are produced in this zone. Coal, prior to devolatilization, is dried and heated by the hot gases leaving the gasifier. The zones and the temperature profile is shown in Figure 9. Reactions taking place in each of the above zones are presented in Figure 10.

2.2. KINETICS

Major solid gas reactions involved in coal gasification are pyrolysis, char-hydrogen, char-carbon dioxide, char-steam and char-oxygen reaction. Pyrolysis of coal which releases the moisture and volatile matter in coal, is usually the first to occur and the fastest among these reactions. In addition to the major chemical changes, there is a substantial change in the physical characteristics of the solid during the rapid stage of pyrolysis. The yields of volatiles and its composition are dependent not only on the volatile matter content of coals but also on the temperature level and rate of heating during pyrolysis. The char-hydrogen reaction becomes important only at high pressures. Char-hydrogen, char-carbon dioxide and char-steam reactions are usually much slower and these reactions can take place with considerable gas penetration within the pores of the particles. Volumetric reaction models are, therefore, a proper representation of these reaction systems. The char-oxygen reaction is rapid and takes place at the external surface of the char particles. The rate is controlled by gas film diffusion and/or ash layer diffusion. Unreacted core shrinking model can be applied to the analysis of this reaction. The kinetics of

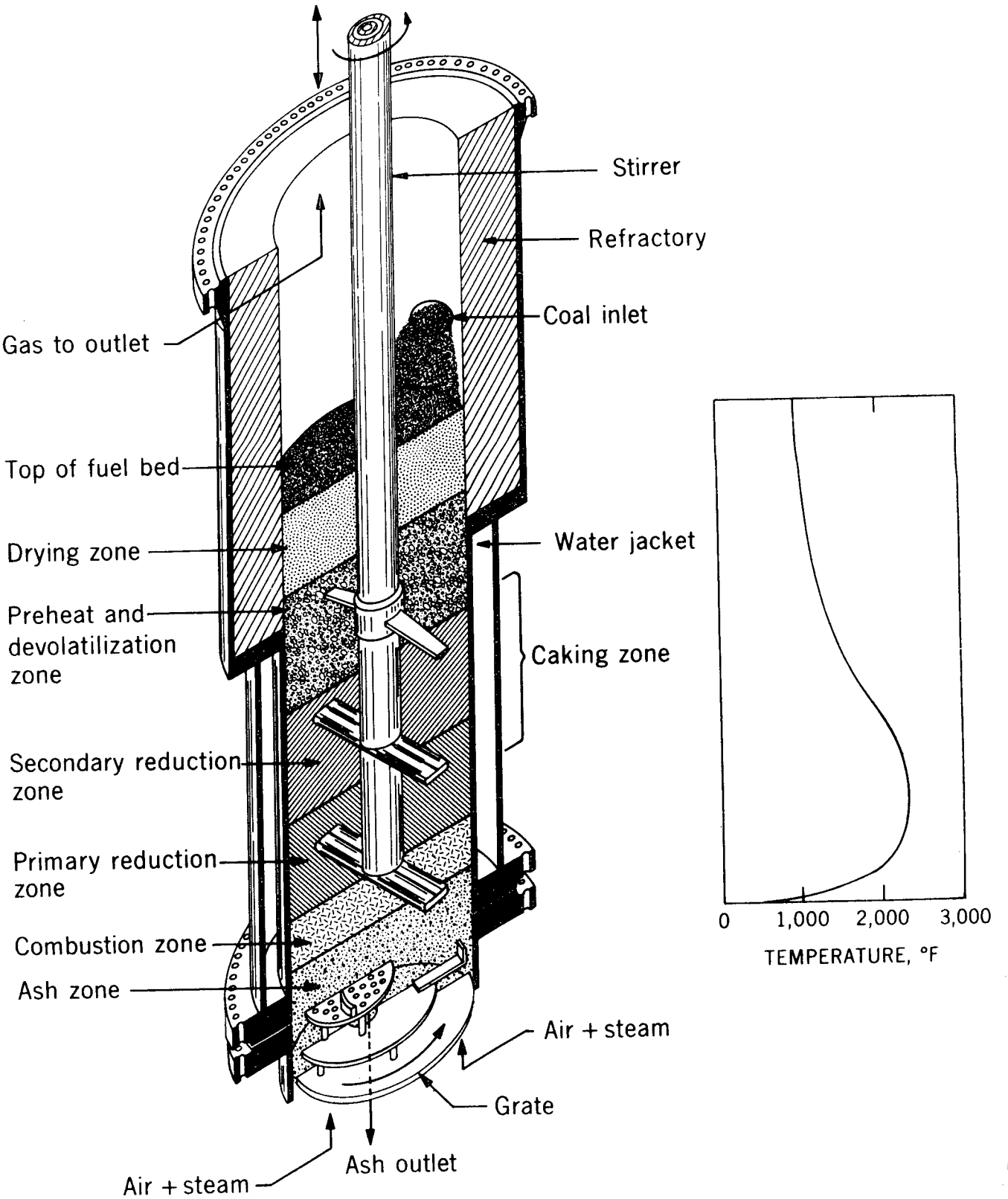


FIGURE 9 - MERC Gasifier Showing Zones and Temperature Profile.

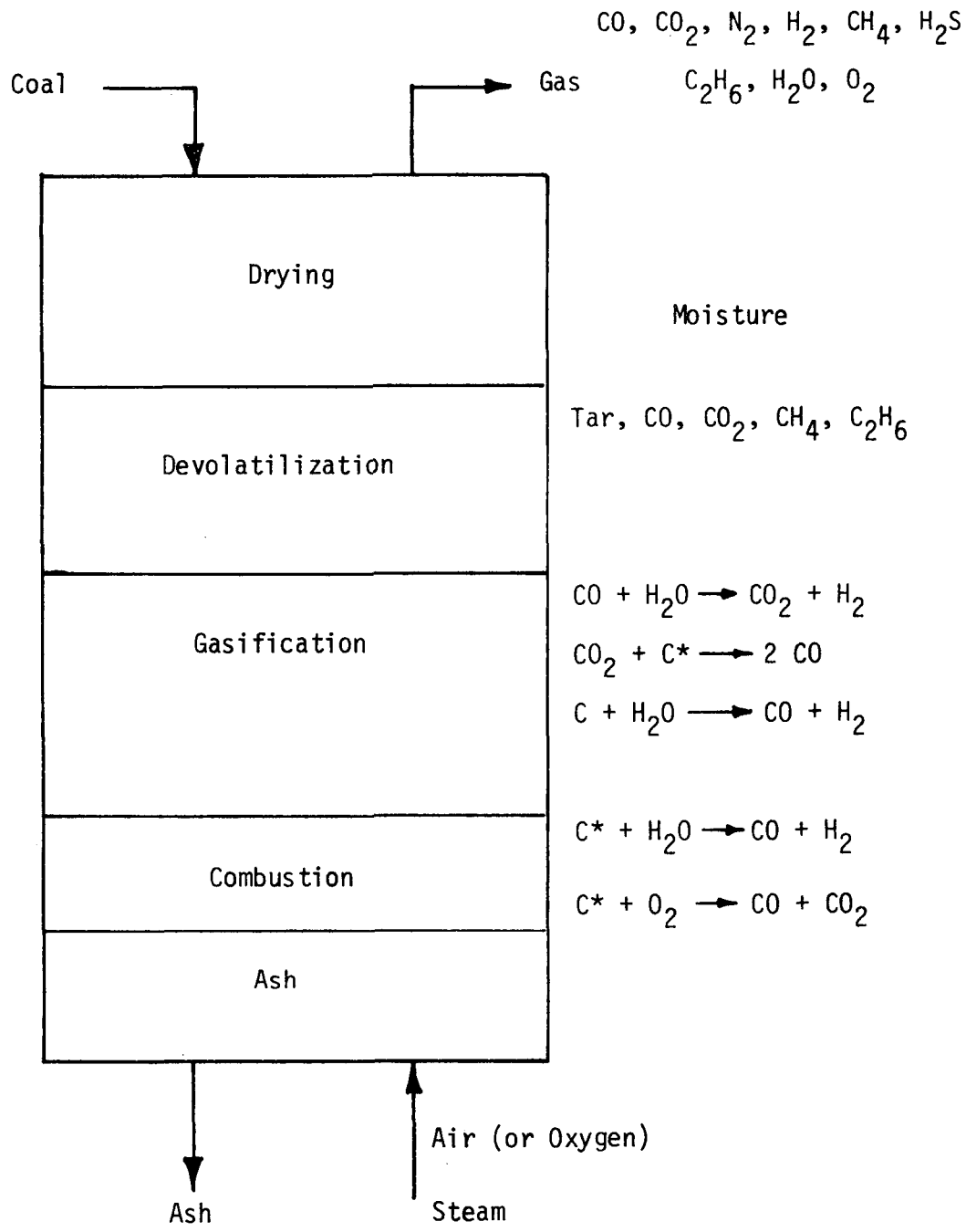


Fig. 10. Chemical Reactions Occurring in a Fixed Bed Gasifier

these reactions will be considered in more detail following the discussion on the reactivity of coal.

2.2.1. REACTIVITY OF COAL

Most commonly, coal is classified into peat, lignite, sub-bituminous, bituminous and anthracite. Lurgi uses a modified method to determine the reactivity of coal (19). In this method, CO_2 is passed through a fixed bed of char produced by carbonization of coal under pressure. This simulated gasification is carried out under pressure and at 1470 °F in a small reactor. The reactivity of coal is estimated by measuring the amount of CO produced as a result of CO_2 decomposition. In Figure 11, reactivity of coal is plotted against the heating value of coal (6). This figure clearly shows that lignite and sub-bituminous coals are more reactive than bituminous coal. High reactivity coals will react at lower temperatures as compared to low reactivity coals. For example, the lowest reaction temperatures at which the reaction rates approaches zero are shown for different coals in the following:

Lignite	1200 °F (approximately)
Sub-bituminous	1350 °F
Semi-anthracite	1450 °F
Coke	1550 °F

Reactivity of a given coal not only depends on its rank, but also on its oxygen content and the composition of mineral matter. It has been demonstrated that a number of inorganic elements present in ash act as catalysts for coal gasification reactions. For example, Ca and Fe are catalysts for the char-carbon dioxide, and char-steam reactions.[23]

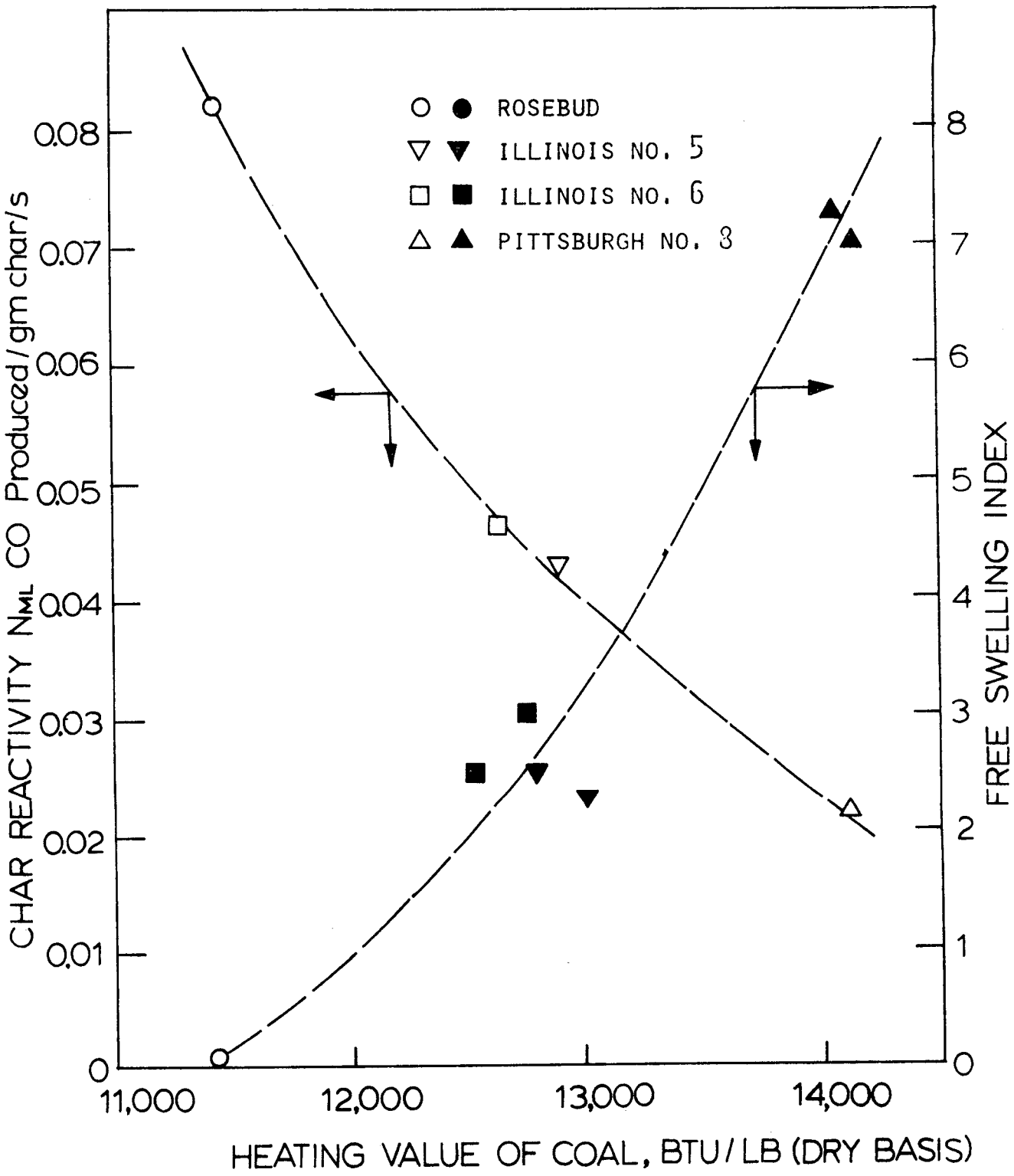


Figure 11 Reactivity vs. type of coal in a Lurgi gasifier (6)

2.2.2. DEVOLATILIZATION:

Devolatilization or pyrolysis of coal is defined as a process by which coal is thermally decomposed into char, gas and liquid products. When coal is heated, most of the uncombined water is driven off below 105 °C. Remaining water (moisture) is removed when the temperature reaches around 300 °C. As the temperature increases, coal particles soften to form a metaplastic then depolymerizes to yield the primary volatile products and semi-coke. These products further decompose to form secondary and tertiary volatiles and coke. The suggested mechanism for pyrolysis is as shown in Figure 12 (23). Devolatilization is a complex phenomena not yet completely understood. Excellent literature reviews can be found in reports by Anthony and Howard (1) and by Dutta and Wen (23).

The composition of products depends on the type of coal, heating rate, residence time of vapor and a host of other factors.

In a fixed bed gasifier, coal is heated slowly (<100 ° C/sec) and hence, the time required for almost complete devolatilization is significantly less than the time required for heating the particles to the final temperature. Therefore, in fixed bed gasifiers, the ultimate yields and the quality of volatiles and chars, rather than the rate of pyrolysis, are important. Figure 13 shows a few typical volatile yields versus temperature curves as observed in the Fischer-Assay of some coal samples. The curves in this figure are calculated based on the equation of Gregory and Littlejohn (1965) shown below (10):

$$V = VM - R - W$$

$$R = 10^{(11.47 - 3.961 \log_{10} T + 0.005\ VM)}$$

$$W = 0.2\ (VM - 10.9)$$

where,

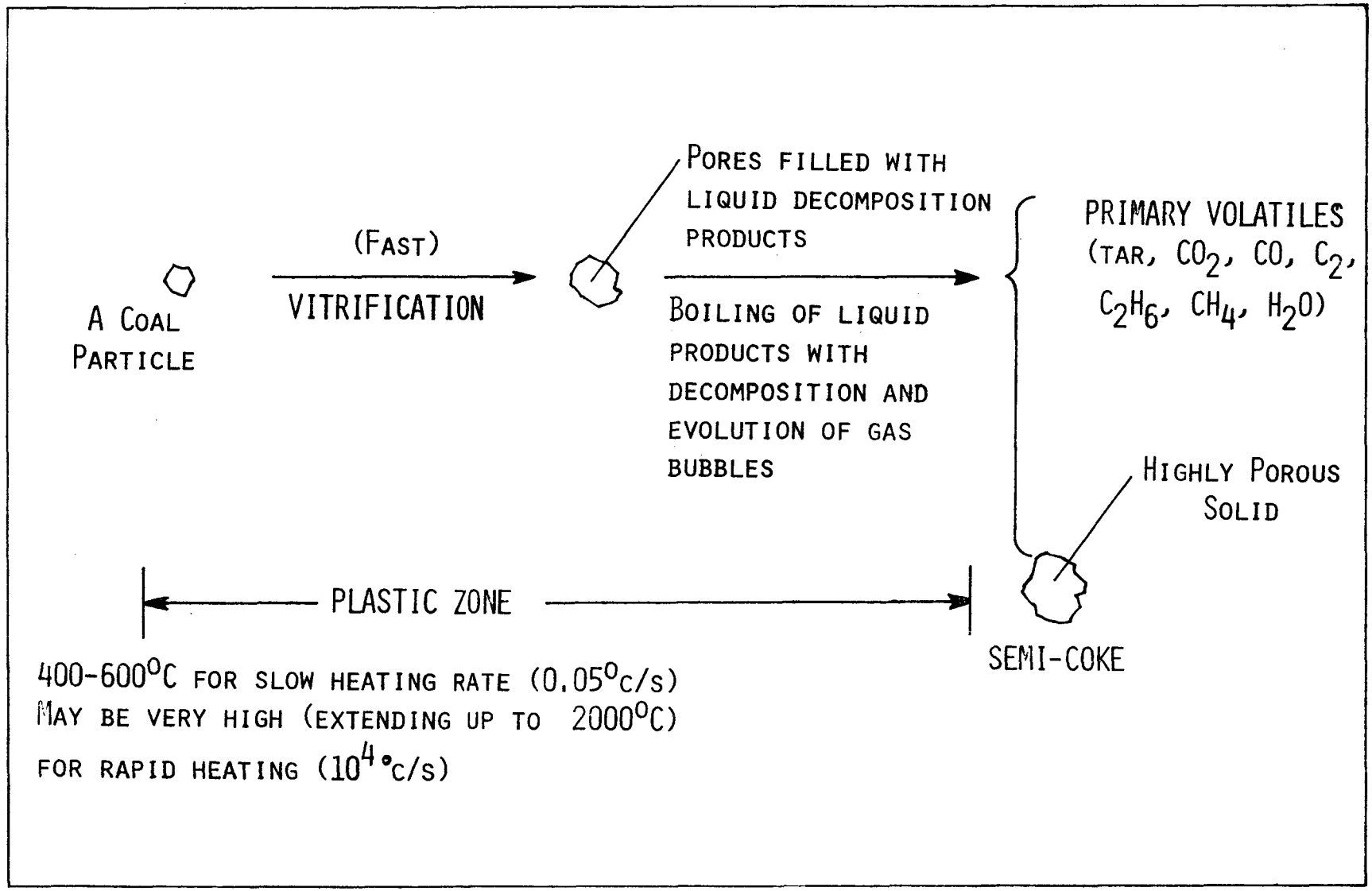


Figure 12 The suggested mechanism for pyrolysis of a single swelling coal particle [23]

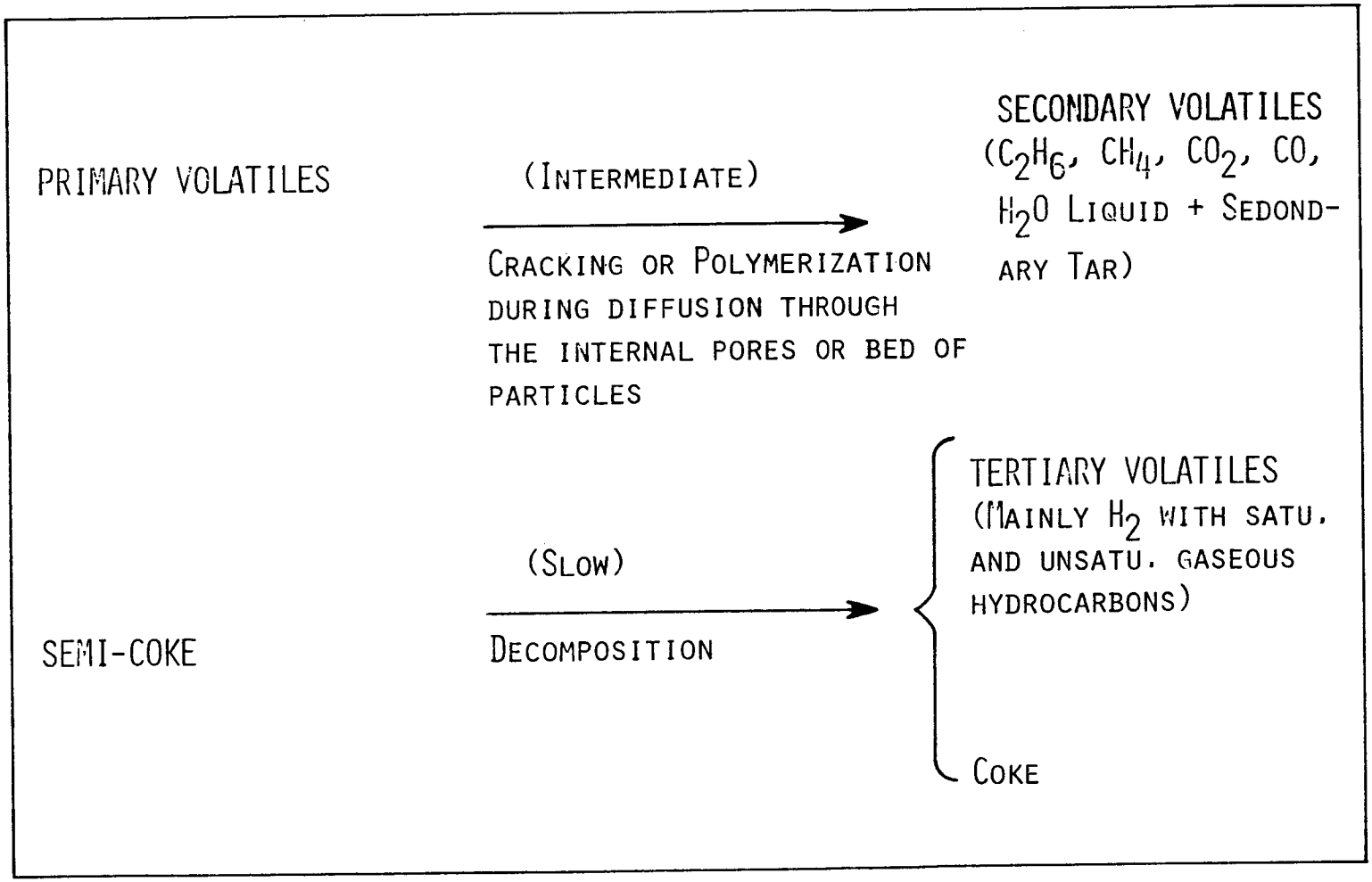


Figure 12 Continued

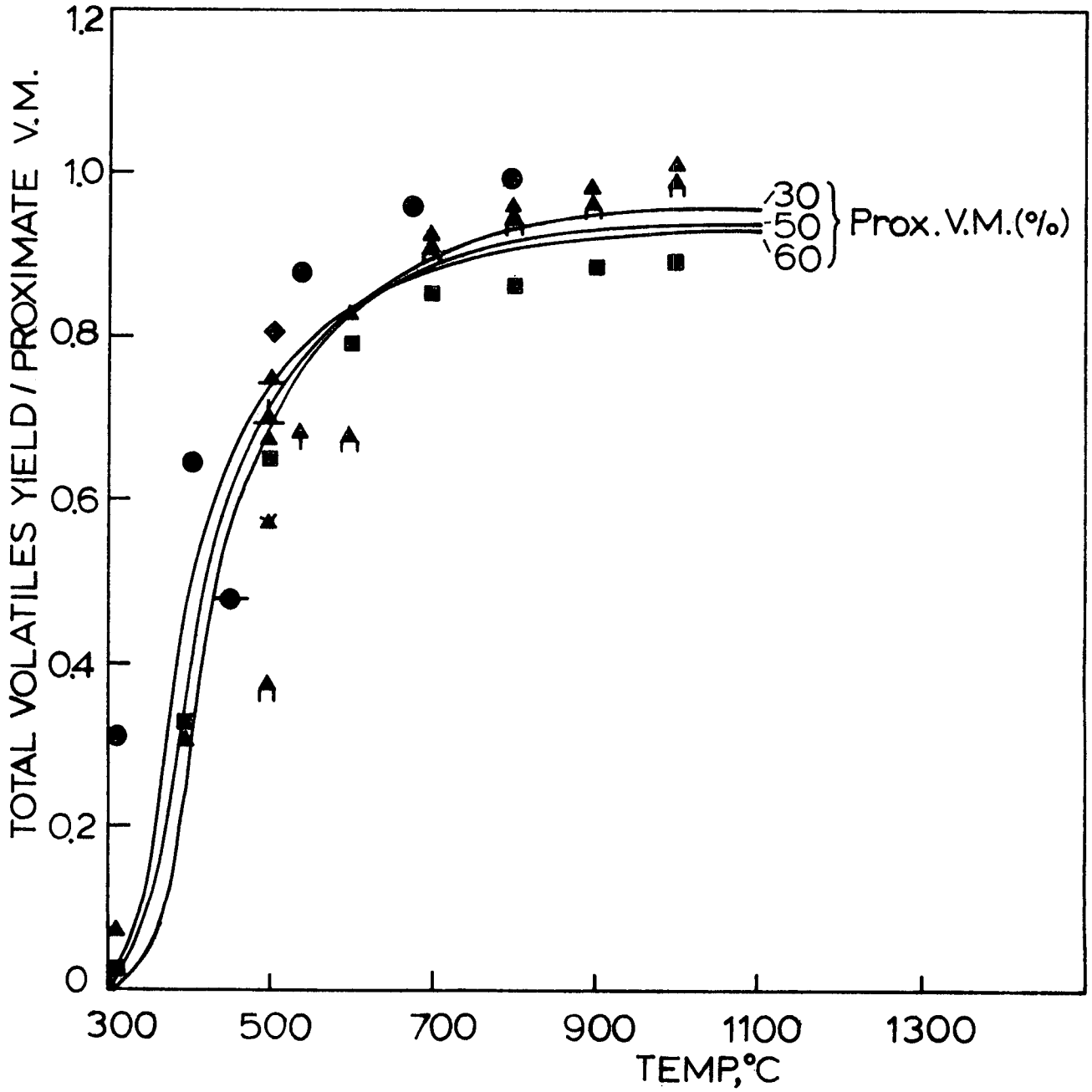


Figure 13 Volatile yield versus temperature

WM = volatile matter, maf %

T = temperature in °C

V = yield of total volatiles, % maf coal

The above equation can be used to predict the total volatile yield. However, estimation of volatile product composition is difficult. For a few coals, the composition of pyrolysis products as a function of temperature is shown in Figure 14. However, the small amount of experimental data available could not be used since the data were obtained under varied conditions.[23] A simplified method was developed to roughly estimate the composition of devolatilization products and is presented in the Appendix.

2.2.3. CHAR-STEAM REACTION:

The char-steam reaction is rather slow when compared to other reactions occurring in a gasifier. This endothermic reaction, along with the char-carbon dioxide reaction, controls the maximum temperature. Therefore, the kinetics of this reaction is very important. Unfortunately, available data for this reaction widely differ as shown in Figure 15.

Most of the earlier investigators used Langmuir-type adsorption equations to express the rate of this reaction. For example, the following mechanism and rate expression was proposed by Walker et al (1959).

$$C_f + H_2O\ (g) \underset{k_g}{\overset{k_8}{\rightleftarrows}} H_2\ (g) + C\ (0)$$

$$C\ (0) \xrightarrow{k_{10}} CO\ (g)$$

$$\text{Rate} = \frac{k_8\ (H_2O)}{1 + k_8/k_{10}\ (H_2O) + \frac{k_g}{k_{10}}\ (H_2)}$$

However, this type of expression requires the knowledge of at least three parameters to include the effect of temperature on the rate.

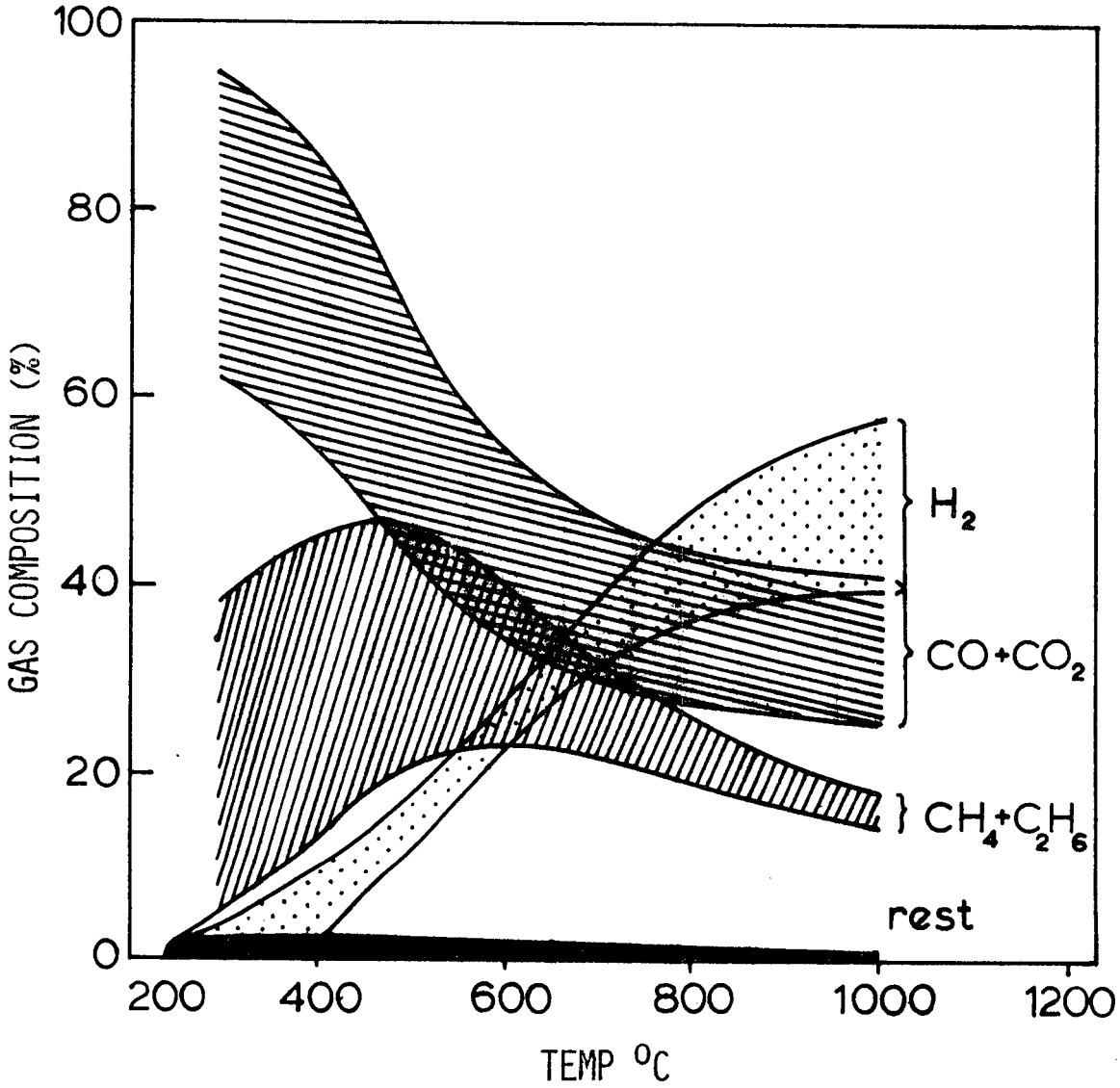


FIGURE 14 Gas composition as a function of temperature in slow pyrolysis

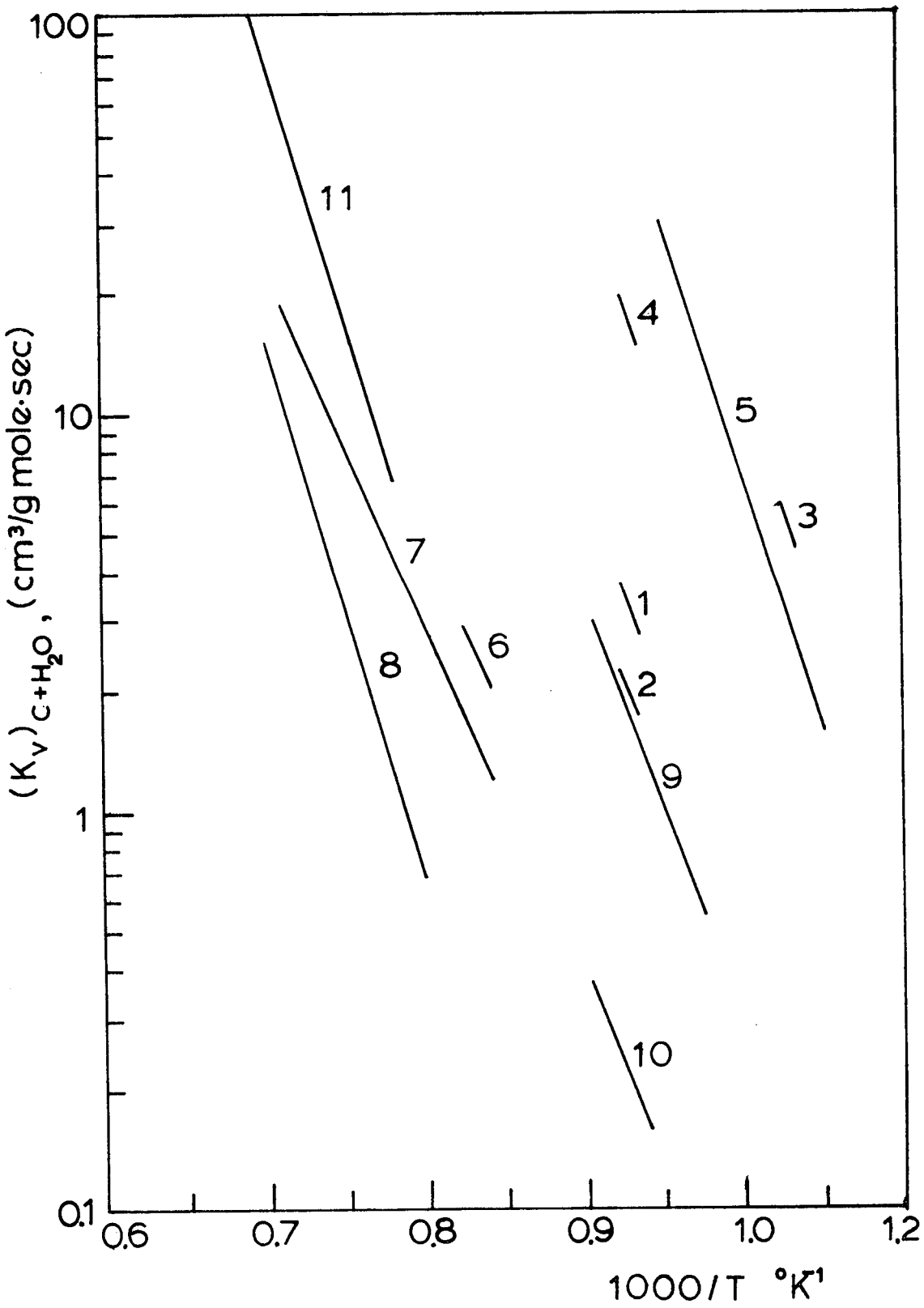


Figure 15 Arrhenius plots for various forms of carbon coal and char in carbon-steam or char-steam reaction (see legend on page 31).

LEGEND TO FIGURE 15

Line	Investigators (Year)	Material	Total Pressure (Atms.)
1, 2	Jolly & Pohl (1953)	Coke	1.0
3, 4	Gadsby et al (1946)	Nut char coal char	1.0
5	Long & Sykes (1948)	Coconut shell charcoal	0.2~1.0
6	Feldkirchner & Linden (1963)	Low temperature bituminous coal char	104
7	Feldkirchner & Huebler (1965)	Low temperature bituminous coal char	70
8	Johnstone et al (1952)	Cylindrical porous graphite rod	1.0
9, 10	Blackwood & McGrory (1958)	Coconut carbon	1.~50.
11	Johnson (1974)	Air-pretreated HVab Pittsburgh No. 8	35.0
12	Jensen (1975)	Coal minerals from Kentucky No. 9 coal	1.0

In this report, a simple rate expression proposed by Wen is used (24):

$$\frac{dx}{dt} = K_v \left(C_{H_2O} - C_{H_2} C_{CO} RT/k_{eq}\right) (1-x)$$

where,

K_{eq} is the equilibrium constant of the reaction,

C's denote the concentration of H_2O, H_2 and CO respectively,

K_v is the rate constant per unit volume.

In Figure 15, values of K_v for various forms of chars are plotted against temperatures. Identification of the different curves is provided on the preceeding page.

2.2.4. CHAR-CARBON DIOXIDE REACTION

The char-carbon dioxide reaction is a relatively slow reaction and is similar to the char-steam reaction. At lower temperatures and for smaller particles, this reaction is controlled by the chemical reaction rate and occurs nearly uniformly throughout the interior surfaces of the char particles. The reaction rate can be expressed as follows (5):

$$\frac{dx}{dt} = a K' C_A^{\eta}(1 - x)$$

$$a = \frac{\text{available pore surface area per unit weight at any stage of conversion}}{\text{initial available pore surface area per unit weight}}$$

C_A = concentration of CO_2

$0 < \eta < 1$, η is order of the reaction with respect to CO_2 concentration.

The rate of the char-carbon dioxide reaction, with respect to CO_2 concentration, is first order up to atmospheric pressure but approaches zeroth - order at high pressure (pressures above 15 atmospheres).

In the model developed, it was assumed that a = 1, η = 1 and $K' = 2. \times 10^{12} \exp\left(^{-59000}/_{RT_s}\right)$

In Figure 16, $(\frac{dx_c}{dt})$ at $x_c = 0.2$ is plotted versus reciprocal of temperature (23). The Legends used are explained on page 35 . The value of K' determined from Figure 16, is applicable only when the chemical reaction controls the rate. At high temperatures, however, diffusion resistance within the particle may become appreciable and, therefore, an effectiveness factor which takes into account the effective diffusivity must be used for such cases.

Then, the rate of gasification is expressed as:

$$\frac{dx}{dt} = \eta \, a \, K' \, C_A \, (1 - x)$$

where, η is the effectiveness factor.

2.2.5. WATER - GAS SHIFT REACTION:

Various rate expressions for the water-gas shift reaction have been proposed. For example, the following correlation for catalytic reaction was developed by Moe (24)

$$\text{Rate} = K \, (P_{CO} P_{H_2O} - P_{CO_2} P_{H_2} / K_{wg})$$

where, P_{CO}, P_{H_2O}, P_{CO} , P_{H_2} are the partial pressures of carbon-monoxide, steam, carbon dioxide and hydrogen respectively. K_{wg} is the equilibrium constant for the shift reaction.

K, based upon the measurement of commercial iron catalyst, is expressed as

$$K = \Theta \, 3.586 \, 10^5 \exp \left(^{-4895}/_{T}\right)$$

where, Θ is used as a factor representing the activity of ash relative to the commercial catalyst (21). In this study, the value of 0.00005 was used for Θ.

2.2.6. CHAR-OXYGEN REACTION:

The burning of char is the fastest among the char gas reactions taking place in a gasifier.

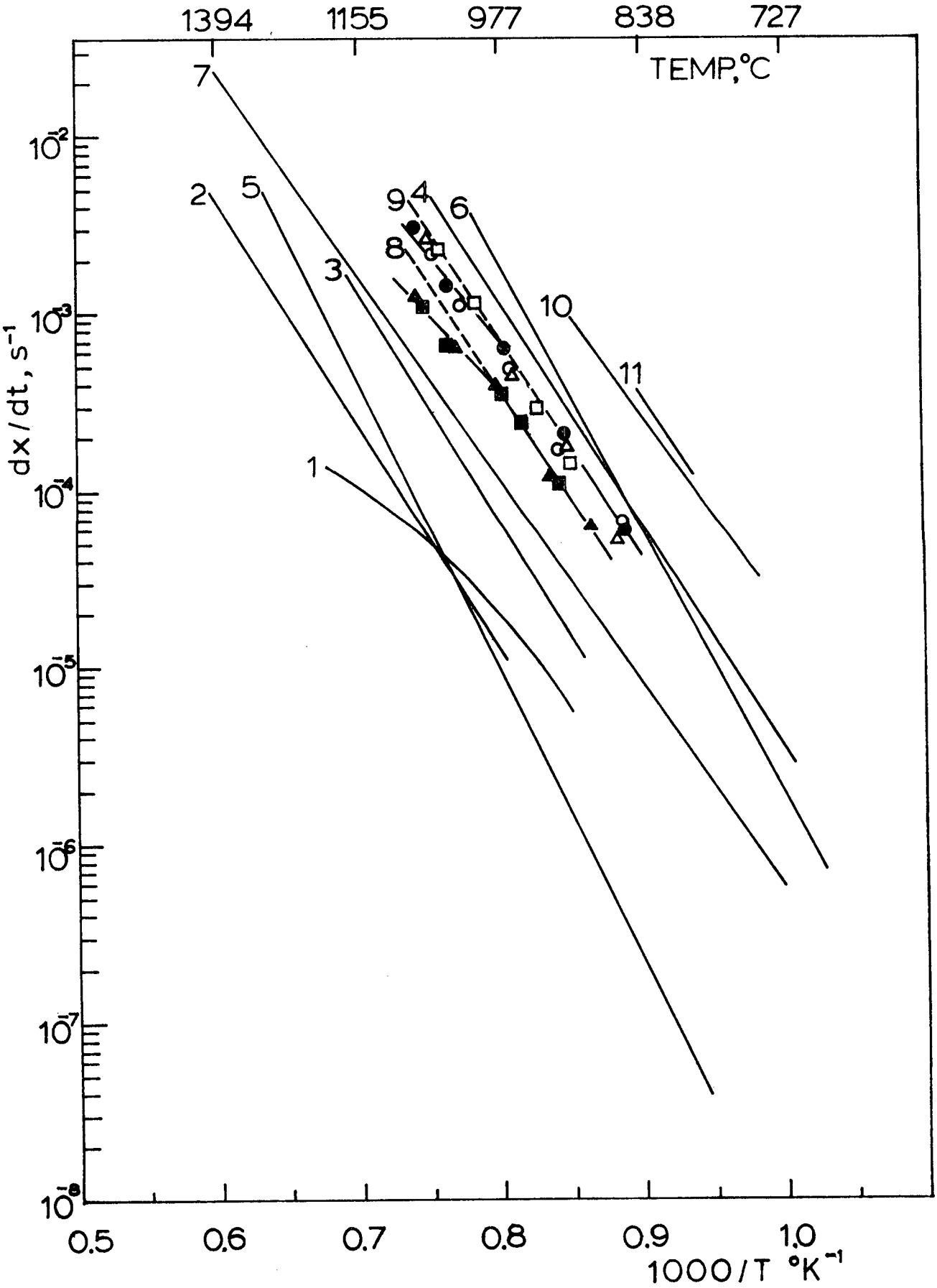


Figure 16 Arrhenius plots for the gasification of various forms of carbon in CO_2 (see legend on page 35)

LEGEND TO FIGURE 16

Line No.	Investigators	Year	Type, Size and Shape of Carbon	Remarks
1	Yoshida and Kunii	(1969)	Graphite Sphere, 1.5 cm. dia.	Initial Rates
2	Ergun	(1956)	Ceylon Graphite, -10+200 mesh	Initial Rate in a fluidized bed.
3	-do-		Activated Graphite, -10+200 mesh	-do-
4	-do-		Activated Carbon, -10+200 mesh	-do-
5	Turkdogan and Vinters	(1969)	Electrode Graphite Particles, -10+40 mesh	Initial Rates
6	-do-		Coconut charcoal particles, -10+40 mesh	Initial Rates
7	Austin and Walker	(1963)	Graphitized Carbon cylinder, 5.1 cm. long and 1.27 cm. dia.	Calculated initial Rates
8 & 9	Dutta et al	(1977)	o - Illinois Coal #6 ● - Synthane Char #122 Δ - Hydrane Char #49 □ - IGT Char #HT155 ▲ - Hydrane Char #150 χ - Pittsburgh HVab Coal All of size -35+60 mesh	Rates at 20% conversion level
10	Fuchs and Yavorsky	(1975)	Hydrane Char from Pittsburgh Coal, -60+100 mesh	Average Rate in a fluidized bed at 16-32 atm. partial pressure of CO_2 with He as diluent
11	-do-		Synthane Char from Illinois Coal #6, -60+100 mesh	Average Rate in a fluidized bed at 32 atm. partial pressure of CO_2 with He as diluent.

$$C^* + a\ O_2 \rightarrow (2 - 2a)\ CO + (-1 + 2a)\ CO_2$$

The stoichiometric coefficient "a" in the char-oxygen reaction shown above depends on the temperature as well as the type of coal. It has been shown that when the temperature is low, the coefficient "a" is approximately unity and carbon dioxide is the prominent product. On the other hand, "a" decreases to 0.5 at high temperatures and carbon monoxide is mostly produced. One such equation correlating the ratio of CO/CO_2 to the temperature is shown below (2).

$$CO/_{CO_2} = 10^{3.4}\ e^{-12400/RT}$$

where T is in °K

In most cases, this reaction takes place at the external surface of the char particles and is controlled by ash layer diffusion. However, if the temperature and/or the particle size increases, the reaction may proceed towards the gas film diffusion control regime.

For such conditions, the char-oxygen reaction rate developed by Field et al (7) can be used

$$\frac{dx}{dt} = \frac{P_{O_2}}{(1/K_s + 1/K_{diff})}$$

where $\frac{dx}{dt}$ = rate per unit area of external particle surface

P_{O_2} = partial pressure of oxygen in free stream

K_{diff} = diffusional reaction rate coefficient

K_s = surface reaction rate coefficient

The diffusional reaction rate coefficient can be approximately calculated by using following formula (7).

$$K_{diff} = \frac{0.292\ \phi\ D}{d_p\ T_m}$$

T_m is the average of particle surface temperature and gas temperature in °K.

d_p = particle diameter in cms

D = diffusion coefficient of oxygen

$$= 4.26 \left(\frac{T_g}{1800}\right)^{1.75} 1/P \quad cm^2/sec$$

P = total pressure in atmospheres

where ϕ is the mechanism factor and takes a value of 2 when CO is the direct product of char-oxygen reaction and a value of 1 when CO_2 is the direct product. Several investigations were made to determine the value of ϕ as a function of temperature, particle size and carbon type. No quantitative conclusions can be drawn from these studies. However, value of 1.0 for ϕ is suggested if the particle diameter is greater than 0.1 cm.

The surface reaction coefficient, K_s, can be calculated from the following equation (7):

$$K_s = K_{so} \exp(-E/R\,T_s)$$

The value of K_{so} varies with the type of coal or carbon. An approximate value for K_{so} is 8710. gm/cm^2 sec atm. cal/gmole. The value of 35.7 Kcal/gmole for the activation energy was reported by Field et al (7).

Recently, an activation energy of 27 Kcal/mole was reported by Seargent and Smith (20) for particle sizes ranging from 0.18 to 0.7 cm for bituminous coal. In this model, this value of activation energy was used for char-oxygen reaction.

In the combustion zone of the moving bed gasifier, char-oxygen reaction, char-steam and char-carbon dioxide reactions are taking place simultaneously. In other words, char-oxygen reaction would take place on the outside surface of the particle reducing the diameter of the unreacted core and at the same time steam and carbon dioxide will penetrate into the particle also reducing the concentration of carbon.

Thus, analysis of char particle in the combustion zone is complex. The particle size in the combustion zone depends on the initial size of the coal feed. In one of MERC's gasifiers, the major fraction of the feed was 3/4" (1.9 cm) in size. In this model, rates were calculated by assuming that the average diameter of the particle is about 0.5 cm in the combustion zone. This assumption, though not valid, simplifies the calculations. The rates of solid gas reactions described above are compared with each other in Figure 17 . Symbols are explained on the page following this figure.

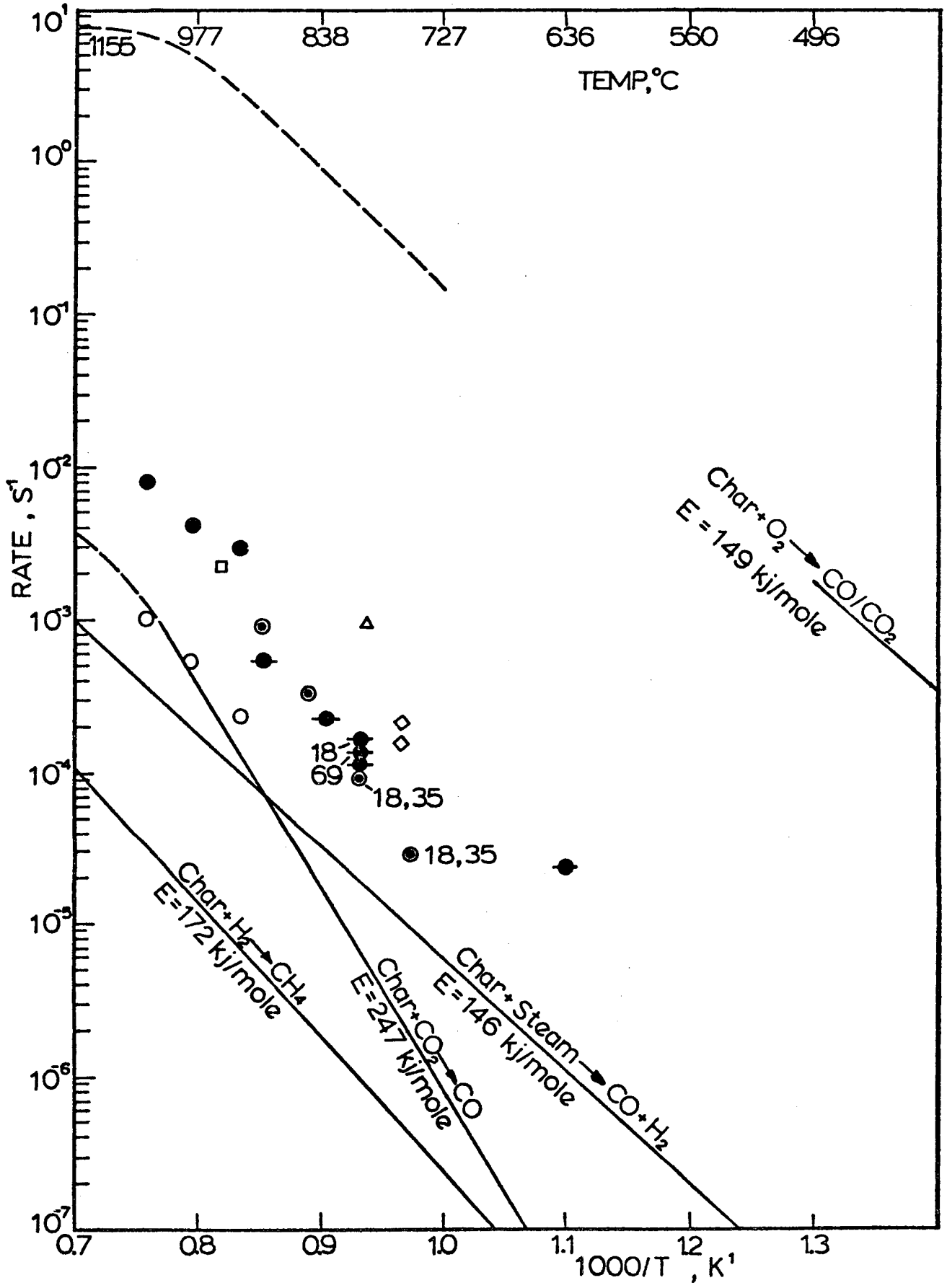


Figure 17 Comparison of char-gas reaction rates

LEGEND TO FIG. 17

Sample for the Arrhenius Lines (atmospheric pressure): Pittsburgh HVab Coal (40.0)

Data points are for initial rates (unless otherwise mentioned) at super-atmospheric pressures. The numbers on points indicate pressures in atm.

○ △ □ ⬡ : Char-H_2 Reaction

● : Char-H_2O Reaction

◉ : Char-CO_2 Reaction

◉ Illinois #6 Coal (32.8), Overall rates at 35 atm. (unless otherwise indicated); Fuchs and Yavorsky (1975).

○ ● Pittsburgh HVab Coal (40.0), 35 atm.; Johnson (1974).

⬡ Concoal Char (19.1), 103 atm. (lower point) and 137 atm. (upper point); Pyrcioch and Linden (1960).

□ Concoal Montour #10 Bit. Coal (37.0), 103 atm.; Feldkirchner and Linden (1963).

△ Wyo. HVcb Coal, 409 atm.; Hiteshue et al (1957).

3. MODEL DEVELOPMENT

One of the reasons why modeling of fixed bed (or moving bed) gasifiers is difficult is that the flows of solid and gas are countercurrent. Complexity of the modeling is further compounded by the complex structure of coal and by the lack of experimental data on rates of gasification for various coals.

3.1 LITERATURE SURVEY

Very few studies on modeling of fixed bed gasifiers are available in literature. An equilibrium model was developed by Gumz in the early fifties [11]. In this model it was assumed that temperature of gas leaving was the same as the temperature of solids entering the reduction zone. There were no further endothermic reactions above this zone because of the low solids temperature. Temperature at the end of the reduction zone was calculated by the heat balance over the bottom half of the reactor for a specified heat loss. It was further assumed that at this temperature, carbon-steam and carbon-dioxide reactions were in equilibrium. In addition, an approach factor (assumed equilibrium constant = approach factor x theoretical equilibrium constant) of 0.25 was used for hydro-gasification reaction for methane production. The effects of devolatilization and the heats required in the drying and devolatilization zone were not included in this model. Material balance equations were solved by initially assuming the values of mole fractions of carbon monoxide and hydrogen and then forcing the sum of the mole fractions to be 1.0.

This model was used by Woodmansee [25] to estimate the composition

and the temperature of the raw gas for Lurgi gasifier and the MERC's gasifier. Products of devolatilization were not included in the calculations of gas composition. The results were in fair agreement with the experimental data; however, certain discrepancies were found in the estimation of heat loss and the temperature of the raw gas.

Recently, a steady state model for Lurgi reactor was developed by Yoon, Wei, and Denn [27]. The main assumptions of this model were as follows:

(1) Plug flow for solid phase and gas phase.
(2) Equal gas and solid phase temperatures.

In this model, the reactor was divided conceptually into two regions, an adiabatic core occupying most of the reactor space and a colder boundary layer occupying an annular portion of the coal bed surrounding the adiabatic core. It was further assumed that the heat loss affected the boundary layer only and that there was no heat transfer between the adiabatic core and the boundary layer. The model predictions were compared with the available plant data for Lurgi reactors. The results seemed to be in good agreement. Some of the conclusions listed in the report were as follows [27]:

(1) The maximum temperature in the bed is determined largely by the steam to oxygen ratio in the feed.

(2) The efficiency at a given steam to oxygen ratio is determined by the carbon-oxygen feed ratio

(3) There is a critical steam and oxygen feed temperature, dependent on the reactivity of coal, below which efficient operation cannot be carried out because of excessive carbon loss in the ash and insufficient extent of gasification.

The model had certain limitations. For instance, conclusion number 3 was based on the assumption that

$$T_{at}\ Z = 0 = T_g$$

where

$$T_{at}\ Z = 0$$

is the temperature at the bottom of the gasifier (i.e. above the grate level) and T_g is the feed gas temperature. From experimental data it has been found that the temperature of the ash is always greater than the temperature of the feed gas. This countercurrent heat exchange between the cold feed gas and hot ash is cited as one of the advantages of the moving bed gasifiers. It has also been shown that during combustion, solid temperature can be higher than the gas temperature by as much as 200-300°c. The rate of oxidation, especially chemical reaction rate constant, is critically dependent on the solid temperature. Therefore, onset of combustion may not be solely dependent on the feed gas temperature.

3.2 SCOPE OF WORK

The main objective of this project, sponsored by the Morgantown Energy Research Center of Department of Energy was to develop a model which can simulate mathematically the phenomena taking place in the fixed bed gasifier. Experimental data covering 81 data periods for three different coals, namely, Arkwright Bituminous, Upper Freeport and Western Kentucky #9 were obtained from MERC.

The entire project was divided into the following three main tasks:

(1) Analysis of experimental data
(2) Development of equilibrium model
(3) Development of steady state model

3.2.1 ANALYSIS OF EXPERIMENTAL DATA

It was logical to analyze the data obtained from MERC gasifier prior to the model development. Therefore, data were examined for the effect of various operating variables, namely, pressure, steam/coal ratio, type of coal, etc. The typical data for this gasifier were then compared with the data obtained from other fixed bed gasifiers. Result of the data analysis are presented in Section 4 of this report.

3.3 EQUILIBRIUM MODEL

In order to develop a comprehensive and realistic gasifier model, it is necessary to start with a simple model to understand and test the sensitivity and the number of the various parameters needed in the model. One simple approach is to assume that all the important reactions are in equilibrium. This simplification will provide insight into the number of gasification reactions necessary for consideration. Even in such approach, calculations are complicated due to the large number of reactions and the gas components involved.

In the equilibrium model developed in this study, the gasifier was conceptually divided into three main zones, combustion zone, gasification zone, and drying and devolatilization zone. The schematic diagram is shown in Figure 10 . In the ash zone, heat is transferred from the hot ash leaving the combustion zone to steam and air streams.

In the combustion zone it was assumed that all the oxygen present in the air reacts with carbon to form CO and CO2. Approach factor of 0.006 was used in this zone for carbon-steam reaction. Carbon is further gasified by steam forming CO and H_2 in the gasification zone. Other minor reactions in which N, S, and O from coal reacts to form N_2, H_2S and H_2O also takes place in this zone. The gas composition is estimated by assuming that the water gas shift reaction is in equilibrium. Approach factor of 0.2-0.5 was used for carbon-steam reation.

In the devolatilization zone, CO, CO_2, H_2, H_2O and CH_4 along with tar are produced from coal. The amounts of pyrolysis products were estimated approximately for a given coal. In the computer program developed, material balance and heat balance equations were solved for each zone. This program calculates the composition and temperature of the gas leaving the gasifier when coal composition, air and steam feed rates are given.

This type of model can be used to predict the gas composition as well as to predict the trends for changes in gas composition when air/coal and steam/coal ratios are changed. However, the model cannot be used for scale-up and optimization purposes and is useful within a given range of the operating conditions only. In addition, due to the lack of experimental data, estimation of pyrolysis products is not accurate. It may be necessary to adjust the approach factors if the program is to be used for different coals or different gasifiers.

3.4 STEADY STATE MODEL

The equilibrium model, as described previously, has limited uses. Therefore, it is necessary to develop a steady state model which can be used for optimization and scale-up purposes. In this type of model, kinetics of various reactions as well as the dimensions of the gasifier are taken into consideration. A good model can also be used for interpolation and minor extrapolation beyond the normal operating conditions. The effect of time variable, which is important during the start-up, is not considered in the steady state model.

Assumptions made in this model were as follows:

(1) Plug flow in solid phase and gas phase;

(2) Steady state;

(3) Drying and devolatilization reactions are instanteneous and devolatilization reactions are thermally neutral;

(4) Carbon-steam and carbon-carbon dioxide reactions are volume reactions while carbon-oxygen reaction is a surface reaction;

(5) The extent of hydrogasification reaction is negligible because of low pressure and low concentration of hydrogen;

(6) Temperature of bed at the bottom of the gasifier is within the range defined by the feed gas temperature and the ash temperature (500°k-650°k);

(7) Heat loss, which includes the heat recovered by cooling water and unaccountable heat, is proportional to the heat of generation.

Development of mathematical representation of gasifier

<u>Material Balance</u>

$$\frac{dF_i}{dZ} = Ar_i$$

where

F_i = flow rate of i, gmole or gm/sec;

A = cross-sectional area, cm^2;

$r_i = \sum_{j=1}^{n} \nu_{ij} R_j$ = net rate of formation of i per unit volume of bed;

R = rate of reaction j, gmole/sec cm^3;

ν_{ij} = Stoichiometric coefficient of component i in reaction j, it is positive if component i is generated, negative if consumed, and is equal to zero for an inert;

F = positive for gas component;

F = negative for solid component;

Z = height, cms.

Heat Balance

For solid phase:

$$\frac{d\, W_s\, C_{ps}\, T_s}{dZ} = -\{ \sum_{j=1}^{n} (-\Delta H_j r_j) A - U\, A\, a\, (T_s - T_g) - H\ell_s \}$$

For gas phase:

$$\frac{d\, W_g\, C_{pg}\, T_g}{dZ} = \{ U\, A\, a\, (T_s - T_g) - H\ell_g \}$$

where

W_s, W_g = flow rate of solids, gms/sec, and flow rate of gas gmoles/sec;

C_{ps} = specific heat of solid, cal/gm ^oK;

C_{pg} = specific heat of gas, cal/gmole ^oK;

T_s = temperature of solid in ^oK;

T_g = temperature of gas in ^oK;

Z = Height, cms;

ΔH_j = heat of reaction j, cal/gmole;

r_j = rate of reaction j, gmole/sec cm^3;

$H_{\ell s}$ = heat loss in solid phase cal/sec/cm;

$H_{\ell g}$ = heat loss in gas phase cal/sec/cm;

U = overall heat transfer coefficient;

A = cross-sectional area of bed, cm^2;

a = contact area/unit volume of bed;
$= \frac{6(1-\varepsilon)}{dp}$;

ε = void fraction;

dp = particle diameter cms.

Stoichiometry of Reactions:

Coal is a complex polymeric compound consisting of C, H, O, N, S and ash. Hence, stoichiometry, assuming coal as graphite carbon, is of little use. Therefore, the stoichiometry as shown below was used. Here α, β, γ, δ and ε are gm-atoms of carbon, hydrogen, oxygen, nitrogen and sulfur present in the coal respectively.

1. char-oxygen reaction:

$$C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon + \left(\frac{a}{2} + b + d + \frac{c + e - \gamma}{2}\right) O_2 \rightarrow a\ CO + b\ CO_2 + CH_2O + d\ SO_2 + eNO$$

2. char-steam reaction:

$$C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon + (\alpha - \gamma) H_2O \rightarrow \alpha\ CO + \left(\alpha - \gamma - \frac{\beta}{2} - \varepsilon\right) H_2 + \delta_2 N_2 + \varepsilon\ H_2S$$

3. water gas shift reaction:

$$CO + H_2O \underset{\text{ash catalyst}}{\rightleftarrows} CO_2 + H_2$$

4. $CO_2 + C \rightarrow 2\ CO$

Unfortunately, experimental data are not available for the production of compounds mentioned above. In addition, composition of char obtained after devolatilization is not known. Hence, it was assumed that H, O, N and S reacting with oxygen or steam are proportional to their amount present relative to the fraction of carbon reacting. For example,

$$\text{Hydrogen reacting} = f \cdot [C_c] \cdot \text{Hydrogen present}$$

where f is 0.5

5. Devolatilization:

$$\underset{\text{(coal)}}{C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon} \rightarrow \underset{\text{(char)}}{C_{\alpha'} H_{\beta'} O_{\gamma'} N_{\delta'} S_{\varepsilon'}} + \underset{\text{(tar)}}{C_{\alpha''} H_{\beta''} O_{\gamma''} N_{\delta''} S_{\varepsilon''}} + U\ CO + v\ CO_2 +$$

$$Z\ C_2H_6 + X\ CH_4 + t\ H_2O + WH_2$$

<u>Method of solution:</u>

Material balance equations were written for the following components:

Gas: CO, CO_2, N_2, H_2, CH_4, C_2H_6, H_2S, O_2, H_2O, SO_2, NO, NH_3

Solids: C, H, O, N, S, Ash

Since it was assumed that temperatures of the solid and gas phases were the same, the heat balance equations reduced to

$$\frac{dT}{dZ} = (H_R A - H_L)/(F_g c_{p_g} - F_s\ c_{ps})$$

where

T = temperature, °K.

Z = height, cms.

H_R = total heat of reactions/unit volume.

H_ℓ = heat loss (This heat loss includes unaccountable heat and heat recovered by cooling water).

F_g = flow rate of gas, gmole/sec.

F_s = flow rate of solid, gm/sec.

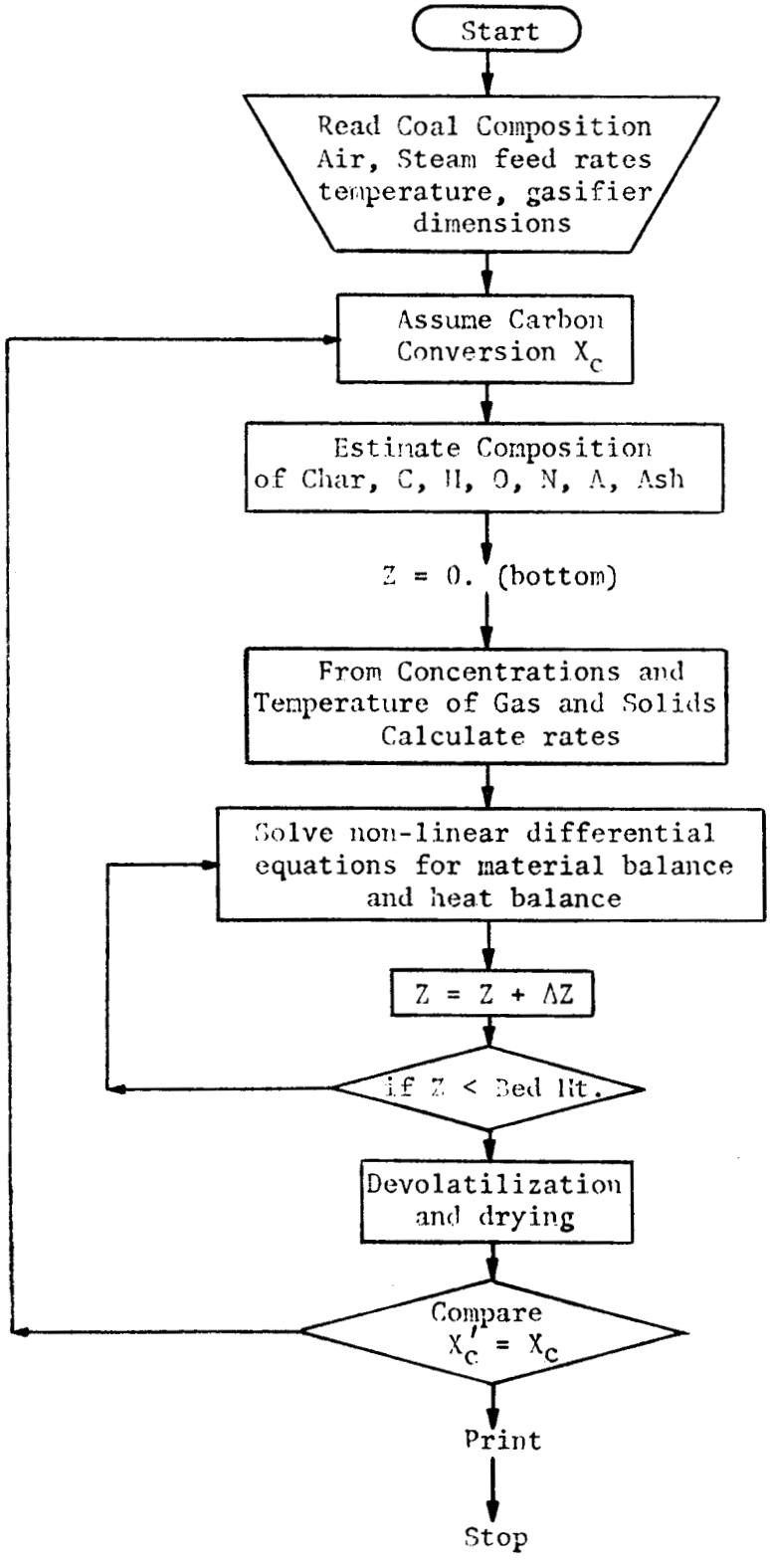
In all, 19 equations were solved which consisted of 18 material balance equations and one heat balance equation.

These 19 simultaneous first order non-linear differential equations were solved using Runge-Kutta with fixed length integration scheme. Initially, the value of carbon conversion is assumed and is used to estimate the solids concentration at the bottom of the gasifier. The integration is started at the point above the grate (Z = 0) using gas and solid concentration as the initial values. The step size of 2 cms is used (total number of steps ≃ 100). The integration is continued over the entire length of the bed. The value of carbon flow rate, gm/sec, at Z = L (where L = height of bed, cms) is compared with the carbon feed rate. If the difference is found to be more than 1.0 gm/sec, the assumed carbon conversion is changed and the entire procedure is repeated. Generally, convergence was obtained within seven to eight iterations. In these calculations, H, O, N, and S flow rates were not compared.

Flow diagram of the model is shown in Figure 18.

FIGURE 18

FLOW DIAGRAM OF STEADY STATE MODEL



4. Results

In this section, a discussion of the results and their significance are presented in the following order:

(1) Results of data analysis

(2) Comparison of equilibrium model results with the experimental data

(3) Results obtained from steady-state model for

(a) air-steam system
and
(b) oxygen-steam system

4.1 Analysis of Data.

Data obtained from MERC (Morgantown Energy Research Center) for 17 Runs (Run 57-80) covering 81 data periods were analyzed. Coal from three different seams namely, Arkwright-Bituminous, Upper Freeport and Western Kentucky #9 were gasified using air and steam at pressures varying from 15 psig to 225 psig. The amount of steam fed per lb of coal ranged from 0.35 lbs to 0.75 lbs and the ratio of air to coal was varied from 2.35 to 3.75. The typical compositions of gas obtained from these three coals are shown in Table 2.

In the analysis of the runs, data periods with time less than 10 hours were neglected because of the possibility that steady state could not have been attained in such a short time.

In the following sections, effects of different operating variables such as pressure, steam to coal ratio, type of coal etc., are discussed.

Effect of Pressure

The gas yield (SCF/lb) and the heating value (BTU/SCF) of the product gas increases slightly with the increase in pressure as shown

TABLE 2

Typical Range of Compositions of Coal and Product gas Covered in Experiments

Type of Coal	Arkwright Pittsburgh	Upper Freeport	Western Kentucky #9
Ultimate Analysis			
C	75.5	66.8	64.5
H	5.9	4.4	5.5
N	1.5	1.2	1.7
S	3.3	3.8	3.9
O	4.0	2.5	4.0
Moisture	1.2	1.0	5.0
Ash	8.7	20.3	15.4
Heating Value BTU/lb	13,860.	11,580.	11,450.
Air/coal, lb/lb	2.5 - 3.75	2.6 - 3.55	2.5 - 2.87
Steam/coal, lb/lb	0.5 - 0.74	0.35 - 0.48	0.39 - 0.5
Steam Temp., °F	990 - 1155	990 - 1115	950 - 1025
Air Temp., °F	88 - 245	206 - 267	220 - 260
Temperature of Gas, °F	722 - 1285	730 - 1050	839 - 1136
Gas Composition			
CO	16. - 23.	18. - 22.	17. - 20.
CO_2	7. - 12.	7. - 8.4	8. - 11.
N_2	48. - 55.	51. - 53.	50. - 55.
H_2	13. - 17.	13. - 15.	13.6 - 15.6
CH_4	2. - 3.5	2.5 - 2.6	2.0 - 2.7
C_2H_6	0.3	—	0.26 - 0.28
H_2S	0.3 - 0.4	0.25	0.87 - 1.95
Heating Value of gas, BTU/SCF	100 - 179	138 - 142	128 - 148

in Figures 19 and 20. However, there is a slight increase in the amount of methane produced (SCF/lb maf coal) with an increase in pressure as shown in Figure 21.

Pressure does not seem to affect the performance of the gasifier, significantly. But more coal can be gasified per unit time at high pressure because of higher air and steam flow rates. Coal feed rate in lb/hr is plotted against gasifier pressure in Figure 22.

Effect of Steam/Coal Ratio

Steam is added in excess not only to absorb heat but to prevent the clinkering of ash particles. The reaction of steam with carbon is endothermic

$$C + H_2O \rightleftharpoons CO + H_2$$

and hence helps to maintain the temperature in the combustion zone below the fusion point of ash.

Excess steam shifts the water gas equilibrium and thus increases the percentage of hydrogen and carbon dioxide and reduces the percentage of carbon monoxide in the product gas.

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

This is shown in Figures 23, 24, and 25.

From gas analysis and weight balance, water-gas equilibrium constant k is calculated for each data period and is plotted against temperature (°F) of the gas in Figure 26.

where $K = (CO_2)(H_2)/(CO)(H_2O)$

The graph shows that the gas composition in the water gas shift equilibrium at temperatures (ranging from 1400-1700 F) is higher than the

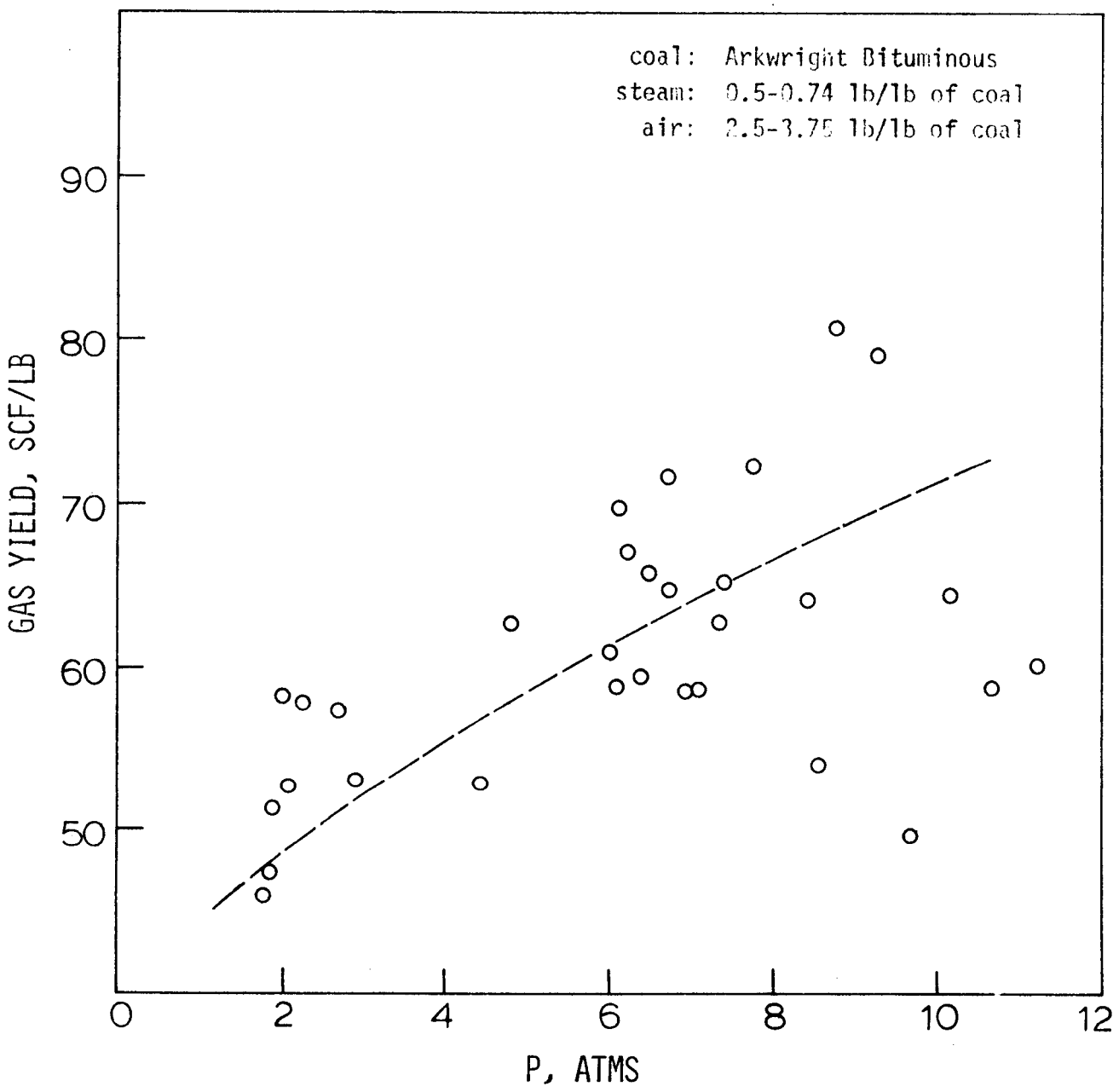


Figure 19 Effect of pressure on gas yield

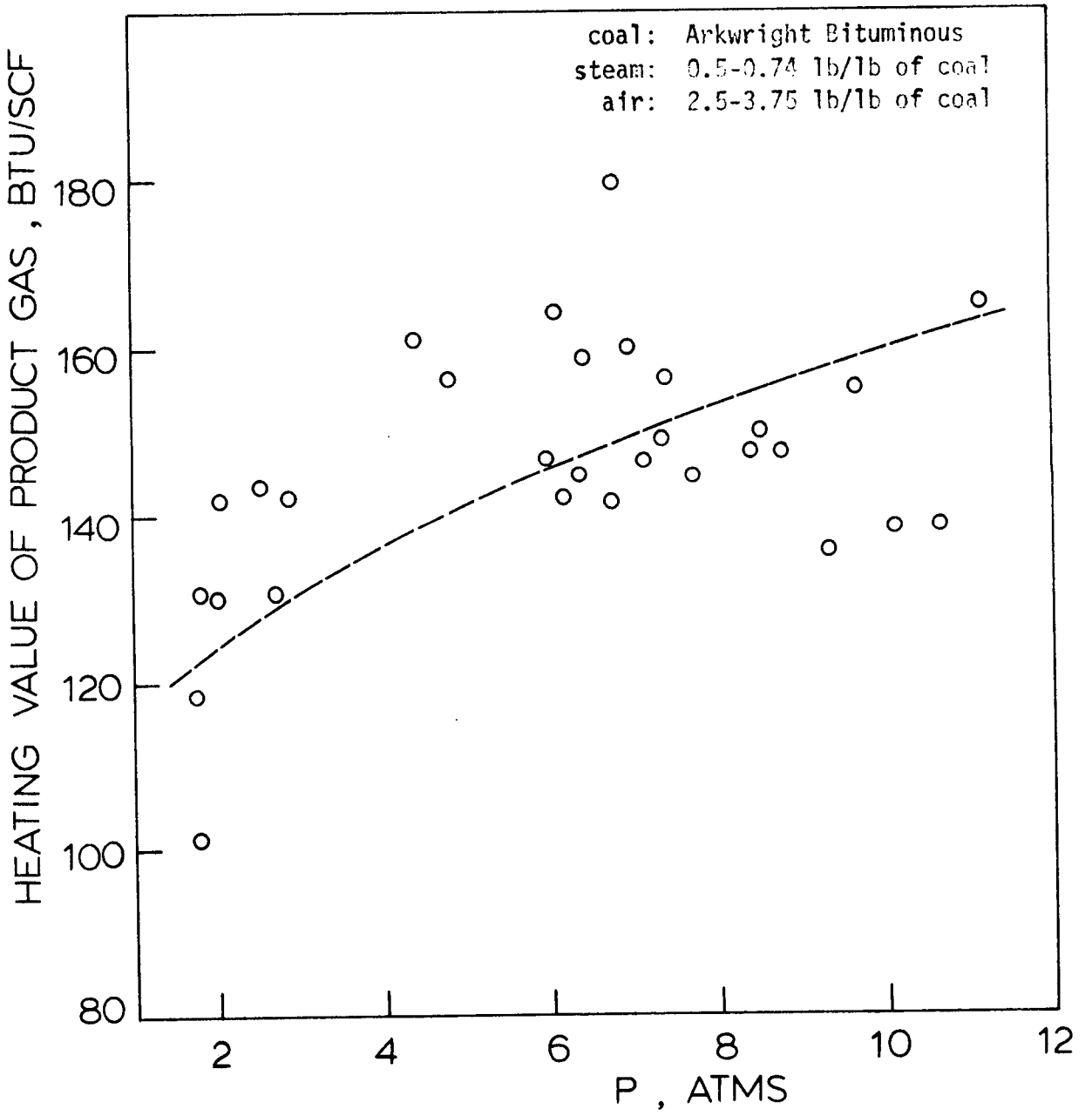


Figure 20 Effect of pressure on the gas heating value

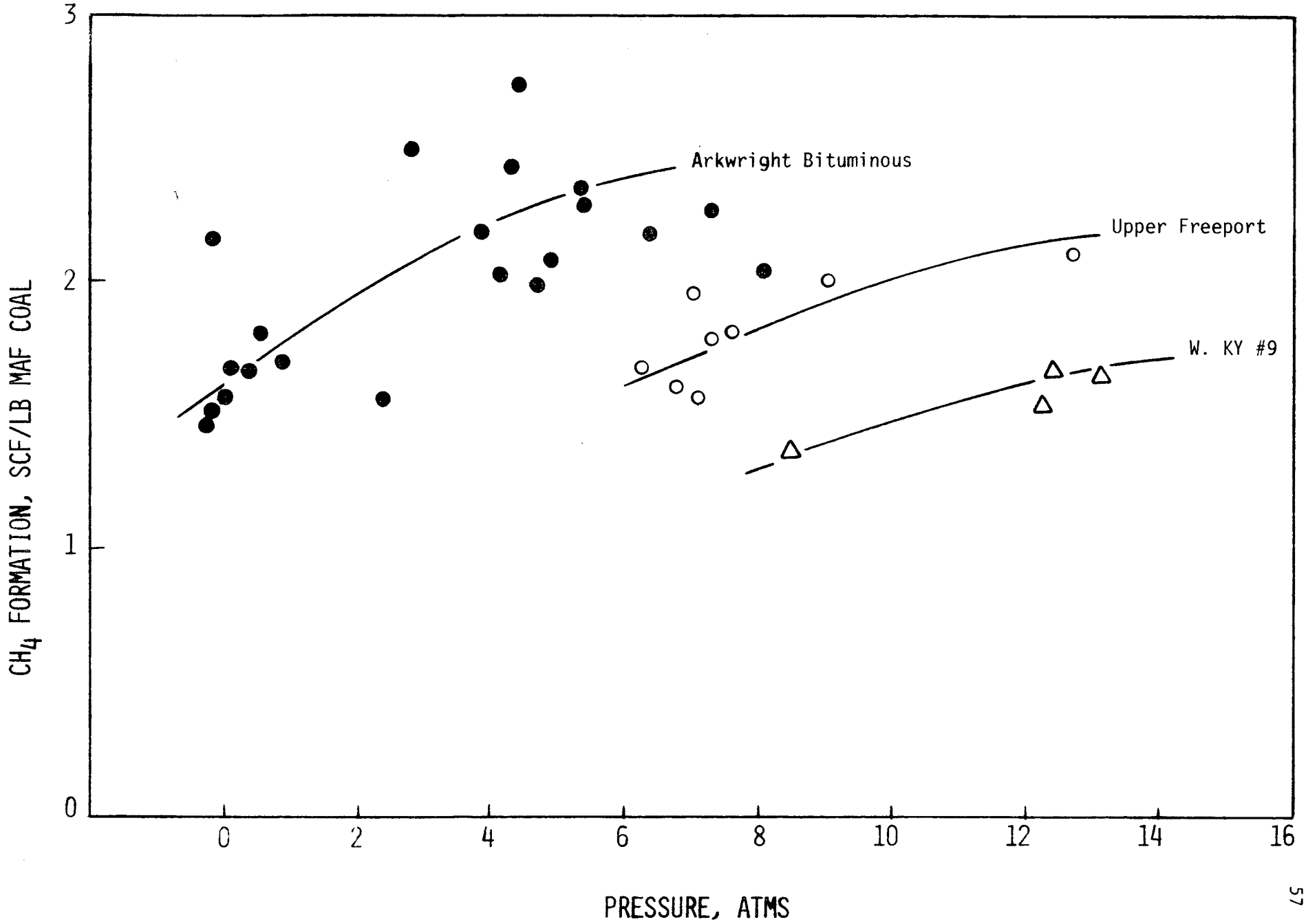


FIGURE 21 Effect of pressure on methane formation

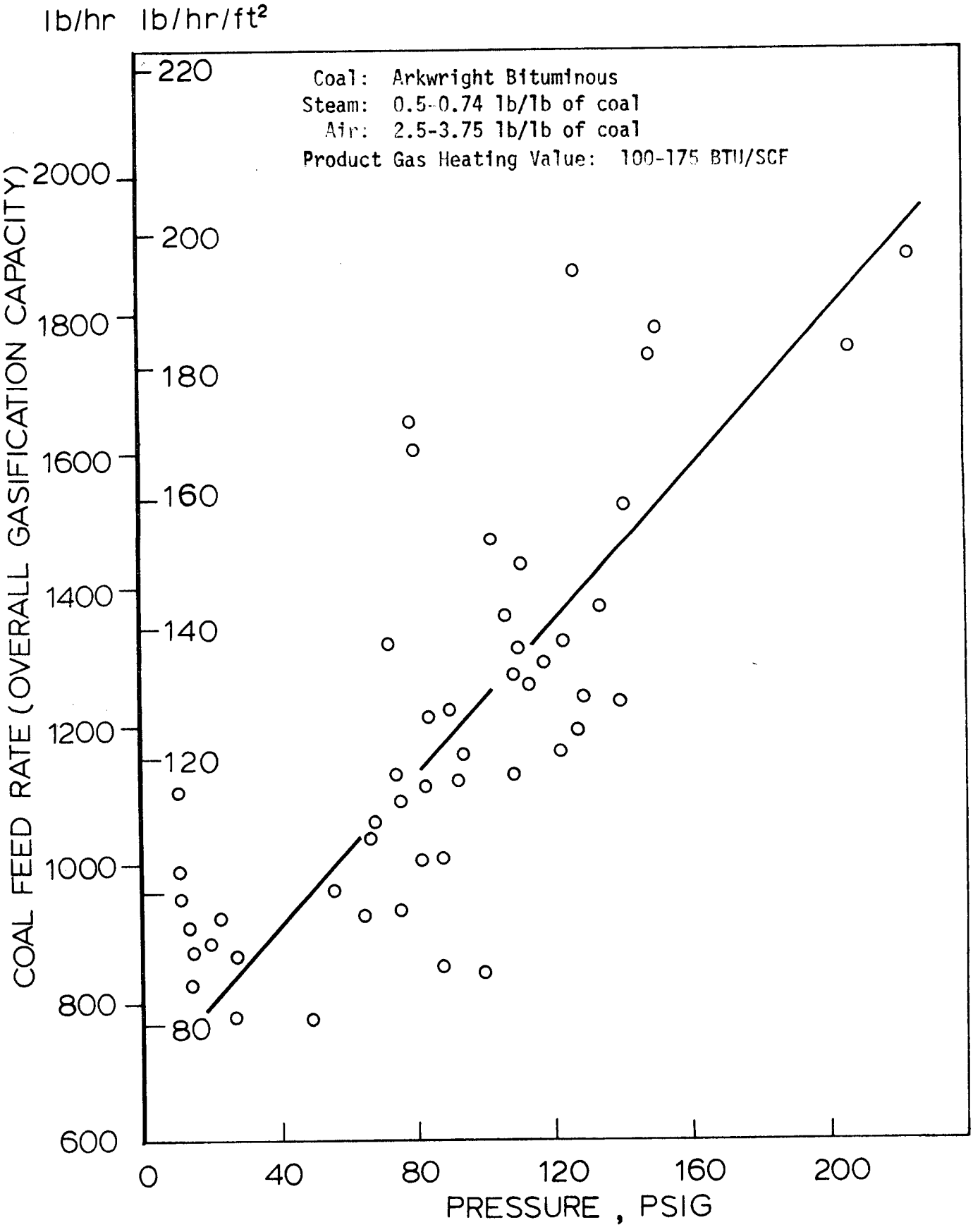


Figure 22 Effect of Pressure on Coal Gasification Rate.

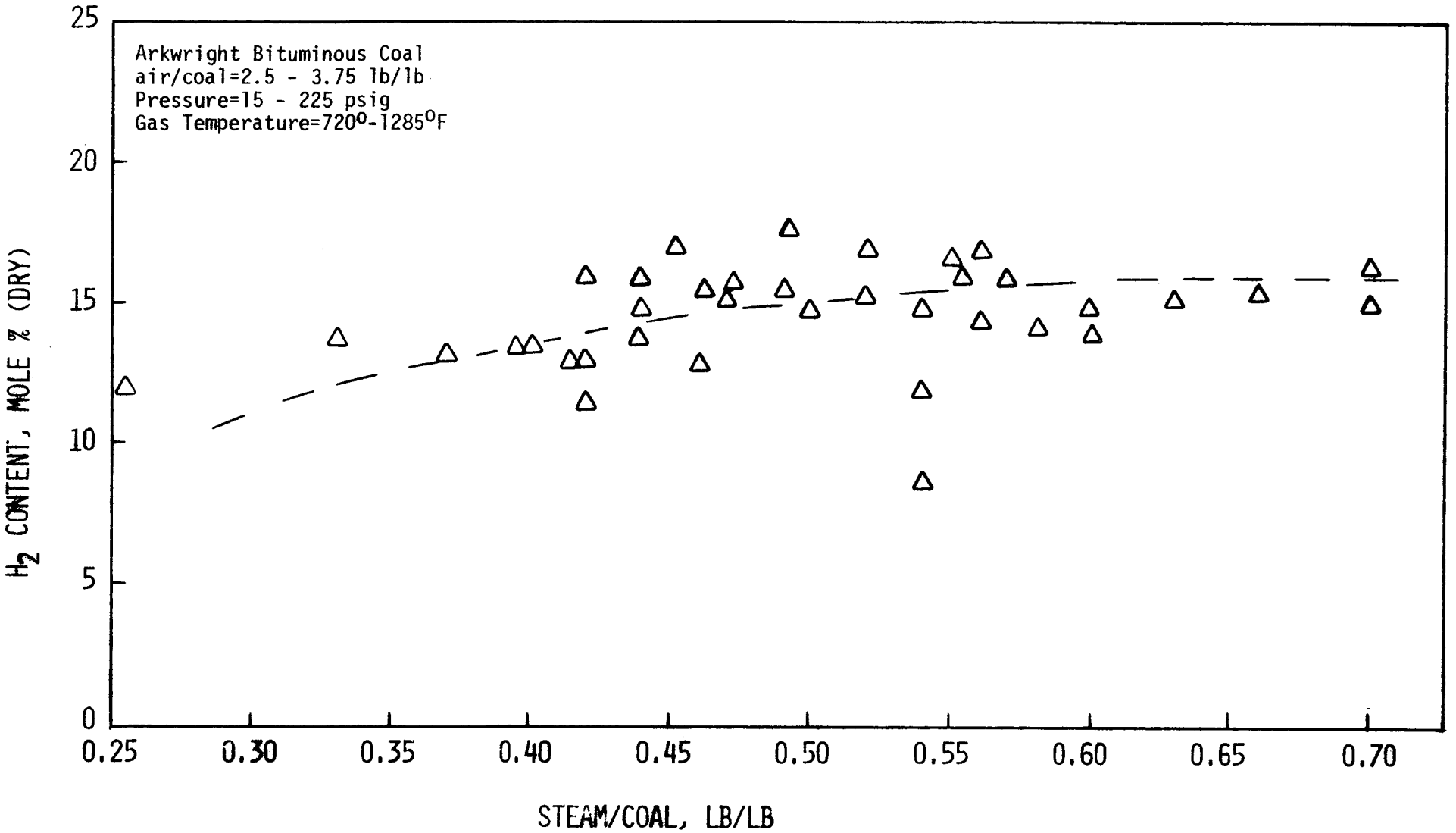


Figure 23 Effect of steam/coal on H_2 content of gas

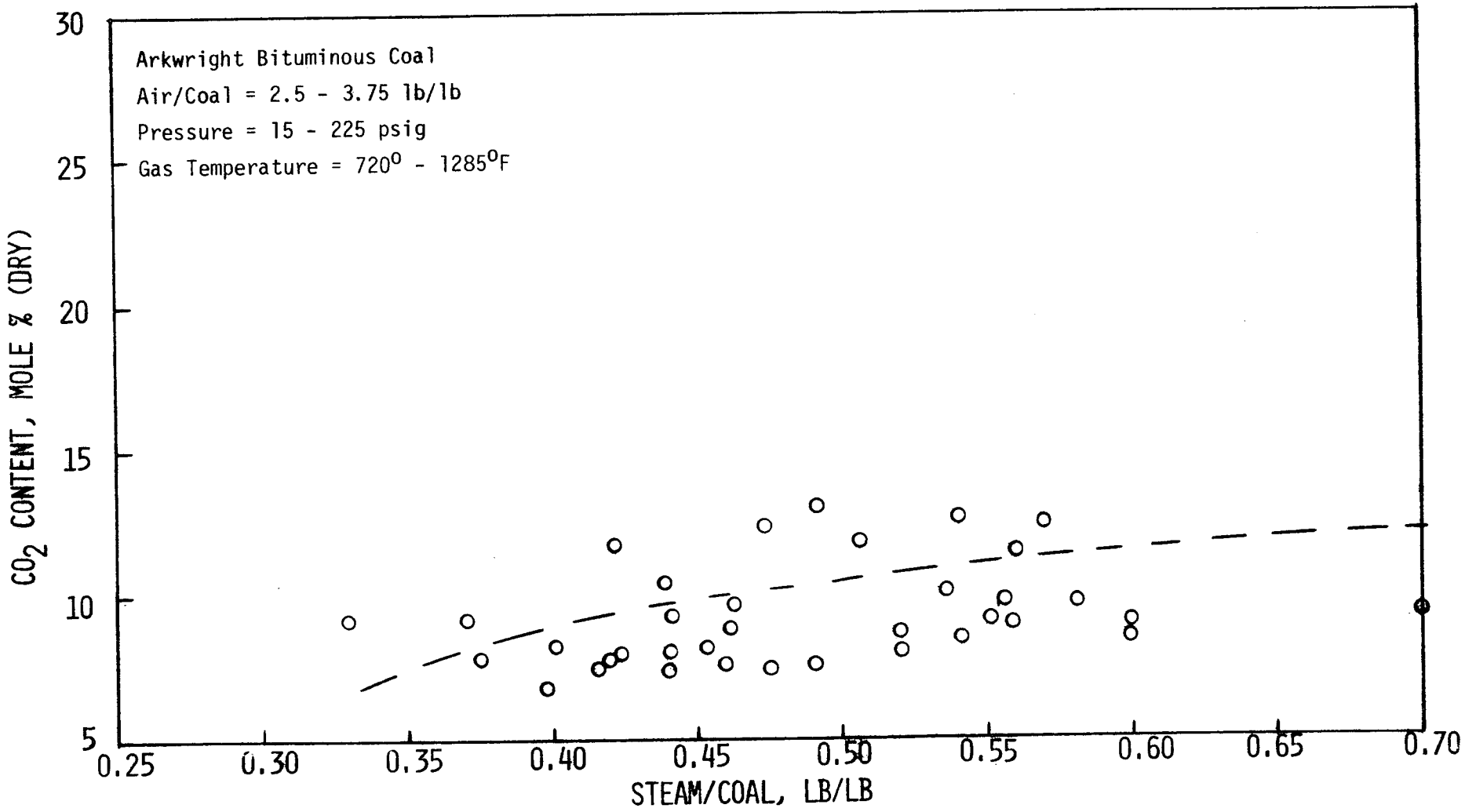


Figure 24 Effect of steam/coal on CO_2 content of gas

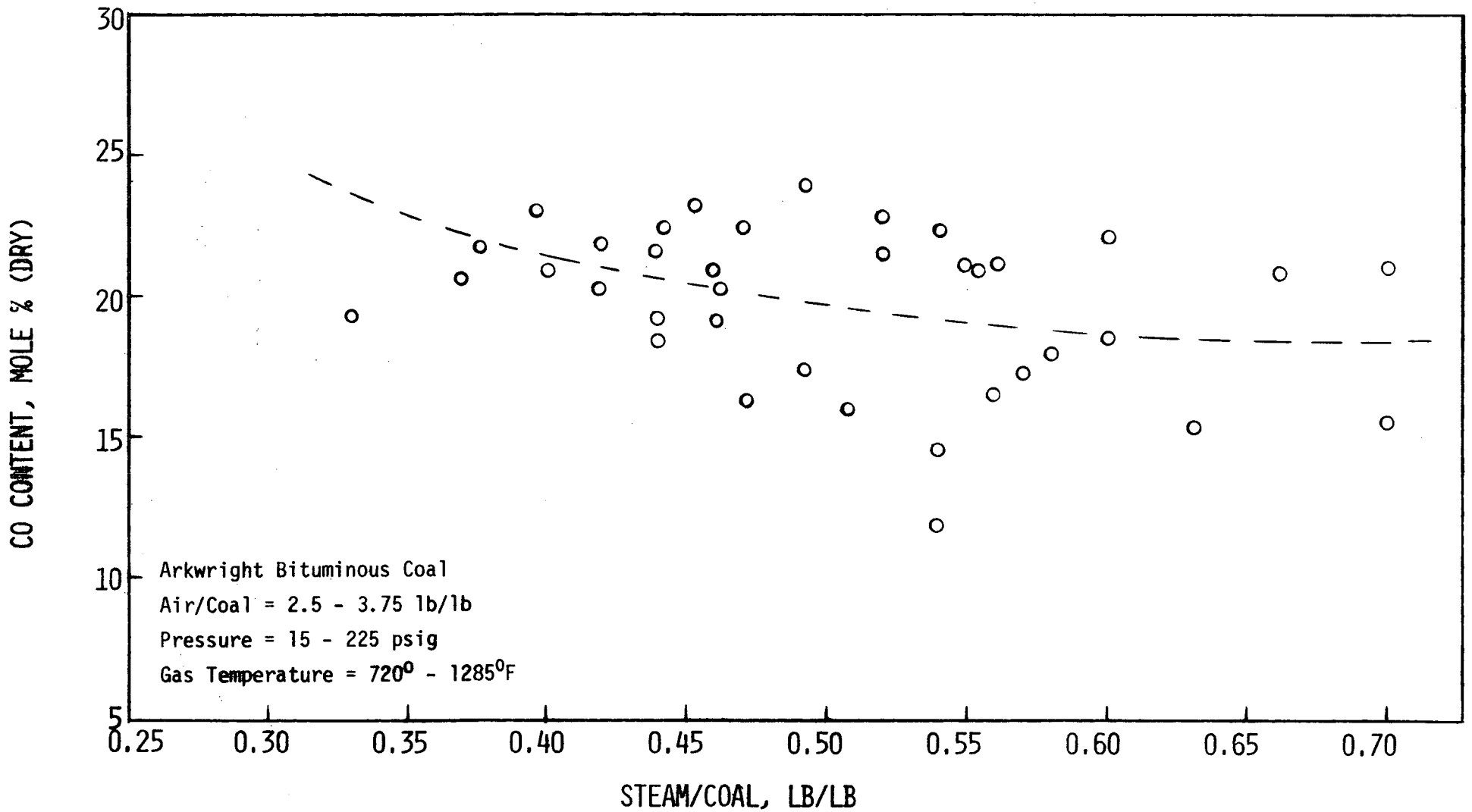


Figure 25 Effect of steam/coal on CO content of gas

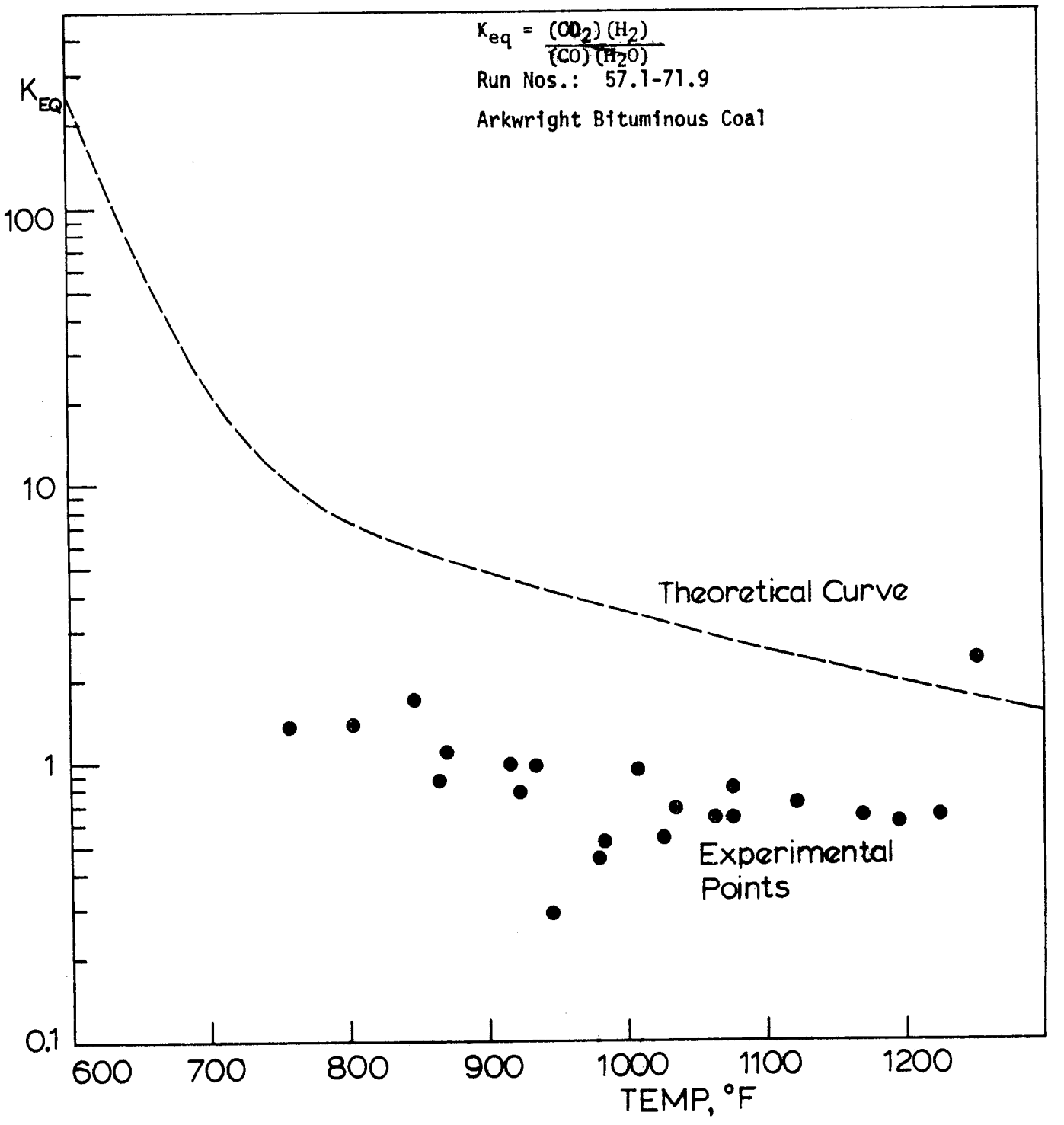


Figure 26 Water gas shift equilibrium at the gasifier exit

exit gas temperatures. It is possible that water gas reaction would not have taken place at low temperatures prevailing in the devolatilization zone.

Effect of Type of Coal

It has been shown that the reactivity of coal decreases with an increase in coal rank. Bituminous coals, e.g. Pittsburgh seam coal, are caking coals and tend to agglomerate on heating. Therefore, it is difficult to gasify Pittsburgh seam coal and higher steam/coal ratio (about 0.5) is required while low ranking coals, e.g. Western Kentucky #9, can be easily gasified at low steam/coal ratio (0.35-0.4). Gas yield is proportional to the carbon throughput which in trun depends on the composition of coal.

An attempt was also made to correlate the amount of tar formed to other variables like the temperature of product gas, coal feed rate, gas flow rate, etc. However, no significant correlation was found.

4.2 Comparison of Equilibrium Model Results with the Experimental Data

In Table 3, the results obtained from the equilibrium model are compared with the experimental data Run 61 Period 4. As can be seen from these tables, the equilibrium model predicts the gas composition rather accurately. However, for reasons mentioned previously, the equilibrium model has very limited use, and it is obvious that approach factors have to be changed for different types of coal. It is nevertheless, a way to begin to quantify the effects of various factors on gasifier performance.

TABLE 3
COMPARISON OF EQUILIBRIUM MODEL RESULTS WITH
EXPERIMENTAL RESULTS FOR UPPER FREEPORT COAL

RUN 61 PERIOD 4

	Experimental	Equilibrium Model
Air/coal, lb/lb	2.83	2.83
Steam/coal, lb/lb	0.35	0.35
Air-steam temp., °F		
Heat loss = % $\frac{\text{Heat loss}}{\text{H.V. of coal in}}$	24.74	
Gas Composition, mole% (dry)		
CO %	18.10	21.29
CO_2	8.35	8.35
N_2	53.24	54.
H_2	14.10	13.23
CH_4	2.55	2.33
C_2H_6	0.00	-
H_2S	0.25	0.8
O_2	0.00	-
	96.59	100.00
Temp. of Gas, °F	730.	1054
H.V. of Gas, BTU/SCF	130.0	139
Cold Gas Efficiency,%	70%	66%
Gas Yield, scf/lb coal[1]		
Steam Decomposition, %[1]		

[1]Based on overall mass balance

4.3 Results of Steady State Model

Results obtained from the steady state model corresponding to Runs 70 Period 6, 71 Period 5, 69 Period 2, and 76 Period 3 are compared with the experimental data in Tables 4, 5, 6, and 7. This comparison shows good agreement except for Run 76 Period 3. The difference in the coal composition between the experimental data and the model results, even though small, is due to the method used for simulation as discussed in Section 3. In Tables 8 and 9, model results are compared to the experimental results for upper Freeport and Western Kentucky coal. These results show good agreement inspite of the fact that same rate constants and similar devolatilization product distribution were used.

Comparison of results in this fashion has certain drawbacks because the experimental data reported are the average values as described in Chapter 1. For example, in one run for Arkwright Bituminous coal, the following lowest and highest values were actually measured.

	Lowest	Highest
Pressure Psig,	85.	137.
Coal Feed Rate lbs/hr	729.	1432.
% CO	16.4	23.1
% CO_2	6.0	9.3
% H_2	11.8	14.7

In addition, for all the runs the output to input ratio for carbon, hydrogen, and oxygen varied from 0.85 to 1.1. However, despite these drawbacks, the comparison is necessary to check the validity of the model. In this exercise, model results are compared with the values reported by MERC without any adjustment.

TABLE 4

COMPARISON OF STEADY-STATE MODEL RESULTS TO
EXPERIMENTAL RESULTS FOR ARKWRIGHT-BITUMINOUS COAL
RUN No: 70 Period 6

	Experimental	Model
Coal feed rate, lbs/hr	1218.	1234.
Composition %		
C	75.92	74.81
H	5.7	5.24
O	4.92	6.22
N	1.38	1.54
S	2.71	2.93
Ash	8.25	8.14
Moisture	1.12	1.12
Pressure, psig	90.	
Steam, lb/hr	576.	576.
Air, lb/hr	3826	3826
Steam, temp., °F	1072.0	—
Air temp., °F	99	—
Product gas lbmoles/hr[a]	199.6	200.5
Gas Composition		
CO	16.2	14.84
CO_2	12.2	12.73
N_2	52.5	52.24
H_2	15.7	15.54
CH_4	3.6	3.34
C_2H_6	0.36	0.27
H_2S	0.58	0.45
O_2	0.1	—
Steam Decomposition; %[b]	69.4	66.2
Gas Temp., °F	1253.	980.
H.V. Gas, BTU/SCF	146.	142.
Carbon Conversion[c]	0.872	0.864
Heat Loss, %(of heating[d] value of coal)	23.0	15.74
Maximum Temperature, °F,[e]		1560.

a: Calculated from the reported value of gas yield, scfh

b: Calculated from amount of water reported in weight balance

c: From material balance (nitrogen basis)

d: From reported heat balance (nitrogen basis)

e: It is the average temperature and not solid temperature

TABLE 5

COMPARISON OF STEADY STATE MODEL RESULTS TO EXPERIMENTAL RESULTS FOR ARKWRIGHT BITUMINOUS COAL
RUN No: 71.5

	Experimental	Model
Coal, lbs/hr	1097.	1098.
Composition,%		
C	75.92	76.4
H	5.7	4.6
O	4.9	5.59
N	1.38	1.36
S	2.71	2.57
Ash	8.25	8.23
Moisture	1.12	1.25
Pressure, psig	76.	
Steam, lbs/hr	501.	501.
Air, lbs/hr	4112.	4112.
Steam temp., °F	1120.	
Air temp., °F	240.	
Product gas, lbmoles/hr[a]	205	206.5
Gas Composition		
CO	20.3	16.86
CO_2	7.7	11.37
N_2	55.2	54.49
H_2	12.9	13.26
CH_4	2.8	2.89
C_2H_6	0.3	0.24
H_2S	0.5	0.39
O_2	0.1	——
Steam Decomposition, %[b]	46.4	66.
H.V. of gas, BTU/SCF	142	135.
Temperature of gas, °F	1062	1110.
Carbon Conversion[c]	0.955	0.976
Heat Loss, %[d]	20.3	17.63
Maximum Temperature, °F[e]		1574.

* a-e See TABLE 4 for legend.

TABLE 6

COMPARISON OF STEADY STATE MODEL RESULTS TO EXPERIMENTAL RESULTS FOR ARKWRIGHT BITUMINOUS COAL RUN No. 69.2 (Bed height = 61")

	Experimental	Model
Coal, lbs/hr	925.	943.0
Composition, %		
C	75.92	74.64
H	5.7	5.32
O	4.92	6.30
N	1.38	1.56
S	2.71	2.97
Ash	8.25	8.10
Moisture	1.12	1.11
Pressure, psig	23.2	
Steam lbs/hr	342.	342.
Air lbs/hr	2887.	2887.
Steam temp., °F	1028.	
Air temp., °F	187.	
Product gas, lbmoles/hr[a]	148.	147.3
Gas Composition		
CO	20.71	17.5
CO_2	9.16	10.57
N_2	53.4	53.67
H_2	13.13	13.64
CH_4	2.86	3.25
C_2H_6	0.3	0.27
H_2S	0.26	0.47
O_2	0.1	—
Steam Decomposition, %[b]	31.4	62.5
H.V. of gas BTU/SCF	144.	143.6
Temperature of gas, °F	948.	1106.0
Carbon Conversion[c]	0.923	0.844
Heat Loss, %[d]	21.5	14.7
Maximum temperature, °F[e]		1644.

*a-e See TABLE 4 for legend.

TABLE 7

COMPARISON OF STEADY STATE MODEL RESULTS TO EXPERIMENTAL RESULTS FOR ARKWRIGHT BITUMINOUS COAL RUN No. 76.3

	Experimental	Model
Coal feed rate, lbs/hr	1240.	1263.
Composition, %		
C	76.8	74.48
H	5.7	5.38
O	4.77	6.34
N	1.19	1.58
S	2.50	2.99
Ash	8.32	8.10
Moisture	0.7	1.23
Pressure, psig	141.	
Steam, lbs/hr	693.	693.
Air, lbs/hr	3756.	3756.
Steam temp. °F	1026	
Air temp. °F	220.	
Product gas, lbmoles/hr[a]	206.	200.
Gas Composition		
CO	21.3	13.11
CO_2	8.9	13.94
N_2	49.4	51.39
H_2	16.9	16.82
CH_4	2.6	3.38
C_2C_6	0.34	0.29
H_2S	0.43	0.46
O_2	——	——
Steam Decomposition[b]	71.6	60.7
H.V. of gas, BTU/SCF	156	141.2
Temperature of gas, °F	1065	987.
Carbon Conversion,[c]	0.907	0.836
Heat Loss, %[d]	24.87	15.30
Maximum temperature, °F[e]		1550.

*a-e See TABLE 4 for legend.

TABLE 8

COMPARISON OF STEADY STATE MODEL RESULTS TO EXPERIMENTAL RESULTS FOR UPPER FREEPORT COAL
RUN 61 Period 6

	Experimental	Model
Coal, lbs/hr	1371	1391
Composition, %		
C	66.8	65.12
H	4.4	4.12
O	3.5	4.5
N	1.2	1.38
S	3.8	4.2
Ash	20.3	19.8
Moisture	1.0	1.0
Pressure, psig	126	126
Steam, lbs/hr	527	527
Air, lbs/hr	4229.	4229.
Air temp., °F	239.	
Steam temp., °F	1058	
Product gas, lbmoles/hr[a]	218.	212.9
Gas Composition, %		
CO	21.8	17.67
CO_2	7.02	10.8
N_2	53.1	54.38
H_2	13.9	11.4
CH_4	2.5	3.97
C_2H_6	0.0	0.33
H_2S	0.25	0.81
O_2	—	—
Steam Decomposition, %[b]	52.7	63.9
Heating Value of Gas, BTU/SCF	140.7	147.
Temperature of gas, °F	1050.	1210.
Carbon Conversion[c]	0.913	0.975
% Heat Loss (% of heating value of coal)[d]	16.1	17.5

*a-e See TABLE 4 for legend.

TABLE 9

COMPARISON OF STEADY STATE MODEL RESULTS TO EXPERIMENTAL RESULTS FOR WESTERN KENTUCKY COAL
RUN 65 Period 1

	Experimental	Model
Coal, lbs/hr	1402.	1422.
Composition, %		
C	64.5	63.8
H	5.5	5.02
O	4.0	4.97
N	1.7	1.89
S	3.9	4.23
Ash	15.4	15.18
Moisture	5.0	4.91
Pressure, psig	139.	139.
Steam, lbs/hr	691.	691.
Air, lbs/hr	4001.	4001.
Air temp., °F	231.	
Steam temp., °F	1024.	
Product gas, lbmoles/hr[a]	200.7	215.
Gas Composition, %		
CO	18.6	14.55
CO_2	9.2	12.61
N_2	54.3	50.93
H_2	14.3	15.86
CH_4	2.11	4.06
C_2H_6	0.17	0.34
H_2S	0.85	0.8
O_2	0.65	——
Steam Decomposition, %[b]	65.4	60.9
Heating value of gas, BTU/SCF	131.	154.
Temperature of gas, °F	839.	1110.
Carbon Conversion[c]	0.843	0.955
Heat Loss (% of heating value of coal)[d]	23.53	16.7

*a-e See TABLE 4 for legend.

In Figure 27 the bed temperature profile is shown as a function of bed height. The maximum temperature is only about 1505°F(1125°K) because of large heat loss. The temperature shown in Figure 27 is the mean between gas and char. It has been demonstrated that in the combustion zone, temperature of coal particles can be higher than gas temperature by as much as (300-500°F) (200-300°C). In Figure 28 concentration profiles for CO, CO_2, H_2, H_2O and O_2 with respect to bed height are shown. The sudden changes in the value of the gas concentration at the exit conditions are because of the assumption of instantaneous devolatilization.

Effect of air/coal ratio on the carbon conversion (defined as fraction of carbon in the feed converted to gas and tar) and the heating value of the product gas are shown in Figure 29. Since the char-oxygen reaction is very fast, and increase in oxygen (or air) increases the carbon conversion, but simultaneously increases the fraction of inert nitrogen in the gas, thereby reducing the heating value of the product.

Effect of air/coal ratio on the product gas composition is shown in Figure 30. The fact that concentration of CO increases while that of H_2 and CO_2 decreases as air/coal ratio is increased is due to one, or a combination of, the following factors.

1. Increase in nitrogen dilutes the concentration of CO and H_2O in the gas stream, thereby reducing the extent of water-gas shift reaction.

2. Increase in oxygen increases the amount of CO and CO_2 formed.

3. Increase in oxygen also tends to decrease the char-steam reaction resulting in the reduction of CO and H_2 formed.

Similarly, effects of steam/coal ratio on the carbon conversion and

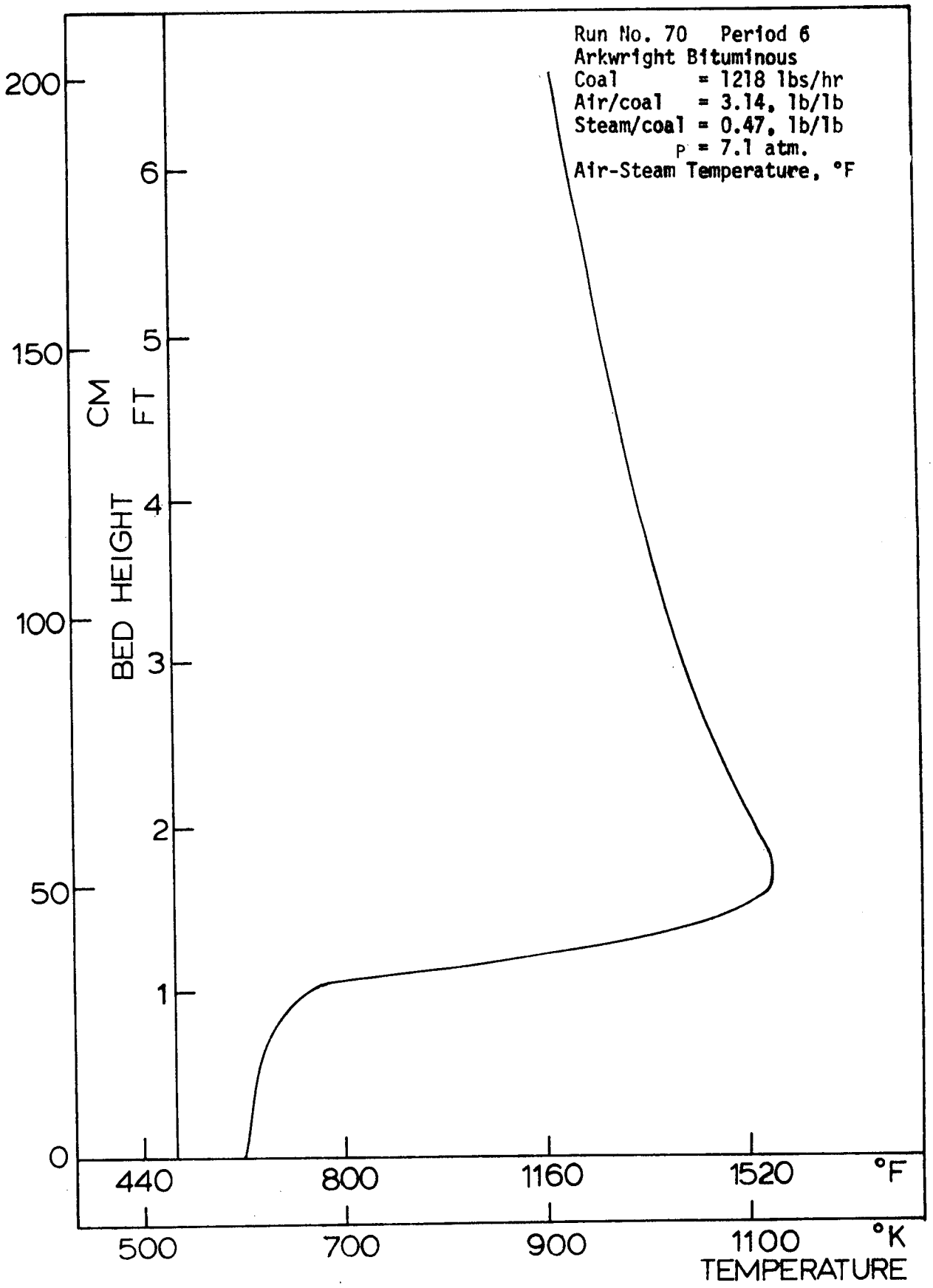


Figure 27 Temperature profile in the fixed bed gasifier

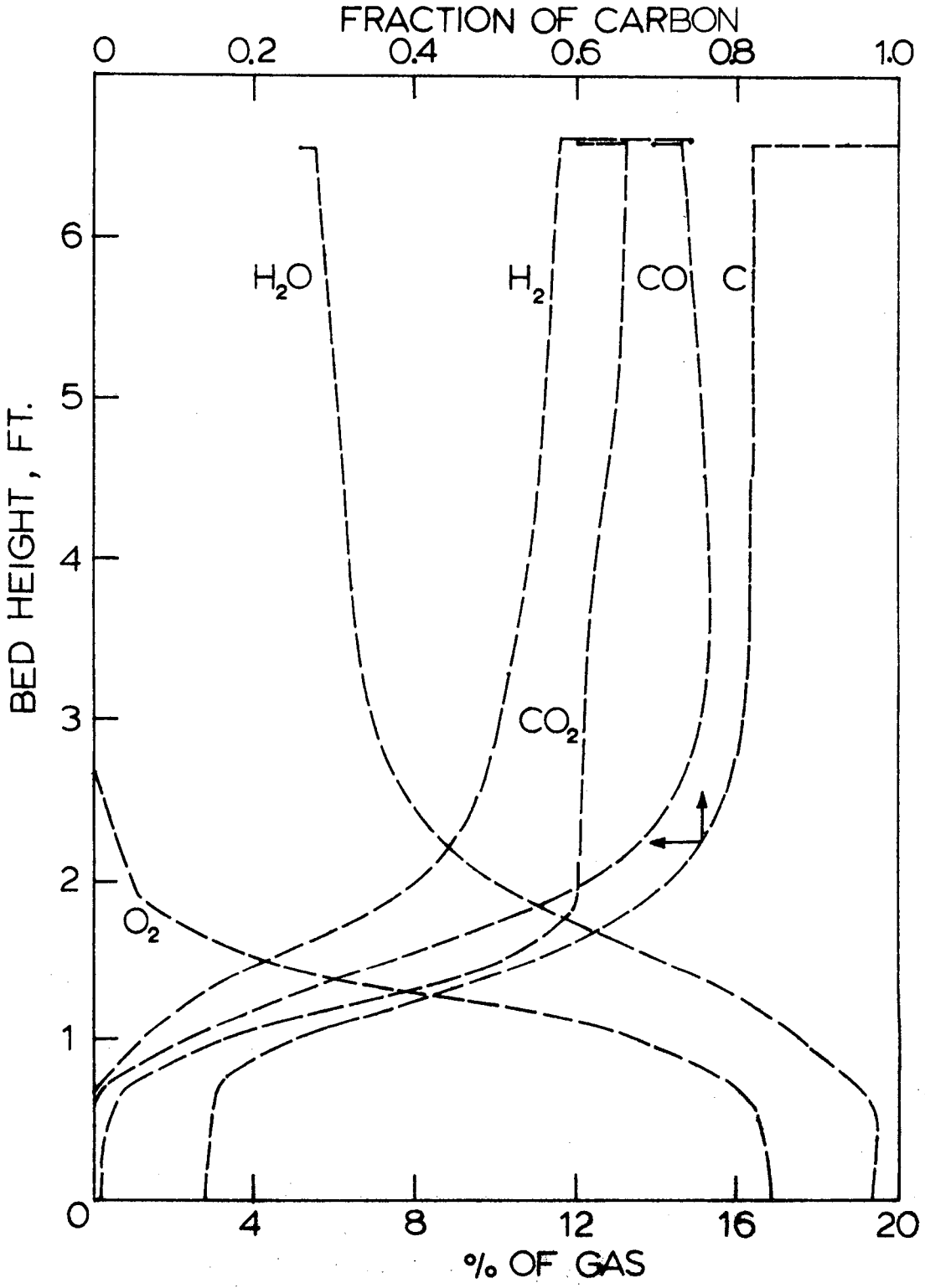


Figure 28 Concentration profile for air-steam stream (Run No. 70 Period 6; Arkwright Bituminous Coal, coal=1218 lbs/hr, air/coal=3.4 lb/lb, steam/coal= 0.47 lb/lb)

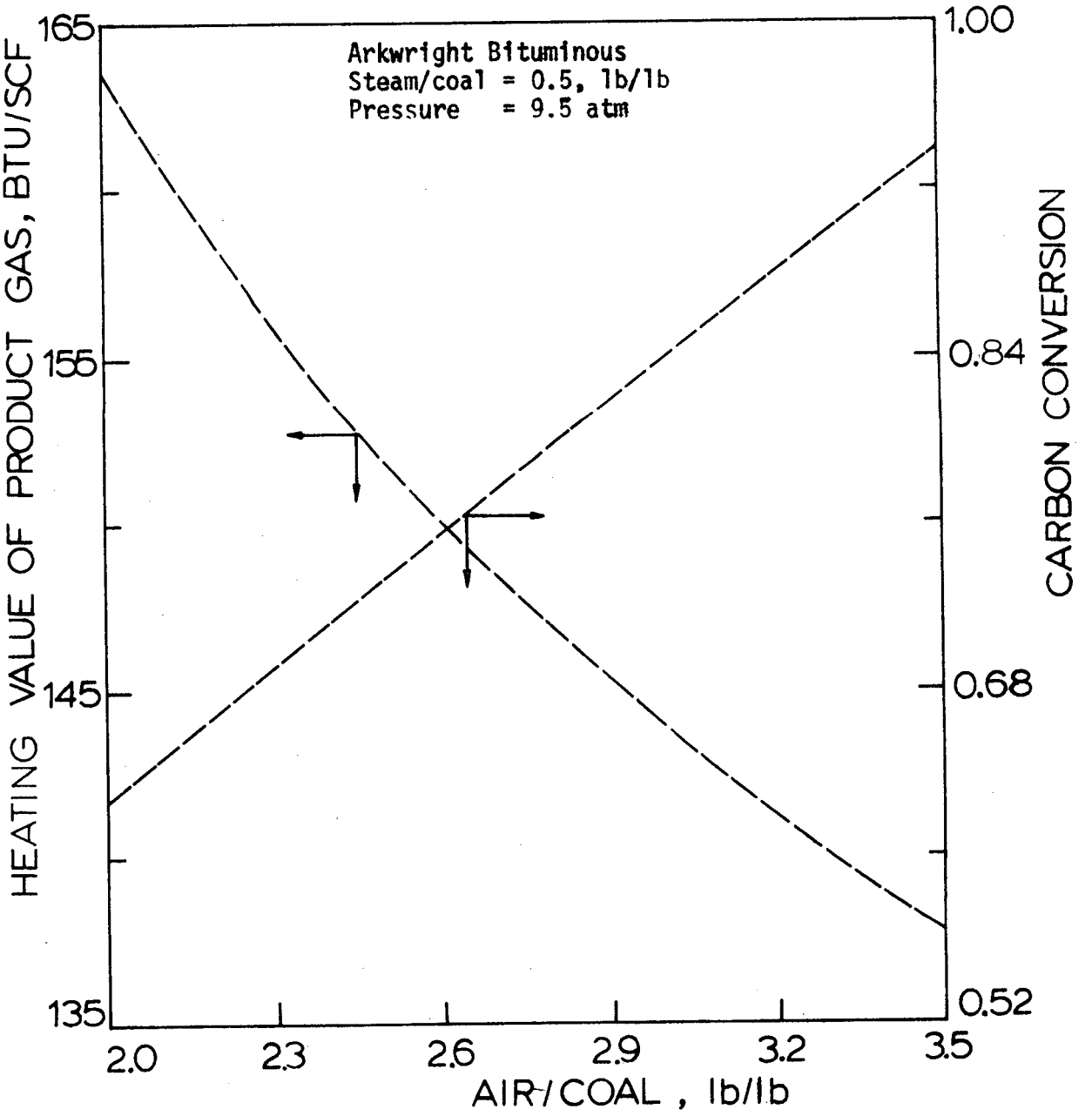


Figure 29 Effect of air/coal ratio on carbon conversion and heating value of the product

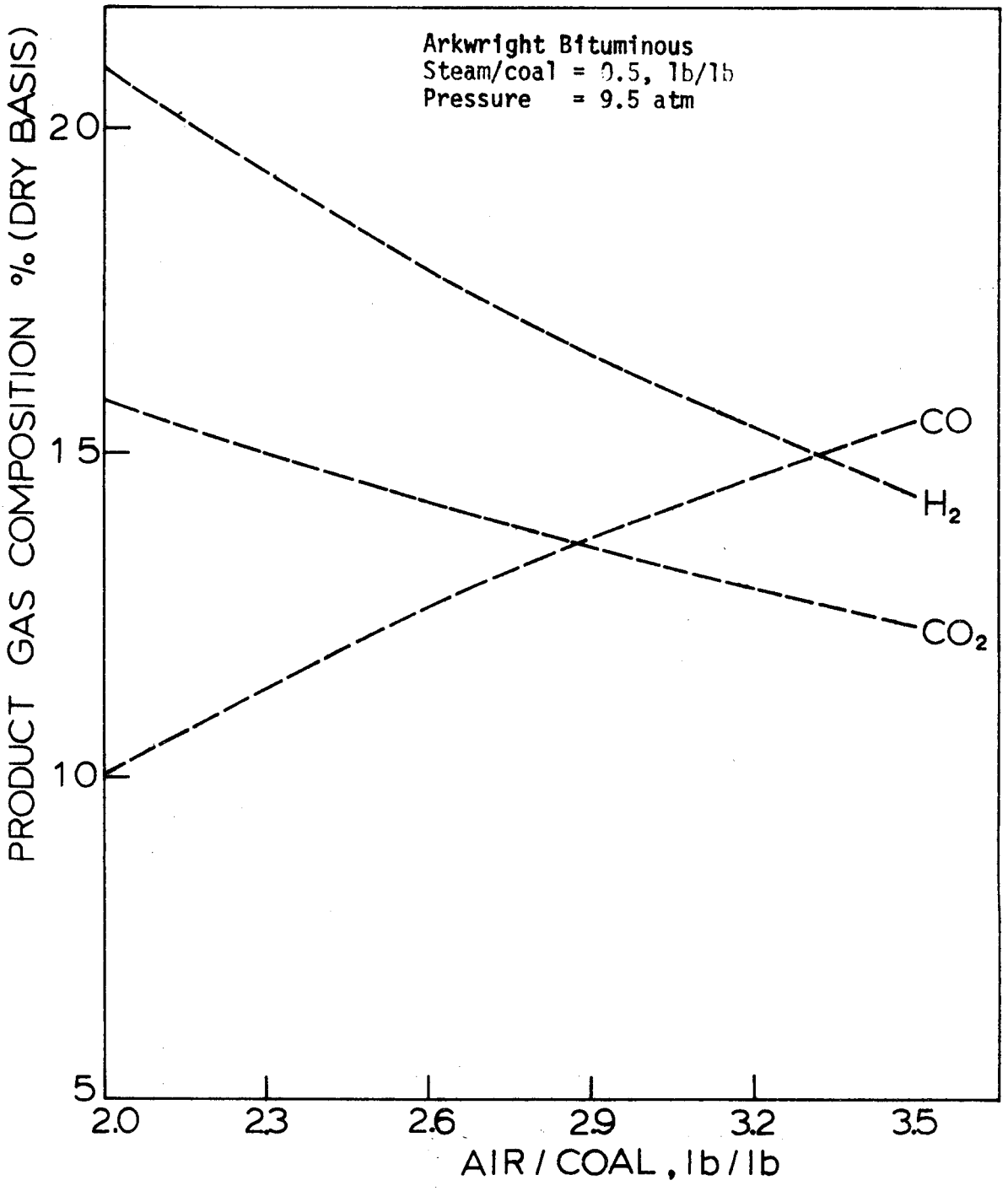


Figure 30 Effect of air/coal ratio on gas composition

heating value of the product, and on gas composition are shown in Figures 31 and 32 respectively.

Excess steam lowers the temperature in the bed and hence reduces the extent of char-CO_2 and char-steam reactions. Furthermore, the heat produced by the oxidation reaction is converted to sensible heat (in heating up the excess of steam) rather than the chemical heat (converting C to CO and H_2).

However, as watergas shift is comparatively fast even at low temperature, excess steam converts CO to CO_2 and H_2 as shown by the following reaction:

$$CO + H_2O \rightleftarrows CO_2 + H_2$$

Effects of pressure on the carbon conversion and the gas composition are presented in Figure 33 and Figure 34.

The rate of char-oxygen reaction is directly proportional to the partial pressure of oxygen. Hence, at low pressures (1-3 atms), oxidation starts late in the upper portion of the bed. This extends the combustion zone, which results in the lower conversion and the extent of shift conversion is also reduced. This can also be explained by the plot of height versus the temperature of bed at different pressures shown in Figure 35. However, higher pressures (5 atm and more) do not have any significant effect on the gasifier performance.

In a fixed bed gasifier, the residence time of coal is long (1-2½ hrs). If the bed height is increased, it increases the height of the drying-

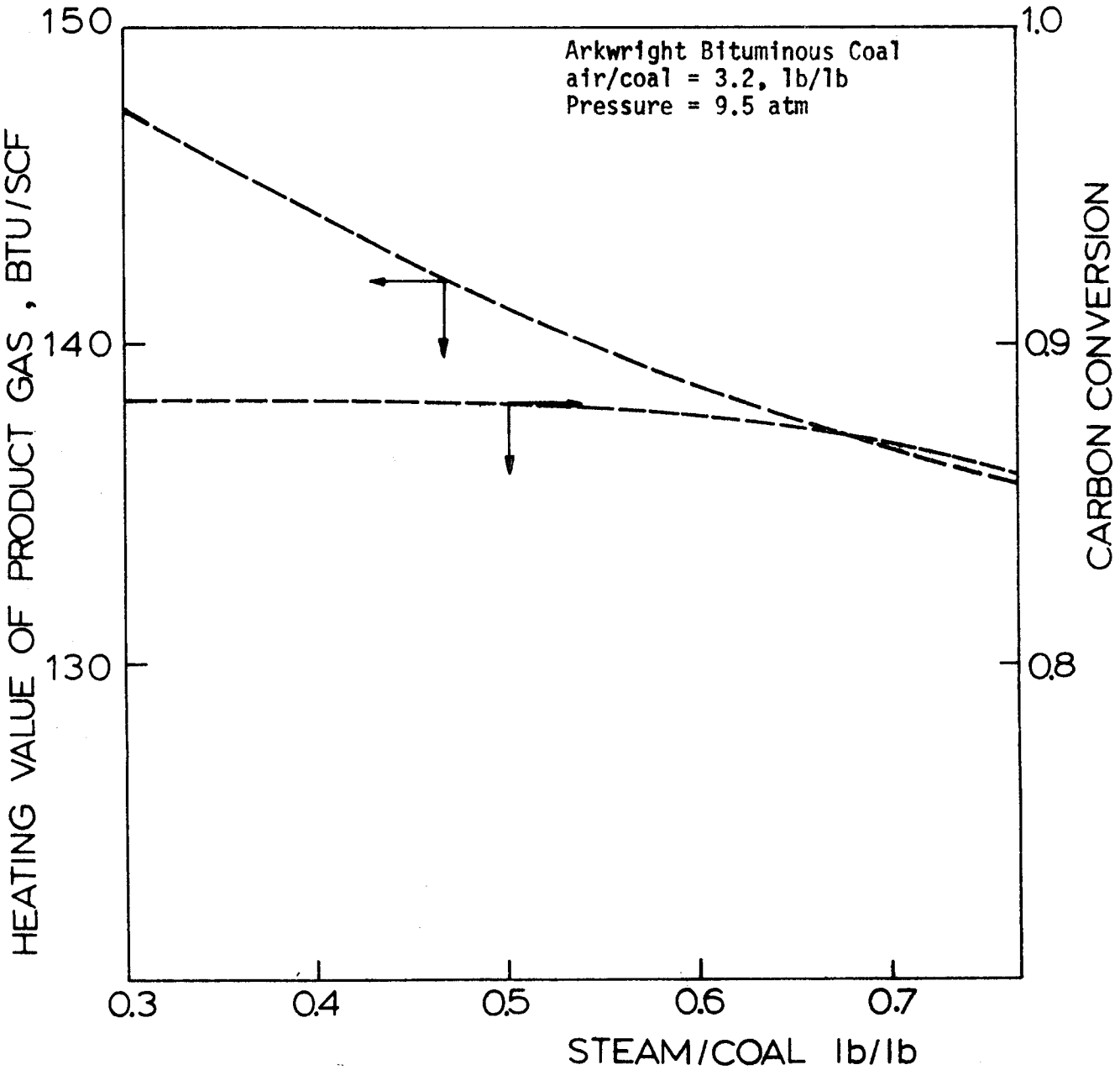


Figure 31 Effect of steam/coal ratio on carbon conversion and the heating value of product gas

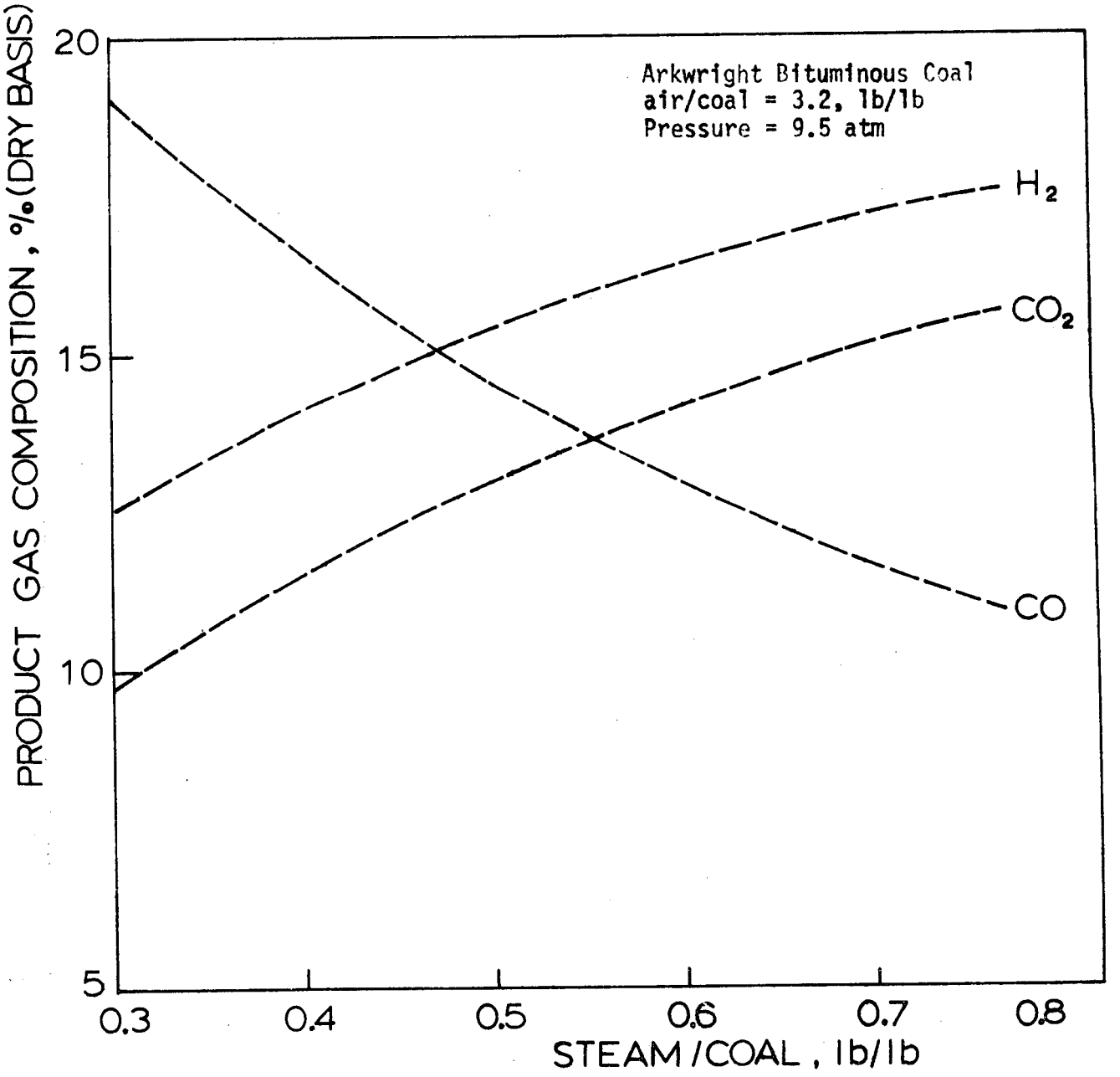


Figure 32 Effect of steam/coal ratio on gas composition

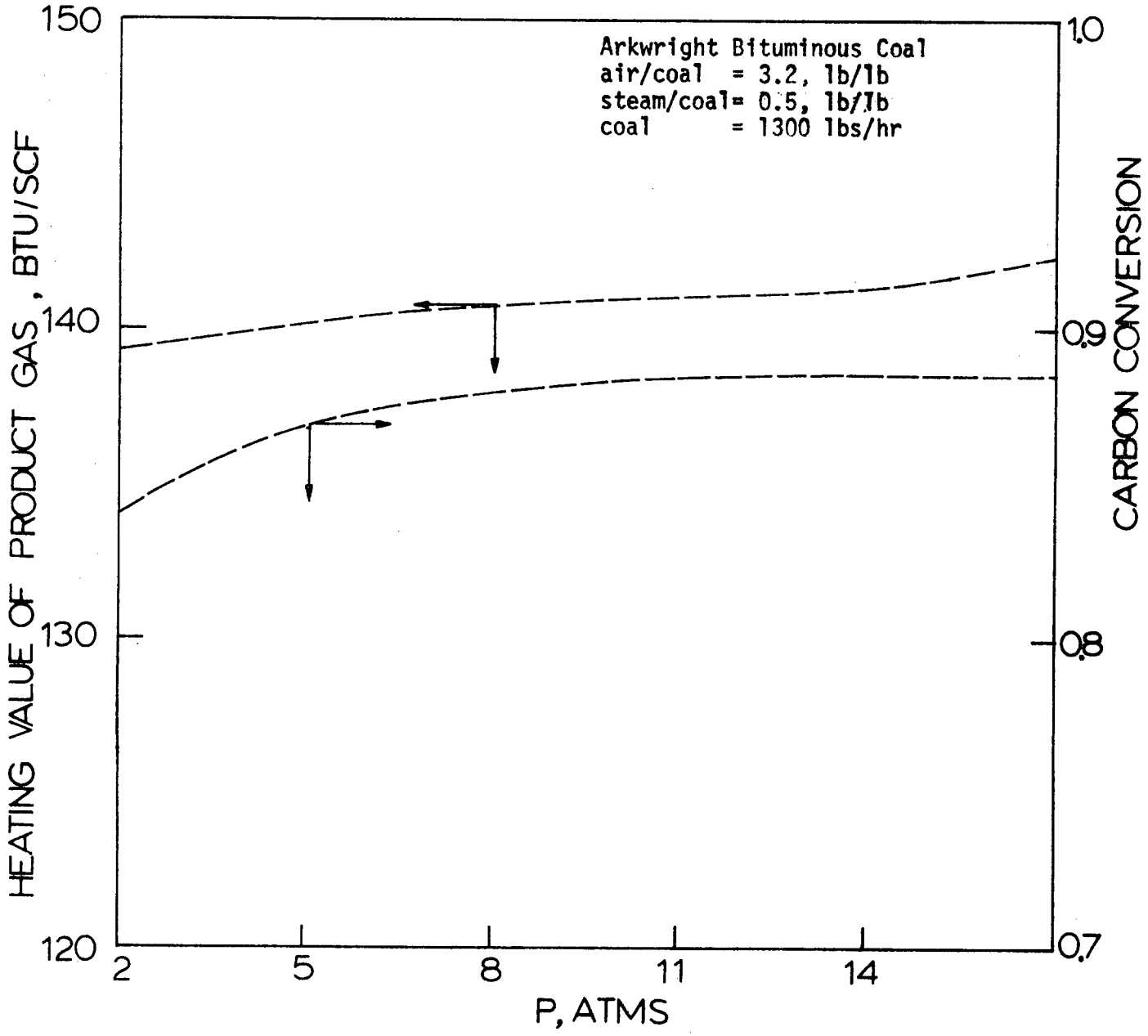


Figure 33 Effect of pressure on carbon conversion and the heating value of the product gas

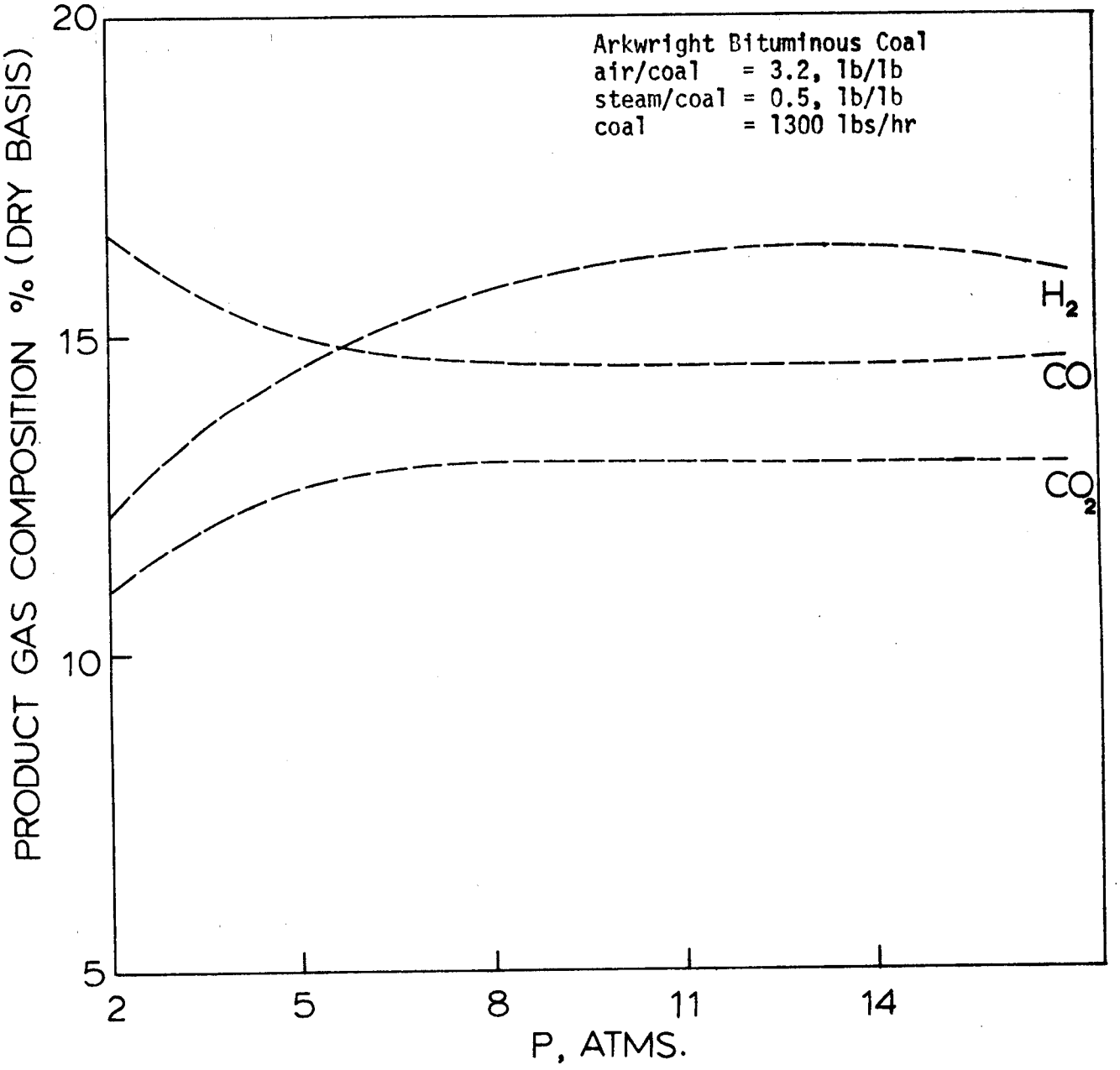


Figure 34 Effect of pressure on gas composition

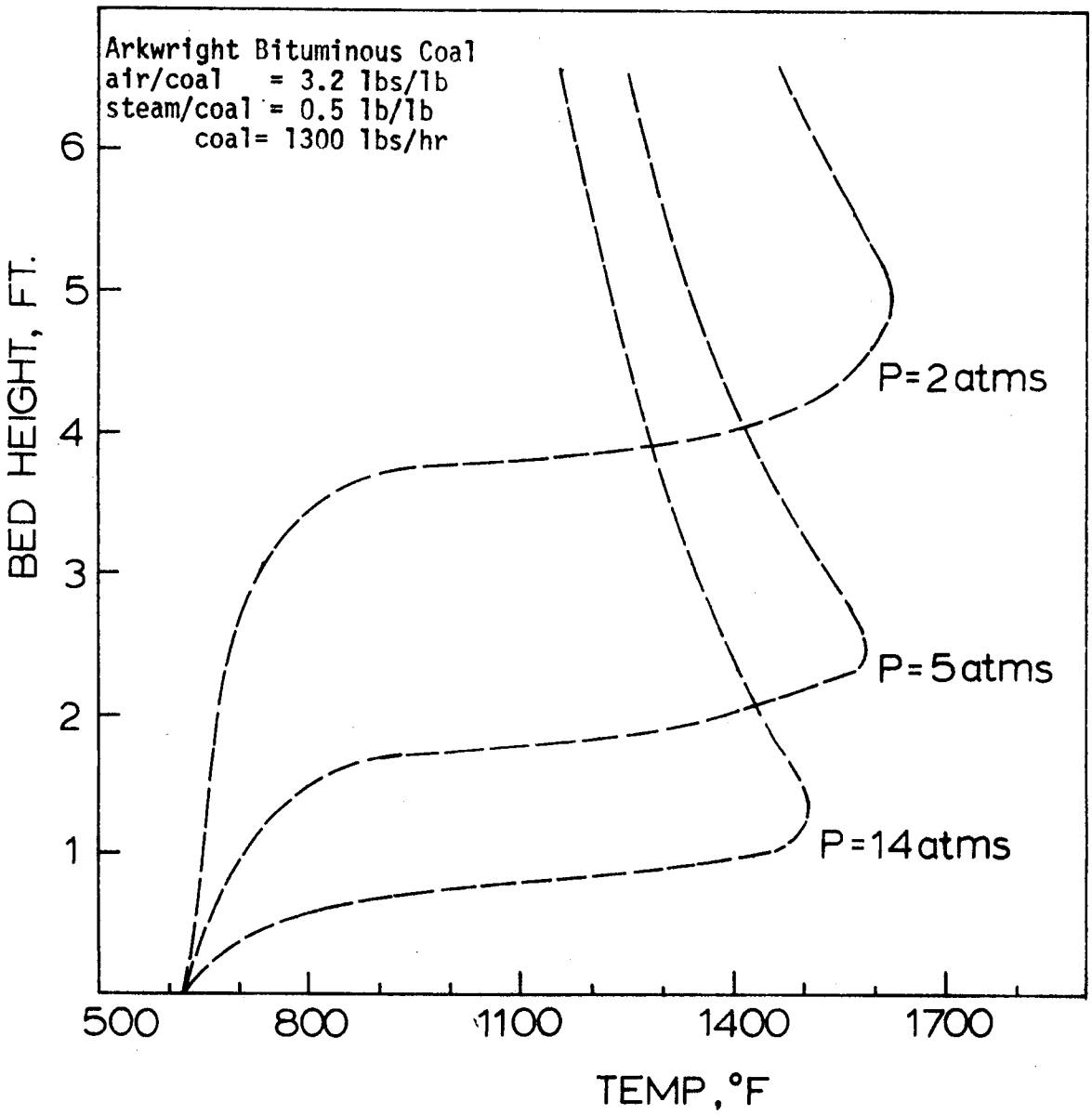


Figure 35 Temperature profiles at different pressures

devolatilization zone. This cools down the outgoing gas and slightly increases the extent of watergas shift reaction. Effect of bed height on gas composition and carbon conversion are shown in Figure 36 and Figure 37. In Table 10, temperatures at different heights are listed for different total bed heights. The operating variables used are same as that for Figures 36 and 37.

Heat loss in the MERC's gasifier is significant because the surface area per unit volume of the gasifier is high and also due to the use of water jacket. This higher heat loss is compensated by the char oxidation reaction requiring more air. In Figure 38, heat loss is plotted as a function of carbon conversion using air/coal ratio as a parameter. It is interesting to note that by reducing the heat loss, the consumption of air can be lowered considerably which is what is done in the GEGAS-D gasifier. Reduced heat loss will not only increase the thermal efficiency but will increase the heating value of the product gas.

4.3.1 Results For Oxygen-Steam System

Results, similar to the air-steam system, are presented for the oxygen-steam gasification system in this section.

In Table 11, composition and the heating value of the product gas are listed for the following feed rates (since experimental data are not available, coal feed rate was arbitrarily selected).

coal = 3000. lbs/hr
Steam = 5250 lbs/hr
oxygen = 2250 lbs/hr

In Figure 40, concentration profiles for CO, CO_2, H_2, H_2O and O_2

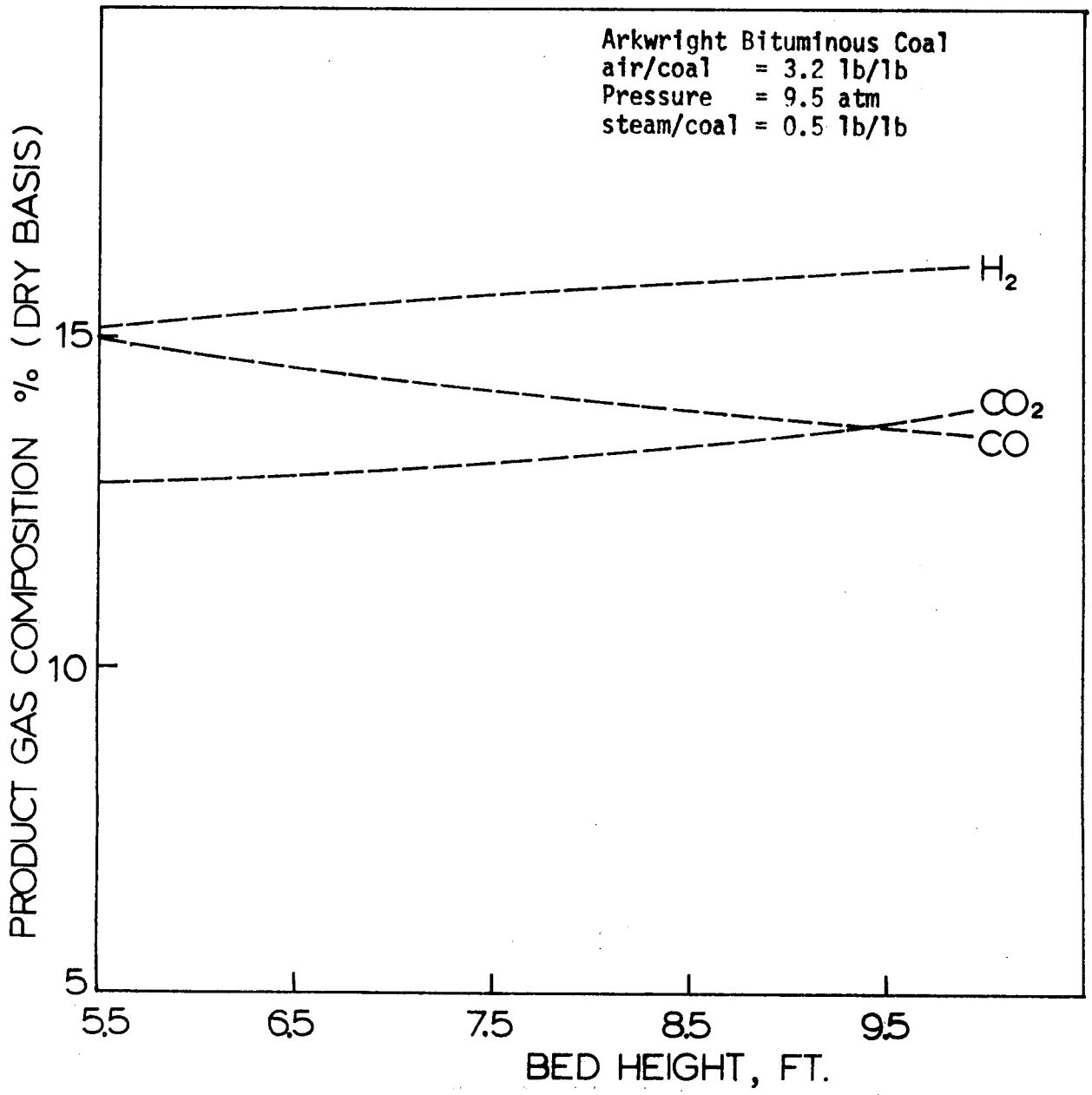


Figure 36 Effect of bed height on gas composition

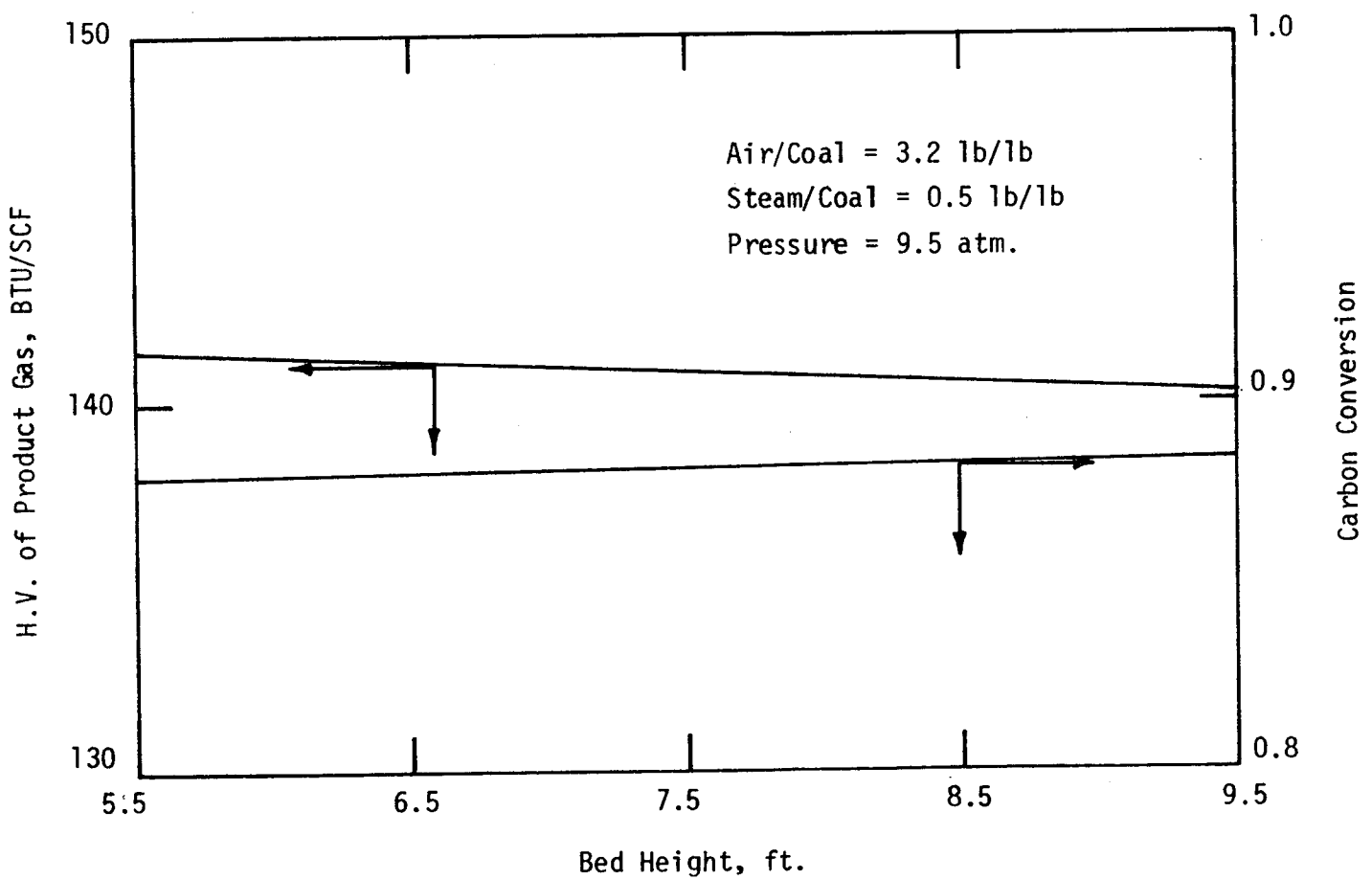


Fig. 37. Effect of bed height on carbon conversion and heating value of the product gas

TABLE 10

TEMPERATURES AS FUNCTION OF HEIGHT
FOR DIFFERENT TOTAL BED HEIGHTS

Total bed height ft.	5.5	7.5	9.5
Height ft.			
0.0	620. (°F)	620. (°F)	620. (°F)
0.5	649.	665.	667.
1.0	1001.	997.	975.
1.5	1486.	1486.	1530.
2.0	1496.	1497.	1498.
2.5	1440.	1442.	1443.
3.0	1398.	1410.	1400.
3.5	1356.	1356.	1358.
4.0	1331.	1322.	1324.
4.5	1300.	1293.	1295.
5.0	1264.	1264.	1266.
5.5	1241.	1240.	1241.
6.0	—	1214.	1217.
6.5	—	1190.	1190.
7.0	—	1167.	1167.
7.5	—	1143.	1144.
8.0	—	—	1124.
8.5	—	—	1101.
9.0	—	—	1080.
9.5	—	—	1063.
Exit Gas Temperature	1045.	950.	870.

Arkwright Bituminous Coal

Air/coal = 3.2 lb/lb

Steam/coal = 0.5 lb/lb

Pressure = 9.5 atms

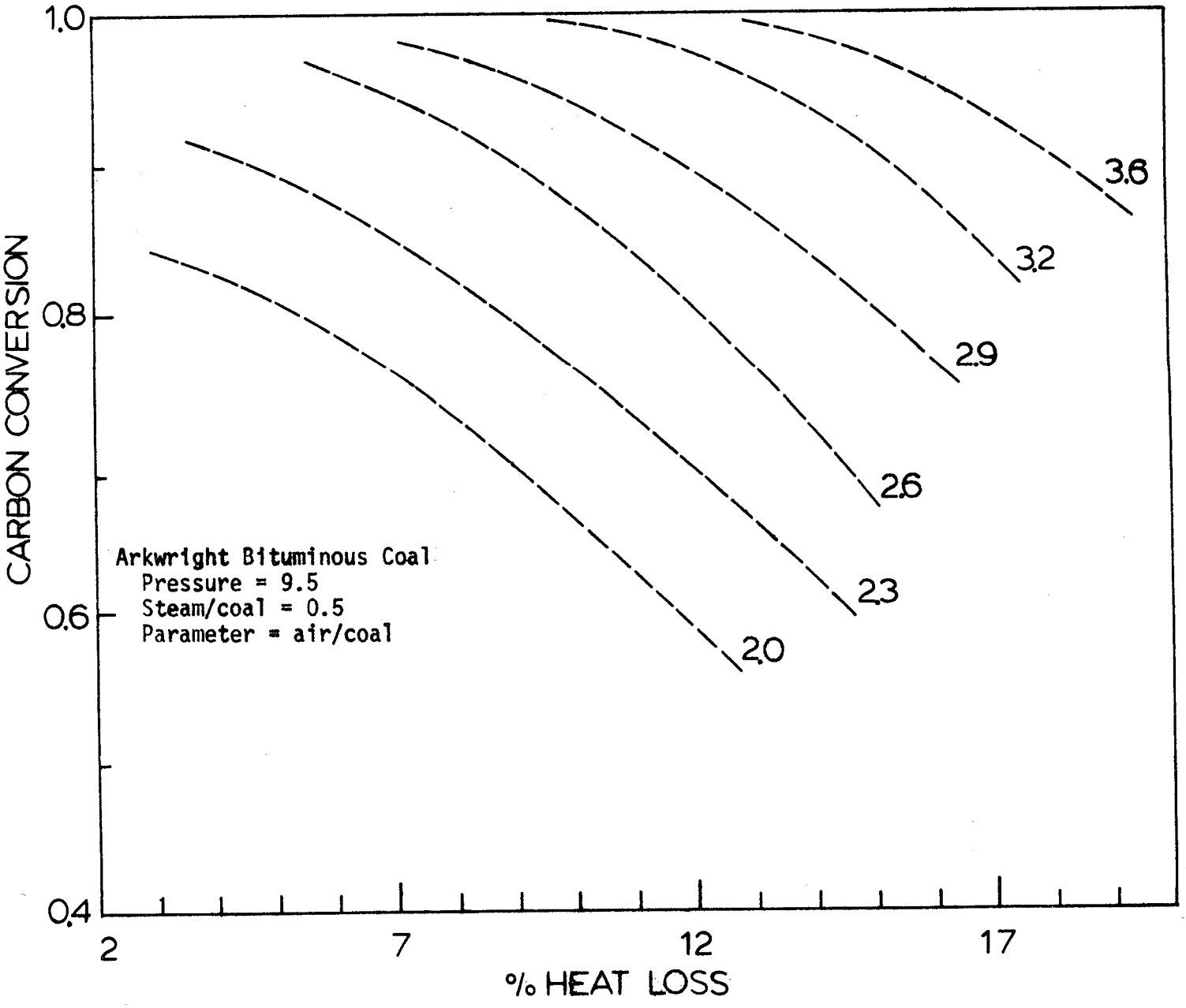


Figure 38 Effect of heat loss on carbon conversion
Heat loss = % of heating value of coal
(unaccountable heat + heat recovered by
cooling water)

TABLE 11

SIMULATION RESULTS OBTAINED FOR
COAL GASIFICATION WITH STEAM AND OXYGEN

Coal Type	Arkwright Bituminous	Upper Freeport	Western Kentucky
Feed Rate, lbs/hr	3000.	3000.	3000.
% Composition			
C	75.9	66.8	64.5
H	5.7	4.4	5.5
O	4.9	3.5	4.0
N	1.4	1.2	1.7
S	2.7	3.8	3.9
Ash	8.2	20.3	15.4
Moisture	1.12	1.0	5.0
Steam, lbs/hr	5250.	4500.	4500.
Oxygen, lbs/hr	2250.	1600.	1600.
Steam-Oxygen temp., °F	620	620	620
Product gas, lbmoles/hr	299.	215.4	231.7
Gas Composition			
CO	13.67	11.63	10.71
CO_2	34.9	34.79	32.61
N_2	0.95	1.41	1.31
H_2	42.16	39.61	43.08
CH_4	6.05	8.6	8.07
C_2H_6	0.5	0.72	0.67
H_2S	0.76	1.76	1.7
Steam decomposition, %	35.8	29.0	29.2
Heating value of gas BTU/SCF	260.	283.	286.
Temperature of gas, °F	995.	964.	980.
Carbon conversion	0.929	0.779	0.806
Heat loss, % (of coal heating value)	18.5	16.37	13.85

are shown for the above conditions.

Effects of various factors are shown in Figures 39 through 46 . Reasoning similar to what was discussed in connection with the air-steam system can be used to explain these effects, and hence need not be repeated.

The model developed in this study can be used to establish the operating variables.

From the Figures, it may be suggested that the following ranges should be used for the operation of oxygen-steam system.

oxygen/coal	0.6 - 0.8	lb/lb
steam/coal	1.5 - 2.0	lb/lb

The information available for Lurgi gasifier shows that the gasifying capacity (in lbs/hr/ft^2)increases 2 to 2.5 times when oxygen is used for gasification in place of air.

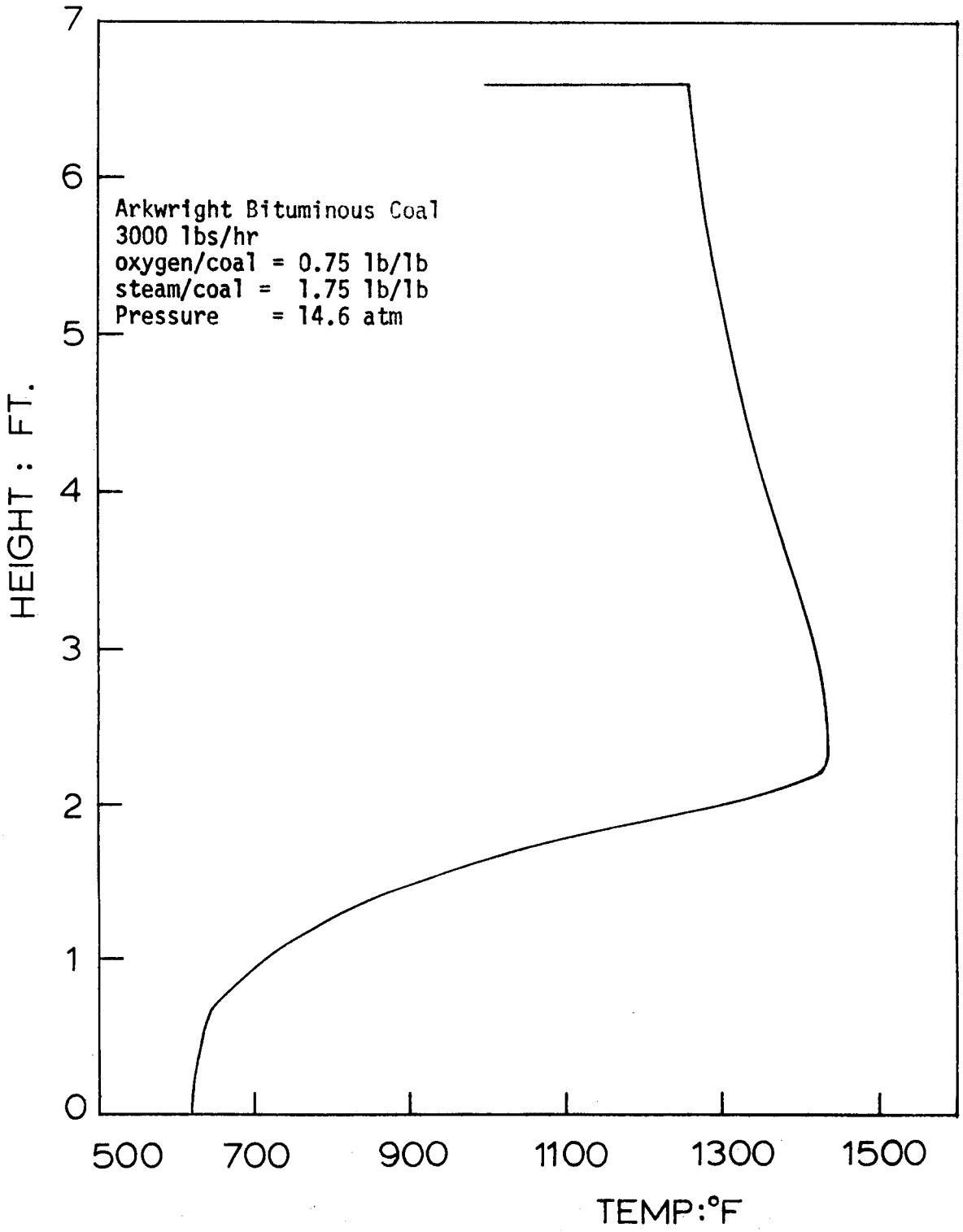


Figure 39 Temperature profile for oxygen-steam system

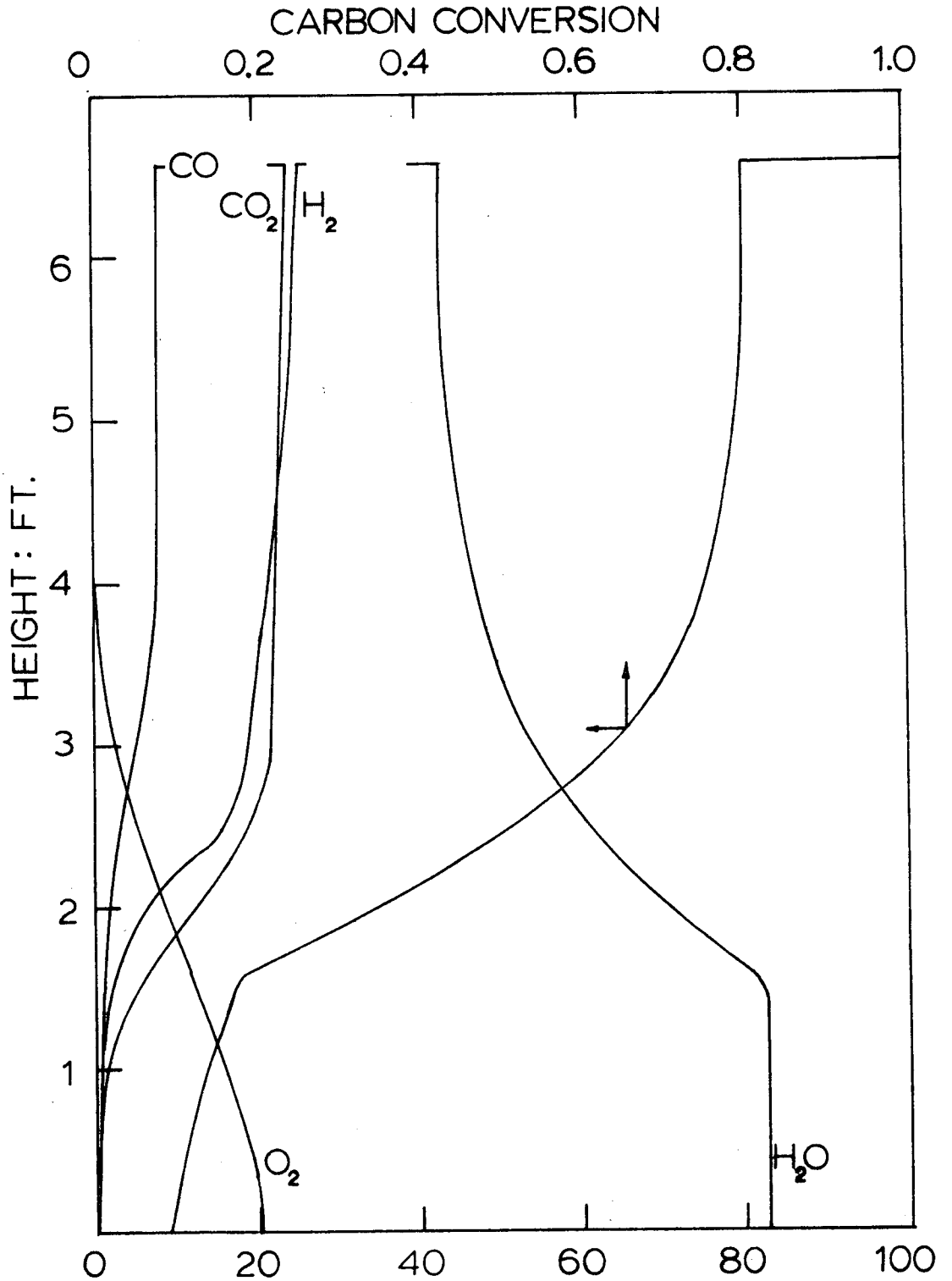


Figure 40 Concentration profiles for oxygen-steam system -

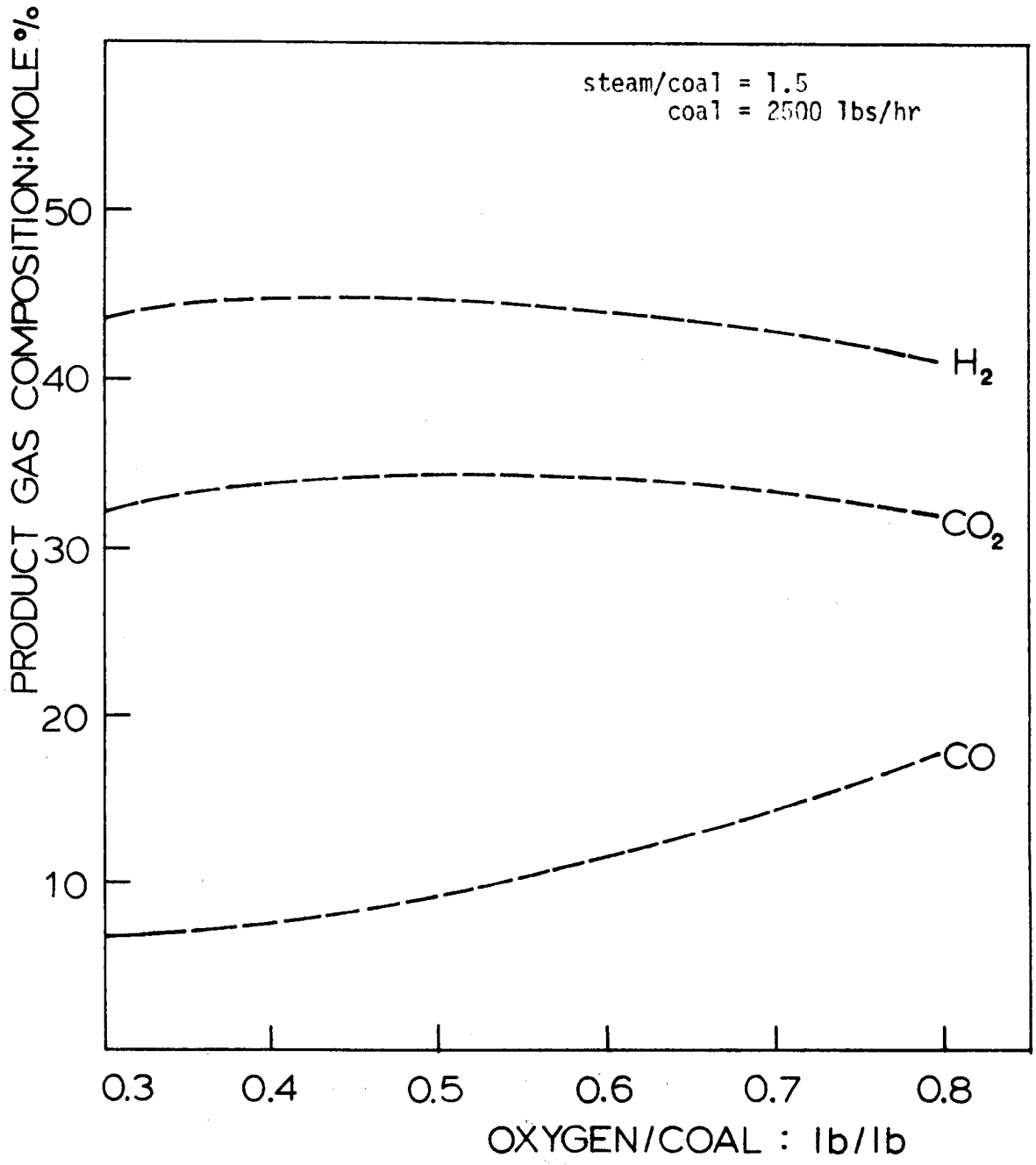


Figure 41 Effect of oxygen/coal ratio on the gas composition

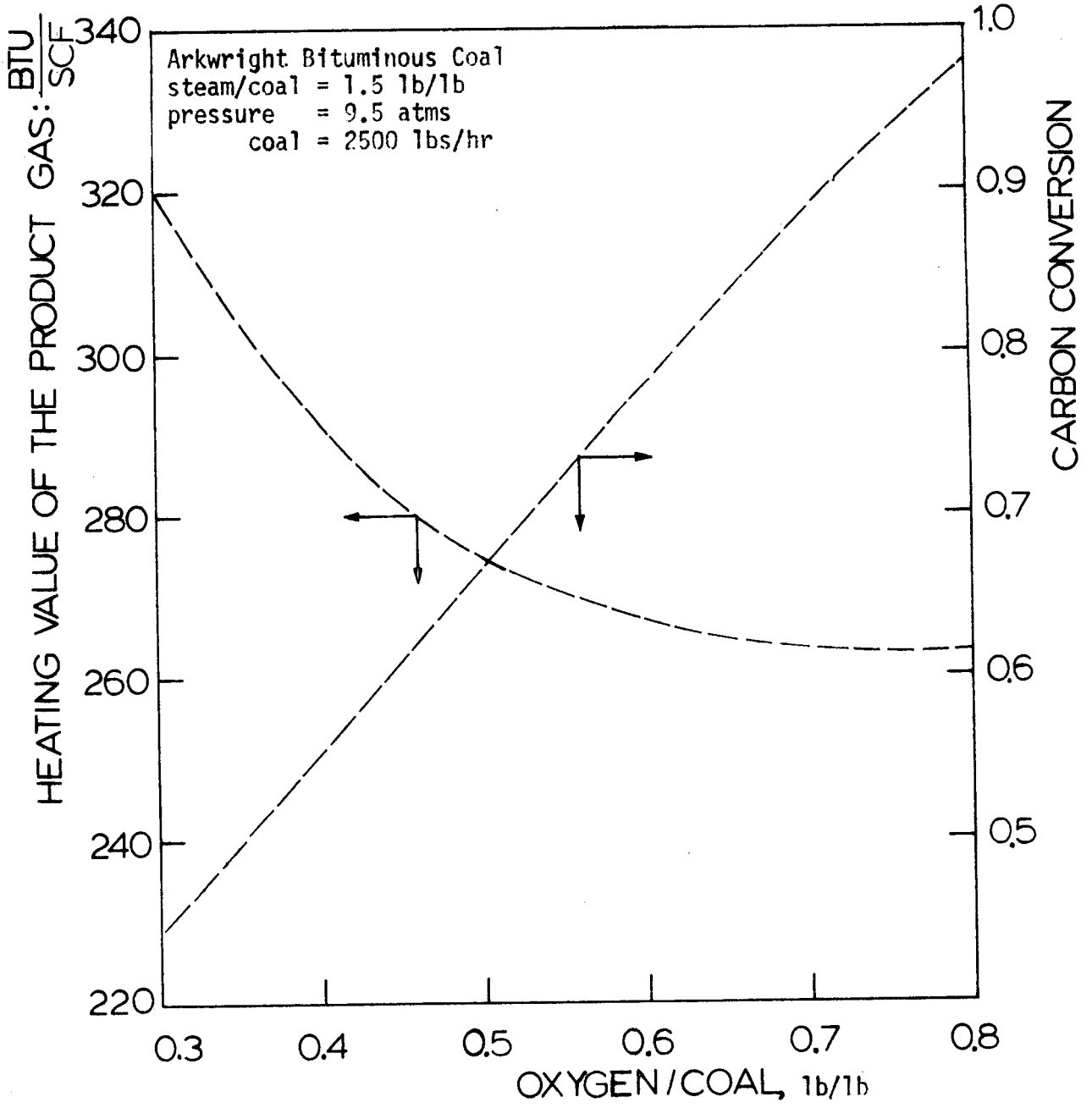


Figure 42 Effect of oxygen/coal ratio on carbon conversion and the heating value of the product gas

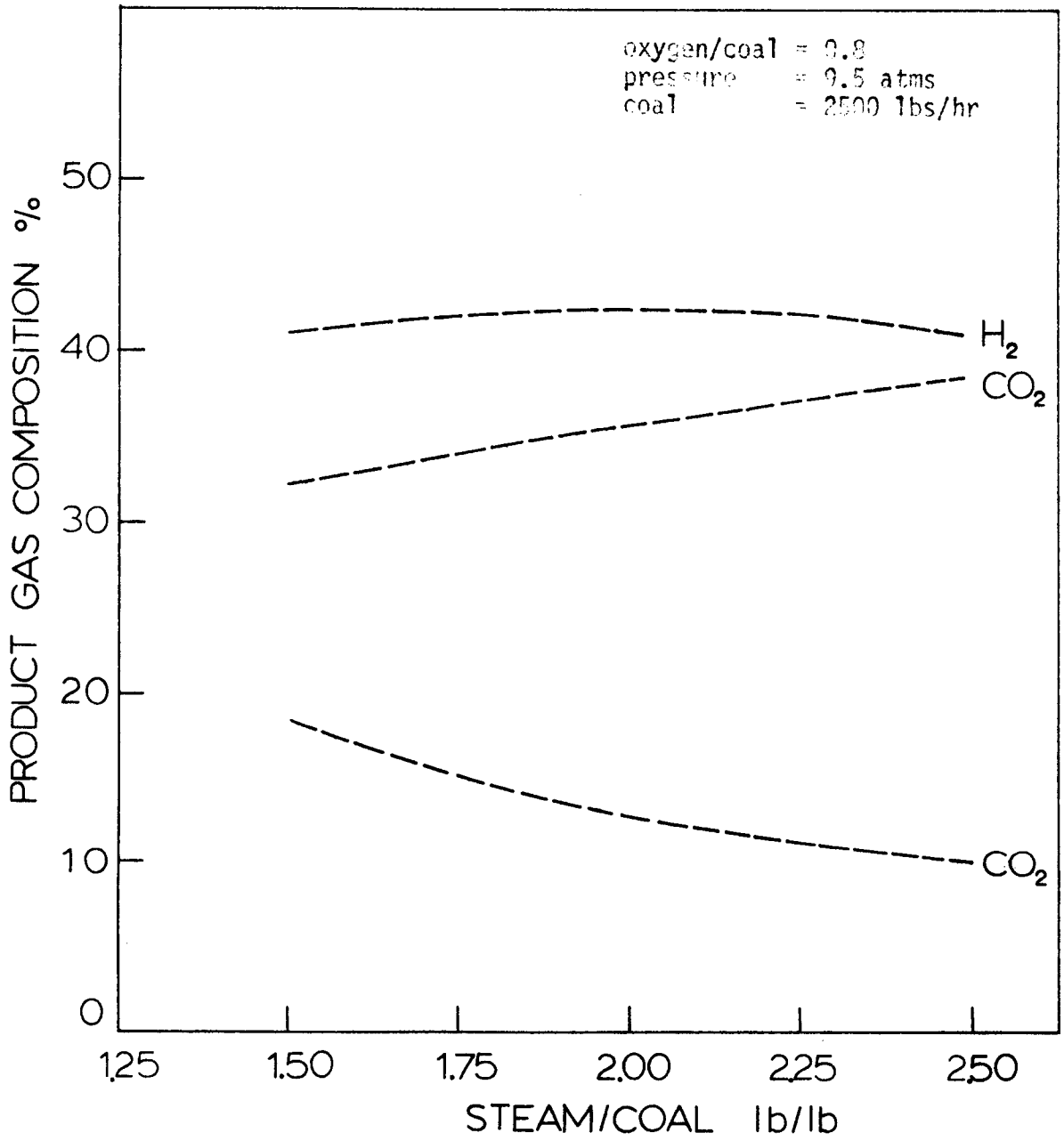


Figure 43 Effect of steam/coal ratio on gas composition

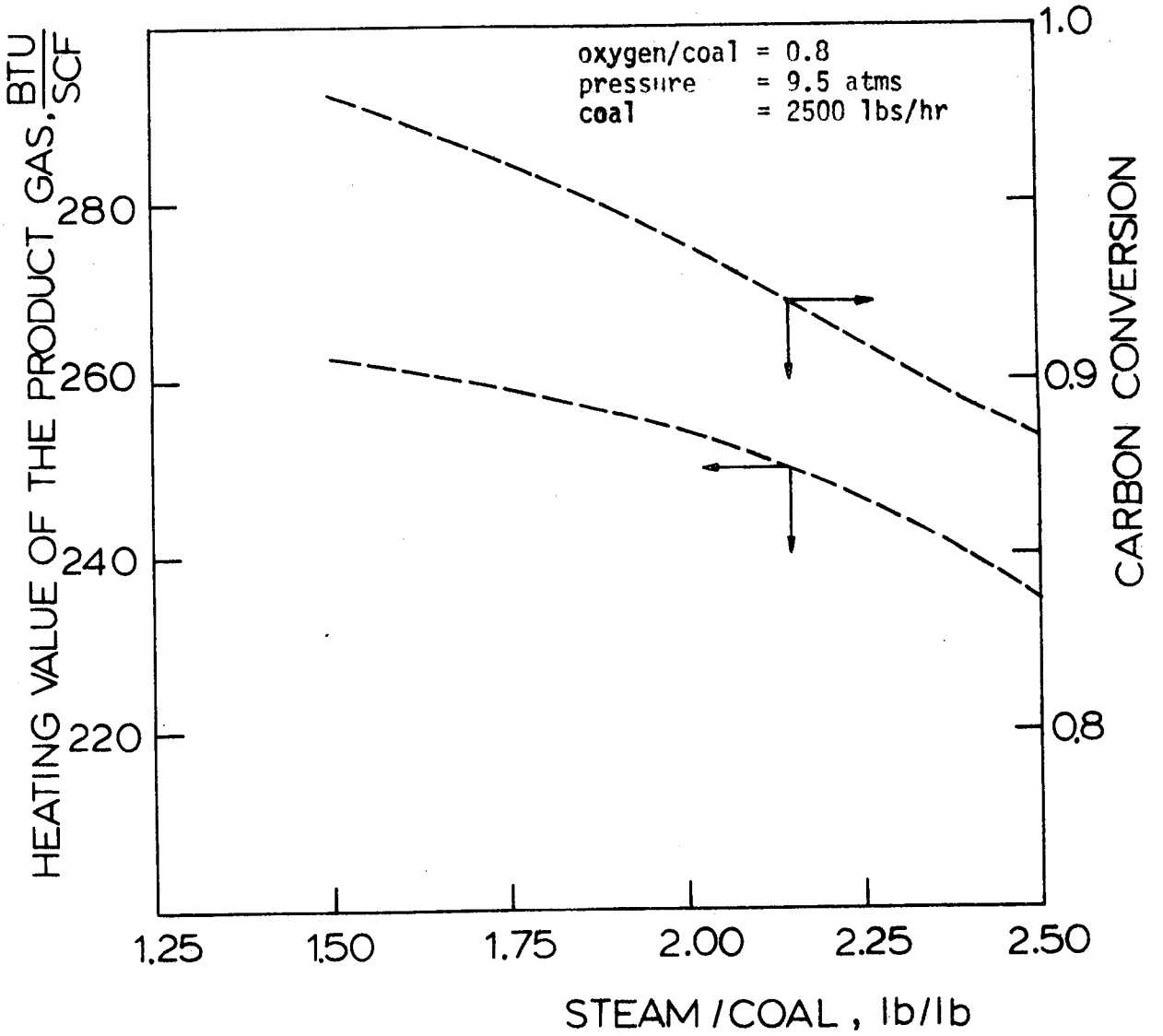


Figure 44 Effect of steam/coal ratio on carbon conversion and the heating value of product gas

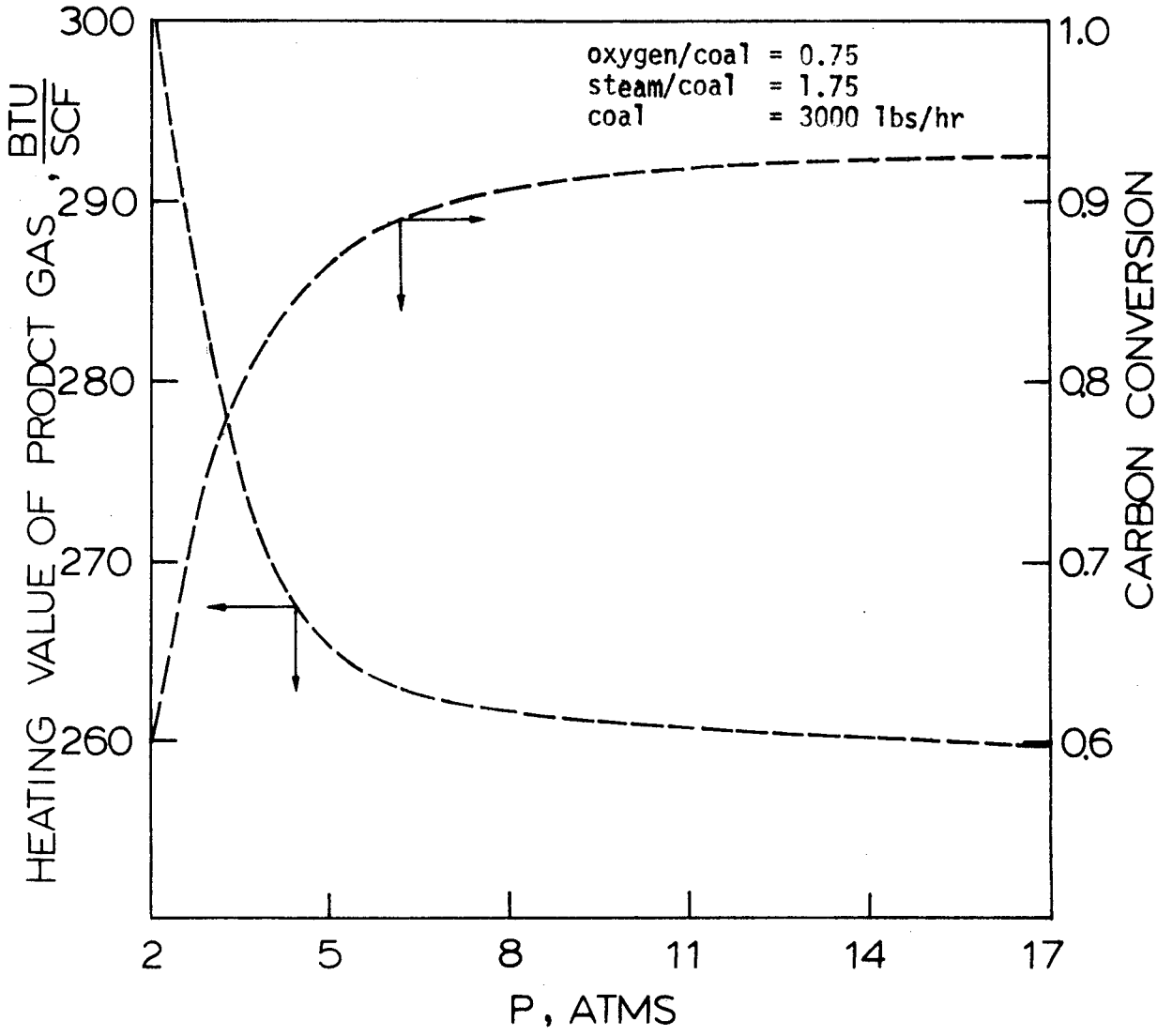


Figure 45 Effect of pressure on carbon conversion and heating value of product gas

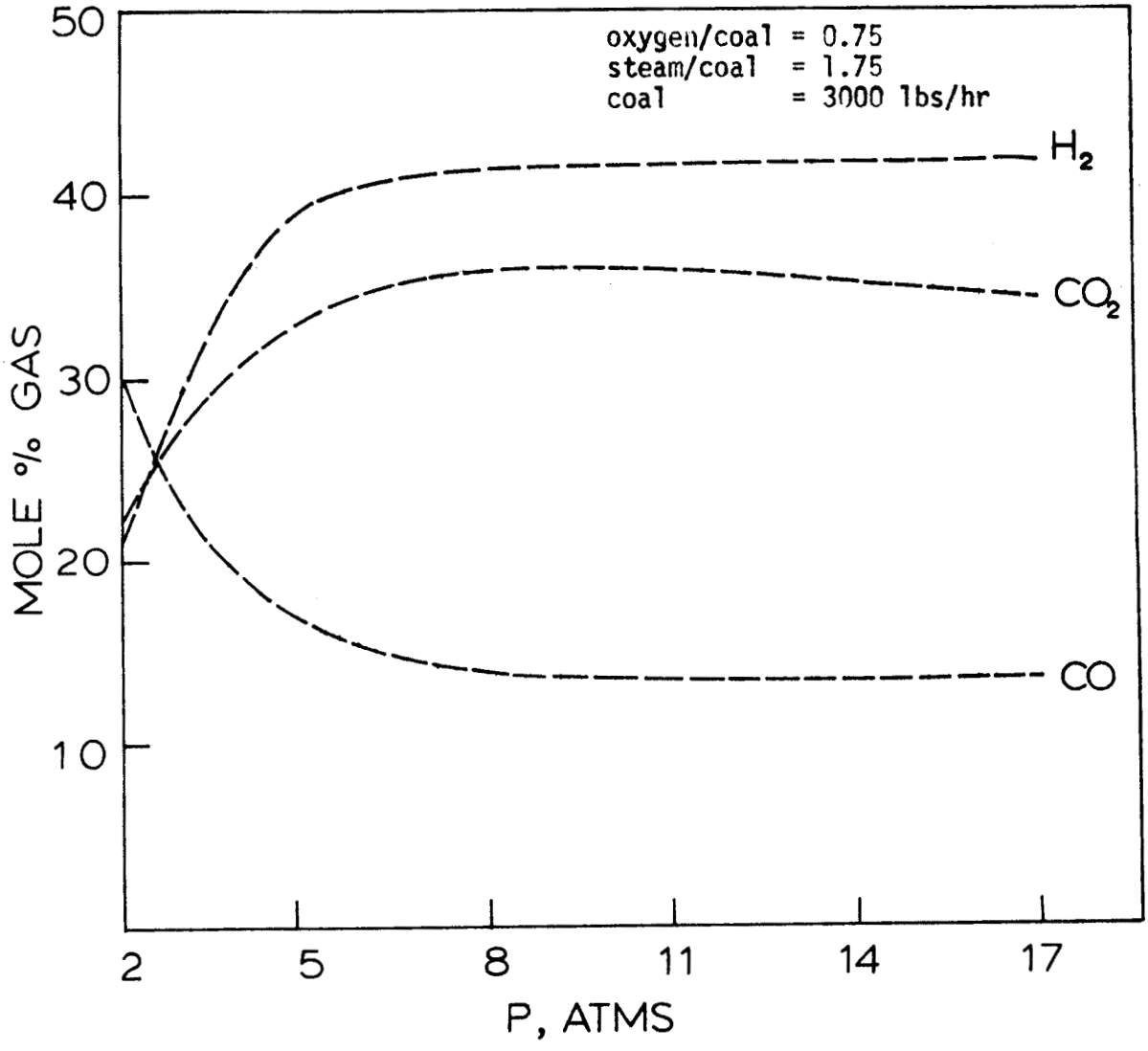


Figure 46 Effect of pressure on the gas composition

5. CONCLUSIONS AND DISCUSSION

5.1 Conclusions

The comparison of results presented in the previous sections show that MERC's fixed bed gasifier has been modeled successfully. Following conclusions can be made from this study:

1. Large amount of air has to be supplied to the gasifier because of the high heat loss.
2. The use of excess air reduces the heating value of the product gas.
3. Excess air increases the percentage of CO and reduces the percentage of CO_2 and H_2 in the product gas.
4. Excess steam does not have a significant effect on carbon conversion, however CO is shifted by the water gas equilibrium to produce more hydrogen.
5. Pressure, (higher than 5 atms and less than 17 atms) does not have a significant effect on the gasifier performance except that more coal can be gasified per unit area.
6. Amount of methane formed is fairly constant and depends mainly on the type of coal.
7. Height of the bed does not significantly affect the carbon conversion or the gas composition. It lowers the temperature of the outgoing gas.

8. There is no apparent correlation between the amount of tar produced and any of the operating variables.
9. This model can also be used to simulate an oxygen-steam system.
10. The estimation of two separate temperature profiles for the gas phase and the solid phase is necessary to predict the actual maximum temperature.

5.2. Suggestions for Improving this Model:

The model developed in this study can be further improved along the lines discussed below.

5.2.1. Temperatue Profile for Gas Phase and Solid Phase:

The initial value of temperature assumed at the bottom of the gasifier (above the grate) in calculation of temperature profile has a significant effect on the accuracy of the temperature profile. Therefore, it would be more useful if separate temperature profiles for both gas phase and the solid phase are estimated. This calculation will be useful especially in the drying-devolatilization zone and the ash zone. It will also indicate the actual maximum temperature of the solid rather than the average temperature of the bed.

5.2.2. Heat Loss:

Heat loss in the MERC pilot plant gasifier is about 13 - 18 % of the heating value of the coal. In this study, heat loss (which includes unaccountable heat loss and the heat recovered by cooling water) was assumed to be proportional to the fraction of heat generated in the combustion zone. This assumption needs further modification. Since the walls of the vessel are cooled by the water jacket, there is a temperature gradient in the radial direction, with

that portion of the bed close to the wall being at a lower temperature. It is possible therefore, that little reaction will occur in this region. Heat loss is important in a MERC's gasifier but is expected to be less significant in case of a larger gasifier.

5.3. Need of Further Information:

It has been mentioned at several places in this report, that experimental data available on the kinetics of coals under varied conditions are scarce. The need for these data cannot be over emphasized. Even the structure of coal is not yet understood completely and needs additional effort to clarify its effect on gasification. In pyrolysis, total yield of volatiles can be estimated with a fair degree of accuracy. However, the composition of product gas or the amount of tar cannot be determined with any certainty. Since product distribution depends on a number of factors; for example, type of coal, particle size, temperature, heating rate, etc., further investigation is needed in this area. Similarly, the rate constants reported by various investigators vary widely because of different experimental conditions and techniques employed.

Very little information is available on the stoichiometry of char-oxygen or char-steam reactions. This type of data will also help in determining the amounts of gasifier products like HCN, NH_3, SO_2 and CO's which are present in small quantities.

The main products of the char-oxygen reaction are carbon monoxide and carbon dioxide. Data available in the literature are insufficient to estimate accurately the ratio of CO to CO_2 formed as a result of oxidation. Part of the CO formed may react with the oxygen in the gas phase producing additional carbon dioxide. This may be significant in the estimation of a gas temperature profile.

Furthermore, the extent of methane formation as a result of gas phase reaction ($CO + 3H_2 \rightarrow CH_4 + H_2O$), or solid gas reaction ($C + 2H_2 \rightarrow CH_4$), or during pyrolysis needs further clarification.

5.4. Suggestions for Further Work:

Other factors, which should be examined in modeling of MERC's gasifier are listed below:

1. Effect of Feed Size:

Coal particles swell to different degrees during pyrolysis depending upon the characteristics of coal. This change in particle size will affect the rates of various reactions. In addition, the heat transfer between solid and gas also depends on the particle diameter.

The composition and physical structure of ash formed during and after coal gasification play an important role in chemical and physical phenomena of coal gasification. Very little if any information is available on this aspect.

2. Effect of Stirrer:

There seems to be a correlation between the stirrer speed and the amount of dust formed. The cooling water circulated through the stirrer may have some effect on the temperature of bed. The effect of stirrer speed on the mixing of the bed should also be examined.

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APPENDIX

Calculation of devolatilization product distribution:

Total yield of volatile products is estimated using Gregory and Little-John equation assuming that solid is at 850°K.

In addition, the following assumptions are made:

(1) Amount of carbon in tar = 4% carbon in coal feed, composition of tar is as follows:

C = 85.0% by wt.

H = 6.0

O = 5.0

N = 1.4

S = 1.9

Ash = 0.7

(2) Amount of methane formed/lb of coal = 0.0035 lbmole

(3) $CH_4/C_2HC = 12.$

(4) $CO/CO_2 = 5.$

(5) $\% \text{ H converted} = \left(0.35 - 0.65 \frac{X_c}{100.}\right)100.$

$\% \text{ N converted} = \left(0.3 - 0.74 \frac{X_c}{100.}\right)100.$

$\% \text{ S converted} = \left(0.3 - 0.74 \frac{X_c}{100.}\right)100.$

where X_c = % of carbon converted.

(6) All the oxygen present in coal is converted to various products during pyrolysis using these assumptions, product distribution of CO, CO_2, H_2S, NH_3, CH_4, C_2H_6, H_2, and H_2O was estimated.

One such calculation gives the following results:

CO	10. %
CO_2	2. %
H_2	38. %
CH_4	33. %
C_2H_6	3.4 %
H_2O	4.4 %
NH_3	5.0 %
H_2S	4.23 %

It is to be noted that this is a rough estimation based on material balance of H, O, N, and S. This calculation cannot be improved, at this time, because of lack of experimental data.

NOMENCLATURE

Main Program

HTBED = height of bed, cm i.e. bed, cm

AREA = cross-sectional area, cm^2

TEMPA = temperature at the bottom of the bed

XC = assumed carbon conversion

XO_2 = mole fraction of oxygen

XH_2O = mole fraction of steam

XCO = mole fraction of carbon monoxide

XCO_2 = mole fraction of carbon dioxide

XH_2 = mole fraction of hydrogen

XCH_4 = mole fraction of methane

XCARB = carbon fraction

XASH = ash fraction

HR = heat of reaction

A_8 = heat of reaction of exothermic reaction

A_9 = heat of reaction of endothermic reaction

A_{10} = heat of reaction in the gas phase

HTLOSS = heat loss in cal/sec/cm

WGEC = water gas equilibrium constant, theoretical

WGEE = water gas equilibrium constant, calculated

XCAL = calculated carbon conversion

STDE = steam decomposition, %

HVG = heating value of the gas, BTU/SCF

PHLOSS = % of heat loss

COLDE = cold gas efficiency, %

TEFF = thermal efficiency, %

CPS = heat capacity of solid, cal/gm°K

CSEQK = char-steam reaction equilibrium constant

AKV = char-steam rate constant

WGEQK = water gas shift equilibrium constant

AK_2 = rate constant for char-carbon dioxide reaction

AK_7 = rate constant for char-hydrogen reaction

EQ_7 = equilibrium constant for char-hydrogen reaction

Subroutine S to 1

$$C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon + (\alpha/2 + \beta/2 + \gamma + \delta/2 + \varepsilon)O_2$$

$$\rightarrow CO + CO_2 + \beta/2\ H_2O + \varepsilon\ SO_2 + \delta\ NO$$

Subroutine S to 2

$$C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon + (\alpha - \gamma)H_2O$$

$$\rightarrow \alpha\ CO + (\alpha - \gamma - \beta/2 - \varepsilon)H_2O + \delta/2\ N_2 + \varepsilon\ H_2S$$

Subroutine FPPLOT

X1 = Array of X variable

Y1 = Array of Y variable

NPT = Number of points

ICHAR = Character for printing

J = Maximum number of points

Subroutine Input

MOIST = moisture in coal, %

VM = volatile matter of coal, %

F1XC = fixed carbon in coal, %

ASH = ash in coal, %

HVCOAL = heating value of coal, BTU/lb

FC = fraction of carbon in coal

FH = fraction of hydrogen in coal

FO = fraction of oxygen in coal

FN = fraction of nitrogen in coal

FS = fraction of sulfur in coal

FASH = fraction of ash in coal

COAL = coal feed rate, lb/hr

AIR = air feed rate, lb/hr

STEAM = steam feed rate, lb/hr

TCOAL = temperature of coal, °F

TAIR = temperature of air, °F

TSTEAM = temperature of steam, °F

P = pressure, psig

DIA = diameter of the vessel, ft.

HT = height of the bed, ft.

HSTEAM = enthalpy of steam

AMW = molecular weight

Subroutine CPH

$C_p = \alpha + \beta T + \gamma T^2$

H_2 = Enthalpy of gas at temperature T

HFO = heat of formation at 298°K

Subroutine CRRECT

XNEW = new assumed value for convergence

INDX = identification number, if equal to 1, the converged value lies between the assumed and the calculated value.

DX = step size

E1 = previous error

E2 = present error

X1, X2 = old and new values of the variable

Subroutine DEVO

XCH_4 = moles of methane formed/lb of coal

YIELD = volatile products yeild

ALPHA = gm-moles of carbon in coal (ash free)

BETA = gm-moles of hydrogen in coal (ash free)

DELTA = gm-moles of nitrogen in coal (ash free)

EPSI = gm-moles of sulfur in coal (ash free)

GAMMA = gm-moles of oxygen in coal (ash free)

ALPHPP = gm-moles of carbon in tar

BETPP = gm-moles of hydrogen in tar

GAMPP gm-moles of oxygen in tar

DELPP = gm-moles of nitrogen in tar

EPSPP = gm-moles of sulfur in tar

ATAR = amount of tar produced, gm/sec

XP = % of carbon conversion in devolatilization

EPSIP = gm-moles of sulfur remaining in char

BETAP = gm-moles of hydrogen remaining in char

DELTAP = gm-moles of nitrogen remaining in char

DCH_4 = gm-moles of methane formed

DH_2S = gm-moles of hydrogen sulfide formed

DC_2H_6 = gm-moles of ethane formed

DH_2O = gm-moles of water formed

DNH_3 = gm-moles of ammonia formed

DH_2 = gm-moles of hydrogen formed

DCO_2 = gm-moles of carbon dioxide formed

DCO = gm-moles of carbon monixide formed

Subroutine RATES

TS = solid temperature, °K

TG = gas temperature, °K

RATE1 = char-oxygen reaction

RATE2 = char-steam reaction

RATE3 = water gas shift reaction

RATE4 = $CO + 1/2\ O_2 \rightarrow CO_2$

RATE5 = $H_2 + 1/2\ O_2 \rightarrow H_2O$

RATE6 = char-carbon dioxide reaction

RATE7 = char-hydrogen reaction

TM = mean temperature

KS = surface reaction coefficient

KDIFF = diffusivity coefficient

```
      REAL MOIST
       DIMENSION DLOSS(300),DLOST(300),DHT(300)
       DIMENSION X3(300),X4(300),X5(300),X6(300),X7(300)
        DIMENSION PGAS(12),PSOLID(6),Y3(300),ICHAR1(5),HG(12),CS(300,20)
        DIMENSION AMW(18),H(12),CP(12)
       DIMENSION X1(300),Y1(300),ICHAR(5)
        DIMENSION  WGEC(300),WGEE(300)
      DIMENSION E(20),F(20),DF(20),FI(20),D(360)
       DIMENSION HV(12)
       COMMON/AA/MOIST,VM,FIXC,ASH,HVCOAL,FC,FH,FO,FN,FS,FASH,COAL,AIR
     1,STEAM,TCOAL,TAIR,TSTEAM,P,DIA,HT,VM1,HSTEAM
      COMMON/FF/F
      COMMON/DD/H,CP
       COMMON/AE/ALPHPP,BETPP,GAMPP,DELPP,EPSPP
      COMMON/BD/AMW
      EQUIVALENCE (E(1),DF(1)),(F(1),FI(1))
       DATA ICHAR/'1111','2222','3333','4444','5555'/
       DATA E/18*0.001,2*2./
      DATA PI,R/3.1415,82.05/
       DATA ICHAR1/'3333','4444','5555','6666','7777'/
         DATA DZ,TB,NSF,ISW,N,N154/2.0,0.0,3,2,20,360/
      DATA DP,EP/0.5,0.4/
       DATA HV/321.1,0.0,0.0,0.0,324.8,1011.6,1772.1,638.9,0.0,0.0,0.0,435.5,0.0
     2,0.0/
C     1=CO,2=CO2,3=N2,4=H2,5=CH4,6=C2H6,7=H2S,8=O2,9=H2O,10=NH3,11=NO
C     12=SO2,13=C,14=H,15=O,16=N,17=S,18=ASH,19=TS,20=TG
C     GASES ARE IN GM-MOLE/SEC
C     SOLIDS ARE IN GM/SEC
C     TEMPERATURE IS IN DEGREE KELVIN
C     INPUTS AND OUTPUTS ARE IN FPS UNITS, HOWEVER ALL THE CALCULATIONS
C     ARE DONE IN CGS UNITS
C     RATE1      C+O2 =CO+CO2
C     RATE2    C+H2O  ---CO+H2
C     RATE3      CO+H2O  ----CO2+H2-
C     RATE4       CO+1/2-O2     _____ CO2
C     RATE5      H2+O2 -----H2O
C     RATE6      CO2+C _____ 2CO
C
C       IF PLOT OF TEMP. VS. HT OR CONC VS HT IS NEEDED THAN PUT NPLOTR=1
C      OTHERWISE SUBSTITUTE NPLOTR=2
C
      CALL INPUT
         COAIR=AIR/COAL
C     CONVERTS UNITS OF COAL,STEAM AND AIR FEEDRATES FROM LBS/HR TO GMS/SEC OR
C     GMOLES/SEC
       COAL=COAL*454.4/3600.
        AIR=AIR*454.4/3600./(0.21*AMW(8)+0.79*AMW(3))
      STEAM=STEAM*454.4/3600./AMW(9)
        VM1=VM
       P=(P+14.7)/14.7
 1009 CONTINUE
       KX=1
   64  CONTINUE
C
C     PRELIMINARY CALCULATIONS E.G. C,H,O,N,S, IN FEED,HEIGHT OF BED,AREA ETC
C
      C=COAL*FC
      HY=FH*COAL
      O=COAL*FO
      AN=COAL*FN
      S=COAL*FS
      ASH=COAL*FASH
       HTBED=HT*30.48
       WRITE(6,105)AIR,COAL,STEAM
        NBED=HTBED+0.5
       HTBED=NBED
      AREA=DIA*DIA*30.48*30.48*PI/4.
       TAIR=(TAIR+460.)/1.8
       TSTEAM=(TSTEAM+460.)/1.8
       CALL CPH(3,TAIR,CP(3),H(3))
       CALL CPH(9,TSTEAM,CP(9),H(9))
       TG=(AIR*CP(3)*(TAIR-298.)+STEAM*CP(9)*(TSTEAM-298.))/(AIR*CP(3)
     2+STEAM*CP(9))+298.
       TEMPA=600.
       XC=0.999
       DX=-0.02
```

```
      L=1
       INDX=0
       U13=PI*DIA*30.48
   61 CONTINUE
C      SETS THE INITIAL VALUES FOR INTEGRATION. AT Z=0. FOR GAS-FEED CONDITIONS
C      FOR SOLIDS-UNCONVERTED SOLIDS MAINLY ASH AND CARBON
C
       FI(1)=0.0
       FI(2)=0.0
      FI(3)=AIR*0.79
       FI(4)=0.0
       FI(5)=0.0
       FI(6)=0.0
       FI(7)=0.0
      FI(8)=AIR*0.21
      FI(9)=STEAM
       FI(10)=0.0
       FI(11)=0.0
      FI(12)=0.0
      FI(13)=C*(1.-XC)
       XCOAL=FI(13)
      FI(14)=HY*(1.-XC)
       FI(15)=O*(1.-XC)
      FI(16)= AN*(1.-XC)
      FI(17)=S*(1.-XC)
      FI(18)=ASH
       FI(19)=TEMPA
       FI(20)=TEMPA
        HLOSS=0.0
       Z=0.0
       KD=1
       J=1
C
C
       TS=FI(19)
       TG=FI(20)
        DP=0.5
       CALL DEVO(TS,DCO,DCO2,DH2,DH2O,DH2S,DC2H6,DCH4,DNH3,ATAR)
       DCARBO=(DCO+DCO2+DC2H6*2.+DCH4)*AMW(13)
C      INITIALIZATION OF  PARAMETERS REQUIRED     IN THE INTEGRATION USING
C     NLDEQS SUBROUTINE
       CALL NLDEQS(1,NSF,E,FI,I,N,ISW,TB,Z,DZ,D,N154)
   29 CONTINUE
   20 CONTINUE
       TS=F(19)
       TG=TS
C      ESTIMATES SPECIFIC HEAT OF COAL DEPENDING ON TEMP.
       CPS=0.32
       IF(TS .GT. 1300.) CPS=0.25
       IF(TS .GE. 1200. .AND. TS .LT. 1300.) CPS=0.25
       IF(TS .GE. 1100. .AND. TS .LT. 1200.) CPS=0.27
       IF(TS .GT. 1000. .AND. TS .LT. 1100.) CPS=0.3
       CPC=(2.673+0.002617*TS-116900./TS/TS)/12.04/1.2
       TOTALG=0.0
       DO 21 K=1,12
   21 TOTALG=TOTALG+F(K)
      IF(F(8) .LE. 0.00001) F(8)=0.00
C      CALCULATES FRACTION OF O2,H2O,CO,CO2,H2,CH4 FOR RATES
       XO2=F(8)/TOTALG
       XH2O=F(9)/TOTALG
       XCO=F(1)/TOTALG
       XCO2=F(2)/TOTALG
       XH2=F(4)/TOTALG
       XCH4=F(5)/TOTALG
       TOTALS=0.0
       DO 22 K=13,18
   22 TOTALS=TOTALS+F(K)
       TESTD=F(13)
       XCARB=F(13)/TOTALS
       XASH=F(18)/TOTALS
        IF(F(8) .EQ. 0.0) DP=2.
       CALL RATES(TS,TG,DP,P,EP,XCO,XCO2,XH2O,XO2,XH2,XCH4,XCARB,XASH,
```

```
     2RATE1,RATE2,RATE3,RATE4,RATE5,RATE6,RATE7)
       IF(RATE7 .LE. 0.0) RATE7=0.0
       IF(RATE2 .LE. 0.0) RATE2=0.0
       RATE4=0.0
       RATE5=0.0
C
C      TEST FOR VARIOUS RATES I.E. IF THE MOLES REACTING ARE MORE THAN AVAILABLE
C     .THEN THE RATES ARE REDUCED PROPORTIONATELY
C
       T1=0.0
       IF(RATE3 .LE. 0.0) T1=-RATE3
      TEST1=(RATE6+T1)*AREA*DZ
       IF(TEST1 .LE. F(2)) GO TO 32
      RATE6=RATE6*F(2)/TEST1
      IF( T1 .EQ. 0.0) GO TO 32
      RATE3=-T1*F(2)/TEST1
   32 CONTINUE
       TEST3=(RATE4+RATE3)*AREA*DZ
       IF(TEST3 .LE. F(1)) GO TO 24
        IF(ABS(TEST3) .LT. 0.00001) GO TO 24
       RATE4=F(1)*RATE4/TEST3
       RATE3=F(1)*RATE3/TEST3
   24 CONTINUE
       TEST4=(RATE2+RATE3)*AREA*DZ
       IF(TEST4 .LE. F(9)) GO TO 26
       RATE2=F(9)*RATE2/TEST4
      RATE3=F(9)*RATE3/TEST4
   26 CONTINUE
       PROCPG=0.0
       DO 25 M=1,12
       CALL CPH(M,TS,CP(M),H(M))
       CALL CPH(M,TG,CP(M),HG(M))
       PROCPG=PROCPG+CP(M)*F(M)
   25 CONTINUE
       HC=CPC*12.*(TS-298.)
C      CALCULATES STOICHIOMETRIC COEFFICIENTS FOR CHAR STEAM REACTION
       CALL STO2(RATE2,TS,HC,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,HR2)
       T3=0.0
      IF(RATE3 .GT. 0.0) T3=RATE3
      RATIO=(10.**3.4)*EXP(-12400./1.987/TS)
       A5=(2.*RATIO+1.)/(2.+2.*RATIO)
       A6=1./(1.+RATIO)
        A7=A6*RATIO
        TEST2=(A5*RATE1+RATE4/2.)*AREA*DZ
      IF(TEST2 .LE. F(8)) GO TO 23
        RATE1=F(8)/TEST2*RATE1
   23 CONTINUE
C      CALCULATES STOICHIOMETRIC COEFFICIENTS FOR CHAR OXYGEN REACTION
C
       CALL STO1(RATE1,TS,HC,C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,HR1)
C      CALCULATION OF HEATS OF REACTIONS
        HR3=HG(2)+HG(4)-HG(1)-HG(9)
       HR4=HG(2)-HG(1)-HG(8)/2.
       HR5=HG(9)-HG(8)/2.-HG(4)
       HR6=2.*H(1)-H(2)-HC
       HR7=HG(5)-2.*HG(4)-HC
       IF(RATE5 .LT. 0.0) RATE5=0.0
       IF(RATE4 .LT. 0.0) RATE4=0.0
        RATE4=0.0
       RATE5=0.0
C
C
C
C      DIFFERENTIAL EQUATIONS ARE DEFINED HERE FOR 12 GAS COMPONENTS,6SOLID
C      COMPONENTS, 1SOLID TEMP. AND 1GAS TEMP.
C
C
C
      DF(1)=AREA*(C7+B7+RATE6*2.-RATE3-RATE4)
       DF(2)=AREA*(C8+RATE3+RATE4-RATE6)
      DF(3)=AREA*B9
       DF(4)=AREA*(B8+RATE3-RATE5-2.*RATE7)
       DF(5)=AREA*RATE7
      DF(6)=0.0
      DF(7)=AREA*B10
      DF(8)=AREA*(-C6-RATE4/2.-RATE5/2.)
```

```
      DF(9)=AREA*(C9-B6-RATE3+RATE5)
      DF(10)=0.0
      DF(11)=AREA*C11
      DF(12)=AREA*C10
       DF(13)=-AREA*(-C1-B1-RATE6*12.-RATE7*12.)
      DF(14)=-AREA*(-C2-B2)
        DF(15)=-AREA*(-C3-B3)
       DF(16)=-AREA*(-C4-B4)
      DF(17)=-AREA*(-C5-B5)
      DF(18)=0.0
       A8=(-HR1-HR3*RATE3-HR7*RATE7)*AREA
        A9=(-HR2-HR6*RATE6)*AREA
        A10=(-HR4*RATE4-HR5*RATE5)*AREA
        TW=400.
       FHLS=0.6
       HTLOSS=FHLS*(A8+A10)
       IF(F(8) .LE. 0.05) HTLOSS=0.0005*U13*(TS-TW)
        DF(19)=(A8+A9+A10-HTLOSS)/(PROCPG-TOTALS*CPS)
       DF(20)=DF(19)
      CALL NLDEQS(2,NSF,DF,F,I,N,ISW,TB,Z,DZ,D,N154)
      GO TO (10,20,10) ,I
   10 CALL NLDEQS(3,NSF,DF,F,I,N,ISW,TB,Z,DZ,D,N154)
       HLOSS=HLOSS+HTLOSS *DZ
       DLOSS(J)=HLOSS
       DLOST(J)=HTLOSS
       DHT(J)=DZ
       TS=F(19)
       TG=TS
       SUMGC=0.0
      DO 28 KK=1,12
   28  SUMGC=SUMGC+F(KK)
C
       VALUES ARE STORED FOR PLOTTING OF CONCENTRATION PROFILES
C
       Y1(J)=Z
       X1(J)=TS
        X3(J)=F(1)/SUMGC
      X4(J)=F(2)/SUMGC
      X5(J)=F(4)/SUMGC
      X6(J)=F(8)/SUMGC
       X7(J)=F(9)/SUMGC
       Y3(J)=Z
       DO 39 KK=1,20
   39 CS(J,KK)=F(KK)
C      ACTUAL AND THEORETICAL WATER GAS EQUILIBRIUM CONSTANTS ARE ESTIMATED
       WGEC(J)=1./(EXP(3.6893-7234./(TS*1.8)))
        WGEE(J)=100000.
       IF(F(1) .NE. 0.0)WGEE(J)=F(2)*F(4)/F(1)/F(9)
   37 CONTINUE
      J=J+1
       TC=DCARBO+F(13)
       IF(TC .LE. (C-1.)) GO TO 1005
       IF(KX .EQ. 1) XC=0.999999
       DX=-0.0005
       KX=KX+1
       IF(KX .GE. 10) GO TO 62
       GO TO 61
 1005 CONTINUE
      IF(KD .EQ. 2) GO TO 31
C
       TESTS FOR COMPLETION OF  BED HEIGHT. IF NOT CONTINUES INTEGRATION
C     OTHERWISECALCULATES DEVOLATILIZATION PRODUCTS
       IF(Z .LT. (HTBED-1.)) GO TO 31
 1002  CONTINUE
      CALL DEVO(TS,DCO,DCO2,DH2,DH2O,DH2S,DC2H6,DCH4,DNH3,ATAR)
       MOIST=COAL-C-HY-O-AN-S-ASH
       KD=KD+1
       DCARBO =(DCO+DCO2+DC2H6*2.+DCH4)*AMW(13)
       DHYDRO=(DH2+DH2O+DH2S+DC2H6*3.+DCH4*2.)*AMW(14)*2.
       DNITRO=DNH3*AMW(16)
        DOXY=(DCO+DCO2*2.+DH2O)*AMW(15)
       DSUL=DH2S*AMW(17)
       F(1)=F(1)+DCO
       F(2)=F(2)+DCO2
       F(4)=F(4)+DH2
       F(5)=F(5)+DCH4
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      F(6)=F(6)+DC2H6
      F(7)=F(7)+DH2S
      F(9)=F(9)+DH2O
      F(10)=F(10)+DNH3
      F(13)=F(13)+DCARBO+ALPHPP*AMW(13)
      F(14)=F(14)+DHYDRO+BETPP*AMW(14)
      F(15)=F(15)+DOXY +GAMPP*AMW(15)
      F(16)=F(16)+DNITRO+DELPP*AMW(16)
      F(17)=F(17)+DSUL +EPSPP*AMW(17)
      F(9)=F(9)+MOIST/18.
      SUMGD=0.0
       WRITE(6,109)DCO,DCO2,DH2,DH2O,DCH4
      DO 51 M=1,12
   51 SUMGD=SUMGD+F(M)
      X1(J)=TS
      Y1(J)=Z
      X3(J)=F(1)/SUMGD
      X4(J)=F(2)/SUMGD
      X5(J)=F(4)/SUMGD
      X6(J)=F(8)/SUMGD
      X7(J)=F(9)/SUMGD
      Y3(J)=Z
      DO 46 K=1,20
   46 CS(J,K)=F(K)
      Z=Z+1.
   31 CONTINUE
      IF(Z .LT. HTBED) GO TO 29
      CCOAL=F(13)
      XCAL=1.-XCOAL/CCOAL
      WRITE(6,109)DP,P,XASH,TOTALS,XCARB
C
C     COMPARISON OF CARBON FLOWRATES -ESTIMATED AMD GIVEN
C     NO AGREEMENT THEN INITIAL VALUE OF CARBON CONVERSION IS CHANGED
C     THE ENTIRE PROCEDURE IS REPEATED
      WRITE(6,109) XCOAL,CCOAL,HLOSS,F(1),F(2)
      WRITE(6,109)F(4),F(9),F(3),F(5),F(14)
     WRITE(6,103)XC,XCAL,HTBED,COAL,Z,TS,F(13),F(8)
      IF(ABS(C-CCOAL) .LT. 1.) GO TO 1004
      XNEW=XCAL
       ERR=XNEW-XC
      IF(KX .GE. 2)XNEW=XC
      IF(KX .GE. 2)ERR=XNEW-XCAL
      CALL CRRECT(L,INDX,DX,XC1,XC2,XNEW,E1,E2,ERR)
      XC=XNEW
      L=L+1
      IF(L .GE. 15) GO TO 62
      GO TO 61
   62 CONTINUE
      WRITE(6,1001)
 1001 FORMAT(5X,'MESSAGE TO THE USER',//,5X,'CHECK THE FOLLOWING',/,5X,
     2'AIR OR THE OXYGEN FEEDRATE AS COMPARED TO THE CARBON FEED RATE',/
     3,5X,'2. HEAT LOSS',/,5X,'ASSUME INITIAL VALUE OF XC=0.9999')
 1004  CONTINUE
C
C     CALCULATION OF HEATING VALUE OF THE PRODUCT GAS,STEAM DECOMPOSITOIN
C     PERCENTAGE HEAT LOSS ETC
C
      DMOIST=F(9)
      SUM1=0.0
      F(9)=0.0
      DO 33 JK=1,12
   33 SUM1=SUM1+F(JK)
      WRITE(6,109)XC,XCAL,STEAM,ERR,SUM1
      HVG=0.0
      SUM3=SUM1+DMOIST
      TS=(SUM3*7.*(TS-298.)-DMOIST*980./1.8-ATAR*6000./1.8)/SUM3/7.+
     2298.
       DO 34 KJ=1,12
      PGAS(KJ)=F(KJ)/SUM1*100.
   34 HVG=HVG+HV(KJ)*PGAS(KJ)/100.
  109 FORMAT(5X,5E12.5)
      SUM1=SUM1*3600./454.4
      F(9)=DMOIST
      STDE=1.-(F(9)-MOIST/AMW(9))/STEAM
      PHLOSS=HLOSS/(COAL*HVCOAL/1.8)*100.
      SUMS=0.0
```

```
      DO 35 LK=13,18
   35 SUMS=SUMS+F(LK)
      DO 36 LK=1,6
   36 PSOLID(LK)=F(LK+12)/(SUMS+MOIST)*100.
      TSOLID=(MOIST+SUMS)*3600./454.4
      WRITE(6,1011)
 1011 FORMAT(1H1,//,5X,'INTERVAL NO. ',5X,'HEAT LOSS',5X,'TOTAL HEAT LO
     2SS')
      DO 111 KK=1,J,5
      WRITE(6,601)KK,DLOST(KK),DLOSS(KK)
  601 FORMAT(5X,I5,15X,2E14.5)
  111 CONTINUE
      WRITE(6,1012)
 1012 FORMAT( 5X,'WATER GAS EQUILIBRIUM CONSTANTS',/,5X,'CALCULATED',
     25X,'THEORETICAL')
      DO 112 KK=1,J,5
      WRITE(6,110)WGEC(KK),WGEE(KK)
  110 FORMAT(5X,2F10.4)
  112 CONTINUE
      WRITE(6,1013)
 1013 FORMAT(5X,'HEIGHT',7X,'CO',7X,'CO2',7X,'N2',7X,'H2',7X,'CH4',7X,
     2'C2H6',7X,'H2S',7X,'H2O',/,5X,'NH3',7X,'NO',7X,'SO2',7X,'C',7X,'H'
     3 ,7X,'O',7X,'N',7X,'S',7X,'ASH',7X,'TEMP. OF SOLID','OF GAS')
      DO 63 KL=1,J,2
      WRITE(6,101)Y3(KL),(CS(KL,M),M=1,10)
  101 FORMAT(2X,11F10.4)
      WRITE(6,102)(CS(KL,M),M=11,20)
  102 FORMAT(11X,10F10.4)
   63 CONTINUE
      WRITE(6,103)DCO,DCO2,DH2,DH2O,DH2S,DC2H6,DCH4,DNH3
  103 FORMAT(5X,8E14.7)
      WRITE(6,1014)
 1014 FORMAT(/,5X,'% OF GAS,DRY BASIS',//)
      WRITE(6,104)PGAS
  104 FORMAT(5X,2(2X,6F10.4,/))
      WRITE(6,1015)SUM1,STDE,PHLOSS
 1015 FORMAT(5X,'TOTAL MOLES OF GAS=',E14.5,/,5X,'STEAM DECOMPOSITION=',
     2E14.5,/,5X,'% OF HEAT LOSS=',E14.5)
  105 FORMAT(/,5X,3E14.5)
      WRITE(6,1016)
 1016 FORMAT(//,5X,'% OF SOLIDS ,C,H,O,N,S,ASH, TOTAL SOLIDS')
      WRITE(6,106)PSOLID,TSOLID
  106 FORMAT(/,5X,7E14.7)
      WRITE(6,107)HLOSS,J,Z,HTBED
  107 FORMAT(5X,E14.7,I3,2E14.7)
      COLDE=HVG*SUM1*359.*100./(HVCOAL*TSOLID)
      THIN=HVCOAL*TSOLID+(AIR*(TEMPA*1.8-537.)*7.+HSTEAM*STEAM*18.)*
     23600./454.4
      THOUT=(HVG*359.+7.*(TS*1.8-537.))*SUM1+18.*F(9)*3600./454.4*((TS*
     21.8-672.)*0.5+980.)+15000.*ATAR*3600./454.4
      HLOSS=HLOSS*3600./252.
      TEFF=THOUT*100./THIN
      WRITE(6,105)THIN,THOUT,HLOSS
      ATAR=ATAR*3600./454.4
      TS=TS*1.8-460.
      WRITE(6,1019)HVG,COLDE,TEFF
 1019 FORMAT(//,5X,'HEATING VALUE OF GAS,BTU/CF=',E14.3,/,5X,'COLD GAS
     2EFFICIENCY=',E14.3,/,5X,'THERMAL EFFICIENCY=',E14.3)
      WRITE(6,105)TS,DMOIST,ATAR
      WRITE(6,1017)TS,ATAR
 1017 FORMAT(/,5X,'TEMP. OF GAS LEAVING THE GASIFIER=',E14.3,/,5X,'AMOUN
     2T OF TAR PRODUCED,LBS/HR=',E14.3)
      IF(NPLOT .NE. 1) GO TO  602
      WRITE(6,108)
      NPT=J
      NPT1=J
C     PLOT OF TEMP. VERSUS HEIGHT
      CALL FPPLOT(X1,Y1,NPT,ICHAR(1),1,J)
  108 FORMAT(1H1)
      WRITE(6,108)
C     PLOT OF CONC. OF CO   VERSUS  HEIGHT
      CALL FPPLOT(X3,Y3,NPT1,ICHAR(1),1,J)
      WRITE(6,108)
C     PLOT OF CONC. OF CO2  VERSUS  HEIGHT
      CALL FPPLOT(X4,Y3,NPT1,ICHAR(2),1,J)
      WRITE(6,108)
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C       PLOT OF CONC. OF H2   VERSUS  HEIGHT
        CALL FPPLOT(X5,Y3,NPT1,ICHAR(3),1,J)
        WRITE(6,108)
C       PLOT OF CONC. OF O2   VERSUS  HEIGHT
        CALL FPPLOT(X6,Y3,NPT1,ICHAR(4),1,J)
        WRITE(6,108)
C       PLOT OF CONC. OF H2O  VERSUS  HEIGHT
        CALL FPPLOT(X7,Y3,NPT1,ICHAR(5),1,J)
 602     CONTINUE
5000    CONTINUE
       STOP
       END
```

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      SUBROUTINE DEVO(TEMP,DCO,DCO2,DH2,DH2O,DH2S,DC2H6,DCH4,DNH3,ATAR)
       REAL MOIST
      COMMON/AA/MOIST,VM,FIXC,ASH,HVCOAL,FC,FH,FO,FN,FS,FASH,COAL,ATR
     1,STEAM,TCOAL,TAIR,TSTEAM,P,DIA,HT,VM1
       COMMON/AE/ALPHPP,BETPP,GAMPP,DELPP,EPSPP
       DATA RATIO1,RATIO2/12.,5./
       XCH4=0.0035*P*0.00007
        VM=VM1*100./(100.-FASH*100.-MOIST)
       WRITE(6,11) VM,FASH,MOIST
       T1=TEMP
        TEMP=850.
      D1=11.47-3.961*ALOG10(TEMP-273.)+0.005*VM
       D2=0.2*(VM-10.9)
      D3=10.**D1
       D4=VM-D3-D2
      YIELD=D4*COAL/100.
       WRITE(6,11)YIELD,D4,D3
      AF=(1.-FASH)
      ALPHA=FC/12.01*COAL/AF
      BETA=FH*COAL/AF
      DELTA=FN*COAL/14./AF
      EPSI=FS*COAL/32./AF
      GAMMA=FO*COAL/16./AF
      TAR=0.04
      ALPHPP=TAR*ALPHA
      BETPP=0.06/0.07083*ALPHPP
      GAMPP=(0.003125/0.07083)*ALPHPP
      DELPP=(0.001/0.07083)*ALPHPP
      EPSPP=0.00059/0.07083*ALPHPP
      ATAR=(ALPHPP*12.+BETPP+GAMPP*16.+DELPP*14.+EPSPP*32.)/0.993
       XP=(YIELD-GAMMA*16.-0.7*DELTA*14.-0.7*EPSI*32.-0.65*BETA)/
     2(0.74*DELTA*14.+0.74*EPSI*32.+ALPHA*12.+0.6573*BETA)*100.
      GAMMAP=0.0
       EPSIP=EPSI*(1.-0.74*XP/100.-0.7)
       BETAP=BETA*(1.-0.65*XP/100.-0.65)
       DELTAP=DELTA*(1.-0.74*XP/100.-0.7)
       KJ=1
  104 CONTINUE
      FOW=0.5
      JK=1
  102 CONTINUE
      DCH4=XCH4*COAL
      DH2S=EPSI-EPSIP-EPSPP
      DC2H6=DCH4/RATIO1
      DH2O=(GAMMA-GAMPP)*FOW
      DNH3=(DELTA-DELTAP)
      DH2=(BETA-BETPP-2.*DH2O-4.*DCH4-6.*DC2H6-2.*DH2S-3.*DNH3-BETAP)/2.
      DCO2=(GAMMA-GAMPP-DH2O)/(2.+RATIO2)
      DCO=DCO2*RATIO2
      ALPHAP=ALPHA-ALPHPP-DCO-DCO2-DCH4-2.*DC2H6
      XP1=(ALPHA-ALPHAP)/ALPHA*100.
      IF (ABS(XP-XP1) .LT. 0.5) GO TO 101
      IF(XP1 .GT. XP) FOW=FOW*1.1
      IF(XP1 .LT. XP) FOW=FOW*0.9
      JK=JK+1
      IF(JK .GT. 25) GO TO 103
      GO TO 102
  103 XCH4=XCH4+0.0005
       KJ=KJ+1
       IF(KJ .GT. 5) GO TO 101
      GO TO 104
  101 CONTINUE
       WRITE(6,11)XP,XP1,XCH4
   11 FORMAT(/,5X,3E14.7)
       IF(DCO .LE. 0.0) DCO=0.0
       IF(DCO2 .LE. 0.0) DCO2=0.0
       IF(DH2 .LE. 0.0) DH2=0.0
       TEMP=T1
      RETURN
      END
```

```
      SUBROUTINE INPUT
      REAL MOIST
      DIMENSION TITLE(15),AMW(18)
       DIMENSION AMW1(18)
      COMMON/AA/MOIST,VM,FIXC,ASH,HVCOAL,FC,FH,FO,FN,FS,FASH,COAL,AIR
     1,STEAM,TCOAL,TAIR,TSTEAM,P,DIA,HT,VM1,HSTEAM
      COMMON/BD/AMW
       DATA AMW1/28.01,44.01,28.02,2.01,16.04,30.07,34.08,32.00,18.02
     2,17.03,30.01,64.06,12.01,1.01,16.00,14.01,32.06,0.000/
      READ(5,101)(TITLE(J),J=1,15)
      READ(5,102)MOIST,VM,FIXC,ASH,HVCOAL
      READ(5,103)FC,FH,FO,FN,FS,FASH
      READ(5,103)COAL,AIR,STEAM,TCOAL,TAIR,TSTEAM
      READ(5,104)P,DIA,HT,HSTEAM
  101 FORMAT(15A4)
  102 FORMAT(5F10.3)
  103 FORMAT(6F10.3)
  104 FORMAT(4F10.3)
      WRITE(6,101)(TITLE(J),J=1,15)
      WRITE(6,11)MOIST,VM,FIXC,ASH,HVCOAL
   11 FORMAT(/,' PROXIMATE ANALYSIS',/,' MOISTURE VOLATILE  FIXED  ASH
     1HEATING VALUE',/,9X,'  MATTER  CARBON        OF COAL',/,4(F8.3,2X),
     25X,F10.2)
      WRITE(6,12)FC,FH,FO,FN,FS,FASH
   12 FORMAT(/,' ULTIMATE ANALYSIS',/,' CARBON HYDROGEN OXYGEN NITROGEN
     1SULFUR ASH ',/,6F7.3)
      WRITE(6,13)COAL,AIR,STEAM,TCOAL,TAIR,TSTEAM
   13 FORMAT(/,' COAL FEED RATE LB/HR',F10.3,/,' AIR FEED RATE LB/HR',
     1F10.3,/,' STEAM FEED RATE LB/HR',F10.3,/,' TEMPERATURE OF COAL F',
     2F10.3,/,  ' TEMPERATURE OF AIR F',F10.3,/,' TEMPERATURE OF STEAM F'
     3,F10.3)
      WRITE(6,14)P,DIA,HT
   14 FORMAT(/,' PRESSURE PSIG',F10.3,/,' DIAMETER OF THE GASIFIER FT',
     1F10.3,/,' HEIGHT OF THE BED FT',F10.3)
      DO 200 K=1,18
  200 AMW(K)=AMW1(K)
      RETURN
      END
```

```
      SUBROUTINE CPH(J,TEMP,CPG,H2)
C     THIS SUBROUTINE CALCULATES MOLAR HEAT CAPACITY AND ENTHALPY OF GAS
C     AT TEMPERATURE T
C     HFO=HEAT OF FORMATION AT 298 DEGREE K
C     UNITS OF ENTHALPY ARE CAL/G-MOLE
C     UNITS OF CP ARE CAL/G-MOLE K
C      T IS IN DEGREEK AND CP= A+BT+CT2
C     1=CO, 2=CO2, 3=N2, 4=H2, 5=CH4, 6=C2H6, 7=H2S, 8=O2, 9=H2O, 10=NH3
C     11=SO2, 12=NO
      DIMENSION AB(12),BC(12),CC(12),HFO(12)
      DATA AB,BC,CC/6.420,6.214,6.524,6.947,3.381,2.247,6.662,6.148,7.25
     16,6.086,7.116,6.524,
     2 1.665,10.396,1.25,-0.2,18.044,38.201,5.134,3.102,2.298,8.812,
     3 9.512,-0.370,
     4-0.196,-3.545,-0.001,-.481,-4.30,-11.049,-0.854,-0.923,0.283,-1.50
     56,3.511,2.546/
      DATA HFO/-26416.,-94052.,0.0,0.0,-17889.,-20236.,-4815.,0.0,
     2-57798.,-11040.,-70960.,21600./
      CX=AB(J)+BC(J)*(1.E-3)*TEMP+CC(J)*(1.E-6)*TEMP*TEMP
      CPG=CX
      A1=(TEMP-298.)
      A2=(TEMP*TEMP-298.*298.)/2.
      A3=((TEMP)**3.-(298.)**3.)/3.
      H2=HFO(J)+AB(J)*A1+BC(J)*(1.E-3)*A2+CC(J)*(1.E-6)*A3
      RETURN
      END
```

```
      SUBROUTINE RATES(TS,TG,DP,P,EP,XCO,XCO2,XH2O,XO2,XH2,XCH4,XCARB,
     2XASH,RATE1,RATE2,RATE3,RATE4,RATE5,RATE6,RATE7)
      REAL KS,KDIFF
      RHOC=1.4
      RHOASH=RHOC
      RATE1=0.0
      RATE2=0.0
      RATE3=0.0
      RATE4=0.0
      RATE5=0.0
      RATE6=0.0
      RATE7=0.0
      TG=TS
     IF(TS .LT. 300.) GO TO 301
      TM=(TS+TG)/2.
      DIFF=4.26*((TG/1800.)**1.75)/P
       KS=8710.*EXP(-27000./1.987/TS)
      PHI=1.
      KDIFF=0.292*DIFF*2.*PHI/DP/(TS+TG)
      RATE1=P/(1./KS+1./KDIFF)*XO2*6./DP*(1.-EP)*XCARB/12.
C
      CSEQK=EXP(17.6444-30260./(TS*1.8))
      AKV=2.26*(1.E+7)/12.*EXP(-35000./1.987/TS)
      A1=AKV*(1.-EP)*RHOC*XCARB/82.05/TS
      A2=P*XH2O-XH2*XCO*P*P/CSEQK
      RATE2=A1*A2
C
      WGEQK=1./(EXP(3.6893-7234./(TG*1.8)))
      A3= 0.00005*3.586*(1.E+5)*EXP(-4895./TS)*P*P/60.
      A3=A3*0.1
      A4=(XCO*XH2O-XCO2*XH2/WGEQK)
      A5=(1.-EP)*XASH*RHOASH
      RATE3=A3*A4*A5
C
      RATE4=0.0
C
      RATE5=0.0
C
      AK2=2.*(1.E+12)*EXP(-59600./1.987/TS)
      AK2=AK2/12.
     A10=(1.-EP)*RHOC*XCARB/82.05/TS*XCO2*P
      RATE6=A10*AK2
C
      AK7=0.1013*EXP(6.974-19460./TS)
      EQ7=0.4/34173.*EXP(18400./TS)
      A11=AK7*(1.-EP)*RHOC*XCARB/82.05/TS/12.
      A12=0.0
      IF(XCH4 .GT. 0.0)A12=SQRT(XCH4*P/EQ7)
      RATE7=A11*(P*XH2-A12)
      IF(RATE7 .LE. (0.1E-8))RATE7=0.0
C
  301 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE STO2(RATE2,TS,HC,B1,B2,B3,B4,B5,B6,B7,B8,B9,B10,HR2)
      DIMENSION F(20),H(12),CP(12),AMW(18)
      COMMON/FF/F
      COMMON/DD/H,CP
      COMMON/BD/AMW
C     C AL HBE O GA N DE S EP + (AL-GA)H2O----------------AL CO +(AL-GA
C     -BE/2-EP) H2 +DE/2 N2 +EP H2S-----------
C     CB1 HB2 OB3 NB4 SB5 + B6 H2O------------- B7 CO+ B8 H2+ B9 N2+ B10 H2S
      XR2=0.2
      B1=RATE2*AMW(13)
      C100=B1/F(13)*XR2
      B2=C100*F(14)
      B3=C100*F(15)
      B4=C100*F(16)
      B5=C100*F(17)
      B7=B1/AMW(13)
      B6=B7-B3/AMW(15)
      B8=(B7-B3/AMW(15)+B2/AMW(14)/2.-B5/AMW(17))
      B9=B4/AMW(16)/2.
      B10=B5/AMW(17)
      HR2=B9*H(3)+B10*H(7)+B8*H(4)+B7*H(1)-B6*H(9)-HC*(B1+B2+B3+B4+B5)
     2/12.
      RETURN
      END
```

```
      SUBROUTINE STO1(RATE1,TS,HC,C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,
     2HR1)
      DIMENSION F(20),H(12),CP(12),AMW(18)
      COMMON/DD/H,CP
      COMMON/FF/F
      COMMON/BD/AMW                                          ------------
C     C AL H BE O GA N DE S EP +(A/2+B+D+(C+E-GA)) O2 ----------------
C     ACO +B CO2+ C H2O+ DSO2 +E NO---
C     CC1HC2OC3NC4SC5  + C6O2 ________C7CO +C8CO2 +C9H2O+ C10SO2+ C11NO
      RATIO=(10.**3.4)*EXP(-12400./1.987/TS)
       XR1=0.2
      C1=RATE1*AMW(13)
      B100=C1/F(13)*XR1
       C2=B100*F(14)*0.05
      C3=B100*F(15)
      C4=B100*F(16)
      C5=B100*F(17)
      C8=RATE1/(1.+RATIO)
      C7=C8*RATIO
      C9=C2/AMW(14)/2.
      C10=C5/AMW(17)
      C11=C4/AMW(16)
      C6=C7/2.+C8+C10+(C9+C11-C3/16.)/2.
      HR1=C11*H(12)+C10*H(11)+C9*H(9)+C8  *H(2)+C7*H(1)-C6*H(8)-HC*(C1+
     2C2+C3+C4+C5)/12.
      RETURN
      END
```

RUN NO. 70.6 BITUMINOUS ARKWRIGHT COAL

PROXIMATE ANALYSIS

MOISTURE	VOLATILE MATTER	FIXED CARBON	ASH	HEATING VALUE OF COAL
1.100	35.100	55.100	8.700	13675.00

ULTIMATE ANALYSIS

CARBON	HYDROGEN	OXYGEN	NITROGEN	SULFUR	ASH
0.759	0.057	0.049	0.014	0.027	0.082

COAL FEED RATE LB/HR 1097.000
AIR FEED RATE LB/HR 4112.000
STEAM FEED RATE LB/HR 501.000
TEMPERATURE OF COAL F 77.000
TEMPERATURE OF AIR F 240.000
TEMPERATURE OF STEAM F 1120.000

PRESSURE PSIG 79.000
DIAMETER OF THE GASIFIER FT 3.500
HEIGHT OF THE BED FT 6.580

0.17997E 02 0.13847E 03 0.35093E 01

0.3872034E 02 0.8249998E-01 0.1099999E 01

0.3853226E 02 0.2782802E 02 0.5328241E 01

0.1700058E 02 0.1654321E 02 0.5446181E-02

0.3872034E 02 0.8249998E-01 0.1099999E 01

0.3853226E 02 0.2782802E 02 0.5328241E 01

0.1700058E 02 0.1654321E 02 0.5446181E-02
0.26376E 00 0.52752E-01 0.10481E 01 0.77971E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.94849E 00 0.12044E 02 0.49381E-01
0.10510E 00 0.19550E 02 0.22231E 04 0.26501E 00 0.92790E-01
0.10500E 01 0.36731E 01 0.14210E 02 0.75411E 00 0.62432E 01
0.9990000E 00 0.9946241E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.6092654E 03 0.1955037E 02 0.3737473E 01

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11397E 00 0.10023E 03 0.87774E 00
0.26669E 01 0.10709E 03 0.17761E 06 0.45598E 01 0.28744E 01
0.34404E 01 0.12915E 01 0.14210E 02 0.75411E 00 0.64540E 01
0.9746241E 00 0.9750972E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.9962761E 03 0.1070918E 03 0.1633342E-04

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11440E 00 0.99858E 02 0.87795E 00
0.24170E 01 0.10678E 03 0.17721E 06 0.45579E 01 0.28714E 01
0.34323E 01 0.12993E 01 0.14210E 02 0.75411E 00 0.64345E 01
0.9770023E 00 0.9773660E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.9989417E 03 0.1067838E 03 0.2395976E-04

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

```
0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11470E 00 0.99595E 02 0.87811E 00
0.22396E 01 0.10657E 03 0.17697E 06 0.45582E 01 0.28681E 01
0.34259E 01 0.13054E 01 0.14210E 02 0.75411E 00 0.64207E 01
0.9786901E 00 0.9789851E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.1001217E 04 0.1065703E 03 0.3271378E-04

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11496E 00 0.99366E 02 0.87820E 00
0.21048E 01 0.10638E 03 0.17662E 06 0.45548E 01 0.28668E 01
0.34197E 01 0.13114E 01 0.14210E 02 0.75411E 00 0.64102E 01
0.9799725E 00 0.9802142E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.1003049E 04 0.1063789E 03 0.4256239E-04

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11516E 00 0.99196E 02 0.87829E 00
0.20002E 01 0.10624E 03 0.17635E 06 0.45539E 01 0.28648E 01
0.34146E 01 0.13164E 01 0.14210E 02 0.75411E 00 0.64020E 01
0.9809682E 00 0.9811731E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.1004733E 04 0.1062387E 03 0.5317718E-04

0.3892593E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11533E 00 0.99051E 02 0.87834E 00
0.19154E 01 0.10612E 03 0.17615E 06 0.45525E 01 0.28632E 01
0.34100E 01 0.13208E 01 0.14210E 02 0.75411E 00 0.63954E 01
0.9817746E 00 0.9819504E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.1006201E 04 0.1061188E 03 0.6454549E-04

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02

0.3892583E 02 0.8249998E-01 0.1578523E 01

0.3874243E 02 0.2797980E 02 0.5340863E 01

0.1716916E 02 0.1667635E 02 0.5446181E-02
0.27434E 00 0.54869E-01 0.10672E 01 0.63156E-01 0.75411E 00
0.50000E 00 0.63741E 01 0.11547E 00 0.98927E 02 0.87839E 00
0.18455E 01 0.10601E 03 0.17600E 06 0.45509E 01 0.28620E 01
0.34059E 01 0.13248E 01 0.14210E 02 0.75411E 00 0.63899E 01
0.9824398E 00 0.9825920E 00 0.2010000E 03 0.1384657E 03 0.2020000E 03 0.1007486E 04 0.1060143E 03 0.7649702E-04
0.98244E 00 0.98259E 00 0.35093E 01 0.17577E-03 0.26076E 02
```

INTERVAL NO.	HEAT LOSS	TOTAL HEAT LOSS
1	0.54990E 02	0.10998E 03
6	0.63713E 02	0.71045E 03
11	0.75149E 02	0.14136E 04
16	0.90729E 02	0.22544E 04
21	0.11306E 03	0.32887E 04
26	0.14739E 03	0.46124E 04
31	0.20604E 03	0.64102E 04
36	0.32514E 03	0.91080E 04
41	0.66586E 03	0.14062E 05
46	0.32438E 04	0.31157E 05
51	0.68452E 04	0.10599E 06
56	0.26480E 04	0.14700E 06
61	0.97643E 03	0.16210E 06
66	0.37335E 03	0.16777E 06
71	0.11376E 03	0.16959E 06
76	0.11110E 03	0.17071E 06
81	0.10868E 03	0.17181E 06
86	0.10661E 03	0.17288E 06
91	0.10483E 03	0.17393E 06
96	0.10329E 03	0.17497E 06
101	0.10192E 03	0.17600E 06

WATER GAS EQUILIBRIUM CONSTANTS

CALCULATED	THEORETICAL
20.2120	0.0000
19.6536	0.0003
19.0255	0.0012
18.3086	0.0028
17.4751	0.0054
16.4803	0.0092
15.2463	0.0144
13.6163	0.0214
11.1863	0.0304
6.2524	0.0394
1.2671	0.2468
0.8728	0.6749
0.9130	0.8005
0.9833	0.9042
1.0420	0.9852
1.1017	1.0508
1.1599	1.1122
1.2134	1.1683
1.2624	1.2190
1.3075	1.2652
1.3495	1.3076

HEIGHT	CO	CO2	N2	H2	CH4	C2H6	H2S	H2O		
NH3	NO	SO2	C	H	O	N	S	ASH	TEMP. OF	SOLIDOF GAS
1.0000	0.0001	0.0009	14.2096	0.0000	0.0	0.0	0.0000	3.7763	3.5093	0.0
	0.0000	0.0000	1.8578	0.1386	0.1198	0.0336	0.0660	11.4234	600.2310	600.2310
5.0000	0.0004	0.0049	14.2096	0.0000	0.0	0.0	0.0000	3.7721	3.5093	0.0
	0.0000	0.0000	1.9090	0.1386	0.1204	0.0338	0.0663	11.4234	601.1951	601.1951
9.0000	0.0007	0.0091	14.2096	0.0000	0.0	0.0	0.0000	3.7678	3.5093	0.0
	0.0000	0.0000	1.9633	0.1387	0.1211	0.0340	0.0667	11.4234	602.2175	602.2175
13.0000	0.0010	0.0137	14.2096	0.0001	0.0	0.0	0.0000	3.7631	3.5092	0.0
	0.0000	0.0000	2.0211	0.1387	0.1218	0.0342	0.0671	11.4234	603.3044	603.3044
17.0000	0.0013	0.0185	14.2096	0.0002	0.0	0.0	0.0000	3.7582	3.5092	0.0
	0.0001	0.0001	2.0828	0.1388	0.1226	0.0344	0.0675	11.4234	604.4636	604.4636
21.0000	0.0016	0.0237	14.2096	0.0003	0.0	0.0	0.0000	3.7529	3.5091	0.0
	0.0001	0.0001	2.1489	0.1388	0.1233	0.0346	0.0679	11.4234	605.7034	605.7034
25.0000	0.0019	0.0292	14.2096	0.0004	0.0	0.0	0.0000	3.7472	3.5090	0.0
	0.0001	0.0001	2.2199	0.1389	0.1241	0.0348	0.0684	11.4234	607.0347	607.0347
29.0000	0.0023	0.0353	14.2096	0.0006	0.0	0.0	0.0000	3.7410	3.5089	0.0
	0.0001	0.0001	2.2966	0.1389	0.1250	0.0351	0.0688	11.4234	608.4692	608.4692
33.0000	0.0027	0.0418	14.2096	0.0007	0.0	0.0	0.0000	3.7344	3.5087	0.0
	0.0001	0.0001	2.3798	0.1389	0.1259	0.0353	0.0693	11.4234	610.0225	610.0225
37.0000	0.0031	0.0489	14.2096	0.0010	0.0	0.0	0.0000	3.7272	3.5085	0.0
	0.0001	0.0001	2.4704	0.1390	0.1268	0.0356	0.0699	11.4234	611.7131	611.7131
41.0000	0.0036	0.0567	14.2096	0.0012	0.0	0.0	0.0000	3.7192	3.5083	0.0
	0.0002	0.0001	2.5699	0.1391	0.1278	0.0359	0.0704	11.4234	613.5640	613.5640
45.0000	0.0041	0.0654	14.2096	0.0015	0.0	0.0	0.0000	3.7105	3.5080	0.0
	0.0002	0.0002	2.6797	0.1391	0.1289	0.0362	0.0710	11.4234	615.6040	615.6040
49.0000	0.0047	0.0750	14.2096	0.0018	0.0	0.0	0.0000	3.7007	3.5077	0.0
	0.0002	0.0002	2.8021	0.1392	0.1301	0.0365	0.0716	11.4234	617.8708	617.8708
53.0000	0.0054	0.0857	14.2096	0.0022	0.0	0.0	0.0000	3.6898	3.5074	0.0
	0.0002	0.0002	2.9398	0.1392	0.1313	0.0368	0.0723	11.4234	620.4133	620.4133
57.0000	0.0062	0.0980	14.2096	0.0027	0.0	0.0	0.0000	3.6774	3.5069	0.0
	0.0003	0.0002	3.0966	0.1393	0.1327	0.0372	0.0731	11.4234	623.2979	623.2979
61.0000	0.0072	0.1120	14.2096	0.0033	0.0	0.0	0.0000	3.6631	3.5064	0.0
	0.0003	0.0003	3.2777	0.1394	0.1342	0.0376	0.0739	11.4234	626.6167	626.6167
65.0000	0.0085	0.1285	14.2096	0.0039	0.0	0.0	0.0000	3.6463	3.5058	0.0
	0.0003	0.0003	3.4908	0.1395	0.1359	0.0381	0.0749	11.4234	630.5017	630.5017
69.0000	0.0101	0.1482	14.2096	0.0048	0.0	0.0	0.0000	3.6261	3.5050	0.0

	0.0004	0.0003	3.7475	0.1396	0.1378	0.0387	0.0759	11.4234	635.1541	635.1541
73.0000	0.0124	0.1726	14.2096	0.0058	0.0	0.0	0.0000	3.6012	3.5040	0.0
	0.0004	0.0004	4.0660	0.1397	0.1401	0.0393	0.0772	11.4234	640.8950	640.8950
77.0000	0.0157	0.2038	14.2096	0.0072	0.0	0.0	0.0000	3.5689	3.5027	0.0
	0.0005	0.0004	4.4819	0.1398	0.1429	0.0401	0.0787	11.4234	648.2034	648.2034
81.0000	0.0210	0.2465	14.2096	0.0091	0.0	0.0	0.0000	3.5245	3.5009	0.0
	0.0005	0.0005	5.0589	0.1400	0.1464	0.0411	0.0806	11.4234	658.4043	658.4043
85.0000	0.0312	0.3109	14.2096	0.0120	0.0	0.0	0.0000	3.4565	3.4980	0.0
	0.0006	0.0005	5.9540	0.1402	0.1512	0.0424	0.0833	11.4234	673.7480	673.7480
89.0000	0.0570	0.4270	14.2096	0.0177	0.0	0.0	0.0000	3.3303	3.4926	0.0
	0.0008	0.0007	7.6582	0.1406	0.1591	0.0446	0.0876	11.4234	701.7319	701.7319
93.0000	0.1753	0.7103	14.2096	0.0358	0.0	0.0	0.0000	2.9967	3.4748	0.0
	0.0011	0.0010	12.4808	0.1413	0.1756	0.0493	0.0967	11.4234	772.3118	772.3118
97.0000	0.6870	1.2516	14.2096	0.1538	0.0	0.0	0.0000	2.2584	3.3573	0.0
	0.0016	0.0014	25.1281	0.1423	0.2020	0.0567	0.1113	11.4234	910.5774	910.5774
101.0000	1.2620	1.8297	14.2096	0.5109	0.0	0.0	0.0000	1.5713	3.0006	0.0
	0.0020	0.0017	38.9774	0.1430	0.2203	0.0618	0.1213	11.4234	1023.6445	1023.6445
105.0000	1.7157	2.3200	14.2096	0.9303	0.0	0.0	0.0000	1.0638	2.5814	0.0
	0.0022	0.0019	50.3135	0.1435	0.2316	0.0650	0.1275	11.4234	1095.3101	1095.3101
109.0000	2.2052	2.5815	14.2096	1.2365	0.0	0.0	0.0000	0.7105	2.2754	0.0
	0.0024	0.0020	59.3334	0.1440	0.2386	0.0669	0.1314	11.4234	1126.5286	1126.5286
113.0000	2.6840	2.6870	14.2096	1.4502	0.0	0.0	0.0000	0.4724	2.0619	0.0
	0.0024	0.0021	66.3502	0.1444	0.2431	0.0682	0.1339	11.4234	1131.3633	1131.3633
117.0000	3.0707	2.7324	14.2096	1.6110	0.0	0.0	0.0000	0.3141	1.9012	0.0
	0.0025	0.0021	71.5379	0.1447	0.2460	0.0690	0.1355	11.4234	1125.6790	1125.6790
121.0000	3.3594	2.7550	14.2096	1.7350	0.0	0.0	0.0000	0.2091	1.7773	0.0
	0.0025	0.0022	75.2756	0.1449	0.2478	0.0695	0.1365	11.4234	1116.8826	1116.8826
125.0000	3.5712	2.7670	14.2096	1.8317	0.0	0.0	0.0000	0.1395	1.6807	0.0
	0.0025	0.0022	77.9634	0.1451	0.2490	0.0699	0.1372	11.4234	1107.5757	1107.5757
129.0000	3.7274	2.7735	14.2096	1.9083	0.0	0.0	0.0000	0.0932	1.6042	0.0
	0.0026	0.0022	79.9158	0.1452	0.2499	0.0701	0.1376	11.4234	1098.6443	1098.6443
133.0000	3.8439	2.7768	14.2096	1.9699	0.0	0.0	0.0000	0.0624	1.5426	0.0
	0.0026	0.0022	81.3555	0.1453	0.2504	0.0702	0.1379	11.4234	1090.2520	1090.2520
137.0000	3.9327	2.7782	14.2096	2.0204	0.0	0.0	0.0000	0.0418	1.4921	0.0
	0.0026	0.0022	82.4381	0.1454	0.2508	0.0704	0.1382	11.4234	1083.3743	1083.3743
141.0000	4.0049	2.7765	14.2096	2.0617	0.0	0.0	0.0000	0.0280	1.4509	0.0
	0.0026	0.0022	83.2842	0.1454	0.2511	0.0704	0.1383	11.4234	1077.3125	1077.3125
145.0000	4.0623	2.7747	14.2096	2.0971	0.0	0.0	0.0000	0.0188	1.4155	0.0
	0.0026	0.0022	83.9520	0.1455	0.2513	0.0705	0.1384	11.4234	1070.9016	1070.9016
149.0000	4.1076	2.7738	14.2096	2.1282	0.0	0.0	0.0001	0.0127	1.3845	0.0
	0.0026	0.0022	84.4842	0.1455	0.2515	0.0705	0.1385	11.4234	1064.5552	1064.5552
153.0000	4.1433	2.7738	14.2096	2.1557	0.0	0.0	0.0001	0.0085	1.3570	0.0
	0.0026	0.0022	84.9135	0.1456	0.2516	0.0706	0.1386	11.4234	1058.4553	1058.4553
157.0000	4.1717	2.7746	14.2096	2.1802	0.0	0.0	0.0001	0.0057	1.3324	0.0
	0.0026	0.0022	85.2643	0.1456	0.2517	0.0706	0.1386	11.4234	1052.6765	1052.6765
161.0000	4.1944	2.7762	14.2096	2.2022	0.0	0.0	0.0001	0.0039	1.3105	0.0
	0.0026	0.0022	85.5548	0.1456	0.2518	0.0706	0.1387	11.4234	1047.2378	1047.2378
165.0000	4.2126	2.7782	14.2096	2.2220	0.0	0.0	0.0001	0.0026	1.2907	0.0
	0.0026	0.0022	85.7982	0.1457	0.2518	0.0706	0.1387	11.4234	1042.1333	1042.1333
169.0000	4.2274	2.7806	14.2096	2.2399	0.0	0.0	0.0001	0.0018	1.2728	0.0
	0.0026	0.0022	86.0043	0.1457	0.2519	0.0706	0.1387	11.4234	1037.3435	1037.3435
173.0000	4.2394	2.7833	14.2096	2.2561	0.0	0.0	0.0001	0.0012	1.2566	0.0
	0.0026	0.0022	86.1806	0.1457	0.2519	0.0707	0.1387	11.4234	1032.8445	1032.8445
177.0000	4.2490	2.7863	14.2096	2.2710	0.0	0.0	0.0001	0.0008	1.2417	0.0
	0.0026	0.0022	86.3324	0.1457	0.2519	0.0707	0.1388	11.4234	1028.6101	1028.6101
181.0000	4.2569	2.7894	14.2096	2.2846	0.0	0.0	0.0001	0.0005	1.2281	0.0
	0.0026	0.0022	86.4641	0.1457	0.2519	0.0707	0.1388	11.4234	1024.6155	1024.6155
185.0000	4.2631	2.7927	14.2096	2.2971	0.0	0.0	0.0001	0.0004	1.2156	0.0
	0.0026	0.0022	86.5788	0.1457	0.2520	0.0707	0.1388	11.4234	1020.8367	1020.8367
189.0000	4.2680	2.7962	14.2096	2.3087	0.0	0.0	0.0001	0.0002	1.2040	0.0
	0.0026	0.0022	86.6792	0.1457	0.2520	0.0707	0.1388	11.4234	1017.2524	1017.2524
193.0000	4.2718	2.7997	14.2096	2.3194	0.0	0.0	0.0001	0.0002	1.1933	0.0
	0.0026	0.0022	86.7672	0.1457	0.2520	0.0707	0.1388	11.4234	1013.8438	1013.8438
197.0000	4.2746	2.8034	14.2096	2.3294	0.0	0.0	0.0001	0.0001	1.1833	0.0
	0.0026	0.0022	86.8445	0.1458	0.2520	0.0707	0.1388	11.4234	1010.5933	1010.5933
201.0000	4.2765	2.8071	14.2096	2.3387	0.0	0.0	0.0001	0.0001	1.1740	0.0
	0.0026	0.0022	86.9124	0.1458	0.2520	0.0707	0.1388	11.4234	1007.4858	1007.4858

0.2743427E 00 0.5486854E-01 0.1067165E 01 0.6315619E-01 0.1025253E 00 0.6284243E-01 0.7541094E 00 0.1230325E 00

% OF GAS,DRY BASIS

17.4525	10.9756	54.4937	13.0615	2.8920	0.2410
0.3934	0.0003	0.0	0.4718	0.0099	0.0085

TOTAL MOLES OF GAS= 0.20659E 03
STEAM DECOMPOSITION= 0.64744E 00
% OF HEAT LOSS= 0.16731E 02

% OF SOLIDS ,C,H,O,N,S,ASH, TOTAL SOLIDS

0.7655530E 02 0.4614305E 01 0.5543788E 01 0.1350242E 01 0.2547388E 01 0.8249104E 01 0.1097118E 04
0.1759979E 06102 0.2020000E 03 0.2010000E 03

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   0.16270E 08    0.12637E 08    0.25143E 07

HEATING VALUE OF GAS,BTU/CF=      0.137E 03
COLD GAS EFFICIENCY=      0.675E 02
THERMAL EFFICIENCY=      0.777E 02

   0.11782E 04    0.13248E 01    0.42665E 02

TEMP. OF GAS LEAVING THE GASIFIER=      0.118E 04
AMOUNT OF TAR PRODUCED,LBS/HR=      0.427E 02
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