

**DOE/MC/16474-1390  
(DE83009533)  
Distribution Category UC-90e**

USER'S MANUAL FOR COMPUTER SIMULATION AND  
DESIGN OF THE MOVING BED COAL GASIFIER

Final Report Task Order No. 41

BY

C.Y. Wen, H. Chen, M. Onozaki  
Department of Chemical Engineering  
West Virginia University  
Morgantown, W. Va. 26505

January 1982

Prepared For

United States Department of Energy  
Morgantown Energy Technology Center  
Morgantown, West Virginia

Under Contract No. DE-AT21-79MC16474

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

## ABSTRACT

A computer model of countercurrent moving bed coal gasifier developed previously has been updated. This manual presents in detail how the computer program developed is used. The unique feature of the present gasifier model is the treatment of the pyrolysis of coal. The estimation of product gas and tar distributions during devolatilization is usually difficult. In addition, tar and high molecular hydrocarbons produced during devolatilization may be subsequently cracked and reacted in the vapor phase in the presence of char and minerals. A semi-empirical approach is taken in the present model to represent the pyrolysis zone of the bed. The pyrolysis reactions are represented by three simple chemical reactions: devolatilization, cracking and carbon deposition with empirically estimated reaction rate constants. The amount of gas and tar formed is estimated based on these reactions together with the transport processes taking place within and around coal particles.

Since the time required for devolatilization is much shorter than that required for gasification, the height of bed needed for devolatilization is negligibly short. The height of the bed is thus composed of the combustion zone and the gasification zone. Combustion is an exothermic reaction while the gasification reactions are endothermic so that the temperature profile along the bed height reaches a maximum in the combustion zone and falls in the gasification zone.

The gasification reactions are assumed to be heterogeneous reactions. For fast reactions, diffusion is the rate controlling step while for slow reactions, the surface reactions within the pores of particles is the rate controlling step. Therefore, the rates of gasification reactions used in the

model are composed of two terms, the reaction term and the diffusion term.

The computer program developed can be used for both simulation and design. It can be used to simulate a gasifier to obtain the gas product distributions and coal conversion and calculate the required bed height for a given carbon conversion. A map of feasible operation ranges can then be constructed for the optimum design of a gasifier.

Kinetic parameters for three different kinds of coal are specified in the program. However, the program users may change these parameters according to the guides listed in the manual if the coal used is different. In addition, the reaction rate equations may be replaced if better rate expressions become available.

It is important that the user checks the assumptions, the simplifications and the limitations of this computer program before applying in order to assure that the applicability of the model is within the range specified. The scale-up and extrapolation from normal operating conditions should be done with caution and, if possible, verified through additional experimentations.

## TABLE OF CONTENTS

	Page
ABSTRACT . . . . .	ii
LIST OF FIGURES . . . . .	vi
LIST OF TABLES . . . . .	vii
I. INTRODUCTION . . . . .	1
II. MODEL . . . . .	2
II-1. Assumptions . . . . .	2
II-2. Pyrolysis . . . . .	5
II-3. Gasification Reactions . . . . .	10
II-3.1. Char-Oxygen Reaction . . . . .	12
II-3.2. Char-Steam Reaction . . . . .	13
II-3.3. Water-Gas Shift Reaction . . . . .	14
II-3.4. Hydrogen-Oxygen Reaction . . . . .	15
II-3.5. Char-Carbon Dioxide Reaction . . . . .	15
II-3.6. Char-Hydrogen Reaction . . . . .	16
III. CALCULATION PROCEDURES . . . . .	17
III-1. Structure of the Computer Program . . . . .	17
III-2. Flow Chart of the Computer Program . . . . .	21
III-3. Kinetic Constants . . . . .	24
IV. INPUT DATA . . . . .	34
V. SAMPLE PROBLEM . . . . .	38
V-1. Output of the Computer Program . . . . .	38
V-2. Interpretation of Graphs . . . . .	38

TABLE OF CONTENTS (cont.)

	Page
VI. APPLICATION AND RANGE OF VALIDITY . . . . .	50
VI-1. Design Map . . . . .	50
VI-2. How to Change Data and Equations in the Program . . .	57
VI-3. Validation of Range of Applicability . . . . .	57
NOMENCLATURE . . . . .	63
REFERENCES . . . . .	65
APPENDIXES	
A. NOMENCLATURE FOR THE PROGRAM . . . . .	67
B. PROGRAM LIST . . . . .	76

## LIST OF FIGURES

Figure	Page
II-1. Moving Bed Coal Gasifier . . . . .	3
II-2. Model of Moving Bed Coal Gasifier . . . . .	3
III-1. Program Structure . . . . .	18
III-2. Computer Flow Diagram . . . . .	22
V-1. Temperature as a Function of Bed Height in Sample Calculation . . . . .	42
V-2. CO Concentration as a Function of Bed Height in Sample Calculation . . . . .	43
V-3. CO <sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation . . . . .	44
V-4. O <sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation . . . . .	45
V-5. H <sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation . . . . .	46
V-6. CH <sub>4</sub> Concentration as a Function of Bed Height in Sample Calculation . . . . .	47
V-7. H <sub>2</sub> O Concentration as a Function of Bed Height in Sample Calculation . . . . .	48
VI-1. Design Map for Moving Bed Coal Gasification (Case 1) . . . . .	51
VI-2. Design Map for Moving Bed Coal Gasification (Case 2) . . . . .	52
VI-3. Design Map for Moving Bed Coal Gasification (Case 3) . . . . .	53
VI-4. Design Map for Moving Bed Coal Gasification (Case 4) . . . . .	54
VI-5. Design Map for Moving Bed Coal Gasification (Case 5) . . . . .	55

## LIST OF TABLES

Table	Page
II-1. Reaction-Rate Constants for Coal Pyrolysis Model . . . . .	9
III-1. List of Subroutines . . . . .	19
III-2. Kinetic Constants . . . . .	25
III-3. Comparison of Simulation Results to Experimental Results for Arkwright Bituminous Coal . . . . .	26
III-4. Comparison of Simulation Results to Experimental Results for Pittsburgh No. 8 Bituminous Coal . . . . .	28
III-5. Comparison of Simulation Results to Experimental Results for Illinois No. 6 Bituminous Coal . . . . .	30
III-6. Comparison of Simulation Results to Experimental Results for Rosebud Subbituminous Coal . . . . .	32
IV-1. Typical Input Data . . . . .	35
V-1. Output from Sample Calculation . . . . .	39
V-2. Output from Sample Calculation . . . . .	40
V-3. Output from Sample Calculation . . . . .	41
VI-1. Assumed Constants and Equations . . . . .	58

## I. INTRODUCTION

The objective of this manual is to assist program users in effectively utilizing the computer program that has been developed for moving bed coal gasifiers. The computer program, developed by West Virginia University, consists of two functions - design and simulation, for a counter-current moving bed coal gasifier. One of the unique characteristics of the program is the capability of the program to estimate the amount of the tar formed in the gasifier. The estimation of gas and tar formed during pyrolysis is based on a set of chemical reactions and transport processes taking place within a particle. This manual includes design maps and a guide to change the parameters and the constants in the program so that the user can apply this program to various operating conditions as well as the different types of coal used. This program is written in such a way that the program user can modify the basic program to fit different types of coal easily.

Although mathematical models are often used for scale-up and optimization as well as extrapolation beyond the range of normal operating conditions, the user should take extreme caution in applying the model developed here for such purposes. Before using the program, the assumptions, simplifications and limitations of models should be examined and clearly understood.

## II. MODEL

### II-1 Assumptions

The moving bed coal gasifier shown in Figure I-1 is a countercurrent gas-solid reactor. Coal is fed to the top of the gasifier and undergoes devolatilization first evolving tar and gases. The remaining char (here represented by C) reacts with gases in the reaction zone in which the following reactions take place:

1.  $C + \frac{1}{\Psi} O_2 \rightarrow (2 - \frac{2}{\Psi}) CO + (\frac{2}{\Psi} - 1) CO_2$
2.  $C + H_2O \rightarrow CO + H_2$
3.  $H_2O + CO \rightleftharpoons H_2 + CO_2$
4.  $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$
5.  $C + CO_2 \rightarrow 2 CO$
6.  $C + 2 H_2 \rightarrow CH_4$

The following assumptions are made in the model

1. Gas in the reactor consists of CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>S, N<sub>2</sub> (including Ar) and CH<sub>4</sub>. The amount of C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> is normally less than 1% and therefore combined into CH<sub>4</sub>.
2. Temperature and gas composition are uniform along the radial direction. (Flat profiles)
3. Coal and gas flow as plug flow.
4. Devolatilization takes place separately from other reactions.

The gasifier model is therefore composed of two sections, as shown in Figure I-2. Since devolatilization takes place in a relatively short time (an order of seconds) as compared with the total residence time of coal in the gasifier (an order of minutes

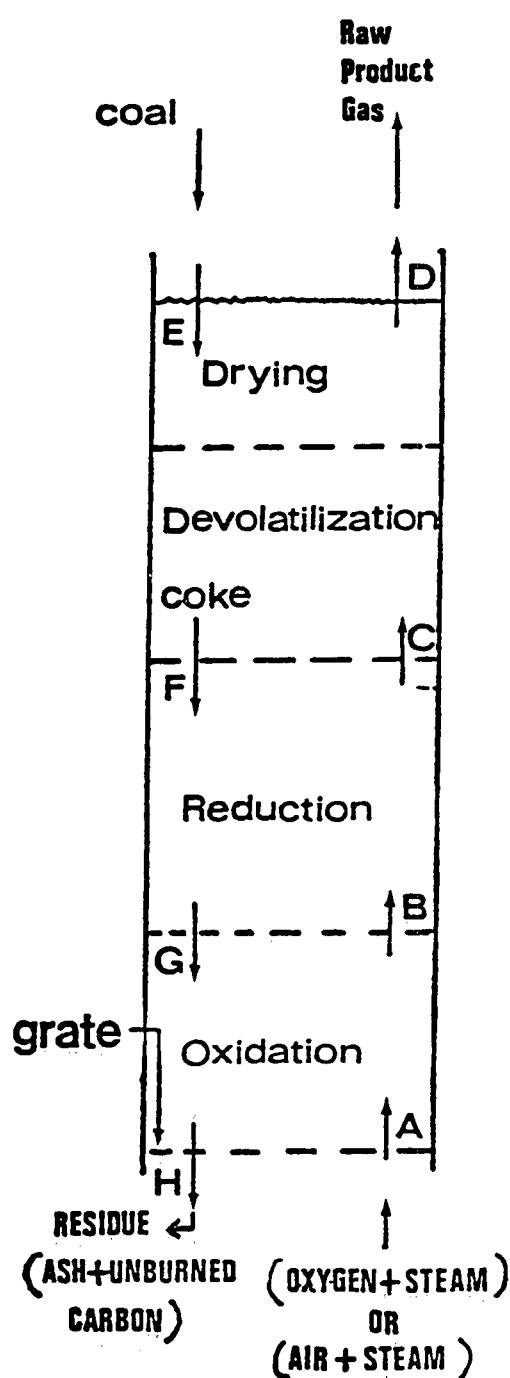


FIGURE I-1  
MOVING BED COAL GASIFIER

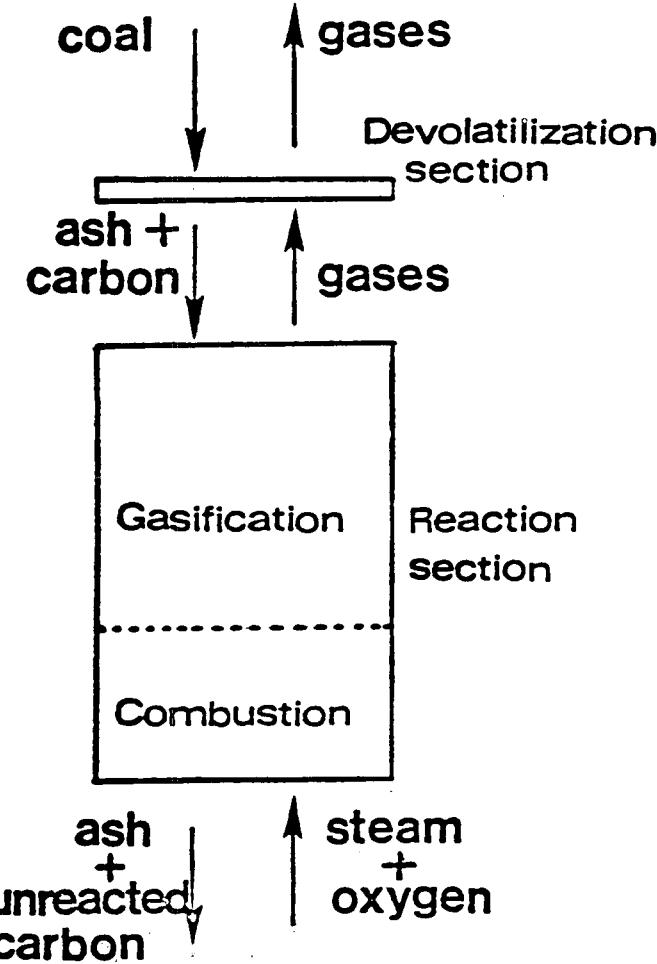


FIGURE I-2  
MODEL OF MOVING BED  
COAL GASIFIER

- to hours), it is further assumed that the length of the devolatilization section is negligible. The length of the reaction section is therefore equal to the length of the gasifier.
5. Volumetric reaction represents all gas-solid reactions except combustion which is according to the shrinking core model.
  6. Gas temperature is the same as solid temperature at every point in the gasifier (i.e. heat transfer between gas and solid is instantaneous).
  7. Temperature at the bottom of the gasifier is equal to the inlet temperature of the gas mixture.
  8. The heat transfer coefficient and the gasifier wall temperature are constant.
  9. All elemental hydrogen, oxygen, nitrogen and sulfur in coal is released during devolatilization; and therefore, the char formed contains only carbon and ash.
  10. The total amount of devolatilized carbon is specified by the program user in accordance with the type of coal fed and is independent of the operating conditions.
  11. Elemental nitrogen is distributed among tar and volatile gas in proportion to their amount.
  12. The C:H:O ratio in tar is the same as that in the original coal.
  13. All nitrogen in volatile gas appears as nitrogen gas, and all sulfur appears as H<sub>2</sub>S. Composition of the remaining volatile gas is the same as that of the exit gas from the reaction section with the amount of hydrogen gas adjusted to satisfy material balance.
  14. All of the additional gas evolved during devolatilization in the presence of hydrogen (hydropyrolysis) is methane.

15. Devolatilization is thermally neutral.

16. The gasifier pressure is constant.

## II-2 Pyrolysis

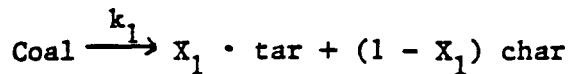
When heated to high temperatures, coal decomposes and produces volatiles which consist of a mixture of combustible gases, carbon dioxide, water vapor and tar. The degree of coal devolatilization depends not only on the type of coal but also on the operating conditions, such as the heating rate, temperature and pressure.

Desai and Wen (3) used equations presented by Gregory and Littlejohn (9) to estimate volatile yield. However, Gregory and Littlejohn's equations were correlated without taking into consideration the effect of the particle size and the temperature between the core and the surface.

Later, Wen and Chen (26) proposed a new mathematical model for single-particle coal pyrolysis in an inert atmosphere based on the combination of chemical reactions and transport processes. Wen and Chen's model is adopted here to estimate the amount of tar and gas formed during the pyrolysis.

Three chemical reactions are assumed to occur simultaneously within a coal particle which is undergoing pyrolysis. These are devolatilization, cracking and deposition:

### \* Devolatilization



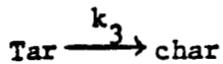
$$\text{Rate} = k_{10} \exp(-E_{10}/R_g T) C_{\text{coal}}$$

### \* Cracking



$$\text{Rate} = k_{20} \cdot \exp(-E_{20}/R_g T) C_{\text{tar}}$$

\* Deposition



$$\text{Rate} = k_{30} \cdot \exp(-E_{30}/R_g T) C_{\text{tar}}$$

The products of pyrolysis are categorized as char, tar and gas. Char is defined as undistillable material which remains in the form of solids. Tar is defined as the distillable liquid which has a molecular weight larger than C<sub>6</sub>. Gas is defined as those components lighter than C<sub>6</sub>, i.e. CO, CH<sub>4</sub>, CO<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, H<sub>2</sub>O, etc. Both tar and gas occur in the form of vapor at the gasifier temperature when coal is pyrolyzed. All of the rates of reactions are assumed to be first order with respect to the concentration of reactants, and rate constants are expressed in Arrhenius form. The rates of formation of tar, product gas, and inert gas can then be expressed as:

$$R_{\text{tar}} = X_1 \cdot k_1 \cdot C_{\text{coal}} - (k_2 + k_3) \cdot C_{\text{tar}}$$

$$R_{\text{gas}} = k_2 \cdot C_{\text{tar}} \quad (\text{and } R_{\text{inert gas}} = 0)$$

#### MASS TRANSFER

The coal particle can be considered as a porous sphere, which retains its integrity while pyrolysis reaction proceeds. The conservation equation for the gaseous species, *i*, inside the particle having a mass concentration, C<sub>i</sub>, can be formulated as:

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \cdot N_i) = R_i$$

where  $R_i$  is the rate of generation of the species  $i$  due to the chemical reactions.

$N_i$  is the mass flux of the species  $i$  and can be expressed as the sum of the rate of diffusion in the radial direction plus bulk flow through the pores. Thus,

$$N_i = -D_{eff,i} \frac{\partial C_i}{\partial r} + w_i \sum_j N_j$$

$w_i$ , the weight fraction of the species  $i$  in the gas phase, can be expressed as:

$$w_i = C_i / \sum_j C_j$$

The solid concentration,  $C_i$ , which is necessary for calculating the reaction rate  $R_i$ , can be obtained from the material balance equation as:

$$\frac{dC_i}{dt} = R_i$$

The conservation equation for the gaseous species  $i$  across the gas film can be written as:

$$N_i = k_{gi} [C_{i,s} - C_{i,b}]$$

where  $C_{i,s}$  and  $C_{i,b}$  are the concentrations of the gas species  $i$  at the particle surface and at the bulk gas stream outside, respectively.

Here  $k_{gi}$  is the mass-transfer coefficient across the gas film and can be estimated from an appropriate mass-transfer correlation.

#### HEAT TRANSFER

The energy-balance equation for the particle is derived by taking

into account convective, radiative, and conductive heat transfer with the heating devices and the heat of reaction of the pyrolysis process:

$$C_{ps} \cdot \rho_s \cdot \frac{dT}{dt} = \frac{3}{r_o} h_c (T_w - T) + \frac{3\sigma F_e}{r_o} (T_w^4 - T^4) + \frac{3km}{r_o^2} (T_w - T) + \sum_i H_i R_i$$

where  $m$  represents the fraction of the surface area of the particle in contact with the heating element, and  $T_w$  is the temperature of the heating element.  $H_i$  is assumed to be zero.

The mass-transfer equations and the heat-transfer equations discussed above can be solved numerically based on the following initial and boundary conditions:

$$\begin{aligned} t = 0, C_i &= C_{i0}, \quad \text{and } T = T_0 \\ r = 0, N_i &= 0, \quad \text{and } r = r_o, C_i = C_{is} \end{aligned}$$

#### WEIGHT-LOSS CALCULATIONS

The observable phenomena for pyrolysis are particle weight loss, WL, and product distribution. The amount of tar and gas formed at any time,  $t$ , can be estimated by integrating the mass flux for tar and gas generated by the particle for a given time interval:

$$(WL)_i = 4\pi r_o^2 \int_0^t N_i(t, r_o) \cdot dt$$

The total weight loss of the particle can be calculated either by the addition of the weight loss of tar and gas or by the subtraction of the weight of unreacted coal and char remaining in the particle during pyrolysis, from the original weight of the coal. Thus,

$$\text{Total weight loss} = \sum_i (\text{WL})_i$$

= (Original weight of coal) - (Weight of unreacted coal) - (Weight of char formed)

#### DETERMINATION OF RATE CONSTANTS

The pyrolysis data of Anthony and Howard (1, 2) for bituminous coal and those of Suuberg et al. (20) for lignite were used to determine the reaction-rate constants for the devolatilization step and the deposition step. The cracking-reaction rate constants for bituminous and subbituminous coal and lignite were chosen on the basis of the product-distribution data of Solomon (18, 19). The reaction-rate constants obtained for different ranks of coals are tabulated in Table II-1.

Table II-1  
Reaction-Rate Constants for Coal Pyrolysis Model

Reaction-rate constant	Bituminous coal	Subbituminous coal	Lignite
$k_{10}$ (1/sec)	$1.1 \times 10^5$	$7.5 \times 10^4$	$5.1 \times 10^4$
$E_{10}$ (cal/g-mole)	21,200	18,700	16,200
$k_{20}$ (1/sec)	$9.7 \times 10^9$	$3.5 \times 10^{10}$	$8 \times 10^{10}$
$E_{20}$ (cal/g-mole)	29,000	27,750	26,500
$k_{30}$ (1/sec)	$5.3 \times 10^4$	$2.5 \times 10^4$	$1.1 \times 10^3$
$E_{30}$ (cal/g-mole)	7,000	5,500	4,000

The amount of tar formed in the devolatilization step,  $X_i$ , can be correlated with the volatile matter content (based on dry, ash-free coal) for

various types of coal as follows:

Bituminous and subbituminous coals:  $X_1 = 1.30 \text{ (V.M.)} + 0.025$

Lignite:  $X_1 = 0.95 \text{ (V.M.)} + 0.025$

This model is useful for predicting the amounts of tar and gas produced during pyrolysis in coal gasifiers.

Estimation of volatile product composition is difficult. Using assumptions 10 to 14, the gas composition and hydropyrolysis are calculated in the program. The amount of devolatilized carbon should be specified by the program user in accordance with the type of coal employed, and particle weight loss by pyrolysis without hydropyrolysis can be calculated by Subroutine DEVOL. In estimating the amount of tar and gas formed during the pyrolysis stage, the temperature must be between 400°C and 1000°C while the pressure must be between 0.01 atm and 35 atm.

### II-3 Gasification Reactions

In order to simulate the reaction section, differential equations with respect to distance are set up for each of the eight variables considered in the program, namely, flow rates of char, CO, CO<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>O and temperature. For example, for the temperature and the molar flow rate of CO, the differential equations have the following form:

$$(\rho C_p U A) \frac{dT}{dZ} = A \sum_{i=1}^6 H_i R_i - h \pi D (T - T_w)$$

$$\frac{d \bar{V}_{CO}}{A d Z} = (2 - \frac{2}{\Psi}) R_1 + R_2 - R_3 + 2R_5$$

where D is the diameter of the gasifier, T<sub>w</sub> is the wall temperature, h is the heat transfer coefficient, H<sub>i</sub> is the heat of reaction of reaction i,

$R_i$  is the rate of reaction  $i$ ,  $A$  is the cross-sectional area of the gasifier,  $C_p$  is the heat capacity of bed materials,  $\rho$  is the density of bed materials,  $U$  is the superficial linear velocity and  $\bar{V}_{CO}$  is the molar flow rate of CO. The rates of various gasification reactions,  $R_i$  are expressed depending on the rate controlling steps.

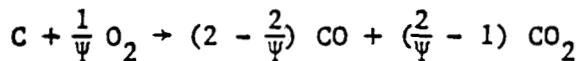
The char-gas reactions are heterogeneous, following volumetric reaction and surface reaction. In the volumetric reaction, the gas can quickly diffuse into the particles and the reaction can take place throughout the interior of the particle. For surface reactions, the reacting gas does not penetrate into the particles but is confined at the surface of the "shrinking core of unreacted solid" (22). Generally, the volume reaction occurs when chemical reaction is slow compared to diffusion while the surface reaction occurs when the chemical reaction is very fast, and diffusion is the rate controlling step. In the char-gas reactions, the burning of char is the fastest among the char-gas reactions taking place in a gasifier. Therefore it is necessary to consider diffusion and to apply an unreacted-core shrinking model to the char-oxygen reaction. The reaction rate considering gas film diffusion, ash diffusion and chemical reaction is shown as:

$$\text{Rate} = \frac{1}{\frac{1}{k_{\text{film}}} + \frac{1}{k_s Y^2} + \frac{1}{k_{\text{ash}}}} (P_i - P_i^*)$$

where  $k_{\text{film}}$  is the gas film diffusion coefficient,  $k_s$  is the chemical reaction constant,  $k_{\text{ash}}$  is the ash diffusion coefficient,  $P_i$  is the partial pressure of reactant  $i$  and  $P_i^*$  is the back reaction equilibrium pressure of reactant  $i$ .

### II-3-1 Char-Oxygen Reaction (Reaction 1)

The stoichiometric coefficient equation of char-oxygen reaction can be expressed as:



The stoichiometric coefficient " $\Psi$ " in the reaction shown above depends on the temperature and particle diameter, as well as the type of coal. Wen and Dutta (24) proposed a correlation for a rough estimation of " $\Psi$ " by a linear interpolation between small and large particle sizes. The value of " $\Psi$ " ranges from zero to one. For large particles ( $>1mm$ ) the value of  $\Psi$  is close to one.

Field et al. (7) presented a chemical reaction rate and gas film diffusion constants for the char-oxygen reaction. Desai and Wen (3) studied the char-oxygen reaction without considering the ash diffusion. In the moving bed gasifier, coal particle sizes are of the order of 10 mm, and in most cases, the gas film and ash diffusions are the rate controlling steps. Therefore the rate equation shown below considering gas film and ash diffusion resistances without reaction resistance are adopted in the program: (22)

$$R_i = P_{O_2} / (1/k_{film} + 1/k_{ash})$$

$$k_{film} = 0.292 \cdot 4.26 (T/1800)^{1.75} / (d_p T)$$

$$k_{ash} = k_{film} \cdot \epsilon_p^{2.5} (Y/(1 - Y))$$

$$Y = r_{core}/r_{particle}$$

where  $R_1$  = the reaction rate (gm-mole/cm<sup>3</sup> · sec)

$\epsilon_p$  = porosity of ash (-)

$k_{film}$  = mass transfer coefficient for gas film diffusion  
 $(\text{gm-mole}/\text{cm}^3 \cdot \text{sec} \cdot \text{atm})$

$k_{ash}$  = mass transfer coefficient for ash diffusion  
 $(\text{gm-mole}/\text{cm}^3 \cdot \text{sec} \cdot \text{atm})$

$r_{core}$  = average radius of shrinking unreacted coal particles (cm)

$r_{particle}$  = average radius of feed coal particles (cm)

### II-3-2 Char-Steam Reaction (Reaction 2)

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 follows the "volumetric reaction" and controls the maximum temperature. Therefore, the kinetics of this reaction are very important.

Wen (23) proposed a simple rate expression shown as follows:

$$\text{Rate} = K_V (P_{H_2O} - P_{H_2} P_{CO} RT/k_{eq}) [C]$$

where [C] = concentration of char

$k_{eq}$  = the equilibrium constant of the reaction

$K_V$  = the rate constant per unit volume

In the program, the following expressions based on the above equation are used:

$$R_2 = k_{O2} \exp(-E_2/RT) [C] (P_{H_2O} - P_{H_2O}^*)$$

$$P_{H_2O}^* = P_{H_2} P_{CO} / \exp(17.29 - 16330/T)$$

where  $R_2$  = the reaction rate ( $\text{g-mol}/\text{cm}^3 \cdot \text{sec}$ )

$k_{O_2}$  = the reaction rate coefficient (1/atm · sec)

$E_2$  = the activation energy for the reaction (cal/g-mol)

The values of  $k_{O_2}$  and  $E_2$  are different for different forms of chars (5, 6, 8, 10, 11, 12). In this program three sets of kinetic constants for different ranks of coals are presented. These constants are listed in III-3 and are determined from experimental data (4). Since the char-steam reaction is affected by diffusion through pores of char for temperatures above 1200°C (10, 13, 14), the above rate expression should not be used when the temperature exceeds 1200°C.

### II-3-3 Water-Gas Shift Reaction (Reaction 3)

This reaction is quick, especially in the presence of a catalyst.

Most water-gas shift reactors employ an iron-base or chromium-base catalyst to produce hydrogen from CO and  $H_2O$ . Desai and Wen (3) used a second order rate expression developed by Moe (15) to describe this reaction. Singh and Sarah (17) also proposed a first order rate equation taking into account the effect of temperature, pressure, age of catalyst, and  $H_2S$  content in the reacting gas on a catalyst.

By assuming a correction factor, b, which represents the reactivity of ash in the char as a catalyst, the following equations were used in the program:

$$R_3 = b \cdot 2.877 \times 10^5 \times \exp(-27760/RT)$$

$$\begin{aligned} & \cdot (X_{CO} X_{H_2O} - X_{CO_2} X_{H_2} / k_{wgs}) X_{ash} \rho_c \\ & \cdot P^{0.5-P/250} (1 - \varepsilon_{bed}) \exp(-8.91 + 5553/T) \end{aligned}$$

$$k_{wgs} = \exp(-3.6890 + 7234/1.8 T)$$

where  $R_3$  = the reaction rate ( $\text{g-mol}/\text{cm}^3 \cdot \text{sec}$ )

$k_{wgs}$  = the equilibrium constant of the water-gas shift reaction

$b$  = the correction factor taking into account the relative reactivity of ash to the iron-base catalyst.

In this program three different correction factors,  $b$ , were used. They are listed in Table III-1.

#### II-3-4 Hydrogen-Oxygen Reaction (Reaction 4)

This reaction is extremely fast, particularly in the presence of minerals that can act as catalysts. Therefore, it is assumed that no hydrogen exists in the presence of oxygen. Although some investigators simulating gasifiers (3, 27) neglected the hydrogen-oxygen reaction, this reaction was included in the program. Using the following reaction rate expression, a good concentration distribution curve has been obtained.

$$R_4 = 3 \cdot 10^{10} \exp(-16000/RT) (P_{O_2}/82.06 \cdot T)^{0.3} \\ \cdot (P_{H_2}/82.06 \cdot T)^{0.5} \epsilon_{bed}$$

where  $R_4$  = the reaction rate ( $\text{gm-mole}/\text{cm}^3 \cdot \text{sec}$ )

$\epsilon_{bed}$  = the porosity of the bed (-)

#### II-3-5 Char-Carbon Dioxide Reaction (Reaction 5)

Gasification of carbon by carbon dioxide is somewhat analogous to steam gasification: 2 mols of CO are made from 1 mol of reactant gas,  $CO_2$ , leading qualitatively to the same conclusion drawn for steam gasification about the effect of temperature and pressure. Wen and Tone (21) suggested that the reaction rate seems to obey the Langmuir type adsorption relation and to be a first order reaction with respect to  $CO_2$  at a

low CO<sub>2</sub> partial pressure and at a temperature below 1300°C.

Three sets of reaction coefficients and apparent activation energies are used based on the following equations similar to the rate equation used for carbon-steam reaction.

$$R_5 = k_{05} \exp (-E_5/RT) [C] (P_{CO_2} - P_{CO_2}^*)$$

$$P_{CO_2}^* = P_{CO_2} / \exp (20.92 - 20280/T)$$

where R<sub>5</sub> = the reaction rate (g-mole/cm<sup>3</sup> · sec)

k<sub>05</sub> = the reaction rate coefficient (1/atm · sec)

E<sub>5</sub> = the activation energy for the reaction (cal/g-mole)

### II-3-6 Char-Hydrogen Reaction (Reaction 6)

The reaction of char and hydrogen is exothermic and produces mainly methane. This reaction is very slow when the hydrogen partial pressure and temperature are low. At high hydrogen partial pressures and at temperatures above 700°C, the rate of this reaction becomes appreciable.

Wen and Huebler (20) proposed empirical equations for the rates of first and second stage hydrogasification. The initial phase of reaction between hydrogen and coal is rapid and has been considered in the devolatilization section in the gasifier. The reaction of hydrogen with the remaining char is much slower. In this program the following rate expressions are used:

$$R_6 = \exp (-7.087 - 8078/T) (P_{H_2} - P_{H_2}^*) [C]$$

$$P_{H_2}^* = [P_{CH_4} / \exp (-13.43 + 10100/T)]^{0.5}$$

### III. CALCULATION PROCEDURES

#### III-1. Structure of the computer program

The computer code consists of the main program, eleven original subroutines and three library subroutines. The structure of the computer program is shown in Figure III-1, and the functions of the subroutines are listed in Table III-1.

Shown in Figure I-2 are the conditions of the inlet gas and the coal feed. The amount of ash is specified by the proximate analysis. The boundary value problem can be solved by first assuming a value for the carbon flow rate in the solid output and then using the fourth order Runge-Kutta method to solve the resulting initial value problem from the bottom to the top of the reaction section. The secant method is used to adjust the assumed value until the calculated flow rate of solid input into the reaction section matches the prescribed flow rate (see assumption 10).

For the devolatilization section of the gasifier, a separate subroutine (DEVOL) is used to calculate the amount of tar and gases formed as a result of pyrolysis. The amount is a function of gasifier pressure, molecular weight and the temperature of the effluent gas from the reaction section. An additional amount of devolatilized carbon due to the presence of hydrogen (hydropyrolysis) in the vapor phase cannot be estimated at this time. This amount must therefore be a user-adjusted parameter (assumption 10).

The program can also be used to design a moving bed coal gasifier if the fraction of unconverted carbon is specified. The initial value problem can be solved for the reaction section from the bottom upward until the calculated coal input rate is equal to the specified value. The distance calculated is then the required bed height. In this calculation, iteration is not required.

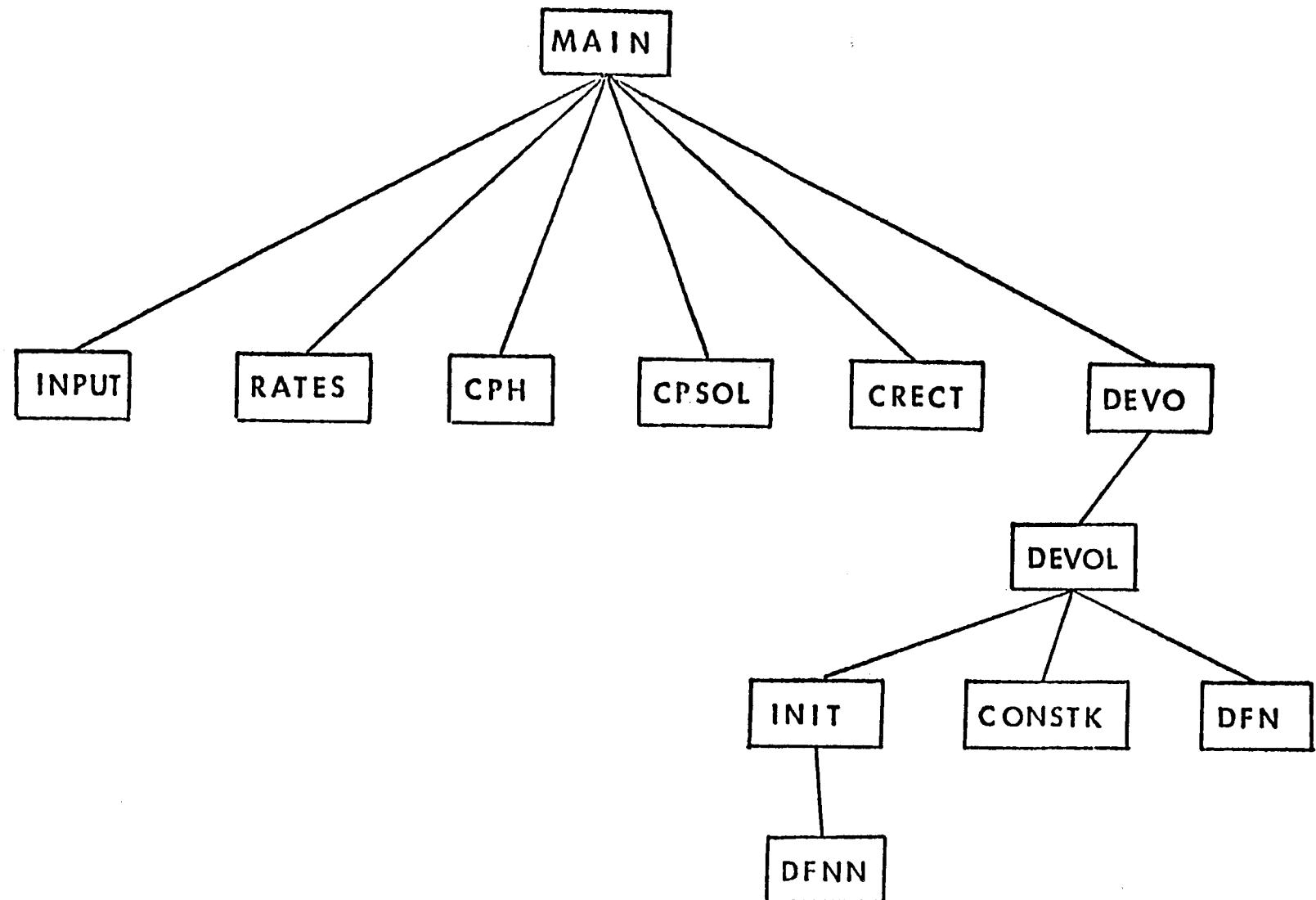


Figure III-1 Program Structure

Table III-1. List of Subroutines

Subroutine	Function	Controlling Program	Input to Subroutines	Output to Subroutines
INPUT	to read and print input data	Main Program	all input data except data given by data statements & block data	same as left
CPH	to calculate the heat capacities and enthalpies of gaseous species	Main Program	temperature	heat capacity & enthalpy of each gas
CPSOL (Function)	to calculate the heat capacity of coal	Main Program	temperature, carbon and ash ratio in devolatilized coal	heat capacity of coal
RATES	to calculate six reaction rates	Main Program	temperature, gas composition particle diameter and amount of combusted carbon	six reaction rates
DEVO	to calculate the amount and composition of volatile products	Main Program	temperature, composition of coal, amount of coal fed and fraction of pyrolyzed volatile matter	amount and composition of tar and gases
DEVOL	to calculate the amount of volatile products	DEVO	temperature, composition of coal and amount of coal fed	amount of tar and gas
DFN	to supply the differential equations for solving mass flux and concentration of species	DEVOL	coefficients of differential equations	differential values

Table III-1. (continued)

Subroutine	Function	Controlling Program	Input to Subroutines	Output from Subroutines
INIT	to calculate the initial conditions for solving the differential equations	DEVOL	devolatilization rate and coal concentration	initial conditions
DFNN	to calculate the coal concentration	INIT	devolatilization rate and coal concentration	change of coal concentration
CONSTK	to fetch the rate constants for three kinds of coal	DEVOL	type of coal	reaction rate coefficients and activation energies for pyrolysis
CRECT	to adjust carbon conversion by Secant Method	Main Program	calculated carbon conversion and difference between assumed and calculated values	modified carbon conversion

Library Subroutine

DREBS	to solve the first order non-linear differential equations by Burlisch-Stoer extrapolation method	DEVOL INIT	*developed by International Mathematical & Statistical Libraries, Inc.
NLDEQS	to solve the first order non-linear differential equations by Runge-Kutta method with fixed step-length	Main Program	*developed by University of Waterloo Computing Center
NBAM	-----	NLDEQS	*developed by University of Waterloo Computing Center
FPPLLOT	to plot diagram	Main Program	

### III-2. Flow chart of the computer program

Figure III-2 shows the computer flow diagram. When IND has a value of 2, the function of the program is simulation, and the carbon conversion has to be found by trial and error in the program; while IND is not equal to 2, the carbon conversion at the bottom of the reactor should be specified by the user.

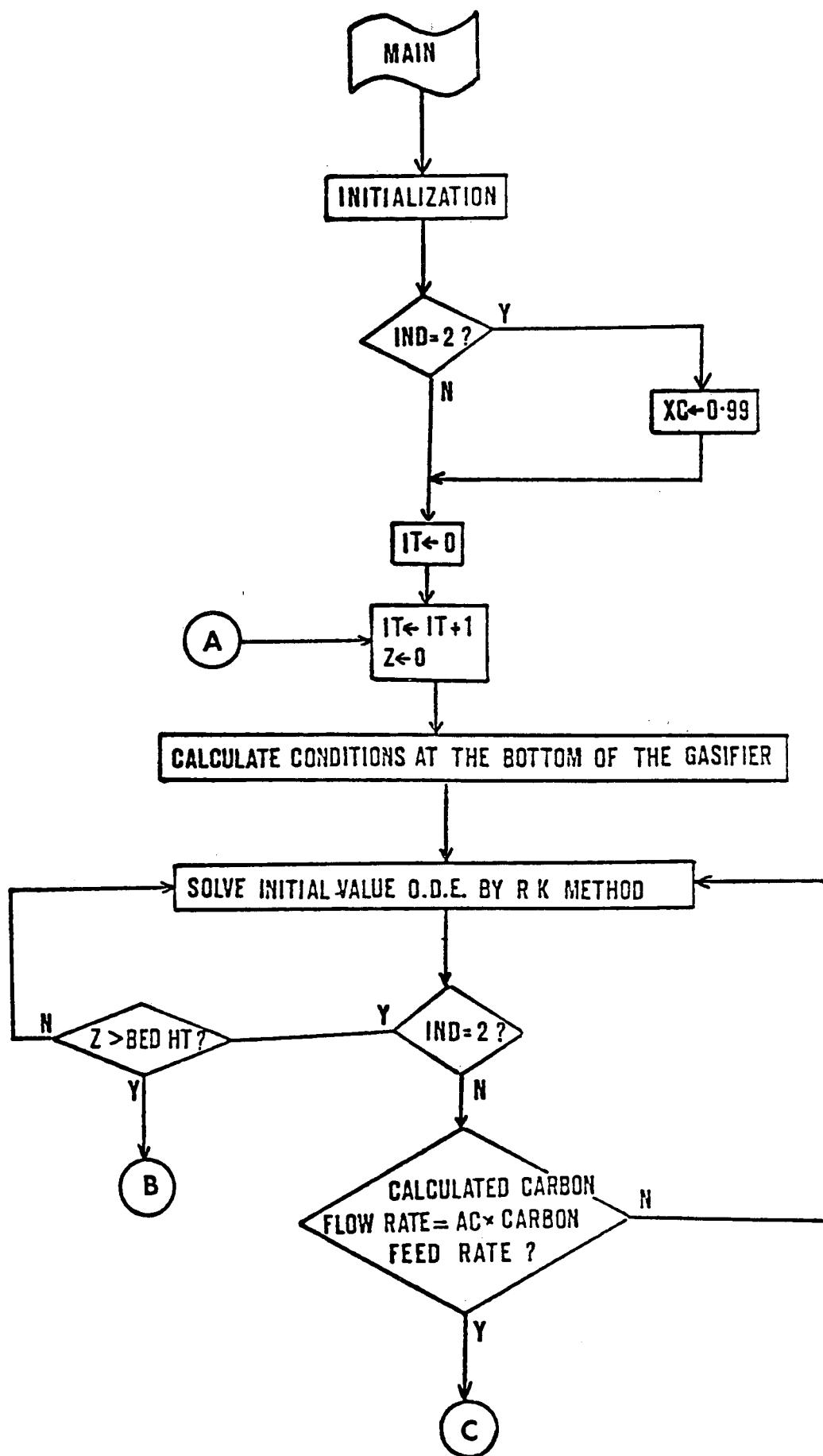


Figure III-2 Computer Flow Diagram

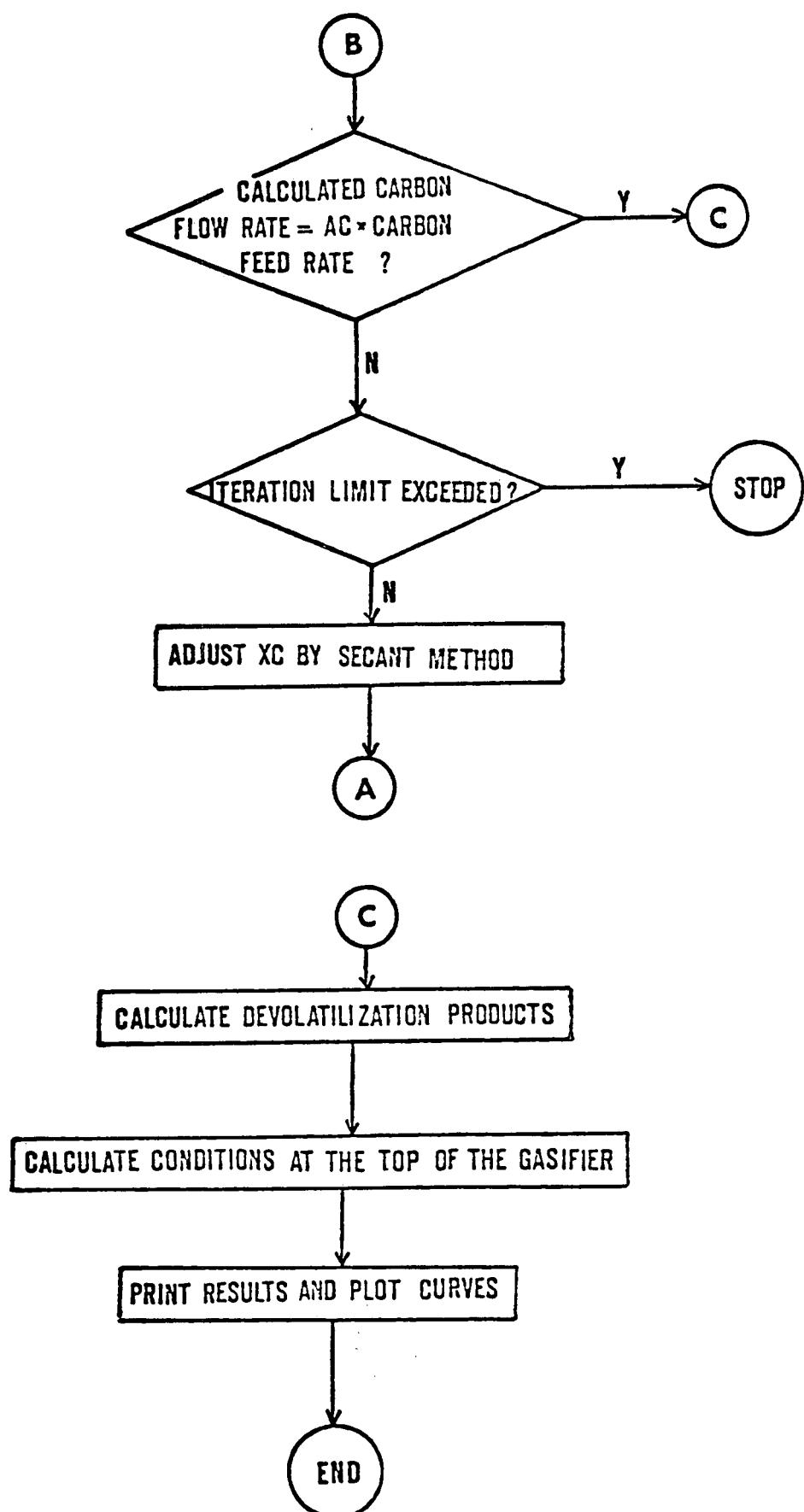


Figure III-2 (continued)

### III-3. Kinetic constants

The simulation program was used to determine kinetic constants. Simulations using oxygen as input gas were compared with the experimental data from the Lurgi Pressure-gasification plant (4) to obtain suitable kinetic constants. The experimental data by the METC fixed bed gasifier (3) were used in comparison for a gasifier using air as feed gas.

Four different kinds of coal--Arkwright, Pittsburgh No. 8, Illinois No. 6 (Bituminous) and Rosebud--were chosen for comparison. Reaction rate coefficients and apparent activation energies for char-steam and char-carbon dioxide reactions, the correction factor for water-gas shift reaction and fraction of volatile matter released by pyrolysis were obtained by simulation, as shown in Table III-2. Tables III-3 to III-6 show good agreement between simulation and experiment.

Table III-2. Kinetic Constants

	Arkwright Pittsburgh (Bituminous)	Pittsburgh No. 8 (Bituminous)	Illinois No. 6 (Bituminous)	Rosebud (Subbituminous)
$K_{O_2}$ , l/atm · sec	600	930	3000	70.0
$E_2$ , cal/g-mole	45000	45000	42000	30000
b	0.0068	0.0068	0.0155	0.014
$k_{05}$ , l/atm · sec	600	930	3000	70.0
$E_5$ , cal/g-mole	45000	45000	42000	30000
$k_{10}$ , l/sec	$1.1 \times 10^5$	$1.1 \times 10^5$	$1.1 \times 10^5$	$5.1 \times 10^4$
$E_{10}$ , cal/g-mole	21200	21200	21200	16200
$k_{20}$ , l/sec	$9.7 \times 10^9$	$9.7 \times 10^9$	$9.7 \times 10^9$	$8 \times 10^{10}$
$E_{20}$ , cal/g-mole	29000	29000	29000	26500
$k_{30}$ , l/sec	$5.3 \times 10^4$	$5.3 \times 10^4$	$5.3 \times 10^4$	$1.1 \times 10^3$
$E_{30}$ , cal/g-mole	7000	7000	7000	4000
Fraction of volatile matter released by pyrolysis	0.870	0.976	0.919	1.22

Table III-3. Comparison of Simulation Results to  
Experimental Results for Arkwright  
Bituminous Coal

<u>Experimental Conditions (3)</u>		
Coal feed rate, lbs/hr		1218.0
Proximate analysis of coal, wt %		
Moisture, 1.12	Volatile matter, 38.63	
Fixed carbon, 52.00	Ash,	8.25
Ultimate analysis of coal, wt %		
C, 75.9	H, 5.7	O, 4.9
N, 1.4	S, 2.7	H <sub>2</sub> O, 1.12
Ash, 8.25		
Heating value of coal, Btu/lb-wet coal		13860.0
Steam feed rate, lbs/hr		576.0
Air feed rate, lbs/hr		3826.0
Temperature of coal, °F		62.95
Temperature of steam, °F		1072.0
Temperature of air, °F		99.0
Temperature of wall		1253.0
Pressure, psig		90.0
Bed diameter, ft		3.5
Bed height, ft		6.5
Initial coal particle size, inches		0.75
<u>Input Data</u>		
Heat transfer coefficient, Btu/ft <sup>2</sup> • hr • °R		90.0
Bed voidage		0.40

Table III-3. (cont.)

	<u>Experimental Results</u>	<u>Simulated Results</u>
Total dry product gas, lbs mole/hr	199.6	200.1
Product gas composition, mole %		
CO	16.2	16.9
CO <sub>2</sub>	12.2	10.2
H <sub>2</sub>	15.7	16.1
CH <sub>4</sub>	4.7	3.6
N <sub>2</sub>	52.5	52.7
H <sub>2</sub> S	0.58	0.52
Exit steam rate, lb mole/hr	17.7*	17.4
Amount of tar, lb/hr	15.0	73.8
Temperature of exit gas, °F	1253.0	1169.0
Maximum temperature, °F	--	2380.0
Carbon conversion, %	87.2	87.0
Heating value of dry product gas, Btu/SCF	146.0	145.0
Heat loss, 10 <sup>6</sup> Btu/hr	5.7	9.5

---

\*Calculated by material balance of hydrogen

Table III-4. Comparison of Simulation Results to Experimental Results for Pittsburgh No. 8 Bituminous Coal

		<u>Experimental Conditions (4)</u>
Coal feed rate, lbs/hr		8058.0
Proximate analysis of coal, wt %		
Moisture,     4.58	Volatile matter, 37.37	
Fixed carbon, 50.31	Ash,               7.74	
Ultimate analysis of coal, wt %		
C,   74.2	H, 5.0	O,   4.5
N,   1.4	S, 2.5	H <sub>2</sub> O, 4.58
Ash, 7.74		
Heating value of coal, Btu/lb-wet coal		13441.8
Steam feed rate, lbs/hr		26145.0
Oxygen feed rate, lbs/hr		5005.0
Oxygen content, mole ratio		0.94
Temperature of coal, °F		77.0
Temperature of steam, °F		700.0
Temperature of oxygen, °F		700.0
Temperature of wall, °F		700.0
Pressure, psig		350.0
Bed diameter, ft		10.0
Bed height, ft		10.0
Initial coal particle size, inches		0.79
		<u>Input Data</u>
Heat transfer coefficient, Btu/ft <sup>2</sup> • hr • °R		30.0
Bed voidage		0.40

Table III-4. (cont.)

	<u>Experimental Results</u>	<u>Simulated Results</u>
Total dry product gas, lbs mole/hr	771.0	796.0
Product gas composition, mole %		
CO	16.8	16.0
CO <sub>2</sub>	31.3	31.0
H <sub>2</sub>	39.2	40.2
CH <sub>4</sub>	10.3	10.3
N <sub>2</sub>	1.6	1.7
H <sub>2</sub> S	0.7	0.8
Exit steam rate, lbs mole/hr	1189.0	1170.0
Amount of tar, lbs/hr	425.0	456.0
Temperature of exit gas, °F	1196.0	1208.0
Maximum temperature, °F	--	1923.0
Carbon conversion, %	98.9	98.3
Heating value of dry product gas, Btu/SCF	285.0	280.0
Heat loss, 10 <sup>6</sup> Btu/hr	--	30.0

Table III-5. Comparison of Simulation Results to Experimental Results for Illinois No. 6 Bituminous Coal

		<u>Experimental Conditions (4)</u>
Coal feed rate, lbs/hr		13270.0
Proximate analysis of coal, wt %		
Moisture, 10.23	Volatile matter, 34.70	
Fixed carbon, 45.97	Ash, 9.10	
Ultimate analysis of coal, wt %		
C, 64.2	H, 4.3	O, 8.1
N, 1.2	S, 2.8	H <sub>2</sub> O, 10.23
Ash, 9.10		
Heating value of coal, Btu/lb-wet coal		11463.598
Steam feed rate, lbs/hr		33331.0
Oxygen feed rate, lbs/hr		6396.0
Oxygen content, mole ratio		0.94
Temperature of coal, °F		77.0
Temperature of steam, °F		700.0
Temperature of oxygen, °F		700.0
Temperature of wall, °F		700.0
Pressure, psig		335.0
Bed diameter, ft		10.0
Bed height, ft		10.0
Initial coal particle size, inches		0.93
		<u>Input Data</u>
Heat transfer coefficient, Btu/ft <sup>2</sup> • hr •°R		30.0
Bed voidage		0.40

Table III-5. (cont.)

	<u>Experimental Results</u>	<u>Simulated Results</u>
Total dry product gas, lbs mole/hr	1061.0	1074.0
Product gas composition, mole %		
CO	17.2	18.0
CO <sub>2</sub>	31.1	30.0
H <sub>2</sub>	38.9	38.3
CH <sub>4</sub>	10.6	10.9
N <sub>2</sub>	1.2	1.7
H <sub>2</sub> S	1.0	1.1
Exit steam rate, lbs mole/hr	1565.0	1528.0
Amount of tar, lbs/hr	558.0 (recycle)	943.0
Temperature of exit gas, °F	1122.0	1119.0
Maximum temperature, °F	--	1814.0
Carbon conversion, %	99.0	98.5
Heating value of dry product gas, Btu/SCF	290.0	288.0
Heat loss, 10 <sup>6</sup> Btu/hr	--	24.0

Table III-6. Comparison of Simulation Results to Experimental Results for Rosebud Subbituminous Coal

	<u>Experimental Conditions (4)</u>
Coal feed rate, lbs/hr	13580.0
<b>Proximate analysis of coal, wt %</b>	
Moisture,     26.48	Volatile matter, 29.10
Fixed carbon, 35.45	Ash,           8.97
<b>Ultimate analysis of coal, wt %</b>	
C,    49.8	H,  3.4
N,    0.8	O,   9.5
	S,  1.0       H <sub>2</sub> O, 26.48
Ash,   8.97	
Heating value of coal, Btu/lb-wet coal	8611.297
Steam feed rate, lbs/hr	13673.0
Oxygen feed rate, lbs/hr	3336.0
Oxygen content, mole ratio	0.94
Temperature of coal, °F	77.0
Temperature of steam, °F	700.0
Temperature of oxygen, °F	700.0
Temperature of wall, °F	700.0
Pressure, psig	344.0
Bed diameter, ft	10.0
Bed height, ft	10.0
Initial coal particle size, inches	0.27
 <u>Input Data</u>	
Heat transfer coefficient, Btu/ft <sup>2</sup> • hr • °R	30.0
Bed voidage	0.40

Table III-6. (cont.)

	<u>Experimental Results</u>	<u>Simulated Results</u>
Total dry product gas, lbs mole/hr	768.0	772.0
Product gas composition, mole %		
CO	20.2	19.0
CO <sub>2</sub>	28.7	28.0
H <sub>2</sub>	36.4	36.2
CH <sub>4</sub>	13.0	15.0
N <sub>2</sub>	1.3	1.3
H <sub>2</sub> S	0.4	0.5
Exit steam rate, lbs mole/hr	672.0	651.0
Amount of tar, lbs/hr	597.0	900.0
Temperature of exit gas, °F	617.0	889.0
Maximum temperature, °F	--	1831.0
Carbon conversion, %	98.7*	95.5
Heating value of dry product gas, Btu/SCF	312.0	325.0
Heat loss, 10 <sup>6</sup> Btu/hr	--	19.0

---

\*This number includes liquid product.

#### IV. INPUT DATA

Three sets of typical input data are shown in Table IV-1. However, the input data can be changed as described in Chapter VI if the properties of coal are different from those three sets listed in Table IV-1.

The contents of the input data are shown as follows:

##### 1st Row:

A title or comment statement for the data set to follow should be entered in columns 1-20.

##### 2nd Row:

In the 1st column: "1" indicates a design case; the bed height required will be calculated. "2" indicates a simulation case; the product composition and distribution will be calculated.

The 2nd column shows the feed stock. A "1" is for bituminous coal, "2" for subbituminous coal and "3" for lignite. According to this code, kinetic constants for pyrolysis will be chosen. If the coal sample is different from the standard, program users should specify different values in the subroutine "BLOCK DATA" and obtain better simulation.

##### 3rd Row (Proximate Analysis):

from the 2nd column; moisture content (wt %)

from the 12th column; volatile matter content (wt %)

from the 22nd column; fixed carbon content (wt %)

from the 32nd column; ash content (wt %)

The summation of the above four numbers should be 100 percent.

Table IV-1. Typical Input Data

Row	Column	2	12	22	32	42	52	62
<b>1 10/9 (PITTSBURGH 8)</b>								
2	21							
3	4.58	37.37	50.31	7.74				
4	0.742	0.050	0.045	0.014	0.025			
5	8058.0	26145.0	5005.0	0.94	77.0	700.0	700.0	
6	13441.8	350.0	10.0	0.79	0.976	10.0		
7	0.4	30.0	700.0					
8								
<b>1 10/9 (ILLINOIS 6)</b>								
2	21							
3	10.23	34.70	45.97	9.10				
4	0.642	0.043	0.081	0.012	0.028			
5	13270.0	33331.0	6396.0	0.94	77.0	700.0	700.0	
6	11463.6	335.0	10.0	0.93	0.919	10.0		
7	0.4	30.0	700.0					
8	3000.0	42000.0	0.0155	3000.0	42000.0			
<b>1 10/9 (ROSEBUD)</b>								
2	23							
3	26.48	29.1	35.45	8.97				
4	0.498	0.034	0.095	0.008	0.01			
5	13580.0	13673.0	3336.0	0.94	77.0	700.0	700.0	
6	8611.3	344.0	10.0	0.27	1.22	10.0		
7	0.4	30.0	700.0					
8	70.0	30000.0	0.014	70.0	30000.0			

4th Row (Ultimate Analysis):

from the 2nd column; carbon content (wt ratio)  
from the 12th column; hydrogen content (wt ratio)  
from the 22nd column; oxygen content (wt ratio)  
from the 32nd column; nitrogen content (wt ratio)  
from the 42nd column; sulfur content (wt ratio)

These numbers should be based on the total weight of coal, including moisture and ash.

5th Row (Operating Condition)

from the 2nd column; coal feed rate (lbs/hr)  
from the 12th column; steam feed rate at the bottom of the gasifier (lbs/hr)  
from the 22nd column; air/oxygen feed rate including nitrogen and argon at the bottom of the gasifier (lbs/hr)  
from the 32nd column; oxygen content of the above air/oxygen feed (mole ratio)  
from the 42nd column; temperature of feed coal (°F)  
from the 52nd column; temperature of steam (°F)  
from the 62nd column; temperature of air/oxygen (°F)

6th Row (Operating Condition and Dimension):

from the 2nd column; heating value of feed coal (Btu/lb-wet coal)  
from the 12th column; pressure inside the gasifier (psig)  
from the 22nd column; bed diameter (ft)  
from the 32nd column; initial particle size of feed coal (inch)  
from the 42nd column; fraction of volatile matter released during pyrolysis, including hydropyrolysis (-)  
from the 52nd column; carbon conversion ratio (-) for "Design Case";  
bed height (ft) for "Simulation Case"

7th Row (Operating Condition)

from the 2nd column; bed voidage (-)

from the 12th column; heat transfer coefficient through the wall of  
the gasifier (Btu/hr • ft<sup>2</sup> • °F)

from the 22nd column; wall temperature (°F)

8th Row (Kinetic Constants)

from the 2nd column; reaction rate coefficient of char-steam  
reaction (g-mole/mole C • atm • sec)

from the 12th column; activation energy of char-steam reaction  
(cal/g-mole)

from the 22nd column; effective factor of steam-gas shift reaction

from the 32nd column; reaction rate coefficient of char-carbon dioxide  
reaction (g-mole/mole C • atm • sec)

from the 42nd column; activation energy of char-carbon dioxide reaction  
(cal/g-mole)

If a program user does not make a specification in this row, the default  
values will be used. The default values for bituminous coal are those of  
Pittsburgh No. 8 seam coal. If another kind of seam coal is used, kinetic  
constants for gasification should be specified by the user with reference  
to Table III-2.

## V. SAMPLE PROBLEM

### V-1. Output of the computer program

The calculations for a sample problem to design a gasifier of Pittsburgh No. 8 seam coal are shown in Tables V-1 to V-3. The computer outputs are shown after the next section.

Since this example illustrates the design of a gasifier, the final output is the bed height needed for a given carbon conversion (see Table V-3). If the program is for the simulation of a gasifier, the nature of the output is slightly altered: the bed height is replaced by carbon conversion. The input information also appears on the first page so that users can read it and avoid unnecessary errors.

When "OUTER LOOP LIMIT OF - ITERATIONS EXCEED" follows the input data, some of the data exceeds the available range for this program. If this happens, the input data should be checked or the step size for integration DZ (in line 22 of the main program) should be reduced. When "MAXIMUM LENGTH OF - FT EXCEED . . ." is printed, the bed diameter should be increased or the specified carbon conversion should be reduced. If users want to increase the limit of bed height, the upper limit of iteration (line 209 of the main program) should be increased.

The number with "HEATING VALUE OF GAS" includes the portion of the tar formed. It is necessary to make slight adjustments if a program user wants to obtain a heating value for only the gas ( $\text{CO}$ ,  $\text{H}_2$  and  $\text{CH}_4$ ). "MAXIMUM TEMPERATURE" should be less than  $2000^{\circ}\text{F}$  to avoid slag formation.

### V-2. Interpretation of graphs

Figures V-1 through V-7 show concentration and temperature profiles in the gasifier along the bed height. The temperature profile is shown in

Table V-1 Output from Sample Calculation

```

*****  

8/7/80 ( PITTSBURGH 8 ) 1303.  

*****  

PROGRAM FUNCTION = DESIGN  

COAL TYPE = BITUMINOUS  

*****  

INPUT DATA  

*****  

PROXIMATE ANALYSIS -  

MOISTURE VOLATILE MATTER FIXED CARBON ASH  

4.580 37.370 50.310 7.740  

*****  

ULTIMATE ANALYSIS -  

CARBON HYDROGEN OXYGEN NITROGEN SULFUR  

0.742 0.050 0.045 0.014 0.025  

COAL FEED RATE = 43204.000 LB/HR  

SIEVE FEED RATE = 133133.000 LB/HR  

AIR FEED RATE = 25923.000 LB/HR  

MOL % FRACTION OF OXYGEN IN AIR = 0.040  

TEMPERATURE OF COAL = 77.000 F  

TEMPERATURE OF STEAM = 700.000 F  

TEMPERATURE OF AIR = 700.000 F  

HEATING VALUE OF COAL = 13441.797 BTU/LB  

PRESSURE = 500.000 PSIG  

BED DIA/FIRE = 12.000 FT  

PARTICLE SIZE = 0.790 INCH  

FRACTION IN REVOL'D = 0.576  

CARBON CONVERSION = 0.980  

BED VELOCITY = 0.400  

HEAT TRANSFER COEFF = 33.000 BTU/HR-FT^2-R  

WALL TEMPERATURE = 700.000 F  

KINETIC CONSTANTS  

REACTION 2 I K = 930.00 E = 45000.00  

REACTION 3 I K = 0.006800  

REACTION 5 I K = 930.00 E = 45000.00  

OUTER LOOP ITERATION:  

F = 112897E 04 0.27691E 04 0.122239E 03 0.102705E 03 0.0 0.132043E 03 0.731591E 00 0.727603E 03  

J = 12 80 6 475, RTG, TH, T, AX  

I = 0.25330E 03 0.1/9229E 04 0.491471E 04 0.846910E 01 0.258419E 07 0.137045E 04  

DEVIATION ITERATION = 1 = 0.112897E 04 -0.396730E 02  

DEVIATION ITERATION = 2 = 0.132043E 03 0.148685E 03 0.661679E 01 -0.387484E 02 0.272185E 01 0.426209E 01  

- 0.26799E 03 -0.236517E 03 -0.154376E 02 -0.143440E 02  

*****  

OUTPUT DATA  

*****  

PROFILES OF FLOW RATES AND TEMPERATURES (UNITS ARE F (1), LB/HR (2), LB/MOLE/LB (3-8))  

2 C H6 CO2  

C H2 CH4 H2O  

0.0 0.699999E 03 0.641148E 03 0.0 0.0  

0.767243E 03 0.0 0.640666E 04  

-0.295 0.123557E 04 0.46534E 03 0.179535E 03 0.179789E 03  

0.191123E 03 0.716159E-01 0.103409E-14 0.684059E 04  

0.623 0.177511E 04 0.984344E-04 0.380693E-03 0.386201E 03  

0.193099E 03 0.490966E 01 0.357954E-11 0.683584E 04

```

Table V-2 Output from Sample Calculation

0.951	0.200061E 04	0.128849E 05	0.537183E 03	0.483129E 03
1.230	0.194950E 04	0.152996E 05	0.709789E 03	0.511748E 03
1.600	0.209866E 04	0.199719E 03	0.204518E 07	0.664142E 04
1.936	0.187546E 04	0.167225E 05	0.802814E 03	0.537875E 03
2.264	0.155546E 02	0.344049E 03	0.334023E 06	0.849955E 04
2.592	0.182623E 04	0.175744E 05	0.857594E 03	0.552378E 03
2.920	0.115426E 04	0.447470E 03	0.273242E 05	0.639316E 04
3.248	0.178932E 04	0.183750E 05	0.893233E 03	0.584611E 03
3.576	0.455972E 07	0.526015E 03	0.170441E 04	0.631261E 04
3.904	0.174010E 04	0.186706E 05	0.917470E 03	0.605309E 03
4.232	0.634776E 09	0.594167E 03	0.949232E 04	0.624684E 04
4.560	0.173614E 04	0.193679E 05	0.935424E 03	0.624733E 03
4.888	0.0	0.649621E 03	0.399216E 00	0.619020E 04
5.217	0.171576E 04	0.197433E 05	0.948205E 03	0.642883E 03
5.545	0.0	0.697869E 03	0.782454E 00	0.614111E 04
5.873	0.169804E 04	0.206648E 05	0.957510E 03	0.654614E 03
6.201	0.0	0.740555E 03	0.116270E 01	0.509713E 04
6.529	0.166835E 04	0.205914E 05	0.969191E 03	0.691258E 03
6.857	0.0	0.813497E 03	0.191877E 01	0.602377E 04
7.185	0.165563E 04	0.208114E 05	0.972856E 03	0.705667E 03
7.513	0.0	0.845171E 03	0.229641E 01	0.599084E 04
7.841	0.164400E 04	0.210091E 05	0.975172E 03	0.719479E 03
8.169	0.0	0.874304E 03	0.267374E 01	0.596694E 04
8.507	0.163327E 04	0.211981E 05	0.978542E 03	0.732651E 03
8.835	0.0	0.901264E 03	0.305017E 01	0.593372E 04
9.163	0.162332E 04	0.213512E 05	0.971156E 03	0.745255E 03
9.491	0.0	0.926338E 03	0.342649E 01	0.590739E 04
9.819	0.161402E 04	0.215067E 05	0.977150E 03	0.757337E 03
10.147	0.0	0.945744E 03	0.380165E 01	0.588323E 04
10.475	0.160530E 04	0.216382E 05	0.976613E 03	0.766440E 03
10.803	0.0	0.971669E 03	0.417577E 01	0.586053E 04
11.131	0.159708E 04	0.217653E 05	0.975691E 03	0.780099E 03
11.459	0.0	0.992320E 03	0.454872E 01	0.583915E 04
11.787	0.158930E 04	0.218941E 05	0.974345E 03	0.790846E 03
12.115	0.0	0.101177E 01	0.492036E 01	0.581895E 04
12.443	0.158191E 04	0.219978E 05	0.972800E 03	0.801209E 03
12.771	0.0	0.103017E 04	0.529057E 01	0.579901E 04
13.100	0.157487E 04	0.220951E 05	0.970454E 03	0.811214E 03
13.428	0.0	0.104754E 04	0.565924E 01	0.574164E 04
13.756	0.145456E 04	0.320661E 05	0.112737E 04	0.947377E 03
14.084	0.0	0.158147E 04	0.347539E 01	0.557703E 04
PERCENTAGE OF GAS PRODUCT (DRY BASIS)				
CO	CO <sub>2</sub>	H <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub> O
27.16153	22.83783	0.0	38.12358	0.34217
PERCENTAGE OF TAR PRODUCT				
C	H			
46.6499	5.9737	5.3763		
TOTAL GAS OUTLET			0.414827E 04	LBMOLE/HR
HEAT G VALUE OF GAS			0.313174E 03	BTU/SCF
GAS EXIT TEMPERATURE			0.145456E 04	F
AVERAGE OF TARI			0.217745E 04	LB/HR
TOTAL SOLID WEIGHT			0.348513E 04	LB/HR
SOLID EXIT TEMP			0.649949E 03	F
TOTAL HEAT LOSS			0.369169E 04	BTU/HR

Table V-3 Output from Sample Calculation

THERMAL EFFICIENCY	=	0.752456E 02 PERCENT
STEAM DECOMPOSITION	=	0.155839E 00
MAXIMUM TEMPERATURE	=	0.202122E 04 F
BED HEIGHT	=	0.764436E-01 MT

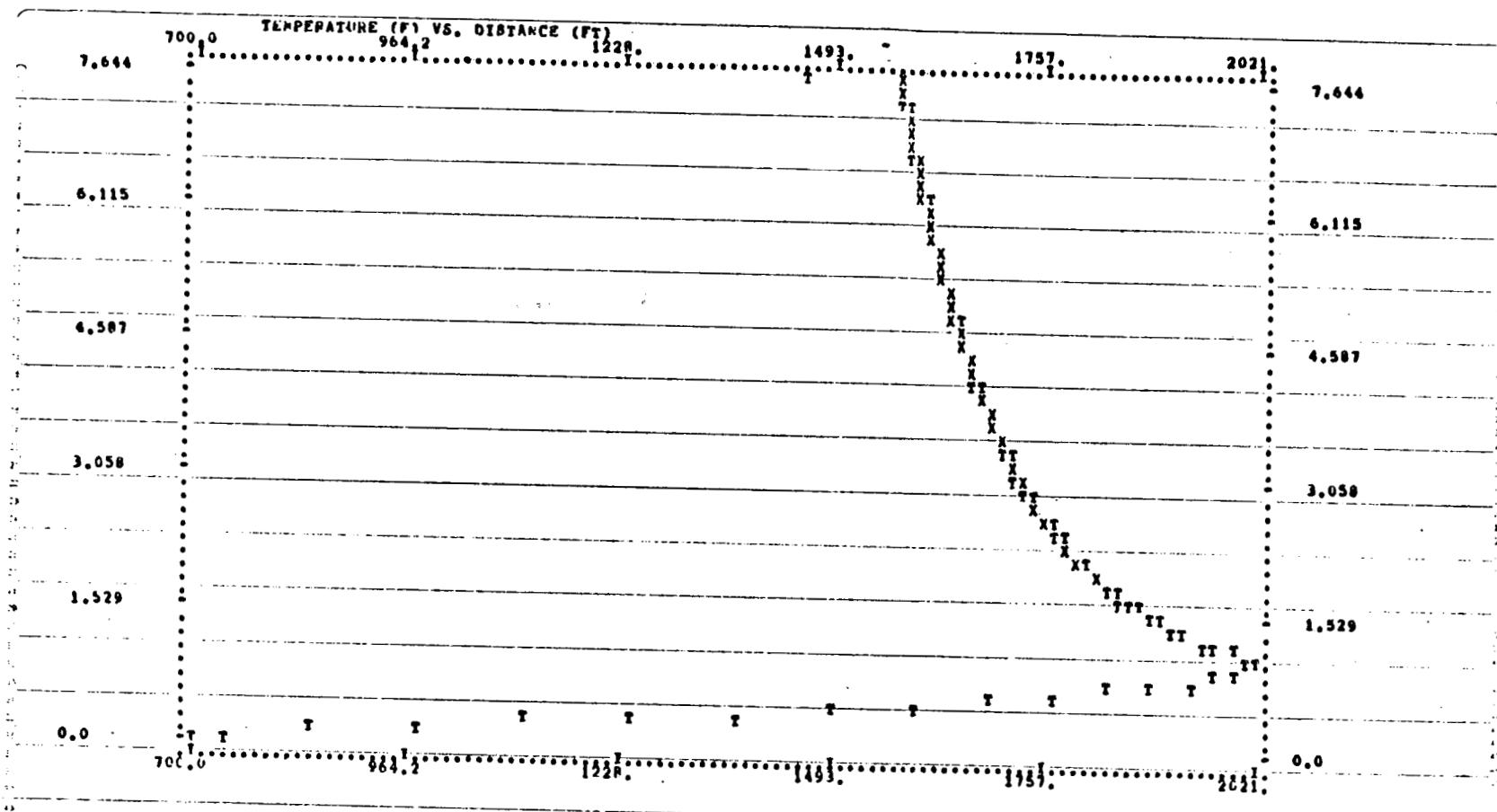


Figure V-1 Temperature as a Function of Bed Height in Sample Calculation

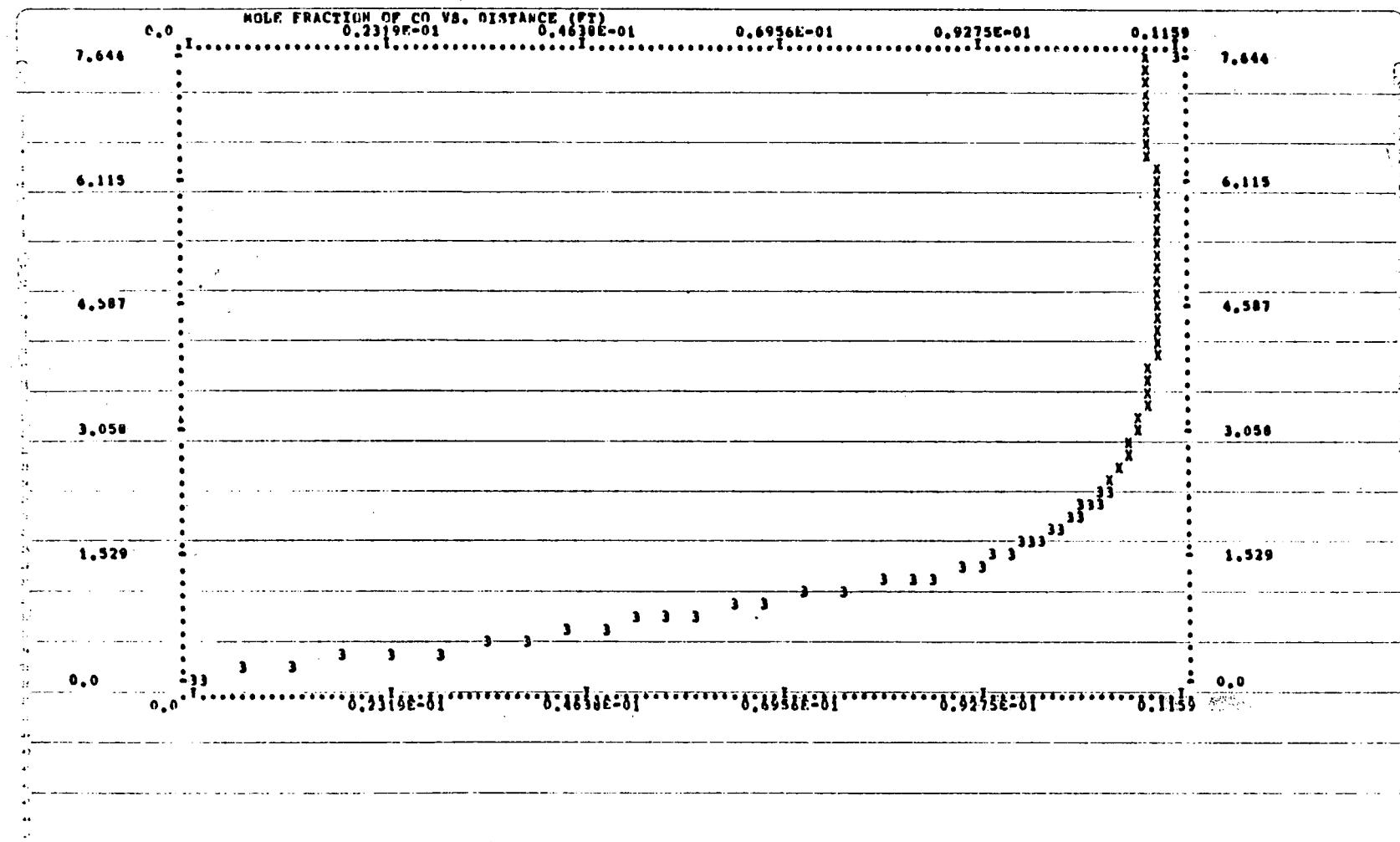


Figure V-2 CO Concentration as a Function of Bed Height in Sample Concentration

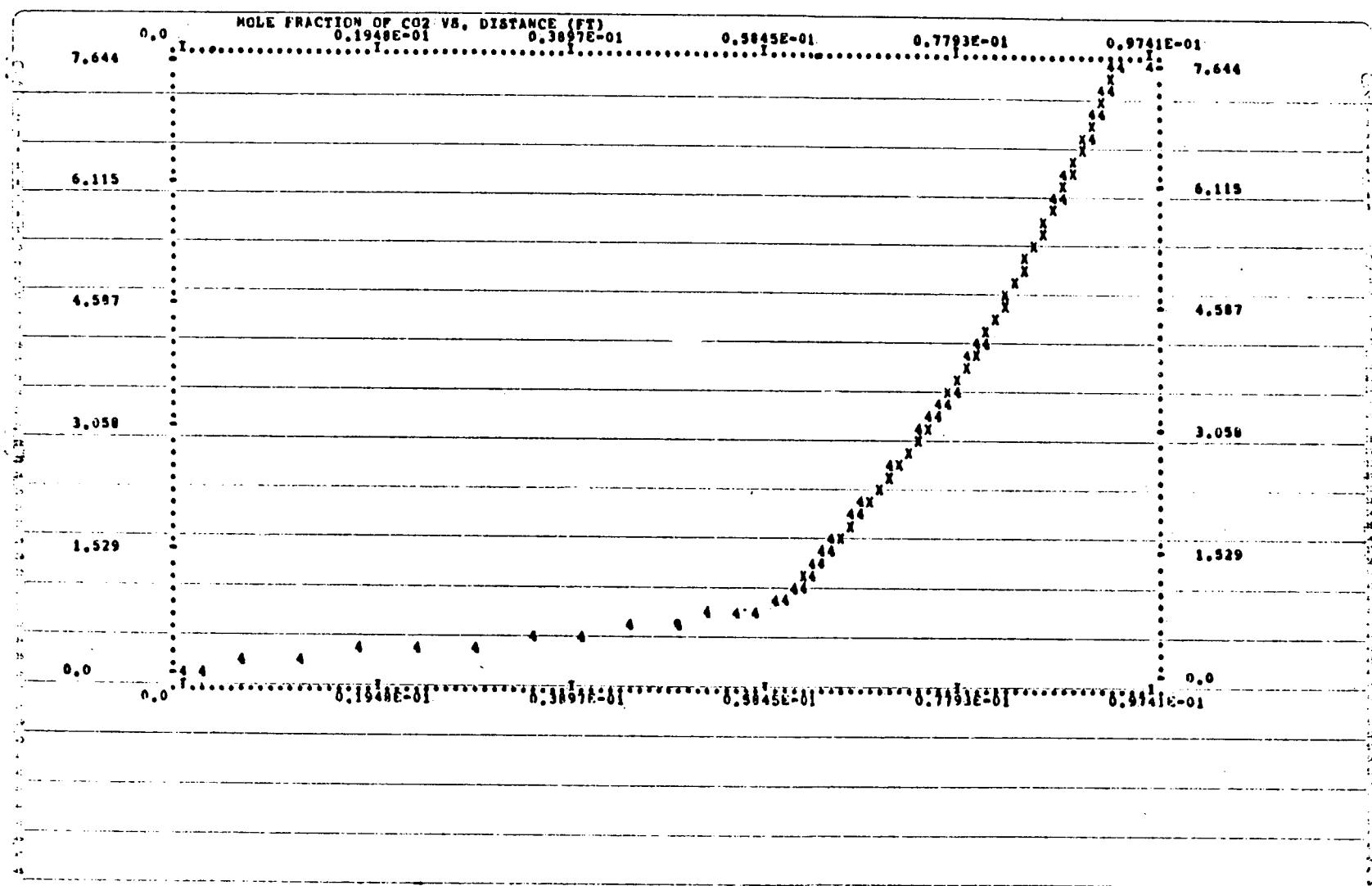


Figure V-3 CO<sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation

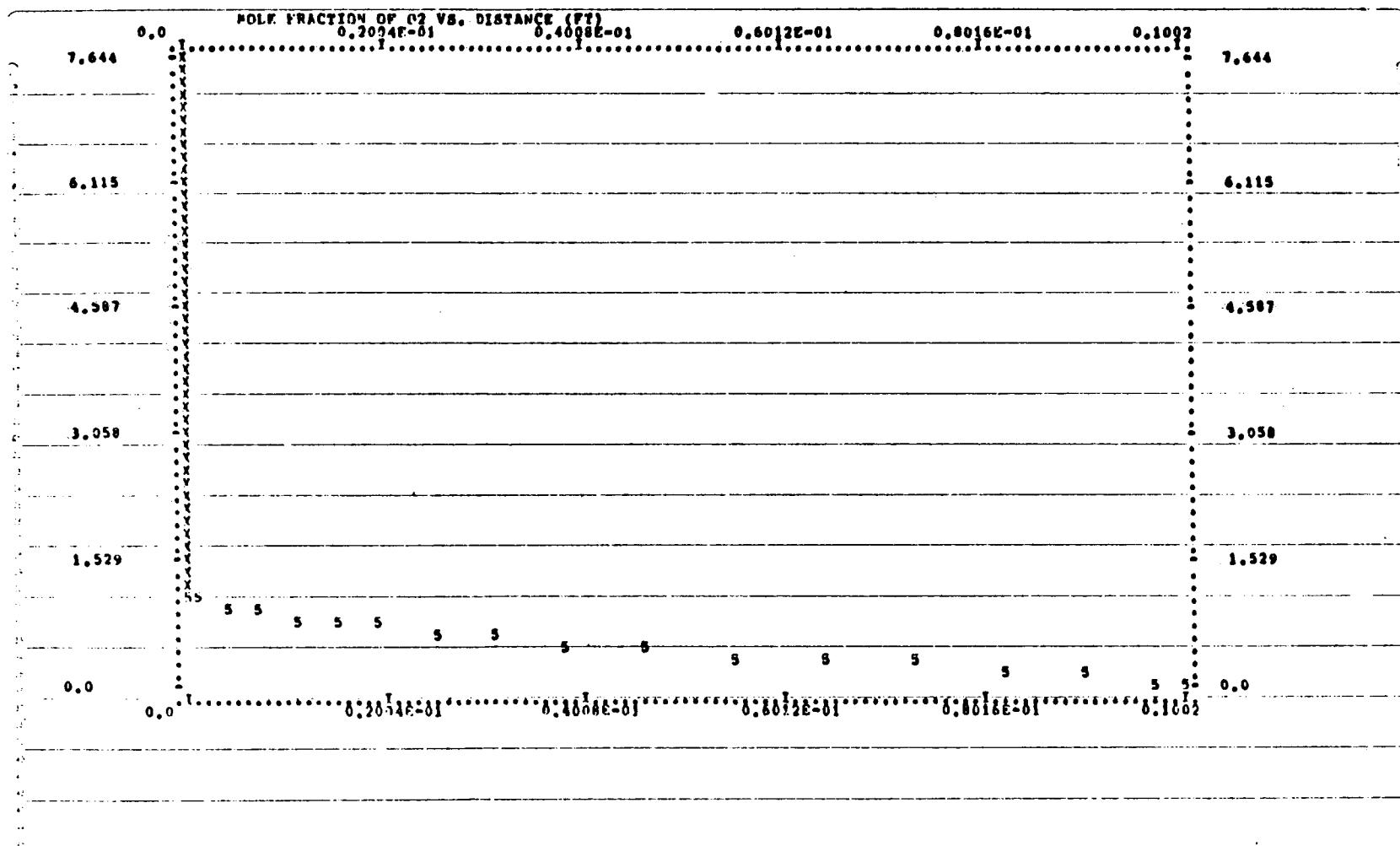


Figure V-4 O<sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation.

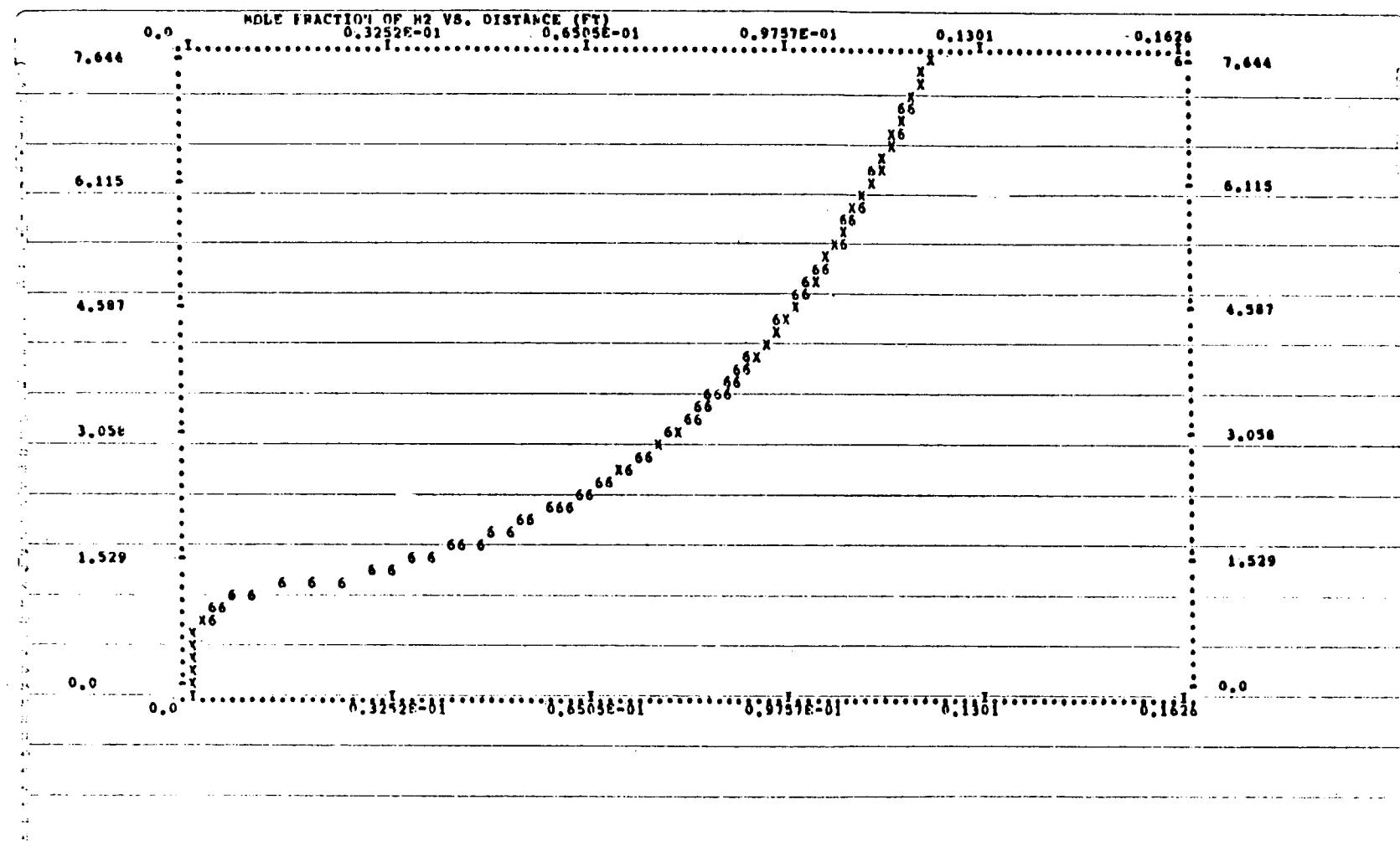


Figure V-5 H<sub>2</sub> Concentration as a Function of Bed Height in Sample Calculation

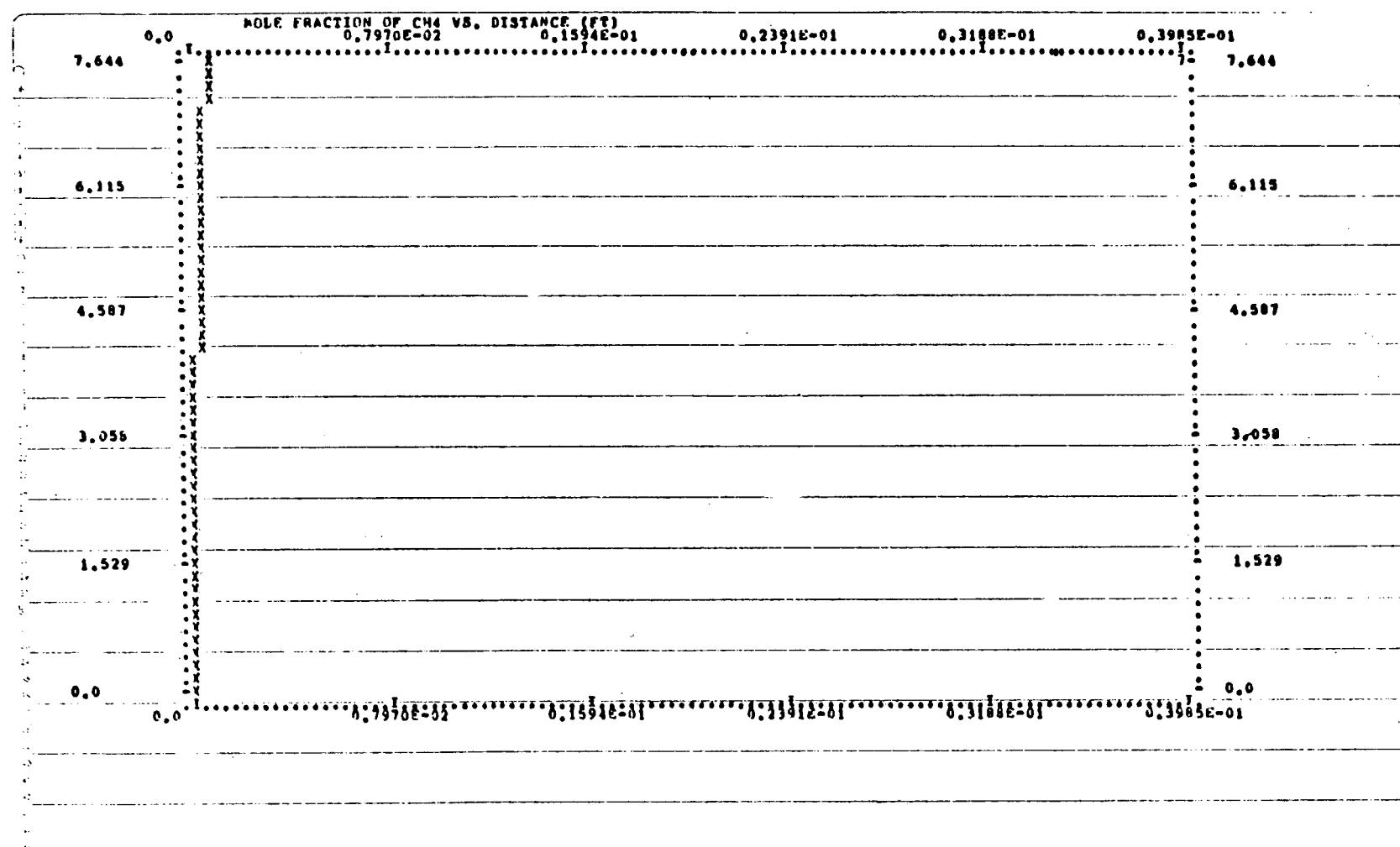


Figure V-6 CH<sub>4</sub> Concentration as a Function of Bed Height in Sample Calculation

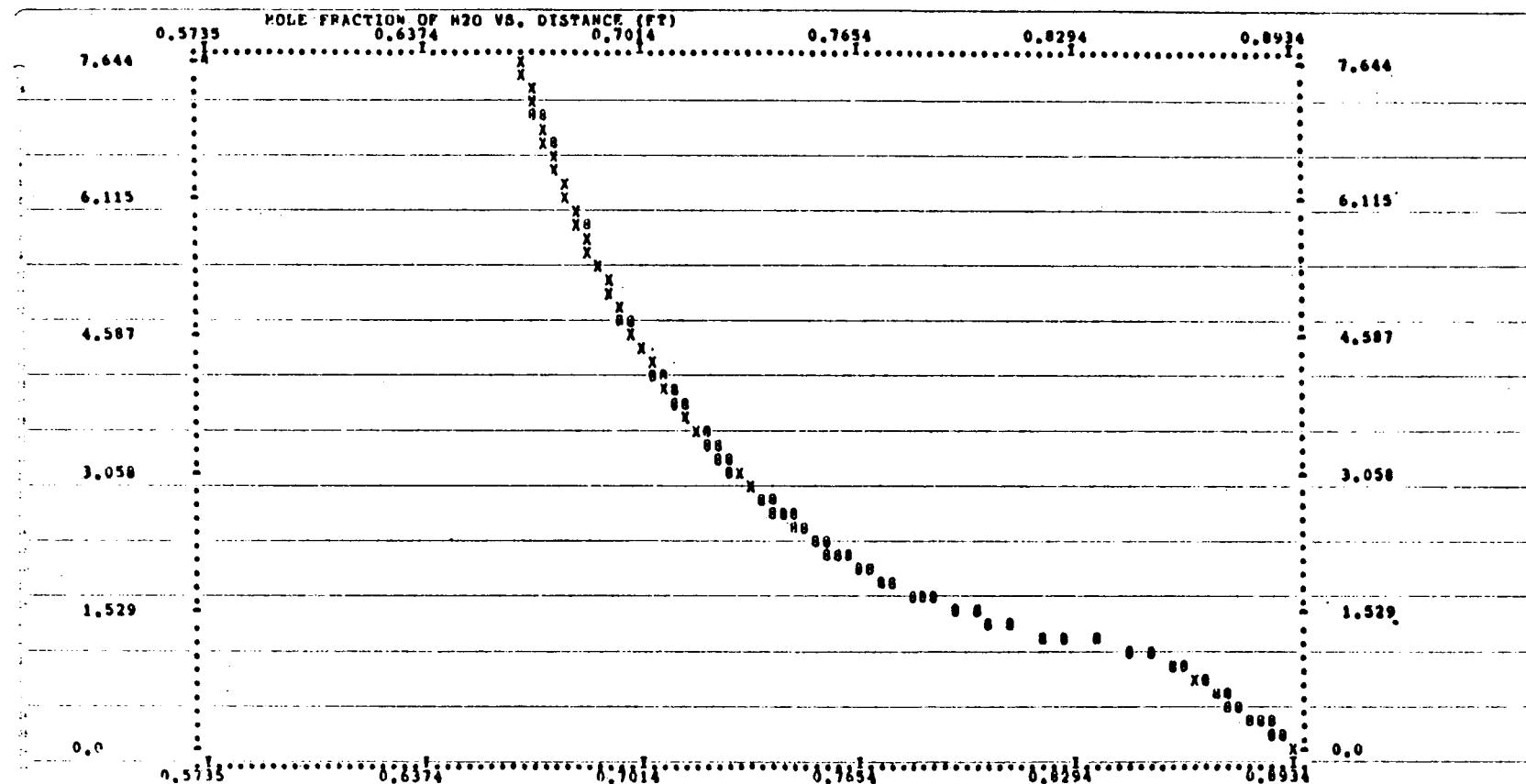


Figure V-7 H<sub>2</sub>O Concentration as a Function of Bed Height in Sample Calculation

Figure V-1. In this figure the section from 0.0 to 1.1 ft represents the combustion zone, and the section from 1.1 to 7.6 ft represents the gasification zone. These figures do not include drying and devolatilization zones (see assumption 4). In Figure V-1, at a bed height of 7.644 ft, "X" is the inlet temperature of the gas entering the devolatilization zone, and "T" is the exit gas temperature.

In Figure V-2, the concentration of CO increases gradually along the bed height because of combustion and char-steam reaction from 0.0 to 4.0 ft. Over 4.0 ft the concentration of CO is almost constant despite the char-steam reaction. This is because the steam-gas shift reaction consumes CO and produces  $H_2$  and  $CO_2$ . The shape of Figure V-5 is related to that of Figure V-7 because one mole of  $H_2O$  produces one mole of  $H_2$ . In the combustion zone,  $H_2$  concentration is almost zero because of complete hydrogen-oxygen reaction as shown in Figure V-5. Figure V-6 shows that the amount of  $CH_4$  produced by gasification is very small in comparison with that by devolatilization.

## VI. APPLICATION AND RANGE OF VALIDITY

Two applications are described in Sections VI-1 and VI-2: the construction of design maps and the modification of the reaction mechanism or parameters in the program. In Section VI-3, the valid range of application is discussed.

### VI-1. Design map

For a given range of temperature and a given range of heating value for coals, design maps can be constructed based on a set of operating conditions. The designer then can choose a correct oxygen/coal flow rate for the gasifier.

Five design maps (Figures VI-1 to VI-5) were constructed based on the following conditions:

<u>Case</u>	<u>Coal Flow Rate (lbs/ft<sup>2</sup> • hr)</u>	<u>Air/Oxygen</u>	<u>Pressure (psig)</u>	<u>Carbon Conversion (%)</u>
1	637	Oxygen	500	98
2	191	Oxygen	500	98
3	637	Air	500	98
4	637	Air	40	95
5	191	Air	40	95

Other conditions are as follows:

Coal:	Pittsburgh No. 8
Mole fraction of oxygen:	Oxygen, 0.94 Air, 0.21
Particle size:	0.79 in.
Bed voidage:	0.4

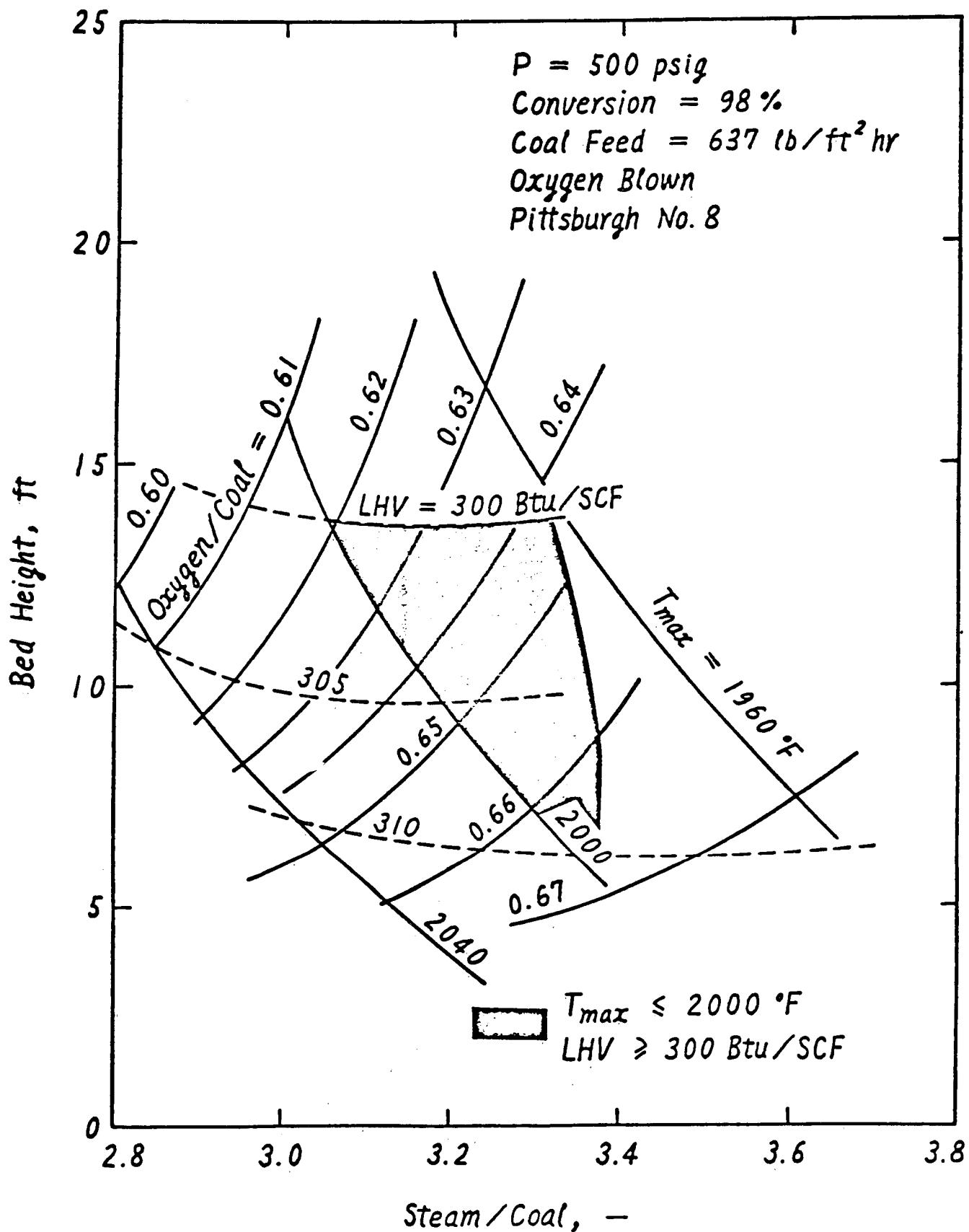


Figure VI-1. Design Map for Moving Bed Coal Gasifier (Case 1)

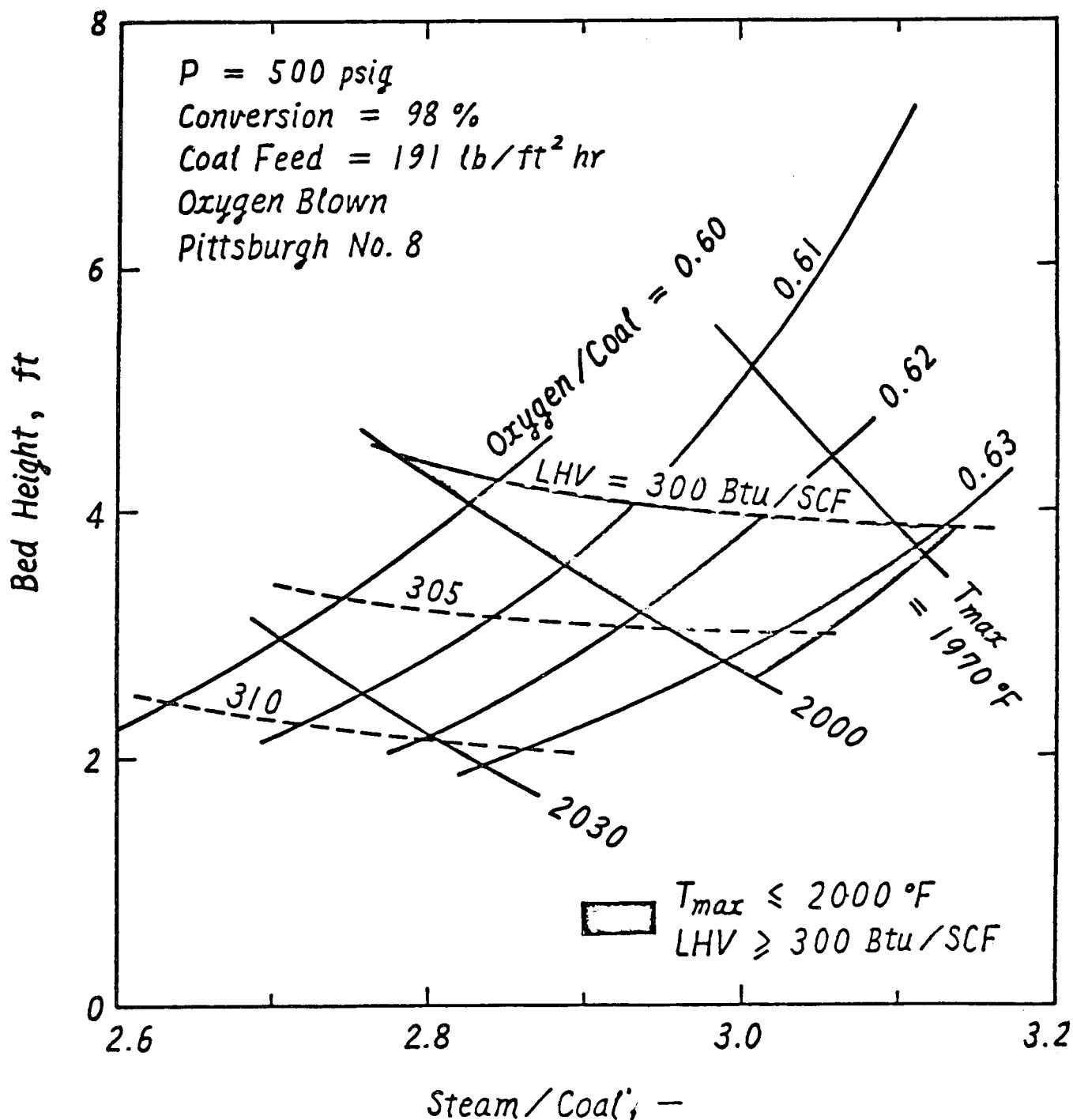


Figure VI-2. Design Map for Moving Bed Coal Gasifier (Case 2)

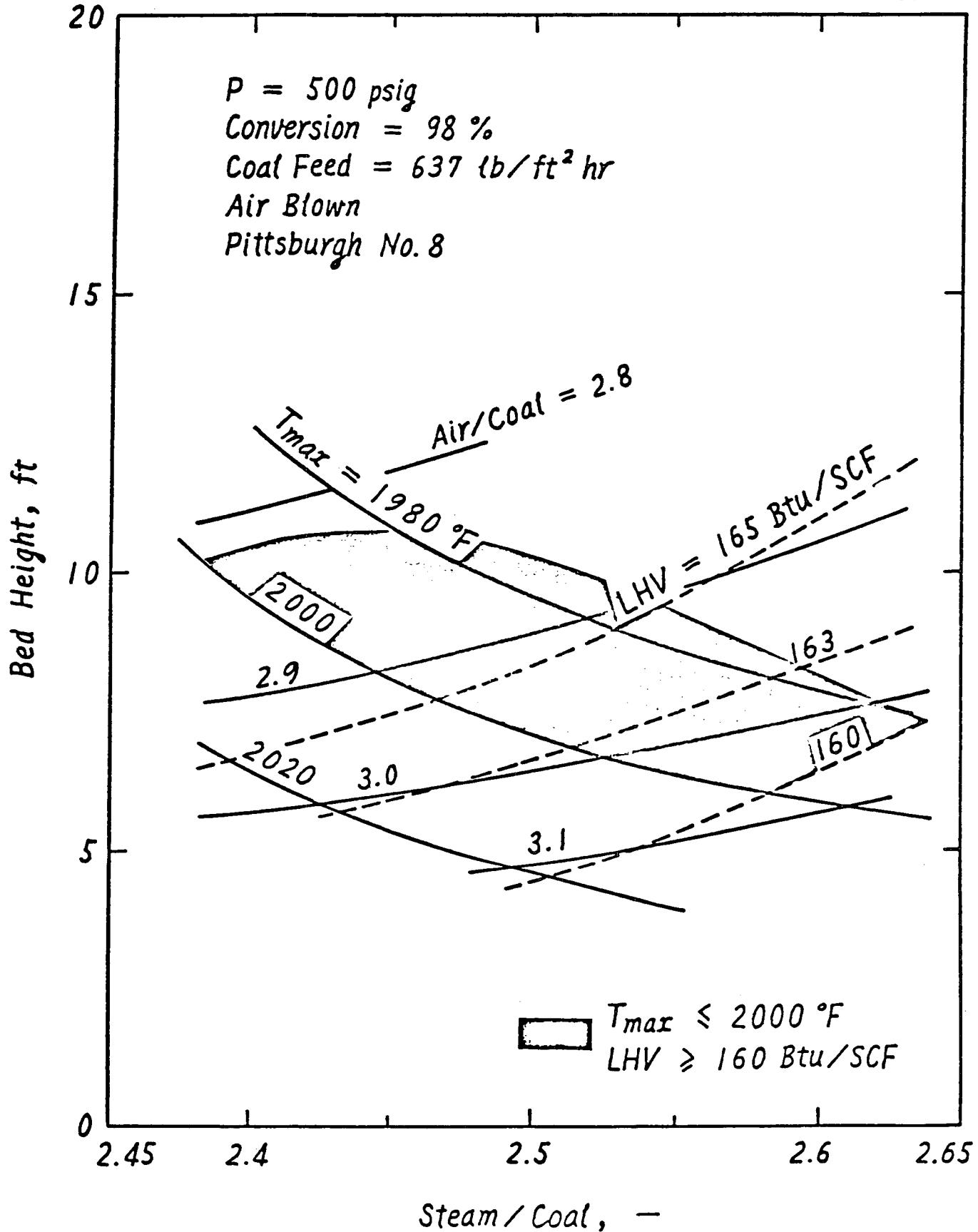


Figure VI-3. Design Map for Moving Bed Coal Gasifier (Case 3)

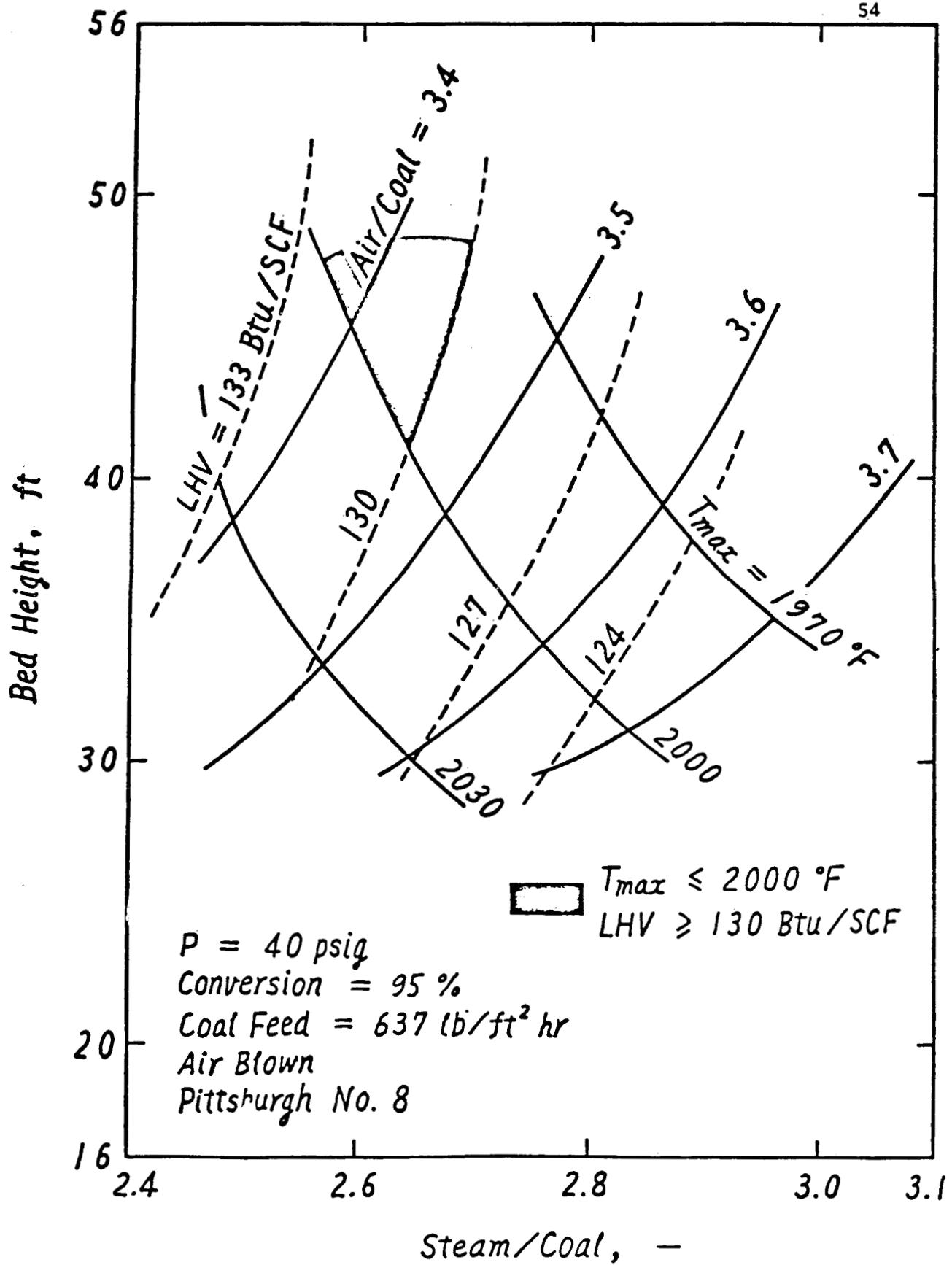


Figure VI-4. Design Map for Moving Bed Coal Gasifier (Case 4)

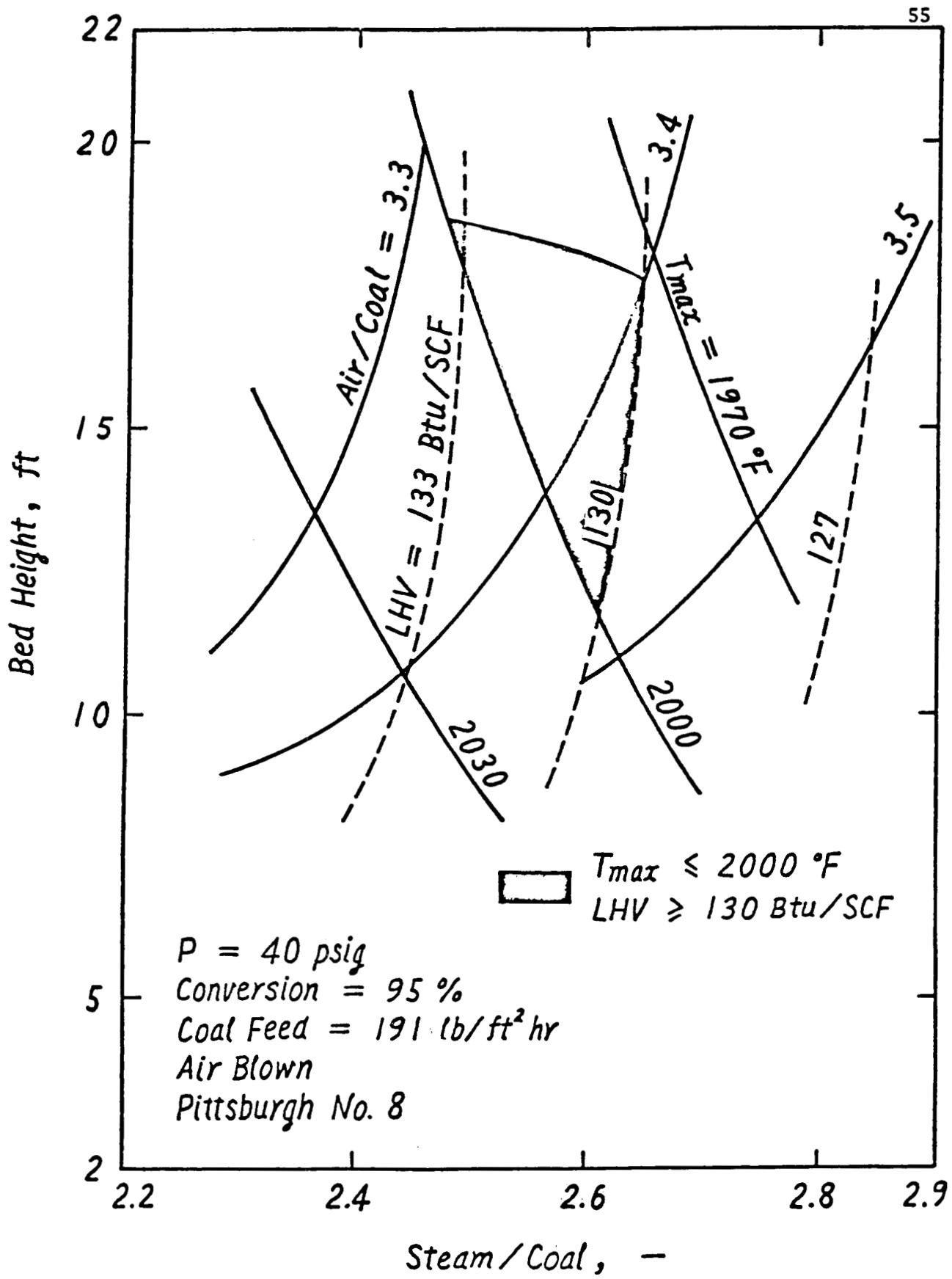


Figure VI-5. Design Map for Moving Bed Coal Gasifier (Case 5)

Heat transfer coefficient:	33.0 Btu/hr • ft <sup>2</sup> • °R
Temperature of wall, steam and air:	700°F
Temperature of inlet coal:	77°F

The shaded area in the maps indicates the feasible region of design satisfying the following two design conditions: the maximum temperature is less than 2000°F, and the minimum heating value of product gas is larger than 300 Btu/SCF. The most suitable design point should be decided by economical consideration identifiable within the shaded area.

## VI-2. How to change data and equations in the program

The moving bed gasifier computer model presented here includes many reaction rate equations, heat and mass balance differential equations and coefficients and parameters for these equations. Although these equations and constants are usually applicable to most of the cases, a program user may want to change some values or replace some equations with those that are more appropriate. Some of the changes may become necessary when special coals different from that indicated in the program are used or when the gasifier is operated in a special mode not described in the program. Table VI-1 provides some of the information for the user to make these changes such that the program can be used more effectively and accurately.

This program consists of a main program and many subroutines, each of which has a clear function described in Table III-1. A program user can use other information for his own calculation by changing the appropriate subroutines, for example, determining the tar amount by devolatilization and reaction rate expressions other than by the method used in this model.

## VI-3. Validation of range of applicability

With proper arrangement and careful usage, the program may be used for scale-up and optimization purposes as well as for extrapolation beyond the normal operating conditions. However, the program contains a number of simplifications, assumptions and empirically evaluated kinetic constants and transport coefficients based on the data obtained from actual gasifier operation. Therefore, when the program is to be used for design, simulation and scale-up for operating conditions and feed stocks not yet validated by reliable field data, the user must consider the problem of applicability. For example, in subroutine DEVO, coal is classified in

Table VI-1. Assumed Constants and Equations

Subroutine /Line No.		Variable /Equation	Expression	Default Value
MAIN	22	DZ	Step size for integration along bed height	2.0 (cm)
MAIN	25	DEB	Print all intermediate steps if true.	FALSE
MAIN	25	MON	Print iteration history if true.	TRUE
MAIN	26	NPLOT	Plot figures if NPLOT is one.	1
MAIN	29	IRT. GT. __	Number of input data set	- (-)
MAIN	147	Equation	Specific heat of carbon	(cal/g-mole°K)
MAIN	148	Equation	Enthalpy of carbon	(cal/g-mole°K)
MAIN	209	J. LT. __	Upper limit of iteration along bed height Maximum height = __ DZ	348 (-)
MAIN	240	AMW	Molecular weight of tar	78.0 (-)
CPSOL	2-3	Equations	Heat capacity of coal	(cal/gm°K)
RATES	25-37	Equations	Rate of char-oxygen reaction	
RATES	38-41	Equations	Rate of char-steam reaction	
RATES	42-46	Equations	Rate of water-gas shift reaction	
RATES	47-52	Equations	Rate of hydrogen-oxygen reaction	
RATES	53-55	Equations	Rate of char-carbon dioxide reaction	
RATES	56-58	Equations	Rate of char-hydrogen reaction	

Table VI-1. (cont.)

Subroutine /Line No.	Variable /Equation	Expression	Default Value
CONSTK 4	CK10	Reaction rate coefficient of devolatilization for lignite	$5.1 \times 10^4$ (1/sec)
CONSTK 5	E1	Activation energy of devolatilization for lignite	16,200 (cal/g-mole)
CONSTK 6	CK20	Reaction rate coefficient of cracking for lignite	$8 \times 10^{10}$ (1/sec)
CONSTK 7	E2	Activation energy of cracking for lignite	26,500 (cal/g-mole)
CONSTK 8	CK30	Reaction rate coefficient of deposition for lignite	$1.1 \times 10^3$ (1/sec)
CONSTK 9	E3	Activation energy of deposition for lignite	4,000 (cal/g-mole)
CONSTK 13	CK10	Reaction rate coefficient of devolatilization for subbituminous coal	$7.5 \times 10^4$ (1/sec)
CONSTK 14	E1	Activation energy of devolatilization for subbituminous coal	18,700 (cal/g-mole)
CONSTK 15	CK20	Reaction rate coefficient of cracking for subbituminous coal	$3.5 \times 10^{10}$ (1/sec)
CONSTK 16	E2	Activation energy of cracking for subbituminous coal	27,750 (cal/g-mole)
CONSTK 17	CK30	Reaction rate coefficient of deposition for subbituminous coal	$2.5 \times 10^4$ (1/sec)
CONSTK 18	E3	Activation energy of deposition for subbituminous coal	5,500 (cal/g-mole)

Table VI-1. (cont.)

Subroutine /Line No.		Variable /Equation	Expression	Default Value
CONSTK	22	CK10	Reaction rate coefficient of devolatilization for bituminous coal	$1.1 \times 10^5$ (1/sec)
CONSTK	23	E1	Activation energy of devolatilization for bituminous coal	21,200 (cal/g-mole)
CONSTK	24	CK20	Reaction rate coefficient of cracking for bituminous coal	$9.7 \times 10^9$ (1/sec)
CONSTK	25	E2	Activation energy of cracking for bituminous coal	29,000 (cal/g-mole)
CONSTK	26	CK30	Reaction rate coefficient of deposition for bituminous coal	$5.3 \times 10^4$ (1/sec)
CONSTK	27	E3	Activation energy of deposition for bituminous coal	7,000 (cal/g-mole)
BLOCK DATA	6	RHOC	Density of coal	0.8 (gm/cm <sup>3</sup> )
BLOCK DATA	7-9	AB BC CC	Coefficients of Cp in Subroutine CPH (for CO, CO <sub>2</sub> , O <sub>2</sub> , H <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> O, N <sub>2</sub> )	- (cal/g-mole • °K)
BLOCK DATA	10	HFO	Heat of formation at standard state (for (CO, CO <sub>2</sub> , O <sub>2</sub> , H <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> O, N <sub>2</sub> )	- (cal/g-mole)
BLOCK DATA	11	THK	Thermal conductivity of the particle for subroutine DEVO	$4.0 \times 10^{-4}$ (cal/cm • °K • sec)
BLOCK DATA	14	DENSO	Initial coal density for subroutine DEVO	1.0 (gm/cm <sup>3</sup> )
BLOCK DATA	15	CP	Heat capacity of coal for subroutine DEVO	0.4 (cal/gm • °K)

Table VI-1. (cont.)

Subroutine /Line No.	Variable /Equation	Expression	Default Value
BLOCK DATA 19	RK2	Reaction rate coefficients of char-steam reaction for three kinds of coal	930.0 (g-mole/mole 2250.0 C • atm 70.0 • sec)
BLOCK DATA 20	AE2	Activation energies of char-steam reaction for three kinds of coal	45,000 (cal/g-mole) 42,000 30,000
BLOCK DATA 21	WG3	Effective factors of steam-gas shift reaction to account for the dif- ferent type of ash	0.0068 0.0155 0.014
BLOCK DATA 22	RKS	Reaction rate coefficients of char-carbon dioxide reaction for three kinds of coal	930.0 2250.0 70.0
BLOCK DATA 23	AES	Activation energies of char-carbon dioxide reaction for three kinds of coal	45,000.0 42,000.0 30,000.0

three ranks, each having several kinetic constants for devolatilization. Since such classification by rank is very approximate, the program user may have to replace these constants with more suitable ones when data is available for more specific coal seams. The following statements may be a useful guide in determining the validity range:

1. Char-steam and char-CO<sub>2</sub> reactions are not affected by diffusion because the chemical reaction rates are the rate controlling steps at temperatures lower than 2200°F.
2. Subroutines for devolatilization are valid between 750°F and 1800°F.
3. In the combustion zone, the temperature must be higher than 1700°F; otherwise, the reaction within pores must be included in the rate expression.
4. Some fixed bed gasifiers use mixing agitators to prevent the agglomeration of coal (most of them use rotating grates). The program user may have to modify the computer code to account for the effect of particle breakup and temperature distribution due to the mixing agitators.
5. The temperature distribution also depends on steam jackets around the bed wall. Hence the program user needs to check in detail the type of gasifier to be used.
6. Based on the volatile analysis of coal, the total amount of devolatilized carbon is specified by the program user. Most kinetic constants in Table III-1 depend on the type of coal. However, the total amount of devolatilized carbon may also depend on the operating conditions. Therefore, the program user should be careful in specifying the amount of devolatilized carbon when extrapolating the operating conditions.

## NOMENCLATURE

$b$	= effectiveness factor to account for the different type of ash
$[c]$	= carbon concentration ( $\text{g-mole}/\text{cm}^3$ )
$C_{ij}$	= mass concentration of species $i$ at position $j$ ( $\text{g}/\text{cm}^3$ )
$C_{pi}$	= heat capacity of species $i$ ( $\text{cal/g} \cdot {}^\circ\text{K}$ )
$D$	= diameter of gasifier (cm)
$D_{\text{eff}}$	= effective diffusivity ( $\text{cm}^2/\text{sec}$ )
$d_p$	= particle diameter (cm)
$E_i$	= activation energy of reaction $i$ ( $\text{cal/g-mole}$ )
$E_{io}$	= activation energy of step $i$ in pyrolysis ( $\text{cal/g-mole}$ )
$e$	= emissivity of the particle
$F$	= geometric factor related with radiation heat transfer
$H_i$	= heat of reaction of reaction $i$ ( $\text{cal/g-mole}$ )
$h$	= heat transfer coefficient ( $\text{cal}/\text{cm}^2 \cdot {}^\circ\text{K} \cdot \text{sec}$ )
$h_c$	= convective heat transfer coefficient ( $\text{cal}/\text{cm}^2 \cdot {}^\circ\text{K} \cdot \text{sec}$ )
$k$	= thermal conductivity of coal particle ( $\text{cal}/\text{cm} \cdot {}^\circ\text{K} \cdot \text{sec}$ )
$k_{oi}$	= reaction rate coefficient of reaction $i$
$k_{io}$	= reaction rate coefficient of step $i$ in pyrolysis (1/sec)
$k_{\text{ash}}$	= mass transfer coefficient for gas film diffusion ( $\text{g-mole}/\text{cm}^3 \cdot \text{sec} \cdot \text{atm}$ )
$k_{\text{film}}$	= mass transfer coefficient for ash diffusion ( $\text{g-mole}/\text{cm}^3 \cdot \text{sec} \cdot \text{atm}$ )
$k_s$	= surface reaction rate constant ( $\text{gm}/\text{cm}^2 \cdot \text{atm} \cdot \text{sec}$ )
$m$	= fraction of the contact surface area of the particle with heating elements
$N_i$	= mass flux of gas species $i$ ( $\text{gm}/\text{cm}^2 \cdot \text{sec}$ )
$R_i$	= rate of generation of species $i$ ( $\text{gm}/\text{cm}^3 \cdot \text{sec}$ )
$R_j$	= reaction rate of reaction $j$ ( $\text{g-mole}/\text{cm}^3$ )

## NOMENCLATURE (cont.)

$R_g$	= gas constant (atm • cm <sup>3</sup> /gm-mole • °K)
T	= temperature (°K)
$T_w$	= temperature of heating devices or on the wall (°K)
t	= time (sec)
$\bar{V}$	= flow rate (g-mole/sec)
V.M.	= weight fraction of volatile matter in daf coal
$w_i$	= weight fraction of species i in the gas phase
$(WL)_i$	= weight loss of coal due to formation of gaseous species i
$X_1$	= weight fraction of coal that converted to tar during devolatilization step
x	= mole fraction
z	= distance (cm)
$\epsilon_{bed}$	= bed voidage
$\rho_c$	= density of coal (gm/cm <sup>3</sup> )
$\rho_i$	= density of species i (g/cm <sup>3</sup> )
$\sigma$	= Stefan-Boltzman constant (cal/cm <sup>2</sup> • °K <sup>4</sup> • sec)

## REFERENCES

1. Anthony, D. B., J. B. Howard, H. C. Hottel, and H. P. Meissner, *Proceedings of the 15th Symposium on Combustion (International)*, Combustion Institute, Pittsburgh, Pa., 1974, p. 1303.
2. Anthony, D. B., and J. B. Howard, *AIChE J.*, 22 (4); 625 (1976).
3. Desai, P., and C. Y. Wen, "Computer Modeling of MERC's Fixed Bed Gasifier," Report prepared for Morgantown Energy Research Center, Morgantown, W. Va., February 1978.
4. Elgin, D. C., "Results of Trials of American Coals in Lurgi Pressure Gasification Plant of Westfield, Scotland," *Proceedings of Sixth Synthetic Pipeline Gas Symposium*, Chicago, Ill., October 1974.
5. Feldkirchner, H. L., and H. R. Linden, *Ind. Eng. Chem. Process Des. Dev.*, 2, 153 (1963).
6. Feldkirchner, H. L., and J. Huebler, *Ind. Eng. Chem. Process Des. Dev.*, 4, 134 (1965).
7. Field, M. A., D. W. Gill, B. B. Morgan, and P. B. W. Hawksley, "Combustion of Pulverized Coal," BCURA, Leatherhead, 1967.
8. Gadsby, J. C., N. Hinshelwood, and K. W. Sykes, *Proc. Royal Soc. (London)*, A187, 129 (1946).
9. Gregory, D. R., and R. F. Littlejohn, *The BWRA Monthly Bulletin*, 29 (6), 173 (1965).
10. Jensen, G. A., *Ind. Eng. Chem. Process Des. Dev.*, 14, 314 (1975).
11. Johnson, J. L., *Adv. Chem. Ser.* 131, 145 (1974).
12. Jolly, L. J., and A. Pohl, *J. Inst. Fuel*, 26, 33 (1953).
13. Kayembe, N., and A. H. Pulsifer, *Fuel*, 55, 211 (1976).
14. Klei, H. E., J. Sahagian, and D. W. Sundstrom, *Ind. Eng. Chem., Process Des. Dev.*, 14, 470 (1975).
15. Moe, J. M., *Chem. Eng. Prog.*, 58 (3), 33 (1962).
16. Russell, W. B., D. A. Saville, and M. I. Greene, *AIChE J.*, 25, 65 (1979).
17. Singh, C. P. P., and D. N. Saraf, *Ind. Eng. Chem. Process Des. Dev.*, 16 (3), 313 (1977).

## REFERENCES (cont.)

18. Solomon, P. R., "The Evolution of Pollutants During the Rapid Devolatilization of Coal," Rep. NSF/RA-770422, NTIS PB 278496/AS, 1977.
19. Solomon, P. R., "The Evolution of Pollutants During the Rapid Devolatilization of Coal," Rep. R76-952588-2, United Technologies Research Center, East Hartford, Conn., 1977.
20. Suuberg, E. M., W. A. Peters, and J. B. Howard, Ind. Eng. Chem. Process Des. Dev., 17, 37 (1978).
21. Wen, C. Y., and J. Heubler, Ind. Eng. Chem. Process Des. Dev., 4, 142 (1965).
22. Wen, C. Y., Ind. Eng. Chem., 60, 34 (1968).
23. Wen, C. Y., "Optimization of Coal Gasification Processes," R & D Report No. 66, 1972.
24. "Coal Conversion Technology," edited by Wen and Lee, Addison Wesley Publishing Co., 1978.
25. Wen, C. Y., and S. Tone, ACS Symposium Series, No. 72, Chemical Reaction Engineering Reviews, Houston (1978).
26. Wen, C. Y., and L. H. Chen, "A Model for Coal Pyrolysis," paper presented at ACS National Meeting, Washington, D.C., Sept. 9-14, 1979.
27. Yoon, H., J. Wei, and M. Denn, AIChE J., 24, 885 (1978).

**Appendix A**

**NOMENCLATURE FOR THE PROGRAM**

Main Program and Subroutine INPUT, RATES, CPH, CPSOL, CRECT and DEVO

AB, BC, CC	= coefficient of specific heat correlations
AC	= fraction of undevolatilized carbon to fixed carbon
AF	= ash flow rate (gm/sec)
AIR	= flow rate of air (lb/hr, g-mole/sec)
AMF	= fraction of fixed carbon and volatile matter in coal
AMW	= molecular weight of tar
AREA	= cross-sectional area of bed ( $\text{cm}^2$ )
ASH	= ash content in coal (wt %)
C	= carbon feed rate (gm/sec)
CAR	= concentration of carbon ( $\text{g-mole}/\text{cm}^3$ )
CC	= carbon feed rate into the reaction section (gm/sec)
CCOM	= estimated amount of carbon consumed by combustion (gm/sec)
CDEVOL	= amount of carbon consumed by pyrolysis (gm/sec)
CIR	= bed circumference (cm)
CMET	= amount of carbon consumed by hydropyrolysis (g-mole/sec)
COAL	= coal feed rate (lb/hr, gm/sec)
COLDE	= thermal efficiency (%)
CORE	= core radius/particle radius
COUT	= amount of unreacted carbon at the exit (gm/sec)
CP, CPS	= specific heat of gas and solid (cal/g-mole $\cdot$ $^{\circ}\text{K}$ , cal/gm $\cdot$ $^{\circ}\text{K}$ )
CPGIN	= molar average specific heat of inlet gas (cal/g-mole $\cdot$ $^{\circ}\text{K}$ )
CPMGIN	= molar average heat capacity of inlet gas (cal/ $^{\circ}\text{K}$ )
CS	= array for table output

D = array used by library subroutine NLDEQS

DCARBO = amount of carbon consumed by pyrolysis (gm/sec)

DCO, DCO<sub>2</sub>, --- = amount of CO, CO<sub>2</sub>, --- formed during pyrolysis (g-mole/sec)

DEB = logical variable. Print all intermediate steps if its content is true.

DF(I) = derivative of F with respect to Z

DGAS = amount of gas formed during pyrolysis (gm/sec)

DIA = diameter of bed (ft, cm)

DP = particle size (inch, cm)

DTAR = amount of tar formed (gm/sec)

DZ = step size for solving the initial value problem (cm)

E = variable used by library subroutine NLDEQS

EP = bed voidage

EQ2, EQ3, --- = equilibrium constant for reaction 2, 3, ---

ER = residue in the secant method for solving the boundary value problem

F(I) = calculated values: temp, flow rates of carbon, CO, CO<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>O, (°F, gm/sec, g-mole/sec)

FC, . . . , FASH = mass fraction of C, . . . , ash in coal

FI(I) = same as F

FILM = film layer mass transfer coefficient (g-mole/cm<sup>3</sup> · sec · atm)

FIXC = fixed carbon content in coal (wt %)

FN2 = flow rate of nitrogen (g-mole/sec)

GAN, GS = amount of nitrogen and sulfur in volatile gas excluding methane (gm/sec)

GC, GH, GOXY = amount of carbon, hydrogen and oxygen in volatile gas excluding methane (gm/sec)

H = heat of formation (cal/g-mole)

HFO	= heat of formation at standard state (cal/g-mole)
HLOS	= heat loss rate (cal/sec • cm)
HR	= heat of reaction (cal/g-mole)
HT	= bed height (ft, cm)
HTC	= heat transfer coefficient (Btu/hr • ft <sup>2</sup> • °F, cal/sec • cm <sup>2</sup> • °K)
HV	= heating value of gas species (cal/g-mole)
HVCOAL	= heating value of coal (Btu/lb)
HVG	= heating value of product gas (cal/g-mole, Btu / SCF)
IND	= Indicator of program function: DESIGN if IND = 1, SIMULATION if IND = 2
ISW	= variable used in library subroutine NLDEQS
IT	= iteration counter
ITYPE	= coal type
J	= counter for array CS
KASH	= ash layer mass transfer coefficient (g-mole/atm • cm <sup>3</sup> • sec)
MON	= logical variable. Print iteration history if its constant is true.
N, NSF, N154	= variables used in library subroutine NLDEQS
OAIR	= fraction of oxygen in air
P	= pressure (psig, atm)
PA	= design parameters, either carbon conversion in fraction or bed height in feet
PGAS	= fractions of components in product gas (g-mole %)
PI	= 3.141592
PVOID	= particle voidage
R	= gas constant
RATE	= reaction rate (g-mole/sec • cm <sup>3</sup> )

RHOC	= density of coal (gm/cm <sup>3</sup> )
RMOIST	= moisture content in coal (wt %)
RTG, RTS	= residence time of gas and solid in bed (sec)
SH	= Sherwood number
SOUT	= total solid output (gm/sec)
STEAM	= steam feed rate (lb/hr, g-mole/sec)
SUMG	= total gas flow rate (g-mole/sec)
SUMS	= total solid flow rate (gm/sec)
T	= temperature (°K)
TAIR	= feed temperature of air (°F)
TAR	= composition of tar - C, H, O, N
TB	= variable used in library subroutine NLDEQS
TCOAL	= feed temperature of coal (°F)
TEST3, . . .	= rate of consumption of each gas species (g-mole/sec)
TGIN	= feed temperature of gas mixture (°F)
THL	= total heat loss (cal/sec, Btu/hr)
TMAX	= maximum temperature in bed (°K, °F)
TSTEAM	= feed temperature of steam (°F)
TW	= wall temperature (°F, °K)
VEL	= superficial velocity of gas or solid
VM	= volatile matter content in coal (wt %)
VMD	= fraction of volatile matter released during pyrolysis
WMI	= molar average molecular weight of gas
XC	= carbon conversion
XCAR, XASH	= mass fraction of carbon and ash in char
XCO, . . .	= molar fraction of CO, . . . , H <sub>2</sub> O in gas

X1, ..., X8 = array to store temperature and concentration profiles  
Z = distance from bottom of the bed (cm)

I = 1, Temperature	I = 2, carbon	I = 3, CO
I = 4, CO <sub>2</sub>	I = 5, O <sub>2</sub>	I = 6, H <sub>2</sub>
I = 7, CH <sub>4</sub>	I = 8, H <sub>2</sub> O	

## Subroutine DEVOL, INIT, CONSTK, DFN and DFNN

CK1 = reaction rate constant of devolatilization (1/sec)  
 CK10 = reaction rate coefficient of devolatilization (1/sec)  
 CK2 = reaction rate constant of cracking (1/sec)  
 CK20 = reaction rate coefficient of cracking (1/sec)  
 CK3 = reaction rate constant of deposition (1/sec)  
 CK30 = reaction rate coefficient of deposition (1/sec)  
 CNST = heat transfer constant for coal (1/sec)  
 CNSTW = heat transfer constant for heating elements (1/sec)  
 COAL0 = initial concentration of coal (gm/cm<sup>3</sup>)  
 CP = heat capacity of coal (cal/gm • °K)  
 CPW = heat capacity of the heating elements (cal/gm • °K)  
 DEFF = effective diffusivity (cm<sup>2</sup>/sec)  
 DEML = molecular diffusivity (cm<sup>2</sup>/sec)  
 DENSO = initial coal density (gm/cm<sup>3</sup>)  
 DENW = density of the heating elements (gm/cm<sup>3</sup>)  
 DH = heat of reaction (cal/gm)  
 DP = particle diameter (cm)  
 DY(I) = dependent variables in differential equations (gm/cm<sup>2</sup>)  
 E1 = activation energy of devolatilization (cal/g-mole)  
 E2 = activation energy of cracking (cal/g-mole)  
 E3 = activation energy of deposition (cal/g-mole)  
 EPS = error tolerance in library subroutine DREBS  
 FR = fraction of the contact surface area of the particle  
with heating elements  
 H = current step size (sec)

HMIN = smallest permissible step size in library subroutine DREBS

HOV = overall heat transfer coefficient of the particle (cal/cm<sup>2</sup> • °K • sec)

HOVW = overall heat transfer coefficient of the heating elements (cal/cm<sup>2</sup> • °K • sec)

IER = error indicator in library subroutine DREBS

IND = convergence indicator in library subroutine DREBS

INDP = indicator for printing the results

JM = the maximum order of the rational approximation in library subroutine DREBS

JSTART = input indicator in library subroutine DREBS

N = the number of equations in the system

P = pressure (atm)

RT = dimensionless radius of the particle

S(I) = variables in library subroutine DREBS

SHN = Sherwood number

SIGM = Stefan-Boltzman constant (cal/cm<sup>2</sup> • °K • sec)

STEP = step size in the time scale (sec)

T = time (sec)

TCD = char concentration (gm/cm<sup>3</sup>)

TCM = calculation parameter (gm)

TEM = solid temperature (°K)

TEMF = final temperature of the system (°K)

TEMO = initial temperature of the system (°K)

TEMWP = temperature change due to the heat of reaction (°K)

THK = thermal conductivity of the particle (cal/cm • °K • sec)

TWLG = total weight loss of gas (gm/gm-feed coal)

TWLV = total weight loss of tar (gm/gm-feed coal)

WD, WDP	= mass concentration of char (gm/cm <sup>3</sup> )
WGB	= mass concentration of gas at the bulk stream outside the particle (gm/cm <sup>3</sup> )
WGS	= mass concentration of gas at the particle surface (gm/cm <sup>3</sup> )
WLG	= weight loss of gas at time T (gm/gm-coal)
WLR	= total weight loss at time T (gm/gm-coal)
WLV	= weight loss of tar at time T (gm)
WMI	= molecular weight of inert gas (gm/g-mole)
WMG	= molecular weight of gas (gm/g-mole)
WMV	= molecular weight of tar (gm/g-mole)
WVB	= mass concentration of tar at the bulk stream outside the particle (gm/cm <sup>3</sup> )
WVS	= mass concentration of gas at the particle surface (gm/cm <sup>3</sup> )
X1	= weight fraction of tar formed during devolatilization step
X2	= weight fraction of gas formed during devolatilization step
Y(I)	= dependent variables
	I = 1, tar mass flux
	I = 2, gas mass flux
	I = 3, inert gas mass flux
	I = 4, tar mass concentration
	I = 5, gas mass concentration
	I = 6, inert gas mass concentration
YY(1)	= coal concentration (gm/cm <sup>3</sup> )

**Appendix B****PROGRAM LIST**

PROGRAM MBS ( MOVING BED COAL GASIFIER SIMULATOR ) WAS DESIGNED TO SIMULATE A COUNTER-CURRENT MOVING BED COAL GASIFIER OF THE LURGI TYPE. IT HAS TWO FUNCTIONS : CALCULATE CARBON CONVERSION IF BED HEIGHT IS SPECIFIED, OR CALCULATE BED HEIGHT IF CARBON CONVERSION IS SPECIFIED.

### LIST OF SUBROUTINES

INPUT	TO HANDLE DATA INPUT
RATES	TO CALCULATE REACTION RATES (GMOLE/CM <sup>3</sup> -S)
CPH	TO CALCULATE THE HEAT CAPACITIES AND ENTHALPIES OF GASEOUS SPECIES
CPSOL	TO CALCULATE THE HEAT CAPACITY OF COAL
CRECT	TO ADJUST XC BY SECANT METHOD
DEVO	TO CALCULATE THE AMOUNT AND COMPOSITION OF VOLATILE PRODUCTS
DEVOL	TO CALCULATE THE AMOUNT OF VOLATILE PRODUCTS
INIT	TO CALCULATE THE INITIAL CONDITIONS FOR SOLVING THE DIFFERENTIAL EQUATIONS (PYROLYSIS)
DFNN	TO CALCULATE THE COAL CONCENTRATION (PYROLYSIS)
DFN	TO SUPPLY THE DIFFERENTIAL EQUATIONS FOR SOLVING MASS FLUX AND CONCENTRATION OF SPECIES (PYROLYSIS)
CONSTK	TO GET THE RATE CONSTANTS FOR SPECIFIED KIND OF COAL (PYROLYSIS)

```

J001      C LOGICAL DEB, MON, OK
J002      C
J003      COMMON / D1 / RMOIST, VM, FIXC, ASH
J004      COMMON / D2 / FC, FH, FO, FN, FS, FASH
J005      COMMON / D3 / COAL, STEAM, AIR, DAIR, TCOAL, TSTEAM, TAIR
J006      COMMON / D4 / IND, ITYPE
J007      COMMON / D5 / HVCOAL, P, DIA, DP, VMD, PA
J008      COMMON / D6 / EP, HTC, TW
J009      COMMON / RP / RATE(6)
J010      COMMON / XX / XCO, XCO2, XO2, XH2, XCH4, XH2O, XCAR, XASH
J011      COMMON / FF / F(8)
J012      COMMON / HE / H(9), CP(9)
J013      COMMON / RHO / RHOC
J014      COMMON / RD / C, CCOM, AC
J015      COMMON / DEB / UK
J016      DIMENSION X1(350),X3(350),X4(350),X5(350),X6(350),X7(350),X8(350)
J017      DIMENSION Y1(350), ICHAR()
J018      DIMENSION PGAS(8), CS(350,8), HV(6), TAR(3), HR(6)
J019      DIMENSION E(8), DF(8), FI(8), D(124)
J020      C EQUIVALENCE ( E(1), DF(1) ), ( F(1), FI(1) )
J021      C
J022      DATA ICHAR / '13333', '44441', '55551', '66661', '77771', '88881', 'TTTT' /
J023      DATA E / 8*0.001 /
J024      DATA DZ, TB, NSF, ISW, N, N154 / 2.0, 0.0, 3, 2, 8, 180 /
J025      DATA PI, R / 3.14159, 82.057 /
J026      DATA HV / 67636.0, 0.0, 0.0, 57798.0, 191759.0, 0.0 /
J027      DATA DEB, MON / .FALSE., .TRUE. /
J028      C
J029      C 1 = T      2 = C      3 = CO      4 = CO2      5 = O2
J030      C 6 = H2     7 = CH4     8 = H2O     9 = N2
J031      C
J032      C NPLOT = 1
J033      C IRT = 0
J034      111    IRT = IRT + 1
J035      C IF ( IRT .GT. 1 ) STOP
J036      C CALL INPUT
J037      C IF ( DEB ) WRITE ( 6,68 )
J038      C
J039      C CONVERSION OF UNITS TO CGS SYSTEM
J040      C
J041      COAL = COAL * 453.6 / 3600.0

```

```

0033     AIR = AIR * 453.6 / ( 3600.0 * ( ( 1.0 - OAIR ) * 28.0 + 78
0034     + OAIR * 32.0 )
0035     STEAM = STEAM * 453.6 / ( 3600.0 * 18.0 )
0036     TCOAL = ( TCOAL + 460.0 ) / 1.8
0037     TSTEAM = ( TSTEAM + 460.0 ) / 1.8
0038     TAIR = ( TAIR + 460.0 ) / 1.8
0039     TW = ( TW + 460.0 ) / 1.8
0040     P = ( P + 14.7 ) / 14.7
0041     HTC = HTC * 252.0 * 1.8 / ( 3600.0 * 30.48 * 30.48 )
0042     DP = DP * 2.54
0043     C
0044     IF ( DEB ) WRITE (6,10) COAL, STEAM, AIR, TCOAL, TSTEAM, TAIR,
0045     + P, HTC, TW
0046     C TO EVALUATE OTHER CONSTANTS
0047     C
0048     AREA = DIA * DIA * 30.48 * 30.48 * PI / 4.0
0049     CIR = PI * DIA * 30.48
0050     AC = ( 100.0 - VM * VMD - RMOIST - ASH ) / ( 100.0 * FC )
0051     FASH = ASH / 100.0
0052     C
0053     IF ( DEB ) WRITE (6,12) AREA, CIR, AC
0054     C
0055     C = COAL * FC
0056     AF = COAL * FASH
0057     CCOM = AIR * OAIR * 12.0
0058     CC = C * AC
0059     FN2 = AIR * ( 1.0 - OAIR )
0060     IF { IND.EQ. 1 } XC = PA
0061     IF { IND.EQ. 2 } HT = PA * 30.48
0062     IF { IND.EQ. 2 } XC = 0.99
0063     C INLET GAS TEMPERATURE
0064     CALL CPH { 9, TAIR }
0065     CALL CPH { 5, TAIR }
0066     CALL CPH { 8, TSTEAM }
0067     C
0068     CPGIN = ( 1.0 - OAIR ) * CP(9) + OAIR * CP(5)
0069     CPMGIN = AIR * CPGIN + STEAM * CP(8)
0070     TGIN = ( AIR * CPGIN * TAIR + STEAM * CP(8) * TSTEAM ) / CPMGIN
0071     C
0072     IF ( DEB ) WRITE (6,16) TGIN
0073     C INITIALIZATION
0074     C
0075     IT = 0
0076     C BEGINNING OF OUTER LOOP OF ADJUSTING XC
0077     C
0078     100 IT = IT + 1
0079     TMAX = 0.0
0080     THL = 0.0
0081     Z = 0.0
0082     J = 1
0083     COUT = C * ( 1.0 - XC )
0084     RTG = 0.0
0085     RTS = 0.0
0086     C
0087     FI(1) = TGIN
0088     FI(2) = COUT
0089     FI(3) = 0.0
0090     FI(4) = 0.0
0091     FI(5) = AIR * OAIR
0092     FI(6) = 0.0
0093     FI(7) = 0.0
0094     FI(8) = STEAM
0095     C
0096     IF { MN } WRITE (6,20) IT
0097     IF { DEB } WRITE (6,32) FI
0098     C GRAPHICAL AND TABLE OUTPUT
0099     C
0100    SUMG = AIR + STEAM
0101    Y1(J) = 0.0
0102    X1(J) = TGIN * 1.8 - 460.0

```

```

0085      X3{J} = 0.0
0086      X4{J} = 0.0
0087      X5{J} = F1(5) / SUMG
0088      X6{J} = 0.0
0089      X7{J} = 0.0
0090      X8{J} = STEAM / SUMG
0091      C
0092      DO 120 K = 2, 8
0093      120  CS{J,K} = FI{K} * 3600.0 / 453.6
0093      CS{J,1} = FI{1} * 1.8 / 460.0
0094      C FIRST CALL NLDEQS, INTEGRATION INITIALIZATION
0094      CALL NLDEQS ( 1, NSF, E, FI, I, N, ISW, TB, Z, DZ, D, N154 )
0095      C BEGINNING OF INNER LOOP OF INITIAL VALUE PROBLEM
0095      140  CONTINUE
0096      C TOTAL GAS FLOW RATE
0096      SUMG = FN2
0097      C
0098      DO 160 K = 3, 6
0098      IF ( F(K) .LT. 1.0E-10 ) F(K) = 0.0
0099      160  SUMG = SUMG + F(K)
0100      C
0101      IF ( F(8) .LT. 1.0E-10 ) F(8) = 0.0
0101      SUMG = SUMG + F(7) + F(8)
0102      C MOLE FRACTION OF GAS
0102      XC0 = F(3) / SUMG
0103      XC02 = F(4) / SUMG
0104      X02 = F(5) / SUMG
0105      XH2 = F(6) / SUMG
0106      XCH4 = F(7) / SUMG
0107      XH2O = F(8) / SUMG
0108      C TOTAL SOLID FLOW RATE
0108      SUMS = AF + F(2)
0109      C MASS FRACTION OF SOLID
0109      XCAR = F(2) / SUMS
0110      XASH = AF / SUMS
0111      C EVALUATE RATE CONSTANTS
0111      T = F(1)
0112      CALL RATES ( T )
0113      C
0114      DO 180 K = 1, 2
0114      IF ( RATE(K) .LT. 0.0 ) RATE(K) = 0.0
0115      DO 200 K = 4, 6
0115      IF ( RATE(K) .LT. 0.0 ) RATE(K) = 0.0
0116      200
0117      C CO2
0117      T4 = 0.0
0118      IF ( RATE(3) .LE. 0.0 ) T4 = -RATE(3)
0119      TEST4 = ( RATE(5) + T4 ) * AREA * DZ
0120      IF ( TEST4 .LE. F(4) ) GO TO 220
0121      IF ( TEST4 .LE. 0.00001 ) GO TO 220
0122      RATE(5) = RATE(5) * F(4) / TEST4
0123      IF ( T4 .EQ. 0.0 ) GO TO 220
0124      RATE(3) = -T4 * F(4) / TEST4
0125      C H2
0125      220  TEST6 = ( T4 + RATE(4) + 2.0 * RATE(6) ) * AREA * DZ
0126      IF ( TEST6 .LE. F(6) ) GO TO 240
0127      IF ( TEST6 .LE. 0.00001 ) GO TO 240
0128      RATE(4) = RATE(4) * F(6) / TEST6
0129      RATE(6) = RATE(6) * F(6) / TEST6

```

130 IF ( T4 ,GT, 0.0 ) RATE(3) = RATE(3) \* F(6) / TEST6

80

C CO

131 240 TEST3 = RATE(3) \* AREA \* DZ  
132 IF ( TEST3 .LE. F(3) ) GO TO 260  
133 IF ( TEST3 .LE. 0.00001 ) GO TO 260  
134 RATE(3) = F(3) \* RATE(3) / TEST3

C H2O

135 260 TEST8 = ( RATE(2) + RATE(3) ) \* AREA \* DZ  
136 IF ( TEST8 .LE. F(8) ) GO TO 280  
137 IF ( TEST8 .LE. 0.00001 ) GO TO 280  
138 RATE(2) = F(8) \* RATE(2) / TEST8  
139 RATE(3) = F(8) \* RATE(3) / TEST8

C O2

140 280 RATIO = 1.0  
141 AS = ( RATIO + 2.0 ) / ( 2.0 + 2.0 \* RATIO )  
142 TEST5 = ( AS \* RATE(1) + RATE(4) / 2.0 ) \* AREA \* DZ  
143 IF ( TEST5 .LE. F(5) ) GO TO 300  
144 IF ( TEST5 .LE. 0.00001 ) GO TO 300  
145 RATE(1) = RATE(1) \* F(5) / TEST5  
146 RATE(4) = RATE(4) \* F(5) / TEST5

C SPECIFIC HEAT OF COAL

147 300 CP(2) = 2.673 + 0.002617 \* T - 116900.0 / ( T \* T )  
148 H(2) = 2.673 \* (T-298) + 0.002617 \* (T\*T-298.\*298.) / 2.  
+ + 116900./T - 116900./298.

C CPMG = SUM OF ( MOLAR FLOW RATE \* CP )

C CALL CPH { 9, T }  
CPMG = CP(9) \* FN2

C DO 320 K = 3, 8  
CALL CPH { K, T }  
CPMG = CPMG + CP(K) \* F(K)

320 CONTINUE

C HEAT OF REACTION

C RATIO = 1.0  
156 HR(1) = ( H(4) + H(3) \* RATIO - H(5) \* ( 1.0 + RATIO/2. ) )  
+ / ( 1.0 + RATIO ) \* H(2)  
157 HR(2) = H(3) + H(6) - H(8) - H(2)  
158 HR(3) = H(4) + H(6) - H(3) - H(8)  
159 HR(4) = H(8) - H(5) / 2.0 - H(6)  
160 HR(5) = 2.0 \* H(3) - H(4) - H(2)  
161 HR(6) = H(7) - 2.0 \* H(6) - H(2)

C DF

C DF(2) = AREA \* ( RATE(1) + RATE(2) + RATE(5) + RATE(6) ) \* 12.0  
162 DF(3) = AREA \* ( RATE(1) \* RATIO / ( 1.0 + RATIO ) + RATE(2)  
+ - RATE(3) + 2.0 \* RATE(5) )  
163 DF(4) = AREA \* ( RATE(1) / ( 1.0 + RATIO ) + RATE(3)  
+ - RATE(5) )  
164 DF(5) = AREA \* ( - RATE(1) \* ( 1.0 + RATIO / 2.0 ) / ( 1.0  
+ + RATIO ) - RATE(4) / 2.0 )  
165 DF(6) = AREA \* ( RATE(2) + RATE(3) - RATE(4) - 2.0 \* RATE(6) )  
166 DF(7) = AREA \* RATE(6)  
167 DF(8) = AREA \* ( RATE(4) - RATE(2) - RATE(3) )

C HEAT GENERATION

C A8 = ( -HR(1) \* RATE(1) - HR(3) \* RATE(3) - HR(6) \* RATE(6) )  
+ \* AREA  
A9 = ( -HR(2) \* RATE(2) - HR(5) \* RATE(5) ) \* AREA  
A10 = - HR(4) \* RATE(4) \* AREA

C HEAT LOSS

```

0172 HLOS = HTC * CIR * ( T - TW )
0173 IF ( HLOS .LT. 0.0 ) HLOS = 0.0
0174 THL = THL + HLOS * DZ
0175
0176 C SPECIFIC HEAT OF SOLID
0177 CF = F(2)
0178 CPS = CPSOL (T,CF,AF)
0179 C DF
0180 C SECOND CALL NLDEQS
0181 C
0182 C
0183 CALL NLDEQS ( 2, NSF, DF, I, N, ISW, TB, Z, DZ, D, N154 )
0184 GO TO ( 340, 140, 340 ) I
0185 340 CALL NLDEQS ( 3, NSF, DF, I, N, ISW, TB, Z, DZ, D, N154 )
0186 C
0187 J = J + 1
0188 C DEBUGGING
0189 C
0190 IF ( .NOT. DEB ) GO TO 360
0191 K = J = ( J / 5 ) * 5
0192 IF ( K .NE. 1 ) GO TO 360
0193 WRITE ( 6,88 ) J, Z
0194 WRITE ( 6,86 ) RATE
0195 WRITE ( 6,84 ) HR
0196 WRITE ( 6,92 ) F
0197 C TOTAL GAS FLOW RATE
0198 C
0199 360 SUMG = FN2
0200 DO 380 K = 3, 8
0201 IF ( F(K) .LT. 0.0 ) F(K) = 0.0
0202 380 SUMG = SUMG + F(K)
0203 C
0204 T = F(1)
0205 IF ( T .GT. TMAX ) TMAX = T
0206 VEL = SUMG * 22400.0 * T / ( P * 273.0 * AREA )
0207 RTG = DZ / VEL + RTG
0208 C TOTAL SOLID FLOW RATE
0209 C
0210 SUMS = AF + F(2)
0211 VEL = SUMS / ( RHOC * ( 1.0 - EP ) * AREA )
0212 RTS = DZ / VEL + RTS
0213 C FOR GRAPHICAL OUTPUT
0214 C
0215 400 Y1(J) = Z / 30.48
0216 C
0217 X1(J) = T * 1.8 - 460.0
0218 X3(J) = F(3) / SUMG
0219 X4(J) = F(4) / SUMG
0220 X5(J) = F(5) / SUMG
0221 X6(J) = F(6) / SUMG
0222 X7(J) = F(7) / SUMG
0223 X8(J) = F(8) / SUMG
0224 C TABLE OUTPUT
0225 C
0226 420 DO 420 K = 2, 8
0227 420 CS(J,K) = F(K) * 3600.0 / 453.6
0228 C
0229 CS(J,1) = F(1) * 1.8 - 460.0
0230 C
0231 IF ( J .LT. 348 ) GO TO 460
0232 C MAXIMUM LENGTH EXCEEDED
0233 C
0234 Z = Z / 30.48
0235 WRITE ( 6,56 ) Z
0236 IF ( MON ) WRITE ( 6,60 )
0237 WRITE ( 6,22 ) F

```

)214 WRITE (6,24) J, Z, SUMG, RTS, RTG, THL, TMAX

)215 C GO TO 111

82

C TERMINATION CRITERION

)216 460 IF ( IND .EQ. 2 ) GO TO 480  
))217 IF ( F(2) .LT. CC ) GO TO 140  
))218 GO TO 500

)219 480 IF ( Z .LT. HT ) GO TO 140

C END OF INNER LOOP

C DEBUGGING

)220 500 IF ( .NOT. MON ) GO TO 520

)221 WRITE (6,22) F

)222 WRITE (6,24) J, Z, SUMG, RTS, RTG, THL, TMAX

C TERMINATION CRITERION FOR OUTER LOOP

)223 520 IF ( IND .EQ. 1 ) GO TO 540  
))224 ER = CC - F(2)  
))225 IF ( MON ) WRITE (6,38) IT, XC, ER  
))226 IF ( ABS(ER) .LT. 1.0 ) GO TO 540  
))227 CALL CRECT ( IT, XC, ER )  
))228 IF ( .NOT. OK ) GO TO 111  
))229 IF ( MON ) WRITE (6,26) XC  
))230 IF ( IT .LT. 15 ) GO TO 100  
))231 WRITE (6,40) IT  
))232 GO TO 111

C END OF OUTER LOOP

C DEVOLATILIZATION

)233 540 WMI = 28.0 \* F(3) + 44.0 \* F(4) + 32.0 \* F(5) + 2.0 \* F(6) +  
+ 16.0 \* F(7) + 18.0 \* F(8) + 28.0 \* FN2  
))234 WMI = WMI / SUMG  
))235 IF ( MON ) WRITE (6,52) T, WMI  
))236 CALL DEVO ( WMI, T, CMET, DCO, DC02, DH2, DCH4, DH20, DN2,  
+ DH2S, DTAR, TAR )  
))237 IF ( MON ) WRITE (6,18) DCO, DC02, DH2, DCH4, DH20, DN2,  
+ DH2S, DTAR, TAR  
))238 DMOIST = COAL \* RMOIST / ( 100.0 \* 18.0 )  
))239 DCARBO = ( DCO + DC02 + DCH4 ) \* 12.0  
))240 AMW=78.0

C GAS FLOW RATE AT TOP OF GASIFIER

)241 F(3) = F(3) + DCO  
))242 F(4) = F(4) + DC02  
))243 F(6) = F(6) + DH2  
))244 F(7) = F(7) + DCH4  
))245 F(8) = F(8) + DMOIST + DH20  
))246 F(2) = F(2) + DCARBO + TAR(1) + CMET \* 12.0

)247 SUMG = FN2 + DN2 + DH2S + DTAR / AMW

)248 DO 560 K = 3, 8

)249 560 SUMG = SUMG + F(K)

C GAS EXIT TEMPERATURE

)250 CF = C  
))251 CPS = CPSOL ( TCOAL, CF, AF )

)252 C  
))253 CALL CPH ( 9, T )  
))254 CPMG = CP(9) \* ( FN2 + DN2 )  
))255 DO 580 K = 3, 8  
))256 CALL CPH ( K, T )  
))257 CPMG = CPMG + F(K) \* CP(K)  
))258 CPMG = CPMG \* SUMG / ( SUMG - DTAR / AMW - DH2S )  
))259 T = T - CPS \* COAL \* ( T - TCOAL ) / CPMG  
))260 F(1) = T

## C GRAPHICAL OUTPUT

83

```

0260      J = J + 1
0261      Y1(J) = Z / 30.48
0262      SUMG = SUMG - DTAR / AMW
0263      X1(J) = T * 1.8 - 460.0
0264      X3(J) = F(3) / SUMG
0265      X4(J) = F(4) / SUMG
0266      X5(J) = F(5) / SUMG
0267      X6(J) = F(6) / SUMG
0268      X7(J) = F(7) / SUMG
0269      X8(J) = F(8) / SUMG

C TABLE OUTPUT
0270      DO 660 K = 2, 8
0271      660      CS(J,K) = F(K) * 3600.0 / 453.6
0272      CS(J,1) = T * 1.8 - 460.0
C EVALUATION OF EFFICIENCY, ETC.
0273      STDE = 1.0 - ( F(8) = DMOIST = DH2O ) / STEAM
0274      SUMG = SUMG - F(8) + DTAR / AMW
0275      HVG = ( 94052.0 * TAR(1) + 57798.0 * TAR(2) ) / ( SUMG * AMW )
0276      DO 680 K = 1, 6
0277      680      HVG = HVG + HVG(K) * F(K+2) / SUMG
0278      HVG = HVG * 537.0 / ( 252.0 * 0.791 * 520.0 )
C
0279      SUMG = SUMG - DTAR / AMW
0280      DO 700 K = 1, 5
0281      PGAS(K) = F(K+2) * 100.0 / SUMG
0282      700      CONTINUE
C
0283      PGAS(6) = 0.0
0284      PGAS(7) = ( FN2 + DN2 ) * 100.0 / SUMG
0285      PGAS(8) = DH2S * 100.0 / SUMG

C CPS = CPSOL ( TGIN )
C
0286      SUMG = SUMG * 3600.0 / 453.6
0287      SOUT = ( COUT + AF ) * 3600.0 / 453.6
0288      COAL = COAL * 3600.0 / 453.6
0289      THL = THL * 3600.0 / 252.0
0290      T = T * 1.8 - 460.0
0291      TGIN = TGIN * 1.8 - 460.0
0292      TMAX = TMAX * 1.8 - 460.0
0293      COLDE = HVG * SUMG * 347.46 * 100.0 / ( HVCOAL * COAL )
0294      DO 720 K = 1, 4
0295      720      TAR(K) = TAR(K) * 100.0 / DTAR
0296      DTAR = DTAR * 3600.0 / 453.6
0297      IF ( IND .EQ. 1 ) HT = Z / 30.48

C OUTPUT
C
0298      WRITE ( 6, 66 )
0299      WRITE ( 6, 44 )
C
0300      DO 740 K = 1, J, 5
0301      WRITE ( 6, 46 ) Y1(K)
0302      WRITE ( 6, 48 ) ( CS(K,M), M = 1, 8 )
0303      740      CONTINUE
C
0304      IF ( K .EQ. J ) GO TO 760
0305      WRITE ( 6, 46 ) Y1(J)
0306      WRITE ( 6, 48 ) ( CS(J,M), M = 1, 8 )

C
0307      760      WRITE ( 6, 50 ) PGAS
0308      WRITE ( 6, 54 ) TAR
0309      WRITE ( 6, 52 ) SUMG, HVG, T, DTAR, SOUT, TGIN, THL,
+     COLDE, STDE, TMAX
0310      IF ( IND .EQ. 1 ) WRITE ( 6, 58 ) HT
0311      IF ( IND .EQ. 2 ) WRITE ( 6, 64 ) XC
C
0312      IF ( NPLOT .NE. 1 ) GO TO 780

```

```

C
      WRITE (6,70)
      CALL FPPLOT ( X1, Y1, J, ICHAR(7), 1, J )
      WRITE (6,72)
      CALL FPPLOT ( X3, Y1, J, ICHAR(1), 1, J )
      WRITE (6,74)
      CALL FPPLOT ( X4, Y1, J, ICHAR(2), 1, J )
      WRITE (6,76)
      CALL FPPLOT ( X5, Y1, J, ICHAR(3), 1, J )
      WRITE (6,78)
      CALL FPPLOT ( X6, Y1, J, ICHAR(4), 1, J )
      WRITE (6,82)
      CALL FPPLOT ( X7, Y1, J, ICHAR(5), 1, J )
      WRITE (6,80)
      CALL FPPLOT ( X8, Y1, J, ICHAR(6), 1, J )

C
780  GO TO 111
C
10   FORMAT (' COAL, STEAM, AIR, TCOAL, TSTEAM, TAIR ',
+        ' 1X, 6E20.6 / P, HTc, TW = ', 3E20.6 )
12   FORMAT (' AREA, CIR, AC ', 3E20.6 )
16   FORMAT (' TGIN = ', E20.6 )
18   FORMAT (' DEVOLATILIZATION RESULT - CO, CO2, H2, CH4, H2O, ',
+        ' N2, H2S / 7E15.6 / 27X, TAR, C, H, O, N / 5E15.6 ')
20   FORMAT (' / OUTER LOOP ITERATION 1, IS ')
22   FORMAT (' F, 8E15.6 ')
24   FORMAT (' J, Z, SUMG, RTS, RTG, THL, TMAX / IS, 6E15.6 ')
26   FORMAT (' / UPDATED XC = ', E15.6 )
32   FORMAT (' FI, 8E15.6 ')
38   FORMAT (' / OUTER LOOP ITERATION - IT, XC, ER ', IS, 2E15.6 )
40   FORMAT (' / / OUTER LOOP LIMIT OF ', IS, ' ITERATIONS EXCEEDED ')
44   FORMAT (' / / PROFILES OF FLOW RATES AND TEMPERATURES ',
+        '(UNITS ARE F (1), LB/HR (2), LBMOLE/HR (3-8))',
+        ' 5X, 1Z, 11X, T, 19X, C, 18X, CO, 17X, CO2,
+        ' 16X, O2, 18X, H2, 17X, CH4, 17X, H2O ')
46   FORMAT (1X, F6.3 )
48   FORMAT (6X, 4E20.6 / 6X, 4E20.6 )
50   FORMAT (' / PERCENTAGE OF GAS PRODUCT (DRY BASIS) / 4X, CO,
+        ' 7X, CO2, 8X, O2, 8X, H2, 7X, CH4, 7X, H2O, 8X, N2,
+        ' 7X, H2S / 8F10.5 )
52   FORMAT (' / TOTAL GAS OUTPUT = ', E15.6, ' LBMOLE/HR / '
+        ' HEATING VALUE OF GAS = ', E15.6, ' BTU/SCF / '
+        ' GAS EXIT TEMPERATURE = ', E15.6, ' F / '
+        ' AMOUNT OF TAR = ', E15.6, ' LB/HR / '
+        ' TOTAL SOLID OUTPUT = ', E15.6, ' LB/HR / '
+        ' SOLID EXIT TEMP = ', E15.6, ' F / '
+        ' TOTAL HEAT LOSS = ', E15.6, ' BTU/HR / '
+        ' THERMAL EFFICIENCY = ', E15.6, ' PERCENT / '
+        ' STEAM DECOMPOSITION = ', E15.6, ' /
+        ' MAXIMUM TEMPERATURE = ', E15.6, ' F / ')
54   FORMAT (' / PERCENTAGE OF TAR PRODUCT / 4X, C, 9X, H,
+        ' 9X, O, 9X, N / 4F10.4 )
56   FORMAT (' / / MAXIMUM LENGTH OF ', F6.1, ' FT EXCEEDED ',
+        ' INCREASE BED DIAMETER OR DECREASE CARBON CONVERSION ',
+        ' AND TRY AGAIN. ')
58   FORMAT (' / BED HEIGHT = ', E15.6, ' HT ')
60   FORMAT (' / THE FOLLOWINGS ARE THE VALUES AT THE LAST COMPARTMENT ')
62   FORMAT (' / DEVOLATILIZATION = T, WMI = ', 2E15.6 )
64   FORMAT (' / CARBON CONVERSION = ', E15.6 )
66   FORMAT (' / 1X, 11(*) // 1X, OUTPUT DATA // 1X, 11(*) // ')
68   FORMAT (' / 1X, 9(*) // 1X, DEBUGGING // 1X, 9(*) // ')
70   FORMAT (' / 1H1, 20X, TEMPERATURE (F) VS. DISTANCE (FT) ')
72   FORMAT (' / 1H1, 20X, MOLE FRACTION OF CO VS. DISTANCE (FT) ')
74   FORMAT (' / 1H1, 20X, MOLE FRACTION OF CO2 VS. DISTANCE (FT) ')
76   FORMAT (' / 1H1, 20X, MOLE FRACTION OF O2 VS. DISTANCE (FT) ')
78   FORMAT (' / 1H1, 20X, MOLE FRACTION OF H2 VS. DISTANCE (FT) ')
80   FORMAT (' / 1H1, 20X, MOLE FRACTION OF H2O VS. DISTANCE (FT) ')
82   FORMAT (' / 1H1, 20X, MOLE FRACTION OF CH4 VS. DISTANCE (FT) ')
84   FORMAT (' / HR ', 6E15.6 )
86   FORMAT (' / RATE ', 6E15.6 )
88   FORMAT (' / J, IS, Z, E15.6 )
92   FORMAT (' / F, 8E15.6 )
C
END

```

## C SUBROUTINE INPUT

85

```

C DIMENSION TITLE(20)
COMMON / D1 / RMOIST, VM, FIXC, ASH
COMMON / D2 / FC, FH, FO, FN, FS, FASH
COMMON / D3 / COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR
COMMON / D4 / IND, ITYPE
COMMON / D5 / HVCOAL, P, DIA, DP, VMD, PA
COMMON / D6 / EP, HTC, TW
COMMON / KK / RK2(3), AE2(3), WG3(3), RK5(3), AE5(3)

```

```

C READ(5,10)(TITLE(J),J = 1,20)
READ(5,15)IND, ITYPE
READ(5,20)RMOIST, VM, FIXC, ASH
READ(5,20)FC, FH, FO, FN, FS
READ(5,20)COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR
READ(5,20)HVCOAL, P, DIA, DP, VMD, PA
READ(5,20)EP, HTC, TW
READ(5,20)RK2, RAE2, RWG3, RRK5, RAES

```

C 10 FORMAT(20A4)

C 15 FORMAT(2I1)

C 20 FORMAT(7F10.3)

```

C WRITE(6,30)(TITLE(J),J = 1,20)
IF ( IND .EQ. 1 ) WRITE(6,35)
IF ( IND .EQ. 2 ) WRITE(6,36)
IF ( ITYPE .EQ. 1 ) WRITE(6,42)
IF ( ITYPE .EQ. 2 ) WRITE(6,44)
IF ( ITYPE .EQ. 3 ) WRITE(6,46)
WRITE(6,38)

```

C WRITE(6,40)RMOIST, VM, FIXC, ASH

```

C 30 FORMAT(1H1, 80('*')//1X, 20A4// 1X, 80('*')// )
C 35 FORMAT( / ! PROGRAM FUNCTION = DESIGN ! )
C 36 FORMAT( / ! PROGRAM FUNCTION = SIMULATION ! )
C 38 FORMAT( 1X, 10('*')// 1X, ! INPUT DATA ! // 1X, 10('*')// )
C 40 FORMAT( / ! PROXIMATE ANALYSIS = ! // 5X, ! MOISTURE ! 2X,
+ 'VOLATILE', 5X, 'FIXED', 7X, 'ASH' / 17X, 'MATTER', 4X,
+ 'CARBON' / 3X, 4F10.3 )
C 42 FORMAT( ! COAL TYPE = BITUMINOUS ! / )
C 44 FORMAT( ! COAL TYPE = SUBBITUMINOUS ! / )
C 46 FORMAT( ! COAL TYPE = LIGNITE ! / )

```

C WRITE(6,50)FC, FH, FO, FN, FS

```

C 50 FORMAT( / ! ULTIMATE ANALYSIS = ! // 7X, 'CARBON HYDROGEN',
+ 'OXYGEN NITROGEN SULFUR' / 3X, 5F10.3 )

```

C WRITE(6,60)COAL, STEAM, AIR, OAIR, TCOAL, TSTEAM, TAIR

```

C 60 FORMAT( / ! COAL FEED RATE      = !, F10.3, ! LB/HR ! /
+ ! STEAM FEED RATE      = !, F10.3, ! LB/HR ! /
+ ! AIR FEED RATE        = !, F10.3, ! LB/HR ! /
+ ! MOLE FRACTION OF OXYGEN IN AIR = !, F10.3, ! /
+ ! TEMPERATURE OF COAL    = !, F10.3, ! E ! /
+ ! TEMPERATURE OF STEAM   = !, F10.3, ! E ! /
+ ! TEMPERATURE OF AIR     = !, F10.3, ! E ! )

```

C WRITE(6,70)HVCOAL, P, DIA, DP, VMD

IF ( IND .EQ. 1 ) WRITE(6,72) PA

IF ( IND .EQ. 2 ) WRITE(6,74) PA

WRITE(6,78) EP, HTC, TW

```

C IF ( RRK2 .NE. .OD1 ) RK2(ITYPE) = RRK2
C IF ( RAE2 .NE. .OD1 ) AE2(ITYPE) = RAE2
C IF ( RWG3 .NE. .OD1 ) WG3(ITYPE) = RWG3
C IF ( RRK5 .NE. .OD1 ) RK5(ITYPE) = RRK5
C IF ( RAE5 .NE. .OD1 ) AE5(ITYPE) = RAE5

```

```

C WRITE(6,80) RK2(ITYPE), AE2(ITYPE), WG3(ITYPE),
+ RK5(ITYPE), AE5(ITYPE)

```

```

C 70 FORMAT( / ! HEATING VALUE OF COAL = !, F10.3, ! BTU/LB ! /
+ ! PRESSURE             = !, F10.3, ! PSIG ! )

```

```

+      ! BED DIAMETER          S !, F10.3, ! FT !
+      ! PARTICLE SIZE          S !, F10.3, ! INCH !, 86
+      ! 25H FRACTION VM DEVOL'D S !, F10.3 )
72   FORMAT ( ! CARBON CONVERSION S !, F10.3 )
74   FORMAT ( ! BED HEIGHT      S !, F10.3, ! FT !
78   FORMAT ( ! BED VOIDAGE     S !, F10.3 )
+      ! HEAT TRANSFER COEFF    S !, F10.3, ! STU/HR-FT2-R !
+      ! WALL TEMPERATURE       S !, F10.3, ! F !
80   FORMAT ( / ! KINETIC CONSTANTS ! /
+      ! REACTION 2 : K = !, F10.2, ! E = !, F10.2 /
+      ! REACTION 3 : A = !, F10.6, ! /
+      ! REACTION 5 : K = !, F10.2, ! E = !, F10.2 )

C   RETURN
END

```

```

C   SUBROUTINE CPH(M,T)
C
COMMON / HCAP / AB(7),BC(7),CC(7),HFO(7)
COMMON / HE / H(9), CP(9)
C
TT = T
IF(T.LT. 298.) T= 298.
IF(T.GT. 2000.) T= 2000.
J = M = 2
C
IF ( M .EQ. 8 ) GO TO 100
CP(M) = AB(J)+BC(J)*(1.E-3)*T+CC(J)*(1.E+6)/(T*T)
GO TO 200
100 CP(M) = AB(J)+BC(J)*1.E-3*T+CC(J)*1.E-6*T*T
C
200 IF ( M .EQ. 8 ) GO TO 300
H(M) = HFO(J) + AB(J)*(T-298.) + BC(J)*1.E-3*(T*T-298.*298.)/2.-
+ CC(J)*1.E+6*( 1./T-1./298.)
GO TO 400
300 H(8) = HFO(6) + AB(6)*(T-298.) + BC(6)*1.E-3*(T*T-298.*298.)/2.-
+ CC(6)*1.E-6*(T**3-298.***3)/3.
C
400 T = TT
RETURN
END

```

```

1   C   FUNCTION CPSOL ( T, CF, AF )
2   C
3   CPSOL = ( 2.673 + 0.002617 * T - 116900.0 / T / T ) * CF / 12.0
4   CPSOL = CPSOL + { 10.87 + 0.008712 * T - 241200.0 / T / T } * AF / 60.0
C
5   CPSOL /= ( CF + AF )
6   RETURN
END

```

```

053 400 IF ( XCO2 , LE , 0.0 ) GO TO 500
054 EQ5 = EXP ( -20.9238 - 20281.8 / T )
055 RATE(5)=RK5(ITYPE)*EXP(-AE5(ITYPE)/(1.987*T))*CAR
+ *P* (XCO2 = P * XCO * XCO / EQ5 )
C
C RATE(6)
C
056 500 IF ( XH2 .LE. 0.0 ) GO TO 600
057 EQ6 = EXP ( -13.4289 + 10998.5 / T )
058 RATE(6) = EXP ( -7.0869 - 8077.5 / T ) * ( P * XH2 -
+ SQRT ( P * XCH4 / EQ6 ) ) * CAR
C
059 600 T = TT
C
060 IF ( DEB ) WRITE (6,10) ( T, RATE )
C
061 RETURN
C
062 10 FORMAT (' FROM RATES = T, RATE = ', 7E15.6 )
063 END

```

```

C
001 SUBROUTINE DEVO ( WMI, T, CMET, DCO, DC02, DH2, DCH4, DH2O, DN2
+ DH2S, DTAR, TAR )
C
002 DIMENSION TAR(3)
003 COMMON / D1 / RMOIST, VM, FIXC, ASH
004 COMMON / D2 / FC, FH, FO, FN, FS, FASH
005 COMMON / D3 / COAL, STEAM, AIR, DAIR, TCOAL, TSTEAM, TAIR
006 COMMON / FF / F(8)
007 COMMON / RD / C, CCOM, AC
C
008 T0 = TCOAL
009 TT = T
010 CALL DEVOL ( WMI, T, T0, DTAR, DGAS )
C
011 DTAR=0.2
012 DGAS=0.5
T = TT
AMF = ( VM + FIXC ) / 100.0
DGAS = DGAS * AMF * COAL
DTAR = DTAR * AMF * COAL
TOTAL = DGAS + DTAR
C
016 CDEVOL = TOTAL - ( FH + FO + FN + FS ) * COAL
017 CMET = ( 1.0 - AC ) * FC * COAL - CDEVOL
018 IF ( CMET .GE. 0.0 ) GO TO 100
019 DGAS = ( TOTAL + CMET ) * DGAS / TOTAL
020 DTAR = ( TOTAL + CMET ) * DTAR / TOTAL
021 TOTAL = TOTAL + CMET
022 CMET = 0.0
023 GO TO 200
C
024 100 CMET = CMET / 12.0
025 F{7} = F{7} + CMET
026 F{6} = F{6} - CMET * 2.0
C
027 200 GAN = FN * COAL
C
028 TOTAL = DTAR / ( FC + FH + FO )
029 TAR{1} = FC * TOTAL
030 TAR{2} = FH * TOTAL
031 TAR{3} = FO * TOTAL
C
032 DN2 = GAN / 28.0
033 DH2S = FS * COAL / 32.0
C
034 GH = FH * COAL - TAR{2} - 2.0 * DH2S
035 GOXY = FO * COAL - TAR{3}
036 GC = DGAS - GOXY - GH - DN2 * 28.0 - DH2S * 34.0
C
037 R = GC / ( F{3} + F{4} + F{7} )
038 R = R / 12.0
039 DCO = F{3} * R
040 DCO2 = F{4} * R
041 DCH4 = F{7} * R
042 DH2O = GOXY / 16.0 - DCO - DC02 * 2.0
043 DH2 = ( GH - 2.0 * DH2O - 4.0 * DCH4 ) / 2.0
C
044 RETURN
C

```

C

```

0001      SUBROUTINE DEVOL(WMI,TEMF,TEMO,TTWLV,TTWLG)          88
0002      LOGICAL DEB
0003      REAL Y(6),R(6),WK(174),YY(1)
0004      COMMON /D1/ RMOIST, VM1, FIXC, ASH
0005      COMMON /D4/ JND, ITYPE
0006      COMMON /D5/ HVCAL, P, DIA, DP1, VMD, PA
0007      COMMON /DE/ THK, FR, DH, DENSO, CP, DENW, CPW, HOVW
0008      COMMON /AA/ X1, X2, CK1, COAL, CK2, CK3, DEF, CNST, COALO
0009      COMMON /CC/ DP
0010      DATA DEB / .FALSE. /
0011      DATA HMIN,EPS/1.0E-8,1.0E-5/
0012      DATA N,JM,IND,JSTART/6,6,3,0/
0013      EXTERNAL DFN
0014      DP = DP1
0015      IF ( DP .GT. 0.01 ) DP = 0.01
0016      IF ( TEMF .GT. 1000.0 ) TEMF = 1000.0
0017      VM = VM1 / ( VM1 + FIXC )
0018      STEP=0.010
0019      SIGM=1.355E-12
0020      DEF=5.0E-3
0021      CNSTW=HOVW/CPW/DENW
0022      WGB=0.0
0023      WVb=0.0
0024      WVS=0.0
0025      WGS=0.0
0026      SHN=2.0+6.024*DP**0.5
0027      DEML=7.2E-2
0028      COALO=1.0
0029      TWLV=0.0
0030      TWLG=0.0
0031      TEMWP=0.0
0032      TEMW=TEMO
0033      CALL CONSTK(ITYPE,VM,X1,X2,CK10,CK20,CK30,E1,E2,E3)
0034      HOV=THK*(1.0+FR)/DP/2.0+SIGM*(TEMW*TEMW+TEMO*TEMO)*(TEMW+TEMO)
0035      CNST=6.0*HOV/DP/CP/DENSO
0036      COAL=COALO
0037      DO 3 J=1,1000
0038      TCM=0.0
0039      T=STEP*FLOAT(J-1)
0040      TEMW=TEMF-(TEMF-TEMO)*EXP(-CNSTW*T)
0041      CNSTT=CNST*T
0042      IF(CNSTT.GT.15.0)CNSTT=15.0
0043      TEM=TEMW+TEMWP-(TEMW+TEMWP-TEMO)*EXP(-CNSTT)
0044      CK1=CK10*EXP(-E1/1.987/TEM)
0045      CK2=CK20*EXP(-E2/1.987/TEM)
0046      CK3=CK30*EXP(-E3/1.987/TEM)
0047      CALL INIT(TEM,J,STEP,YY,WL)
0048      Y(1)=DP/2.0*(X1*CK1*COAL-(CK2+CK3)*WVS)/3.0
0049      Y(2)=(CK2*WVS)*DP/6.0
0050      Y(3)=0.0
0051      Y(4)=WVS
0052      Y(5)=WGS
0053      Y(6)=P*WMI/82.06/TEM/COALO
0054      S(1)=Y(1)
0055      S(2)=Y(2)
0056      S(3)=Y(3)
0057      S(4)=Y(4)
0058      S(5)=Y(5)
0059      S(6)=Y(6)
0060      RT=0.0
0061      IF(J.EQ.1)GO TO 30
0062      TCM=TCM+Y(4)*0.1
0063      DO 2 I=1,10
0064      H=0.001
0065      B=0.1*FLOAT(I)
0066      1 IF(H.GT.B-RT)H=B-RT
0067      CALL DRBSCDFN(Y,RT,N,JM,IND,JSTART,H,HMIN,EPS,R,S,WK,IER)
0068      IF(IER.NE.0)RETURN
0069      IF(RT.LT.B-HMIN) GO TO 1
0070      IF(Y(1).LT.0.0)Y(1)=0.0
0071      IF(Y(2).LT.0.0)Y(2)=0.0
0072      IF(Y(5).LT.0.0)Y(5)=0.0
0073      IF(Y(4).LT.0.0)Y(4)=0.0
0074      TCM=TCM+(1.0*B)**2*Y(4)*0.1
0075      2 CONTINUE

```

```

      IF(J,NE,1)GO TO 15
30 DO 31 KL=1,6
      Y(KL)=0.0
31 CONTINUE
15 WLV=(DP/2.0*(X1*CK1*COAL/3.0-(CK2+CK3)*TCM))/DP*6.0
      WLG=(DP/2.0*CK2*TCM)/DP*6.0
      IF(WLV,GE,0.0)GO TO 37
      WLG=3.0*CK2*TCM+CK2/(CK2+CK3)*WLV
      WLV=0.0
37 TWLV=TWLV+WLV
      TWLG=TWLG+WLG
      TWL=(TWLG+TWLV)*STEP
      WVS=WLV*DP/6.0*DP/DEM/SHN+WVB
      WGS=WLG*DP/6.0*DP/DEM/SHN+WGB
      WLR=WLV+WLG
      TEMWP=-DH*DP/6.0/HOV*WLR*COALO
      HOV=THK*(1.0+FR)/DP/2.0+SIGM*(TEMW*TEMW+TEMO*TEMO)*(TEMW+TEMO)
      DENS=(1.0-TWL)*DENO
      CNST=6.0*HOV/DP/CP/DENS
      IF(WLV,EQ,0.0.AND.WLG,LT,5.0E-2) GO TO 88
      3 CONTINUE
88 TTWLV=STEP*TWLV
      TTWLG=STEP*TWLG
      IF ( DEB ) WRITE ( 6,10 ) T,TTWLV,TTWLG,TWL
      RETURN
10 FORMAT(//,4X,'TIME FOR PYROLYSIS = ',F10.3,' SEC'
*,4X,'WEIGHT LOSS OF TAR = ',F10.4,' FRACTION OF ORIGINAL WEIGHT
*OF COAL'
*,4X,'WEIGHT LOSS OF GAS = ',F10.4,' FRACTION OF ORIGINAL WEIGHT
*OF COAL'
*,4X,'TOTAL WEIGHT LOSS OF COAL = ',F10.4,' FRACTION OF ORIGINAL
*WEIGHT OF COAL')
      RETURN
      END

```

C

```

SUBROUTINE DFN(N,RT,Y,DY)
REAL Y(6),DY(6)
COMMON /AA/X1,X2,CK1,COAL,CK2,CK3,DEFF,CNST,COALO
COMMON/CC/DP
IF(RT,LE,0.9)GO TO 1
RT2=20.0
GO TO 2
1 RT2=2.0/(1.0-RT)
2 DY(1)=-DP/2.0*(X1*CK1*COAL-(CK2+CK3)*Y(4))+RT2*Y(1)
      DY(2)=-DP/2.0*(X2*CK1*COAL+CK2*Y(4))+RT2*Y(2)
      DY(3)=RT2*Y(3)
      DY(4)=-DP/2.0/DEFF*(-Y(1)+Y(4)/(Y(4)+Y(5)+Y(6))*((Y(1)+Y(2)+Y(3)))
      DY(5)=-DP/2.0/DEFF*(-Y(2)+Y(5)/(Y(4)+Y(5)+Y(6))*((Y(1)+Y(2)+Y(3)))
      DY(6)=-DP/2.0/DEFF*(-Y(3)+Y(6)/(Y(4)+Y(5)+Y(6))*((Y(1)+Y(2)+Y(3)))
      RETURN
      END

```

```

C
0001      SUBROUTINE INIT(TEM,I,STEP,Y,WL)
0002      REAL Y(1),R(1),S(1),WK(29)
0003      COMMON /AA/X1,X2,CK1,COAL,CK2,CK3,DEFF,CNST,COALO
0004      COMMON/CC/DP
0005      DATA HMIN,EPS/1.0E-5,1.0E-6/
0006      DATA N,JM,IND/1,6,3/
0007      EXTERNAL DFNN
0008      IF(FLOAT(I).NE.1.0)GO TO 11
0009      10 Y(1)=1.0
0010      COALEY(1)
0011      DO 12 K=1,N
0012      S(K)=Y(K)
0013      12 CONTINUE
0014      RT=0.0
0015      JSTART=0
0016      11 H=0.001
0017      B=STEP*FLOAT(I-1)
0018      1 IF(H.GT.B-RT)H=B-RT
0019      CALL DRESS(DFNN,Y,RT,N,JM,IND,JSTART,H,HMIN,EPS,R,S,WK,IER)
0020      IF(IER.NE.0)RETURN
0021      IF(RT.LT.B-HMIN)GO TO 1
0022      COAL=Y(1)
0023      RETURN
0024      END

```

```

C
0001      SUBROUTINE DFNN(N,RT,Y,DY)
0002      REAL Y(1),DY(1)
0003      COMMON /AA/X1,X2,CK1,COAL,CK2,CK3,DEFF,CNST,COALO
0004      COMMON/CC/DP
0005      DY(1)=-CK1*Y(1)
0006      RETURN
0007      END

```

```

C
0001      SUBROUTINE CONSTK(ITYPE,VM,X1,X2,CK10,CK20,CK30,E1,E2,E3)
0002      IF(ITYPE.EQ.1)GO TO 3
0003      IF(ITYPE.EQ.2)GO TO 2
0004      CK10=5.1E4
0005      E1=16200.0
0006      CK20=8.0E10
0007      E2=26500.0
0008      CK30=1.1E3
0009      E3=4000.0
0010      X1=0.95*VM+0.025
0011      X2=0.0
0012      RETURN
0013      2 CK10=7.5E4
0014      E1=18700.0
0015      CK20=3.5E10
0016      E2=27750.0
0017      CK30=2.5E4
0018      E3=5500.0
0019      X1=1.13*VM+0.025
0020      X2=0.0
0021      RETURN
0022      3 CK10=1.1E5
0023      E1=21200.0
0024      CK20=9.7E9
0025      E2=29000.0
0026      CK30=5.3E4
0027      E3=7000.0
0028      X1=1.3*VM+0.025
0029      X2=0.0
0030      RETURN
0031      END

```

```

)001      C      SUBROUTINE CRECT ( IT, X, E )          91
)002      C      LOGICAL OK
)003      C      COMMON / DEB / OK
)004      C      OK = TRUE
)005      C      IF ( IT .GT. 1 ) GO TO 100
)006      C      X1 = X
)007      C      E1 = E
)008      C      X = X - 0.01
)009      C      RETURN
)010      C      100   ACC = 1.0
)011      C      IF ( ( E * E1 ) .GT. 0.0 ) ACC = 0.5
)012      C      X2 = X - E * ACC * ( X - X1 ) / ( E - E1 )
)013      C      E1 = E
)014      C      X1 = X
)015      C      X = X2
)016      C      IF ( X .LE. 0.999 ) GO TO 200
)017      C      X = 0.999
)018      C      IF ( X .GT. X1 ) RETURN
)019      C      WRITE ( 6, 10 ) X, X1
)020      C      OK = FALSE
)021      C      RETURN
)022      C      200   IF ( X .GE. 0.0 ) RETURN
)023      C      X = 0.0
)024      C      IF ( X .LT. X1 ) RETURN
)025      C      WRITE ( 6, 10 ) X, X1
)026      C      OK = FALSE
)027      C      RETURN
)028      C      10    FORMAT ( ' OUTER LOOP ITERATION - ANSWER OUT OF BOUND ! '
)029      C      + / ' CURRENT XC = ', E20.6 / ' PREVIOUS XC = ', E20.6 )
END

```

```

C      BLOCK DATA
)001      COMMON / RHO / RHOC
)002      COMMON / HCAP / AB(7), BC(7), CC(7), HFO(7)
)003      COMMON / DE / THK, FR, DH, DENSO, CP, DENW, CPW, HOVW
)004      COMMON / KK / RK2(3), AE2(3), WG3(3), RK5(3), AE5(3)
)005      REAL RHOC / 0.8 /
)006      REAL AB / 6.6, 10, 34, 8, 27, 6, 62, 5, 34, 8, 22, 6.5 /
)007      REAL BC / 1.2, 2, 74, 258, 81, 11, 5, 15, 1 /
)008      REAL CC / 0, 1955, 1877, 0, 0, 1, 34, 0 /
)009      REAL HFO / -26416, -94052, 0.0, 0.0, -17889, -57798, 0.0 /
)010      REAL THK / 4.0E-4 /
)011      REAL FR / 0.0 /
)012      REAL DH / 166, 67 /
)013      REAL DENSO / 1.0 /
)014      REAL CP / 0.4 /
)015      REAL DENW / 8.027 /
)016      REAL CPW / 0.12 /
)017      REAL HOVW / 0.96 /
)018      REAL RK2 / 930.0, 2250.0, 70.0 /
)019      REAL AE2 / 45000.0, 42000.0, 30000.0 /
)020      REAL WG3 / 0.0068, 0.0155, 0.014 /
)021      REAL RK5 / 930.0, 2250.0, 70.0 /
)022      REAL AE5 / 45000.0, 42000.0, 30000.0 /
)023      END

```