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MATHEMATICAL MODELING OF THE SYNTHANE GASIFIER
FOR NON-CAKING COALS

By
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ABSTRACT

A mathematical model based on IGT kinetics has been developed to simulate the gasification of coal in the Synthane gasifier. Two computer codes have been prepared that incorporate this model. The first, called the analytical code, has been designed primarily to evaluate model parameters from runs on the 4-inch Synthane PDU gasifier. The second, called the predictive code, has been designed to predict temperatures for the zones within the model as well as the effluent products from a stipulation of run conditions.

In the present report some 35 Synthane runs for the non-caking western coal Montana Rosebud have been analyzed. Parity plots have been prepared to check the efficacy of the model and of the computer codes developed.

INTRODUCTION

Due to the dwindling supplies of natural gas and petroleum, it has become imperative to seek alternate sources of energy. The abundance of coal in our nation has made this fuel a good candidate. Gasification of the carbon in the coal can lead to compounds that can supplement natural supplies. Hence, an extremely high national priority has been placed on the development of technology for coal gasification.

Several high Btu gas processes are currently under development nationwide; the SYNTHANE process is in the developmental phase at PETC. The present report deals with the mathematical simulation of the SYNTHANE Process Development Unit (PDU) gasifier. An important aspect of this simulation is the kinetics and reactor design model for coal gasification. There are a number of studies which have been carried out on the kinetics of coal gasification for the important coal-hydrogen and coal-steam reactions. ¹⁻¹⁵ The kinetics of char gasification developed by Johnson at IGT, ^{1,2} together with the three-zone backmixed reactor model for the gasifier presented by Dobner et al., ^{16,17} has been the basis for the model presented in this report.

PERC SYNTHANE PDU

The flow diagram of the Synthane PDU is given in Figure 1. The PDU and its operation are described below, with particular attention being given to the measurements used as input to the mathematical model. The proposed three-zone reactor model is depicted in Figure 30.

Solids Flow

Before the start of a typical PDU run for a non-caking coal, the coal is weighed and charged to the feedhopper. During operation, the coal is fed to the 6-foot carbonizer, where it is contacted countercurrently with the gas rising from the gasifier.

After passing downward through the carbonizer, the coal enters the top of the fluidized bed in the gasifier, which is six feet long and four inches in diameter. Bed density is determined from pressure drop measurements through the bed. The bed is maintained at a height of 68 inches by maintaining the pressure drop from that point in the gasifier to the top of the carbonizer at a small value just above zero. From the combustion of a portion of the char at the bottom of the gasifier and from the inlet gases, a gaseous mixture results which fluidizes the char in the gasifier.

The char is continuously transferred from the gasifier to the ash hopper. After the run, char removed during gasification, char left in the gasifier, and coal and char collected in the dust filter of the product gas stream are weighed.

Gas Flow

A mixture of steam and oxygen is fed to the bottom of the gasifier. Steam is formed in a steam generator from water stored in a reservoir which is weighed periodically throughout the run. Oxygen is drawn from a cylinder which is weighed before and after the run. The flow rate of each of these

two gas feeds is measured by a rotameter before the mixture is formed for injection to the gasifier.

Nitrogen is used to convey the coal to the carbonizer. It is drawn from a cylinder and its flow rate is also measured by a rotameter. This nitrogen is assumed to mix immediately with the gas stream rising from the carbonizer as it leaves the reactor system.

Small amounts of nitrogen are introduced at a number of points in the coal feed and reactor systems to prevent plugging by the coal particles and loss of reactive gases. These points are located in the feed hopper, in the three pressure taps on the reactor system, in the jacket around the gasifier, and in the extractor. The flow rates of these nitrogen streams are not measured, except for the stream introduced to the ash hopper, which is monitored with a rotameter. The total nitrogen gas fed to the system is set equal to the nitrogen appearing in the product gas.

The product gas leaving the carbonizer is treated to remove dust, tar, and moisture. The flow rate of the treated product gas is measured by a wet-test meter. The tar and condensate, collected in a simple receiver from the bottom of both condensers, are separated and weighed.

Other Measurements

Temperatures are measured at many points in the system. A thermowell, along the axis of the reactor, carries the thermocouples that measure temperatures at eight points in the gasifier and four points in the carbonizer. The temperatures are noted periodically, and those in the gasifier are averaged over time and space to give an average gasifier

temperature. The temperature of the steam is measured before the steam is mixed with oxygen and fed to the gasifier.

Pressure is measured at several points in the system, the most important measurement point being the pressure inside the gasifier.

A number of analyses are performed on feeds and products of the system. Ultimate analyses are obtained for the coal fed; the chars in the extractor, gasifier, and filter; and the tar. Proximate analyses, sieve analyses, and bulk density measurements are obtained for all of these except the tar. The sulfur and carbon content of the condensate for the total run are measured. The final product gas is sampled periodically for chemical analysis by an on-line gas chromatographic column.

Start-up and Shut-down Transients

During approximately the first hour of each run, the gasifier is filling with solids, and the temperatures are coming to their steady-state values. Consequently, the compositions of all of the product streams are changing with time during this period.

A similar unsteady-state operation is experienced during approximately the last half-hour of the run when large amounts of nitrogen are used to lower the temperature of the reactor rapidly. During both of these periods, non-steady state char, tar, and condensate are being produced and ultimately blended in with the steady-state contributions of each of these streams.

Computer Facilities

The U.S. Bureau of Reclamation Cyber 74128 Computer System at Denver with a Control Data Corporation 6600 mainframe has been used in the development of the program for the model. Access to this computer facility has been through a remote job entry terminal located at the U.S. Bureau of Mines Bruceton station, which is available to the staff of the Pittsburgh Energy Technology Center. The Operating System is NOS1.0, and programs have been written in Control Data's Extended Fortran.

For parity plots, the System 17 Computer was used. The plotter was a Houston Model DP-5 incremental plotter.

MATHEMATICAL COMPUTATIONS

Steady-State Material Balance

A number of adjustments to various flow rates are required to account for gas flows during unsteady-state operation, char flow during unsteady-state operation, and special nitrogen injections.

Gas Flows During Unsteady-State Operation

In a given run, the PDU operates at steady state for approximately one hour less than the total run time. Several of the gas flows to and from the unit are monitored every half hour, and their steady-state rates can be precisely determined. Other gas flows are measured as total quantities for the entire run. The rates of many of these are constant for the entire run and also may be precisely calculated.

However, the rates of three of the gas flows, whose total quantities are measured for the entire run, are not constant during the run. These flows are the oxygen and steam fed to the system and the (once gaseous) condensate from the system. At the beginning of the period when the PDU is being cooled, which is at the end of the run, the oxygen flow is stopped. About halfway through this cool-down period, the steam flow also is stopped. The calculation for the steady-state flow rates therefore are adjusted for oxygen by setting the time of oxygen injection at 0.4 hour less than the time of the entire run and for steam by setting the time of steam injection at 0.2 hour less than the time of the entire run. The

rate of accumulation of condensate is calculated in a manner similar to that used for the steam flow rate. These times were selected as generally applicable as per discussion with the PDU operators.

Char Flow During Unsteady-State Operation

Two methods of establishing the flow of solids are used during the period when the PDU is brought up to temperature at the start of each run. In the first method a precharge is placed in the gasifier before the start of the run. In the second method the gasifier is empty at the start of the run and fills during the first period of the run, equal to the residence time of the char. In both methods the gas flow begins several minutes before the coal feed is initiated. The run is ended by cooling the gasifier with a large flow of cold nitrogen. During this brief period the coal and char flow remain unchanged, and the run ends with a full charge of char in the gasifier.

The effect on char composition of the difference in composition of the precharge is taken into account by subtracting the precharge from the component masses of the solids in the ash hopper. The effect of the precharge on total char accumulated is taken into account by subtracting the total mass of the precharge from the total mass of the solids in the ash hopper. In effect, this creates an initially empty gasifier in the model. The effect on the calculated steady-state char flow rate of the initially empty gasifier and the brief period of zero coal flow is taken into account by reducing the total time of char flow by the residence time of the char plus 0.025 hour.

The char produced during the two periods of unsteady-state operation is assumed to be identical with the char produced during the period of steady-state operation, as per discussion with the operators.

Special Nitrogen Injections

The unmeasured flows to the unit are accounted for in the analytical mode of the program by adding 60 SCFH to the nitrogen flow into the gasifier.

IGT Kinetics

The kinetic model developed by J. L. Johnson ^{1,2} has been used to describe the rate of carbon conversion and the selectivity to various major components in the product gas. According to the IGT analysis, the total carbon content of the coal is composed of a volatile fraction, which can be devolatilized merely by a thermal treatment, and a residual base carbon fraction,

$$C_t = C_v + C_b \quad (1)$$

where,

C_t = total carbon in the feed coal, in units of lbs. carbon 1 lb. feed coal MAF (i.e., Moisture-Ash-Free Basis)

C_v = carbon in the volatile fraction, in units of lbs. carbon/lb. feed coal MAF

C_b = Carbon remaining after standard devolatilization in lbs.

carbon/lb. feed coal MAF

The volatile fraction is composed of a fraction that forms carbon oxides from "available oxygen" in the coal, C_{ox} ; a fraction which is converted to tar, C_{tar} ; and a fraction from which methane equivalent is formed, C_m :

$$C_v = C_{ox} + C_{tar} + C_m \quad (2)$$

Again, units are lbs. carbon/lb. feed coal MAF. "Available oxygen" is defined as oxygen in the coal minus oxygen in the char, fines, and tars. "Methane equivalent" represents methane and higher alkanes which appear in the product gas.

When all volatile carbon has been gasified, the base carbon conversion fraction is defined as follows:

$$X = \frac{C_g - C_v}{C_t - C_v} = \frac{C_g - C_v}{C_b} \quad (3)$$

where

X = base carbon conversion fraction

C_g = total carbon gasified in units of lbs. carbon/lb. feed coal MAF.

According to Johnson's kinetics there are essentially three mechanisms for gasification. The first is devolatilization, which consists of a very rapid-rate process at elevated temperatures for the thermal decomposition of coal into char and gases such as CO , CO_2 , H_2 , H_2O , CH_4 and higher alkanes. The second is rapid-rate methane formation, which is a rapid process at elevated temperatures for the evolution of CH_4 in the presence of gaseous hydrogen. The third is low-rate gasification, which is a slower process than the above two and results in the formation of

hydrogen, methane, and carbon oxides from the reactions of steam and hydrogen with char. Johnson's kinetics are available for the rapid and low rate gasification processes but not for the devolatilization process.

For temperatures above 1500° F, the base carbon conversion to the so-called "rapid rate" methane, X_R , is correlated with the hydrogen partial pressure by the equation:

$$\int_0^{X_R} \frac{\exp(BX^2) dx}{(1-X)^{2/3}} = 0.0092 f_R P_{H_2} \quad (4)$$

where P_{H_2} is the hydrogen partial pressure in atm., f_R is a relative reactivity factor dependent on the particular coal undergoing gasification, and B is a kinetic parameter dependent on gas composition and pressure. For the present report, f_R was assigned a value of 1.25, and B , a value of 1.7, as suggested by Dobner et al. 16,17

With respect to low-rate gasification, Johnson's kinetics are based on the three reactions:

The rate of base carbon conversion is given by the following:

$$\frac{dX}{dt} = f_o \exp \frac{8467}{T_p} \cdot (1 - X)^{2/3} \exp(-BX^2) \cdot k_T \quad (6)$$

where f_0 is a relative reactivity factor dependent on the specific carbonaceous solid, T_p is the coal pretreatment temperature, and k_T is given by the following:

$$k_T = k_I + k_{II} + 2k_{III}$$

The three individual rate constants, k_I , k_{II} , and k_{III} , for the above three reactions are defined as follows:

$$k_I = \frac{\exp(9.0201 - 31,705/T) (1 - P_{CO} P_{H_2} / P_{H_2O} K_I)}{[1 + \exp(-22.2160 + 44,787/T) (1/P_{H_2O} + 16.35 P_{H_2} / P_{H_2O} + 43.5 P_{CO} / P_{H_2})]^2} \quad (7)$$

$$k_{II} = \frac{P_{H_2}^2 \exp(2.6741 - 33,076/T) (1 - P_{CH_4} / P_{H_2}^2 K_{II})}{[1 + P_{H_2} \exp(-10.4520 + 19,976/T)]} \quad (8)$$

$$k_{III} = \frac{P_{H_2}^{1/2} P_{H_2O} \exp(12.4463 - 44,544/T) (1 - P_{CH_4} P_{CO} / P_{H_2} P_{H_2O} K_{III})}{[1 + \exp(-6.6696 + 15,198/T) (P_{H_2}^{1/2} + 0.85 P_{CO} + 18.62 P_{CH_4} / P_{H_2})]^2} \quad (9)$$

where K_I , K_{II} , and K_{III} are equilibrium constants for the above three reactions considering carbon as graphite; T is the reaction temperature in $^{\circ}R$; and P_{H_2} , P_{H_2O} , P_{CO} , and P_{CH_4} are partial pressures of H_2 , H_2O , CO , and CH_4 in atm.

The rates at which carbon is gasified to CH_4 and CO are given as follows:

$$\frac{dX_{CH_4}}{dt} = \frac{k_{II} + \frac{1}{2}k_{III}}{k_T} \left(\frac{dX}{dt} \right) \quad (10)$$

$$\frac{dX_{CO}}{dt} = \frac{k_I + \frac{1}{2}k_{III}}{k_T} \left(\frac{dX}{dt} \right) \quad (11)$$

In the low and rapid-rate gasification expressions, the term $(1-X)^{2/3}$ represents the effective surface area of the coal particles, and the term $\exp(-BX^2)$ represents the reactivity of the effective surface area.

Evaluation of Rapid Rate Methane

The fraction of base carbon converted to rapid rate methane, X_R , has been evaluated from equation (4) with the use of Simpson's rule. ¹⁸ In general, the area under the curve $y = f(x)$ between a and b is

$$I = \int_a^b f(x) dx \quad (12)$$

According to Simpson's rule, if the interval for this integral is divided into n equal intervals, where n is even, and each interval is of size $h = (b - a)/n$, the integral in (12) can be approximated by the following:

$$I = \frac{h}{3} (y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \dots + 2y_{n-4} + 4y_{n-3} + 2y_{n-2} + 4y_{n-1} + y_n) \quad (13)$$

Applying this equation to the integral expression for rapid rate methane in equation (4) with $h = X_R/n$ ($b = X_R$, $a = 0$), $y_1 = e^{Bx_1^2/(1-x_1)^{2/3}}$, and $x_1 = 1h$ results in the following expression for Simpson's rule:

$$I = \frac{X_R}{3n} \left[1 + 4 \sum_{\substack{j=1 \\ j=\text{odd}}}^{n-1} \frac{e^{\alpha \left(\frac{jX_R}{n} \right)^2}}{\left(\frac{1-jX_R}{n} \right)^{2/3}} + 2 \sum_{\substack{j=2 \\ j=\text{even}}}^{n-2} \frac{e^{\alpha \left(\frac{jX_R}{n} \right)^2}}{\left(\frac{1-jX_R}{n} \right)^{2/3}} + \frac{e^{\alpha \left(\frac{X_R}{n} \right)^2}}{\left(\frac{1-X_R}{n} \right)^{2/3}} \right] \quad (14)$$

Normally, values are substituted in the expression for Simpson's formula to obtain an approximation for the integral. In equation (14), however, X_R is unknown while the area is known. The area can simply be calculated from the right hand expression in equation (4), namely,

$$I = 0.0092 f_R^{PH_2} \quad (15)$$

By substituting (15) into (14), an equation in only one unknown, X_R , results. A value for n is somewhat arbitrary, except that it must be even, and in the present report has been set equal to 20.

Equation (14) is highly non-linear in X_R . In order to solve for X_R , a computer oriented algorithm developed by Brown¹⁹ called NONLIN has been used. NONLIN was designed to solve a series of real non-linear simultaneous equations. This method is at least quadratically convergent and requires only $(N^2/2 + 3N/2)$ functional evaluations for each iteration as compared to Newton's method which requires $(N^2 + N)$ functional evaluations; this results in considerable savings in computational requirement for complicated functions. Also, the user does not need to supply any derivatives. Only a function subprogram must be supplied which defines the function where zeroes are sought. In the present study, this subprogram is called RAPID and incorporates equations (14) and (15). The zero of the function defined in RAPID for the variable X_R is evaluated in this way. Units of X_R are lbs. carbon in rapid rate CH_4 /lb. base carbon.

Evaluation of Equilibrium Constants for Low Rate Gasification Reactions

The three equilibrium constants that appear in the kinetic rate constant equations (7) - (9) are evaluated from the relationship of the temperature effect on the Gibbs free-energy change. ²¹ Essentially, if data is available for $\Delta \bar{G}^\circ_f$ (Gibbs Free Energy of Formation at 25°C), $\Delta \bar{H}^\circ_f$ (enthalpy of formation at 25°C), and $\bar{C}_p$ (heat capacity) for reactants and products as a function of temperature, it is then possible to evaluate ΔG° at any temperature within this range. From ΔG° , the equilibrium constant can readily be evaluated.

The enthalpy of a reaction at temperature T is given by the following:

$$\Delta H_T = \Delta H_0 + \int_0^T \Delta \bar{C}_p \, dT \quad (16)$$

where ΔH_0 is the hypothetical enthalpy at absolute zero. $\Delta \bar{C}_p$ is the change in heat capacity of products from the reactants and can be expressed as follows:

$$\Delta \bar{C}_p = \Delta a + (\Delta b)T + (\Delta c)T^2 + \dots \quad (17)$$

where a, b, and c are the coefficients in the equation for heat capacity as a function of temperature. Substituting (17) into (16) and integrating leads to the following:

$$\Delta H = \Delta H_0 + (\Delta a)T + \frac{1}{2}(\Delta b)T^2 + \frac{1}{3}(\Delta c)T^3 + \dots \quad (18)$$

Substituting this into the Gibbs-Helmholz equation,

$$\frac{\partial (\Delta G^\circ/T)}{\partial T} = \frac{-\Delta H_T}{T^2} \quad (19)$$

where $\Delta H_T = H_{298}^\circ$ and integrating the following general relationship for ΔG° as a function of T results in the following:

$$\Delta G^\circ = \Delta H_0 - (\Delta a)T \ln T - \frac{1}{2}(\Delta b)T^2 - \frac{1}{6}(\Delta c)T^3 + \dots + CT \quad (20)$$

In the present work, the three equilibrium constants are evaluated in the following manner. ΔH_{298}° and ΔG_{298}° for each reaction are evaluated using values of ΔH_f° and ΔG_f° from tables. Heat capacity tables are used to supply values for coefficients, and ΔH_0 is then evaluated from equation (18). Substituting values for ΔH_0 , heat capacity coefficients, ΔG_{298}° , and $T = 298$ into equation (20) results in the determination of the integration constant C. Substituting this value of the integration constant into equation (20) results in a general equation for calculating ΔG_T° at any temperature for which the heat capacity equations are valid. Once the temperature is specified and ΔG° hence evaluated, the equilibrium constant is simply calculated from the relationship:

$$\Delta G^\circ = -RT \ln K \quad (21)$$

Evaluation of Water-Gas Shift Equilibrium

Since the model assumes the water-gas shift equilibrium to be in effect in the fluid bed and carbonizer, it has been necessary to evaluate the corresponding equilibrium constant and adjust the water-gas shift species

accordingly. The equilibrium constant is evaluated from the expression:

$$K = e^{-3.823 + 4224.8/T} \quad (22)$$

where T is the temperature and is taken to be the fluid bed temperature in the present study. This equation was derived from the above equations and the use of standard thermodynamic constants.^{21,27} The water-gas shift reaction together with the species concentrations is given as follows:

where a, b, c, and d represent concentration of species prior to undergoing the shift reactions, and x represents the amount undergoing reaction. The equilibrium constant can then be defined as follows:

$$K = \frac{(c+x)(d+x)}{(a-x)(b-x)} \quad (24)$$

After expanding and rearranging this expression, it can be written in terms of a quadratic in x,

$$(K-1)x^2 - (Kb + Ka + d + c)x + Kab - cd = 0 \quad (25)$$

which can be readily solved for x. Since two values of x will be obtained, that value is chosen which insures that the species in (23) will be positive. It is in this manner, then, that the equilibrium concentrations for the water-gas shift species are calculated.

Physical Characteristics of the Bed

Correlations from the literature can be used to compute various physical characteristics of the bed provided the bulk density and the particle size distribution are known for coal and char. This information has been available in the present study. From the particle size distribution, a weighted average has been taken for the particle size diameter. From the bulk density, the particle density has been determined using a value of 0.42 for ϵ_m , the voidage of coal.

The minimum fluidization velocity, u_{mf} , has been calculated using equation 3-21 of Kunii and Levenspiel, ²²

$$u_{mf} = \frac{d_p^2(\rho_s - \rho_g)g}{1650 \mu} \quad (26)$$

where d_p is the average particle diameter, ρ_s is solids particle density, ρ_g is gas density, μ is viscosity, and g is gravitational acceleration.

According to Table 2.5 of Botterill, ²³ ϵ_{mf} , the voidage at u_{mf} , minus ϵ_m , the slumped voidage, is 0.3. Since ϵ_m for coal has been taken as 0.42, ϵ_{mf} is 0.45. It follows then that H_{mf} , the bed height at minimum fluidization is 1.055 times H_0 , the slumped bed height.

Equation 5.32 of Hovmand and Davidson²⁴ gives a correlation between H , the expanded bed height, and H_{mf} . A modification of this equation to fit experimental data which is given in Figure 5.21 of the same reference has

been used in the present study and can be written as follows:

$$\frac{H}{H_{mf}} = \frac{2(u - u_{mf})}{0.35(gD)^{1/2}} + 1 \quad (27)$$

from which it follows that

$$\frac{H}{H_0} = \frac{2.11(u - u_{mf})}{0.35(gD)^{1/2}} + 1.055 \quad (28)$$

where u is the superficial gas velocity and D is the vessel diameter.

The bed density is then given by

$$\rho_{bed} = \rho_s \left(\frac{H_0}{H} \right) \quad (29)$$

and the average residence time is given by

$$\tau = \frac{\rho_{bed} \cdot V_{bed}}{F_{coal}} \quad (30)$$

where V is bed volume and F_{coal} is the coal feedrate.

In this study, H is known to be fixed at 68 inches. Equation (28) is used to correlate H_0 . Then equation (29) is used to find ρ_{bed} , and equation (30) is used to find τ .

Entrainment and elutriation correlations have been compared with the weight of fines collected in the filter. The largest particle entrained by the gas issuing from the gasifier can be calculated by equation 3-30 of Kunii and Levenspiel:²²

$$dp_{\max} = \frac{u_t}{\left[\frac{4}{225} \frac{(\rho_s - \rho_g)^2 g^2}{\rho_g \mu} \right]^{1/3}} \quad (31)$$

where u_t is the terminal velocity. The weight of char which has a size less than $dp_{\max}$ is then determined.

For comparison with entrainment correlations this weight of char is set equal to F_g in the abscissi of Figure 31 from Figure 3 of Chapter 10 of Kunii and Levenspiel.²² Then the values of the abscissa and ordinate are computed and the experimental data point is ready for graphical comparison with the entrainment correlation. For comparison with elutriation correlations, the weight of char is set equal to K^* via the ordinate of Figure 32 from Figure 12 of Chapter 10, Kunii and Levenspiel.²² Again, the values of the abscissa and ordinate are computed and the experimental data point is ready for graphical comparison with the elutriation correlation.

Energy Balance

A subroutine entitled ENERGY has been developed to perform energy balance calculations. The calculations are essentially based on evaluating the enthalpy change of each step in a three-step process. These steps include the following: cooling the reactants at one atmosphere from their inlet temperatures T_1 , to 298°K (ΔH_r°); allowing the reactions to proceed isothermally at 298°K to yield the reaction products (ΔH_{298}°); and heating the reaction products at one atmosphere from 298°K to temperature T (ΔH_p°). The effect of pressure on the enthalpies of each step are neglected.

The enthalpy change for cooling the reactants is calculated from heat capacities:

$$H_r^\circ = \sum_i \left(n \int_{T_i}^{298} C_p^\circ dT \right) \quad (32)$$

reactants

Similarly, for the products,

$$H_p^\circ = \sum_j \left(n \int_{298}^T C_p^\circ dT \right) \quad (33)$$

products

where n is concentration and C_p° is the heat capacity expressed as a function of T . The functions for C_p° were obtained from Daniels and Alberti²¹ for gases, from Lee²⁵ for coal and char, and from Kirov and Stephens for tar.²⁶

In order to evaluate ΔH_{298}° , the reaction of coal or char with steam and oxygen to form the various reaction products was broken down into the decomposition of coal or char and steam into their elements and the formation of the products from these elements. Values for heats of formation for the gas products were obtained from Smith and Van Ness.²⁷ Heating values for coal, char and tar were calculated using the Dulong formula obtained from the Chemical Engineer's Handbook.²⁸

An overall enthalpy balance is achieved with the subroutine ENERGY, and this can be stated as follows:

$$\Delta H_r^\circ + \Delta H_{298}^\circ + \Delta H_p^\circ - Q = 0 \quad (34)$$

where Q is the heat loss. The subroutine can be operated in several modes. Either the heat loss may be determined if all inlet and outlet temperatures are specified, or the outlet temperature may be determined if the heat loss is specified. To evaluate this outlet temperature, equation (34) becomes a cubic in T , and the solution for T is obtained merely by solving the cubic equation. An option also exists in the program to either specify the temperature of the exit char or assume it to be the same as the temperature of the gas products. Also, heating values for coal, char, and tar may be specified, as opposed to being calculated by the Dulong Formula.

Algorithm for Parameter Adjustment

The computer oriented algorithm used for parameter adjustment in both the analytical and predictive code was developed by Brown.^{20,29} It is called SSQMIN and is based on a non-linear finite difference Levenberg-Marquadt least squares approximation. From an initial estimate of the parameters X_1 , $1 = 1$, and N , SSQMIN minimizes the sum of the squares of the residuals, $[F_j (X_1 \dots X_N)]_j^2$, $j = 1, M$, where M is the number of residuals. In terms of the non-linear model G and the data Y , this can be expressed:

$$\sum_{j=1}^M [F_j (X_1 \dots X_N)]_j^2 = \sum_{j=1}^M [G_j (X_1 \dots X_N)_j - Y_j]^2 \quad (35)$$

These residuals are defined in a user supplied subroutine called FUNC.
Convergence is achieved if any of the following three criteria are met:

- (1) All components of two successive iterations agree to a specified number of digits.
- (2) The sum of squares of residuals for two successive iterations agree to a specified number of digits.
- (3) The Euclidean norm of the approximate gradient vector is less than a specified value.

Estimation of Conversion Parameter for Devolatilization Products

Since the mechanisms are not available for reactions in the devolatilization zone, it has been necessary to make estimates for a number of the products formed in this zone from runs in the analytical code for use in the predictive code. On the basis of over 30 Montana Rosebud runs, average values for parameters have been estimated for the following: H_2S , CH_4 , C_2H_6 , and H_2 formed in zone 1 and the base carbon in the coal, C_b .

The amount of H_2S formed is known in the analytical code and is assumed to be entirely formed in zone 1. For use in the predictive code, the parameter is defined as the fraction of sulfur in the coal evolved as H_2S . An average value of about 78% has been obtained.

The amount of carbon evolved as CH_4 equivalent in the carbonizer, C_m , is evaluated in the analytical code. Since C_2H_6 is known and is assumed to be entirely formed in zone 1, the balance of CH_4 equivalent is attributed to CH_4 . The percent of CH_4 equivalent evolved as CH_4 has been found to be 76% and evolved as C_2H_6 , 24%.

Johnson ^{1,30} has suggested that the base carbon fraction, C_b , be estimated as a fraction of the fixed matter in the coal and that the value is generally around 95%. In the present study, this estimate has been calculated as 94%.

In his gasification model studies, Johnson ³⁰ has assumed that the ratio of H_2 evolved to the carbon devolatilized in zone 1 is a constant. This assumption has been adopted in the present study and the ratio found to be 0.11.

REACTOR MODEL

A three-zone reactor model similar to that presented by Dobner et al.^{16,17} has been formulated in the present study and is depicted in the reactor design configuration of the sample computer printout in Appendices III and IV and also in Figure 30. Zone 1 is the carbonizer in which all of the devolatilization of the coal is assumed to occur during free fall to the top of the gasifier. Zone 2, the gasification region, has been divided into two sections. Zone 2A is the volumeless upper border of the gasifier where it is assumed that the rapid-rate formation of methane occurs essentially instantaneously. Zone 2B is basically the entire gasifier in which the low-rate gasification of the carbon in the char takes place. As in other studies of a similar nature, it is assumed that the gas and solids in Zone 2 are completely mixed. Finally, Zone 3 is the volumeless lower border of the gasifier where it is assumed that all of the oxygen entering the unit reacts essentially instantaneously with char.

It is also assumed that the water-gas shift equilibrium is in effect in the gasification and devolatilization zones. The shift temperature from which the equilibrium constant is calculated is taken to be the average temperature of the gasifier bed, zone 2. The value of the equilibrium constant so determined is also applied to zone 1.

COMPUTER PROGRAMS

Three computer programs have been written to carry out the mathematical simulation of the Synthane gasifier. The first is called the Analytical Computer Code which contains 5000 Fortran statements and is stored on the update file named ANKIN6 at the Bureau of Reclamation computer facilities in Denver. Its purpose is essentially to evaluate the parameters f_0 and A_m so that parametric studies for a variety of process conditions can be carried out using the Predictive Computer Code where f_0 and A_m are stipulated.

The second is called the Predictive Computer Code which also contains over 5000 Fortran statements and is stored in the update file named MPRED19 in Denver. As stated above its purpose is to carry out parametric studies. From a stipulation of f_0 and A_m and a set of run conditions, the composition of the product stream and the temperatures of the carbonization region (zone 1) and the fluid bed region (zone 2) are calculated. Run conditions can be varied and hence parametric studies can be carried out.

The third is a short plotting program which is designed to construct the parity plots presented in this text.

Copies of these programs are available from the authors.

Analytical Computer Code

Function

The purpose of the analytical computer code is to determine the kinetic parameter f_0 in equation (6) and the parameter A_m , which is the fraction of carbon in coal evolved as methane and higher alkanes in the devolatilization zone (zone 1), i.e.,

$$A_m = \frac{C_m}{C_T} \quad (36)$$

Also evaluated are any heat losses in the devolatilization and gasification zones (zones 1 and 2).

Input Data

Data from the PDU runs, which is input to this program, consists essentially of the following: proximate and ultimate analysis of the coal, tar, and char composition; particle size distribution for coal and char as well as bulk densities of the same; flowrates of all streams including coal, steam, O_2 , and N_2 ; effluent product compositions, including H_2O , CO , H_2 , CO_2 , CH_4 , C_2H_6 , N_2 , NH_3 , H_2S , tar, and char; total system pressure; temperatures for inlet and outlet streams as well as the average temperature for the gasification region, zone 2, and for the devolatilization region, zone 1; total run time and steady-state run time; bed height and diameter.

All input information is included in the computer printout for each run. A sample of output is given in Appendix III for Montana Rosebud Run No. 229.

Evaluation of Product Composition for Reactor Zones

The evaluation of the product compositions in each zone of the model in general follows the formulation of Dobner et. al. 30,31

For zone 1, the following assumptions have been made prior to any water-gas shift adjustment: CO is formed from "available" oxygen, i.e., oxygen in coal minus oxygen in char, fines and tar; the quantities of H₂S, C₂H₆, and tar observed in the effluent stream are assumed to be formed entirely in this zone; H₂O produced is from moisture in the coal; NH₃ is formed from 90% of the "available" nitrogen (defined similar to "available" oxygen) as suggested by in-house experimental findings; N₂ is from N₂ fed with coal and 10% "available" nitrogen; for CH₄, C_m is evaluated from equation (36) using an assumed value of A_m and then corrected for methane equivalent evolved as C₂H₆; H₂ is equal to hydrogen in coal minus hydrogen in char, fines, tar, H₂S, C₂H₆, and devolatilized CH₄; the volatile carbon fraction C_v is calculated from equation (2); the base carbon fraction C_b is calculated from equation (1).

For zone 2A, rapid rate CH₄ is evaluated from equation (4) according to the procedure previously discussed.

For zone 2B, the following assumptions have been made prior to any water-gas shift adjustment: CO is equal to the sum of CO and CO₂ in the effluent stream minus CO₂ formed in zone 1 and minus CO formed in zone 3; H₂O equals input steam minus the amount used in the steam-carbon reaction, i.e., minus CO formed in this zone; CH₄ equals CH₄ in effluent stream minus devolatilized CH₄ from zone 1 and minus rapid rate CH₄ from zone 2A; H₂ equals the amount formed from the steam carbon reaction minus the amount that reacts with carbon to form CH₄ in this zone.

For zone 3, it is assumed that the O_2 reacts stoichiometrically with char to form CO_2 .

The char effluent for each zone is calculated by performing a material balance around each zone. This is accomplished by calling a subroutine entitled MATBAL. These values are also given on the computer printout for the sample reactor design configuration.

Calculation Procedure and Flowsheet

In Appendix I, the flowsheet is given for the analytical computer code and indicates the procedure followed in development of the computer code. More details are presented in certain areas than in others, especially for the iterative processes, the energy balance calculations, and the product composition evaluations.

The computer code begins in PROGRAM MAIN. Here the PDU data is read into the input file from data cards. Various physical characteristics of the bed and a steady-state materials balance are computed.

To begin the evaluation of rapid-rate CH_4 , X_R in equation (4), an estimate of the partial pressure of hydrogen P_{H_2} is made from the effluent product stream. An initial guess is supplied for X_R . The iterative algorithm NONLIN is called which in turn calls the user-supplied subroutine RAPID that defines the rapid rate CH_4 expression. The parameter X_R is incremented until the right- and left-hand terms in equation (4) agree to a preset tolerance level.

Once convergence has been achieved, program control is transferred back to MAIN, and subroutine KIN1 is then called. Here those products which are not dependent on the iterative parameters f_0 and A_m are evaluated; no attempt is made as yet to adjust for the water-gas shift equilibrium. For zone 1 these include CO , H_2S , N_2 , C_2H_6 , and tar; for zone 2B, CO , CO_2 , and H_2O ; for zone 3, CO_2 .

Program control is returned back to MAIN in order to evaluate the parameters A_m and f_o . To accomplish this task, initial guesses are made for these parameters, and the iterative algorithm SSQMIN is then called. The user-supplied subroutine FUNC is called by SSQMIN to first calculate carbon conversion and product concentrations dependent on the iterative parameters and then to define the residuals. Carbon conversions calculated include C_m , C_v and C_b . The following product compositions prior to any water-gas shift adjustment are calculated: for zone 1, CH_4 and H_2 ; for zone 2B, before water-gas shift adjustment, CH_4 and H_2 , and after water-gas shift adjustment, H_2 , CO , CO_2 , and H_2O . The residuals are defined as follows:

$$F(1) = \frac{dX}{dt} - \frac{X}{\tau} \quad (37)$$

$$F(2) = \frac{dX_{co}}{dt} - \frac{X_{co}}{\tau} \quad (38)$$

where dX/dt and dX_{co}/dt are rates calculated from the Johnson kinetic equations (6) and (11); and the rate terms x/τ and X_{co}/τ are rates based on equation (3) for X and X_{co} and equation (30) for τ . Essentially the algorithm involves solving the above two equations in two unknowns, namely, A_m and f_o . Results are written to output for the first and last iteration. At this point, program control is transferred back to SSQMIN and a test for convergence, as previously discussed, is made. If convergence has not been achieved, A_m and f_o are adjusted, and the iteration procedure begun again. Once convergence is achieved, program control is transferred back to MAIN.

In MAIN, adjustment is made for the water-gas shift equilibrium in zone 1, and new values are calculated for CO, CO₂, H₂O, and H₂. With all gas product compositions now evaluated for all zones, the subroutine MATBAL is called to carry out a material balance for each zone and hence to compute the char exiting each zone. The material balance for each zone is written to output.

Program control is transferred back to MAIN and information - essentially inlet and outlet stream composition and temperatures, and program operation mode - is prepared for an energy balance around zone 3. It is assumed that there is no heat loss from that zone. The inlet char temperature is taken to be equal to the average gasifier bed temperature. Experimental values for the temperatures of the feed streams for N₂, O₂ and steam are available. The subroutine ENERGY is called to calculate the outlet product gas temperature, which is assumed equal to the exit char temperature.

Program control is transferred back to MAIN where information is prepared for an energy balance calculation around zone 2 (sum of zones 2A and 2B). It is assumed that the outlet product gas temperature and the inlet and outlet char temperatures are equal. The inlet gas temperature is simply the outlet product gas temperature from zone 3 which has been determined above. A call is made to subroutine ENERGY and the heat loss is evaluated for zone 2.

Program control is once again transferred back to MAIN where information is prepared for an energy balance around zone 1. It is assumed that the temperature of the exit char is equal to the temperature of the inlet

product gas from zone 2, which has already been determined above.

Experimental values for the inlet temperatures of the coal and N_2 feed streams and for the outlet temperature of the product effluent stream are available. ENERGY is called and the heat loss for zone 1 calculated. An option exists to printout the details of the three-step process for each zone. Program control is returned to MAIN.

At this point, the subroutine RXDSGN is called to print out the reactor model with the following information: the reactions assumed to occur in each zone; the inlet and outlet product compositions - both before and after adjustment for the water-gas shift equilibrium - and temperatures for each zone; and heat losses for each zone. All information is printed on one page of output, a sample of which is included in the sample output on the page entitled Reactor Design Configuration in Appendix III.

Program control is returned to MAIN. Data which can be used as input to the predictive computer code is written to an update data file as well as to output. A test is made to determine whether any additional runs remain to be processed. If so, the above described procedure is repeated for each remaining run. When all runs are processed, a summary table is written to output and contains values for a select number of variables for all the runs processed. Two descriptive statistics subroutines DSCRPT and DSCRPT2³¹ are called to calculate such statistics as the minimum, maximum, median, range, mean, standard deviation, and variance of a number of select variables for all of the runs processed. Program control is returned to MAIN and these statistics written to output. Finally, values for effluent products and zone temperatures for generating - together with similar information from the predictive code-parity plots are written to yet another data update file. The program is now terminated.

Sample Output

As previously indicated, a sample of the computer output for specifically Montana Rosebud Run No. 229 is given in Appendix III. The output for each run is about 15 pages and includes all input information for that run as well as a large number of computed results.

The output for each run analyzed consists essentially of the following information: ultimate and proximate analysis of the coal; char and tar compositions; feed flow rates of O_2 , steam, N_2 , and coal; steady-state product gas flow rates; stream and zone temperatures; total run time and steady-state run time; system pressure; coal and char particle size distributions, average particle sizes, bulk and particle densities; separate material balance for the entire run period and for the steady-state run period; bed dimensions; superficial gas velocity; residence time; rates of gasification and product distribution for initial estimates and final convergence values of A_m and f_o ; material balance around each reactor zone displayed for convenience on one page of output; optional printout of the details of the energy balance calculations for each zone - one page of output for each zone - and also including the heating values for coal, char, and tar; a reactor design configuration specially prepared to present a maximum amount of information for the reactor model on one page of output - details have previously been described; parameter estimates of devolatilization products for use in the predictive code; and input data for use in the predictive code.

Predictive Computer Code

Function

The purpose of the predictive computer code is basically to predict product composition in the effluent stream and average fluid bed and carbonizer temperatures given values for f_o and A_m determined from the analytical code. There are five variables to be evaluated and these are defined as follows:

- X(1) - Percent coal conversion
- X(2) - Temperature of fluid bed, zone 2
- X(3) - Percent of total carbon in coal converted to low and rapid rate CH_4
- X(4) - Percent of total carbon in coal converted to CO in zone 2.
- X(5) - Fraction of base carbon converted to rapid rate CH_4

Input Data

Input data is read from an update file generated by the analytical code, or created separately, and includes the following information: proximate and ultimate analysis for the coal; particle size distribution and bulk density for coal; flowrates and inlet temperatures of all feed streams including coal, steam, O_2 , and N_2 ; total system pressure; bed height and diameter; amount of tar formed; initial guesses for the five variables, previously defined; heat losses for zones 1 and 2; values for the kinetic parameters, A_m and f_o .

As in the case with the analytical code, input information is listed in the computer output. Since output for the predictive code is similar to that for the analytical code, only sample output for the reactor design configuration giving all products in each zone is given in Appendix IV.

As previously discussed, a number of parameters related to product formation in the devolatilization zone, namely C_b , H_2S , CH_4 , C_2H_6 , and H_2 , are evaluated in the analytical code for use in the predictive code. Values for these parameters are not entered with the above data but rather inserted with the Fortran program statements.

Evaluation of Product Composition for Reactor Zones

For zone 1, the products formed have been calculated as follows: CH_4 is 76% of C_m and C_2H_6 is 24% of C_m where C_m is calculated from equation (36); CO is calculated from C_{ox} in equation (2) where C_v is calculated from equation (1); 78% of sulfur in coal is assumed devolatilized as H_2S ; all moisture in the coal is taken to be devolatilized here; N_2 is from N_2 fed with coal plus 10% N_2 in coal; NH_3 is formed from 90% of N_2 in coal; H_2 is calculated to be 11% of C_v ; the amount of tar is an input parameter; and no CO_2 is assumed to be formed.

For zone 2A, rapid rate CH_4 is evaluated from equation (4) using the iterative algorithm NONLIN as previously discussed.

For zone 2B, the following procedure has been adopted: CO is calculated from the variable $X(4)$; H_2O equals the input steam minus CO; CH_4 is evaluated from differences in two of the variables, i.e., $X(3) - X(5)$; H_2

equals CO minus CH₄ formed in this zone.

For zone 3, it is assumed that the O₂ reacts stoichiometrically with char to form CO₂.

The calculations discussed thus far are for the products formed in each zone. Evaluation of the total products in each zone as well as the computation for char formation in each zone is essentially the same as in the analytical code and has been discussed previously and in Appendix III.

Calculation Procedure and Flowsheet

In Appendix II, the flowsheet is given for the predictive computer code and indicates the general procedure followed in development of the computer code. Again, as with the analytical code, certain areas are presented in more detail than others.

The computer code begins in PROGRAM EXEC. Here the PDU data for run conditions for a particular run is read into the input file from an update file, which may or may not be generated from the analytical code. Various physical characteristics of the bed are computed.

To begin the iteration process, initial guesses are supplied for the five variables listed under the section entitled Function. Estimates of these variables for the various runs analyzed are made from the corresponding runs analyzed in the analytical code. In order to evaluate the variables, the iterative process is carried out by calling SSQMIN.

The user-supplied subroutine, FUNC, is called by SSQMIN to calculate product distributions for all zones and evaluate the residuals. Within FUNC, the iterative algorithm NONLIN is used to calculate X_R in a manner similar to that described in the analytical code. After convergence has been achieved in NONLIN, program control is returned to FUNC. Adjustment is made for the water-gas shift equilibrium, and the following residuals are defined:

$$F(1) = \frac{dX}{dt} - \frac{X}{\tau} \quad (39)$$

$$F(2) = \frac{dX_{CH_4}}{dt} - \frac{X_{CH_4}}{\tau} \quad (40)$$

$$F(5) = X(5) - X_R \quad (41)$$

In order to evaluate the fourth residual, the subroutine MATBAL is called to carry out a material balance for each zone and hence evaluate the char exiting each zone. The material balance is written to output for each zone for the first and last iteration only. Program control is returned to FUNC, and the residual $F(3)$ is defined as the quantity of char exiting zone 3 as calculated in MATBAL minus the quantity of char calculated as a function of the variable $X(1)$.

The fifth residual is evaluated with the aid of the energy balance subroutine ENERGY. In FUNC, information is prepared for the energy balance calculated around zone 3 as described in the analogous section for the analytical code.

A call is made to ENERGY, and the exit product gas temperature calculated. Program control is returned to FUNC. Information for the energy balance calculation around zone 2 is prepared in a manner similar to that described in the analogous section of the analytical code. The heat loss, however, is not calculated but is rather an input parameter. A call is made to ENERGY, and the temperature for the exit product gas is computed. Program control is returned to FUNC, and the fourth residual is evaluated as the difference between the exit product gas temperature for zone 2 and the variable X(2). At this point, an energy balance is carried out for zone 1, again in a manner similar to that described in the calculation procedure for the analytical code. As with zone 2, a value for the heat loss is supplied, a call made to ENERGY, and the exit product gas temperature computed. If the option is chosen, the details of the energy balance calculations for each zone will be written to output for the first and last iteration only (the default is no printout of the energy balance calculations). Program control is returned to FUNC.

The subroutine RXDSGN is now called to print out the reactor model with almost all the same information as in the analytical code. A sample printout is given in Appendix IV. The only difference is that the column headed "EXP" in the analytical code and representing the experimental values for the effluent stream is now replaced by the predicted values. (These predicted values, of course, embody the water-gas shift adjusted values, and hence there is no need for a separate column for shift-adjusted values.)

Program control is returned to FUNC and results written to output for the first and last iterations only. Program control is then transferred back

to SSQMIN, and a test for convergence made as previously discussed. If convergence has not been achieved, the five variables X(1) through X(5) are incremented and the iteration process is repeated. When convergence is finally achieved, program control is transferred back to EXEC.

A test is now made to determine whether any additional runs remain to be processed. If so, the above described procedure is repeated for each remaining run. When all runs are processed, the summary table and descriptive statistics discussed in the analytical codes are evaluated and written to output. Finally, values for effluent products and zone temperature which are used for generating parity plots are written to a data update file. The program is now terminated.

Plotting Program

A plotting program has been developed for the preparation of the parity plots presented in this report. The program has been designed to read input data for effluent products and zone temperatures from data files generated by the analytical code and the predictive code. The data file generated from the analytical code contains principally the experimentally observed values, while that from the predictive code contains the predicted values. Various plotting subroutines are called in the program to carry out such functions as labeling the axes, setting the height of the letters and numbers, drawing the plots, setting the physical origin, and choosing the symbols for points plotted.

RESULTS AND DISCUSSION

In the present study, some 35 Montana Rosebud runs have been analyzed using the analytical and predictive computer codes. Copies of the computer printouts for summary tables of some of the more important system variables are given in Appendix VI for the analytical code and Appendix VII for the predictive code. These system variables include much of the input information as well as calculated results. Definitions for symbols of the variables appearing in the summary tables are given in Appendix V. Parity plots are given in Figures 5-29.

Analytical Code

The summary table for the analytical code in Appendix VI consists of the following variables: gas products in effluent stream; effluent char; temperatures for each of the three zones; heat losses for zones 1 and 2; conversion parameters for devolatilization products previously discussed which serve as input to the predictive code; estimates of the five variables for the predictive code which will serve as the initial guesses; the variables f_0 and A_m ; all input feed streams; the assumed water-gas shift temperatures and the corresponding equilibrium constant; the percent of carbon gasified and converted; properties of the coal and char, namely the bulk and particle densities and the average particle diameter; bed properties such as the superficial gas velocity; minimum fluidization velocity, bed volume, fluid bed height, slumped bed height, and residence time; heating values for coal, char, and tar; and finally, total system pressure.

Most runs have been carried out at 40 atm pressure and a few at 10, 20, and 30 atm. Coal feedrates have been varied from 10 to 45 lbs/hr; steam feedrates, 6 to 44 lbs/hr; and O₂ feedrates, 3 to 12 lbs/hr.

For the devolatilization zone (zone 1), the average experimental value for temperature has been 743° F with a minimum of 522° F and a maximum of 853° F. For the gasification zone (zone 2), the average experimental value for the temperature has been 1570° F with a minimum of 1495° F and a maximum of 1623° F. For the combustion region (zone 3), the average calculated temperature has been 2349° F with a minimum of 1842° F and a maximum of 3126° F. These are much higher temperatures than can possibly exist at the bottom of the PDU, because the ash of coal forms clinkers at about 1900° F and slags at somewhat higher temperatures. Clinker and slag formation were not observed in any of the 35 runs examined here, and therefore this temperature must have been below 1900° F at all times during these runs. This indicates that considerable convective heat transfer must be taking place at the bottom of the gasifier which renders this region far from being adiabatic. The computation of the adiabatic temperature in this region has been included to indicate the potential for clinkering and slagging, particularly if the bed defluidizes for any reason in this region.

While the variance in temperature for zones 1 and 2 has been moderate from run to run, the variance in the corresponding calculated heat losses has been substantial. This can be attributed to a lack of adequate control of heaters around these regions of the gasifiers from run to run.

With respect to properties of the coal, the average particle diameter is 325 microns; the bulk density, 0.794 gm/cc; and the particle density, 1.42 gm/cc. For the effluent char, the average particle diameter is 297 microns; the bulk density, 0.475 gm/cc; and the particle density, 0.819 gm/cc.

Average values for some of the bed properties are as follows, with ranges given in parenthesis: fluid bed height, 67.4 inches (62.0 - 71.7); slumped bed height, 42.6 inches (39.7 - 45.7); bed volume, 0.489 ft³ (0.450 - 0.508); bed density, 28.3 lbs/ft³ (19.0 - 35.6); residence time, 31 minutes (9 - 46); superficial gas velocity, 0.316 ft/sec (0.285-0.361).

For the seven runs 203 - 221, a number of values for particle and bed properties are zero on the summary table printout, which can be misleading. This occurs merely because bed densities have been input information and, together with some of the particle and bed properties, are not calculated by the program. In the listing of the values of these properties, zeroes are therefore included which, however, should not be interpreted literally.

Heating values for coal, char, and tar have been calculated from the Dulong formula in the computer code. The average value for coal is 10664 Btu/lb; for effluent char, 8238 Btu/lb; and for tar, 16474 Btu/lb.

In addition to the experimental values for the gas products in the effluent stream, the calculated water-gas shift values have also been included in the summary table. As previously discussed, these values have been calculated by first adding the products formed in zone 1 to those

formed in zone 2 and then adjusting for the water-gas shift equilibrium. From an inspection of the parity plots in Figures 5-8, it can be seen that there is in general good agreement between the experimental values and the calculated water-gas shift values. (See section under parity plots for interpretation of the plots.)

Three values for effluent char are given for each run. The first is the experimental value. The second and third values are calculated from a material balance around the gasifier in the subroutine MATBAL. The second value is corrected for ash loss while the third is not. For about two-thirds of the runs, agreement with the experimental value is better when ash loss is taken into account, as would be expected. The lack of similar agreement among more of the runs may be due to the difficulties involved in evaluating ash loss.

Parity plots in Figures 9 and 10 reflect the better correlation when ash loss is included.

Values based on all 35 runs have been calculated for the variables f_0 and A_m . Averages have been taken for each variable and serve as input values for each of the 35 runs in the predictive code. For f_0 , an average value of 24.6 with a standard deviation of 16.9 has been obtained; and for A_m , an average value of 0.103 with a standard deviation of 0.01 has been calculated.

Comparison of the observed elutriation from the fluidized bed gasifier with the entrainment and elutriation correlations described earlier is shown in Figures 2 and 3 for 28 of the 35 runs. Figure 2 shows a portion

of the entrainment correlation of Figure 31 (from Figure 3, Chapter 10, of Kunii and Levenspiel²²). The lower solid line represents the correlation for a gas-fluidized bed. The clustering of data points around this line implies that all of the particles which can be entrained by the gas flowing from the gasifier are indeed being entrained by that gas. Figure 3 shows a portion of the elutriation correlation of Figure 32 (from Figure 12, Chapter 10, of Kunii and Levenspiel²²). Again, the clustering of data points about the correlation line implies that every particle that is entrained is elutriated. A final look at elutriation is given in Figure 4. Here the amount of elutriation predicted by the correlation of Figure 12, Chapter 10, of Kunii and Levenspiel, is shown on a parity plot versus the amount of elutriation actually observed. Not being a log-log plot as are Figures 2 and 3, Figure 4 has considerable scatter, but generally the scatter is symmetrical with the parity line.

Predictive Code

The summary table for the predictive code in Appendix VII consists of many of the variables given in the summary table for the analytical code as discussed in the preceding section. There are a few differences, however.

All values for gas effluent products are, of course, calculated (with the exception of tar which is input from the analytical code).

The first value for char is not an experimental value but rather is calculated from the first variable $X(1)$, the percent coal conversion. As in the case with the analytical code, the third value of char is computed from a material balance around the gasifier in the subroutine MATBAL.

These two values for char are equal since this is one of the convergence criteria. The second value for char takes into account ash loss by correcting the third value by the value for ash loss that is calculated in the analytical code for the corresponding run.

Values of heat losses in zones 1 and 2 for each run are the values calculated in the analytical code for the corresponding runs. The temperatures for the product gas streams in zones 1 and 2 are calculated values (which is, of course, the case for zone 3 where no heat loss is assumed).

For the variables X(1) thru X(5), values given are the final convergence values.

Since information was not available for particle size distribution of coal for runs 203 - 221, an average of values from the other runs was used to calculate the average particle size for coal for these runs.

Parity Plots

Figures 5-29 contain parity plots for all effluent gas products except tar, for effluent char, and for temperatures of the three reaction zones. The plots presented have been prepared directly from the plotter as discussed in the Computer Facilities section. Calculated values from the predictive code, which are the ordinate values, are plotted against some calculated but mostly experimental values in the analytical code, which are the abscissa values. The straight lines in the plots do not represent least square lines but rather the region where the points should fall.

Parity plots are given for the calculated water-gas shift species H_2O , CO , H_2 , and CO_2 in the effluent stream in Figures 11-14. Here, experimental values are not included. Rather, values from the predictive code are plotted against values calculated from the shift adjustment in the analytical code as previously discussed. The good agreement in these plots indicates that the predictive code is effectively duplicating the analytical code in calculating the water-gas shift species.

In Figures 15-18, plots are given for the water-gas shift species, but for these plots the abscissa contains the experimentally observed values. These plots indicate how well the predictive code is duplicating the experimental values. Predicted values are somewhat on the low side for H_2O and CO_2 and on the high side for CO and H_2 .

Figures 19 and 20 contain plots for CH_4 and C_2H_6 where the points are evenly distributed about the parity line.

Figure 21 contains the parity plot for N_2 in which there is no scatter of points. This would be expected since essentially the N_2 in the effluent stream is defined to be the same as the N_2 input to the system, since very little N_2 is evolved from the coal. This equality was required because no independent measure was made of N_2 input to the PDU.

Parity plots for NH_3 and H_2S are given in Figures 22 and 23 where the scatter of points is somewhat on the high side.

In Figures 24-26 three different plots for char are given. In Figure 24 the effluent char calculated in the predictive code and corrected for ash loss is plotted against the experimental char; there is a fair spread in the points but a random scatter about the parity line. There is less scatter in the plot in Figure 25 where the experimental values for char in the abscissa are replaced by values calculated in the analytical code and corrected for ash loss. Again, compared with Figure 24, there is less scatter in the plot in Figure 26 where the effluent char calculated in the predictive code and not corrected for ash loss is plotted against that calculated in the analytical code and not corrected for ash loss. The larger spread when plotting the experimental char is not surprising when it is taken into consideration that only a rough estimate of the char flowrate at steady state is made.

The last three plots in Figures 27-29 are for temperatures of the reaction zones. Figure 27 contains the plot for the temperature in Zone 1, the devolatilization region (also called the low temperature region); here results are somewhat on the high side possibly due to a slight underestimation of steam produced in the predictive code, which means less enthalpy tied up with the steam and hence a higher temperature. Figure 28 contains the plot for the temperature of zone 2, the gasification region (also called the high temperature region); there is some scatter in results here. Figure 29 contains the plot for the temperature of zone 3, the combustion zone. There is little scatter but this would be expected since the temperature in the abscissa is not experimentally determined but rather calculated in the analytical code the same way it is calculated in the predictive code.

From the parity plots presented in this report, then, there is, in general, good agreement between values for effluent products and zone temperatures calculated in the predictive code and the corresponding experimental and calculated values from the analytical code. This attests to the adequacy of the model developed in this report for the simulation of the SYNTHANE gasifier for non-caking coals.

SUMMARY

A model for the Synthane gasifier has been developed and incorporated into two computer codes. These codes have been used for the simulation of some 35 gasification runs for Montana Rosebud. The analytical computer code has been designed to accept raw data from SYNTHANE PDU coal gasification runs and, essentially, to evaluate the model parameters. The predictive computer code has been designed to accept as input these model parameters, together with run conditions, for the purpose of predicting the product stream and zone temperatures.

From an analysis of the results and the parity plots, product streams and zone temperatures have been reasonably well predicted. Hence, the model developed thus far has potentials for further use in design and parametric studies.

A study has been made of the effect of operating conditions on product yield and gasifier performance using the Predictive Computer Code.

Briefly, the results, which have been presented at the 71st Annual AIChE Meeting, indicate that an increase in total system pressure and in steam/coal ratio would improve gasifier performance.

NOMENCLATURE

- A_m = Parameter which represents the fraction of carbon in coal evolved as methane and higher alkanes in the devolatilization zone.
- C_b = Carbon in the mixed carbon fraction of the feed coal char as determined by a proximate analysis, lbs/lb feed coal
- C_g = Total carbon gasified, lbs/lb feed coal
- C_m = Volatile carbon from which methane equivalent is formed, lbs/lb feed coal
- C_{ox} = Volatile carbon that forms carbon oxides, lbs/lb feed coal
- C_t = Total carbon in the feed coal char as determined by an ultimate analysis, lbs/lb feed coal
- C_{tar} = Volatile carbon that is connected to tar, lbs/lb feed coal
- C_v = Volatile carbon in feed coal, lbs/lb feed coal
- D = Vessel diameter, inches
- ΔC_p = Change in heat capacity of products from the reactants, Btu/lb. $^{\circ}$ F
- ΔG° = Gibbs free energy for a reaction, Btu/lb
- ΔH_o = Hypothetical enthalpy at absolute zero, Btu/lb
- ΔH_p° = Enthalpy change for heating the reaction products at one atmosphere from 298 $^{\circ}$ K to temperature T, Btu/lb
- ΔH_r° = Enthalpy change for cooling the reactants at one atmosphere from their inlet temperatures T_i , to 298 $^{\circ}$ K, Btu/lb
- ΔH_T = Enthalpy of a reaction at temperature T, Btu/lb
- ΔH_{298}° = Enthalpy change for allowing the reactions to proceed isothermally at 298 $^{\circ}$ K to yield the reaction products, Btu/lb
- dp_{max} = Largest particle entrained by the gas issuing from the gasifier, microns
- F_{coal} = Coal feedrate, lbs/hr
- f_o = Relative reactivity factor for low-rate gasification dependent on the particular carbonaceous solid
- f_R = Relative reactivity factor for rapid-rate methane formation, dependent on the particular carbonaceous solid

- g = Gravitational acceleration, cm/sec^2
 H = Expanded bed height, inches
 H_{mf} = Bed height at minimum fluidization, inches
 H_o = Slumped bed height, inches
 k_I = Overall rate constant for low-rate gasification, min^{-1}
 k_I, k_{II}, k_{III} = Rate constants for Reactions I, II, and III, min^{-1}
 K_I, K_{II}, K_{III} = Equilibrium constants for Reactions I, II, and III considering carbon as graphite
 $P_{H_2}, P_{H_2O}, P_{CO}, P_{CO_2}, P_{CH_4}$ = Partial pressures of H_2, H_2O, CO, CO_2 and CH_4 , atm
 T = Reaction temperature, $^{\circ}\text{R}$
 T_p = Pretreatment temperature, $^{\circ}\text{R}$
 X = Total base carbon conversion fraction
 X_R = Base carbon conversion fraction after reaction in rapid-rate methane formation stage is completed
 V = Bed volume, ft^3

GREEK SYMBOLS

ϵ_m = Slumped voidage

ϵ_{mf} = Voidage at u_{mf}

ρ_{bed} = Bed density, lbs/ft³

ρ_f = Fluid density, gm/cm³

ρ_s = Density of solids, gm/cm³

τ = The average residence time, min

μ = Viscosity of gas, gm/cm·sec

u = Superficial gas velocity, cm/sec

u_{mf} = Superficial fluid velocity at minimum fluidizing conditions,
cm/sec

u_t = Terminal velocity of a falling particle, cm/sec

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Figure 1 - Schematic diagram of the fluid bed gasifier .

Figure 2. Comparison with entrainment correlation

Figure 3. Comparison with elutriation correlation

Figure 4. Parity plot for elutriation calculated from correlation vs. that observed.

FIGURE 5. PARITY PLOT FOR H_2O CALCULATED FROM THE ANALYTICAL CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 5. PARITY PLOT FOR CO CALCULATED FROM THE ANALYTICAL CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 7. PARITY PLOT FOR H_2 CALCULATED FROM THE ANALYTICAL CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 8. PARITY PLOT FOR CO₂ CALCULATED FROM THE ANALYTICAL CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 9. PARITY PLOT FOR CHAR CALCULATED FROM THE ANALYTICAL CODE AND CORRECTED FOR ASH LOSS VS. THE EXPERIMENTAL VALUE.

FIGURE 10. PARITY PLOT FOR CHAR CALCULATED FROM THE ANALYTICAL CODE AND NOT CORRECTED FOR ASH LOSS VS. THE EXPERIMENTAL VALUE.

FIGURE 11. PARITY PLOT FOR H_2O CALCULATED FROM THE PREDICTIVE CODE VS. THAT CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 12. PARITY PLOT FOR CO CALCULATED FROM THE PREDICTIVE CODE VS. THAT CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 13. PARITY PLOT FOR H₂ CALCULATED FROM THE PREDICTIVE CODE VS. THAT CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 14. PARITY PLOT FOR CO₂ CALCULATED FROM THE PREDICTIVE CODE VS. THAT CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 15. PARITY PLOT FOR H_2O , CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 16. PARITY PLOT FOR CO CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 17. PARITY PLOT FOR H_2 CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 18. PARITY PLOT FOR CO₂ CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 19. PARITY PLOT FOR CH_4 CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 20. PARITY PLOT FOR C_2H_6 CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 21. PARITY PLOT FOR N_2 CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 22. PARITY PLOT FOR NH_3 CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 23. PARITY PLOT FOR H_2S CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 24. PARITY PLOT FOR CHAR CALCULATED FROM THE PREDICTIVE CODE AND CORRECTED FOR ASH LOSS VS. THE EXPERIMENTAL VALUE.

FIGURE 25. PARITY PLOT FOR CHAR CALCULATED FROM THE PREDICTIVE CODE AND CORRECTED FOR ASH LOSS VS. THE SAME CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 26. PARITY PLOT FOR CHAR CALCULATED FROM THE PREDICTIVE CODE ASSUMING NO ASH LOSS VS. THE SAME CALCULATED FROM THE ANALYTICAL CODE.

FIGURE 27. PARITY PLOT FOR THE TEMPERATURE ZONE 1 (ALSO THE DEVOLATILIZATION ZONE OR LOW TEMPERATURE REGION) CALCULATED FROM THE PREDICTIVE CODE VS. THE EXPERIMENTAL VALUE.

FIGURE 29. PARITY PLOT FOR THE TEMPERATURE OF ZONE 3 (ALSO, THE COMBUSTION ZONE OR COMBUSTION TEMPERATURE REGION) CALCULATED FROM THE PREDICTIVE CODE VS. THE SAME CALCULATED FROM THE ANALYTICAL CODE.

Figure 30- Reactor model for SYNTHANE gasifier

Figure 31. Empirical correlation of the saturation carrying capacity with superficial gas velocity u_o for uniform-sized particles in either horizontal or vertical cocurrent dispersed flow.

Figure 32. Elutriation correlation. Continuous operations: sand, zinc blende, pyrite, cinder, pyrrhotite, calcium carbide, coke. Unsteady operations: sand, glass spheres, iron catalyst, magnesium oxide.

APPENDIX I

FLowsHEET FOR THE
ANALYTICAL COMPUTER CODE

FLWSHEET FOR ANALYTICAL CODE

APPENDIX II

**FLowsheet for the
PREDICTIVE COMPUTER CODE**

FLWSHEET FOR PREDICTIVE CODE

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APPENDIX III

SAMPLE COMPUTER PRINTOUT FROM THE
ANALYTICAL CODE FOR
MONTANA ROSEBUD RUN NO. 229

Explanation of Entries for Page Entitled

REACTOR DESIGN CONFIGURATION

Values in the left-most column of numbers are product compositions calculated according to the procedure discussed under Evaluation of Product Composition for Reactor Zones for the Analytical Computer Code in the text. The total gas product composition for each zone is equal to the products formed in that zone plus the gas products which have moved upward from the next lower zone. These values are given in the second and third column from the left (the second column has units of lb-moles/hr. and the third column of atm). Once the total product composition is calculated, adjustment is made in zones 1 and 2 for the water-gas shift equilibrium. These values are the two columns of numbers to the right of the blocks representing the zones, with the exception of zone 1 where these columns represent the experimental values of the effluent stream. The right-most column for zone 1 gives calculated values for the water-gas shift species after adjustment for the corresponding equilibrium.

INPUT DATA

ULTIMATE ANALYSIS

	AS RECEIVED	MOISTURE FREE	MOISTURE-ASH-FREE
HYDROGEN	5.00	4.46	5.00
CARBON	61.50	66.92	75.00
NITROGEN	1.00	1.09	1.22
OXYGEN	21.90	15.99	17.93
SULFUR	.70	.76	.85
ASH	9.90	10.77	*****

PROXIMATE ANALYSIS

	AS RECEIVED	MOISTURE-FREE	MOISTURE-ASH-FREE
MOISTURE	8.10	*****	*****
VOLATILE MATTER	34.80	37.87	42.44
FIXED MATTER	47.20	51.36	57.56
ASH	9.90	10.77	*****

TOTAL PRODUCT GAS FLOW= 930.70 SCFH (STEADY STATE PERIODS 3 THROUGH 18 INCLUSIVE)

TOTAL PRODUCT GAS FOR STEADY STATE PERIODS 3 THROUGH 18 INCLUSIVE

	PERCENT	SCFH	LB-MOLES/HR	LBS/HR
HYDROGEN	30.14	280.50	.78135	1.575
CARBON MONOXIDE	11.81	109.89	.30609	8.574
METHANE	8.81	81.99	.22837	3.664
CARBON DIOXIDE	24.95	232.22	.64685	28.469
ETHANE	.53	4.89	.01361	.409
HYDROGEN SULFIDE	.19	1.79	.00498	.170
NITROGEN	23.58	219.45	.61128	17.126
OXYGEN	0.00	0.00	0.00000	0.000

CHAR COMPOSITION

C = 93.50
H = 1.20
S = 0.00
O = 4.30
N = .50

PERCENT VOLATILE MATTER IN CHAR = 4.73

SPECIFIC GRAVITY OF TAR = 1.100 GM/CC

TAR COMPOSITION--COMPOSITE FOR ALL BALANCES (01 THROUGH 20 INCLUSIVE)

RUN 229

HYDROGEN 7.9
CARBON 83.7
OXYGEN 7.0
SULFUR .4

INPUT (LBS/HR) STEADY STATE VALUES

O2 = 10.21
CO2 = 0.00
COAL = 32.04
STEAM = 41.64
H2O(COAL) = 2.59
N2 (GASIFIER) = 10.28
N2 (WITH COAL) = 6.85

INLET TEMPERATURES

	FAHRENHEIT	CENTIGRADE	KELVIN
OXYGEN	700.00	371.11	644.11
COAL	100.00	37.78	310.78
STEAM	700.00	371.11	644.11
STEAM	100.00	37.78	310.78
CO2	0.00	-17.78	255.22

ZONE TEMPERATURES

	FAHRENHEIT	CENTIGRADE	KELVIN
LTR	773.60	412.00	685.00
HTR	1554.80	846.00	1119.00

RUN TIME = 8.67 HRS
TIME AT STEADY STATE = 7.50 HRS

TOTAL SYSTEM PRESSURE = 40.0 ATM

WATER IN CHAR = .60 PERCENT
WATER IN GASIFIER = .60 PERCENT
WATER IN FILTER = 1.10 PERCENT
BED DENSITY = 31.243 LBS/FT3

BED HEIGHT = 68.00 IN

PARTICLE SIZE DISTRIBUTION

MESH SIZE	10	20	50	100	140	200	325	****
MICRONS	2000	841	297	149	105	74	44	0
					PERCENT			
CHAR	0.0	5.6	30.6	19.4	11.1	11.1	11.1	
COAL	0.0	3.6	35.7	21.4	8.9	8.9	8.9	12.5

-----INPUT-----

	TOTAL WEIGHT IN GMS.	PRETREATER (GMS)	GASIFIER (GMS)
OXYGEN	38350.01	0.00	38350.01
AIR	0.00	0.00	0.00
COAL	126095.53	126095.53	0.00
STEAM	160121.08	0.00	160121.08
NITROGEN	88187.00	35274.80	52912.20
PRECHG	0.00	0.00	0.00
TOTAL	412753.62	161370.33	251383.29

BASIS - 1 HR. WEIGHT IN LBS.

	WEIGHT	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	ARRAY AIN
OXYGEN	9.74	0.00	9.74	0.00	0.00	0.00	0.00	
AIR	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
COAL	32.04	1.60	7.02	19.70	.32	.22	3.17	
STEAM	40.68	4.52	36.16	0.00	0.00	0.00	0.00	
NITROGEN	22.40	0.00	0.00	0.00	22.40	0.00	0.00	
PRECHG	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
TOTAL	****	6.12	52.92	19.70	22.72	.22	3.17	

BASIS - 1 HR. QUANTITY IN LB MOLES

	LB-MOLES	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	ARRAY BIN
OXYGEN	.3045	0.0000	.3045	0.0000	0.0000	0.0000	0.0000	
AIR	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
COAL	*****	.7945	.2192	1.6403	.0114	.0070	*****	
STEAM	2.2580	2.2398	1.1301	0.0000	0.0000	0.0000	0.0000	
NITROGEN	.7997	0.0000	0.0000	0.0000	.7997	0.0000	0.0000	
PRECHG	*****	0.0000	0.0000	0.0000	0.0000	0.0000	*****	
TOTAL	*****	3.0343	1.6538	1.6403	.8111	.0070	*****	

-----OUTPUT-----

RUN 229

WEIGHT IN GMS

	WEIGHT	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	ARRAY TOUT
CONDENSATE	124169.	13534.	108027.	1987.	0.	0.	0.	
EXTRACTOR	27013.	324.	1162.	16613.	135.	0.	8779.	
GASIFIER	0.	0.	0.	0.	0.	0.	0.	
FILTER	2077.	44.	114.	1572.	17.	4.	326.	
TAR	660.	46.	46.	548.	0.	18.	0.	
GAS	249128.	9724.	96034.	54562.	88187.	621.	0.	
TOTAL	403047.	23672.	205383.	75281.	88339.	643.	9105.	

BASIS - 1 HR, WEIGHT IN LBS

	WEIGHT	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	ARRAY AOUT
CONDENSATE	31.55	3.44	27.44	.50	0.00	0.00	0.00	
EXTRACTOR	6.86	.08	.30	4.22	.03	0.00	2.23	
GASIFIER	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
FILTER	.53	.01	.03	.40	.00	.00	.08	
TAR	.17	.01	.01	.14	0.00	.00	0.00	
GAS	63.29	2.47	24.40	13.86	22.40	.16	0.00	
TOTAL	****	6.01	52.18	19.13	22.44	.16	2.31	
PCT. RECOVERY	97.65	98.32	98.59	97.08	98.76	72.86	72.94	

BASIS - 1 HR, QUANTITY IN LB MOLES

	LB-MOLFS	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	ARRAY BOUT
CONDENSATE	*****	1.7056	.8576	.0420	0.0000	0.0000	0.0000	
EXTRACTOR	*****	.0408	.0092	.3514	.0012	0.0000	*****	
GASIFIER	*****	0.0000	0.0000	0.0000	0.0000	0.0000	*****	
FILTER	*****	.0055	.0009	.0333	.0002	.0000	*****	
TAR	*****	.0058	.0004	.0116	0.0000	.0001	0.0000	
GAS	*****	1.2254	.7624	1.1541	.7997	.0049	0.0000	
TOTAL	*****	2.9832	1.6306	1.5923	.8011	.0051	*****	

(10) STEADY STATE MASS BALANCE (PERIODS 3 THROUGH 18 INCLUSIVE)

RUN - 229

-----INPUT-----

WEIGHT IN GMS

	WEIGHT	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	MOISTURE	ARRAY..TSIN
OXYGEN	34779.	0.	34779.	0.	0.	0.	0.	0.	
AIR	0.	0.	0.	0.	0.	0.	0.	0.	
COAL	100244.	4473.	16034.	67084.	1091.	764.	10799.	0.	
STEAM	141784.	15738.	126046.	0.	0.	0.	0.	141784.	
NITROGEN	34988.	0.	0.	0.	34988.	0.	0.	0.	
PRETREAT GAS	32161.	981.	7855.	0.	23325.	0.	0.	8835.	
TOTAL	343955.	21192.	184713.	67084.	59404.	764.	10799.	150619.	

-----OUTPUT-----

WEIGHT IN GMS

	WEIGHT	HYDROGEN	OXYGEN	CARBON	NITROGEN	SULFUR	ASH	MOISTURE	ARRAY..TSOUT
CONDENSATE	109949.	11984.	95656.	1759.	0.	0.	0.	107599.	
EXTRACTOR	23368.	280.	1005.	14371.	117.	0.	7594.	140.	
GASIFIER	0.	0.	0.	0.	0.	0.	0.	0.	
FILTER	1797.	38.	99.	1360.	14.	4.	282.	20.	
TAR	571.	40.	40.	474.	0.	15.	0.	46.	
GAS	204253.	8795.	87183.	49418.	58313.	544.	0.	0.	
TOTAL	339937.	21138.	183982.	67383.	58444.	563.	7877.	107805.	

PERCENT								
RECOVERY	98.83	99.74	99.60	100.45	98.38	73.69	72.94	71.57

COMPUTED VALUES

RUN 229

PERCENT STEAM DECOMPOSITION = 30.20

PERCENT CARBON GASIFIED = 73.67

PERCENT CARBON CONVERTED = 77.00

CARBON INVENTORY = 9.483 LBS

COAL FEEDRATE ON MAF BASIS = 26.26870 LBS/HR

BED VOLUME = .494 FT³

BED AVERAGE (AVERAGE OF COAL ON MF BASIS AND STEADY STATE CHAR OUT) = 18.15 LBS/HR

STEADY STATE FRESH COAL FEED AVERAGE = 32.04 LBS/HR

PARTICLE DENSITY OF COAL = 1.379 GM/CM³PARTICLE DENSITY OF CHAR = .690 GM/CM³

AVERAGE PARTICLE DENSITY = 1.03440 GM/CC

CHAR BULK DENSITY = .400 GM/CM³COAL BULK DENSITY = .800 GM/CM³

SUPERFICIAL GAS VELOCITY = .32 FT/SEC

RESIDENCE TIME = 28.88 MIN

WEIGHT ARITHMETIC MEAN PARTICLE SIZE (CHAR) = 329.95 MICRONS

WEIGHT ARITHMETIC MEAN PARTICLE SIZE (COAL) = 329.26 MICRONS

GAS FLOW RATE = .0983 METERS PER SECOND OR .3224 FT/SEC

MINIMUM FLUIDIZATION VELOCITY = .0083 METERS PER SECOND OR .0274 FT/SEC

BED HEIGHT AT GAS FLOW RATE OF .0983 METERS PER SECOND = 68.00 INCHES

BED HEIGHT AT ZERO GAS FLOW RATE = 1.0806 METERS OR 42.54 INCHES

LARGEST PARTICLE ENTRAINED BY GAS FLOW OF .0983 M/SEC IS 60.06 MICRONS I.D.

WT PERCENT CHAR IN GASIFIER HAVING PARTICLES LESS THAN 60.06 MICRONS = 22.35

ORDINATE FOR FIG 3, CHAPTER 10, KUNII AND LEVENSPIEL = 30.64749 CM³/GM²

ABSCISSA FOR FIG 3, CHAPTER 10, KUNII AND LEVENSPIEL = .04153

CALCULATED ENTRAINMENT = 5.15089E-05 KG/SEC

OBSERVED ELUTRIATION = 6.65450E-05 KG/SEC

ORDINATE FOR FIG 12, CHAPTER 10, KUNII AND LEVENSPIEL = .0029504

ABSCISSA FOR FIG 12, CHAPTER 10, KUNII AND LEVENSPIEL = .291236

EQUILIBRIUM CONSTANTS FOR THE THREE BASIC REACTIONS ASSUMED TO OCCUR IN THE LOW-RATE GASIFICATION STAGE,

ZONE 2, HIGH-TEMPERATURE REGION - 1554.8 F 846.0 C 1119.0 K

H₂O + C = CO + H₂ 1.02966E-012H₂ + C = CH₄ 2.21645E-02H₂ + H₂O + 2C = CO + CH₄ 8.98348E-01

FINAL VALUES FOR NONLIN

I = 1 X(I) = .79386269667133E-01 F(I) = -.44406920985006E-15

SS = .19721522630525E-30 IT = 3 IERROR = 1

PRODUCTS INDEPENDENT OF PARAMETER VARIATION

RUN 229

PRODUCTS FORMED IN ZONE 1 (LTR)

CO	.27331	LB-MOLES/HR			
H2S	.00480	LB-MOLES/HR			
N2	.01006	LB-MOLES/HR			
H2O	.14080	LB-MOLES/HR			
C2H6	.01361	LB-MOLES/HR			
C ENTERING	1.64179	LB-MOLES/HR	.75000	LB C/LB COAL MAE	C IS TOTAL C IN COAL
C IN TAR	.01159	LB-MOLES/HR	.00530	LB C/LB COAL MAE	C IS DEVL C GOING TO TAR
C IN OXIDES	.27306	LB-MOLES/HR	.12485	LB C/LB COAL MAE	C IS DEVL C GOING TO CO

PRODUCTS FORMED IN ZONE 2 (HTR)

C OXIDES	.67963	LB-MOLES/HR			
CO	.36044	LB-MOLES/HR			
CO2	.31919	LB-MOLES/HR			
H2O	1.95289	LB-MOLES/HR			
C OUT	.67091	LB-MOLES/HR			
EFF EO K	.95362	---			

PRODUCTS FORMED IN ZONE 3

CO2	.31919	LB-MOLES/HR			
-----	--------	-------------	--	--	--

105

RATE CONSTANT FLKT 4.36198E-04 MIN-1
PRODUCTS DEPENDENT ON PARAMETER VARIATION

MEQ IS METHANE EQUIVALENT, I.E., CH₄, C₂H₆, ETC.

RUN 229

PRODUCTS FORMED IN ZONE 1 (LTR)

C-MEQ	.17436	LB-MOLES/HR	.07973	LB C/LB COAL MAF	C IS DEVOL C GOING TO MEQ
C-DEVOL	.45901	LB-MOLES/HR	.20988	LB C/LB COAL MAF	C IS TOTAL DEVOL C IN COAL
C-BASE	1.18128	LB-MOLES/HR	.54012	LB C/LB COAL MAF	C IS TOTAL BASE C IN COAL
CH ₄	.14717	LB-MOLES/HR			
H ₂	.26431	LB-MOLES/HR			
C OUT (TO ZONE 2)	1.18250	LB-MOLES/HR			

PRODUCTS FORMED IN ZONE 2 (HTR)

C IN	1.18250	LB-MOLES/HR
C USED	.51159	LB-MOLES/HR
CH ₄	.08121	LB-MOLES/HR
H ₂	.38558	LB-MOLES/HR

PARTIAL PRESSURE
BEFORE EQUILIBRIUM ADJUSTMENT

H ₂ O	22.53577	ATM	1.95289	LB-MOLES/HR
CO	4.15937	ATM	.36044	LB-MOLES/HR
H ₂	4.44953	ATM	.38558	LB-MOLES/HR
CO ₂	3.68341	ATM	.31919	LB-MOLES/HR
CH ₄	.93709	ATM	-.01257	LB-MOLES/HR
N ₂	4.23483	ATM	.61128	LB-MOLES/HR

PARTIAL PRESSURE
AFTER EQUILIBRIUM ADJUSTMENT

H ₂ O	20.36904	ATM	1.76512	LB-MOLES/HR
CO	1.99265	ATM	.17268	LB-MOLES/HR
H ₂	6.61625	ATM	.57335	LB-MOLES/HR
CO ₂	5.85013	ATM	.50696	LB-MOLES/HR

F0 VARIABLE X(1)	.31300			
AM-VARIABLE X(2)	.10630	LBS C IN MEQ/LB TOTAL C IN COAL		
CH ₄ RAPID-RATE	.09378	LB MOLES/HR		
CH ₄ LOW-RATE	-.01257	LB MOLES/HR		
XR FROM NONLIN	.07939	LBS C IN RAPID RATE MEQ/LB BASE C		
X-EXP	.37387	LBS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C		
CH ₄ HRC	.00234	LB-MOLES/HR		
CH ₄ DVC	.22603	LB-MOLES/HR		
DX/DT CAL	2.51805E-04	LBS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C/MIN		
DX/DT EXP	1.29460E-02	LBS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C/MIN		
DX/DT-MEQ CAL	6.84750E-05	LBS C IN LOW AND RAPID RATE MEQ/LB BASE C/MIN		
DX/DT-MEQ EXP	2.38038E-03	LBS C IN LOW AND RAPID RATE MEQ/LB BASE C/MIN		
DX/DT-CO CAL	1.83330E-04	LBS C IN LOW RATE CO/LB BASE C/MIN		
DX/DT-CO EXP	1.05656E-02	LBS C IN LOW RATE CO/LB BASE C/MIN		

ICONV= 3
ITER= 8
X=

.1822238393E+02 .1010326718E+00

SUM OF SQUARES OF FITS AT FINAL X = .34274720887756E-10

MEQ IS METHANE EQUIVALENT, I.E., CH₄, C₂H₆, ETC.

RUN 229

PRODUCTS FORMED IN ZONE 1 (LTR)

C-MEQ	.16572	LB-MOLES/HR	.07577	LB C/LB COAL MAF	C IS DEVOL C GOING TO MEQ
C-DEVOL	.45037	LB-MOLES/HR	.20593	LB C/LB COAL MAF	C IS TOTAL DEVOL C IN COAL
C-BASE	1.18992	LB-MOLES/HR	.54407	LB C/LB COAL MAF	C IS TOTAL BASE C IN COAL
CH ₄	.13853	LB-MOLES/HR			
H ₂	.28159	LB-MOLES/HR			
C OUT (TO ZONE 2)	1.19114	LB-MOLES/HR			

PRODUCTS FORMED IN ZONE 2 (HTR)

C IN	1.19114	LB-MOLES/HR
C USED	.52023	LB-MOLES/HR
CH ₄	.08985	LB-MOLES/HR
H ₂	.36968	LB-MOLES/HR

PARTIAL PRESSURE
BEFORE EQUILIBRIUM ADJUSTMENT

H ₂ O	22.58312	ATM	1.95289	LB-MOLES/HR
CO	4.16811	ATM	.36044	LB-MOLES/HR
H ₂	4.27492	ATM	.36968	LB-MOLES/HR
CO ₂	3.69115	ATM	.31919	LB-MOLES/HR
CH ₄	1.03897	ATM	.00462	LB-MOLES/HR
N ₂	4.24373	ATM	.61128	LB-MOLES/HR

PARTIAL PRESSURE
AFTER EQUILIBRIUM ADJUSTMENT

H ₂ O	20.37982	ATM	1.76235	LB-MOLES/HR
CO	1.96481	ATM	.16991	LB-MOLES/HR
H ₂	6.47822	ATM	.56021	LB-MOLES/HR
CO ₂	5.89445	ATM	.50973	LB-MOLES/HR

F0 VARIABLE X(1) 18.22238

AM-VARIABLE X(2) .10103

CH₄ RAPID-RATE .09446

CH₄ LOW-RATE -.00462

XR FROM NONLIN .07939

X-EXP .37842

CH₄HRC .09014

CH₄DVC .13823

DX/DT CAL 1.31039E-02

DX/DT EXP 1.31034E-02

DX/DT-MEQ CAL 2.62083E-03

DX/DT-MEQ EXP 2.61452E-03

DX/DT-CO CAL 1.04A30E-02

DX/DT-CO EXP 1.04889E-02

LHS C IN MEQ/LB TOTAL C IN COAL

LB MOLES/HR

LB MOLES/HR

LHS C IN RAPID RATE MEQ/LB BASE C

LHS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C

LB-MOLES/HR

LB-MOLES/HR

LHS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C/MIN

LHS C IN LOW AND RAPID RATE MEQ AND IN LOW RATE CO/LB BASE C/MIN

LHS C IN LOW AND RAPID RATE MEQ/LB BASE C/MIN

LHS C IN LOW AND RAPID RATE MEQ/LB BASE C/MIN

LHS C IN LOW RATE CO/LB BASE C/MIN

LHS C IN LOW RATE CO/LB BASE C/MIN

MATERIALS IN
LB-MOLES/HR

MATERIAL BALANCE (ASH ASSUMED CONSTANT AND NOT INCLUDED BELOW)

RUN 229

MATERIALS OUT
LB-MOLES/HR

	C	H2	O2	N2	S			C	H2	O2	N2	S	
COAL	1.640	.795	.219	.011	.007	*****	ZONE 1	CHAR	1.190	.017	.012	.001	.002
GAS	.769	2.295	1.476	.612	0.000	*	DEVOLATILIZATION	GAS	1.219	3.071	1.683	.622	.005
TAR	0.000	0.000	0.000	0.000	0.000	*	2H2 + C = CH4	TAR	.001	.003	.000	.000	.000
SUM	2.409	3.089	1.695	.623	.007	*	3H2 + 2C = C2H6	SUM	2.410	3.090	1.695	.623	.007

H2 + S = H2S
C + O = CO
N2 + 2H3 = 2NH3
C+H+O+N+S = TAR
MOISTURE = STEAM

	C	H2	O2	N2	S			C	H2	O2	N2	S	
CHAR	1.190	.017	.012	.001	.002	*****	ZONE 2A	CHAR	1.096	.017	.012	.001	.002
GAS	.674	2.295	1.476	.367	0.000	*	RAPID-RATE GASIFICATION	GAS	.769	2.295	1.476	.367	0.000
SUM	1.864	2.312	1.488	.368	.002	*	2H2 + C = CH4	SUM	1.864	2.312	1.488	.368	.002

REC V 100.000 100.000 100.000 100.000 100.000

	C	H2	O2	N2	S			C	H2	O2	N2	S	
CHAR	1.096	.017	.012	.001	.002	*****	ZONE 2B	CHAR	.740	.017	.012	.001	.002
GAS	.319	2.295	1.476	.367	0.000	*	LOW-RATE GASIFICATION	GAS	.674	2.295	1.476	.367	0.000
SUM	1.415	2.312	1.488	.368	.002	*	H2O + C = CO + H2	SUM	1.415	2.312	1.488	.368	.002

2H2 + C = CH4
H2 + H2O + 2C = CO + CH4

REC V 100.000 100.000 100.000 100.000 100.000

	C	H2	O2	N2	S			C	H2	O2	N2	S	
CHAR	.740	.017	.012	.001	.002	*****	ZONE 3	CHAR	.421	.017	.012	.001	.002
GAS	0.000	2.295	1.434	.367	0.000	*	COMBUSTION	GAS	.319	2.295	1.476	.367	0.000
SUM	.740	2.312	1.446	.368	.002	*	C + O2 = CO2	SUM	.740	2.312	1.488	.368	.002

REC V 100.000 100.000 97.217 100.000 100.000

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CALCULATIONS FOR TEMPERATURE = 1632.7 K

2478.8 F

HEAT LOSS = 0.0 BTU/HR

ENTHALPY CHANGE FOR COOLING REACTANTS FROM TEMPERATURE T TO 298 DEGREES KELVIN

	BTU/HR
CARBON DIOXIDE	0.
STEAM2	0.
NITROGEN	-5.828E+01
STEAM3	0.
OXYGEN	-1.470E+03
MOISTURE IN COAL	0.
COAL	-1.199E+04
STEAM	-1.211E+04
METHANE	0.
HYDROGEN	0.
CARBON MONOXIDE	0.
TOTAL	-2.563E+04

ENTHALPY CHANGE FOR REACTION PROCEEDING ISOTHERMALLY AT 298 DEGREES K

	BTU/HR
AMMONIA	0.
CHAR FORMATION	-3.45 E+02
COAL DECOMPOSITION	1.064E+03
HYDROGEN FORMATION	0.
CARBON MONOXIDE **	0.
METHANE **	0.
CARBON DIOXIDE **	-5.404E+04
ETHANE **	0.
HYDROGEN SULFIDE **	0.
TAR **	0.
STEAM DECOMPOSITION	0.
TOTAL	-5.545E+04

ENTHALPY CHANGE FOR HEATING PRODUCTS FROM 298 DEGREES KELVIN TO TEMPERATURE T

	BTU/HR
AMMONIA	0.
OXYGEN	0.
HYDROGEN	0.
NITROGEN	6.815E+03
CARBON MONOXIDE	0.
METHANE	0.
CARBON DIOXIDE	9.528E+03
ETHANE	0.
HYDROGEN SULFIDE	0.
CHAR	1.038E+04
STEAM	5.435E+04
TAR	0.
TOTAL	8.107E+04

ADDITIONAL HEAT REQUIREMENTS OF SYSTEM 0. BTU/HR

STANDARD HEAT OF REACTION = -1.728E+00 BTU/HR

HEATING VALUE OF COAL CALCULATED FROM DULONG FORMULA 10233.4 BTU/LB (AS REC. OR MF. DEPENDING ON INPUT COAL)

HEATING VALUE OF CHAR CALCULATED FROM DULONG FORMULA 8346.6 BTU/LB-MF

HEATING VALUE OF TAR FROM DULONG FORMULA 16545.2 BTU/LB

ENERGY BALANCE FOR ZONE 2

RUN 229

ENTHALPY CHANGE FOR COOLING REACTANTS FROM TEMPERATURE T TO 298 DEGREES KELVIN

	BTU/HR
CARBON DIOXIDE	-9.526E+03
STEAM2	0.
NITROGEN	-6.813E+03
STEAM3	0.
OXYGEN	0.
MOISTURE IN COAL	0.
COAL	-1.714E+04
STEAM	-5.434E+04
METHANE	0.
HYDROGEN	0.
CARBON MONOXIDE	0.
TOTAL	-8.781E+04

ENTHALPY CHANGE FOR REACTION PROCEEDING ISOTHERMALLY AT 298 DEGREES K

	BTU/HR
AMMONIA	0.
CHAR FORMATION	1.371E+03
COAL DECOMPOSITION	-3.467E+03
HYDROGEN FORMATION	0.
CARBON MONOXIDE **	-8.079E+03
METHANE	-2.893E+03
CARBON DIOXIDE **	-3.226E+04
ETHANE	0.
HYDROGEN SULFIDE **	0.
TAR **	0.
STEAM DECOMPOSITION	5.732E+04
TOTAL	1.200E+04

ENTHALPY CHANGE FOR HEATING PRODUCTS FROM 298 DEGREES KELVIN TO TEMPERATURE T

	BTU/HR
AMMONIA	0.
OXYGEN	0.
HYDROGEN	3.897E+03
NITROGEN	4.018E+03
CARBON MONOXIDE	1.881E+03
METHANE	1.828E+03
CARBON DIOXIDE	8.741E+03
ETHANE	0.
HYDROGEN SULFIDE	0.
CHAR	7.039E+03
STEAM	2.355E+04
TAR	0.
TOTAL	5.095E+04

ADDITIONAL HEAT REQUIREMENTS OF SYSTEM 0. BTU/HR

STANDARD HEAT OF REACTION = -2.486E+04 BTU/HR

HEATING VALUE OF COAL CALCULATED FROM DULONG FORMULA 11528.5 BTU/LB (AS REC. OR MF DEPENDING ON INPUT COAL)

HEATING VALUE OF CHAR CALCULATED FROM DULONG FORMULA 10233.4 BTU/LB-MF

HEATING VALUE OF TAR FROM DULONG FORMULA 16545.2 BTU/LB

ENTHALPY CHANGE FOR COOLING REACTANTS FROM TEMPERATURE T TO 298 DEGREES KELVIN

	BTU/HR
CARBON DIOXIDE	-8.741E+03
STEAM2	0.
NITROGEN	-6.697E+03
STEAM3	0.
OXYGEN	0.
MOISTURE IN COAL	-5.968E+01
COAL	-2.771E+02
STEAM	-2.355E+04
METHANE	-1.828E+03
HYDROGEN	-3.897E+03
CARBON MONOXIDE	-1.881E+03
TOTAL	-4.693E+04

ENTHALPY CHANGE FOR REACTION PROCEEDING ISOTHERMALLY AT 298 DEGREES K

	BTU/HR
AMMONIA	-3.995E+02
CHAR FORMATION	3.791E+03
COAL DECOMPOSITION	2.639E+04
HYDROGEN FORMATION	0.
CARBON MONOXIDE **	-7.006E+03
METHANE **	-4.461E+03
CARBON DIOXIDE **	-2.132E+04
ETHANE **	-4.958E+02
HYDROGEN SULFIDE **	-4.859E+01
TAR **	-1.192E+01
STEAM DECOMPOSITION	1.345E+04
TOTAL	9.887E+03

ENTHALPY CHANGE FOR HEATING PRODUCTS FROM 298 DEGREES KELVIN TO TEMPERATURE T

	BTU/HR
AMMONIA	4.021E+02
OXYGEN	0.
HYDROGEN	3.782E+03
NITROGEN	3.041E+03
CARBON MONOXIDE	1.589E+03
METHANE	1.775E+03
CARBON DIOXIDE	4.616E+03
ETHANE	1.727E+02
HYDROGEN SULFIDE	3.502E+01
CHAR	1.006E+04
STEAM	1.047E+04
TAR	4.673E+01
TOTAL	3.599E+04

ADDITIONAL HEAT REQUIREMENTS OF SYSTEM 2.72198E+03 BTU/HR

STANDARD HEAT OF REACTION = 1.671E+03 BTU/HR

HEATING VALUE OF COAL CALCULATED FROM DULONG FORMULA 10376.6 BTU/LB (AS REC. OR MF. DEPENDING ON INPUT COAL)

HEATING VALUE OF CHAR CALCULATED FROM DULONG FORMULA 11528.5 BTU/LB-MF

HEATING VALUE OF TAR FROM DULONG FORMULA 16545.2 BTU/LB

PRODUCTS FORMED IN ZONE LB-MOLES/HR			TOTAL PRODUCTS IN ZONE LB-MOLES/HR			REACTOR DESIGN CONFIGURATION			PRODUCTS EXITING ZONE AFTER WATER-GAS SHIFT LB-MOLES/HR			RUN 229		
			ATM			COAL (+ASH) = * 32.04 LBS/HR * (AS REC) * N2 = 6.85 *** T = 100. F * *****								
BEFORE WATER-GAS SHIFT IN ZONE 1						T = 774. F *****								
H2O	=	.1408	1.9032	17.35		ZONE 1			H2O	=	1.7556	16.20	SHFT ADJ	
CO	=	.2733	.4432	4.04		DEVOLATILIZATION			CO	=	.3061	2.89	1.7772	
H2	=	.2816	.6529	5.95		2H2 + C = CH4			H2	=	.7813	7.10	.3173	
CO2	=	0.0000	.5097	4.65		3H2 + 2C = C2H6			CO2	=	.6469	5.80	.778A	
CH4	=	.1385	.2284	2.08		H2 + S = H2S			CH4	=	.2284	2.08	.6357	
C2H6	=	.0136	.0136	.12		C + O = CO			C2H6	=	.0136	.12	SHFT TEMP =	
N2	=	.2447	.6116	5.58		N2 + 2H3 = 2NH3			N2	=	.6116	5.58	1555. F	
NH3	=	.0201	.0201	.18		C+H+O+N+S = TAR			NH3	=	.0201	.18	K = .95	
H2S	=	.0048	.0048	.04		MOISTURE = STEAM			H2S	=	.0048	.04		
TAR	=	.0001	.0001	.00					TAR	=	.0001	.00		

CHAR (+ASH) = * 17.98 LBS/HR * *****														
*HEAT LOSS = -1571. BTU/HR														

AFTER WATER-GAS SHIFT IN ZONE 2B														
T = 1555. F * *****														
ZONE 2A														
H2O	=	0.0000	1.7624	20.38		RAPID-RATE GASIFICATION			H2O	=	1.7624	20.38		
CO	=	0.0000	.1699	1.96		2H2 + C = CH4			CO	=	.1699	1.96		
H2	=	0.0000	.5602	6.48					H2	=	.3713	6.48		
CO2	=	0.0000	.5097	5.89					CO2	=	.5097	5.89		
CH4	=	.0945	.0898	1.04					CH4	=	.0898	1.04		
N2	=	0.0000	.3670	4.24					N2	=	.3670	4.24		

CHAR (+ASH) = * 16.85 LBS/HR * *****														
HEAT LOSS = 24863. BTU/HR														

BEFORE WATER-GAS SHIFT IN ZONE 2B														

ZONE 2B														
H2O	=	0.0000	1.9529	22.58		LOW-RATE GASIFICATION			H2O	=	1.7624	20.38		
CO	=	.3604	.3604	4.17		H2O + C = CO + H2			CO	=	.1699	1.96		
H2	=	.3697	.3697	4.27		2H2 + C = CH4			H2	=	.5602	6.48		
CO2	=	0.0000	.3192	3.69		H2 + H2O + 2C = CO + CH4			CO2	=	.5097	5.89		
CH4	=	-.0046	-.0046	1.04					CH4	=	-.0046	1.04		
N2	=	0.0000	.3670	4.24					N2	=	.3670	4.24		

SHFT ADJ														
TEMP = 1554.8 F														
K = .9536														

CHAR (+ASH) = * 12.58 LBS/HR * *****														
T = 1555. F * *****														
T = 2479. F														

ZONE 3														
CO2	=	.3192	.3192	4.08		COMBUSTION			CO2	=	.3192	4.08		
N2	=	0.0000	.3670	4.92		C + O2 = CO2			N2	=	.3670	4.92		

*HEAT LOSS = 0. BTU/HR														

T = 2479. F * *****														
CHAR (+ASH) = * 6.86 LBS/HR * 6.15 LBS/HR***														
O2 = 10.21 LBS/HR														
H2O = 41.64 LBS/HR														
N2 = 10.28 LBS/HR														

EXP														
(ASSUMING .30 ASH LOSS)														
T = 700. F														
T = 700. F														
T = 100. F														

WATER-GAS SHIFT K CALCULATION BASED ON TEMPERATURE OF ZONE 2

CHAR COMPOSITION (ASH-FREE BASIS) EXITING ZONE -- CALCULATED

RUN 229

ZONE	C	H	S	O	N
1	96.50	.23	.47	2.55	.25
2	94.49	.36	.74	4.02	.39
3	90.70	.60	1.25	6.78	.66

ZONE 1 PRODUCT EVOLUTION ESTIMATES

FRACTION OF FIXED MATTER THAT IS BASE CARBON = .945
 FRACTION OF MEQ EVOLVED AS CH₄ = .836
 FRACTION OF MEQ EVOLVED AS C₂H₆ = .164
 FRACTION OF CDV EQUIVALENT TO H₂ DEVOLATIZED = .105
 FRACTION OF S EVOLVED AS H₂S = .712

INPUT DATA FOR PREDICTIVE MODE

MONTANA ROSEBUD	RUN-40CHPM-2	PREDICTIVE MODEL	
8.100	34.800	47.200	9.900 4.730 229.1
5.00	61.50	1.00	21.90 .70 229.2
7.90	83.70	7.00	.40 1.00 1.10 229.3
10.21	0.00	32.04	41.64 10.28 6.85 0.00 0.00 229.4
100.	700.	700.	0. 100. 1555. 229.5
93.5	1.2	0.0	4.3 .5 229.6
3.6	35.7	21.4	8.9 8.9 8.9 12.5 229.7
.400	.333	68.0	40. .005298 .703 229.8
72.69	1555.	5.472	21.954 .07931 229.9
-1671.	24863.		
.1010	1.2500	18.2224	

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APPENDIX IV

SAMPLE COMPUTER PRINTOUT OF
REACTOR MODEL FROM THE
PREDICTIVE CODE FOR
MONTANA ROSEBUD RUN NO. 229

APPENDIX V

**DEFINITIONS OF SYMBOLS USED IN
SUMMARY TABLES GIVEN IN
APPENDIX VI and VII**

Definitions of Symbols* Used in Summary Tables
Given in Appendices VI and VII

- EQ SHFT - Suffix for products calculated assuming water-gas shift equilibrium
- CHAR EXP - In analytical code, experimental value of effluent char (lbs/hr); in predictive code, calculated from variable X(1)
- CHAR ASH LOSS - Calculated value of effluent char with correction for ash loss as estimated from material balance.
- CHAR NO ASH LOSS - Calculated value of effluent char without any correction for ash loss
- LTR TEMP - Temperature ($^{\circ}\text{F}$) for low temperature region - zone 1
- HTR TEMP - Temperature ($^{\circ}\text{F}$) for high temperature region - zone 2
- CTR TEMP - Temperature ($^{\circ}\text{F}$) for combustion region - zone 3
- FR FM CB - Fraction of fixed matter that is base carbon
- FR CH_4 - Fraction of paraffinic carbon evolved as CH_4 in zone 1
- FR C_2H_6 - Fraction of paraffinic carbon evolved as C_2H_6 in zone 1
- FR H_2 - Fraction of H_2 evolved in zone 1
- FR H_2S - Fraction of sulfur evolved as H_2S in zone 1
- X1 - Initial estimate of variable for percent coal conversion
- X2 - Initial estimate of variable for temperature of zone 2
- X3 - Initial estimate of variable for percent of total carbon in coal converted to low and rapid rate CH_4
- X4 - Initial estimate of variable for percent of total carbon in coal converted to CO in zone 2
- X5 - Initial estimate of variable for fractional base carbon conversion to rapid rate CH_4
- X(1) - X(5) - Convergence values for above variables in predictive code
- FO - Reactivity parameter dependent on type of coal; a variable in the analytical code and a constant in the predictive code
- AM - Fraction of devolatilized carbon evolved as CH_4 ; a variable in the analytical code and a constant in the predictive code.
- SHF K - Water-gas shift equilibrium constant
- SHF TEMP F - Temperature ($^{\circ}\text{F}$) for which SHF K is evaluated

COAL BULK DN - Coal bulk density in gm/cc

PR DN COAL - Particle density for coal in gm/cc

COAL DM MICRONS - Average coal particle diameter in microns

SUPGASVEL FT/SC - Superficial gas velocity in ft/sec.

SLMPD BEDHT IN - Slumped bed height in inches

BED AVG LBS/HR - Average of coal and char flowrates in lbs/hr.

BED DN LBS/FT³ - Bed density in lbs/ft³

H COAL BTU/LB - Heating value of coal in Btu/lb on MAF basis.

* Symbols not defined can be deduced from those given here.

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APPENDIX VI

SUMMARY TABLE OF SELECT VARIABLES FOR RUNS PROCESSED IN THE ANALYTICAL COMPUTER CODE

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SUMMARY LIST FOR RUNS PROCESSED

RUN NO.	203	204	205	218	219	220	221
H2O - EQ SHFT	1.524	1.512	1.532	1.856	1.357	1.698	1.538
CO - EQ SHFT	.239	.228	.271	.222	.530	.481	.459
H2 - EQ SHFT	.656	.633	.664	.700	.989	1.061	.866
CO2 - EQ SHFT	.478	.456	.506	.568	.574	.631	.654
H2O	1.668	1.553	1.540	1.872	1.627	1.732	1.506
CO	.218	.211	.266	.208	.419	.416	.449
H2	.580	.559	.619	.609	.823	.843	.840
CO2	.499	.473	.511	.582	.685	.696	.643
CH4	.188	.150	.199	.278	.296	.296	.274
C2H6	.013	.012	.018	.028	.016	.026	.022
N2	.928	1.009	.933	.743	.609	.682	.543
NH3	.015	.015	.020	.018	.024	.022	.020
H2S	.002	.003	.003	.006	.008	.007	.007
TAR	.001	.001	.001	.001	.000	.001	.000
CHAR EXP	4.000	3.000	4.400	15.806	11.158	10.059	6.973
CHAR ASH LOSS	3.671	3.808	4.578	14.551	9.104	9.938	8.232
CHAR NO ASH LOS	5.195	5.095	7.669	19.678	15.065	13.884	11.096
LTR TEMP	779.	833.	784.	653.	682.	698.	721.
HTR TEMP	1569.	1589.	1589.	1495.	1584.	1584.	1598.
CTR TEMP	1842.	2157.	2272.	2055.	2312.	2112.	2747.
HEAT LOSS Z1	4607.	3368.	1004.	-7792.	-10057.	-6112.	-4691.
HEAT LOSS Z2	106.	8526.	11306.	19602.	11821.	8797.	29132.
FR FM CB	.850	.885	.929	.920	1.009	.959	.949
FR CH4	.815	.782	.772	.791	.835	.760	.798
FR C2H6	.185	.218	.228	.209	.166	.240	.202
FR H2	.061	.089	.066	.063	.135	.115	.101
FR H2S	.433	.730	.376	.798	.532	.604	1.121
X1	78.352	77.315	73.565	57.068	64.990	67.678	71.148
X2	1569.	1589.	1589.	1495.	1584.	1584.	1598.
X3	6.202	5.477	5.309	2.662	6.222	5.933	4.967
X4	27.845	25.747	23.461	8.582	23.568	22.989	21.039
X5	.063	.063	.067	.062	.081	.079	.086
F0	33.422	13.391	19.076	21.795	72.359	42.238	38.306
AM	.110	.095	.107	.114	.086	.095	.108
COAL FD LBS/HR	24.000	22.460	29.010	45.834	43.031	42.955	38.457
STEAM FD	37.259	35.572	36.218	40.066	36.410	43.958	38.232
O2 FD	5.430	6.155	7.059	7.075	8.170	7.823	11.412
N2 FD WITH COAL	12.428	22.960	21.300	8.320	6.817	7.633	7.278
N2 FD BOTTOM	13.558	5.278	4.823	12.480	10.225	11.449	7.939
SHF K	.928	.895	.895	1.070	.904	.904	.881
SHF TEMP F	1569.200	1589.000	1589.000	1495.400	1583.600	1583.600	1598.000
O/O CARB GASFD	75.017	73.886	68.984	47.326	64.965	64.998	70.933
O/O CARB CONV	85.755	83.271	79.664	53.531	67.256	69.317	74.027
COAL BULK DN	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CHAR BULK DN	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PR DN COAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PR DN CHAR	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AVG PR DN GM/CC	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL DM MICRONS	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CHAR DM MICRONS	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SUPGASVEL FT/SC	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MINFLUVEL FT/SC	0.000	0.000	0.000	0.000	0.000	0.000	0.000
BED VOL FT3	.486	.456	.478	.450	.496	.518	.508
FLUID BEDHT IN	66.960	62.800	65.920	62.000	68.400	71.440	70.000
SLMPD BEDHT IN	0.000	0.000	0.000	0.000	0.000	0.300	0.000
BED AVG LBS/HR	12.956	11.790	15.284	29.079	25.503	25.025	21.465
RED DN LBS/FT3	19.000	19.000	19.010	19.000	19.000	19.000	11.565
RES TIME MIN	23.084	23.134	18.811	11.192	13.152	13.760	9.167
H COAL BTU/LB	10472.	10484.	10371.	10590.	10517.	10753.	10761.
H CHAR BTU/LB	7145.	7586.	7509.	10520.	9050.	9272.	8953.
H TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.

RUN NO.	229	231	238	246	248	249	250
H2O - EQ SHFT	1.777	1.815	1.393	1.433	1.230	1.782	1.519
CO - EQ SHFT	.317	.345	.313	.384	.479	.504	.372
H2 - EQ SHFT	.779	.822	.798	.778	.814	1.155	.851
CO2 - EQ SHFT	.636	.699	.487	.582	.566	.589	.600
H2O	1.756	1.721	1.446	1.318	1.214	1.635	1.393
CO	.305	.319	.257	.330	.363	.419	.329
H2	.781	.780	.699	.752	.829	.818	.774
CO2	.647	.725	.562	.635	.682	.673	.643
CH4	.229	.267	.174	.263	.256	.248	.228
C2H6	.014	.018	.019	.027	.022	.024	.023
N2	.612	.527	.669	.622	.581	.596	.638
NH3	.020	.026	.015	.022	.022	.021	.016
H2S	.005	.006	.004	.005	.006	.005	.005
TAR	.000	.000	.001	.000	.000	.000	.000
CHAR EXP	6.863	9.740	4.671	9.786	9.736	7.073	6.312
CHAR ASH LOSS	6.154	8.596	4.408	13.383	9.479	9.105	6.712
CHAR NO ASH LOS	8.751	12.370	5.646	9.955	10.108	9.716	7.668
LTR TEMP	.774	.770	.853	.716	.781	.786	.822
HTR TEMP	1555.	1524.	1580.	1573.	1587.	1623.	1569.
CTR TEMP	2479.	2598.	2430.	2776.	3126.	2439.	2299.
HEAT LOSS Z1	-1673.	-8708.	4230.	-6062.	-11380.	-6363.	-9356.
HEAT LOSS Z2	24865.	32190.	14419.	30797.	36196.	18938.	17740.
FR FM CB	.945	.912	1.199	.876	.927	.990	.815
FR CH4	.836	.823	.645	.777	.801	.756	.769
FR C2H6	.164	.178	.356	.224	.200	.244	.232
FR H2	.105	.098	.209	.107	.137	.194	.094
FR H2S	.712	.611	.853	1.003	.926	.924	.762
X1	72.684	68.706	78.046	72.261	72.495	73.936	75.754
X2	1555.	1524.	1580.	1573.	1587.	1623.	1569.
X3	5.475	4.926	8.002	3.983	4.335	5.282	4.642
X4	21.954	17.108	34.140	16.294	18.116	24.655	19.722
X5	.079	.079	.080	.084	.092	.082	.080
FO	18.233	50.239	41.022	10.872	18.606	10.848	12.307
AM	.101	.100	.081	.134	.117	.102	.123
COAL FD LBS/HR	32.035	39.527	25.716	35.889	36.751	37.277	31.626
STEAM FD	41.640	2.043	35.189	32.869	28.713	42.438	38.618
O2 FD	10.214	11.541	8.467	10.653	12.181	9.744	8.111
N2 FD WITH COAL	6.850	5.897	7.489	6.968	6.512	6.676	7.146
N2 FD BOTTOM	10.275	8.846	11.233	10.452	9.768	10.014	10.719
SHF K	.954	1.011	.910	.922	.898	.842	.928
SHF TEMP F	1554.800	1524.200	1580.000	1572.800	1587.200	1623.200	1569.200
O/O CARB GASFD	73.667	66.528	78.204	70.209	71.954	72.916	77.159
O/O CARB CONV	76.995	70.516	85.417	72.619	73.974	75.449	79.556
COAL BULK DN	.800	.800	.780	.795	.796	.775	.789
CHAR BULK DN	.400	.400	.455	.509	.491	.468	.275
PR DN COAL	1.379	1.379	1.345	1.371	1.372	1.336	1.360
PR DN CHAR	.690	.690	.784	.878	.846	.807	.474
AVG PR DN GM/CC	1.034	1.034	1.065	1.124	1.109	1.071	.917
COAL DM MICRONS	329.263	329.263	437.772	355.016	286.886	389.527	342.649
CHAR DM MICRONS	329.947	329.947	230.386	255.564	231.764	314.019	437.544
SUPGASVEL FT/SC	.322	.322	.285	.275	.254	.336	.301
MINFLUVEL FT/SC	.027	.027	.015	.022	.017	.030	.031
BED VOL FT3	.494	.487	.500	.503	.450	.467	.482
FLUID BEDHT IN	68.000	67.120	68.880	69.360	62.000	64.320	66.480
SLMPD BEDHT IN	42.542	42.542	44.385	45.599	41.576	39.739	42.810
BED AVG LBS/HR	18.151	23.072	14.229	21.420	21.796	20.548	18.605
BED DN LBS/FT3	31.243	19.000	31.376	32.626	33.321	29.890	31.717
RES TIME MIN	28.879	14.050	36.596	27.458	24.479	22.459	29.033
H COAL BTU/LB	10377.	10404.	12349.	10905.	10945.	11257.	10293.
H CHAR BTU/LB	8347.	9089.	7217.	9673.	9159.	9155.	8329.
H TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.
PRESSURE ATU	40.000	40.000	40.000	40.000	40.000	40.000	40.000

RUN NO.	251	252	253	254	255	256	257
M20 - EQ SHFT	1.620	1.837	1.806	1.583	1.666	1.808	.827
CO - EQ SHFT	.294	.314	.291	.351	.322	.334	.247
M2 -EQ SHFT	.769	.872	.734	.916	.792	.888	.444
CO2 -EQ SHFT	.535	.559	.606	.525	.569	.582	.355
M20	1.983	1.637	1.575	1.702	1.656	1.683	.862
CO	.239	.262	.275	.261	.249	.284	.242
M2	.681	.695	.691	.684	.662	.684	.482
CO2	.590	.612	.622	.615	.642	.632	.361
CH4	.171	.222	.199	.198	.200	.216	.100
C2H6	.020	.022	.021	.019	.020	.021	.010
N2	.601	.567	.432	.425	.411	.415	.351
NH3	.016	.021	.019	.025	.018	.020	.010
H2S	.004	.004	.004	.005	.004	.004	.003
TAR	.000	.000	.000	.000	.000	.000	.000
CHAR EXP	4.638	7.400	5.700	5.300	5.682	6.667	3.633
CHAR ASH LOSS	3.726	11.189	7.966	9.085	8.230	8.732	3.895
CHAR NO ASH LOS	7.100	11.716	9.293	10.784	8.731	9.271	4.531
LTR TEMP	820.	797.	828.	802.	835.	820.	698.
HTR TEMP	1567.	1569.	1575.	1584.	1576.	1564.	1575.
CTR TEMP	2216.	2465.	2472.	2290.	2354.	2501.	2686.
HEAT LOSS Z1	50.	-7321.	-6621.	-1855.	-6291.	-7156.	-3925.
HEAT LOSS Z2	12445.	27541.	24492.	10998.	18066.	24734.	14538.
FR FM C8	1.057	1.106	.931	1.208	1.020	.923	.793
FR CH4	.664	.778	.758	.692	.736	.767	.767
FR C2H6	.336	.222	.243	.308	.264	.233	.233
FR H2	.139	.153	.092	.255	.115	.158	.084
FR H2S	.744	.619	.673	.142	.732	.715	1.011
X1	73.129	67.025	71.166	63.842	71.578	71.874	76.422
X2	1567.	1569.	1575.	1584.	1576.	1564.	1575.
X3	6.662	3.666	4.221	6.756	5.395	4.735	3.257
X4	27.782	15.228	18.067	27.111	22.198	15.319	22.411
X5	.070	.076	.080	.077	.076	.077	.045
F0	19.713	4.978	6.683	18.932	11.628	10.526	12.989
AM	.084	.110	.104	.075	.095	.106	.096
COAL FD LBS/HR	26.422	35.531	32.228	29.826	30.827	32.962	19.217
STEAM FD	39.341	39.792	40.833	40.000	39.583	40.546	20.439
O2 FD	7.648	9.457	9.565	8.587	8.261	9.748	5.959
N2 FD WITH COAL	6.734	6.354	4.842	4.762	4.604	4.650	3.929
N2 FD BOTTOM	10.101	9.531	7.263	7.143	6.906	6.975	5.894
SHF K	.932	.928	.919	.904	.916	.938	.919
SHF TEMP F	1567.400	1569.200	1574.600	1583.600	1576.400	1563.800	1574.600
O/O CARB GASFD	74.531	62.799	69.128	67.090	70.069	70.001	76.985
O/O CARB CONV	78.564	65.564	72.500	69.873	72.822	72.909	82.786
COAL BULK DN	.786	.908	.786	.769	.782	.803	.772
CHAR BULK DN	.634	.431	.422	.380	.458	.429	.543
PR DN COAL	1.355	1.565	1.355	1.326	1.348	1.384	1.331
PR DN CHAR	1.093	.743	.728	.655	.790	.740	.936
AVG PR DN GM/CC	1.224	1.154	1.041	.990	1.069	1.062	1.134
COAL DM MICRONS	393.992	307.002	273.667	182.391	400.154	321.660	298.163
CHAR DM MICRONS	388.474	240.118	260.698	235.731	190.033	237.866	367.001
SUPGASVEL FT/SC	.301	.308	.307	.299	.294	.303	.333
MINFLUVEL FT/SC	.063	.016	.018	.013	.011	.015	.048
BED VOL FT3	.467	.493	.476	.480	.490	.492	.480
FLUID BEDHT IN	64.400	67.920	65.520	66.160	67.520	67.840	66.160
SLMPD BEDHT IN	43.133	42.623	41.293	41.818	42.828	42.810	41.882
BED AVG LBS/HR	14.447	19.952	17.659	16.937	16.991	18.387	10.768
BED DN LRS/FT3	32.863	35.570	30.923	30.342	30.964	31.632	30.507
RES TIME MIN	34.880	29.609	27.376	29.309	29.533	28.350	45.737
H COAL BTU/LB	10777.	10991.	10196.	12046.	10514.	10898.	9463.
H CHAR BTU/LB	8710.	9945.	9142.	8861.	9481.	9262.	6315.
H TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.

RUN NO.	281	290	291	292	306	307	310
H2O - EQ SHFT	1.765	1.632	1.225	1.697	.243	.670	1.252
CO - EQ SHFT	.234	.266	.320	.183	.190	.391	.451
H2 - EQ SHFT	.638	.719	.671	.617	.273	.587	.907
CO2 - EQ SHFT	.566	.550	.499	.493	.134	.338	.526
H2O	2.013	1.548	1.276	1.736	.221	.742	1.419
CO	.208	.169	.296	.157	.152	.356	.411
H2	.593	.691	.625	.552	.308	.553	.752
CO2	.593	.647	.522	.519	.172	.373	.565
CH4	.166	.205	.176	.155	.038	.127	.219
C2H6	.018	.019	.018	.016	.007	.014	.021
N2	.794	.748	.670	.634	.477	.621	.614
NH3	.011	.014	.016	.014	.005	.012	.019
H2S	.003	.004	.004	.003	.001	.003	.005
TAR	.000	.000	.001	.001	.000	.001	.000
CHAR EXP	3.600	3.000	8.250	6.583	2.161	5.322	9.818
CHAR ASH LOSS	1.321	1.802	8.466	6.037	1.349	3.566	5.793
CHAR NO ASH LOS	2.623	3.741	7.844	7.577	2.642	5.415	10.675
LTR TEMP	761.	853.	682.	696.	527.	664.	522.
HTR TEMP	1576.	1553.	1569.	1515.	1575.	1594.	1575.
CTR TEMP	2304.	2092.	2456.	2154.	2740.	2674.	2181.
HEAT LOSS Z1	10463.	4075.	-2099.	2402.	-86.	-3198.	-520.
HEAT LOSS Z2	16555.	9068.	17302.	16399.	5367.	10052.	7580.
FR FM CB	.863	.926	.882	.906	.936	.922	.935
FR CH4	.742	.754	.770	.758	.656	.751	.745
FR C2H6	.258	.247	.230	.242	.345	.250	.255
FR H2	.068	.090	.077	.094	.131	.093	.110
FR H2S	1.142	1.363	.911	.673	.596	.883	.717
X1	87.398	83.447	72.821	70.018	73.824	76.246	69.044
X2	1576.	1553.	1569.	1515.	1575.	1594.	1575.
X3	5.957	7.612	3.901	4.031	1.876	3.581	5.324
X4	30.453	32.000	20.230	16.440	25.554	28.138	25.357
X5	.060	.076	.058	.065	.025	.044	.063
F0	13.818	35.237	15.174	9.670	31.586	46.068	38.799
AM	.126	.129	.102	.103	.082	.097	.095
COAL FD LBS/HR	20.818	22.603	28.859	25.272	10.093	22.795	34.485
STEAM FD	41.458	40.603	30.345	37.845	6.827	18.779	34.528
O2 FD	8.913	7.232	7.768	7.143	3.090	6.220	6.667
N2 FD WITH COAL	8.890	8.374	7.502	7.098	5.338	6.951	6.875
N2 FD BOTTOM	13.335	12.561	11.252	10.646	8.007	10.427	10.312
SHF K	.916	.957	.928	1.029	.919	.887	.919
SHF TEMP F	1576.400	1553.000	1569.200	1515.200	1574.600	1594.400	1574.600
O/O CAH8 GASFD	92.525	89.603	68.863	65.995	72.391	75.746	70.105
O/O CARB CONV	100.634	93.100	76.081	73.218	77.218	80.777	72.987
COAL BULK DN	.792	.818	.818	.794	.842	.818	.831
CHAR BULK DN	.351	.410	.474	.493	.531	.473	.476
PR DN COAL	1.365	1.410	1.410	1.369	1.452	1.410	1.433
PR DN CHAR	.605	.707	.817	.850	.915	.815	.821
AVG PR DN GM/CC	.985	1.059	1.114	1.109	1.184	1.113	1.127
COAL DM MICRONS	299.115	328.051	328.051	337.759	326.197	377.821	309.892
CHAR DM MICRONS	195.810	136.514	244.571	271.353	396.517	371.792	342.746
SUPGASVEL FT/SC	.332	.315	.336	.285	.331	.353	.361
MINFLUVEL FT/SC	.008	.005	.018	.023	.054	.042	.036
BED VOL FT3	.492	.516	.511	.505	.499	.503	.508
FLUID BEDHT IN	7.760	71.040	70.400	69.520	68.800	69.280	70.000
SLMPD BEDHT IN	41.025	43.697	42.901	45.232	43.990	42.565	42.327
BED AVG LBS/HR	11.457	12.087	17.619	15.175	5.804	13.132	21.183
BED DN LBS/FT3	29.934	31.410	31.118	32.249	33.607	31.373	31.368
RES TIME MIN	42.428	42.988	33.056	38.630	99.758	41.522	27.727
H COAL RTU/LB	10726.	10859.	10595.	10732.	10704.	10542.	10538.
H CHAR RTU/LB	3774.	6048.	9381.	9652.	8819.	8837.	9186.
H TAR RTU/LB	16545.	16545.	16290.	16290.	15894.	15894.	15894.

APPENDIX VII

SUMMARY TABLE OF SELECT VARIABLES FOR RUNS PROCESSED IN THE PREDICTIVE COMPUTER CODE

SUMMARY LIST FOR RUNS PROCESSED

222-2-6-23, 1978

(2) 2-6-23

RUN-NO.	203	204	205	218	219	220	221
H2O - EQ SHFT	1.545	1.503	1.524	1.876	1.383	1.723	1.551
CO - EQ SHFT	.242	.221	.320	.264	.585	.498	.474
H2 - EQ SHFT	.701	.637	.784	.851	1.004	1.062	.897
CO2 - EQ SHFT	.431	.438	.486	.538	.574	.620	.652
CH4	.180	.167	.202	.262	.290	.301	.257
C2H6	.016	.015	.019	.030	.028	.028	.026
N2	.928	1.009	.913	.743	.609	.681	.544
NH3	.014	.014	.019	.024	.025	.022	.020
H2S	.005	.004	.011	.009	.014	.011	.006
TAR	.001	.001	.001	.001	.000	.001	.000
CHAR EXP	6.643	5.897	6.762	19.181	13.456	13.241	10.971
CHAR ASH LOSS	8.802	8.563	6.938	15.306	9.554	10.752	8.985
CHAR NO ASH LOS	6.643	5.897	6.762	19.181	13.456	13.241	10.971
LTR TEMP	913.	934.	821.	649.	825.	746.	736.
HTR TEMP	1602.	1584.	1605.	1515.	1641.	1620.	1602.
CTR TEMP	1875.	2163.	2306.	2071.	2356.	2136.	2747.
HEAT LOSS Z1	4607.	3368.	1004.	-7792.	-10057.	-6112.	-4691.
HEAT LOSS Z2	106.	8526.	11306.	19602.	11821.	8797.	29132.
X(1)	69.682	71.336	74.158	54.706	56.230	66.893	69.491
X(2)	1602.104	1583.565	1604.448	1514.648	1640.802	1619.828	1602.012
X(3)	6.733	6.629	6.000	3.271	5.381	5.608	4.991
X(4)	30.573	28.608	25.923	9.532	22.607	22.602	20.604
X(5)	.084	.076	.087	.086	.109	.104	.097
COAL FD LBS/HR	24.000	22.460	29.010	45.830	43.030	42.960	38.460
STEAM FD	37.260	35.570	36.220	40.070	36.410	43.960	38.230
O2 FD	5.430	6.160	7.060	7.070	8.170	7.820	11.410
N2 FD WITH COAL	12.430	22.960	21.300	8.320	6.820	7.630	7.280
N2 FD BOTTOM	13.560	5.280	4.820	12.480	10.230	11.450	7.940
SHF K	.874	.904	.871	1.030	.817	.847	.875
SHF TEMP F	1602.104	1583.565	1604.448	1514.648	1640.802	1619.828	1602.012
PR DN GM/CC	.690	.690	.690	.690	.690	.690	.690
COAL BULK DN	.400	.400	.400	.400	.400	.400	.400
SUPGASVEL FT/SC	.295	.258	.263	.302	.288	.338	.303
MINFLUVEL FT/SC	.027	.027	.027	.027	.027	.027	.027
BED VOL FT3	.486	.456	.478	.450	.496	.518	.508
FLUID BEDHT IN	67.000	62.800	65.900	62.000	58.400	71.400	70.000
SLMPD BEDHT IN	43.284	42.449	44.257	39.730	44.539	43.897	44.764
BED AVG LBS/HR	13.328	12.620	16.543	30.263	26.898	26.461	23.167
BED DN LBS/FT3	16.132	16.878	16.769	16.001	16.259	15.352	15.968
RES TIME MIN	19.510	20.551	16.588	9.426	11.255	11.111	12.656
H COAL BTU/LB	10470.	10482.	10369.	10589.	10516.	10751.	10760.
H CHAR BTU/LB	4265.	4683.	5200.	9771.	8680.	9186.	8835.
H TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.
PRESSURE ATM	40.000	40.000	40.000	40.000	40.000	40.000	40.000
COAL DM MICRONS	329.263	329.263	329.263	329.263	329.263	329.263	329.263

RUN NO.	229	231	238	246	248	249	250
H2O - EQ SHFT	1.764	1.840	1.356	1.399	1.199	1.686	1.478
CO - EQ SHFT	.327	.332	.436	.360	.458	.507	.352
H2 - EQ SHFT	.801	.813	.866	.733	.735	1.006	.821
CO2 - EQ SHFT	.640	.672	.558	.595	.595	.670	.583
CH4	.224	.261	.206	.233	.232	.266	.225
C2H6	.021	.026	.018	.023	.024	.024	.020
N2	.612	.527	.669	.622	.581	.596	.638
NH3	.021	.028	.015	.021	.022	.021	.016
H2S	.005	.008	.004	.005	.006	.004	.005
TAR	.000	.000	.001	.000	.000	.000	.000
CHAR EXP	8.300	13.291	2.829	11.383	10.501	8.845	9.845
CHAR ASH LOSS	5.835	9.237	2.209	15.299	9.850	8.288	8.615
CHAR NO ASH LOS	8.300	13.291	2.829	11.383	10.501	8.845	9.845
LTR TEMP	770.	856.	1233.	701.	764.	888.	934.
HTR TEMP	1546.	1536.	1595.	1543.	1574.	1597.	1559.
CTR TEMP	2480.	2600.	2448.	2746.	3112.	2431.	2297.
HEAT LOSS Z1	-1673.	-8708.	4230.	-6062.	-11380.	-6363.	-9356.
HEAT LOSS Z2	24865.	32190.	14419.	30797.	36196.	18938.	17740.
X(1)	71.813	63.493	88.111	65.562	68.982	74.005	68.140
X(2)	1546.660	1536.172	1593.819	1543.000	1574.051	1596.571	1559.088
X(3)	5.913	5.122	7.096	4.972	4.627	6.190	6.183
X(4)	22.702	17.694	31.298	17.637	18.305	25.575	23.386
X(5)	.084	.087	.096	.088	.093	.097	.091
COAL FD LBS/HR	32.040	39.530	25.720	35.890	36.750	37.280	31.630
STEAM FD	41.640	42.040	35.190	32.870	28.710	42.440	38.620
O2 FD	10.210	11.540	8.470	10.650	12.180	9.740	8.110
N2 FD WITH COAL	6.850	5.900	7.490	6.970	6.510	6.680	7.150
N2 FD BOTTOM	10.280	8.850	11.230	10.450	9.770	10.010	10.720
SHF K	.968	.988	.888	.975	.920	.883	.946
SHF TEMP F	1546.660	1536.172	1593.819	1543.000	1574.051	1596.571	1559.088
PR DN GM/CC	1.379	1.379	1.345	1.371	1.372	1.336	1.360
COAL BULK DN	.800	.800	.780	.795	.796	.775	.789
SUPGASVEL FT/SC	.322	.319	.285	.275	.254	.336	.301
MINFLUVEL FT/SC	.059	.059	.101	.068	.044	.079	.062
BED VOL FT3	.494	.487	.500	.504	.450	.467	.483
FLUID BEDMT IN	68.000	67.100	68.900	69.400	62.000	64.300	66.500
SLMPD BEDMT IN	44.127	43.732	49.400	48.320	43.023	42.105	44.496
BED AVG LBS/HR	18.745	23.899	14.507	21.112	21.582	21.446	19.198
BED DN LBS/FT3	32.407	32.548	34.911	34.554	34.481	31.680	32.956
RES TIME MIN	29.951	24.059	40.725	29.096	25.332	23.794	30.172
M COAL BTU/LB	10375.	10402.	12348.	10903.	10943.	11255.	10292.
M CHAR BTU/LB	8002.	8140.	-2428.	10541.	10863.	11083.	7130.
M TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.
PRESSURE ATM	40.000	40.000	40.000	40.000	40.000	40.000	40.000
COAL DM MICRONS	329.263	329.263	437.772	355.016	286.886	389.527	342.649

RUN NO.	251	252	253	254	255	256	26A
120 - EQ SHFT	1.598	1.699	1.748	1.429	1.619	1.733	.850
10 - EQ SHFT	.337	.423	.311	.562	.372	.313	.140
12 - EQ SHFT	.816	.976	.790	1.027	.865	.775	.427
102 - EQ SHFT	.572	.678	.621	.625	.609	.622	.318
CH4	.201	.226	.223	.241	.226	.231	.110
CH6	.018	.023	.021	.021	.020	.021	.012
V2	.601	.567	.432	.425	.411	.415	.351
VH3	.017	.021	.019	.023	.018	.020	.011
125	.004	.006	.005	.027	.004	.005	.002
TAR	.000	.000	.000	.000	.000	.000	.000
CHAR EXP	5.403	8.793	8.601	5.532	6.999	9.434	7.579
CHAR ASH LOSS	2.837	8.397	7.371	4.658	6.600	8.887	6.518
CHAR NO ASH LOS	5.403	8.793	8.601	5.532	6.999	9.434	7.579
TR TEMP	963.	1055.	828.	1334.	943.	858.	1015.
1TR TEMP	1564.	1518.	1539.	1625.	1553.	1541.	1546.
CTR TEMP	2218.	2462.	2469.	2384.	2353.	2496.	2625.
HEAT LOSS Z1	50.	-7321.	-6621.	-1855.	-6291.	-7156.	-3925.
HEAT LOSS Z2	12445.	27541.	24492.	10998.	18066.	24734.	14538.
K(1)	77.721	72.948	70.960	80.642	75.269	68.664	57.673
K(2)	1563.525	1518.019	1538.610	1624.825	1553.351	1542.175	1546.487
K(3)	6.665	4.677	5.751	6.770	6.215	5.986	3.913
K(4)	26.925	16.331	20.862	30.484	22.892	21.522	24.171
K(5)	.087	.087	.087	.106	.093	.087	.045
COAL FD LBS/HR	26.420	35.530	32.230	29.830	30.830	32.960	19.220
STEAM FD	39.340	39.790	40.830	40.000	39.580	40.550	20.440
Z2 FD	7.650	9.460	9.570	8.590	8.260	9.750	5.960
V2 FD WITH COAL	6.730	6.350	4.840	4.760	4.600	4.650	3.930
V2 FD BOTTOM	10.100	9.530	7.260	7.140	6.910	6.980	5.890
SHF K	.938	1.023	.983	.840	.956	.977	.969
SHF TEMP F	1563.525	1518.019	1538.610	1624.825	1553.351	1542.175	1546.487
PR DN GM/CC	1.355	1.565	1.355	1.326	1.348	1.384	1.331
COAL BULK DN	.786	.908	.786	.769	.782	.803	.772
SUPGASVEL FT/SC	.301	.308	.307	.299	.294	.303	.333
MINFLUVEL FT/SC	.082	.058	.040	.017	.084	.056	.046
3ED VOL FT3	.467	.493	.475	.480	.490	.492	.480
FLUID BEDHT IN	64.400	67.900	65.500	66.200	67.500	67.800	66.200
SLMPD BEDHT IN	44.164	44.813	42.337	42.039	46.861	44.919	41.830
3ED AVG LBS/HR	15.385	21.611	19.079	19.455	18.159	19.287	11.064
BED DN LBS/FT3	33.648	37.409	31.715	30.485	33.890	33.211	30.451
RES TIME MIN	35.716	31.132	28.067	29.460	32.311	29.749	45.673
H COAL BTU/LB	10775.	10989.	10194.	12045.	10513.	10897.	9462.
H CHAR BTU/LB	6512.	9047.	7878.	4049.	7714.	10344.	4112.
H TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.
PRESSURE ATM	40.000	40.000	40.000	40.000	40.000	40.000	20.000
COAL DN MICRONS	393.992	307.002	273.667	182.391	400.154	322.370	298.163

RUN NO.	272	273	275	277	278	279	280
M20 - EQ SHFT	1.347	1.185	1.888	1.616	1.658	1.729	1.693
CO - EQ SHFT	.344	.504	.158	.286	.241	.275	.249
M2 - EQ SHFT	.761	.902	.641	.728	.696	.764	.708
CO2 - EQ SHFT	.550	.498	.491	.565	.482	.531	.509
CH4	.225	.221	.182	.204	.159	.174	.164
C2H6	.026	.021	.019	.018	.013	.014	.013
N2	.742	.615	.893	.821	.873	.858	.748
NH3	.023	.019	.017	.016	.012	.012	.012
H2S	.004	.006	.003	.004	.003	.004	.003
TAR	.000	.000	.001	.000	.000	.000	.000
CHAR EXP	15.452	8.388	10.885	7.901	4.060	3.272	3.164
CHAR ASH LOSS	12.099	4.697	9.731	4.061	3.337	2.271	1.840
CHAR NO ASH LOS	15.452	8.388	10.885	7.901	4.060	3.272	3.164
LTR TEMP	674.	648.	828.	807.	833.	789.	798.
HTR TEMP	1518.	1618.	1471.	1549.	1599.	1588.	1586.
CTR TEMP	2546.	2298.	2000.	2308.	1906.	1928.	2018.
HEAT LOSS Z1	-10540.	-3292.	-1134.	1084.	9918.	9483.	10065.
HEAT LOSS Z2	26839.	6706.	16052.	17621.	689.	1360.	4380.
X(1)	58.503	72.547	59.710	69.886	78.190	83.345	82.838
X(2)	1517.428	1617.841	1470.897	1549.055	1598.675	1588.274	1585.932
X(3)	3.116	5.269	4.218	6.241	7.896	8.100	8.219
X(4)	12.331	27.867	14.308	24.796	38.406	37.805	38.369
X(5)	.065	.080	.066	.080	.078	.079	.079
COAL FD LBS/HR	40.040	33.030	29.210	28.470	20.020	21.200	19.940
STEAM FD	30.730	32.400	40.630	38.660	40.630	42.830	41.350
O2 FD	9.240	6.960	6.970	8.700	6.230	6.670	6.890
N2 FD WITH COAL	8.310	6.890	10.000	9.200	9.780	9.610	8.380
N2 FD BOTTOM	12.460	10.330	15.000	13.800	14.670	14.410	12.570
SHF K	1.023	.850	1.124	.964	.880	.897	.900
SHF TEMP F	1517.828	1617.841	1470.897	1549.055	1598.675	1588.274	1585.932
PR DN GM/CC	1.396	1.426	1.388	1.379	.945	1.384	1.346
COAL BULK DN	.810	.827	.805	.800	.548	.803	.781
SUPGASVEL FT/SC	.350	.346	.314	.315	.323	.340	.323
MINFLUVEL FT/SC	.048	.041	.046	.050	.050	.049	.052
BED VOL FT3	.483	.504	.467	.507	.498	.486	.485
FLUID BEDHT IN	66.600	69.400	64.300	69.800	68.600	67.000	66.800
SLMPD BEDHT IN	41.302	42.900	41.483	45.223	44.072	42.103	42.984
BED AVG LBS/HR	25.580	19.557	18.158	16.473	10.555	11.297	10.336
BED DN LBS/FT3	31.358	31.913	32.420	32.356	21.977	31.500	31.372
RES TIME MIN	22.713	29.199	31.077	34.544	32.793	43.351	45.765
M COAL BTU/LB	10497.	10296.	10561.	10357.	10355.	10661.	10429.
M CHAR BTU/LB	10159.	8150.	8834.	7101.	2443.	4426.	785.
M TAR BTU/LB	16545.	16545.	16545.	16545.	16545.	16545.	16545.
PRESSURE ATM	30.000	30.000	40.000	40.000	40.000	40.000	40.000
COAL DN MICRONS	295.159	269.919	289.402	304.392	375.255	299.338	313.209

RUN NO.	281	290	291	292	306	307	310
H2O - EQ SHFT	1.753	1.649	1.238	1.663	.243	.694	1.272
CO - EQ SHFT	.236	.273	.305	.186	.182	.383	.445
H2 - EQ SHFT	.675	.746	.701	.637	.255	.600	.896
CO2 - EQ SHFT	.553	.546	.469	.493	.132	.321	.512
CH4	.163	.178	.185	.173	.050	.130	.230
C2H6	.014	.015	.019	.017	.007	.015	.022
N2	.794	.748	.670	.634	.477	.621	.614
NH3	.013	.013	.018	.016	.006	.013	.021
H2S	.002	.003	.004	.004	.002	.003	.007
TAR	.000	.000	.001	.001	.000	.001	.000
CHAR EXP	3.436	4.125	9.065	7.699	2.756	5.836	10.823
CHAR ASH LOSS	1.729	1.988	9.781	6.136	1.409	3.846	5.877
CHAR NO ASH LOS	3.436	4.125	9.065	7.699	2.756	5.836	10.823
LTR TEMP	775.	832.	787.	748.	672.	745.	600.
HTR TEMP	1559.	1556.	1555.	1497.	1590.	1618.	1596.
CTR TEMP	2296.	2087.	2445.	2153.	2751.	2679.	2196.
HEAT LOSS Z1	10463.	4075.	-2099.	2402.	-86.	-3198.	-520.
HEAT LOSS Z2	16555.	9068.	17302.	16399.	5367.	10052.	7580.
X(1)	82.210	80.517	66.412	67.602	70.814	72.140	66.750
X(2)	1558.631	1556.682	1555.291	1496.420	1589.968	1618.036	1596.242
X(3)	7.315	7.315	4.633	5.469	1.824	3.405	5.265
X(4)	33.094	30.910	21.751	19.302	26.223	27.916	25.449
X(5)	.074	.079	.069	.075	.022	.051	.078
COAL FD LBS/HR	20.820	22.600	28.860	25.270	10.090	22.800	34.490
STEAM FD	41.460	40.600	30.340	37.840	6.830	18.780	34.530
O2 FD	8.910	7.230	7.770	7.140	3.090	6.220	6.670
N2 FD WITH COAL	8.890	8.370	7.500	7.100	5.340	6.950	6.870
N2 FD BOTTOM	13.340	12.560	11.250	10.650	8.010	10.430	10.310
SHF K	.947	.950	.953	1.067	.894	.850	.884
SHF TEMP F	1558.631	1556.682	1555.291	1496.420	1589.968	1618.036	1596.242
PR DN GM/CC	1.365	1.410	1.410	1.369	1.452	1.410	1.433
COAL BULK DN	.792	.818	.818	.794	.842	.818	.831
SUPGASVEL FT/SC	.332	.315	.336	.285	.331	.353	.361
MINFLUVEL FT/SC	.048	.060	.060	.061	.061	.079	.054
BED VOL FT3	.492	.515	.511	.504	.499	.503	.508
FLUID BEDHT IN	67.800	71.000	70.400	69.500	68.800	69.300	70.000
SLMPD BEDHT IN	42.946	46.561	44.991	47.360	44.310	44.437	43.192
BED AVG LBS/HR	10.875	12.338	17.163	15.444	5.958	12.961	21.315
BED DN LBS/FT3	31.316	33.487	32.634	33.776	33.852	32.743	32.008
RES TIME MIN	44.409	45.811	34.665	40.452	108.514	43.338	28.289
H COAL BTU/LB	10725.	10857.	10594.	10731.	10703.	10541.	10537.
H CHAR BTU/LB	2354.	2586.	2586.	8039.	7517.	7376.	8546.
H TAR BTU/LB	16545.	16545.	16290.	16290.	15894.	15894.	15894.
PRESSURE ATM	40.000	40.000	30.000	40.000	10.000	20.000	30.000
COAL DM MICRONS	299.115	328.051	328.051	337.759	326.197	377.821	309.892