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MORGANTOWN LOW-BTU GASIFIER SIMULATION PROGRAM

October 1978

Work Performed Under Contract No. EY-77-C-21-8085

Morgantown Energy Technology Center
Morgantown, West Virginia

and

TRW Systems and Energy Group
Redondo Beach, California

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UNITED STATES DEPARTMENT OF ENERGY

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MORGANTOWN LOW-BTU GASIFIER SIMULATION PROGRAM

ABSTRACT

This project's overall purpose is to develop a Morgantown low-Btu gasifier system simulation program. The gasifier system consists of a moving bed gasifier and a gas clean-up system, and the present report concerns steady-state simulation of the gasifier.

Since the gasifier output controls the performance of the gas clean-up system, it is necessary to investigate the effects of steam/coal and oxygen/coal ratios and of feed temperature on the gasifier output. Simulation of the gasifier performance, therefore, was undertaken to gain quantitative understanding of these effects.

This gasifier simulation program will be coupled with a gas clean-up system simulation program now under development. Simulation of the entire gasifier system will serve as a guideline in planning experiments to enable its optimum overall operation.

1. SUMMARY

Two-dimensional partial differential equations were derived to describe the concentration change of hydrogen, carbon, methane, carbon monoxide, carbon dioxide, water and oxygen, and temperature profile in both longitudinal and radial directions.

This system of partial differential equations is non-linear and stiff, and therefore can only be solved numerically. Because of the non-linearity and stiffness of the equations, careful selection of the computational algorithm was essential to ensure a numerical solution. In addition, the computer program had to be general enough so that whenever the system equation was modified, it would not impose a major program modification. The PDECOL program package developed at Lawrence Livermore Laboratory appeared to meet these requirements. This program was acquired from Lawrence Livermore Laboratory and installed at the West Virginia Network Computer Center, to which METC has access. The program was tested and is running satisfactorily.

As a preliminary test of the gasifier model's validity, all physical parameters including mass-transfer coefficients and diffusivities were evaluated at an average condition within the gasifier and used as data input. We found that the gasifier model does describe the general trend of the gasifier behavior.

As in almost all chemical process simulations, a system model seldom matches the experimentally obtained values exactly. However, if the model can describe the general trend of system behavior, we then can adjust those theoretically estimated physical and chemical parameters -- in the sense of tuning -- to match the theoretically predicted values with those experimentally obtained within the accuracy of experimental data.

The following suggestions are made for project extension:

- Develop an experimental program to generate necessary data.
- Statistically analyze the data.
- Adjust physical and chemical parameters to match theoretical and experimental values within the statistically estimated accuracy of experimental data.
- Having obtained the aforesaid information, predict the gasifier performance by changing steam/coal ratio, oxygen (or air)/coal ratio, and temperature of steam/oxygen feed mixture.

2. INTRODUCTION

The purpose of Task 006 is to develop a computer simulation program. This will expedite the development and aid in optimization and scale-up of the Morgantown Energy Technology Center (METC) low-Btu coal gasifier system, which includes the METC low-Btu fixed-bed gasifier and the producer gas clean-up system.

The program consists of two parts:

- Steady-State Gasifier Simulation Program

Subject of this report, this program develops the mathematical models and computer program for calculation of the concentration profiles for hydrogen, carbon, methane, carbon monoxide, carbon dioxide, water and oxygen, and temperature profiles in both longitudinal and radial directions in the METC low-Btu gasifier.

- Producer Gas Clean-up System Simulation Program

This program develops the mathematical models and computational procedures for the material balance calculations around each of the major process units constituting the METC producer gas clean-up system.

This report presents the mathematical models and computer programs for simulation of the METC low-Btu gasifier. During the course of their development, certain simplifying assumptions were made to alleviate some difficulties involved in mathematical simulation of this complex system. These assumptions, and the subsequent limitations of the mathematical models, should be fully understood by users of the models and the computer program.

2.1 ORGANIZATION OF THIS REPORT

After the description of the METC low-Btu gasifier given below in Section 2.2, this report is organized in the following manner:

- Section 3: THEORY

Discusses the equilibrium and behavioral methods generally used in calculating the composition of chemical components and temperature profiles within a chemical reactor.

- Section 4: GASIFIER MODEL

Discusses the model's five conceptualized zones, their functions, and the methods used to derive mathematical equations for the various reactions.

- Section 5: NUMERICAL TECHNIQUE

Discusses use of the PDECOL program package in numerical solution of non-linear partial differential equations for the METC steady-state, two-dimensional model.

- Section 6: DISCUSSION AND CONCLUSIONS

Summarizes advantages and limitations of methods employed, assumptions made in formulating a workable preliminary model and computer program; gives computational results and suggests extensions to the current program.

- Four Appendices complete the report:

Appendix A. Additional Assumptions and Rearrangement of Equations

Appendix B. Estimation of Effective Diffusivity, D_{effi} , and Mass-Transfer Coefficient, k_{pi}

Appendix C. PDECOL Program User's Guide

Appendix D. Computer Program and Sample Inputs and Outputs

2.2 METC LOW-BTU GASIFIER

The METC experimental producer shown in Figure 1 is similar to commercial fixed-bed gas producers, except for its smaller diameter, (42 inches ID) and provision for stirring deeply within the coal bed. The coal bed has a depth of six to seven feet; it is supported on a grate that can be rotated at a slow rate adjusted to ash production. Ash is removed through a lock hopper, weighed, and sampled for analysis.

Air mixed with superheated steam is introduced below the grate and flows upward through the descending fuel. Gas is withdrawn through an off-take in the top cover. Pressure in the gasifier is developed by the resistance to gas flow through two orifices. A cyclone separator, located between the two orifices, removes most of the dust entrained in the gas. The cyclone dust is removed through a lock hopper, sampled, and analyzed. A small gas flow is diverted from the main stream, cooled, cleaned of dust, tar and water, and measured before it is analyzed for CO, H₂, N₂, CO₂ and CH₄.

The water-cooled, two-armed stirrer rotates at one-half revolution per minute, and moves vertically up to two feet. A continuous stirring maintains a dense coal bed to ensure better contact between coal and gas. Nuclear density gauges are used to indicate bed depth and voids in the bed. A portion of heat is released to cooling water circulating within a jacket located in the lower part

of the gasifier. The upper portion of the gasifier is insulated with 13-inch-thick refractory.

FIGURE 1. 42-INCH STIRRED-BED HIGH PRESSURE GAS PRODUCER

3. THEORIES AND APPROACHES

Composition of chemical components and temperature profile within a chemical reactor are calculated generally by either one of the following two methods:

- Equilibrium calculation
- Behavioral calculation

3.1 EQUILIBRIUM CALCULATION

The assumption made with this method is that all conceivable chemical reactions are in equilibrium. If all the chemical equilibrium constants are known, chemical composition can be calculated.⁽¹¹⁾ Theoretically, these chemical equilibrium constants can be calculated from a thermodynamic relationship:

$$\Delta F_i = - RT \ln K_i$$

In this equation, ΔF_i is the free energy change associated with i-th chemical reaction, K_i is the chemical equilibrium constant associated with the i-th chemical reaction, R is the gas constant, and T is the temperature.

With a known temperature, K_i is computed for each reaction step, and subsequently, the equilibrium composition of each chemical constituent can be calculated. Actually, however, the chemical reactions hardly reach the equilibrium, and therefore an "approach to equilibrium" factor, α_i , is often used:

$$\tilde{K}_i = \alpha_i K_i$$

Here: K_i = theoretically calculated chemical equilibrium constant (using the thermodynamic relation shown above).

$\tilde{K}_i$ = actual chemical equilibrium constant used in the equilibrium calculation.

α_i = approach to equilibrium factor.

The factor α_i is essentially a "parameter" manipulated to match the calculated chemical composition with those of experimentally obtained values. In this sense, α_i depends on the reactor type, residence time and transport phenomenon. This relationship is generally unknown.

Consequently, the weakness of this approach is clear. If an operating variable changes, such as the steam or air flow rate, or coal size and coal flow rate, the reactor behavior changes, and consequently α_i changes.

Unless all α_i 's are insensitive to changes in the operating conditions, or the relationship between α_i and operating conditions are established, equilibrium calculation is less useful for a gasifier simulation.

3.2 BEHAVIORAL CALCULATION

This approach differs from the equilibrium calculation, mathematical equations being derived according to the fundamental understanding of the physical and chemical reactions taking place within a reactor.

The behavioral approach requires an elaborate numerical calculation because the reactor system equations are usually non-linear and stiff. Despite the mathematical sophistication that requires computer assistance, a few "parameters" remain in the reactor system equations. These "parameters" are manipulated to match computed results with experimentally obtained values. Such "parameters" are expected to be less dependent on the reactor configuration, gas and solid flow rates, and temperature compared to the α_i factor mentioned earlier in the equilibrium calculation.

Yoon, Wei and Denn^(36,37) at the University of Delaware, Desai and Wen⁽⁷⁾ at West Virginia University, and Kosky⁽¹⁶⁾ at the General Electric Company made independent steady-state simulations of moving-bed gasifiers using the behavioral approach.

Table 1 summarizes assumptions and chemical components considered by each of these investigators.

West Virginia University's and GE's models are one-dimensional. The University of Delaware's model is a modified version of a one-dimensional model. The Lurgi gasifier, for which the University of Delaware's model was originally developed, is equipped with a water-cooling jacket. Therefore, the bed temperature in the vicinity of the gasifier wall should drop to that of the cooling water, which means that the radial temperature is non-uniform. Taking this fact into consideration, the University of Delaware investigators assumed two regions in the radial direction: adiabatic core and boundary layer. The adiabatic core represents the region where the major portion of gasification occurs. The boundary layer is a region close to the gasifier wall. In each region, the model is one-dimensional.

As the Lurgi gasifier, the METC gasifier is equipped with a water-cooling jacket. According to the experimental evidence, shown in Figure 2, the temperature distribution in the radial direction is bell-shaped. Therefore, we derived

TABLE 1. SUMMARY OF ASSUMPTIONS AND CHEMICAL COMPONENTS CONSIDERED BY DIFFERENT INVESTIGATORS

	Univ. of Delaware	W. Virginia Univ.	General Electric Co.
Reactor	Lurgi gasifier	METC gasifier	GEGAS gasifier
State	Steady-state	Steady-state	Steady-state
Model	Plug-flow (one-dimensional)	Plug-flow (one-dimensional)	Plug-flow (one-dimensional)
Chemical Component	H ₂ , H ₂ O, O ₂ , CO, CO ₂ , CH ₄ , and C	H ₂ , H ₂ O, O ₂ , CO, CO ₂ , N ₂ , CH ₄ , C ₂ H ₆ , H ₂ S, SO ₂ , NO, NH ₃ , C, H, O, N, S,	H ₂ , H ₂ O, O ₂ , CO, CO ₂ , CH ₄ , and C
Temperature	Assumed identical gas phase and solid phase temperature	Equations are derived for gas phase and solid phase, but, apparently, single phase equations were adapted in the calculation	Assumed identical gas phase and solid phase temperature
Reference	36,37	7	16

two-dimensional equations to describe the distribution of gas concentration and temperature in longitudinal and radial directions.

FIGURE 2. TEMPERATURE PROFILE IN THE 42-INCH GAS PRODUCER

4. GASIFIER MODEL

Conceptually, the gasifier consists of five zones (Figure 3):

- Drying Zone
- Devolatilization Zone
- Gasification Zone
- Combustion Zone
- Ash Zone

Figure 3. Conceptual Drawing of the Gasifier

- Drying Zone

This is located at the top of the bed. The major portion of the moisture content in the coal feed, as determined by a proximate analysis, is vaporized as it comes into contact with the ascending product gas (at approximately 1000°F). The remaining portion will be vaporized as the coal feed continues to descend in the gasifier.^(21,22)

This simulation program assumes that the coal moisture content will be completely removed in this zone.

- Devolatilization Zone

This is located somewhere between the drying zone above and the gasification zone below. The devolatilization proceeds at fairly constant temperature because of negligible net heat of devolatilization.

Coal is a complex network of organic polymers consisting of heteroatomic clusters. When a coal is heated to 750°F, weaker linkages of these polymers begin to break up into smaller molecules and free radicals which then react with neighboring active atoms or free radicals to form more stable molecules. As the temperature increases, these complex depolymerization and repolymerization reaction processes proceed more actively. As a result of these reactions, volatiles, consisting of tar and coal-gas, are released into the gas-phase while the remaining portion of the original coal remains in the solid-phase as char.⁽²⁾

Tar is a mixture of benzene, toluene, naphthalene, anthracene, and many other hydrocarbons. Coal-gas is a mixture of methane, carbon oxides, and low-boiling-point hydrocarbons. The quantity and composition of tar and coal-gas depend strongly on the coal type and operating conditions within a gasification reactor. Table 2 is an example of typical devolatilization data given in the University of Delaware report.⁽³⁶⁾

Instead of attempting to derive a mathematical model for these complex devolatilization processes, the quantity and composition of volatiles, and also of tar and coal-gas are estimated from the devolatilization data for a coal type. Methane, hydrogen, carbon monoxide and carbon dioxide devolatilized in this zone are added to those gases produced in the gasification and combustion zones to make-up the total gas produced in the gasifier.

Table 2. Typical Devolatilization Data⁽³⁶⁾

Fractional Composition of Volatiles (% by weight)

Tar plus liquor	50
Coal-Gas	50

Chemical Constituent of Coal-Gas (% by volume)

CH ₄	42.9
H ₂	17.1
CO	9.5
CO ₂	9.5
Others	21.0

● Gasification and Combustion Zones

The most drastic changes in gas composition and temperature distribution take place in these zones. Conceptually, the gasification zone is located above the combustion zone, and the temperature rise will be fastest in this combustion zone while most of the oxygen feed will be consumed. Actually, however, a distinct demarcation line between these two zones can hardly be drawn because some gasification reaction may already have been proceeding in the combustion zone. Therefore, rate equations were derived for the combined gasification and combustion zone. We considered only methane, carbon dioxide, carbon monoxide, oxygen, hydrogen, carbon and water concentration changes because these are the major constituents currently of main concern. In the later stage of the simulation program, one might add equations for other chemical constituents that were considered significant.

To derive heat and material balance equations, the following assumptions were made:

For gas phase:

- (i) Convective mass- and heat-flow in the longitudinal direction
- (ii) Diffusive mass- and heat-flow in the radial direction

For Solid Phase:

- (i) Convective mass-flow in the longitudinal direction, and no diffusive mass-flow in the radial direction
- (ii) Solid-phase temperature is equal to the gas-phase temperature

Unlike other simulation models shown in Table 1, the chemical composition and temperature changes in a radial direction were considered in our model. Experimental evidence, shown in Figure 4 (Sec. 6), seems to indicate there is a bell-shaped temperature distribution in the radial direction. Consequently, there must also be a non-uniform concentration distribution in the radial direction. In addition, the inspection of the physical structure of the METC gasifier (see Figure 1) also indicates the possibility of radial temperature distribution because approximately 15% of heat input (heat content of coal, air, and steam) is released into the cooling water running within the cooling jacket. Our first attempt, therefore, was to incorporate the diffusive mass- and heat-transfer terms to account for this experimental fact.

The last assumption on the solid-phase temperature requires explanation.

Although the solid-phase temperature was assumed equal to that of gas-phase, realistically, these two temperatures will be different, particularly in the lower part of the combustion zone (the difference will be substantial in the ash zone). However, in most parts of the gasification and combustion zones, where the majority of gasification and combustion reactions occur, the temperature difference is expected to be small.

With these assumptions, the following material balance and heat balance equations were derived:

Material Balance Equations:

For oxygen:

$$\frac{\partial(VC_1)}{\partial z} = D_1 \left[\frac{\partial^2 C_1}{\partial r^2} + \frac{1}{r} \frac{\partial C_1}{\partial r} \right] - R_2 \quad (1)$$

For steam:

$$\frac{\partial(VC_2)}{\partial z} = D_2 \left[\frac{\partial^2 C_2}{\partial r^2} + \frac{1}{r} \frac{\partial C_2}{\partial r} \right] - R_1 \quad (2)$$

For Methane:

$$\frac{\partial (VC_3)}{\partial z} = D_3 \left[\frac{\partial^2 C_3}{\partial r^2} + \frac{1}{r} \frac{\partial C_3}{\partial r} \right] + R_4 \quad (3)$$

For Carbon Monoxide:

$$\frac{\partial (VC_4)}{\partial z} = D_4 \left[\frac{\partial^2 C_4}{\partial r^2} + \frac{1}{r} \frac{\partial C_4}{\partial r} \right] + R_1 + 2(\lambda-1)R_2 + 2R_3 \quad (4)$$

For Carbon Dioxide:

$$\frac{\partial (VC_5)}{\partial z} = D_5 \left[\frac{\partial^2 C_5}{\partial r^2} + \frac{1}{r} \frac{\partial C_5}{\partial r} \right] + (2-\lambda)R_2 - R_3 \quad (5)$$

For Hydrogen:

$$\frac{\partial (VC_6)}{\partial z} = D_6 \left[\frac{\partial^2 C_6}{\partial r^2} + \frac{1}{r} \frac{\partial C_6}{\partial r} \right] + R_1 - 2R_4 \quad (6)$$

For Carbon:

$$F_c^0 \frac{\partial W}{\partial z} = R_1 + \lambda R_2 + R_3 + R_4 \quad (7)$$

Energy Balance Equation:

$$\begin{aligned} & \left[G_{char} C_{p, char} + G_{ash} C_{p, ash} - \sum_i VC_i C_{pi} \right] \frac{\partial T}{\partial z} \\ & = \sum_i R_i \Delta H_i - \lambda_{eff} \left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right] \end{aligned} \quad (8)$$

Boundary Conditions:

$$C_1 = C_{10}$$

$$C_2 = C_{20}$$

$$C_3 = 0.$$

$$C_4 = 0.$$

$$C_5 = 0.$$

$$C_6 = 0.$$

$$T = T_0$$

at $\{z=0 \text{ and } 0 < r \leq r_w\}$

$$W = 1.0$$

at $\{z=L \text{ and } 0 \leq r \leq r_w\}$

$$\frac{\partial T}{\partial r} = 0$$

$$\frac{\partial C_i}{\partial r} = 0$$

at $\{r=0 \text{ and } 0 \leq z \leq L\}$

$$\frac{\partial T}{\partial r} = \frac{-h_w}{\lambda_{er}} (T - T_c)$$

$$\frac{\partial C_i}{\partial r} = 0$$

at $\{r=r_w \text{ and } 0 < z \leq L\}$

In the equations, R_1 , R_2 , R_3 and R_4 are the net reaction rates, each corresponding to the four gas-solid phase reactions.

Gas-solid phase reaction

Gas-gas phase reaction

The first four steps are gas-solid phase reactions. Among them, the first two reactions are characteristically different from the last two reaction steps. Unlike carbon dioxide and hydrogen, steam and oxygen are being fed into the gasifier. These feed gases must migrate through a thin layer of gas film, an ash layer covering the coal surface, and finally react with carbon. Furthermore, the gases may migrate deeper into pore spaces within the coal and react. Carbon dioxide and hydrogen are not the feed, but rather part of a product formed in the previous two reaction steps. These gases are formed as a result of reaction between carbon and steam and oxygen. Because of this difference in transport mechanism, the apparent reaction rate of steam and oxygen, therefore, depends on the migration rates of the gas reactant through the gas and ash layers and the rate of chemical reaction. As the residence time of coal increases, the thickness of ash layer also increases to the extent that the exterior of the ash coat may be constantly reduced by attrition, finally reaching a constant thickness of ash layer. Ultimate ash coat thickness would be the function of such factors as gas flow rate, temperature, coal type and bed motion.

Based on this rate mechanism, the apparent reaction rate is given by ⁽³⁷⁾:

$$R_i = \frac{(1-\epsilon)(P_i - P_i^*)}{\frac{R_p}{3k_{pj}} + \frac{R_p(R_p - r_c)}{3\left(\frac{r_c}{R_p}\right) \frac{\overline{RT}}{D_{effi}} + \frac{1}{\eta\left(\frac{r_c}{R_p}\right)^3 k_i C_c^0}}$$

in g-mole/cm³ bed volume-sec

Three terms in the denominator are the resistance to the apparent reaction rate, each represented by k_{pj} , D_{effi} and k_i . k_{pj} is associated with the mass-transfer through gas film, D_{effi} is the effective diffusivity of a gas component in the ash layer, and k_i is an intrinsic reaction rate constant. P_i^* is the partial pressure of i -th component at equilibrium.

If the ash layer is so small as to be negligible, the second resistance term in the denominator becomes zero, and we have the "ash segregated" model.

For carbon dioxide and hydrogen, we assumed that the apparent reaction rate is equal to the intrinsic reaction rate because, as mentioned earlier, these gases are formed on the coal surface and should be readily available for chemical reaction.

The only gas-gas phase reaction considered is the water-gas shift reaction. This tends to quickly reach an equilibrium, and does not explicitly contribute to the net reaction rate.

The five reaction steps described here do not exhaust all possible chemical reactions occurring within the gasifier. Because of the complex nature of coal, hundreds of chemical constituents might be identified, and consequently hundreds of possible chemical reaction steps could be considered. As mentioned earlier, we are currently interested only in those chemical constituents considered as relevant. If other components are considered significant, an additional equation could be introduced.

5. NUMERICAL TECHNIQUE

The numerical solution of non-linear partial differential equations is often a highly complicated and non-trivial process: a different set of partial differential equations may require development of separate and different programs, and the programming is generally complicated, tedious and time-consuming. However, the difficulty has been eased somewhat by development of an automated partial differential equation solution software package^(20,27) such as PDECOL.⁽²⁰⁾ The PDECOL program was used for the numerical solution of our system of partial differential equations.

The structure of PDECOL uses the "method of lines" approach⁽¹⁷⁾. Its basic idea is to reduce a partial differential equation into a simpler ordinary differential equation by "discretizing" all but one of the independent variables.⁽²⁰⁾ Among several existing discretizing techniques such as the finite difference technique,⁽¹⁾ Galerkin technique⁽³⁾ or collocational technique, PDECOL has adapted the collocational.⁽²³⁾ Once the partial differential equation has been approximated by a simpler ordinary differential equation, the differential equation may either be approximated numerically or solved analytically.⁽²⁰⁾ Recently, sophisticated and reliable computer programs for the solution of non-linear and stiff systems of ordinary differential equations have become available.^(10,13,14) The method of lines is an attempt to take advantage of these recent developments in computer software packages for solution of ordinary differential equations.

PDECOL was developed by the Mathematics Group at Lawrence Livermore Laboratory for the solution of transient one-dimensional partial differential equations. For our steady-state two-dimensional model, the program was readily usable.

The user interfaces with the program by writing a MAIN program and three subprograms:

MAIN Program: Defines the region for the problem and initializes several variables.

Subprograms:

SUBROUTINE F: Defines the desired partial differential equations to be solved.

SUBROUTINE BNDRY: Provides needed information about boundary conditions.

SUBROUTINE UINIT: Provides needed initial condition function values.

The user also may provide an optional subroutine, DERIVF, which specifies derivatives of the aforementioned function F. Details of the formats to be used in the MAIN program and subprograms are presented in Appendix C, User's Guide. Lists of computer input data and output are presented in Tables 3 and 4 respectively.

The MAIN program and subprograms for our problem were prepared by the Computer/Math Branch of Morgantown Energy Technology Center. These are presented in Appendix D together with the sample inputs and outputs.

Table 3. List of Computer Input Data

Description	Program Code	Description	Program Code
$\bar{R}$	RBAR	D_1/r_w^2	D1
R	R	D_2/r_w^2	D2
ϵ	EPSX	D_3/r_w^2	D3
R_p	RP	D_4/r_w^2	D4
k_{p1}	AKP1	D_5/r_w^2	D5
k_{p2}	AKP2	D_6/r_w^2	D6
r_c	RC	$V_o/(T_o \cdot L)$	D7
$D_{eff.1}$	DEFF1	λ_{er}	ERLAMB
$D_{eff.2}$	DEFF2	$\Delta \check{C}_p r_w^2 / L$	DELCp
η	ETA	ΔH_1	D10
C_c^o	CCO	ΔH_2	D11
λ	ALAMB	ΔH_3	D12
U_w	UW	ΔH_4	D13
T_c	TC	$r_w^2/(F_c^o)/L$	D14
r_w	RWALL		
k_1^o	AK10	C_{10}/α_1	U10
k_2^o	AK20	C_{20}/α_1	U20
k_3^o	AK30	C_{30}/α_1	U30
k_4^o	AK40	C_{40}/α_1	U40
k_5^o	AK50	C_{50}/α_1	U50
E_1	E1	C_{60}/α_1	U60
E_2	E2	T_o	U70
E_3	E3	W	U80
E_4	E4	α_1	ALPHA1
E_5	E5	$\alpha_2 = \alpha_1 r_w^2$	ALPHA2
		β	BETA

Table 4. List of Computer Output

C_1 ... Concentration of oxygen in lb-mol/ft³

C_2 ... Concentration of water in lb-mol/ft³

C_3 ... Concentration of methane in lb-mol/ft³

C_4 ... Concentration of carbon monoxide in lb-mol/ft³

C_5 ... Concentration of Carbon Dioxide in lb-mol/ft³

C_6 ... Concentration of Hydrogen in lb-mol/ft³

W Fraction of carbon

T ... Temperature in °F

6. DISCUSSION AND CONCLUSIONS

A two-dimensional steady-state gasifier model was derived, describing the temperature profile and concentration distribution of six components: methane, oxygen, hydrogen, carbon monoxide, carbon dioxide, and carbon.

PDECOL was adapted because, in addition to its capability of providing the numerical solution to partial differential equations, it alleviated many difficulties involved in the preparation of a computer program to solve for this type of problem. Simulation of a chemical reactor system often requires revisions of mathematical models and computer programs, and the PDECOL package was useful in easing tedious programming efforts.

Despite its advantages, the PDECOL program is limited to a system of two-dimensional PDE (time and one-dimensional space, or a two-dimensional space), and a substantial modification will be needed to extend its capability to handle a two-dimensional transient PDE system.

One important aspect of using PDECOL is that the boundary conditions must be consistent. In our case, a boundary condition was not consistent at $z = 0$ (at the top of the grate), because the temperature of the mixture of steam and oxygen (or air) feed was T_0 °F and the temperature of reactor vessel cooling jacket water was set at T_c °F ($T_0 \neq T_c$). This situation created a discontinuity at $z = 0$. To deal with this problem, a function, $f(z)$, was introduced.

$$\left\{ \begin{array}{ll} f(z) = \frac{1}{2} (1 + \cos(az)) & \text{for } 0 \leq z \leq \pi/a \\ \text{and} & \\ f(z) = 0 & \text{for } z \geq \pi/a \end{array} \right.$$

so that the boundary condition

$$\frac{\partial T}{\partial r} = - \frac{U_w}{\lambda_{er}} (T - T_c)$$

was rearranged as

$$\frac{\partial T}{\partial r} + \frac{U_w}{\lambda_{er}} T = (1 - f(z)) \left\{ \frac{U_w}{\lambda_{er}} T_c \right\} + f(z) \left\{ \frac{U_w}{\lambda_{er}} T \right\}$$

at $z = 0$

where "a" is a preassigned numerical parameter.

What we did was to force $\frac{\partial T}{\partial r} = 0$ at $z = 0$, and then gradually restore the boundary condition,

$$\frac{\partial T}{\partial r} = -\frac{U_w}{\lambda_{er}} (T - T_c),$$

to eliminate the discontinuity.

To obtain a preliminary gasifier model and a workable computer program, and to reduce the computational efforts, the following additional assumptions were made (see Appendix A):

- Gas linear flow rate is proportional to bed temperature
- Mass-transfer coefficients and specific heats evaluated at an average gasifier condition can be used throughout
- Diffusivity is proportional to (bed temperature)^{3/2}
- Constant pressure

We were aware that these additional assumptions could oversimplify the view of system behavior. However, considering the availability and accuracy of experimental data and the weakness in understanding the devolatilization mechanism, these assumptions might not be unrealistic.

Generally available data are:

1. Coal proximate analysis, coal feed rate and temperature
2. Steam and oxygen (or air) feed rate and temperature
3. Product gas flow rate and composition
4. Temperature measurement within the gasifier.

Computationally, items 1 and 2 are the data input, based on which items 3 and 4 are computed. We may adjust such parameters as the mass-transfer coefficients, diffusivities and reaction rate parameters, which depend on the coal type, to match the predicted product gas composition and temperature with those experimentally obtained within the accuracy of the experimental data.

On the other hand, the product gas is composed of those gases released in the devolatilization zone and those produced in the gasification and combustion zones. Because of the conflicting opinions on the devolatilization mechanism, the amount and composition of gas released in the devolatilization zone can only be roughly estimated, and subsequently the computed amount and composition of product gas

could be affected by the estimated releases occurring in the devolatilization zone.

With these considerations, the additional assumptions listed in Appendix A were used in formulating a workable preliminary gasifier model and a computer program.

The model is acceptable if it predicts the experimentally determined gas composition and temperature distribution within the accuracy of experimental data; otherwise, the revisions to the model should be made.

Results of computation, based on the gasifier model, are demonstrated in the following figures.

- Figure 4: Temperature distribution in the longitudinal direction
- Figure 5: Temperature distribution in the radial direction at $z = 8.48$ in.
- Figure 6: Concentration distribution of chemical constituents in the longitudinal direction

These results were based on hypothetical data input and should be regarded as a test case only to demonstrate the model's operational adequacy.

One important aspect of a process simulation program is the development of an experimental program to acquire accurate data with which the predicted values will be matched.

The following suggestions are, therefore, made to extend this program:

- Design an experimental program to generate data such as bed temperature distribution and composition and flow rate of input and output streams.
- Statistically analyze the experimental data to test their consistency and accuracy.
- With this data available, adjust the gasifier parameters, such as the mass-transfer coefficients, diffusivities, and reaction rate parameters that depend on coal type.
- Reexamine those additional assumptions listed in Appendix A, and revise the model and the computer program if necessary.
- Finally, if it can predict the experimental data within the estimated accuracy, the model will be used to predict gasifier performance with respect to changes in operating conditions, such as the steam/coal and oxygen/coal ratios.

FIGURE 4. COMPUTED TEMPERATURE PROFILE IN THE LONGITUDINAL DIRECTION AT CENTER

FIGURE 5. COMPUTED TEMPERATURE PROFILE IN THE RADIAL DIRECTION AT 8.48 INCHES ABOVE THE GRATE

FIGURE 6. COMPUTED CONCENTRATION DISTRIBUTION IN THE LONGITUDINAL DIRECTION AT CENTER

Nomenclature:

C_i	= Concentration of i-th component, g-mole/cm ³
C_{pi}	= Heat capacity of i-th gas component, cal/g-mole °K
$C_{p,ash}$	= Heat capacity of ash, cal/g. °K
$C_{p,char}$	= Heat capacity of char, cal/g. °K
D_i	= Diffusivity of i-th gas component in the gas phase, cm ² /sec
E_j	= Activation energy, cal/g-mol
F_c^0	= Molar feed flux of fixed carbon, g-mol/cm ² /sec
G_{ash}	= Mass flux of ash, g/cm ² . sec
G_{char}	= Mass flux of char, g/cm ² . sec
H_j	= Heat of reaction in j-th reaction step, cal/g-mole
k_j	= Intrinsic reaction rate constant, g-mole/mole of carbon.atm.sec
k_j^0	= Arrhenius const, g-mole/mole of carbon.atm.sec
k_{pj}	= Mass transfer coefficient, g-mole/cm ² .atm.sec
L	= Bed height, cm
P	= System operating pressure, atm
r	= Radial distance from the center of the gasifier, cm
r_w	= Inside radius of gasifier, cm
R_j	= Apparent reaction rate, g-mole/cm ³ . sec
r_c	= Radius of unreacted coal, cm
R_p	= Initial coal radius, cm
R	= Gas constant, 1.987 cal/g-mol. °K
$\bar{R}$	= Gas constant, 82.057 cm ³ . atm/g-mol. °K

T	= Bed temperature, $^{\circ}\text{K}$
T_c	= Coolant temperature, $^{\circ}\text{K}$
U_w	= Overall heat-transfer coefficient, $\text{cal}/\text{cm}^2 \cdot \text{sec. } ^{\circ}\text{K}$
V	= Linear gas flow rate, $\text{cm}/\text{sec.}$
W	= Fraction of remaining carbon in coal particles
z	= Longitudinal distance, cm
λ_{er}	= Thermal conductivity of gas mixture, $\text{cal}/\text{cm} \cdot \text{sec. } ^{\circ}\text{K}$

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Appendix A

Additional Assumptions and Rearrangement of Equations

Equations (1) to (8) were unsuitable for computation. Additional assumptions were made and the equations rearranged.

These additional assumptions were:

- Linear gas flow rate is a linear function of temperature only, i.e.,

$$v = v_0 \frac{T}{T_0}$$

where:

v, v_0 = linear gas flow rate (in ft./sec.) respectively at temperature T and T_0 .

- Physical constants, such as gas-phase diffusivities, D_i , mass transfer coefficients, k_{pi} , are evaluated at an average bed condition, and used throughout the simulation.
- Effective diffusivity, D_{effi} , is proportional to $\sqrt{T^3}$

These assumptions are undoubtedly too strong. We supplemented this weakness with the sensitivity test, plan to modify the formula for the calculation of linear gas flow rate, if necessary, and also incorporate the program package for the calculation of physical constants so that each physical constant will be computed at each local condition.

We then introduced variables:

$$C_i = \alpha_i U_i \quad \text{for } i = 1, 2, \dots, 6$$

$$z = L X$$

$$r = r_w y$$

$$T = U_7$$

$$W = U_8$$

and

$$\tilde{D}_i = D_i / r_w^2 \quad \text{for } i = 1, 2, \dots, 6$$

$$\tilde{D}_7 = D_7 / L = \left(\frac{V_o}{T_o} \right) / L$$

$$\tilde{D}_8 = D_8$$

$$\tilde{D}_9 = \left[G_{\text{char}} C_{p, \text{char}} + G_{\text{ash}} \cdot C_{p, \text{ash}} - \sum_{i=1}^n VC_i C_{pi} \right] \frac{r_w^2}{L}$$

$$\alpha_2 = \alpha_1 \frac{r_w^2}{F_c^o r_w^2}$$

$$D_{14} = \frac{F_c^o r_w^2}{L}$$

the material and heat balance equations, then, became

$$\frac{\partial U_1}{\partial X} = - \left(\frac{U_1}{U_7} \right) \frac{\partial U_7}{\partial X} + \left(\frac{\tilde{D}_1}{\tilde{D}_7} \right) \left(\frac{1}{U_7} \right) \left(\frac{\partial^2 U_1}{\partial y^2} + \frac{1}{y} \frac{\partial U_1}{\partial y} \right) - \left(\frac{1}{\tilde{D}_7} \right) \left(\frac{R_2}{U_7} \right)$$

$$\frac{\partial U_2}{\partial X} = - \left(\frac{U_2}{U_7} \right) \frac{\partial U_7}{\partial X} + \left(\frac{\tilde{D}_2}{\tilde{D}_7} \right) \left(\frac{1}{U_7} \right) \left(\frac{\partial^2 U_2}{\partial y^2} + \frac{1}{y} \frac{\partial U_2}{\partial y} \right) - \left(\frac{1}{\tilde{D}_7} \right) \left(\frac{1}{U_7} \right)$$

$$\frac{\partial U_3}{\partial X} = - \left(\frac{U_3}{U_7} \right) \frac{\partial U_7}{\partial X} + \left(\frac{\tilde{D}_3}{\tilde{D}_7} \right) \left(\frac{1}{U_7} \right) \left(\frac{\partial^2 U_3}{\partial y^2} + \frac{1}{y} \frac{\partial U_3}{\partial y} \right) + \left(\frac{1}{\tilde{D}_7} \right) (\alpha_1) \left(\frac{R_4}{U_7} \right)$$

$$\frac{\partial U_4}{\partial X} = - \left(\frac{U_4}{U_7} \right) \frac{\partial U_7}{\partial X} + \left(\frac{\tilde{D}_4}{\tilde{D}_7} \right) \left(\frac{1}{U_7} \right) \left(\frac{\partial^2 U_4}{\partial y^2} + \frac{1}{y} \frac{\partial U_4}{\partial y} \right) + \left(\frac{1}{\tilde{D}_7} \right) \left(\frac{1 + 2(\lambda-1)R_2 + 2R_3}{U_7} \right)$$

$$\frac{\partial U_5}{\partial X} = -\left(\frac{U_5}{U_7}\right)\left(\frac{\partial U_7}{\partial X}\right) + \left(\frac{\tilde{D}_5}{\tilde{D}_7}\right)\left(\frac{1}{U_7}\right)\left(\frac{\partial^2 U_5}{\partial y^2} + \frac{1}{y} \frac{\partial U_5}{\partial y}\right) + \left(\frac{1}{\tilde{D}_7}\right)\left(\frac{(2-\lambda) R_2 - R_3}{U_7}\right)$$

$$\frac{\partial U_6}{\partial X} = -\left(\frac{U_6}{U_7}\right)\left(\frac{\partial U_7}{\partial X}\right) + \left(\frac{\tilde{D}_6}{\tilde{D}_7}\right)\left(\frac{1}{U_7}\right)\left(\frac{\partial^2 U_6}{\partial y^2} + \frac{1}{y} \frac{\partial U_6}{\partial y}\right) + \left(\frac{1}{\tilde{D}_7}\right)\left(\frac{R_1 - 2\alpha_1 R_4}{U_7}\right)$$

$$\frac{\partial U_7}{\partial X} = \left(\frac{\tilde{D}_8}{\tilde{D}_9}\right)\left(\frac{\partial^2 U_7}{\partial y^2} + \frac{1}{y} \frac{\partial U_7}{\partial y}\right) + \left(\frac{\alpha_2}{\tilde{D}_9}\right)(R_1 D_{10} + R_2 D_{11} + R_3 D_{12} + \alpha_1 R_4 D_{13})$$

$$\frac{\partial U_8}{\partial X} = \left(\frac{\alpha_2}{\tilde{D}_{14}}\right)[R_1 D_{10} + R_2 D_{11} + R_3 D_{12} + \alpha_1 R_4 D_{13}]$$

with the boundary conditions that

$$\left\{ \begin{array}{ll} U_j = U_{j0} & \text{at } X=0, \text{ and } 0 < y \leq 1. \\ & \text{for } j=1, 2, \dots, 7 \\ U_8 = U_{8L} & \text{at } X=1 \text{ and } 0 < y \leq 1. \end{array} \right.$$

$$\left\{ \begin{array}{ll} \frac{\partial U_j}{\partial y} = 0 & \text{at } 0 < X \leq 1 \text{ and } y = 0. \\ & \text{for } j = 1, 2, \dots, 7 \\ \frac{\partial U_j}{\partial y} = 0 & \text{at } 0 < x \leq 1 \text{ and } y = 1. \\ & \text{for } j = 1, 2, \dots, 6 \\ \frac{\partial U_7}{\partial y} = \left(\frac{\tilde{U}_w}{\lambda_{er}}\right)(U_7 - T_c) & \text{at } 0 < x \leq 1 \text{ and } y = 1. \end{array} \right.$$

the apparent reaction rates, R_i , are

$$R_1 = \frac{\bar{R} (1-\epsilon) (U_2 - U_2^*) U_7}{\frac{R_p}{3k_{p2}} + \frac{R_p (R_p - r_c) (\beta)}{3 \left(\frac{r_c}{R_p}\right) (D_{eff.1})_o} \sqrt{\frac{\beta}{U_7}} + \frac{1}{\eta \left(\frac{r_c}{R_p}\right)^3 k_1 C_c^o}}$$

$$R_2 = \frac{\bar{R} (1-\epsilon) (U_1) (U_7)}{\frac{R_p}{3k_{p1}} + \frac{R_p (R_p - r_c) (\beta)}{3 \left(\frac{r_c}{R_p}\right) (D_{eff.2})_o} \sqrt{\frac{\beta}{U_7}} + \frac{1}{\eta \left(\frac{r_c}{R_p}\right)^3 k_2 C_c^o}}$$

$$R_3 = \eta k_3 C_c^o \bar{R} (1-\epsilon) (U_5) (U_7)$$

$$R_4 = \eta k_4 C_c^o \bar{R}^2 (1-\epsilon) (U_6)^2 (U_7)^2$$

$$\text{and } U_2^* = \frac{U_5 U_6}{K_5 U_4}$$

where

$$k_j = k_j^0 e^{-E_j/RT_7} \quad \text{for } j = 1, 2, \dots, 4.$$

are the intrinsic reaction rate constant respectively associated with

- $$\left\{ \begin{array}{l} j = 1. \dots \text{carbon-steam reaction} \\ j = 2. \dots \text{carbon-oxygen reaction} \\ j = 3. \dots \text{carbon-carbon dioxide reaction} \\ j = 4. \dots \text{carbon-hydrogen reaction} \end{array} \right.$$

$$K_5 = K_5^o e^{-\Delta H_5/RT_7} \quad \text{is the equilibrium constant for the water-gas shift reaction}$$

$D_{10} = \Delta H_1 \dots$ heat of reaction associated with C-H₂O reaction

$D_{11} = \Delta H_2 \dots$ heat of reaction associated with C-O₂ reaction

$D_{12} = \Delta H_3 \dots$ heat of reaction associated with C-CO₂ reaction

$D_{13} = \Delta H_4 \dots$ heat of reaction associated with C-H₂ reaction

$$\left\{ \begin{array}{l} k_{pj} \dots \text{mass transfer coefficient} \\ D_{effj} \dots \text{effective diffusivity for } j\text{-th gas component in the ash core} \end{array} \right.$$

These values are computed by the method described in Appendix B.

Appendix B

Estimation of Effective Diffusivity, D_{eff} ,
And Mass Transfer Coefficient k_{pi}

- (1) Estimation of effective diffusivity, D_{effi} .

The effective diffusivity, D_{effi} , is computed by the following equations:

$$D_{effi} = D_{im} \theta_s^2 \quad (B-1-1)$$

in which D_{im} is computed by

$$D_{im} = \frac{1 - x_i}{\sum_{j=1}^n \frac{x_j}{D_{ij}}} \quad (B-1-2)$$

and D_{ij} is computed by

$$D_{ij} = 1.8583 \times 10^{-3} \frac{\sqrt{T^3 \left(\frac{1}{M_i} + \frac{1}{M_j} \right)}}{P \sigma_{ij}^2 \Omega_D} \quad (B-1-3)$$

where

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \quad (B-1-4)$$

and σ_i and σ_j are tabulated in Table 5, Ω_D is read from Table 6 in

which $\frac{\kappa T}{\epsilon_{ij}}$ is defined as $\frac{\kappa T}{\epsilon_{ij}} = \sqrt{\frac{\kappa T}{\epsilon_i} \times \frac{\kappa T}{\epsilon_j}}$ (B-1-5)

$\frac{\kappa T}{\epsilon_i}$ and $\frac{\kappa T}{\epsilon_j}$ are tabulated in Table 5

θ_s in Equation (B-1-1) is the void fraction in the ash layer embracing a coal particle.

- (2) Estimation of mass transfer coefficient, k_{pi} .

The mass transfer coefficient, k_{pi} , is computed by the following equations:

$$k_{pi} = \frac{2.06}{\epsilon P} S_c^{-.092} \left(\frac{P D_{im}}{2R_p RT} \right)^{.575} F_G^{.425} \quad (B-2-1)$$

in which

$$S_c = \left(\frac{\mu_m}{D_{im} \frac{PM}{RT}} \right) \quad (B-2-2)$$

D_{im} is computed by Equation (B-1-2), and the viscosity of gas mixture, μ_m , is computed by

$$\mu_m = \frac{\sum_{i=1}^n \frac{X_i \mu_i}{\sum_{j=1}^n X_j \phi_{ij}}}{\sum_{j=1}^n X_j \phi_{ij}} \quad (B-2-3)$$

and

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-\frac{1}{2}} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left(\frac{M_j}{M_i} \right)^{\frac{1}{4}} \right]^2 \quad (B-2-4)$$

viscosity of each specie i , μ_i , is computed by

i) For non-polar gases ... Chapman-Enskog equation

$$\mu_i = 2.6693 \times 10^{-5} \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega_\mu} \quad (B-2-5)$$

Here, σ_i and Ω_μ are obtained from Table 5 and Table 6 respectively.

ii) For polar gases ...

The equation used for a calculation of carbon monoxide viscosity is

$$\mu_i = 0.012385 + 0.001712 \sqrt{T}. \quad (B-2-6)$$

TABLE 5. INTERMOLECULAR FORCE PARAMETERS

Substance	Molecular Weight M	Lennard-Jones Parameters	
		σ (Å)	ϵ/κ (°K)
H ₂	2.016	2.915	38.0
Air	28.97	3.617	97.0
N ₂	28.02	3.681	91.5
O ₂	32.00	3.433	113.
CO	28.01	3.590	110.
CO ₂	44.01	3.996	190.
SO ₂	64.07	4.290	252.
CH ₄	16.04	3.822	137.
C ₂ H ₄	28.05	4.232	205.
C ₂ H ₆	30.07	4.418	230.
COS	60.08	4.13	335.
CS ₂	76.14	4.430	488.

Table 6.

FUNCTIONS FOR PREDICTION OF TRANSPORT PROPERTIES OF GASES AT
LOW DENSITIES^a

$\kappa T/\epsilon$ or $\kappa T/\epsilon_{AB}$	$\Omega_\mu = \Omega_k$ (For viscosity and thermal conductivity)	$\Omega_{\mathcal{D},AB}$ (For mass diffusivity)	$\kappa T/\epsilon$ or $\kappa T/\epsilon_{AB}$	$\Omega_\mu = \Omega_k$ (For viscosity and thermal conductivity)	$\Omega_{\mathcal{D},AB}$ (For mass diffusivity)
0.30	2.785	2.662	2.50	1.093	0.9996
0.35	2.628	2.476	2.60	1.081	0.9878
0.40	2.492	2.318	2.70	1.069	0.9770
0.45	2.368	2.184	2.80	1.058	0.9672
0.50	2.257	2.066	2.90	1.048	0.9576
0.55	2.156	1.966	3.00	1.039	0.9490
0.60	2.065	1.877	3.10	1.030	0.9406
0.65	1.982	1.798	3.20	1.022	0.9328
0.70	1.908	1.729	3.30	1.014	0.9256
0.75	1.841	1.667	3.40	1.007	0.9186
0.80	1.780	1.612	3.50	0.9999	0.9120
0.85	1.725	1.562	3.60	0.9932	0.9058
0.90	1.675	1.517	3.70	0.9870	0.8998
0.95	1.629	1.476	3.80	0.9811	0.8942
1.00	1.587	1.439	3.90	0.9755	0.8888
1.05	1.549	1.406	4.00	0.9700	0.8836
1.10	1.514	1.375	4.10	0.9649	0.8788
1.15	1.482	1.346	4.20	0.9600	0.8740
1.20	1.452	1.320	4.30	0.9553	0.8694
1.25	1.424	1.296	4.40	0.9507	0.8652
1.30	1.399	1.273	4.50	0.9464	0.8610
1.35	1.375	1.253	4.60	0.9422	0.8568
1.40	1.353	1.233	4.70	0.9382	0.8530
1.45	1.333	1.215	4.80	0.9343	0.8492
1.50	1.314	1.198	4.90	0.9305	0.8456
1.55	1.296	1.182	5.0	0.9269	0.8422
1.60	1.279	1.167	6.0	0.8963	0.8124
1.65	1.264	1.153	7.0	0.8727	0.7896
1.70	1.248	1.140	8.0	0.8538	0.7712
1.75	1.234	1.128	9.0	0.8379	0.7556
1.80	1.221	1.116	10.0	0.8242	0.7424
1.85	1.209	1.105	20.0	0.7432	0.6640
1.90	1.197	1.094	30.0	0.7005	0.6232
1.95	1.186	1.084	40.0	0.6718	0.5960
2.00	1.175	1.075	50.0	0.6504	0.5756
2.10	1.156	1.057	60.0	0.6335	0.5596
2.20	1.138	1.041	70.0	0.6194	0.5464
2.30	1.122	1.026	80.0	0.6076	0.5352
2.40	1.107	1.012	90.0	0.5973	0.5256
			100.0	0.5882	0.5170

^a Taken from J. O. Hirschfelder, R. B. Bird, and E. L. Spotz, *Chem. Revs.*, **44**, 205 (1949).

Nomenclature

D_{effi}	= Effective diffusivity of i-th gas component in the shell of coal, cm^2/sec
D_{ij}	= Binary diffusivity, cm^2/sec
D_{im}	= Gas diffusivity in multicomponent gas mixture, cm^2/sec
F_G	= Total molar flux of gas phase, $\text{g-mol}/\text{cm}^2 \cdot \text{sec}$
M_i	= Molecular weight of i-th component, g/g-mole
P	= Reactor operating pressure, atm
$\bar{R}$	= Gas constant, $82.057 \text{ cm}^3\text{-atm/g-mole} \cdot ^\circ\text{K}$
R_p	= Coal particle radius, cm
T	= Temperature, $^\circ\text{K}$
X_i	= Mole fraction of i-th component in a mixture
ϵ	= Void fraction of moving bed
$\sigma_i, \epsilon_i/\text{K}$	= Lennard-Jones parameters (see Table 5.)
Ω_μ, Ω_D	= Function for prediction of transport properties (See Table 6.)
μ_i	= Viscosity of i-th component, $\text{g}/\text{cm} \cdot \text{sec}$
θ_s	= Void fraction in the shell of particle
S_c	= Schmidt number

Appendix C
PDECOL Program User's Guide⁽²⁰⁾

The methods in PDECOL are based on the method of lines with collocation that converts partial differential equations into ordinary differential equations. The structure of PDECOL includes a driver subroutine, a core integrator which advances the time by a single time step, and routines which assist in setting up and solving nonlinear and linear equations.

The interconnections and line of communication in PDECOL are quite complicated and difficult to understand when viewed as a whole. However, when the driver program and the core integrator are isolated, the pictures become clear. Figure 7 illustrates all of the package and user subroutines and their interconnections. A brief summary of the basic functions of all of the packages is contained in this Appendix.

FIGURE 7. LINES OF COMMUNICATION BETWEEN USER ROUTINES AND PDECOL PACKAGE ROUTINES (USER ROUTINES ARE INDICATED BY HEAVY BORDERS)

```

C      SUBROUTINE PDECOL(T0,T0U1,DT,XHKPT,EPS,NINT,KORD,NCC,NPDE,MF,
C      *      INDEX,WORK,TWORK)
C
C      -----
C
C      THIS IS THE SEPT 23, 1977 VERSION OF PDECOL.
C
C      THIS PACKAGE WAS CONSTRUCTED SO AS TO CONFORM TO AS MANY ANSI-FORTRAN
C      RULES AS WAS CONVENIENTLY POSSIBLE. THE FORTRAN USED VIOLATES ANSI
C      STANDARDS IN THE TWO WAYS LISTED BELOW....
C
C      1. SUBSCRIPTS OF THE GENERAL FORM C*V1 + V2 + V3 ARE USED
C      (POSSIBLY IN A PERMUTED ORDER), WHERE C IS AN INTEGER CONSTANT
C      AND V1, V2, AND V3 ARE INTEGER VARIABLES.
C
C      2. ARRAY NAMES APPEAR SINGLY IN DATA STATEMENTS IN THE ROUTINES
C      BSPLVN AND COSET.
C
C      -----
C
C      PDECOL IS THE DRIVER ROUTINE FOR A SOPHISTICATED PACKAGE OF
C      SUBROUTINES WHICH IS DESIGNED TO SOLVE THE GENERAL SYSTEM OF
C      NPDE NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS OF AT MOST SECOND
C      ORDER ON THE INTERVAL (XLEFT,XRIGHT) FOR T.GT. TO WHICH IS OF THE
C      FORM....
C
C      
$$\frac{DU}{DT} = F(T, X, U, UX, UXX)$$

C
C      WHERE
C
C      
$$U = (U(1), U(2), \dots, U(NPDE))$$

C      
$$UX = (UX(1), UX(2), \dots, UX(NPDE))$$

C      
$$UXX = (UXX(1), UXX(2), \dots, UXX(NPDE))$$

C
C      EACH U(K) IS A FUNCTION OF THE SCALAR QUANTITIES T AND X.
C      UX(K) REPRESENTS THE FIRST PARTIAL DERIVATIVE OF U(K) WITH RESPECT
C      TO THE VARIABLE X, UXX(K) REPRESENTS THE SECOND PARTIAL DERIVATIVE
C      OF U(K) WITH RESPECT TO THE VARIABLE X, AND DU/DT IS THE VECTOR OF
C      PARTIAL DERIVATIVES OF U WITH RESPECT TO THE TIME VARIABLE T.
C      F REPRESENTS AN ARBITRARY VECTOR VALUED FUNCTION WHOSE NPDE
C      COMPONENTS DEFINE THE RESPECTIVE PARTIAL DIFFERENTIAL EQUATIONS OF
C      THE PDE SYSTEM. SEE SUBROUTINE F DESCRIPTION BELOW.
C
C      BOUNDARY CONDITIONS
C
C      DEPENDING ON THE TYPE OF PDE(S), 0, 1, OR 2 BOUNDARY CONDITIONS
C      ARE REQUIRED FOR EACH PDE IN THE SYSTEM. THESE ARE IMPOSED AT XLEFT
C      AND/OR XRIGHT AND EACH MUST BE OF THE FORM....
C
C      
$$B(U,UX) = Z(T)$$

C
C      WHERE B AND Z ARE ARBITRARY VECTOR VALUED FUNCTIONS WITH
C      NPDE COMPONENTS AND U, UX, AND T ARE AS ABOVE. THESE BOUNDARY
C      CONDITIONS MUST BE CONSISTENT WITH THE INITIAL CONDITIONS WHICH ARE
C      DESCRIBED NEXT.
C
C      INITIAL CONDITIONS
C
C      EACH SOLUTION COMPONENT U(K) IS ASSUMED TO BE A KNOWN (USER
C      PROVIDED) FUNCTION OF X AT THE INITIAL TIME T = T0. THE

```


C INITIAL CONDITION FUNCTIONS MUST BE CONSISTENT WITH THE BOUNDARY
C CONDITIONS ABOVE, I.E. THE INITIAL CONDITION FUNCTIONS MUST
C SATISFY THE BOUNDARY CONDITIONS FOR $T = T_0$. SEE SUBROUTINE UINIT
C DESCRIPTION BELOW.

C-----

C
C REQUIRED USER SUPPLIED SUBROUTINES

C THE USER IS REQUIRED TO CONSTRUCT THREE SUBPROGRAMS AND A MAIN
C PROGRAM WHICH DEFINE THE PDE PROBLEM WHOSE SOLUTION IS TO BE
C ATTEMPTED. THE THREE SUBPROGRAMS ARE...

C
C 1) SUBROUTINE F(T, X, U, UX, UXX, FVAL, NPDE)

```

C      DIMENSION U(NPDE), UX(NPDE), UXX(NPDE), FVAL(NPDE)
C      THIS ROUTINE DEFINES THE DESIRED PARTIAL DIFFERENTIAL
C      EQUATIONS TO BE SOLVED. THE PACKAGE PROVIDES VALUES OF THE
C      INPUT SCALARS T AND X AND INPUT ARRAYS (LENGTH NPDE) U, UX,
C      AND UXX, AND THE USER MUST CONSTRUCT THIS ROUTINE TO COMPUTE
C      THE OUTPUT ARRAY FVAL (LENGTH NPDE) WHICH CONTAINS THE
C      CORRESPONDING VALUES OF THE RIGHT HAND SIDES OF THE DESIRED
C      PARTIAL DIFFERENTIAL EQUATIONS, I.E.
C
C      FVAL(K) = THE VALUE OF THE RIGHT HAND SIDE OF THE K-TH PDE IN
C      THE PDE SYSTEM ABOVE, FOR K = 1 TO NPDE.
C
C      THE INCOMING VALUE OF THE SCALAR QUANTITY X WILL BE A
C      COLLOCATION POINT VALUE (SEE INITIAL AND COLPMI) AND THE
C      INCOMING VALUES IN THE ARRAYS U, UX AND UXX CORRESPOND TO THIS
C      POINT X AND TIME T.
C      RETURN
C      END
C 2) SUBROUTINE BNDRY( T, X, U, UX, DBDU, DBDUX, DZDT, NPDE )
C      DIMENSION U(NPDE), UX(NPDE), DZDT(NPDE)
C      DIMENSION DBDU(NPDE,NPDE), DBDUX(NPDE,NPDE)
C      THIS ROUTINE IS USED TO PROVIDE THE PDE PACKAGE WITH NEEDED
C      INFORMATION ABOUT THE BOUNDARY CONDITION FUNCTIONS B AND Z
C      ABOVE. THE PACKAGE PROVIDES VALUES OF THE INPUT VARIABLES
C      T, X, U, AND UX, AND THE USER IS TO DEFINE THE CORRESPONDING
C      OUTPUT VALUES OF THE DERIVATIVES OF THE FUNCTIONS B AND Z
C      WHERE....
C      DBDU(K,J) = PARTIAL DERIVATIVE OF THE K-TH COMPONENT OF THE
C      VECTOR FUNCTION B(U,UX) ABOVE WITH RESPECT TO
C      THE J-TH VARIABLE U(J).
C      DBDUX(K,J) = PARTIAL DERIVATIVE OF THE K-TH COMPONENT OF THE
C      VECTOR FUNCTION B(U,UX) ABOVE WITH RESPECT TO
C      THE J-TH VARIABLE UX(J).
C      DZDT(K) = DERIVATIVE OF THE K-TH COMPONENT OF THE VECTOR
C      FUNCTION Z(U) ABOVE WITH RESPECT TO THE
C      VARIABLE T.
C      NOTE... THE INCOMING VALUE OF X WILL BE EITHER XLEFT OR XRIGHT.
C      IF NO BOUNDARY CONDITION IS DESIRED FOR SAY THE K-TH PDE AT
C      ONE OR BOTH OF THE ENDPOINTS XLEFT OR XRIGHT, THEN DBDU(K,K)
C      AND DBDUX(K,K) SHOULD BOTH BE SET TO ZERO WHEN BNDRY IS
C      CALLED FOR THAT POINT. WE REFER TO THIS AS A NULL BOUNDARY
C      CONDITION. THIS ROUTINE CAN BE STRUCTURED AS FOLLOWS...
C      THE COMMON BLOCK /ENDPT/ IS NOT A PART OF PDECOL AND
C      MUST BE SUPPLIED AND DEFINED BY THE USER.
C      COMMON /ENDPT/ XLEFT
C      IF( X.NE. XLEFT ) GO TO 10
C      HERE DEFINE AND SET PROPER VALUES FOR DBDU(K,J), DBDUX(K,J),
C      AND DZDT(K) FOR K,J = 1 TO NPDE FOR THE LEFT BOUNDARY POINT
C      X = XLEFT.
C      RETURN
C 10 CONTINUE
C      HERE DEFINE AND SET PROPER VALUES FOR DBDU(K,J), DBDUX(K,J),
C      AND DZDT(K) FOR K,J = 1 TO NPDE FOR THE RIGHT BOUNDARY POINT
C      X = XRIGHT.
C      RETURN
C      END
C 3) SUBROUTINE UINIT( X, U, NPDE ) :
C      DIMENSION U(NPDE)
C      THIS ROUTINE IS USED TO PROVIDE THE PDE PACKAGE WITH THE
C      NEEDED INITIAL CONDITION FUNCTION VALUES. THE PACKAGE
C      PROVIDES A VALUE OF THE INPUT VARIABLE X, AND THE USER IS TO

```

```

C      DEFINE THE PROPER INITIAL VALUES (AT  $T = T_0$ ) FOR ALL OF THE
C      PDE COMPONENTS, I.E.
C       $U(K) =$  DESIRED INITIAL VALUE OF PDE COMPONENT  $U(K)$  AT
C       $X$  AND  $T = T_0$  FOR  $K = 1$  TO NPDE.
C      NOTE... THE INCOMING VALUE OF  $X$  WILL BE A COLLOCATION POINT
C      VALUE. THE INITIAL CONDITIONS AND BOUNDARY CONDITIONS
C      MUST BE CONSISTENT (SEE ABOVE).
C      RETURN
C      END
C-----
C
C  OPTIONAL USER SUPPLIED SUBROUTINE
C

```

C IF THE USER DESIRES TO USE THE MF = 11 OR 21 OPTION IN ORDER TO SAVE
C ABOUT 10-20 PERCENT IN EXECUTION TIME (SEE BELOW), THEN THE USER MUST
C PROVIDE THE FOLLOWING SUBROUTINE WHICH PROVIDES INFORMATION ABOUT THE
C DERIVATIVES OF THE FUNCTION F ABOVE. THIS PROVIDES FOR MORE EFFICIENT
C JACOBIAN MATRIX GENERATION. ON MOST COMPUTER SYSTEMS, THE USER WILL
C BE REQUIRED TO SUPPLY THIS SUBROUTINE AS A DUMMY SUBROUTINE IF THE
C OPTIONS MF = 12 OR 22 ARE USED (SEE BELOW).

C 1) SUBROUTINE DERIVE(T, X, U, UX, UXX, DFDU, DFDUX, DFDUXX, NPDE)
C DIMENSION U(NPDE), UX(NPDE), UXX(NPDE)
C DIMENSION DFDU(NPDE,NPDE), DFDUX(NPDE,NPDE), DFDUXX(NPDE,NPDE)
C THE PACKAGE PROVIDES VALUES OF THE INPUT VARIABLES T, X, U, UX,
C AND UXX, AND THE USER SHOULD CONSTRUCT THIS ROUTINE TO PROVIDE
C THE FOLLOWING CORRESPONDING VALUES OF THE OUTPUT ARRAYS
C DFDU, DFDUX, AND DFDUXX FOR K,J = 1 TO NPDE...
C DFDU(K,J) = PARTIAL DERIVATIVE OF THE K-TH COMPONENT OF THE
C PDE DEFINING FUNCTION F WITH RESPECT TO THE
C VARIABLE U(J).
C DFDUX(K,J) = PARTIAL DERIVATIVE OF THE K-TH COMPONENT OF THE
C PDE DEFINING FUNCTION F WITH RESPECT TO THE
C VARIABLE UX(J).
C DFDUXX(K,J) = PARTIAL DERIVATIVE OF THE K-TH COMPONENT OF THE
C PDE DEFINING FUNCTION F WITH RESPECT TO THE
C VARIABLE UXX(J).

C NOTE... THE INCOMING VALUE OF X WILL BE A COLLOCATION POINT
C VALUE.

C RETURN
C END

C METHODS USED

C THE PACKAGE PDECOL IS BASED ON THE METHOD OF LINES AND USES A
C FINITE ELEMENT COLLOCATION PROCEDURE (WITH PIECEWISE POLYNOMIALS
C AS THE TRIAL SPACE) FOR THE DISCRETIZATION OF THE SPATIAL VARIABLE
C X. THE COLLOCATION PROCEDURE REDUCES THE PDE SYSTEM TO A SEMI-
C DISCRETE SYSTEM WHICH THEN DEPENDS ONLY ON THE TIME VARIABLE T.
C THE TIME INTEGRATION IS THEN ACCOMPLISHED BY USE OF SLIGHTLY
C MODIFIED STANDARD TECHNIQUES (SEE REFS. 1,2).

C PIECEWISE POLYNOMIALS

C THE USER IS REQUIRED TO SELECT THE PIECEWISE POLYNOMIAL SPACE
C WHICH IS TO BE USED TO COMPUTE HIS APPROXIMATE SOLUTION. FIRST, THE
C ORDER, KORD, OF THE POLYNOMIALS TO BE USED MUST BE SPECIFIED
C (KORD = POLYNOMIAL DEGREE + 1). NEXT, THE NUMBER OF PIECES
C (INTERVALS), NINT, INTO WHICH THE SPATIAL DOMAIN (XLEFT,XRIGHT) IS
C TO BE DIVIDED, IS CHOSEN. THE NINT + 1 DISTINCT BREAKPOINTS OF
C THE DOMAIN MUST BE DEFINED AND SET INTO THE ARRAY XBKPT IN
C STRICTLY INCREASING ORDER, I.E.
C XLEFT=XBKPT(1) .LT. XBKPT(2) .LT.LT. XBKPT(NINT+1)=XRIGHT.
C THE APPROXIMATE SOLUTION AT ANY TIME T WILL BE A POLYNOMIAL OF
C ORDER KORD OVER EACH SUBINTERVAL (XBKPT(I),XBKPT(I+1)). THE
C NUMBER OF CONTINUITY CONDITIONS, NCC, TO BE IMPOSED ACROSS ALL OF
C THE BREAKPOINTS IS THE LAST PIECE OF USER SUPPLIED DATA WHICH IS
C REQUIRED TO UNIQUELY DETERMINE THE DESIRED PIECEWISE POLYNOMIAL
C SPACE. FOR EXAMPLE, NCC = 2 WOULD REQUIRE THAT THE APPROXIMATE
C SOLUTION (MADE UP OF THE SEPARATE POLYNOMIAL PIECES) AND ITS FIRST
C SPATIAL DERIVATIVE BE CONTINUOUS AT THE BREAKPOINTS AND HENCE ON
C THE ENTIRE DOMAIN (XLEFT,XRIGHT). NCC = 3 WOULD REQUIRE THAT THE
C APPROXIMATE SOLUTION AND ITS FIRST AND SECOND SPATIAL DERIVATIVES
C BE CONTINUOUS AT THE BREAKPOINTS, ETC. THE DIMENSION OF THIS LINEAR
C SPACE IS KNOWN AND FINITE AND IS NCPIS = KORD*NINT - NCC*(NINT-1).

C THE WELL-KNOWN B-SPLINE BASIS (SEE REF. 3) FOR THIS SPACE IS USED
C BY PDECOL AND IT CONSISTS OF NCPTS KNOWN PIECEWISE POLYNOMIAL
C FUNCTIONS $BF(I,X)$, FOR $I=1$ TO NCPTS, WHICH DO NOT DEPEND ON THE
C TIME VARIABLE T . WE WISH TO EMPHASIZE THAT THE PIECEWISE POLYNOMIAL
C SPACE USED IN PDECOL (WHICH IS SELECTED BY THE USER) WILL DETERMINE
C THE MAGNITUDE OF THE SPATIAL DISCRETIZATION ERRORS IN THE COMPUTED
C APPROXIMATE SOLUTION. THE PACKAGE HAS NO CONTROL OVER ERRORS
C INTRODUCED BY THE USER'S CHOICE OF THIS SPACE. SEE INPUT PARAMETERS
C BELOW.
C
C COLLOCATION OVER PIECEWISE POLYNOMIALS
C
C THE BASIC ASSUMPTION MADE IS THAT THE APPROXIMATE SOLUTION

C SATISFIES

C NCPIS

C $U(T,X) = \sum_{I=1} C(I,T) * BF(I,X)$

C WHERE THE UNKNOWN COEFFICIENTS C DEPEND ONLY ON THE TIME T AND
C THE KNOWN BASIS FUNCTIONS DEPEND ONLY ON X (WE HAVE ASSUMED THAT
C $NPDF = 1$ FOR CONVENIENCE). SO, AT ANY GIVEN TIME T THE APPROX-
CIMATE SOLUTION IS A PIECEWISE POLYNOMIAL IN THE USER CHOSEN SPACE.
C THE SEMI-DISCRETE EQUATIONS (ACTUALLY ORDINARY DIFFERENTIAL
C EQUATIONS) WHICH DETERMINE THE COEFFICIENTS C ARE OBTAINED BY
C REQUIRING THAT THE ABOVE APPROXIMATE $U(T,X)$ SATISFY THE PDE AND
C BOUNDARY CONDITIONS EXACTLY AT A SET OF NCPTS COLLOCATION POINTS
C (SEE COLPNT). THUS, PDECOL ACTUALLY COMPUTES THE BASIS FUNCTION
C COEFFICIENTS RATHER THAN SPECIFIC APPROXIMATE SOLUTION VALUES.

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C USE OF PDECOL

C PDECOL IS CALLED ONCE FOR EACH DESIRED OUTPUT VALUE (TOUT) OF THE
C TIME T, AND IT IN TURN MAKES REPEATED CALLS TO THE CORE INTEGRATOR,
C STIFIB, WHICH ADVANCES THE TIME BY TAKING SINGLE STEPS UNTIL
C $T \geq TOUT$. INTERPOLATION TO THE EXACT TIME TOUT IS THEN DONE.
C SEE TOUT BELOW.

C SUMMARY OF SUGGESTED INPUT VALUES

C IT IS OF COURSE IMPOSSIBLE TO SUGGEST INPUT PARAMETER VALUES WHICH
C ARE APPROPRIATE FOR ALL PROBLEMS. THE FOLLOWING SUGGESTIONS ARE TO
C BE USED ONLY IF YOU HAVE NO IDEA OF BETTER VALUES FOR YOUR PROBLEM.

C $DT = 1.E-10$

C $XBKPT =$ CHOOSE NINT+1 EQUALLY SPACED VALUES SUCH THAT $XBKPT(1) =$
C $XLEFT$ AND $XBKPT(NINT+1) = XRIGHT$.

C $EPS = 1.E-4$

C $NINT =$ ENOUGH SO THAT ANY FINE STRUCTURE OF THE PROBLEM MAY BE
C RESOLVED.

C $KORD = 4$

C $NCC = 2$

C $MF = 22$

C $INDEX = 1$ (ON FIRST CALL ONLY, THEN 0 THEREAFTER).

C THE INPUT PARAMETERS ARE..

C $T0 =$ THE INITIAL VALUE OF T, THE INDEPENDENT VARIABLE
C (USED ONLY ON FIRST CALL).

C $TOUT =$ THE VALUE OF T AT WHICH OUTPUT IS DESIRED NEXT. SINCE

```

C      THE PACKAGE CHOOSES ITS OWN TIME STEP SIZES, THE
C      INTEGRATION WILL NORMALLY GO SLIGHTLY BEYOND TOUT
C      AND THE PACKAGE WILL INTERPOLATE TO T = TOUT.
C      DT      = THE INITIAL STEP SIZE IN 1, IF INDEX = 1, OR, THE
C      MAXIMUM STEP SIZE ALLOWED (MUST BE .GT. 0), IF INDEX = 3.
C      USED FOR INPUT ONLY WHEN INDEX = 1 OR 3. SEE BELOW.
C      XBKPT = THE ARRAY OF PIECEWISE POLYNOMIAL BREAKPOINTS.
C      THE NINT+1 VALUES MUST BE STRICTLY INCREASING WITH
C      XBKPT(1) = XLEFT AND XBKPT(NINT+1) = XRIGHT (USED ONLY
C      ON FIRST CALL).
C      EPS      = THE RELATIVE TIME ERROR BOUND (USED ONLY ON THE
C      FIRST CALL, UNLESS INDEX = 4). SINGLE STEP ERROR
C      ESTIMATES DIVIDED BY CMAX(I) WILL BE KEPT LESS THAN 1

```

```

C      FPS IN ROOT-MEAN-SQUARE NORM. THE VECTOR CMAX OF WEIGHTS
C      IS COMPUTED IN PDECOL. INITIALLY CMAX(I) IS SET TO
C      ABS(C(I)), WITH A DEFAULT VALUE OF 1 IF ABS(C(I)) .LT. 1.
C      THEREAFTER, CMAX(I) IS THE LARGEST VALUE
C      OF ABS(C(I)) SEEN SO FAR, OR THE INITIAL CMAX(I) IF
C      THAT IS LARGER. TO ALTER EITHER OF THESE, CHANGE THE
C      APPROPRIATE STATEMENTS IN THE DO-LOOPS ENDING AT
C      STATEMENTS 50 AND 130 BELOW. THE USER SHOULD EXERCISE
C      SOME DISCRETION IN CHOOSING FPS. IN GENERAL, THE
C      OVERALL RUNNING TIME FOR A PROBLEM WILL BE GREATER IF
C      FPS IS CHOSEN SMALLER. THERE IS USUALLY LITTLE REASON TO
C      CHOOSE FPS MUCH SMALLER THAN THE ERRORS WHICH ARE BEING
C      INTRODUCED BY THE USER'S CHOICE OF THE POLYNOMIAL SPACE.
C      SEE RELATED COMMENTS CONCERNING CMAX BELOW STATEMENT 40.
C      NINT = THE NUMBER OF SUBINTERVALS INTO WHICH THE SPATIAL DOMAIN
C      (XLEFT,XRIGHT) IS TO BE DIVIDED (MUST BE .GE. 1)
C      (USED ONLY ON FIRST CALL).
C      KORD = THE ORDER OF THE PIECEWISE POLYNOMIAL SPACE TO BE USED.
C      ITS VALUE MUST BE GREATER THAN 2 AND LESS THAN 21. FOR
C      FIRST ATTEMPTS WE RECOMMEND KORD = 4. IF THE SOLUTION
C      IS SMOOTH AND MUCH ACCURACY IS DESIRED, HIGHER VALUES
C      MAY PROVE TO BE MORE EFFICIENT. WE HAVE SELDOM USED
C      VALUES OF KORD IN EXCESS OF 8 OR 9, THOUGH THEY ARE
C      AVAILABLE FOR USE IN PDECOL (USED ONLY ON FIRST CALL).
C      NCC = THE NUMBER OF CONTINUITY CONDITIONS TO BE IMPOSED ON THE
C      APPROXIMATE SOLUTION AT THE BREAKPOINTS IN XRP1.
C      NCC MUST BE GREATER THAN 1 AND LESS THAN KORD. WE
C      RECOMMEND THE USE OF NCC = 2 (WITH NOGAUS = 0, SEE
C      BELOW), SINCE THEORY PREDICTS THAT DRAMATICALLY MORE
C      ACCURATE RESULTS CAN OFTEN BE OBTAINED USING THIS CHOICE
C      (USED ONLY ON FIRST CALL).
C      NPDE = THE NUMBER OF PARTIAL DIFFERENTIAL EQUATIONS IN THE SYSTEM
C      TO BE SOLVED (USED ONLY ON FIRST CALL).
C      MF = THE METHOD FLAG (USED ONLY ON FIRST CALL, UNLESS
C      INDEX = 4). ALLOWED VALUES ARE 11, 12, 21, 22.
C      FOR FIRST ATTEMPTS WE RECOMMEND THE USE OF MF = 22.
C      MF HAS TWO DECIMAL DIGITS, METH AND MITER
C      (MF = 10*METH + MITER).
C      METH IS THE BASIC METHOD INDICATOR..
C      METH = 1 MEANS THE ADAMS METHODS (GENERALIZATIONS OF
C      CRANK-NICOLSON).
C      METH = 2 MEANS THE BACKWARD DIFFERENTIATION
C      FORMULAS (BDF), OR STIFF METHODS OF GEAR.
C      MITER IS THE ITERATION METHOD INDICATOR
C      AND DETERMINES HOW THE JACOBIAN MATRIX IS
C      TO BE COMPUTED..
C      MITER = 1 MEANS CHORD METHOD WITH ANALYTIC JACOBIAN.
C      FOR THIS USER SUPPLIES SUBROUTINE DERIVE.
C      SEE DESCRIPTION ABOVE.
C      MITER = 2 MEANS CHORD METHOD WITH JACOBIAN CALCULATED
C      INTERNALLY BY FINITE DIFFERENCES. SEE
C      SUBROUTINES RSETH AND DIFE.
C      INDEX = INTEGER USED ON INPUT TO INDICATE TYPE OF CALL,
C      WITH THE FOLLOWING VALUES AND MEANINGS..
C      1 THIS IS THE FIRST CALL FOR THIS PROBLEM.
C      0 THIS IS NOT THE FIRST CALL FOR THIS PROBLEM,
C      AND INTEGRATION IS TO CONTINUE.
C      2 SAME AS 0 EXCEPT THAT TOUT IS TO BE SET
C      EXACTLY (NO INTERPOLATION IS DONE). SEE NOTE
C      BELOW. ASSUMES TOUT .GE. THE CURRENT T.
C      IF TOUT IS .11, THE CURRENT TIME, THEN TOUT IS
C      RESET TO THE CURRENT TIME AND CONTROL IS
C      RETURNED TO THE USER. A CALL TO VALUES WILL

```


C PRODUCE ANSWERS FOR THE NEW VALUE OF TOUT.
 C 3 SAME AS 0 EXCEPT CONTROL RETURNS TO CALLING
 C PROGRAM AFTER ONE STEP. TOUT IS IGNORED AND
 C DT MUST BE SET .GT. 0 TO A MAXIMUM ALLOWED
 C DT VALUE. SEE ABOVE.
 C 4 THIS IS NOT THE FIRST CALL FOR THE PROBLEM,
 C AND THE USER HAS RESET FPS AND/OR MF.
 C SINCE THE NORMAL OUTPUT VALUE OF INDEX IS 0,
 C IT NEED NOT BE RESET FOR NORMAL CONTINUATION.
 C
 C NOTE.. THE PACKAGE MUST HAVE TAKEN AT LEAST ONE SUCCESSFUL TIME
 C STEP BEFORE A CALL WITH INDEX = 2 OR 4 IS ALLOWED.
 C AFTER THE INITIAL CALL, IF A NORMAL RETURN OCCURRED AND A NORMAL

```

C CONTINUATION IS DESIRED, SIMPLY RESET IOUT AND CALL AGAIN.
C ALL OTHER PARAMETERS WILL BE READY FOR THE NEXT CALL.
C A CHANGE OF PARAMETERS WITH INDEX = 4 CAN BE MADE AFTER
C EITHER A SUCCESSFUL OR AN UNSUCCESSFUL RETURN PROVIDED AT LEAST
C ONE SUCCESSFUL TIME STEP HAS BEEN MADE.
C
C   WORK = FLOATING POINT WORKING ARRAY FOR PDECOL. WE RECOMMEND
C           THAT IT BE INITIALIZED TO ZERO BEFORE THE FIRST CALL
C           TO PDECOL. ITS TOTAL LENGTH MUST BE AT LEAST
C
C           KORD + 4*NPDE + 9*NPDE**2 + NCPTS*(3*KORD + 2) +
C           NPDE*NCPTS*(3*ML + MAXDER + 7).
C
C           WHERE ML AND MAXDER ARE DEFINED BELOW (SEE STORAGE
C           ALLOCATION).
C   IWORK = INTEGER WORKING ARRAY FOR PDECOL. THE FIRST TWO
C           LOCATIONS MUST BE DEFINED AS FOLLOWS...
C           IWORK(1) = LENGTH OF USERS ARRAY WORK
C           IWORK(2) = LENGTH OF USERS ARRAY IWORK
C           THE TOTAL LENGTH OF IWORK MUST BE AT LEAST
C           NCPTS*(NPDE + 1).
C OUTPUT
C
C THE SOLUTION VALUES ARE NOT RETURNED DIRECTLY TO THE USER BY PDECOL.
C THE METHODS USED IN PDECOL COMPUTE BASIS FUNCTION COEFFICIENTS, SO
C THE USER (AFTER A RETURN FROM PDECOL) MUST CALL THE PACKAGE ROUTINE
C VALUES TO OBTAIN HIS APPROXIMATE SOLUTION VALUES AT ANY DESIRED SPACE
C POINTS X AT THE TIME T = IOUT. SEE THE COMMENTS IN SUBROUTINE VALUES
C FOR DETAILS ON HOW TO PROPERLY MAKE THE CALL.
C
C THE COMMON BLOCK /GEAR0/ CAN BE ACCESSED EXTERNALLY BY THE USER
C IF DESIRED. IT CONTAINS THE STEP SIZE LAST USED (SUCCESSFULLY),
C THE ORDER LAST USED (SUCCESSFULLY), THE NUMBER OF STEPS TAKEN
C SO FAR, THE NUMBER OF RESIDUAL EVALUATIONS (RES CALLS) SO FAR,
C AND THE NUMBER OF MATRIX EVALUATIONS (PSETIB CALLS) SO FAR.
C DIFFUN CALLS ARE COUNTED IN WITH RESIDUAL EVALUATIONS.
C
C THE OUTPUT PARAMETERS ARE...
C   DT = THE STEP SIZE USED LAST, WHETHER SUCCESSFULLY OR NOT.
C   IOUT = THE OUTPUT VALUE OF T. IF INTEGRATION WAS SUCCESSFUL,
C           AND THE INPUT VALUE OF INDEX WAS NOT 3, IOUT IS
C           UNCHANGED FROM ITS INPUT VALUE. OTHERWISE, IOUT
C           IS THE CURRENT VALUE OF T TO WHICH THE INTEGRATION
C           HAS BEEN COMPLETED.
C   INDEX = INTEGER USED ON OUTPUT TO INDICATE RESULTS,
C           WITH THE FOLLOWING VALUES AND MEANINGS...
C           0   INTEGRATION WAS COMPLETED TO IOUT OR BEYOND.
C           -1  THE INTEGRATION WAS HALTED AFTER FAILING TO PASS THE
C           ERROR TEST EVEN AFTER REDUCING DT BY A FACTOR OF
C           1.E10 FROM ITS INITIAL VALUE.
C           -2  AFTER SOME INITIAL SUCCESS, THE INTEGRATION WAS
C           HALTED EITHER BY REPEATED ERROR TEST FAILURES OR BY
C           A TEST ON EPS. TOO MUCH ACCURACY HAS BEEN REQUESTED.
C           -3  THE INTEGRATION WAS HALTED AFTER FAILING TO ACHIEVE
C           CORRECTOR CONVERGENCE EVEN AFTER REDUCING DT BY A
C           FACTOR OF 1.E10 FROM ITS INITIAL VALUE.
C           -4  SINGULAR MATRIX ENCOUNTERED. PROBABLY DUE TO STORAGE
C           OVERWRITES.
C           -5  INDEX WAS 4 ON INPUT, BUT THE DESIRED CHANGES OF
C           PARAMETERS WERE NOT IMPLEMENTED BECAUSE IOUT
C           WAS NOT BEYOND T. INTERPOLATION TO T = IOUT WAS
C           PERFORMED AS ON A NORMAL RETURN. TO TRY AGAIN,
C           SIMPLY CALL AGAIN WITH INDEX = 4 AND A NEW IOUT.

```

C	-6	ILLEGAL INDEX VALUE.
C	-7	ILLEGAL EPS VALUE.
C	-8	AN ATTEMPT TO INTEGRATE IN THE WRONG DIRECTION. THE
C		SIGN OF DT IS WRONG RELATIVE TO TO AND TOUT.
C	-9	DT .EQ. 0.0.
C	-10	ILLEGAL MINT VALUE.
C	-11	ILLEGAL KORD VALUE.
C	-12	ILLEGAL NCC VALUE.
C	-13	ILLEGAL NPDE VALUE.
C	-14	ILLEGAL ME VALUE.
C	-15	ILLEGAL BREAKPOINTS - NOT STRICTLY INCREASING.
C	-16	INSUFFICIENT STORAGE FOR WORK OR IWORK.
C		-----

```

C
C
C SUMMARY OF ALL PACKAGE ROUTINES
C
C PDECOL - STORAGE ALLOCATION, ERROR CHECKING, INITIALIZATION, REPEATED
C          CALLS TO STIFIR TO ADVANCE THE TIME.
C
C INTERP - INTERPOLATES COMPUTED BASIS FUNCTION COEFFICIENTS TO THE
C          DESIRED OUTPUT TIMES, TOUT, FOR USE BY VALUES.
C
C INITIAL - INITIALIZATION, GENERATION AND STORAGE OF PIECEWISE POLY-
C          NOMIAL SPACE BASIS FUNCTION VALUES AND DERIVATIVES, DET-
C          ERMINES THE BASIS FUNCTION COEFFICIENTS OF THE PIECEWISE
C          POLYNOMIALS WHICH INTERPOLATE THE USERS INITIAL CONDITIONS.
C
C COLPNT - GENERATION OF REQUIRED COLLOCATION POINTS.
C
C BSPLVD - B-SPLINE PACKAGE ROUTINES WHICH ALLOW FOR EVALUATION OF
C          ANY B-SPLINE BASIS FUNCTION OR DERIVATIVE VALUE.
C
C INTERV
C
C VALUES - GENERATION AT ANY POINT(S) OF VALUES OF THE COMPUTED
C          APPROXIMATE SOLUTION AND ITS DERIVATIVES WHICH ARE
C          PIECEWISE POLYNOMIALS. THE SUBROUTINE IS CALLED ONLY BY
C          THE USER.
C
C STIFIR - CORE INTEGRATOR, TAKES SINGLE TIME STEPS TO ADVANCE THE
C          TIME. ASSEMBLES AND SOLVES THE PROPER NONLINEAR EQUATIONS
C          WHICH ARE RELATED TO USE OF ADAMS OR GEAR TYPE INTEGRATION
C          FORMULAS. CHOOSES PROPER STEP SIZE AND INTEGRATION FORMULA
C          ORDER TO MAINTAIN A DESIRED ACCURACY. DESIGNED FOR ODE
C          PROBLEMS OF THE FORM  $A * (DY/DT) = G(I,Y)$ .
C
C COSET - GENERATES INTEGRATION FORMULA AND ERROR CONTROL COEFFICIENTS.
C
C RES - COMPUTES RESIDUAL VECTORS USED IN SOLVING THE NONLINEAR
C          EQUATIONS BY A MODIFIED NEWTON METHOD.
C
C DIFFUN - COMPUTES  $A**(-1) * G(I,Y)$  WHERE A AND G ARE AS ABOVE (STIFIR).
C
C ADDA - ADDS THE A MATRIX TO A GIVEN MATRIX IN BAND FORM.
C
C EVAL - EVALUATES THE COMPUTED PIECEWISE POLYNOMIAL SOLUTION AND
C          DERIVATIVES AT COLLOCATION POINTS.
C
C GFUN - EVALUATES THE FUNCTION  $G(I,Y)$  BY CALLING EVAL AND THE USER
C          SUBROUTINES F AND BNDRY.
C
C PSETIB - GENERATES PROPER JACOBIAN MATRICES REQUIRED BY THE MODIFIED
C          NEWTON METHOD.
C
C DIFFE - PERFORMS SAME ROLE AS THE USER ROUTINE DERIVE. COMPUTES
C          DERIVATIVE APPROXIMATIONS BY USE OF FINITE DIFFERENCES.
C
C DECB - PERFORM AN LU DECOMPOSITION AND FORWARD AND BACKWARD
C          SUBSTITUTION FOR SOLVING Banded SYSTEMS OF LINEAR EQUATIONS.
C
C -----
C
C STORAGE ALLOCATION
C
C SINCE PDECOL IS A DYNAMICALLY DIMENSIONED PROGRAM, MOST OF ITS

```

C WORKING STORAGE IS PROVIDED BY THE USER IN THE ARRAYS WORK AND IWORK.
 C THE FOLLOWING GIVES A LIST OF THE ARRAYS WHICH MAKE UP THE CONTENTS
 C WORK AND IWORK, THEIR LENGTHS, AND THEIR USES. WHEN MORE THAN ONE
 C NAME IS GIVEN, IT INDICATES THAT DIFFERENT NAMES ARE USED FOR THE
 C SAME ARRAY IN DIFFERENT PARTS OF THE PROGRAM. THE DIFFERENT NAMES
 C OCCUR BECAUSE PDECOL IS AN AMALGAMATION OF SEVERAL OTHER CODES
 C WRITTEN BY DIFFERENT PEOPLE AND WE HAVE TRIED TO LEAVE THE SEPARATE
 C PARTS AS UNCHANGED FROM THEIR ORIGINAL VERSIONS AS POSSIBLE.

NAMES	LENGTH	USE
-----	-----	-----

C BC	4*NPDE**2	BOUNDARY CONDITION INFORMATION.
C WORK		
C A	3*KORD*NCPTS	BASIS FUNCTION VALUES AT COLLOCATION POINTS.
C WORK(IW1)		
C XT	NCPTS + KORD	BREAKPOINT SEQUENCE FOR GENERATION OF BASIS
C WORK(IW2)		FUNCTION VALUES.
C XC	NCPTS	COLLOCATION POINTS.
C WORK(IW3)		
C CMAX	NPDE*NCPTS	VALUES USED IN ESTIMATING TIME
C YMAX		INTEGRATION ERRORS.
C WORK(IW4)		
C ERROR	NPDE*NCPTS	TIME INTEGRATION ERRORS.
C WORK(IW5)		
C SAVE1	NPDE*NCPTS	WORKING STORAGE FOR THE TIME INTEGRATION
C WORK(IW6)		METHOD.
C SAVE2	NPDE*NCPTS	WORKING STORAGE FOR THE TIME INTEGRATION
C WORK(IW7)		METHOD.
C SAVE3	NPDE*NCPTS	WORKING STORAGE FOR THE TIME INTEGRATION
C WORK(IW8)		METHOD.
C UVAL	3*NPDE	WORKING STORAGE FOR VALUES OF U, UX, AND
C WORK(IW9)		USS AT ONE POINT.
C C	NPDE*NCPTS*	CURRENT BASIS FUNCTION COEFFICIENT VALUES
C Y	(MAXDER+1)	AND THEIR SCALED TIME DERIVATIVES.
C WORK(IW10)		
C DFDU	NPDE**2	WORKING STORAGE USED TO COMPUTE THE
C WORK(IW11)		JACOBIAN MATRIX.
C DFDUX	NPDE**2	WORKING STORAGE USED TO COMPUTE THE
C WORK(IW12)		JACOBIAN MATRIX.
C DFDUXX	NPDE**2	WORKING STORAGE USED TO COMPUTE THE
C WORK(IW13)		JACOBIAN MATRIX.
C DBDU	NPDE**2	BOUNDARY CONDITION INFORMATION.
C WORK(IW14)		
C DBDUX	NPDE**2	BOUNDARY CONDITION INFORMATION.
C WORK(IW15)		
C DZDT	NPDE	BOUNDARY CONDITION INFORMATION.
C WORK(IW16)		
C PW	NPDE*NCPTS*	STORAGE AND PROCESSING OF THE JACOBIAN
C WORK(IW17)	(3*ML+1)	MATRIX.
C ILEFT	NCPTS	POINTERS TO BREAKPOINT SEQUENCE FOR
C IWORK		GENERATION OF BASIS FUNCTION VALUES.
C IPIV	NPDE*NCPTS	PIVOT INFORMATION FOR THE LU DECOMPOSED
C IWORK(IW18)		JACOBIAN MATRIX PW.
C WHERE...		

```

C
C      NCPTS = KORD*NINT - NCC*(NINT-1)
C      ML = NPDE*(KORD+IQAD-1) - 1
C      IQAD = 1 IF KORD = 3 AND A NULL BOUNDARY CONDITION EXISTS
C      IQAD = 0 OTHERWISE
C      MAXDER = 5 UNLESS OTHERWISE SET BY THE USER INIO /OPTION/.
C
C THE COMMON BLOCK /OPTION/ CONTAINS THE VARIABLES NOGAUS AND MAXDER.
C NOGAUS IS SET .EQ. 0 IN THE BLOCK DATA. IT CAN BE CHANGED TO BE
C SET .EQ. 1 IF THE GAUSS-LEGENDRE COLLOCATION POINTS ARE NOT
C DESIRED WHEN NCC = 2 (SEE ABOVE AND COLPNT). MAXDER IS SET
C .EQ. 5 IN THE BLOCK DATA AND ITS VALUE REPRESENTS THE
C MAXIMUM ORDER OF TIME INTEGRATION FORMULA ALLOWED. ITS VALUE

```

```

C AFFECTS THE STORAGE REQUIRED IN WORK AND MAY BE CHANGED IF
C DESIRED. SEE COSET FOR RESTRICTIONS. THESE CHANGES MAY BE MADE BY
C THE USER BY ACCESSING /OPTION/ IN HIS CALLING PROGRAM (BEFORE THE
C FIRST CALL TO PDECOL) OR BY CHANGING THE DATA STATEMENT IN
C THE BLOCK DATA.
C
C-----
C
C COMMUNICATION
C
C EACH SUBROUTINE IN THE PACKAGE CONTAINS A COMMUNICATION SUMMARY
C AS INDICATED BELOW.
C
C PACKAGE ROUTINES CALLED.. EVAL,INITIAL,INTERP,STIFIR
C USER ROUTINES CALLED.. BNDRY
C CALLED BY.. USERS MAIN PROGRAM
C FORTRAN FUNCTIONS USED.. ABS,AMAX1,FLOAT, SORT
C-----
0001 SUBROUTINE PDECOL(TO,TOUT,DT,XRKPT,EPS,NINT,KORD,NCC,NPDE,MF,
* INDEX,WORK,IWORK)
0002 DIMENSION WORK(1),IWORK(1),XRKPT(1)
0003 COMMON /GEAR0/ DTUSED,NQUSED,NSTEP,NFF,NJF
0004 COMMON /GEAR1/ T,DTG,DTMN,DTMX,EPSC,UROUND,N,MFC,KFLAG,ISTART
0005 COMMON /GEAR9/ EPSJ,R0,ML,MU,MW,NM1,NOML,NOW
0006 COMMON /OPTION/ NOGAUS,MAXDER
0007 COMMON /SIZES/ NIN,KOR,NC,NPD,NCPIS,NEQN,IQUAD
0008 COMMON /ISTART/ IW1,IW2,IW3,IW4,IW5,IW6,IW7,IW8,IW9,IW10,
* IW11,IW12,IW13,IW14,IW15,IW16,IW17,IW18
0009 COMMON /IUNIT/ IOUT
0010 IF (INDEX.EQ. 0) GO TO 60
0011 IF (INDEX.EQ. 2) GO TO 70
0012 IF (INDEX.EQ. 4) GO TO 80
0013 IF (INDEX.EQ. 3) GO TO 90
C-----
C SEVERAL CHECKS ARE MADE HERE TO DETERMINE IF THE INPUT PARAMETERS
C HAVE LEGAL VALUES. ERROR CHECKS ARE MADE ON INDEX, EPS, (TO-TOUT)*DT,
C DT, NINT, KORD, NCC, NPDE, MF, WHETHER THE BREAKPOINT SEQUENCE IS
C STRICTLY INCREASING, AND WHETHER THERE IS SUFFICIENT STORAGE
C PROVIDED FOR WORK AND IWORK. PROBLEM DEPENDENT PARAMETERS ARE
C CALCULATED AND PLACED IN COMMON.
C-----
0014 IERID = -6
0015 IF (INDEX.NE. 1) GO TO 320
0016 IERID = IERID - 1
0017 IF (EPS.LE. 0.) GO TO 320
0018 IERID = IERID - 1
0019 IF ((TO-TOUT)*DT.GT. 0.) GO TO 320
0020 IERID = IERID - 1
0021 IF (DT.EQ. 0.0) GO TO 320
0022 IERID = IERID - 1
0023 NIN = NINT
0024 IF (NIN.LT. 1) GO TO 320
0025 IERID = IERID - 1
0026 KOR = KORD
0027 IF (KOR.LT. 3 .OR. KOR.GT. 20) GO TO 320
0028 IERID = IERID - 1
0029 NC = NCC
0030 IF (NCC.LT. 2 .OR. NCC.GE. KOR) GO TO 320
0031 IERID = IERID - 1
0032 NPD = NPDE
0033 NPDE2 = NPD*NPD
0034 IF (NPDE.LT. 1) GO TO 320

```


Appendix D
Computer Program and Sample Inputs and Outputs

```

0001      IMPLICIT REAL*8 (A-H,O-Z)
0002      COMMON /ENDPT/ XLEFT
0003      COMMON /GEAR/ DTUSED,NO,NSTEPS,NF,NJ
0004      DIMENSION U(8,6),XBKPT(6),SCTCH(10),WORK(15000),IWORK(600)
0005      DIMENSION OXY(11,6),STE(11,6),XMET(11,6),CARM(11,6),
      &CARD(11,6),HYD(11,6),TEM(11,6),ENE(11,6),HGT(11),XBKPT1(6)

      C
      C INITIALIZE PARAMETERS AND PDECOL CALLING ARGUMENTS
      C
0006      CALL ERRSET(206,256,-1,1,1)
0007      NPDE = 8
0008      NINT = 5
0009      NPTS = NINT + 1
0010      KORD = 4
0011      NCC = 2
0012      T0 = 0.0000
0013      TOUT = 1.0-3
0014      DT = 1.0-7
0015      EPS = 1.0-4
0016      MF = 22
0017      INDEX = 1
0018      IWORK(1) = 15000
0019      IWORK(2) = 600
0020      DX = 1. / DFLOAT(NPTS-1)
0021      XBKPT(1) = .01
0022      XBKPT1(1) = XBKPT(1)*21.
0023      DO 10 I=2,NPTS
0024      XBKPT(I) = DFLOAT(I-1) * DX
0025      XBKPT1(I) = XBKPT(I)*21.
0026      10 CONTINUE
0027      XLEFT = XBKPT(1)

      C
      C CALL THE PACKAGE TO INTEGRATE TO TIME T = TOUT
      C
0028      J=0
0029      20 CALL PDECOL(T0,TOUT,DT,XBKPT,EPS,NINT,KORD,NCC,NPDE,MF,INDEX,
      *      WORK,IWORK)
0030      J=J+1

      C
      C C-ECK FOR EXECUTION ERRORS
      C
0031      IF ( INDEX.NE. 0 ) GO TO 70

      C
      C OUTPUT PERFORMANCE DATA AND COMPUTED SOLUTION VALUES
      C
0032      WRITE(6,2)
0033      2  FORMAT('1',/,1X,'X = THE NUMBER OF INCHES FROM THE CENTER OF THE')
0034      WRITE(6,3)
0035      3  FORMAT(/,6X,'PRODUCER TOWARD THE WALL.',/,,,/)
0036      WRITE(6,9)
0037      WRITE(6,9)
0038      TOUT1=TOUT*84.
0039      HGT(J)=TOUT1
0040      WRITE(6,8) TOUT1
0041      8  FORMAT(60X,'HEIGHT IN BED = ',F5.2,' INCHES')
0042      WRITE(6,9)
0043      WRITE(6,9)
0044      9  FORMAT(60X,'*****')
0045      WRITE(6,990)
0046      990 FORMAT(/,,,/,1X,'THE UNITS FOR OXYGEN, STEAM FEED, METHANE,')
0047      WRITE(6,991)
0048      991 FORMAT(1X,'CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN')

```

```

0050      942  FORMAT(1X,'ARE LB-MOLES/FI**3.')
```

```
0051      WRITE(6,993)
```

```
0052      943  FORMAT(1X,'TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE')
```

```
0053      WRITE(6,994)
```

```
0054      944  FORMAT(1X,'IS DIMENSIONLESS.')
```

```
0055      WRITE(6,888)
```

```
0056      888  FORMAT(59X,'R A D I A L D I R E C T I O N',//)
```

```
0057      CALL VALUES(XBKPT,U, SCTCH,NPDE,NPTS,NPTS,0,WORK)
```

```
0058      DO 13 MM=1,NPDE
```

```
0059      DO 13 MMM=1,NPTS
```

```
0060      IF (U(MM,MMM).LT.0.) U(MM,MMM)=0.
```

```
0061      13  CONTINUE
```

```
0062      DO 6 I=1,NPTS
```

```
0063      OXY(J,I)=U(1,I)*.0001*62.422
```

```
0064      STE(J,I)=U(2,I)*.0001*62.422
```

```
0065      XMET(J,I)=U(3,I)*.0001*62.422
```

```
0066      CARM(J,I)=U(4,I)*.0001*62.422
```

```
0067      CARD(J,I)=U(5,I)*.0001*62.422
```

```
0068      HYD(J,I)=U(6,I)*.0001*62.422
```

```
0069      TEM(J,I)=U(7,I)*1.8-460
```

```
0070      ENE(J,I)=U(8,I)
```

```
0071      6  CONTINUE
```

```
0072      WRITE(6,4) (XHKPT1(M),M=1,NPTS)
```

```
0073      4  FORMAT(1X,'E L E M E N T S',6X,6(8X,'X=',F6.1),//)
```

```
0074      DO 91 I=1,NPTS
```

```
0075      U(1,I)=U(1,I)*.0001*62.422
```

```
0076      U(2,I)=U(2,I)*.0001*62.422
```

```
0077      U(3,I)=U(3,I)*.0001*62.422
```

```
0078      U(4,I)=U(4,I)*.0001*62.422
```

```
0079      U(5,I)=U(5,I)*.0001*62.422
```

```
0080      U(6,I)=U(6,I)*.0001*62.422
```

```
0081      U(7,I)=U(7,I)*1.8-460.
```

```
0082      91  CONTINUE
```

```
0083      WRITE(6,51) (U(1,I),I=1,NPTS)
```

```
0084      51  FORMAT(1X,'OXYGEN',6(4X,E12.4),//)
```

```
0085      WRITE(6,52) (U(2,I),I=1,NPTS)
```

```
0086      52  FORMAT(1X,'STEAM FEED',6(4X,E12.4),//)
```

```
0087      WRITE(6,53) (U(3,I),I=1,NPTS)
```

```
0088      53  FORMAT(1X,'METHANE',6(4X,E12.4),//)
```

```
0089      WRITE(6,54) (U(4,I),I=1,NPTS)
```

```
0090      54  FORMAT(1X,'CARBON MONOXIDE',6(4X,E12.4),//)
```

```
0091      WRITE(6,55) (U(5,I),I=1,NPTS)
```

```
0092      55  FORMAT(1X,'CARBON DIOXIDE',6(4X,E12.4),//)
```

```
0093      WRITE(6,56) (U(6,I),I=1,NPTS)
```

```
0094      56  FORMAT(1X,'HYDROGEN',6(4X,E12.4),//)
```

```
0095      WRITE(6,57) (U(7,I),I=1,NPTS)
```

```
0096      57  FORMAT(1X,'TEMPERATURE',6(4X,E12.4),//)
```

```
0097      WRITE(6,58) (U(8,I),I=1,NPTS)
```

```
0098      58  FORMAT(1X,'ENERGY BALANCE',6(4X,E12.4))
```

```

C      SET NEW OUTPUT TIME AND CONTINUE THE INTEGRATION IF TOUT .LT. 1.1
C      OTHERWISE, TERMINATE THE PROBLEM
C
0099      TOUT = TOUT + .1
0100      IF ( TOUT .LE. 1.1 ) GO TO 20
0101      WRITE(6,2)
0102      WRITE(6,3)
0103      WRITE(6,41)
0104      41  FORMAT(50X,'O X Y G E N   P R O F I L E',//)
```

```
0105      WRITE(6,888)
```

```
0106      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
```

```
0107      42  FORMAT(1X,'E L E M E N T S',6(9X,'X=',F6.1),//)
```

```
0108      43  FORMAT(1X,'THE CHY=1.00 IN 1.0/54.45 HRS')
```

```

0109      DO 900 MER=1,11
0110      WRITE(6,43) HGT(12-MER),(OXY(12-MER,I),I=1,NPTS)
0111      900 CONTINUE
0112      WRITE(6,2)
0113      WRITE(6,3)
0114      WRITE(6,141)
0115      141 FORMAT(50X,'S T E A M   P R O F I L E',//)
0116      WRITE(6,888)
0117      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0118      DO 901 MER=1,11
0119      WRITE(6,43) HGT(12-MER),(STE(12-MER,I),I=1,NPTS)
0120      901 CONTINUE
0121      WRITE(6,2)
0122      WRITE(6,3)
0123      WRITE(6,241)
0124      241 FORMAT(50X,'M E T H A N E   P R O F I L E',//)
0125      WRITE(6,888)
0126      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0127      DO 902 MER=1,11
0128      WRITE(6,43) HGT(12-MER),(XMET(12-MER,I),I=1,NPTS)
0129      902 CONTINUE
0130      WRITE(6,2)
0131      WRITE(6,3)
0132      WRITE(6,341)
0133      341 FORMAT(50X,'C A R B O N   M O N O X I D E   P R O F I L E',//)
0134      WRITE(6,888)
0135      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0136      DO 903 MER=1,11
0137      WRITE(6,43) HGT(12-MER),(CARM(12-MER,I),I=1,NPTS)
0138      903 CONTINUE
0139      WRITE(6,2)
0140      WRITE(6,3)
0141      WRITE(6,441)
0142      441 FORMAT(50X,'C A R B O N   D I O X I D E   P R O F I L E',//)
0143      WRITE(6,888)
0144      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0145      DO 904 MER=1,11
0146      WRITE(6,43) HGT(12-MER),(CARD(12-MER,I),I=1,NPTS)
0147      904 CONTINUE
0148      WRITE(6,2)
0149      WRITE(6,3)
0150      WRITE(6,541)
0151      541 FORMAT(50X,'H Y D R O G E N   P R O F I L E',//)
0152      WRITE(6,888)
0153      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0154      DO 905 MER=1,11
0155      WRITE(6,43) HGT(12-MER),(HYD(12-MER,I),I=1,NPTS)
0156      905 CONTINUE
0157      WRITE(6,2)
0158      WRITE(6,3)
0159      WRITE(6,641)
0160      641 FORMAT(50X,'T E M P E R A T U R E   P R O F I L E',//)
0161      WRITE(6,888)
0162      WRITE(6,42) (XBKPT1(M),M=1,NPTS)
0163      DO 906 MER=1,11
0164      WRITE(6,43) HGT(12-MER),(TEM(12-MER,I),I=1,NPTS)
0165      906 CONTINUE
0166      WRITE(6,2)
0167      WRITE(6,3)
0168      WRITE(6,741)
0169      741 FORMAT(50X,'C A R B O N   B A L A N C E   P R O F I L E',//)
0170      WRITE(6,888)
0171      WRITE(6,42) (XBKPT1(M),M=1,NPTS)

```

```

0172      DO 907 MER=1,11
0173      WRITE(6,43) HGT(12-MER),(ENE(12-MER,I),I=1,NPTS)
0174      907 CONTINUE
0175      70 STOP
0176      END
    
```

```

0001      SUBROUTINE F(T,X,U,UX,UXX,FVAL,NPDE)
0002      IMPLICIT REAL*8 (A-H,O-Z)
0003      DIMENSION J(NPDE), UX(NPDE), UXX(NPDE), FVAL(NPDE)
0004      DATA ERLAMB,DELC, H1,H2,H3,H4/.0013,-.512,32457.,-80705.,
      840300.,-21854./
0005      DATA R,EP SX,RP,AKP2,AKP1,RC/1.987,.3,1.27,.000035,.000035,1.0/
0006      DATA DEFF1,DEFF2,ETA,CC0,ALAMB,UW/.07,.07,.8,.0468,1.333,.6/
0007      DATA TC,RWALL,AK10,AK20,AK30,AK40/283.,53.34,613.,1790000.
      8,943.6.,.002184/
0008      DATA AK50,D1,D2,D3,D4,D5,RBAR/.0245,.0000457,
      8.0000562,.0000387,.0000351,.0000351,82.0569/
0009      DATA D6,D7,D8,D9,D10,D11,D12,D13,D14/.0001548
      8,.0000676,.0013,-.512,32457.,-80705.,40300.,-21854.,.0276/
0010      DATA E1,E2,E3,E4,E5/35000.,27000.,35000.,16000.,-7860./
0011      DATA ALPHA1,ALPHA2,BETA/.0001,.285,700./
0012      FVAL(1)=-U(1)/U(7)*(ERLAMB/DELC*(UXX(7)+1./X*UX(7))+(
      8((RBAR*(1.-EP SX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
      8U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      8U(7)))/(3.*(RC/RP)*DEFF2)+1./
      8(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))*H1+
      8((RBAR*(1.-EP SX)*U(1)*U(7))/(RP/(3.*AKP1)
      8+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7)))/(3.*(RC/RP)*
      8DEFF1)+1./((ETA*RC**3/RP**3
      8*(AK20*DEXP(-E2/(R*U(7))))*CC0)))*H2+
      8((RBAR*(1.-EP SX)*U(5)*U(7))/(1./((ETA*RC**3
      8/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0))
      8*H3+
      8((RBAR*RBAR*(1.-EP SX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      8*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0))*H4*ALPHA1))
      8/DELC*ALPHA2)+D1/D7*1./U(7)
      8*(UXX(1)+1./X*UX(1))-1./D7*
      8((RBAR*(1.-EP SX)*U(1)*U(7))/(RP/(3.*AKP1)
      8+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7)))/(3.*(RC/RP)*
      8DEFF1)+1./((ETA*RC**3/RP**3
      8*(AK20*DEXP(-E2/(R*U(7))))*CC0)))/U(7)
      C
0013      FVAL(2)=-U(2)/U(7)*(ERLAMB/DELC*(UXX(7)+1./X*UX(7))+(
      8((RBAR*(1.-EP SX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
      8U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      8U(7)))/(3.*(RC/RP)*DEFF2)+1./
      8(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))*H1+
      8((RBAR*(1.-EP SX)*U(1)*U(7))/(RP/(3.*AKP1)
      8+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7)))/(3.*(RC/RP)*
      8DEFF1)+1./((ETA*RC**3/RP**3
      8*(AK20*DEXP(-E2/(R*U(7))))*CC0)))*H2+
      8((RBAR*(1.-EP SX)*U(5)*U(7))/(1./((ETA*RC**3
      8/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0))
      8*H3+
      8((RBAR*RBAR*(1.-EP SX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      8*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0))*H4*ALPHA1))
      8/DELC*ALPHA2)+D2/D7*1./U(7)
      8*(UXX(2)+1./X*UX(2))-1./D7*
      8((RBAR*(1.-EP SX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
      8U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      8U(7)))/(3.*(RC/RP)*DEFF2)+1./
      8(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))/U(7)
      C
0014      FVAL(3)=-U(3)/U(7)*(ERLAMB/DELC*(UXX(7)+1./X*UX(7))+(
      8((RBAR*(1.-EP SX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
      8U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      8U(7)))/(3.*(RC/RP)*DEFF2)+1./

```

```

      X(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0))
      R*H1+
      R((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
      R*RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*
      &DEFF1)+1./((ETA*RC**3/RP**3
      X*(AK20*DEXP(-E2/(R*U(7))))*CC0)))*H2+
      R((RBAR*(1.-EPSX)*U(5)*U(7))/(1./((ETA*RC**3
      R/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0))
      R*H3+
      R((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      R*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0))
      R*H4*ALPHA1))
      R/DELCP*ALPHA2)+D3/D7*1./U(7)
      R*(UXX(3)+1./X*UX(3))+1./D7*ALPHA1*
      R((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      R*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))/U(7)

```

C
C

0015

```

      FVAL(4)=-U(4)/U(7)*(ERLAMB/DELCP*(UXX(7)+1./X*UX(7)))+(
      R((RBAR*(1.-EPSX)*U(2)-(U(5)*U(6)))/((AK50*DEXP(-E5/(R*U(7))))*
      R*U(4)))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      R*U(7))/(3.*(RC/RP)*DEFF2)+1./((ETA*RC**3/RP**3*(AK10*DEXP(-E1/
      R*(R*U(7))))*CC0)))*H1+((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
      R*RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
      X(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))*H2+
      R((RBAR*(1.-EPSX)*U(5)*U(7))/(1./((ETA*RC**3
      R/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))*H3+
      R((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      R*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))*H4*ALPHA1))
      R/DELCP*ALPHA2)+D4/D7*1./U(7)*(UXX(4)+1./X*UX(4))+1./D7*(
      R(RBAR*(1.-EPSX)*U(2)-(U(5)*U(6)))/((AK50*DEXP(-E5/(R*U(7))))*
      R*U(4)))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      R*U(7))/(3.*(RC/RP)*DEFF2)+1./
      X(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0))+2.*(ALAMB-1.)*
      R((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)+RP*(RP-RC)*BETA*RBAR
      R*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./((ETA*RC**3/RP**3
      R*(AK20*DEXP(-E2/(R*U(7))))*CC0)))+2.*(RBAR*(1.-EPSX)*U(5)*
      R*U(7))/(1./((ETA*RC**3/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))/U(7)

```

C
C

0016

```

      FVAL(5)=-U(5)/U(7)*(ERLAMB/DELCP*(UXX(7)+1./X*UX(7)))+(
      R((RBAR*(1.-EPSX)*U(2)-(U(5)*U(6)))/((AK50*DEXP(-E5/(R*U(7))))*
      R*U(4)))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
      R*U(7))/(3.*(RC/RP)*DEFF2)+1./
      X(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0))
      R*H1+
      R((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
      R*RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
      X(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))*H2+
      R((RBAR*(1.-EPSX)*U(5)*U(7))/(1./((ETA*RC**3
      R/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))*H3+
      R((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./((ETA
      R*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))*H4*ALPHA1))
      R/DELCP*ALPHA2)+D5/D7*1./U(7)
      R*(UXX(5)+1./X*UX(5))+1./D7*((2.-ALAMB)*
      R((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
      R*RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
      X(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))-
      R((RBAR*(1.-EPSX)*U(5)*U(7))/(1./((ETA*RC**3
      R/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))/U(7)

```

C
C

0017

```

      FVAL(6)=-U(6)/U(7)*(ERLAMB/DELCP*(UXX(7)+1./X*UX(7)))+(

```

```

&((RBAR*(1.-EPSX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
&U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
&U(7))/(3.*(RC/RP)*DEFF2)+1./
&(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))H1+
&((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
&+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
&(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))H2+
&((RBAR*(1.-EPSX)*U(5)*U(7))/(1./(ETA*RC**3
&/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))H3+
&((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./(ETA
&*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))H4*ALPHA1)
&/DELCP*ALPHA2)+D6/D7*1./U(7)
&(UX(6)+1./X*UX(6))+1./D7*(
&((RBAR*(1.-EPSX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
&U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
&U(7))/(3.*(RC/RP)*DEFF2)+1./
&(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))=2.*ALPHA1*
&((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./(ETA
&*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))U(7)

```

C

C

0018

FVAL(7)=D8/D9*(UX(7)+1./X*UX(7))+ALPHA2/D9*

```

&(D10*
&((RBAR*(1.-EPSX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
&U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
&U(7))/(3.*(RC/RP)*DEFF2)+1./
&(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))
&+D11*
&((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
&+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
&(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))
&+D12*
&((RBAR*(1.-EPSX)*U(5)*U(7))/(1./(ETA*RC**3
&/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))
&+D13*ALPHA1*
&((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./(ETA
&*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))
&

```

C

C

0019

```

FVAL(8)=ALPHA2/D14*(
&((RBAR*(1.-EPSX)*(U(2)-((U(5)*U(6))/((AK50*DEXP(-E5/(R*U(7)))))*
&U(4))))*U(7))/(RP/(3.*AKP2)+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/
&U(7))/(3.*(RC/RP)*DEFF2)+1./
&(ETA*RC**3/RP**3*(AK10*DEXP(-E1/(R*U(7))))*CC0)))
&+ALPHA*
&((RBAR*(1.-EPSX)*U(1)*U(7))/(RP/(3.*AKP1)
&+RP*(RP-RC)*BETA*RBAR*DSQRT(BETA/U(7))/(3.*(RC/RP)*DEFF1)+1./
&(ETA*RC**3/RP**3*(AK20*DEXP(-E2/(R*U(7))))*CC0)))
&((RBAR*(1.-EPSX)*U(5)*U(7))/(1./(ETA*RC**3
&/RP**3*(AK30*DEXP(-E3/(R*U(7))))*CC0)))ALPHA1*
&((RBAR*RBAR*(1.-EPSX)*U(6)*U(6)*U(7)*U(7))/(1./(ETA
&*RC**3/RP**3*(AK40*DEXP(-E4/(R*U(7))))*CC0)))

```

C

C

0020

RETURN

0021

END

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = F , LINECNT = 65
STATISTICS SOURCE STATEMENTS = 21,PROGRAM SIZE = 13260
STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE HNDRY(T,X,U,UX,DBDU,DBDUX,DZDT,NPDE)
0002      IMPLICIT REAL*8 (A-H,O-Z)
0003      DIMENSION U(NPDE), UX(NPDE), DZDT(NPDE)
0004      DIMENSION DBDU(NPDE,NPDE), DBDUX(NPDE,NPDE)
0005      COMMON /ENDPT/ XLEFT
0006      DATA UW,ERLAMB/.6,.0013/
0007      IF (X.NE.XLEFT) GO TO 10
0008      DO 17 I=1,8
0009      DO 17 J=1,8
0010      DBDU(I,J)=0.
0011      DBDUX(I,J)=0.
0012      IF (I.EQ.J) DBDUX(I,J)=1.
0013      DZDT(I)=0.
0014      17 CONTINUE
0015      RETURN
0016      10 DO 18 I=1,8
0017      DO 18 J=1,8
0018      DBDU(I,J)=0.
0019      DBDUX(I,J)=0.
0020      IF (I.EQ.J) DBDUX(I,J)=1.
0021      18 CONTINUE
0022      DBDU(7,7)=UW/ERLAMB
0023      DO 19 I=1,8
0024      DZDT(I)=0.
0025      19 CONTINUE
0026      IF (I.LE..1) DZDT(7)=-5655.1*DSIN(31.4159*T)*UW/ERLAMB
0027      RETURN
0028      END
```

FORTRAN IV G LEVEL 21

HNDRY

DATE = 78159

15/20754

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
OPTIONS IN EFFECT NAME = HNDRY , LINECNT = 65
STATISTICS SOURCE STATEMENTS = 28, PROGRAM SIZE = 1210
STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE UINIT(X,U,NPDE)
0002      IMPLICIT REAL*8 (A-H,O-Z)
0003      DIMENSION U(NPDE)
0004      C
0005      C SET INITIAL CONDITIONS.
0006      C
0007      DATA U10,U20,U30,U40/0.607,4.131,.0,.0000001/
0008      DATA U50,U60,U70,U80/0.,0.,.643,.1/
0009      U(1)=U10
0010      U(2)=U20
0011      U(3)=U30
0012      U(4)=U40
0013      U(5)=U50
0014      U(6)=U60
0015      U(7)=U70
0016      U(8)=U80
0017      RETURN
0018      END
```

OPTIONS IN EFFECT NOID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP

OPTIONS IN EFFECT NAME = UINIT , LINECNT = 65

STATISTICS SOURCE STATEMENTS = 15, PROGRAM SIZE = 526

STATISTICS NO DIAGNOSTICS GENERATED

```
0001      SUBROUTINE DERIVF(T,X,U,UX,UXX,DFDU,DFDUX,DFDUXX,NPDE)
0002      IMPLICIT REAL*8 (A-H,O-Z)
0003      DIMENSION U(NPDE), UX(NPDE), UXX(NPDE)
0004      DIMENSION DFDU(NPDE,NPDE), DFDUX(NPDE,NPDE), DFDUXX(NPDE,NPDE)
0005      RETURN
0006      END
```

OPTIONS IN EFFECT NOID,ERCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP

OPTIONS IN EFFECT NAME = DERIVF , LINECNT = 65

STATISTICS SOURCE STATEMENTS = 6, PROGRAM SIZE = 596

STATISTICS NO DIAGNOSTICS GENERATED

STATISTICS NO DIAGNOSTICS THIS STEP

F88-LEVEL LINKAGE EDITOR OPTIONS SPECIFIED OVLY,LET
DEFAULT OPTION(S) USED - SIZE=(114688,32768)

IEW0201
*****MAIN

DOES NOT EXIST BUT HAS BEEN ADDED TO DATA SET

DIAGNOSTIC MESSAGE DIRECTORY

IEW0201 WARNING - OVERLAY STRUCTURE CONTAINS ONLY ONE SEGMENT -- OVERLAY OPTION CANCELED.

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 0.08 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.37380-02	0.37380-02	0.37380-02	0.37380-02	0.37380-02	0.37380-02
STEAM FEED	0.25560-01	0.25560-01	0.25560-01	0.25560-01	0.25560-01	0.25560-01
METHANE	0.11010-22	0.11010-22	0.11010-22	0.11010-22	0.11000-22	0.11020-22
CARBON MONOXIDE	0.11890-04	0.11890-04	0.11890-04	0.11890-04	0.11890-04	0.11890-04
CARBON DIOXIDE	0.11910-04	0.11910-04	0.11910-04	0.11910-04	0.11910-04	0.11910-04
HYDROGEN	0.35120-09	0.35120-09	0.35120-09	0.35120-09	0.35120-09	0.35120-09
TEMPERATURE	0.70750 03	0.70750 03	0.70750 03	0.70750 03	0.70690 03	0.69800 03
ENERGY BALANCE	0.10170 00	0.10170 00	0.10170 00	0.10170 00	0.10170 00	0.10170 00

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 8.48 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

82

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.10400-02	0.10400-02	0.10400-02	0.10400-02	0.10430-02	0.10150-02
STEAM FEED	0.14190-01	0.14190-01	0.14190-01	0.14200-01	0.14250-01	0.13760-01
METHANE	0.14450-06	0.14460-06	0.14440-06	0.14210-06	0.13100-06	0.27100-06
CARBON MONOXIDE	0.14100-02	0.14100-02	0.14090-02	0.14060-02	0.13890-02	0.15810-02
CARBON DIOXIDE	0.71050-03	0.71060-03	0.71070-03	0.71120-03	0.71380-03	0.68540-03
HYDROGEN	0.57100-03	0.57100-03	0.57060-03	0.56750-03	0.55250-03	0.72490-03
TEMPERATURE	0.15620 04	0.15620 04	0.15610 04	0.15530 04	0.14530 04	0.15640 03
ENERGY BALANCE	0.36640 00	0.36640 00	0.36630 00	0.36580 00	0.36350 00	0.39020 00

X = THE NUMBER OF INCHES FROM THE CENTER OF THE

PRODUCER TOWARD THE WALL.

 HEIGHT IN BED = 16.88 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
 CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
 ARE LB-MOLES/FT**3.
 TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
 IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.48370-03	0.48370-03	0.48380-03	0.48420-03	0.48600-03	0.46600-03
STEAM FEED	0.13220-01	0.13220-01	0.13220-01	0.13240-01	0.13330-01	0.12340-01
METHANE	0.69090-05	0.69080-05	0.68980-05	0.68040-05	0.63140-05	0.12420-04
CARBON MONOXIDE	0.36070-02	0.36070-02	0.36060-02	0.35930-02	0.35340-02	0.42060-02
CARBON DIOXIDE	0.96350-03	0.96350-03	0.96380-03	0.96560-03	0.97430-03	0.87650-03
HYDROGEN	0.20090-02	0.20090-02	0.20080-02	0.19990-02	0.19520-02	0.24890-02
TEMPERATURE	0.14980 04	0.14980 04	0.14980 04	0.14900 04	0.13920 04	0.15360 03
ENERGY BALANCE	0.65710 00	0.65710 00	0.65690 00	0.65520 00	0.64730 00	0.73610 00

X = THE NUMBER OF INCHES FROM THE CENTER OF THE

PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 25.28 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.23040-03	0.23040-03	0.23040-03	0.23080-03	0.23220-03	0.21650-03
STEAM FEED	0.12980-01	0.12980-01	0.12990-01	0.13020-01	0.13160-01	0.11580-01
METHANE	0.22420-04	0.22420-04	0.22380-04	0.22060-04	0.20290-04	0.42760-04
CARBON MONOXIDE	0.49050-02	0.49050-02	0.49030-02	0.48830-02	0.47880-02	0.58720-02
CARBON DIOXIDE	0.10800-02	0.10800-02	0.10800-02	0.10840-02	0.10990-02	0.92330-03
HYDROGEN	0.28220-02	0.28220-02	0.28210-02	0.28090-02	0.27390-02	0.35580-02
TEMPERATURE	0.14230 04	0.14230 04	0.14220 04	0.14140 04	0.13160 04	0.15000 03
ENERGY BALANCE	0.80290 00	0.80280 00	0.80250 00	0.79970 00	0.78700 00	0.93240 00

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 33.68 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.1105D-03	0.1105D-03	0.1105D-03	0.1108D-03	0.1119D-03	0.1004D-03
85 STEAM FEED	0.1300D-01	0.1300D-01	0.1300D-01	0.1304D-01	0.1324D-01	0.1104D-01
METHANE	0.4078D-04	0.4077D-04	0.4070D-04	0.4007D-04	0.3642D-04	0.8393D-04
CARBON MONOXIDE	0.5702D-02	0.5702D-02	0.5699D-02	0.5674D-02	0.5550D-02	0.6999D-02
CARBON DIOXIDE	0.1140D-02	0.1140D-02	0.1141D-02	0.1146D-02	0.1169D-02	0.9114D-03
HYDROGEN	0.3307D-02	0.3307D-02	0.3306D-02	0.3292D-02	0.3208D-02	0.4249D-02
TEMPERATURE	0.1362D 04	0.1362D 04	0.1361D 04	0.1352D 04	0.1252D 04	0.1478D 03
ENERGY BALANCE	0.8791D 00	0.8791D 00	0.8786D 00	0.8748D 00	0.8574D 00	0.1058D 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 42.08 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	x= 0.2	x= 4.2	x= 8.4	x= 12.6	x= 16.8	x= 21.0
OXYGEN	0.5319E-04	0.5319D-04	0.5321D-04	0.5339D-04	0.5421D-04	0.4634D-04
98 STEAM FEED	0.1310E-01	0.1310D-01	0.1311D-01	0.1316D-01	0.1343D-01	0.1057D-01
METHANE	0.5895E-04	0.5894D-04	0.5883D-04	0.5783D-04	0.5191D-04	0.1314D-03
CARBON MONOXIDE	0.6232D-02	0.6232D-02	0.6229D-02	0.6200D-02	0.6055D-02	0.7826D-02
CARBON DIOXIDE	0.1175E-02	0.1175D-02	0.1176D-02	0.1182D-02	0.1214D-02	0.8726D-03
HYDROGEN	0.3622D-02	0.3622D-02	0.3621D-02	0.3608D-02	0.3516D-02	0.4731D-02
TEMPERATURE	0.1313D 04	0.1313D 04	0.1312D 04	0.1301D 04	0.1198D 04	0.1468D 03
ENERGY BALANCE	0.9222D 00	0.9222D 00	0.9215D 00	0.9167D 00	0.8950D 00	0.1150D 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 50.48 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE, IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.2555D-04	0.2555D-04	0.2557D-04	0.2570D-04	0.2628D-04	0.2112D-04
STEAM FEED	0.1323D-01	0.1323D-01	0.1324D-01	0.1331D-01	0.1365D-01	0.1011D-01
METHANE	0.7594D-04	0.7593D-04	0.7578D-04	0.7438D-04	0.6590D-04	0.1837D-03
CARBON MONOXIDE	0.6610D-02	0.6610D-02	0.6607D-02	0.6577D-02	0.6419D-02	0.8482D-02
CARBON DIOXIDE	0.1196D-02	0.1196D-02	0.1197D-02	0.1206D-02	0.1246D-02	0.8207D-03
HYDROGEN	0.3841D-02	0.3841D-02	0.3840D-02	0.3829D-02	0.3740D-02	0.5090D-02
TEMPERATURE	0.1273D 04	0.1273D 04	0.1272D 04	0.1260D 04	0.1151D 04	0.1466D 03
ENERGY BALANCE	0.9488D 00	0.9487D 00	0.9480D 00	0.9421D 00	0.9162D 00	0.1226D 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 58.88 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.12350-04	0.12350-04	0.12360-04	0.12450-04	0.12850-04	0.96020-05
STEAM FEED	0.13360-01	0.13360-01	0.13370-01	0.13460-01	0.13890-01	0.96360-02
METHANE	0.91590-04	0.91580-04	0.91380-04	0.89550-04	0.78320-04	0.24060-03
CARBON MONOXIDE	0.68930-02	0.68930-02	0.68900-02	0.68610-02	0.67010-02	0.90360-02
CARBON DIOXIDE	0.12100-02	0.12100-02	0.12120-02	0.12230-02	0.12730-02	0.76210-03
HYDROGEN	0.40010-02	0.40010-02	0.40000-02	0.39920-02	0.39160-02	0.53740-02
TEMPERATURE	0.12420 04	0.12410 04	0.12400 04	0.12260 04	0.11100 04	0.14710 03
ENERGY BALANCE	0.96640 00	0.96630 00	0.96540 00	0.95850 00	0.92870 00	0.12960 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 67.28 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE, IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.58850-05	0.58860-05	0.58950-05	0.59540-05	0.62220-05	0.42350-05
68 STEAM FEED	0.13470-01	0.13470-01	0.13490-01	0.13600-01	0.14120-01	0.91510-02
METHANE	0.10600-03	0.10600-03	0.10570-03	0.10340-03	0.89370-04	0.30270-03
CARBON MONOXIDE	0.71150-02	0.71150-02	0.71120-02	0.70860-02	0.69370-02	0.95330-02
CARBON DIOXIDE	0.12210-02	0.12210-02	0.12230-02	0.12360-02	0.12970-02	0.70000-03
HYDROGEN	0.41220-02	0.41220-02	0.41230-02	0.41190-02	0.40660-02	0.56120-02
TEMPERATURE	0.12160 04	0.12160 04	0.12140 04	0.11970 04	0.10720 04	0.14790 03
ENERGY BALANCE	0.97910 00	0.97900 00	0.97790 00	0.96990 00	0.93650 00	0.13630 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 75.68 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	x= 0.2	x= 4.2	x= 8.4	x= 12.6	x= 16.8	x= 21.0
OXYGEN	0.27430-05	0.27440-05	0.27490-05	0.27880-05	0.29670-05	0.17790-05
STEAM FEED	0.13570-01	0.13580-01	0.13590-01	0.13730-01	0.14370-01	0.86470-02
METHANE	0.11930-03	0.11930-03	0.11900-03	0.11620-03	0.99320-04	0.37060-03
CARBON MONOXIDE	0.72940-02	0.72940-02	0.72930-02	0.72730-02	0.71500-02	0.99990-02
CARBON DIOXIDE	0.12280-02	0.12280-02	0.12310-02	0.12470-02	0.13200-02	0.63550-03
HYDROGEN	0.42180-02	0.42180-02	0.42190-02	0.42250-02	0.42060-02	0.58220-02
TEMPERATURE	0.11950 04	0.11950 04	0.11920 04	0.11730 04	0.10370 04	0.14910 03
ENERGY BALANCE	0.98880 00	0.98670 00	0.98740 00	0.97820 00	0.94160 00	0.14310 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HEIGHT IN BED = 84.08 INCHES

THE UNITS FOR OXYGEN, STEAM FEED, METHANE,
CARBON MONOXIDE, CARBON DIOXIDE, AND HYDROGEN
ARE LB-MOLES/FT**3.
TEMPERATURE IS IN DEGREES F AND ENERGY BALANCE
IS DIMENSIONLESS.

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
OXYGEN	0.12800-05	0.12800-05	0.12840-05	0.13100-05	0.14290-05	0.72980-06
16 STEAM FEED	0.13660-01	0.13660-01	0.13690-01	0.13850-01	0.14630-01	0.81220-02
METHANE	0.13170-03	0.13170-03	0.13130-03	0.12800-03	0.10850-03	0.44510-03
CARBON MONOXIDE	0.74420-02	0.74430-02	0.74440-02	0.74330-02	0.73590-02	0.10450-01
CARBON DIOXIDE	0.12340-02	0.12350-02	0.12370-02	0.12570-02	0.13440-02	0.56910-03
HYDROGEN	0.42950-02	0.42950-02	0.42970-02	0.43050-02	0.43450-02	0.60110-02
TEMPERATURE	0.11780 04	0.11780 04	0.11740 04	0.11510 04	0.10030 04	0.15050 03
ENERGY BALANCE	0.99650 00	0.99640 00	0.99490 00	0.98450 00	0.94520 00	0.15000 01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

O X Y G E N P R O F I L E

R A D I A L D I R E C T I O N

E L E M E N T S	x= 0.2	x= 4.2	x= 8.4	x= 12.6	x= 16.8	x= 21.0
HEIGHT=84.1 IN.	0.12800-05	0.12800-05	0.12840-05	0.13100-05	0.14290-05	0.72980-06
HEIGHT=75.7 IN.	0.27430-05	0.27440-05	0.27490-05	0.27880-05	0.29670-05	0.17790-05
HEIGHT=67.3 IN.	0.58850-05	0.58860-05	0.58950-05	0.59540-05	0.62220-05	0.42350-05
HEIGHT=58.9 IN.	0.12350-04	0.12350-04	0.12360-04	0.12450-04	0.12850-04	0.96020-05
HEIGHT=50.5 IN.	0.25550-04	0.25550-04	0.25570-04	0.25700-04	0.26280-04	0.21120-04
HEIGHT=42.1 IN.	0.53190-04	0.53190-04	0.53210-04	0.53390-04	0.54210-04	0.46340-04
HEIGHT=33.7 IN.	0.11050-03	0.11050-03	0.11050-03	0.11080-03	0.11190-03	0.10040-03
HEIGHT=25.3 IN.	0.23040-03	0.23040-03	0.23040-03	0.23080-03	0.23220-03	0.21650-03
HEIGHT=16.9 IN.	0.48370-03	0.48370-03	0.48380-03	0.48420-03	0.48600-03	0.46600-03
HEIGHT= 8.5 IN.	0.10400-02	0.10400-02	0.10400-02	0.10400-02	0.10430-02	0.10150-02
HEIGHT= 0.1 IN.	0.37380-02	0.37380-02	0.37380-02	0.37380-02	0.37380-02	0.37380-02

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

STEAM PROFILE

RADIAL DIRECTION

ELEMENTS	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.1366D-01	0.1366D-01	0.1369D-01	0.1385D-01	0.1463D-01	0.8122D-02
HEIGHT=75.7 IN.	0.1357D-01	0.1358D-01	0.1359D-01	0.1373D-01	0.1437D-01	0.8647D-02
HEIGHT=67.3 IN.	0.1347D-01	0.1347D-01	0.1349D-01	0.1360D-01	0.1412D-01	0.9151D-02
HEIGHT=58.9 IN.	0.1336D-01	0.1336D-01	0.1337D-01	0.1346D-01	0.1389D-01	0.9636D-02
HEIGHT=50.5 IN.	0.1323D-01	0.1323D-01	0.1324D-01	0.1331D-01	0.1365D-01	0.1011D-01
HEIGHT=42.1 IN.	0.1310D-01	0.1310D-01	0.1311D-01	0.1316D-01	0.1343D-01	0.1057D-01
HEIGHT=33.7 IN.	0.1300D-01	0.1300D-01	0.1300D-01	0.1304D-01	0.1324D-01	0.1104D-01
HEIGHT=25.3 IN.	0.1298D-01	0.1298D-01	0.1299D-01	0.1302D-01	0.1316D-01	0.1158D-01
HEIGHT=16.9 IN.	0.1322D-01	0.1322D-01	0.1322D-01	0.1324D-01	0.1333D-01	0.1234D-01
HEIGHT= 8.5 IN.	0.1419D-01	0.1419D-01	0.1419D-01	0.1420D-01	0.1425D-01	0.1376D-01
HEIGHT= 0.1 IN.	0.2556D-01	0.2556D-01	0.2556D-01	0.2556D-01	0.2556D-01	0.2556D-01

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

M E T H A N E P R O F I L E

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.1317D-03	0.1317D-03	0.1313D-03	0.1280D-03	0.1085D-03	0.4451D-03
HEIGHT=75.7 IN.	0.1193D-03	0.1193D-03	0.1190D-03	0.1162D-03	0.9932D-04	0.3706D-03
HEIGHT=67.3 IN.	0.1060D-03	0.1060D-03	0.1057D-03	0.1034D-03	0.8937D-04	0.3027D-03
HEIGHT=58.9 IN.	0.9159D-04	0.9158D-04	0.9138D-04	0.8955D-04	0.7832D-04	0.2706D-03
HEIGHT=50.5 IN.	0.7544D-04	0.7593D-04	0.7578D-04	0.7438D-04	0.6590D-04	0.1837D-03
HEIGHT=42.1 IN.	0.5895D-04	0.5894D-04	0.5883D-04	0.5783D-04	0.5191D-04	0.1314D-03
HEIGHT=33.7 IN.	0.4078D-04	0.4077D-04	0.4070D-04	0.4007D-04	0.3642D-04	0.8393D-04
HEIGHT=25.3 IN.	0.2242D-04	0.2242D-04	0.2238D-04	0.2206D-04	0.2029D-04	0.4276D-04
94 HEIGHT=16.9 IN.	0.6909D-05	0.6908D-05	0.6898D-05	0.6804D-05	0.6314D-05	0.1242D-04
HEIGHT= 8.5 IN.	0.1446D-06	0.1446D-06	0.1444D-06	0.1421D-06	0.1310D-06	0.2710D-06
HEIGHT= 0.1 IN.	0.1101D-22	0.1101D-22	0.1101D-22	0.1101D-22	0.1100D-22	0.1102D-22

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

C A R B O N M O N O X I D E P R O F I L E

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.7442D-02	0.7443D-02	0.7444D-02	0.7433D-02	0.7359D-02	0.1045D-01
HEIGHT=75.7 IN.	0.7294D-02	0.7294D-02	0.7293D-02	0.7273D-02	0.7150D-02	0.9999D-02
HEIGHT=67.3 IN.	0.7115D-02	0.7115D-02	0.7112D-02	0.7086D-02	0.6937D-02	0.9533D-02
HEIGHT=58.9 IN.	0.6893D-02	0.6893D-02	0.6890D-02	0.6861D-02	0.6701D-02	0.9036D-02
HEIGHT=50.5 IN.	0.6610D-02	0.6610D-02	0.6607D-02	0.6577D-02	0.6419D-02	0.8482D-02
HEIGHT=42.1 IN.	0.6232D-02	0.6232D-02	0.6229D-02	0.6200D-02	0.6055D-02	0.7826D-02
HEIGHT=33.7 IN.	0.5702D-02	0.5702D-02	0.5699D-02	0.5674D-02	0.5550D-02	0.6999D-02
HEIGHT=25.3 IN.	0.4905D-02	0.4905D-02	0.4903D-02	0.4883D-02	0.4788D-02	0.5872D-02
56 HEIGHT=16.9 IN.	0.3607D-02	0.3607D-02	0.3606D-02	0.3593D-02	0.3534D-02	0.4206D-02
HEIGHT= 8.5 IN.	0.1410D-02	0.1410D-02	0.1409D-02	0.1406D-02	0.1389D-02	0.1581D-02
HEIGHT= 0.1 IN.	0.1189D-04	0.1189D-04	0.1189D-04	0.1189D-04	0.1189D-04	0.1189D-04

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

CARBON DIOXIDE PROFILE

RADIAL DIRECTION

ELEMENTS	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.1234D-02	0.1235D-02	0.1237D-02	0.1257D-02	0.1344D-02	0.5691D-03
HEIGHT=75.7 IN.	0.1228D-02	0.1228D-02	0.1231D-02	0.1247D-02	0.1320D-02	0.6355D-03
HEIGHT=67.3 IN.	0.1221D-02	0.1221D-02	0.1223D-02	0.1236D-02	0.1297D-02	0.7000D-03
HEIGHT=58.9 IN.	0.1210D-02	0.1210D-02	0.1212D-02	0.1229D-02	0.1273D-02	0.7621D-03
HEIGHT=50.5 IN.	0.1196D-02	0.1196D-02	0.1197D-02	0.1206D-02	0.1246D-02	0.8207D-03
HEIGHT=42.1 IN.	0.1175D-02	0.1175D-02	0.1176D-02	0.1182D-02	0.1214D-02	0.8726D-03
HEIGHT=33.7 IN.	0.1140D-02	0.1140D-02	0.1141D-02	0.1146D-02	0.1169D-02	0.9114D-03
HEIGHT=25.3 IN.	0.1080D-02	0.1080D-02	0.1080D-02	0.1084D-02	0.1099D-02	0.9233D-03
HEIGHT=16.9 IN.	0.9635D-03	0.9635D-03	0.9638D-03	0.9656D-03	0.9743D-03	0.8765D-03
HEIGHT= 8.5 IN.	0.7106D-03	0.7106D-03	0.7107D-03	0.7112D-03	0.7138D-03	0.6854D-03
HEIGHT= 0.1 IN.	0.1191D-04	0.1191D-04	0.1191D-04	0.1191D-04	0.1191D-04	0.1191D-04

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

HYDROGEN PROFILE

RADIAL DIRECTION

ELEMENTS	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.42950-02	0.42950-02	0.42970-02	0.43050-02	0.43450-02	0.60110-02
HEIGHT=75.7 IN.	0.42180-02	0.42180-02	0.42190-02	0.42200-02	0.42060-02	0.58220-02
HEIGHT=67.3 IN.	0.41220-02	0.41220-02	0.41230-02	0.41190-02	0.40660-02	0.56120-02
HEIGHT=58.9 IN.	0.40010-02	0.40010-02	0.40000-02	0.39920-02	0.39160-02	0.53740-02
HEIGHT=50.5 IN.	0.38410-02	0.38410-02	0.38400-02	0.38290-02	0.37400-02	0.50900-02
HEIGHT=42.1 IN.	0.36220-02	0.36220-02	0.36210-02	0.36080-02	0.35160-02	0.47310-02
HEIGHT=33.7 IN.	0.33070-02	0.33070-02	0.33060-02	0.32920-02	0.32080-02	0.42490-02
HEIGHT=25.3 IN.	0.28220-02	0.28220-02	0.28210-02	0.28090-02	0.27390-02	0.35580-02
97 HEIGHT=16.9 IN.	0.20090-02	0.20090-02	0.20080-02	0.19990-02	0.19520-02	0.24890-02
HEIGHT= 8.5 IN.	0.57100-03	0.57100-03	0.57060-03	0.56750-03	0.55250-03	0.72490-03
HEIGHT= 0.1 IN.	0.35120-09	0.35120-09	0.35120-09	0.35120-09	0.35120-09	0.35120-09

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

TEMPERATURE PROFILE

RADIAL DIRECTION

ELEMENTS	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.1178D 04	0.1178D 04	0.1174D 04	0.1151D 04	0.1003D 04	0.1505D 03
HEIGHT=75.7 IN.	0.1145D 04	0.1195D 04	0.1192D 04	0.1173D 04	0.1037D 04	0.1491D 03
HEIGHT=67.3 IN.	0.1216D 04	0.1216D 04	0.1214D 04	0.1197D 04	0.1072D 04	0.1479D 03
HEIGHT=58.9 IN.	0.1242D 04	0.1241D 04	0.1240D 04	0.1226D 04	0.1110D 04	0.1471D 03
HEIGHT=50.5 IN.	0.1273D 04	0.1273D 04	0.1272D 04	0.1260D 04	0.1151D 04	0.1466D 03
HEIGHT=42.1 IN.	0.1313D 04	0.1313D 04	0.1312D 04	0.1301D 04	0.1198D 04	0.1468D 03
HEIGHT=33.7 IN.	0.1362D 04	0.1362D 04	0.1361D 04	0.1352D 04	0.1252D 04	0.1478D 03
HEIGHT=25.3 IN.	0.1423D 04	0.1423D 04	0.1422D 04	0.1414D 04	0.1316D 04	0.1500D 03
HEIGHT=16.9 IN.	0.1498D 04	0.1498D 04	0.1498D 04	0.1490D 04	0.1392D 04	0.1536D 03
HEIGHT= 8.5 IN.	0.1562D 04	0.1562D 04	0.1561D 04	0.1553D 04	0.1453D 04	0.1564D 03
HEIGHT= 0.1 IN.	0.7075D 03	0.7075D 03	0.7075D 03	0.7075D 03	0.7069D 03	0.6980D 03

X = THE NUMBER OF INCHES FROM THE CENTER OF THE
PRODUCER TOWARD THE WALL.

C A R B O N B A L A N C E P R O F I L E

R A D I A L D I R E C T I O N

E L E M E N T S	X= 0.2	X= 4.2	X= 8.4	X= 12.6	X= 16.8	X= 21.0
HEIGHT=84.1 IN.	0.9965D 00	0.9964D 00	0.9949D 00	0.9845D 00	0.9452D 00	0.1500D 01
HEIGHT=75.7 IN.	0.9888D 00	0.9887D 00	0.9874D 00	0.9782D 00	0.9416D 00	0.1431D 01
HEIGHT=67.3 IN.	0.9791D 00	0.9790D 00	0.9779D 00	0.9699D 00	0.9365D 00	0.1363D 01
HEIGHT=58.9 IN.	0.9664D 00	0.9663D 00	0.9654D 00	0.9585D 00	0.9287D 00	0.1296D 01
HEIGHT=50.5 IN.	0.9488D 00	0.9487D 00	0.9480D 00	0.9421D 00	0.9162D 00	0.1226D 01
HEIGHT=42.1 IN.	0.9222D 00	0.9222D 00	0.9215D 00	0.9167D 00	0.8950D 00	0.1150D 01
HEIGHT=33.7 IN.	0.8791D 00	0.8791D 00	0.8786D 00	0.8748D 00	0.8574D 00	0.1058D 01
HEIGHT=25.3 IN.	0.8029D 00	0.8028D 00	0.8025D 00	0.7997D 00	0.7870D 00	0.9324D 00
HEIGHT=16.9 IN.	0.6571D 00	0.6571D 00	0.6569D 00	0.6552D 00	0.6473D 00	0.7361D 00
HEIGHT= 8.5 IN.	0.3664D 00	0.3664D 00	0.3663D 00	0.3658D 00	0.3635D 00	0.3902D 00
HEIGHT= 0.1 IN.	0.1017D 00	0.1017D 00	0.1017D 00	0.1017D 00	0.1017D 00	0.1017D 00

SUMMARY OF ERRORS FOR THIS JOB ERROR NUMBER NUMBER OF ERRORS

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