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A Computer Simulation of the Steam-Graphite Reaction Under Isothermal and Steady-State Conditions

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ABSTRACT

A mathematical model has been formulated to describe the isothermal, steady-state diffusion and reaction of steam in a graphite matrix. A generalized Langmuir-Hinshelwood equation is used to represent the steam-graphite reaction rate. The model also includes diffusion in the gas phase adjacent to the graphite matrix. A computer program, written to numerically integrate the resulting differential equations, is described.

The coupled nonlinear differential equations in the graphite phase are solved using the IBM Continuous System Modeling Program. Classical finite difference techniques are used for the gas-phase calculations. An iterative procedure is required to couple the two sets of calculations. Several sample problems are presented to demonstrate the utility of the model.

1. INTRODUCTION

The core of an HTGR reactor is cooled by passing high pressure helium through the coolant channels. After leaving the core, the hot helium passes through a steam generator and is then recycled to the core.

Under normal operating conditions, the water side of the steam generator is at a higher pressure than the helium side; thus, any leak in the heat exchanger would allow water to be forced into the reactor-coolant stream. The water would be transported to the core where it could react with the hot graphite in accordance with the expression:

$$H_2O(g) + C(s) = H_2(g) + CO(g).$$

Thus, one of the major areas of concern in accident analyses is associated with evaluations of the consequences of steam entering the primary coolant system. While elaborate safeguards have been added to the reactor to detect a steam leak and quickly isolate a leaking steam generator, a significant amount of water could, nonetheless, enter the reactor. The amount of graphite that would be reacted, and the resulting pressure buildup in the primary coolant system, have been the subject of several reports.[1-4]

To analyze the effects of steam ingress, the rate at which the steam-graphite reaction proceeds must be known. A series of experiments studying the steam-graphite reaction have been conducted at the Oak Ridge National Laboratory. This report describes a calculational procedure which was developed to aid in the analysis of the experimental results. Only the calculational techniques are described, and no attempt is made to analyze actual experimental data. To apply the resulting computer program to the experimental program, the actual physical dimensions, reaction conditions, and the desired reaction rate equation must be supplied as input data.

The computer program was developed in three stages. In the first stage, a model was developed to simulate diffusion and reaction in the graphite pores. The second stage consisted of simulating the diffusion of the gaseous components in the coolant channel. The third stage consisted of combining the results of the two previous stages. A brief explanation and listing of the program are included, and several sample problems are described that illustrate how the program could be used.

2. PHYSICAL SYSTEM

A relatively simple apparatus was designed to study the steam-graphite reaction rate. The apparatus is composed of two concentric annuli which surround a quartz core. The graphite matrix forms the inner annulus, and a mixture of helium and steam flows in an axial direction in the outer annulus (Fig. 1). The flow rate of the helium-steam mixture is controlled so that a well-defined laminar flow profile is

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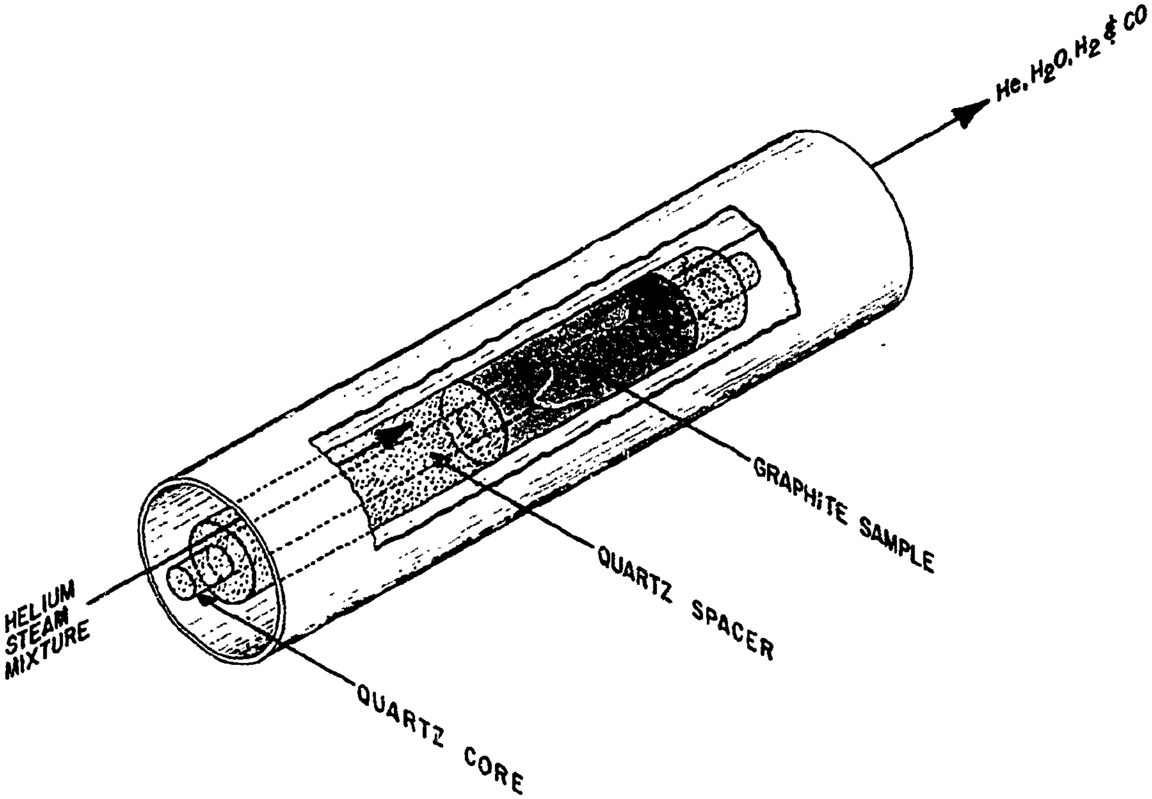

Fig. 1. Simplified drawing of experimental apparatus.

established. The inner quartz core and the outer wall of the gas annulus form impervious barriers. Isothermal conditions are maintained by supporting the entire apparatus in a furnace. The experiments were carried out at essentially atmospheric pressure.

3. GRAPHITE PHASE DIFFUSION MODEL

The generalized equation representing mass transfer and chemical reaction of a gaseous component at constant density and diffusivity in the graphite shell is

$$\frac{\partial c'}{\partial t} + U\cdot\nabla c' = D'\nabla^2 c - R , \qquad (1)$$

where

c' = molar concentration of component based on total volume (volume of graphite + pores), moles/cm^3,

c = molar concentration of component based on pore volume, moles/cm^3,

U = bulk velocity in graphite shell, cm/sec,

D' = diffusion coefficient for the component in He within the graphite matrix, cm^2/sec, and

R = molar rate of reaction of component, based on total volume, moles cm^{-3} sec^{-1}.

Two concentrations are used in Eq. (1). One concentration, c', is based on the total volume of the graphite matrix and includes the volume of the solid graphite and the volume of the voids within the graphite. The other concentration, c, is based only on the void volume. These concentrations are related by the porosity, ε_t, which is the fraction of the total volume which is void. In other words,

$$c' = \varepsilon_t c. \qquad (2)$$

The diffusion coefficient, D', in Eq. (1) contains the correction for porosity; hence, the concentration in that term must be based on the pore volume. If the pore-size distribution is isotropic, the relation between D' and the free-space diffusivity is

$$D' = D(\varepsilon/q), \tag{3}$$

where

D = free-space diffusivity of component in He, cm^2/sec and

(ε/q) = porosity-tortuosity factor, dimensionless.

The porosity-tortuosity factor enters Eq. (3) because the diffusion process takes place in the pores of the graphite matrix. Under these conditions, the diffusional path is not parallel to any of the axes; hence, this effect is accounted for by a porosity-tortuosity factor which must be determined experimentally.

Equation (1) can be simplified by assuming no bulk flow within the graphite matrix, and that the process approaches steady state very rapidly, resulting in

$$D'\nabla^2 c - R = 0. \tag{4}$$

If Eq. (4) is expressed in cylindrical coordinates, and if no axial diffusion and symmetry in the azimuthal direction, θ, is assumed, the following ordinary differential equation is obtained:

$$\frac{d^2c}{dr^2} + \frac{1}{r}\frac{dc}{dr} - \frac{R}{D'} = 0. \tag{5}$$

The molar concentration of the component can be converted to mole fraction by dividing each term by the total molar concentration, $\bar{c}$ (based on pore volume). If X, Y, and Z represent the mole fraction of H_2, H_2O, and CO, respectively, in the graphite pores, the resulting equations are:

$$\frac{d^2Y}{dr^2} + \frac{1}{r}\frac{dY}{dr} - \frac{R}{D_1'\ \bar{c}} = 0, \tag{6a}$$

$$\frac{d^2X}{dr^2} + \frac{1}{r}\frac{dX}{dr} + \frac{R}{D_2'\ \bar{c}} = 0, \text{ and} \tag{6b}$$

$$\frac{d^2Z}{dr^2} + \frac{1}{r}\frac{dZ}{dr} + \frac{R}{D_3' \; \bar{c}} = 0, \tag{6c}$$

where

$\bar{c}$ = total molar concentration, moles/cm^3 and

D_1', D_2', D_3' = diffusion coefficient for H_2O, H_2, and CO, respectively.

Several expressions have been proposed to describe the graphite-water reaction, and any of these expressions could be substituted into Eqs. (6). The rate expression (a generalized Langmuir-Hinshelwood equation) used in this report was presented in ref. 1 as follows:

$$K = \frac{K_1 P_{H_2O}}{1 + K_2 P_{H_2}^{0.75} + K_3 P_{H_2O}} , \tag{7}$$

$$K_j = k_j \exp\,(-E_j/\bar{\bar{R}}T) , \tag{8}$$

where

K = rate of graphite reacted, fraction/sec,

K_j = Arrhenius rate constants,

P_{H_2O} and P_{H_2} = partial pressure of H_2O and H_2, respectively, atm,

E_j = activation energy, cal/mole,

$\bar{\bar{R}}$ = gas constant, 1.9872 cal mole^{-1} °K^{-1}, and

T = temperature, °K

The suggested numerical values of the Arrhenius constants and activation energies are listed in Table 1.

The reaction term in Eqs. (6) can be expressed as

$$R = \frac{K\rho}{M} , \tag{9}$$

where

ρ = density of graphite, g/cm^3 and

M = molecular weight of graphite, g/mole.

Table 1. Values of Arrhenius constants and activation energies[a]

j	Component	k_j[b]	E_j(cal/mole)
1	H_2O	7.417×10^3	40,900
2	H_2	1.66×10^{-2}	-28,600
3	H_2O	5.31×10^{-2}	-27,500

[a] From ref. 1.

[b] The units for the Arrhenius constants are:

k_1 = fraction sec^{-1} atm^{-1},

k_2 = $\text{atm}^{-0.75}$, and

k_3 = atm^{-1}.

If the gas in the voids is assumed to be an ideal gas, the total molar concentration can be expressed as

$$\bar{c} = P/(\bar{R}T), \tag{10}$$

where

P = pressure, atm,

$\bar{R}$ = gas constant, atm cm^{-3} mole^{-1} $^\circ\text{K}^{-1}$.

The partial pressure of water is

$$P_{H_2O} = P \cdot Y. \tag{11}$$

Substituting Eqs. (9)-(11) into Eqs. (6) gives

$$\frac{d^2Y}{dr^2} + \frac{1}{r}\frac{dY}{dr} - \left(\frac{\alpha}{D_1'}\right)Y = 0, \tag{12a}$$

$$\frac{d^2X}{dr^2} + \frac{1}{r}\frac{dX}{dr} + \left(\frac{\alpha}{D_2'}\right)Y = 0, \text{ and} \tag{12b}$$

$$\frac{d^2Z}{dr^2} + \frac{1}{r}\frac{dZ}{dr} + \left(\frac{\alpha}{D_3'}\right)Y = 0, \tag{12c}$$

where

$$\alpha = \left[\frac{K_1}{1 + K_2P_{H_2}^{0.75} + K_3P_{H_2O}}\right]\frac{\rho\overline{R}T}{M} .$$

Equations (12) form a set of three second-order nonlinear differential equations. The equations are coupled through the reaction terms and, thus, must be solved simultaneously.

4. SOLUTION OF GRAPHITE-PHASE DIFFERENTIAL EQUATIONS

A set of nonlinear differential equations representing the diffusion and reaction of H_2O, H_2, and CO in the graphite matrix were derived in the previous section [Eqs. (12)]. At the inner radius of the graphite cylinder, the quartz rod forms an impervious barrier and results in the following boundary conditions:

$$\frac{dY}{dr} = 0, \ \frac{dX}{dr} = 0, \text{ and } \frac{dZ}{dr} = 0. \tag{13}$$

The mole fractions of the components at the gas-graphite interface are assumed to be known; for example,

$$X = X_0, \ Y = Y_0, \text{ and } Z = Z_0. \tag{14}$$

Since the three equations [Eqs. (12)] are coupled, they must be solved simultaneously. A numerical integration of the equations was performed utilizing the IBM Continuous System Modeling Program (CSMP)[5] that enables the user to simulate the operation of an analog computer on a digital computer. The CSMP program assumes the independent variables will have an initial value of zero. In our case, the independent variable is the radial distance and, since the graphite is in the form of a cylindrical shell,

$$RG \le r \le RI ,$$

where

RG = inside radius of graphite shell, and

RI = outside radius of graphite shell or gas-graphite interface.

A simple transformation of variable is shown by

$$\beta = \frac{r - RG}{RI - RG} , \tag{15}$$

which defines a new independent variable, β, whose value equals zero when r = RG, and 1 when r = RI. The substitution of Eq. (15) into Eqs. (12) gives

$$\frac{d^2Y}{d\beta^2} + \frac{(RI - RG)}{\beta(RI - RG) + RG} \frac{dY}{d\beta} - \frac{(RI - RG)^2\alpha}{D_1'} Y = 0 \tag{16a}$$

$$\frac{d^2X}{d\beta^2} + \frac{(RI - RG)}{\beta(BI - RG) + RG} \frac{dX}{d\beta} + \frac{(RI - RG)^2\alpha}{D_2'} Y = 0, \text{ and} \tag{16b}$$

$$\frac{d^2Z}{d\beta^2} + \frac{(RI - RG)}{\beta(RI - RG) + RG} \frac{dZ}{d\beta} + \frac{(RI - RG)^2\alpha}{D_3'} Y = 0. \tag{16c}$$

The boundary conditions become

$$\frac{dX}{d\beta} = \frac{dY}{d\beta} = \frac{dZ}{d\beta} = 0 \text{ at } \beta = 0 , \tag{17}$$

and

$$X = X_0, \ Y = Y_0, \text{ and } Z = Z_0 \text{ at } \beta = 1. \tag{18}$$

Analog computers and, by analogy, the CSMP program can only solve initial condition problems, that is, problems where all the boundary conditions are initial conditions. The problem expressed in Eqs. (16)-(18) is that of a boundary value. Equation (17) is an initial condition defining the concentration gradient at the inner radius of the graphite cylinder. However, Eq. (18), which specifies the mole fractions or concentrations of the components at the outer radius, is not an initial condition. The CSMP program can be used to solve Eqs. (16), but an iterative technique must be employed. A search must be made over a range of estimates for the mole fractions of the components at the inner wall (X, Y, and Z at β = 0) until a value is found that gives the desired final condition, as shown in Eq. (18).

Three sample calculations were made to test the CSMP program. The value of K_1 in Eq. (7) was increased by a factor of 10 in each successive run. Hence, the rate of reaction in case B was ten times that of case A, while in case C it was a hundred times that of case A. The concentration profiles for each run are shown in Figs. 2-4. The numerical values of the various parameters used in the calculations are listed in Table 2.

As shown in Figs. 2-4, the concentration of water reaches a minimum, while the concentrations of H_2 and CO attain a maximum at the inner boundary of the graphite shell. The minimum value of H_2O varies significantly from run to run, showing that it is quite sensitive to a change in the reaction rate.

Chemical reaction is the controlling mechanism in case A. Although only a small amount of graphite is being reacted, the graphite would not act as a protective barrier since the concentration of water is quite high at the inner boundary. If a highly reactive material were in contact with the graphite at this position, it would be subject to attack. Case C represents the other extreme in which diffusion is the controlling mechanism. The mole fraction of water decreases very rapidly and is almost zero (8.5×10^{-6}) at the inner boundary. Thus, while the graphite is being reacted at a higher rate in this case, any reactive material in contact with the graphite at the inner radius would be protected from chemical attack.

In all cases, the mole fraction of H_2 is one-half that of CO. From the assumption of steady state, the molar flux of all components must be equal. As seen from Table 2, the diffusivity of H_2 is assumed to be twice the diffusivity of CO. Hence, the concentration gradient of H_2 must be one-half that of CO to have equal molar fluxes; therefore, the concentration of H_2 will increase at exactly one-half the rate at which the concentration of CO increases.

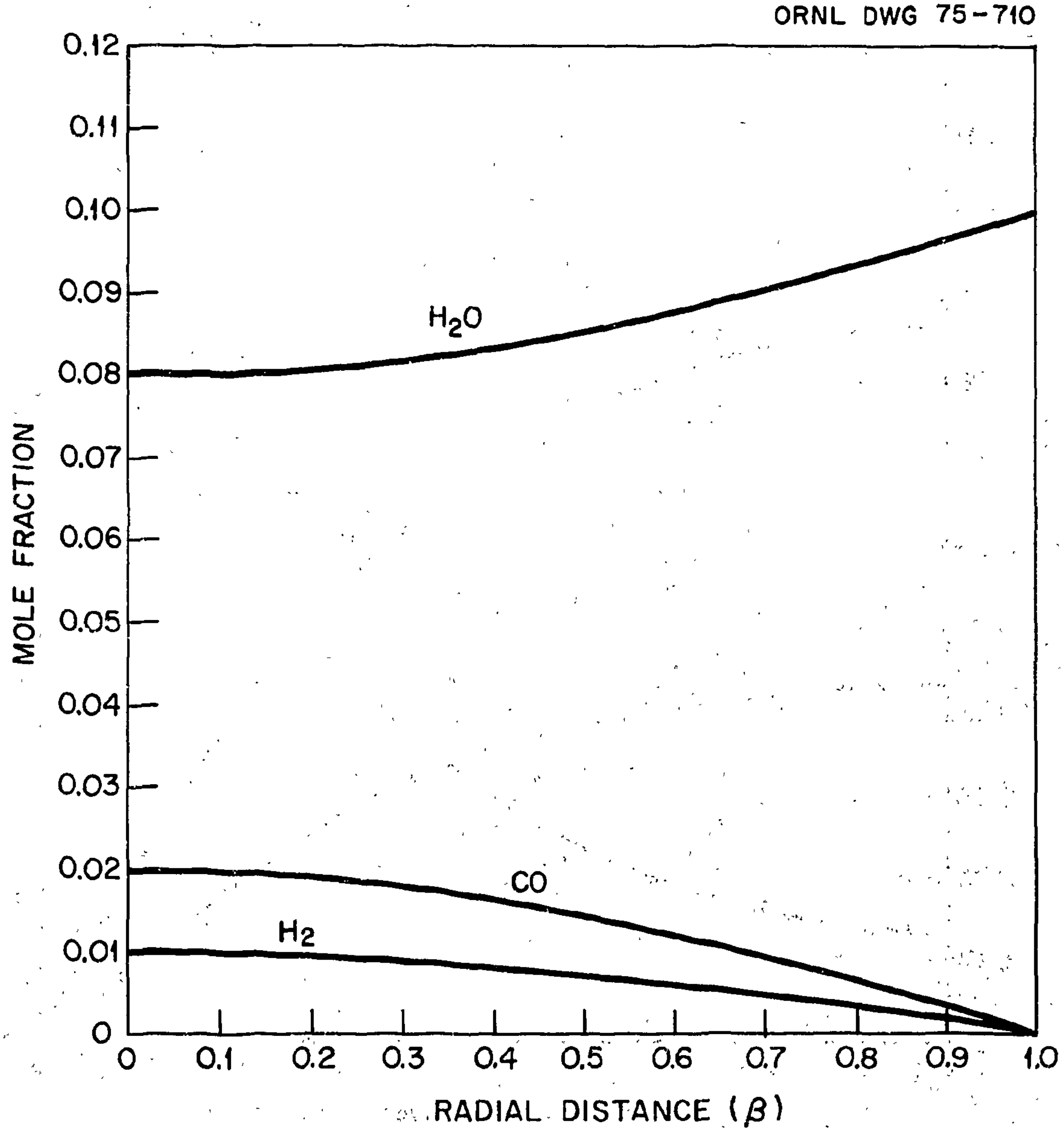

Fig. 2. Concentration profiles – Case A.

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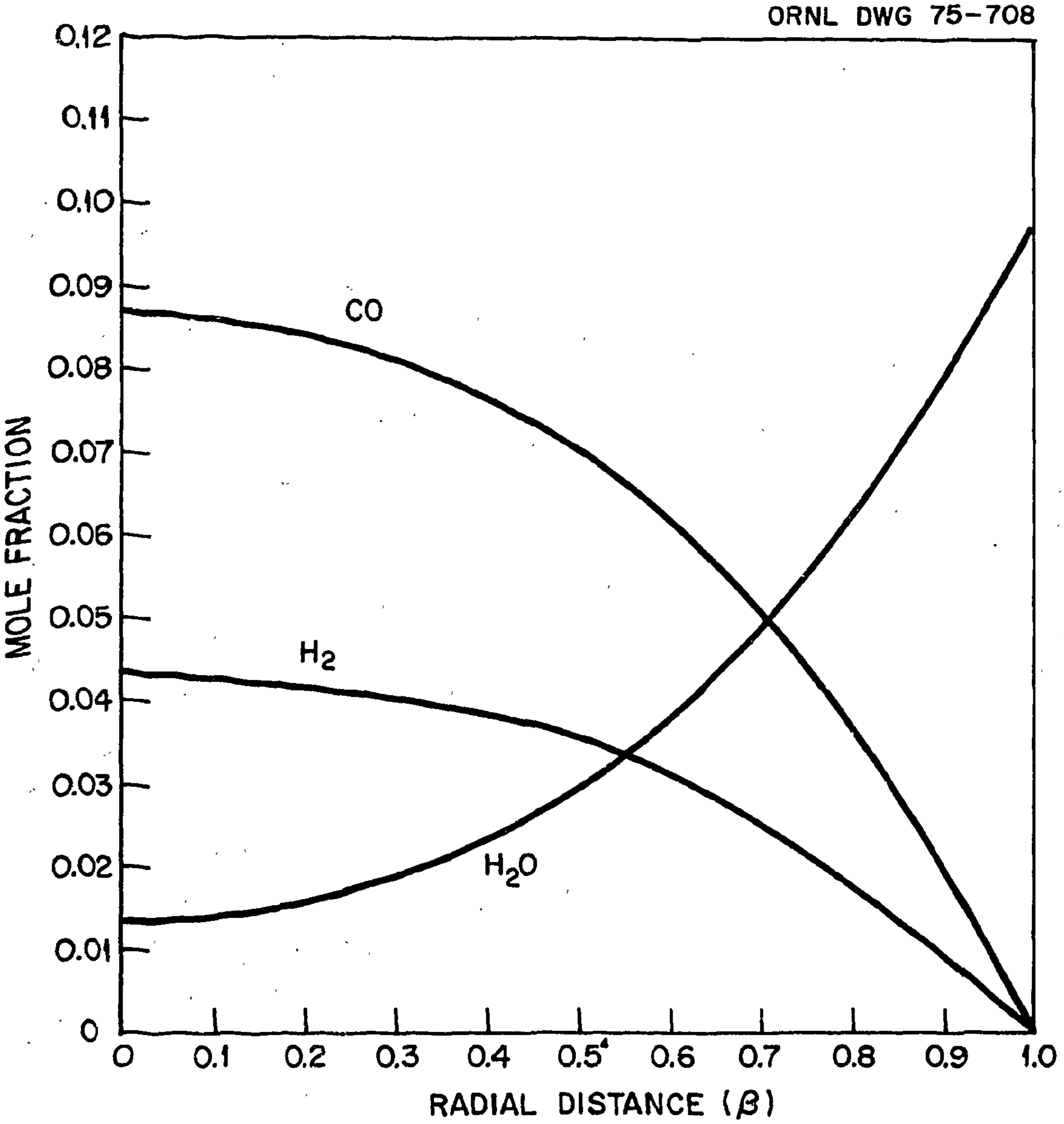

Fig. 3. Concentration profiles – Case B.

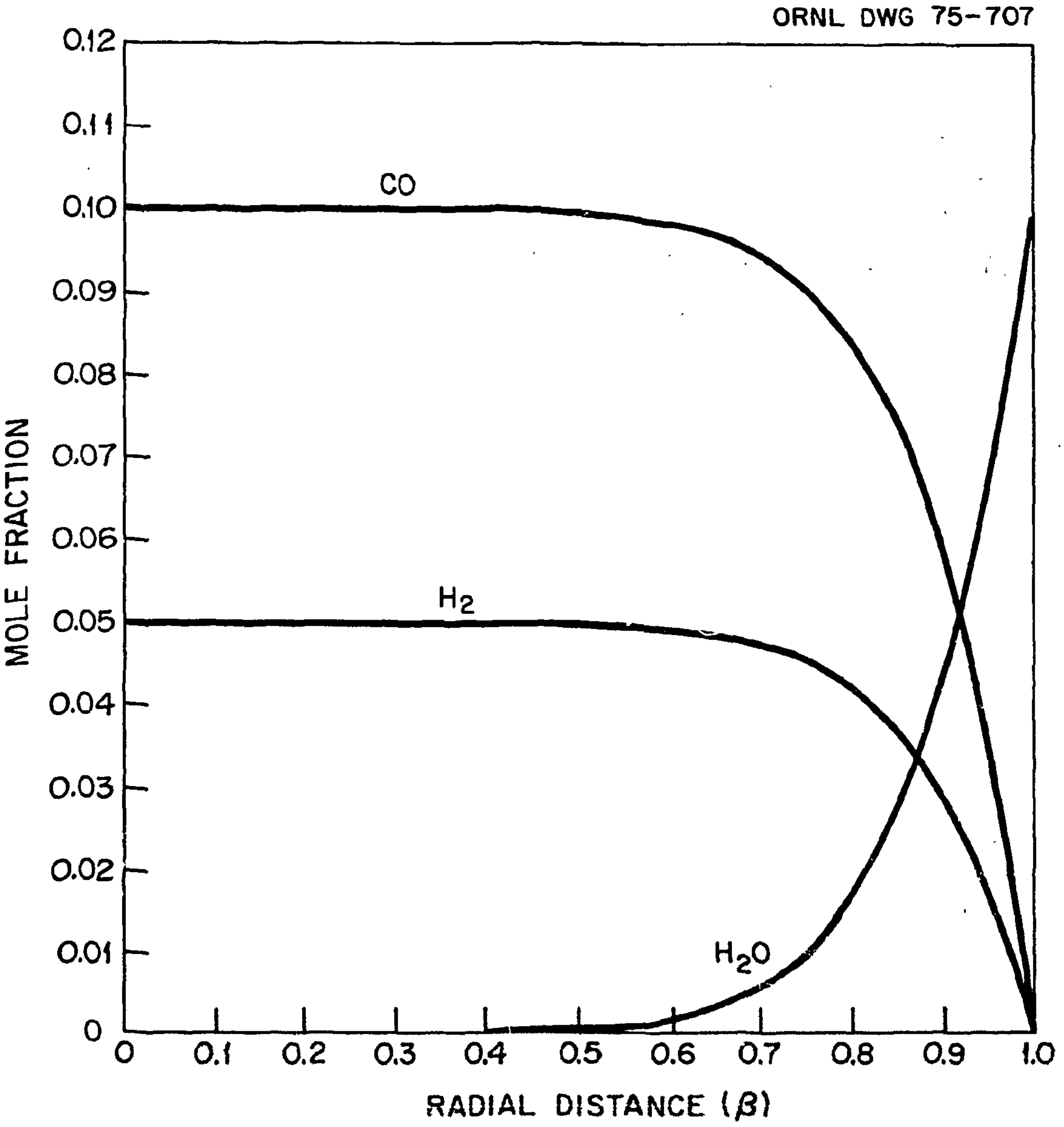

Fig. 4. Concentration profiles – Case C.

Table 2. Values of parameters used in sample problems

$RG = 0.762$ cm or 0.3 in.

$RI = 1.905$ cm or 0.75 in.

$T = 1273°K$

$P = 1$ atm

$\rho = 1.792$ g/cm^3 or 111.87 lb/ft^3

$M = 12.0$ g/mole

$Y_o = 0.1$

$X_o = 0.0$

$Z_o = 0.0$

$D_1' = 0.0853$ cm^2/sec, or 0.0132 in.^{2}/sec[a]

$D_2' = 0.1706$ cm^2/sec, or 0.0264 in.^{2}/sec[a]

$D_3' = 0.0853$ cm^2/sec, or 0.0132 in.^{2}/sec[a]

$k_1 = 7.417 \times 10^3$ fraction sec^{-1} atm^{-1} for Case A

$= 7.417 \times 10^4$ fraction sec^{-1} atm^{-1} for Case B

$= 7.417 \times 10^5$ fraction sec^{-1} atm^{-1} for Case C

$k_2 = 1.66 \times 10^{-2}$ atm$^{-0.75}$

$k_3 = 5.31 \times 10^{-2}$ atm^{-1}

$E_1 = 40{,}900$ cal/mole

$E_2 = -28{,}600$ cal/mole

$E_3 = -27{,}500$ cal/mole

---

[a] Values calculated from ref. 3.

5. GAS PHASE DIFFUSION MODEL

The differential equations representing the diffusion of the gaseous components to or from the graphite interface are:

$$\frac{\partial^2 y}{\partial r^2} + \frac{1}{r}\frac{\partial y}{\partial r} - \frac{U}{D_1}\frac{\partial y}{\partial z} = 0, \tag{19a}$$

$$\frac{\partial^2 x}{\partial r^2} + \frac{1}{r}\frac{\partial y}{\partial r} - \frac{U}{D_2}\frac{\partial x}{\partial z} = 0, \text{ and} \tag{19b}$$

$$\frac{\partial^2 v}{\partial r^2} + \frac{1}{r}\frac{\partial v}{\partial r} - \frac{U}{D_3}\frac{\partial v}{\partial z} = 0, \tag{19c}$$

where

y = mole fraction H_2O in the gas phase,

x = mole fraction H_2 in the gas phase,

v = mole fraction CO in the gas phase,

D_1, D_2, D_3 = free space diffusivity of H_2O, H_2, and CO in He, respectively, cm^2/sec, and

U = velocity in the axial direction, cm/sec.

The gases are flowing in the outer annulus with a well defined laminar velocity profile. The velocity at any radial point is[6]

$$U = \frac{(P_0 - P_L)R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2 + \frac{1 - b^2}{\ln \frac{1}{b}} \ln \left(\frac{r}{R}\right)\right], \tag{20}$$

where

p_o = inlet pressure, $dynes/cm^2$,

P_L = outlet pressure, $dynes/cm^3$,

μ = viscosity, $g\ cm^{-1}\ sec^{-1}$, or poise,

L = length, cm,

R = outside radius of annulus, cm,

r_o = inside radius of annulus, cm,

$b = r_o/R$, dimensionless, and

r = radius, $r_o \leq r \leq R$, cm.

The volume rate of flow is[6]

$$Q = \frac{(P_o - P_L)R^4}{8\mu L}\left[(1 - b^4) - \frac{(1 - b^2)^2}{\ln \frac{1}{b}}\right]. \tag{21}$$

Through combination of Eqs. (20) and (21), the velocity at any radial position can be expressed as a function of the volumetric flow rate.

The partial derivatives in Eqs. (19) can be approximated by difference equations. A grid system is devised by dividing the radial and axial length into a number of segments. The radial index is represented by j, the inner radius (interface between the gas and graphite) is represented by $j = 1$, and $j = J$ represents the outer radius. The distance between the radial points is

$$h = \frac{RO - RG}{J - 1}, \tag{22}$$

where

h = radial step size, cm,

RO = outside radius, cm, and

RG = inside radius, cm.

The axial distance is also divided into N increments where the axial step size is

$$\Delta = \frac{L}{N}, \tag{23}$$

and

Δ = axial step size, in., and

L = length of tube, in.

The mole fraction of water at any point is expressed as $y(j,m)$, with $x(j,n)$ and $v(j,n)$ used to express the mole fractions of H_2 and CO.

The finite-difference expressions used to approximate the various partial derivatives in Eqs. (19) are:

$$\frac{\partial^2 y}{\partial r^2} = \frac{y(j-1, n) - 2y(j, n) + y(j + 1, n)}{h^2}, \tag{24a}$$

$$\frac{\partial y}{\partial r} = \frac{y(j + 1, n) - y(j - 1, n)}{2h}, \tag{24b}$$

and

$$\frac{\partial y}{\partial z} = \frac{y(j, n) - y(j, n - 1)}{\Delta}. \tag{24c}$$

Similar expressions can be written for the terms in Eqs. (19b) and (19c). The substitution of Eqs. (24) into Eq. (19a) gives

$$\left[\frac{2r + h}{2h^2 r}\right] y(j + 1, n) - \left[\frac{2}{h^2} + \frac{U}{D_1 \Delta}\right] y(j, n) + \left[\frac{2r - h}{2h^2\, r}\right] y(j - 1, n)$$

$$= - \left[\frac{U}{D_1 \Delta}\right] y(j, n - 1). \tag{25}$$

It must be remembered that the velocity is a function of the radial position, j, and is evaluated from Eqs. (20) and (21). The radius at any radial position j is

$$r = RG + (j - 1)h. \tag{26}$$

Equation (25) holds for the interior points $2 \leq j \leq J - 1$. At the outer radius, $(j = J)$, the boundary condition is $\partial y/\partial r = 0$. Application of Eq. (24b) to this boundary condition gives

$$y(J + 1, n) = y(J - 1, n). \tag{27}$$

Since the velocity is equal to zero at the outer wall, Eq. (25) reduces to

$$y(J - 1, n) - y(J, n) = 0. \tag{28}$$

At the inner wall, the flux of water must be continuous across the gas-solid interface, that is,

$$D_1 \left.\frac{\partial y}{\partial r}\right|_{r = RI} = D_1' \delta_1 , \tag{29}$$

where $\delta_1 = \left.\frac{dY}{dr}\right|_{r = RI}$ in the graphite phase. By applying Eq. (24b) to Eq. (29),

$$y(0, n) = y(2, n) = \frac{2D_1'\delta_1 h}{D_1} . \tag{30}$$

Evaluation of Eq. (25) at the inner radius, ($j = 1$), substitution of Eq. (30), and utilization of the fact that the velocity is zero at the interface results in:

$$\left[\frac{2}{h^2}\right] y(2, n) - \left[\frac{2}{h^2}\right] y(1, n) = \frac{D_1'\delta_1(2RI - h)}{D_1 bRI} . \tag{31}$$

Equations (25), (28), and (31) form a set of simultaneous linear equations expressing $y(j,n)$ in terms of $y(j, n - 1)$. The coefficient matrix for this set of equations is a tridiagonal matrix. Thus, the concentration profile of water in the gas phase can be calculated once the flux at the interface, (δ_1), is specified.

Similar equations can be written for H_2 and CO. From the stoichiometry of the reaction, one mole of H_2 and CO are formed for each mole of water reacted. Therefore, the flux of H_2 and CO at the interface can be expressed as a function of the flux of water as follows: for H_2

$$D_2' \left.\frac{dX}{dr}\right|_{r = RI} = -D_1'\delta_1$$

or

$$\delta_2 = -\frac{D_1'\delta_1}{D_2'} , \tag{32}$$

and for CO

$$\delta_3 = -\frac{D_1'\delta_1}{D_3'} \tag{33}$$

The equations used to calculate the mole fraction of H_2 and CO are easily derived from the equations used for H_2O by substitution of the appropriate diffusivity (D_2 or D_3) and slope at the interface (δ_2 or δ_3).

6. COMBINED GAS AND GRAPHITE MODEL

The models simulating diffusion and chemical reaction in the graphite cylinder and diffusion across the gas annulus have been discussed. To simulate the experimental apparatus, it is necessary to combine the two sets of calculations. The differential equations, Eqs. (12) and (19), and the boundary conditions, Eqs. (17) and (27), still apply to the combined model. Two additional boundary conditions must be written for each component to represent the continuity of the mole fraction and molar flux at the gas-graphite interface. The additional boundary conditions are:

$$x = X, \quad y = Y, \quad z = Z \qquad (34)$$

and

$$D_1 \frac{\partial y}{\partial r}\Big|_{RI} = D_1' \frac{dY}{dr}\Big|_{RI}, \quad D_2 \frac{\partial x}{\partial r}\Big|_{RI} = D_2' \frac{dX}{dr}\Big|_{RI}, \quad D_3 \frac{\partial z}{\partial r}\Big|_{RI} = D_3' \frac{dZ}{dr}\Big|_{RI} . \qquad (35)$$

The model for the gas phase requires that the molar flux of each component be specified at the interface. Alternately, the graphite-phase calculation requires the specification of the mole fractions at the interface. Each calculation requires quantities calculated in the other phase; therefore, an iterative calculation must be performed until the concentrations and molar fluxes at the interface are identical in each set of calculations. This satisfies the boundary conditions connecting the two models, Eqs. (34) and (35).

The calculational procedure used for each axial node is as follows:

(1) Estimate the concentrations of the components at the graphite surface from the corresponding value calculated in the previous time step. For the first axial step, the initial conditions are used as the estimate.

(2) Calculate the concentration profiles for the components in the graphite annulus.

(3) Use the results of step (2) to calculate the molar flux for the components at the interface.

(4) Calculate the concentration profiles in the gas phase. This calculation also determines the mole fractions at the graphite interface.

(5) Compare the results of step (4) with the previously calculated or estimated compositions. If the results agree, convergence has been obtained and the next axial step is considered. Otherwise another iteration is required and the procedure returns to step (2).

A sample problem was solved to test the combined model. The physical properties for the graphite cylinder are the same as those listed in Table 2. The reaction rate, k, used in the calculations corresponds to Case B (7.417×10^4). The physical properties for the gas phase are listed in Table 3.

Table 3. Gas phase physical properties used in sample problem

Variable	Value
Q	10.0 cm^3/sec
D_1	8.63 cm^2/sec or 1.32 $\text{in.}^2/\text{sec}$
D_2	17.06 cm^2/sec or 2.64 $\text{in.}^2/\text{sec}$
D_3	8.53 cm^2/sec or 1.32 $\text{in.}^2/\text{sec}$
RO	2.54 cm or 1.00 in.
h	0.02116 cm or 0.00833 in.
Δ	0.127 cm or 0.05 in.

The resulting concentration profiles are shown in Figs. 5 and 6. Figure 5 shows the results for the fourth axial step, or 0.15 in. from the leading edge of the graphite cylinder. Figure 6 corresponds to the 24th axial step, which is 1.15 in. from the leading edge. In both figures the concentration profiles in the graphite cylinder are similar to those

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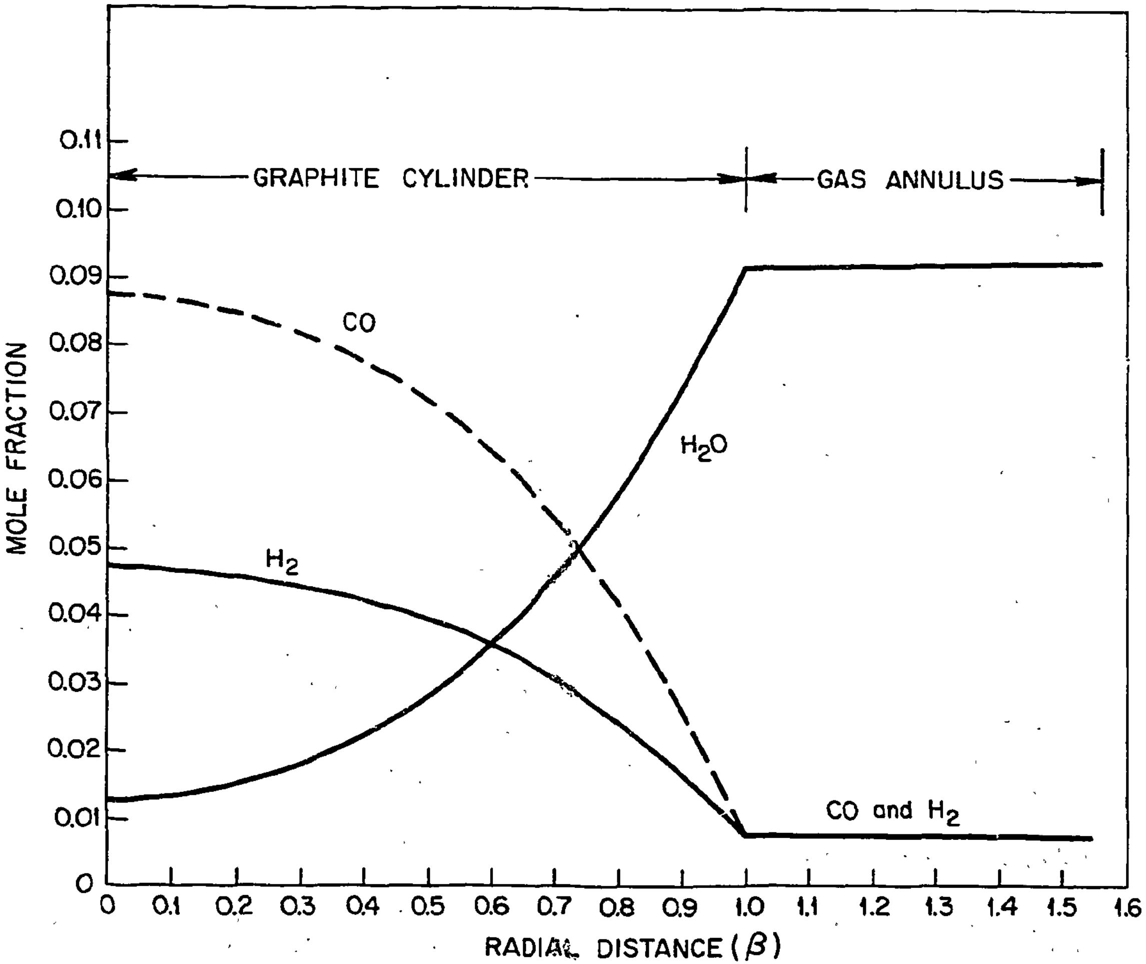

Fig. 5. Concentration profiles for the combined model of sample problem 1 at axial step No. 4.

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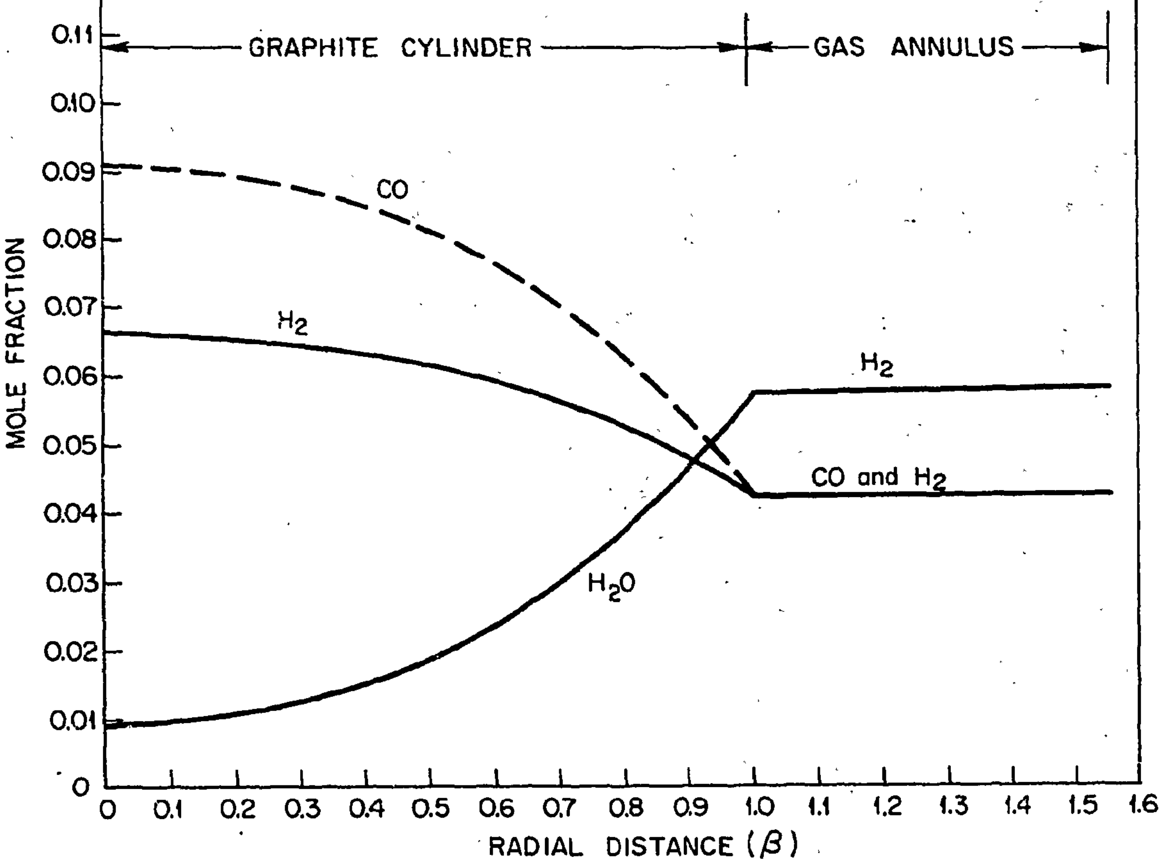

Fig. 6. Concentration profiles for the combined model of sample problem 1 at axial step No. 24.

shown in Fig. 3, except that there is an appreciable concentration of CO and H_2 at the gas-graphite interface. The gas-phase concentration profile of all three components are nearly flat. This is caused by the proportionally larger diffusivities in the gas phase. The gas-phase diffusivities are 100 times larger than the graphite matrix.

In a second sample problem, the gas-phase diffusivities were reduced by a factor of 10. The results of the calculation are shown in Figs. 7 and 8. In this case, there is a small concentration gradient across the gas phase. The wall composition of H_2O is reduced slightly, while the wall compositions of H_2 and CO are increased slightly. This inhibition caused by H_2 results in a slower reaction rate. Hence, the concentration of water does not decrease as rapidly in the graphite cylinder as it did in the previous sample problem.

Each sample problem considered 31 axial steps and divided the gas phase into 31 radial nodes. Computation time on the IBM 360/91 computer was 29 sec for the first problem and 22 sec for the second problem. The core storage requirements are 150K. A description and a listing of the computer program are presented in the Appendix.

7. SUMMARY

A computer program has been developed that predicts the concentration profiles of H_2O, H_2, and CO in a graphite matrix. The program also considers the gas-space diffusion of the components to and from the graphite surface.

The sample problems discussed are presented as illustrations and do not represent actual experimental data. To simulate the experimental data generated at ORNL, the actual physical dimensions and reaction conditions must be supplied as input data. The reaction rate equation presented in ref. 1 was used in the sample problems; it would be a simple matter to insert another expression, if so desired.

The program calculates 31 axial nodes in approximately 21 to 27 sec. Additional nodes can be added if necessary, and the computational requirements would increase linearly. Only 150K of computer memory is required

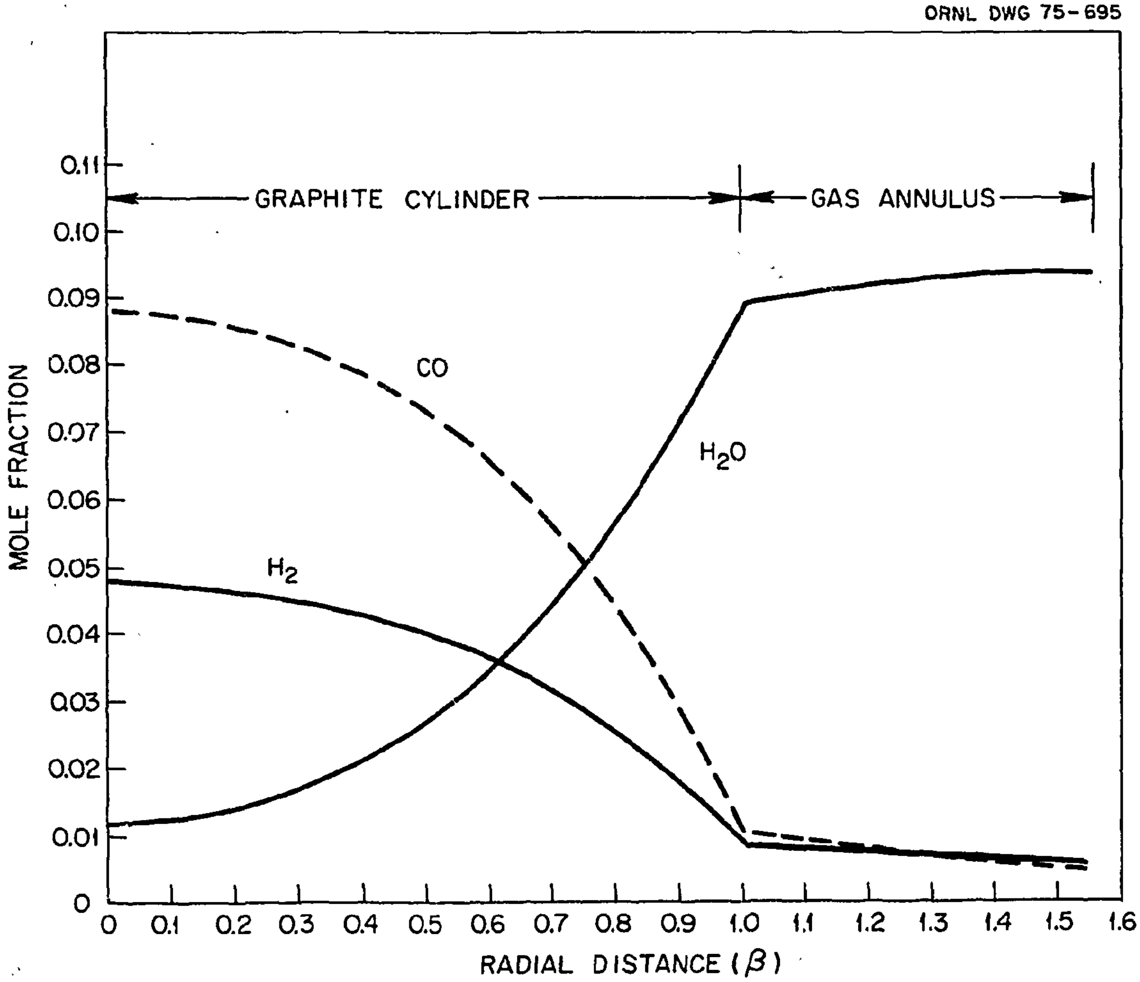

Fig. 7. Concentration profiles for the combined model of sample problem 2 at axial step No. 4.

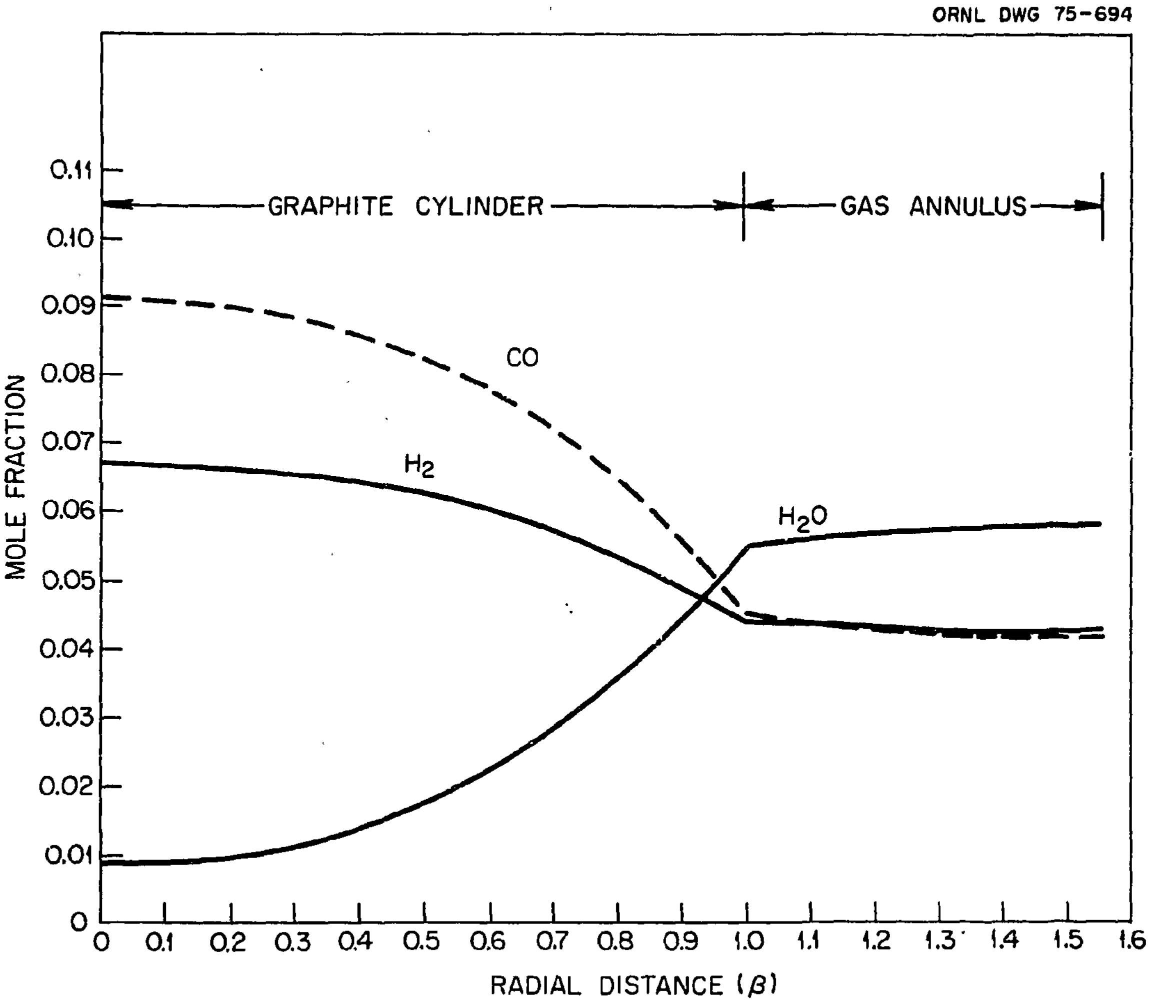

Fig. 8. Concentration profiles for the combined model of sample problem 2 at axial step No. 24.

to execute the program. The program requires the availability of the IBM Continuous System Modeling Program.

8. REFERENCES

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3. P. Hawtin, R. A. Huber, D. Wilmore, "The Calculation of Graphite Corrosion and Coolant Composition in Helium Cooled HTRs," J. Brit. Nucl. Eng. Soc. 11, 71 (1972).
4. P. Hawtin, R. A. Huber, D. Wilmore, A Transient Model for the Calculation of the Corrosion Rate of an HTR Core Under Fault Conditions, AERE-R-7414 (1974).
5. System/360 Continuous System Modeling Program (360A-CX-16X), User's Manual (GH20-0367), IBM Corporation, Data Processing Division, White Plains, N. Y.
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9. APPENDIX: DESCRIPTION OF THE COMPUTER PROGRAM

9. APPENDIX: DESCRIPTION OF THE COMPUTER PROGRAM

The computer program previously discussed is described in more detail. The main part of the program is the CSMP program which performs the graphite-phase calculations. This program calls several subroutines to perform the gas-phase calculations. The subroutines will be discussed first since they appear before the CSMP program in the listing.

9.1 Subroutine GAS

This subroutine calculates the composition of the three components (H_2O, H_2, and CO) in the gas annulus. The calculations are made using the finite-difference equations derived in the section describing the Gas-Phase Diffusion Model, [i.e., Eqs. (25), (28), and (31)]. The subroutine is called from the CSMP program after calculation of the corresponding concentration profiles in the graphite annulus. The following information is passed between the CSMP program and the GAS subroutine:

(1) DYDB - concentration gradient of H_2O in the graphite phase at the solid-gas interface (calculated in the CSMP program);

(2) N - the index for the axial step (set in the CSMP program);

(3) VFIRST, XFIRST and YINT - concentrations of CO, H_2, and H_2O, respectively, at the gas-solid interface (calculated in GAS subroutine); and

(4) NEXIT - variable indicating whether gas-phase calculations have converged.

The GAS subroutine first reads the required data and then calculates the gas phase diffusivities, laminar velocity profile, and finite-difference coefficient matrix. This information is independent of the graphite-phase concentration profiles, reaction rate, or previous gas-phase calculations. Thus, for subsequent calls to the GAS subroutine, these calculations are bypassed. The logic is controlled by the variable, NQUES. The initial value of NQUES is 1 and is set via a data statement. After the above calculations have been performed, the value of NQUES is incremented by 1. During later calls to the subroutine, if NQUES has a value greater than 1, the program will immediately go to the second step.

The second part of the GAS subroutine calculates the right-hand side of the finite difference equations. The right-hand sides are a function of the graphite-phase concentration profiles and, in addition, are a function of the gas-phase calculations for the previous axial step. After setting up the right-hand side, the set of simultaneous equations are solved using the TRIDIA subroutine which must be called three times, once for each component. Once the calculation of the gas-phase concentration profiles is completed, the program compares the result of the wall composition of H_2O with that obtained in the last iteration. If the results agree to within 0.01%, convergence has been obtained, and the variable NEXIT is set to a value of 5. If the results have not converged, the value of NEXIT is left unchanged. In either case, the logic path returns to the CSMP program. A simplified flowsheet of the calculations is shown in Fig. 9, and the variables used in the program are defined in Table 4.

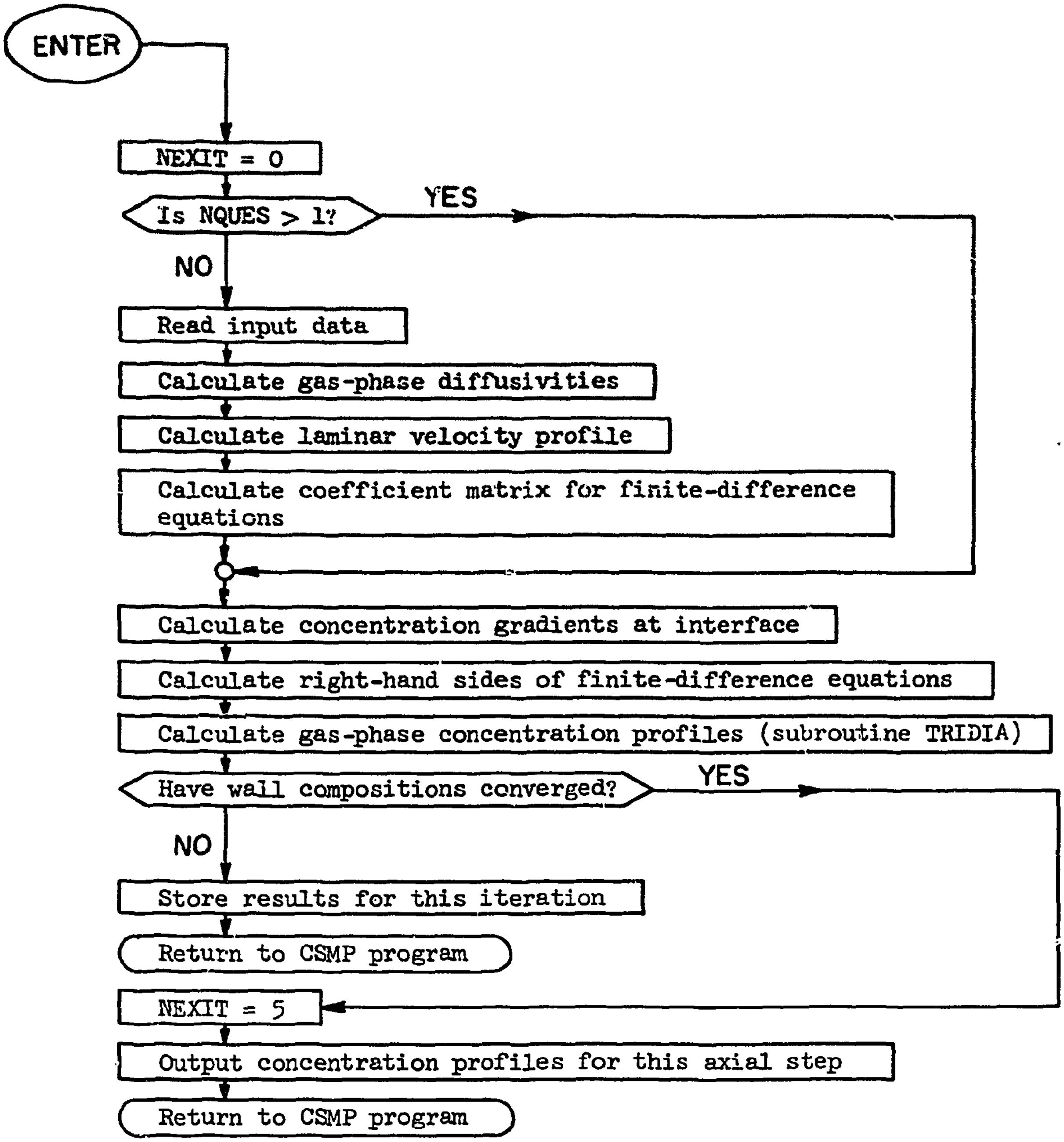

Fig. 9. Simplified flowsheet for subroutine GAS.

Table 4. Definition of variables used in Subroutine GAS

Name	Definition
A(J,K)[a]	Coefficient matrix for H_2O in finite difference equations, Eqs. (25), (28), and (31)
ACO (J,K)[a]	Coefficient matrix for CO in finite difference equations, Eqs. (25), (28), and (31)
AH2(J,K)[a]	Coefficient matrix for H_2 in finite difference equations, Eqs. (25), (28), and (31)
ALP	Concentration gradient of H_2O at gas-graphite interface, in.$^{-1}$
ALP2	Concentration gradient of H_2 as gas-graphite interface, in.$^{-1}$
ALP3	Concentration gradient of CO at gas-graphite interface, in.$^{-1}$
B(J)[b]	Right-hand sides of finite difference equations for H_2O, Eqs. (25), (28), and (31)
BCO(J)[b]	Right-hand sides of finite difference equations for CO, Eqs. (25), (28), and (31)
BH2(J)[b]	Right-hand sides of finite difference equations for H_2 , Eqs. (25), (28), and (31)
DCDR	Double precision value of concentration gradient of H_2O in graphite at interface ($\partial y/\partial \beta$), dimensionless
DCOG	Diffusivity of CO in He in gas annulus, in.^{2}/sec (Note: DCOG is assumed to be equal to DIG)
DCOS	Effective diffusivity of CO in He in graphite pores, in.^{2}/sec (Note: DCOS is assumed to be equal to DIS)
DEL	Axial step size, in.
DENOM	Internal variable which has two definitions and is used for the calculation of velocity profile
DH2G	Diffusivity of H_2 in He in gas annulus, in.^{2}/sec (Note: DH2G is assumed to be twice DIG)

Table 4 (continued)

Name	Definition
DH2S	Effective diffusivity of H_2 in He in graphite pores, in.^{2}/sec (Note: DH2S is assumed to be twice DIS)
DIG	Diffusivity of H_2O in He in gas annulus, in.^{2}/sec
DIS	Effective diffusivity of H_2O in He in graphite pores, in.^{2}/sec
DYDB[d]	Concentration gradient of H_2O in graphite at interface ($\partial y/\partial \beta$), dimensionless
EPT	Temperature exponent in diffusivity equation, dimensionless
FACT	Internal variable used in the calculation of the velocity profile
FLOW	Volumetric flow rate of entering gas stream, cm^3/sec
H	Radial step size, in. (Note: gas annulus is assumed to be divided into 30 equal segments)
J	DO - Loop counter
M	DO - Loop counter
M	DO - Loop counter
N[d]	Index of axial step
NEXIT[e]	Convergence indicator
NQUES	Index which controls program logic to avoid repeating needless calculations
PRES[c]	Pressure, atm
RAD	Dimensionless radius used for calculating velocity profile
RG[c]	Inside radius of graphite annulus, in.
RI[c]	Outside radius of graphite annulus, in. (position of gas-solid interface)

Table 4 (continued)

Name	Definition
RO[c]	Outside radius of gas annulus, in.
RR	Outside radius of gas annulus, cm
TEMP[c]	Temperature, °K
TRIDIA	Subroutine for solving finite difference equations
VFIRST[e]	Mole fraction of H_2 at graphite interface
VZ(J)[b]	Laminar velocity profile in gas annulus, in./sec
X(J)[b]	Concentration of H_2O at current axial position
XCO(J)[b]	Concentration of CO at current axial position
XFIRST[e]	Mole fraction of H_2 at graphite interface
XH2(J)[b]	Concentration of H_2 at current axial position
XKAP	RI/RO, dimensionless; see Eq. (20), variable b
XKK[c]	Constant in diffusivity equation, cm^2 atm^{-1} sec^{-1} $(°K)^{-EPT}$
Y(J,K)[a]	Concentration of H_2O in gas annulus
YCO(J,K)[a]	Concentration of CO in gas annulus
YCOI[c]	Mole fraction CO in entering gas stream
YH2(J,K)	Concentration of H_2 in entering gas stream
YINT[e]	Mole fraction of H_2O at graphite interface
YO[c]	Mole fraction of H_2O in entering gas stream

[a] Position dependent variable; first subscript refers to radial position, and second subscript refers to axial position.

[b] Position dependent variable; subscript refers to radial position.

[c] Input variable whose value must be defined in subroutine.

[d] Value passed from CSMP program as an argument.

[e] Value passed to CSMP program as an argument.

9.2 Subroutine TRIDIA

Subroutine TRIDIA solves the set of simultaneous linear algebraic equations derived from the finite-difference approximations for the partial derivatives. The set of equations can be expressed as

$$Ax = b \tag{36}$$

where

A = coefficient matrix,

x = column vector of compositions, and

b = column vector of right-hand sides.

The coefficient matrix is a tridiagonal matrix with all elements of the major diagonal being nonzero. Sets of equations of this type may be solved by factoring the tridiagonal matrix into two bidiagonal matrices, L and R; thus, Eq. (36) becomes

$$Ax = b = LRx \ . \tag{37}$$

If Rx is written as g, the original system can be broken into two bidiagonal systems:

$$Lg = b \text{ and} \tag{38}$$

$$Rx = g \ . \tag{39}$$

The two bidiagonal matrices can be represented as follows:

$$\underset{L}{\begin{bmatrix} \ell_1 & 0 & 0 & 0 \\ \gamma_2 & \ell_2 & 0 & 0 \\ 0 & \gamma_3 & \ell_3 & 0 \\ 0 & 0 & \gamma_4 & \ell_4 \end{bmatrix}} \underset{R}{\begin{bmatrix} 1 & r_1 & 0 & 0 \\ 0 & 1 & r_2 & 0 \\ 0 & 0 & 1 & r_3 \\ 0 & 0 & 0 & 1 \end{bmatrix}} = \underset{A}{\begin{bmatrix} \alpha_1 & \beta_1 & 0 & 0 \\ \gamma_2 & \alpha_2 & \beta_2 & 0 \\ 0 & \gamma_3 & \alpha_3 & \beta_3 \\ 0 & 0 & \gamma_4 & \alpha_4 \end{bmatrix}}$$

The equations for factoring the tridiagonal matrix are:

$$\ell_1 = \alpha_1 \tag{40}$$

$$\ell_1 r_1 = \beta_1$$

$$\ell_2 + \gamma_2 r_1 = \alpha_2 \tag{41}$$

$$r_2 \ell_2 = \beta_2$$

$$\cdots\cdots$$

$$\ell_4 + \gamma_4 r_3 = \alpha_4 \; . \tag{42}$$

The two bidiagonal systems can be evaluated easily by solving Eq. (38) and substituting the results into Eq. (39). Equation (38) can be written as

$$\begin{bmatrix} \ell_1 & 0 & 0 & 0 \\ \gamma_2 & \ell_2 & 0 & 0 \\ 0 & \gamma_3 & \ell_3 & 0 \\ 0 & 0 & \gamma_4 & \ell_4 \end{bmatrix} \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} ,$$

or as

$$\begin{aligned} \ell_1 g_1 &= b_1 \\ \ell_2 g_2 + \gamma_2 g_1 &= b_2 \\ \ell_3 g_3 + \gamma_3 g_2 &= b_3 \\ \ell_4 g_4 + \gamma_4 g_3 &= b_4 \; , \end{aligned} \tag{43}$$

and may be easily solved for g_1, g_2, g_3, and g_4. The second set of equations, Eq. (39), may be expressed as

$$\begin{bmatrix} 1 & r_1 & 0 & 0 \\ 0 & 1 & r_2 & 0 \\ 0 & 0 & 1 & r_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix}$$

or as

$$\begin{aligned} x_1 + r_1 x_2 &= g_1 \\ x_2 + r_2 x_3 &= g_2 \\ x_3 + r_3 x_4 &= g_3 \\ x_4 &= g_4 \; , \end{aligned} \tag{44}$$

and may be solved by first evaluating x_4, and then x_3, x_2, and x_1. Subroutine TRIDIA simply puts this logic into computer language.

9.3 Subroutine OUTPUT

This subroutine stores the necessary data for printing a summary of the concentration profiles. The same information would be obtained by using the CSMP print statement; however, this statement would print the results for each iteration. Since the user is generally interested in the final result, the output from the CSMP program is suppressed by defining File 6 as a dummy file. To obtain the values of the dependent variables at the desired values of the independent variables, it is necessary to include the CSMP print card in the CSMP program.

After the calculations have converged for a particular axial increment, the OUTPUT Subroutine is again called to calculate the amount of graphite reacted as a function of the radial position. The amount of water or graphite being reacted is easily calculated from a steady-state mass balance over a cylindrical shell:

$$N_r|_1(2\pi r_1 \Delta L) - N_r|_2(2\pi r_2 \Delta L) = R[\pi D\Delta(r_1^2 - r_2^2)] , \tag{45}$$

where

N_r = molar flux across surface, moles in.$^{-2}$ sec^{-1},

r_1 = outside radius of cylindrical shell, in.,

r_2 = inside radius of cylindrical shell, in.,

ΔL = length of segment, in., and

R = molar rate of reaction, moles in.$^{-3}$ sec^{-1}

The right-hand side of Eq. (45) is the rate at which water on graphite is being reacted, and is expressed as moles/sec. The molar flux can be expressed as

$$N_r = D' \frac{dc}{dr} , \tag{46}$$

where

D' = diffusion coefficient of H_2O in He in graphite matrix, in.^{2}/sec, and

c = molar concentration of H_2O based on pore volume, moles/in.^{3}.

Substituting Eq. (46) into Eq. [illegible]) and solving for the rate of reaction yields

$$A = 2\,\pi\,D'\Delta L \left[r_1 \frac{dc}{dr}\Big|_1 - r_2 \frac{dc}{dr}\Big|_2 \right] , \tag{47}$$

where

A = amount of H_2O reacted, moles/sec $A = \{[\pi \Delta L(r_1^2 - r_2^2)] \cdot R\}$.

The molar concentration of H_2O can be converted to a mole fraction by

$$y = \frac{c}{\bar{c}} , \tag{48}$$

where

$\bar{c}$ = total molar concentration, moles/in.^{3}.

The total molar concentration can be expressed as a function of the system temperature and pressure by using the perfect gas law,

$$\bar{c} = \frac{n}{V} = \frac{P}{\bar{R}T} , \tag{49}$$

where

n = total moles,

V = volume, in.^{3},

P = pressure, atm,

$\bar{R}$ = gas constant, 2270.59 atm in.$^{-3}$ mole^{-1} °K^{-1}, and

T = temperature, °K.

Substitution of Eq. (49) into Eq. (47) gives the desired expression,

$$A = \frac{2\pi D'\Delta LP}{\bar{R}T} \left[r_1 \frac{dy}{dr}\Big|_1 - r_2 \frac{dy}{dr}\Big|_2 \right] . \tag{50}$$

The CSMP program calculates the concentration gradient as $dy/d\beta$, where β is a dimensionless radius and is defined as

$$\beta = \frac{r - RG}{RI - RG} . \tag{51}$$

Equation (50) can be expressed in terms of dy/dβ by utilizing the relationship

$$\frac{dy}{dr} = \frac{dy}{d\beta}\frac{d\beta}{dr} = \frac{1}{RI - RG} , \tag{52}$$

to give

$$A = \frac{2\pi D' \Delta LP}{RT(RI-RG)} \left[r_1 \frac{dy}{d\beta}\Big|_1 - r_2 \frac{dy}{d\beta}\Big|_2 \right] . \tag{53}$$

Equation (53) gives the rate of reaction (moles/sec) between any two radial positions. The total rate of reaction for the axial segment is calculated from Eq. (53) by noting that at the inside radius $dy/d\beta|_2 = 0$.

9.4 The CSMP Program

The CSMP Program is designed to solve the differential equations expressing the diffusion and reaction in the graphite annulus. Another feature of the CSMP package is the automatic ordering of the program instructions; hence, the user does not have to concern himself with the ordering and, within broad limits, can place the statements anywhere he wishes. At first glance this program may look confusing because the program instructions are a mixture of standard FORTRAN and special CSMP instructions.

At this point, it is probably worthwhile to review the calculational method. The CSMP program requires two boundary conditions for each differential equation at the inner radius of the graphite annulus, $\beta = 0$. However, only one boundary condition, Eq. (17), is known at $\beta = 0$. The second boundary condition, Eq. (18), applies at the outside radius of the graphite annulus, $\beta = 1$. Hence, it is necessary to estimate the mole fractions at the inside radius, solve the problem, and compare the calculated mole fractions at the outside radius with the desired values. If the results do not agree, it is necessary to adjust the estimated mole fractions and rerun the problem. Iterations are made until the calculated mole fractions agree with the specified boundary condition. The desired boundary conditions are being calculated in Subroutine GAS.

The first statement of the program is

RENAME TIME = B.

The CSMP package defines the independent variable as time. However, this definition can be overridden by the use of the RENAME instruction, which defines B as the independent variable. The variable, B, represents the transformed radial distance [see Eq. (15)].

The INITIAL card defines the start of the initial section of the program. This section is executed only once per run and is used to calculate either parameters or initial conditions that are problem oriented and are not functions of the independent variable. Several items are calculated in this section. DIS and DISSQ are constants introduced into the differential equations by transforming the independent variable [see Eq. (16)]. The reader should be aware at this point of the difference in nomenclature between the CSMP program and Eq. (16). In the CSMP program, RO and RI represent the outside and inside radius of the graphite annulus, while in Eq. (16) the same dimensions are represented by RI and RG. The initial estimates of the mole fraction of H_2 and CO (XFIRST AND VFIRST) at the inner boundary are also calculated from the boundary conditions at the gas-solid interface (XGOAL and VGOAL); the estimate of the mole fraction of H_2O is calculated at both boundaries (YGOAL and YFIRST). The remaining calculations evaluate the reaction constants K_1, K_2, and K_3 in Eq. (8), and the effective diffusivity of H_2O in He in the graphite pores, and then passes the initial conditions to Subroutine OUTPUT. A list of the variables used in this section appears in Table 5.

The DYNAMIC card indicates the end of the initial section and the start of the dynamic or numerical integration section. The numerical integration of a differential equation is easily programmed in the CSMP package. It is only necessary to write a FORTRAN statement defining the highest order derivative, $d^2Y/d\beta^2$ in Eq. (16a). The other derivatives and the dependent variable are obtained by successively integrating the highest-order derivative. These statements appear as follows:

Table 5. Nomenclature for initial section of CSMP Program

Variable	Definition
D	Effective diffusivity of H_2O in He in graphite pores, in.^{2}/sec
DELY	Change in mole fraction of H_2O across graphite annulus
DIS	Thickness of graphite annulus, in.
DISSQ	Square of graphite thickness, in.^{2}
P	Pressure, atm
RATE 1	Reaction rate K_1 in Eq. (8), fraction sec^{-1} atm^{-1}
RATE 2	Reaction rate K_2 in Eq. (8), atm$^{-0.75}$
RATE 3	Reaction rate K_3 in Eq. (8), atm^{-1}
RI	Inside radius of graphite annulus, in.
RO	Outside radius of graphite annulus, in.
R2	Gas constant, cal/mole-°K
T	Temperature, °K
VFIRST	Boundary condition, mole fraction of CO at inner radius
VGOAL	Boundary condition, mole fraction of CO at outer radius
XFIRST	Boundary condition, mole fraction of H_2 at inner radius
XGOAL	Boundary condition, mole fraction of H_2 at outer radius
YFIRST	Boundary conditions, mole fraction of H_2O at inner radius
YGOAL	Boundary conditions, mole fraction of H_2O at outer radius
YK	Constant in diffusivity equation, cm^2 atm^{-1} sec^{-1} (°K)$^{-1.58}$

```
YP = INTGRL(DYDB, YPP) and
YBDY = INTGRL(YFIRST,YP).
```

The INTGRL statement calls a variable-step Runge-Kutta program to perform the numerical integration. The first argument is the initial conditions (at $\beta = 0$) and the second argument is the variable being integrated. In the first examples given above, YP represents the first derivative of the H_2O mole fraction $dY/d\beta$, DYDB represents the value of $dY/d\beta$ at $\beta = 0$, and YPP represents the second derivative, $d^2Y/d\beta^2$. Similar equations are written for the mole fractions of CO and H_2. The differential equations are written assuming the effective diffusivity of H_2 is twice that of H_2O and CO. The equation also assumes that the porosity-tortuosity factor is equal to 0.01 and is independent of the extent of reaction.

The remaining calculations performed in the dynamic section include the calculation of the reaction rate (RATEPS), and a simple combination of the reaction rate and the effective diffusivity. The nomenclature for this section is listed in Table 6.

After the numerical integration is completed, the program moves on to the terminal section. This section checks whether or not the boundary conditions at the outside radius have been satisfied. If this condition is not satisfied, a new estimate is made of the mole fractions at the inner radius and the numerical integration is repeated. Once convergence has been obtained, the program calls SUBROUTINE GAS. The gas-phase calculations define a new problem for the CSMP program.

A rather simple convergence technique is employed in this program. If the boundary condition at the outer radius is not satisfied, the initial estimate is either doubled or halved until the desired values have been bracketed. From this point on, a linear interpolation is used to find the estimated starting conditions.

The series of cards following the terminal section are used to define initial values and certain information required in the CSMP program. The FIXED card defines integer variables. The CONSTANT cards define values of various parameters. Statement TIMER FINTIME = 1.0 defines the value of the independent variable at the end of the problem. OUTDEL

Table 6. Nomenclature for dynamic section of CSMP Program[a]

Variable	Definition
AH2	Absolute value of H_2 partial pressure, atm
AH2O	Absolute value of H_2O partial pressure, atm
B	Independent variable, dimensionless radius [see Eq. (15)]
F	Multiplier of reaction rate to account for different types of graphite, dimensionless
LSQ	Ratio of effective diffusivity and reaction rate for H_2O and CO, in.^{2}
LSQ2	Ratio of effective diffusivity and reaction rate for H_2, in.^{2}
PH2	Partial pressure of H_2, atm
PH2O	Partial pressure of H_2O, atm
RATEPS	Reaction rate [α in Eq. (12)], sec^{-1}
RHO	Graphite density, lb/ft^3
R1	Gas constant, atm cm^{-3} mole^{-1} °K^{-1}
VBDY	Mole fraction of CO
VP	First derivative of CO mole fraction ($d^2V/d\beta^2$)
WT	Molecular weight of graphite
XBDY	Mole fraction of H_2
XP	First derivative of H_2 mole fraction ($dx/d\beta$)
SPP	Second derivative of H_2 mole fraction ($d^2x/d\beta^2$)
YBDY	Mole fraction of H_2O
YP	First derivative of H_2O mole fraction, ($dy/d\beta$)
YPP	Second derivative of H_2O mole fraction ($d^2y/d\beta^2$)

[a] Does not include variables listed in Initial Section, Table 5.

and PRDEL define the increment of the independent variable to be used in the printing and plotting subroutines. The PRINT statement defines the variables to be printed at the specified values of the independent variable during the numerical integration. The FINISH card will terminate the integration if the slope or the value of the H_2O mole fraction becomes negative.

```
LEVEL  21.6  (DEC 72)                            OS/360  FORTRAN H

          COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=60,SIZE=0000K,
                             SOURCE,EBCDIC,NOLIST,DECK,LOAD,MAP,NOEDIT,NOID,XREF
  ISN 0002            SUBROUTINE   GAS(DYDB,N,VFIRST,XFIRST,YINT,NEXIT)
  ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
  ISN 0004            COMMON/ALPHA/ DIS,TEMP,PRES,RG,RI,DEL
  ISN 0005            DIMENSION   A(31,31),X(31)    ,B(31),VZ(31),Y(31,31)
  ISN 0006            DIMENSION AH2(31,31),ACO(31,31),BH2(31),BCO(31),YH2(31,31)
  ISN 0007            DIMENSION YCO(31,31),XH2(31),XCO(31)
  ISN 0008            REAL*4 DYDB,VFIRST,XFIRST,YINT
  ISN 0009            DATA  NOUES/1/
  ISN 0010            WRITE(10,1071)N
  ISN 0011       1071 FORMAT (20X,'ENTRY TO GAS SUBROUTINE N=',I3)
  ISN 0012            NEXIT=0
  ISN 0013            IF(NOUES.GT.1) GO TO 28
                C
                C               READ INPUT DATA
                C
                C                       TEMP = TEMPERATURE, DEG K
                C                       PRES = PRESSURE, ATM
                C
                C     READ 1000, TEMP,PRES
  ISN 0015            TEMP=1273.0
  ISN 0016            PRES=1.0
                C
                C                       XKK = CONSTANT IN DIFFUSIVITY EQN.,
                C                             CM**2 - ATM/ SEC - DEG**EPT
                C                       EPT = TEMPERATURE EXPONENT IN DIFFUSIVITY EQN.,
                C                       DIMENSIONLESS
                C
                C     READ 1001 ,XKK,EPT
  ISN 0017            XKK=1.06D-04
  ISN 0018            EPT=1.58
  ISN 0019       1000 FORMAT(2F10.3)
  ISN 0020       1001 FORMAT( E15.6,F10.3)
                C
                C                       YO = MOLE FRACTION WATER IN INLET GAS
                C                       YH2I = MOLE FRACTION HYDROGEN IN INLET GAS
                C                       YCOI = MOLE FRACTION CO IN INLET GAS
                C
                C     READ 1003, YO,YH2I,YCOI
  ISN 0021            YO=0.1
  ISN 0022            YH2I=0.0
  ISN 0023            YCOI=0.0
  ISN 0024       1003 FORMAT( 3F10.3)
                C
                C                       RG = INSIDE RADIUS OF GRAPHITE ANNULUS, IN
                C                       RI = RADIUS OF GAS - GRAPHITE INTERFACE, IN
                C                       RO = OUTSIDE RADIUS OF GAS ANNULUS, IN
                C
                C     READ 1003, RG,RI,RO
  ISN 0025            RG=0.3
  ISN 0026            RI=0.75
  ISN 0027            RO=1.00
                C
                C                       FLOW = VOLUMETRIC FLOW RATE, CM**3/ SEC
                C
                C     READ 1003, FLOW
  ISN 0028            FLOW=10.0
```

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                  C
                  C              CALCULATE REACTION RATE AND DIFFUSIVITY
                  C              DIG = GAS PHASE DIFFUSIVITY
                  C              DIS = GRAPHITE PHASE DIFFUSIVITY
                  C
ISN 0029                DIG = XKK *(TEMP ** EPT )/ PRES  * .155
ISN 0030                DIS = 0.01 * DIG
                  C
                  C              ASSUME DIFF OF H2 IS TWICE THAT OF H2O AND THAT OF
                  C              CO IS EQUAL TO THAT CF H2O
                  C
ISN 0031                DH2G = 2.0 * DIG
ISN 0032                DCDG = DIG
ISN 0033                DH2S = 2.0 * DIS
ISN 0034                DCOS = DIS
                  C
                  C              SET INITIAL CONDITICN FOR GAS PHASE  AND VELOCITY
                  C              VECTOR
ISN 0035                XKAP = RI/RO
ISN 0036                RR = RO * 2.54
ISN 0037                DENOM = (1.0 - XKAP **4) - (1.0 -XKAP*XKAP)*(1.0 -XKAP*XKAP)/
                       1          DLOG(1.0/XKAP)
ISN 0038                FACT = 2.0 * FLOW/(3.1416 * RR * RR * DENOM)
ISN 0039                WRITE(10.1010)
ISN 0040           1010 FORMAT( 1H1.20X.'RADIUS'.10X.'VELOCITY')
ISN 0041                H = (RO - RI)/30.0
ISN 0042                DO 9 M=1.31
ISN 0043                Y(1.M)=YO
ISN 0044              9 CONTINUE
ISN 0045                DO 10 J=1.31
ISN 0046                RAD = RI + (J-1)* H
ISN 0047                DENOM = 1.0 - RAD*RAD/(RO*RO) + (1.0 -XKAP *XKAP)/DLOG(1.0/XKAP)*
                       1        DLOG(RAD/RO)
ISN 0048                VZ(J) = FACT* DENOM/2.54
ISN 0049                IF( VZ(J) .LT. 0.0) VZ(J) = 0.0
ISN 0051                Y(J.1) = YO
ISN 0052                YH2(J.1) = YH2I
ISN 0053                YCO(J.1) = YCOI
ISN 0054                WRITE(10.1011)RAD.VZ(J)
ISN 0055           1011 FORMAT( 20X.F6.4. 5X.E20.6)
ISN 0056             10 CONTINUE
                  C
                  C              SET UP MATRIX COEFFICIENTS - NOTE THESE REMAIN CONSTANT
                  C              FOR ENTIRE PROBLEM
ISN 0057                DEL = 0.05
ISN 0058                DO 15 J=1.31
ISN 0059                DO 15 K=1.31
ISN 0060                AH2(J.K) = 0.0
ISN 0061                ACO(J.K) = 0.0
ISN 0062             15 A(J.K)   = 0.0
ISN 0063                A(1.1) = -2.0/(H*H)
ISN 0064                A(1.2) = -A(1.1)
ISN 0065                AH2(1.1) = A(1.1)
ISN 0066                ACO(1.1) = A(1.1)
ISN 0067                AH2(1.2) = A(1.2)
ISN 0068                ACO(1.2) = A(1.2)
ISN 0069                DO 20 J =2.30
ISN 0070                A(J.J-1) =(2.0 *RI +(2.0*J -3)*H)/(2.0*H*H*(RI+(J-1)*H))
```

```
ISN 0071          AH2(J.J-1) = A(J.J-1)
ISN 0072          ACO(J.J-1) = A(J.J-1)
ISN 0073          A(J.J) = -(2.0 * DIG * DEL + H*H*VZ(J))/(H*H*DIG * DEL)
ISN 0074          AH2(J.J) = -(2.0 * DH2G * DEL +H*H*VZ(J))/(H*H*DH2G * DEL)
ISN 0075          ACO(J.J) = -(2.0 * DCOG * DEL +H*H*VZ(J))/(H*H*DCOG * DEL)
ISN 0076          A(J.J+1) =(2.0 *RI +(2.0*J -1.)*H)/(2.0*H*H*(RI+(J-1)*H))
ISN 0077          AH2(J.J+1) = A(J.J+1)
ISN 0078          ACO(J.J+1) = A(J.J+1)
ISN 0079       20 CONTINUE
ISN 0080          A(31.30) = 1.0
ISN 0081          A(31.31) = -1.0
ISN 0082          AH2(31.30) = 1.0
ISN 0083          ACO(31.30) = 1.0
ISN 0084          AH2(31.31) = -1.0
ISN 0085          ACO(31.31) = -1.0
ISN 0086     1020 FORMAT( // (5E20.6))
            C
            C               SET UP RIGHT - HAND SIDES   HERE IS WHERE N DC LOOP
            C               BELONGS
ISN 0087       28 CONTINUE
ISN 0088          DO 30 J=2.30
ISN 0089          B(J) = - VZ(J)* Y(J.N-1)/(DIG * DEL)
ISN 0090          BH2(J) = -VZ(J) * YH2(J.N-1)/(DH2G * DEL)
ISN 0091          BCO(J) = -VZ(J) * YCO(J.N-1)/(DCOG * DEL)
ISN 0092       30 CONTINUE
ISN 0093          B(31) = 0.0
ISN 0094          BH2(31) = 0.0
ISN 0095          BCO(31) = 0.0
ISN 0096          DCDR=DBLE(DYDB)
ISN 0097          ALP =DCDR*(-1/(RI-RG))
ISN 0098          ALP2 = ALP * DIS/ DH2S
ISN 0099          ALP3 = ALP * DIS/ DCOS
ISN 0100          B(1) = DIS * ALP *(2.0 * RI -H)/(RI * DIG *H)
ISN 0101          BH2(1) = -DH2S * ALP2*(2.0 * RI-H)/(RI * DH2G * H)
ISN 0102          BCO(1) = - DCOS * ALP3*(2.0*RI -H)/(RI * DCOG *H)
            C
            C               SOLVE EQS
            C
ISN 0103          CALL TRIDIA(A.B.X.31)
ISN 0104          CALL TRIDIA(AH2.BH2.XH2.31)
ISN 0105          CALL TRIDIA(ACO.BCO.XCO.31)
ISN 0106          VFIRST=SNGL(XCO(1))
ISN 0107          XFIRST=SNGL(XH2(1))
ISN 0108          YINT=SNGL (X(1))
ISN 0109          NQUES=NQUES+1
ISN 0110          WRITE( 6.1050)
ISN 0111          WRITE( 6.1020)(Y(J.N).J=1.31)
ISN 0112          WRITE( 6.1051)
ISN 0113          WRITE( 6.1020)(YH2(J.N).J=1.31)
ISN 0114          WRITE( 6.1052)
ISN 0115          WRITE( 6.1020)(YCO(J.N).J=1.31)
ISN 0116          IF(DABS(X(1)-Y(1.N))/Y(1.N).LT.0.0001)GO TO 42
ISN 0118          DO 41 J=1.31
ISN 0119          Y(J.N) = X(J)
ISN 0120          YH2(J.N) = XH2(J)
ISN 0121          YCO(J.N) = XCO(J)
ISN 0122       41 CONTINUE
ISN 0123          RETURN
```

```
   42 CONTINUE
      NEXIT=5
      WRITE(10,1050)
 1050 FORMAT( // 30X,'SOLUTION VECTOR FOR WATER')
      WRITE(10,1020)(Y(J,N),J=1,31)
      WRITE(10,1051)
 1051 FORMAT( // 30X,'SOLUTION VECTOR FOR HYDROGEN')
      WRITE(10,1020)(YH2(J,N),J=1,31)
      WRITE(10,1052)
 1052 FORMAT( // 30X,'SOLUTION VECTOR FOR CO')
      WRITE(10,1020)(YCO(J,N),J=1,31)
  100 CONTINUE
      RETURN
      END
```

```
LEVEL  21.6  (DEC 72)                               OS/360  FORTRAN H

         COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=60,SIZE=0000K,
                            SOURCE,EBCDIC,NOLIST,DECK,LOAD,MAP,NOEDIT,NOID,XREF
  ISN 0002                SUBROUTINE TRIDIA(C,B,X,NEQ)
                 C
                 C              SOLVES A SET OF SIMULTANEOUS EQUATIONS WHERE THE COEFFICIENT
                 C              MATRIX IS A N X N TRIDIAGONAL MATRIX. VECTOR B IS THE RIGHT -
                 C              HAND SIDES AND THE VECTOR X IS THE SOLUTION VECTOR. NEQ IS THE
                 C              NUMBER OF EQUATIONS (MAX = 100). NOTE C AND B ARE NOT
                 C              DESTROYED DURING CALCULATIONS.
                 C
  ISN 0003                IMPLICIT REAL*8(A-H,O-Z)
  ISN 0004                DIMENSION C(31,31),B(31),X(31),R(31),G(31)
  ISN 0005                REAL*8 L(31)
  ISN 0006                NSTOP = NEQ - 1
  ISN 0007                L(1) = C(1,1)
  ISN 0008                R(1) = C(1,2)/L(1)
  ISN 0009                DO 10 J=2,NSTOP
  ISN 0010                L(J) = C(J,J) - C(J,J-1) * R(J-1)
  ISN 0011                R(J) = C(J,J+1)/L(J)
  ISN 0012             10 CONTINUE
  ISN 0013                L(NEQ) = C(NEQ,NEQ) - C(NEQ,NEQ-1) * R(NEQ-1)
  ISN 0014                G(1) = B(1)/L(1)
  ISN 0015                DO 20 J=2,NEQ
  ISN 0016                G(J) = ( B(J) - C(J,J-1)*G(J-1))/L(J)
  ISN 0017             20 CONTINUE
  ISN 0018                X(NEQ) = G(NEQ)
  ISN 0019                DO 30 J=1,NSTOP
  ISN 0020                K = NSTOP - (J-1)
  ISN 0021                X(K) = G(K) - R(K) * X(K+1)
  ISN 0022             30 CONTINUE
  ISN 0023                RETURN
  ISN 0024                END
```

```
LEVEL  21.6  (DEC 72)                              OS/360  FORTRAN H

          COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=60,SIZE=0000K,
                               SOURCE,EBCDIC,NOLIST,DECK,LOAD,MAP,NOEDIT,NOID,XREF
   ISN 0002           SUBROUTINE OUTPT(BT,Y,YP,X,V,NTEST)
   ISN 0003           DIMENSION SAVBT(21), SAVY(21), SAVYP(21),SAVX(21), SAVV(21)
   ISN 0004           COMMON/ALPHA/ DIS,TEMP,PRES,RG,RI,DEL
   ISN 0005           REAL *8  DIS,TEMP,PRES,RG,RI,DEL
   ISN 0006           DATA SUM/0.0/,NBR/1/
   ISN 0007           IF(NTEST.GT.2) GO TO 10
   ISN 0009           IF(NTEST.EQ.0) J=0
   ISN 0011           J=J+1
   ISN 0012           SAVBT(J)=BT
   ISN 0013           SAVY(J)=Y
   ISN 0014           SAVYP(J)=YP
   ISN 0015           SAVX(J)=X
   ISN 0016           SAVV(J)=V
   ISN 0017           NTEST=1
   ISN 0018           RETURN
   ISN 0019        10 CONTINUE
   ISN 0020           NBR = NBR + 1
   ISN 0021           WRITE(10,1000) NBR
   ISN 0022      1000 FORMAT( 1H1,20X,'SUMMARY OF GRAPHITE PHASE CALCULATIONS FOR',
                     1      ' AXIAL STEP NO.',I4/ 10X,'RADIAL',22X,'MOLE FRACTIONS',
                     2      19X,'CONC. GRADIENT'/ 9X,'DISTANCE',8X,'H2O',15X,'H2',15X,
                     3      'CO',12X,'OF H2O',/)
   ISN 0023           DO 20 K=1,J
   ISN 0024        20 WRITE(10,1001) SAVBT(K),SAVY(K),SAVX(K),SAVV(K),SAVYP(K)
   ISN 0025      1001 FORMAT( 10X,F4.2,6X,4(E12.5,5X))
   ISN 0026           NTEST=0
                C
                C                   CALCULATE RATE AT WHICH GRAPHITE IS BEING REACTED
                C
   ISN 0027           WRITE(10,1005)
   ISN 0028      1005 FORMAT(/// 24X,'SUMMARY OF RATE OF GRAPHITE REACTION'/ 22X,
                     1          'RADIUS',14X,'GRAPHITE REACTED'/ 16X,'OUTSIDE',4X,
                     2          'INSIDE',12X,'MOLES/SEC'/)
   ISN 0029           CONST = 2.0 * 3.1416 * DIS * PRES /((RI-RG)*(2270.59*TEMP))
   ISN 0030           IF( NBR .EQ. 2  .OR.  NBR .EQ. 31) GO TO 30
   ISN 0032           CONST = CONST * DEL
   ISN 0033           GO TO 31
   ISN 0034        30 CONST = CONST * 1.5 * DEL
   ISN 0035        31 CONTINUE
   ISN 0036           RIO = ( SAVBT(1) * (RI-RG) + RG) * SAVYP(1)
   ISN 0037           DO 40 J=2,21
   ISN 0038           RIN =( SAVBT(J) * (RI-RG) + RG) * SAVYP(J)
   ISN 0039           A = CONST * (RIN - RIO)
   ISN 0040           WRITE(10,1011) SAVBT(J),SAVBT(J-1),A
   ISN 0041           RIO = RIN
   ISN 0042        40 CONTINUE
   ISN 0043           RRR = CONST * RIO
   ISN 0044           SUM = SUM + RRR
   ISN 0045           WRITE(10,1015) RRR,SUM
   ISN 0046      1011 FORMAT( 16X,F4.2,7X,F3.2,12X,E12.5)
   ISN 0047      1015 FORMAT( // 10X,'TOTAL GRAPHITE REACTION RATE THIS SEGMENT',E15.5,
                     1          // 10X,'ACCUMULATIVE GRAPHITE REACTION RATE',5X,E15.5)
   ISN 0048           RETURN
   ISN 0049           END
```

```
            ****CONTINUOUS SYSTEM MODELING PROGRAM****

      ***PROBLEM INPUT STATEMENTS***

   RENAME   TIME=B
INITIAL
*
*                       USING NEWTON-RAPHSON AND BISECTION TECH
*
*                        RATE1'S EXPONENT IS 4
*
*              V IS CO
*              X IS H2
*              Y IS WATER
*
      DIS=RO-RI
      DISSO=(RO-RI)**2
      DELY=YGOAL-YFIRST
      VFIRST=VGOAL+DELY
      XFIRST=XGOAL+0.5*DELY
      RATE1=7.417E03*EXP(-40900/(R2*T))
      RATE2=1.66E-02*EXP(28600/(R2*T))
      RATE3=5.31E-02*EXP(27500/(R2*T))
      D=0.155*0.01*YK*T**1.58/P *0.5
      NOSORT
      TIME=0.0
      NTEST=0
      CALL OUTPT(TIME,YFIRST,DYDB,XFIRST,VFIRST,NTEST)
      TIME=0.0499
DYNAMIC
      LSQ=D/RATEPS
      LSQ2=2.0*D/RATEPS
      PH2=XBDY*P
      AH2=ABS(PH2)
      PH2O=YBDY*P
      AH2O=ABS(PH2O)
      RATEPS=F*RATE1*RHO*R1*T/(1+RATE2*AH2**0.75+RATE3*AH2O)/WT
      VBDY=INTGRL(VFIRST,VP)
      VP=INTGRL(DVDB,VPP)
      VPP=-VP*DISSO/(B*DISSQ+RI*DIS)-YBDY*DISSO/LSQ
      XBDY=INTGRL(XFIRST,XP)
      XP=INTGRL(DXDB,XPP)
      XPP=-XP*DISSO/(B*DISSQ+RI*DIS)-YBDY*DISSQ/LSQ2
      YBDY=INTGRL(YFIRST,YP)
      YP=INTGRL(DYDB,YPP)
      YPP=-YP*DISSQ/(B*DISSQ+RI*DIS)+YBDY*DISSQ/LSQ
      NOSORT
      IF(KEEP.NE. 1)GO TO 10
      IF(B.LT.TIME) GO TO 10
      CALL OUTPT(B,YBDY,YP,XBDY,VBDY,NTEST)
      TIME=TIME+0.05
   10 CONTINUE
TERMINAL
      IF(HIGHP.NE.0.0.AND.LOWP.NE.0.0) GO TO 61
      IF(YBDY.GT.YGOAL) GO TO 20
      IF(B.LT.0.95) GO TO 5
      LOWS=YBDY
      LOWP=YFIRST
    5 CONTINUE
      LOW=YFIRST
      IF(HIGH.NE.0.0) GO TO 40
      YFIRST=LOW*2.0
```

```
      GO TO 50
   20 CONTINUE
      IF(B.LT.0.95) GO TO 21
      HIGHS=YBDY
      HIGHP=YFIRST
   21 HIGH=YFIRST
      IF(LOW.NE.0.0) GO TO 40
      YFIRST=HIGH/2.0
      GO TO 50
   40 CONTINUE
      IF(HIGHP.NE.0.0.AND.LOWP.NE.0.0) GO TO 60
      YFIRST=(HIGH+LOW)/2.0
      GO TO 50
   60 X1=LOWP
      Y1=LOWS
      X2=HIGHP
      Y2=HIGHS
      GO TO 63
   61 CONTINUE
      X2=YFIRST
      Y2=YBDY
   63 CONTINUE
      SLOPE=(Y2-Y1)/(X2-X1)
      DELX=(YGOAL-Y1)/SLOPE
      YFIRST=X1+DELX
      IF(YFIRST.GT.YGOAL) YFIRST=YGOAL
      IF(ABS(YBDY-YGOAL)/YGOAL.LT.0.0001) GO TO 100
      C1=ABS(X1-YFIRST)
      C2=ABS(X2-YFIRST)
      IF(C1.LT.C2) GO TO 50
      X1=X2
      Y1=Y2
      GO TO 50
  100 CONTINUE
      CALL GAS (YP,N,VBDY,XBDY,YBDY,NEXIT)
      HIGH=0.0
      LOW=0.0
      HIGHP=0.0
      LOWP=0.0
      IF(NEXIT.GT.0)GO TO 7
      YGOAL=YBDY
      XGOAL=XBDY
      VGOAL=VBDY
      GO TO 31
    7 CONTINUE
      NBR=N
      N=NBR+1
      NTEST=5
      CALL OUTPT(B,YBDY,YP,XBDY,VBDY,NTEST)
      IF(N.GT.31)GO TO 6
      YGOAL=YBDY
      XGOAL=XBDY
      VGOAL=VBDY
      GO TO 100
   50 CONTINUE
   31 CALL RERUN
    6 CONTINUE
FIXED N,NBR,NEXIT,NTEST
CONSTANT YGOAL=0.1,XGOAL=0.0,VGOAL=0.0
CONSTANT YFIRST=1.3E-02
CONSTANT   VBDY=0.00, XBDY=0.00, YBDY=0.1 , N=2
CONSTANT   T=1273.00,  F=10, RHO=111.872, R1=1.314,  R2=1.9872,  WT=12.0
CONSTANT   P=1.0,     YK=1.06E-04
 CONSTANT  HIGH=0.0,LOW=0.0,HIGHP=0.0,LOWP=0.0
CONSTANT   VP=0.0, XP=0.0, YP=0.0
CONSTANT    RI=0.3,  RO=0.75
```

```
          TIMER FINTIM=1.0,  OUTDEL=0.05, PRDEL=0.05
          PRINT VBDY,VP,XBDY,XP,YBDY,YP,RATEPS
          FINISH  YP=-1.0E-03, YBDY=-1.0E-05
          TITLE   WATER-GRAPHITE REACTION
          END
          STOP

OUTPUT VARIABLE SEQUENCE
DIS       DISSQ     DELY      VFIRST    XFIRST    RATE1     RATE2     RATE3     D         TIME
NTEST     ZZ0001    TIME      VBDY      PH2O      AH2O      PH2       AH2       RATEPS    LSQ
VPP       VP        XBDY      LSQ2      XPP       XP        YBDY      YPP       YP        ZZ0008
TIME      ZZ0009    LOWS      LOWP      LOW       YFIRST    HIGHS     HIGHP     HIGH      YFIRST
YFIRST    X1        Y1        X2        Y2        X2        Y2        SLCPE     DELX      YFIRST
YFIRST    C1        C2        X1        Y1        HIGH      LOW       HIGHP     LOWP      YGOAL
XGOAL     VGOAL     NBR       N         NTEST     YGOAL     XGOAL     VGCAL

PARAMETERS NOT INPUT OR OUTPUTS NOT AVAILABLE TO SORT SECTION***SET TO ZERO***
DVDB      DXDB      DYDB

 OUTPUTS    INPUTS     PARAMS   INTEGS + MEM BLKS  FORTRAN  DATA CDS
 72(500)  132(1400)  31(400)     6+   0=  6(300)  101(600)      13

          ENDJOB
```