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AEC RESEARCH AND DEVELOPMENT REPORT

A NUMERICAL SOLUTION OF A SYSTEM
OF ORDINARY AND NON-LINEAR
PARTIAL DIFFERENTIAL EQUATIONS

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A NUMERICAL SOLUTION OF A SYSTEM
OF ORDINARY AND NON-LINEAR
PARTIAL DIFFERENTIAL EQUATIONS

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Abstract

A system of two linear first order ordinary and two non-linear second order partial differential equations with mixed boundary conditions is considered. Solutions by both linear and non-linear numerical methods are discussed and compared.

The equations arise from a description of the simultaneous chemical reaction and convective-diffusive transport of water vapor and hydrogen through a graphite cylinder. Although specifically written for the steam-graphite system, the equations may have applications to general systems of fluid flow coupled with chemical reactions.

1. Introduction

The chemical reaction between water vapor and carbon,

is of considerable interest to designers of high-temperature gas cooled nuclear reactors. This interest stems from the widespread use of graphite as fuel cladding and core structural material and the possible presence of water vapor in the coolant either as impurity or through inleakage from the steam generators. Designers consider this "steam-graphite" reaction primarily to determine two quantities:

- (1) the magnitude and distribution of the attack on the core graphite under various conditions of water vapor and hydrogen concentrations, flow, and temperature distribution (the attack may deteriorate core structural integrity and may enhance the release of fission products from the fuel), and
- (2) the amount of water consumed and hydrogen produced (the hydrogen is a potential explosive hazard and the ratio of hydrogen concentration to water vapor concentration has a controlling influence on the amount of carbon transported from the core and deposited in the heat exchangers).

The determination of these quantities involves making mass balances for hydrogen and water vapor throughout the regions of interest. These mass balances result in a system of four differential equations which, along with their boundary conditions, represent the mathematical model [6] treated in this report.

We give the mathematical statement of the problem in Section 2 and the linear and non-linear numerical methods employed to solve the problem in Section 3. The remaining sections are devoted to a discussion and comparison of these numerical methods. Included in the Appendix is a description of a computer program, "Steamcar" written for the IBM 360/75. This program performs the numerical operations needed to solve the system of equations.

2. Statement of the Problem

An inert coolant enters one end and flows turbulently through a cylindrical channel in a long cylindrical piece of graphite that has a non-uniform distribution of temperature. At the channel entrance there is a given constant concentration of water vapor and hydrogen uniformly distributed across the cross section. The exterior boundaries of the graphite cylinder are regions of no flux. Symmetry allows us to express the problem in two-dimensions (see Figure 1).

FIGURE 1

We let $u(r,x)$ and $v(r,x)$ denote the concentrations of water vapor and hydrogen at the point (r,x) in the graphite, and let $\bar{u}(x)$ and $\bar{v}(x)$ denote the average concentrations of water vapor and hydrogen in the convecting stream at the point x along the center line of the cylinder.

The transport and rate mechanisms involved are:

- (1) turbulent convection through the central coolant channel resulting in mass transfer between the coolant stream and the graphite surface.
- (2) permeation throughout the graphite by effective in-pore diffusion, and
- (3) the chemical reaction itself.

Steamcar treats these various rate mechanisms as shown separately below.

Turbulent Convection

The water vapor and hydrogen fluxes in the radial direction between the coolant stream and the graphite surface are each expressed by the product of the average concentration potential and a mass transfer coefficient. For water vapor, the flux in the radial direction is given by

$$\text{flux}_{u,r} \equiv \ell(x) [\bar{u}(x) - u(R_1, x)] ,$$

in which the film coefficient, $\ell(x)$, is obtained from the heat-mass transfer analogy with an arbitrary maximum at the inlet. We, therefore, express $\ell(x)$ by

$$l(x) = \begin{cases} (.046) \frac{D_c}{2R_1} (N_{Re})^{.8} (N_{SC})^{.33}, & 0 \leq x \leq .2R_1, \\ (.029) \frac{D_c}{2R_1} \left(\frac{2R_1}{x}\right)^{.2} (N_{Re})^{.8} (N_{SC})^{.33}, & .2R_1 < x < x^*, \\ (.023) \frac{D_c}{2R_1} (N_{Re})^{.8} (N_{SC})^{.33}, & x \geq x^*, \end{cases}$$

where the value,

$$x^* = 2R_1 \left(\frac{.029}{.023}\right)^5,$$

represents the position of "well-developed" flow.

The flux in the axial direction is simply

$$\text{flux}_{u,x} = \bar{u}(x)Q,$$

where Q is the bulk average coolant velocity.

In-Pore Diffusion

The flux of water vapor and hydrogen in a given direction within the graphite is expressed by a Fickian type equation. For example, for water vapor traveling in the axial direction,

$$\text{flux}_{u,x} = -D_u \frac{\partial u}{\partial x}.$$

The effective diffusion coefficient, D_u , is given by [3]

$$\frac{1}{D_u} = \frac{3}{4K_0 v_u} + \frac{1}{\phi D_{c,u}}, \quad (2.1)$$

in which K_0 and ϕ are constants characteristic of the type of graphite,

$$v_u \equiv \sqrt{\frac{8RT}{\pi W_u}},$$

and $D_{c,u}$ is the normal binary molecular diffusion coefficient for water vapor diffusing through the coolant, c. The binary diffusion coefficient is often expressed [1] as

$$D_{c,u} = \frac{.00185T^{3/2}}{\Omega P \sigma_u^2} \left(\frac{1}{W} + \frac{1}{W_u} \right)^{1/2},$$

where T is the absolute temperature (°K) and P is the pressure (atms.), and W and W_u are the molecular weights of graphite and water.

In the temperature range of interest (greater than 400°C), Equation (2.1) is approximated for water vapor and hydrogen by

$$D_u = \left[\frac{7.317 \times 10^{-5}}{K_0} T^{-.5} + (8.403 \times 10^3) \frac{P}{\phi} T^{-1.67} \right]^{-1}$$

and

$$D_v = \left[\frac{2.187 \times 10^{-4}}{K_0} T^{-.5} + (1.449 \times 10^4) \frac{P}{\phi} T^{-1.67} \right]^{-1}.$$

Representative values of the graphite constants [3,4] for nuclear grade graphite are

$$\phi = 0.01$$

and

$$K_0 = 1.5 \times 10^{-6} \text{ cm.}$$

The pressure, P, is usually in the range 20-100 atmospheres.

Chemical Reaction

Steamcar uses a commonly accepted expression for the chemical reaction rate,

$$\gamma(u,v) = \frac{K_1 P_u}{1 + K_2 P_v + K_3 P_u}, \quad (2.2)$$

where P_u and P_v are the partial pressures of water vapor and hydrogen, and

$$K_i = K_{0i} \exp[-E_i/RT], \quad i = 1, 2, 3,$$

where K_{0i} , E_i , and R are constants.

Using a perfect gas equation of state, Equation (2.2) was expressed in terms of the concentrations rather than the partial pressures,

$$\gamma(u,v) = \frac{K_1(r,x)u(r,x)R_u T(r,x)}{1 + K_2(r,x)v(r,x)R_v T(r,x) + K_3(r,x)u(r,x)R_u T(r,x)}.$$

Representative values for the reaction constants [5,7] are

$$K_{01} = 29.658 \text{ gmoles/g-min.-atm.},$$

$$K_{02} = 0.94185 \times 10^{-10} \text{ atm}^{-1},$$

$$K_{03} = 0.7062 \times 10^{-15} \text{ atm}^{-1},$$

$$E_1 = 32.7 \text{ Kcal/gmole},$$

$$E_2 = -60.8 \text{ Kcal/gmole},$$

$$E_3 = -79.3 \text{ Kcal/gmole},$$

$$R_u = 4.615 \times 10^6 \text{ dyne-cm/g-}^\circ\text{K},$$

$$R_v = 4.124 \times 10^7 \text{ dyne-cm/g-}^\circ\text{K}.$$

The Mathematical System

Based on the preceding transfer and rate mechanisms, mass balances can be made in the graphite and the coolant stream [6].

Within the graphite, the mass balance equations for water vapor and hydrogen are

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} - \rho \frac{W_u}{D_u} \gamma(u,v) &= 0, \\ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial r^2} + \frac{1}{r} \frac{\partial v}{\partial r} + \rho \frac{W_v}{D_v} \gamma(u,v) &= 0, \end{aligned} \quad (2.3)$$

for $0 < x < L$ and $R_1 < r < R_2$.

The three boundary conditions representing no flux at the graphite exterior boundaries are

$$\begin{aligned} \frac{\partial u}{\partial r}(R_2, x) &= \frac{\partial v}{\partial r}(R_2, x) = 0, \quad 0 < x < L, \\ \frac{\partial u}{\partial x}(r, 0) &= \frac{\partial v}{\partial x}(r, 0) = 0, \quad R_1 < r < R_2, \\ \frac{\partial u}{\partial x}(r, L) &= \frac{\partial v}{\partial x}(r, L) = 0, \quad R_1 < r < R_2. \end{aligned} \quad (2.4)$$

The boundary values $u(R_1, x)$ and $v(R_1, x)$, $0 < x < L$, are determined from the two equations for the mass balances in the coolant stream,

$$\rho \frac{d\bar{u}}{dx} + \frac{2\ell(x)}{R_1} [\bar{u}(x) - u(R_1, x)] = 0, \quad 0 < x \leq L, \quad (2.5)$$

$$\rho \frac{d\bar{v}}{dx} + \frac{2\ell(x)}{R_1} [\bar{v}(x) - v(R_1, x)] = 0, \quad 0 < x \leq L, \quad (2.6)$$

coupled with the boundary conditions

$$\bar{u}(0) = c'_1, \bar{v}(0) = c'_2, \quad (2.7)$$

$$D_u \left. \frac{\partial u}{\partial r} \right|_{R_1} + \ell(x) [\bar{u}(x) - u(R_1, x)], \quad 0 < x \leq L, \quad (2.8)$$

$$D_v \left. \frac{\partial v}{\partial r} \right|_{R_1} + \ell(x) [\bar{v}(x) - v(R_1, x)], \quad 0 < x \leq L. \quad (2.9)$$

Once this system of equations is solved for $u(r, x)$ and $v(r, x)$, the local equilibrium rate of chemical reaction is given by

$$\rho W Y(u, v), \quad (2.10)$$

where ρ and W are the density and molecular weight of the graphite (see Appendix A).

The system of equations, (2.3) through (2.9), represents a mathematical description of the attack of water vapor on a graphite cylinder due to convective-diffusive flow and a chemical reaction. The temperature distribution within the graphite, entering through the last terms on the left sides of the equations in (2.3), affects the system in the manner described earlier under the headings "In-Pore Diffusion" and "The Chemical Reaction". The behavior of this system may strongly depend on the temperature distribution, $T(r, x)$, in these non-linear terms. The computer program for the solution will allow any continuous function for $T(r, x)$. However, the analysis of the equations will be for a "test case" using

$$T(r, x) = 1725 + 111 \left(\frac{x}{L} + \frac{r-R_1}{R_2-R_1} \right).$$

Other values needed in the "test case" are

$$L = 60 \text{ cm.},$$

$$R_1 = .635 \text{ cm.},$$

$$R_2 = 3.81 \text{ cm.},$$

$$P = 20.41 \text{ atm.},$$

$$Q = 2395 \text{ cm/sec.},$$

$$W_u = 18.016 \text{ g/gmole},$$

$$W_v = 2.016 \text{ g/gmole},$$

$$W = 12.01 \text{ g/gmole},$$

$$\rho = 1.7 \text{ g/cm.}^3,$$

$$c'_1 = 3.523 \times 10^{-3} \text{ g/cm.}^3,$$

$$c'_2 = 0,$$

$$N_{Re} = 2.54 \times 10^4,$$

$$N_{SC} = 0.38,$$

$$D_c = .53 \text{ cm.}^2/\text{sec.}$$

3. Numerical Methods

In this section we describe the general iterative methods of solution.

Consider the following point sets:

$$S = \{(r,x) / R_1 < r < R_2, 0 < x < L\},$$

$$B_1 = \{(r,x) / x = 0, R_1 \leq r \leq R_2\},$$

$$B_2 = \{(r,x) / x = L, R_1 \leq r \leq R_2\},$$

$$B_3 = \{(r,x) / r = R_2, 0 \leq x \leq L\},$$

$$B_4 = \{(r,x) / r = R_1, 0 \leq x \leq L\},$$

$$B_5 = \{(r,x) / r = 0, 0 \leq x \leq L\}.$$

The region G of the graphite in Figure 1 can then be expressed as

$$G = S \cup B,$$

where

$$B = B_1 \cup B_2 \cup B_3 \cup B_4$$

is the boundary of G .

Subdivide G into rectangular regions formed by lines parallel to the line $x = 0$ and parallel to the line $r = R_1$. The intersection of these lines generates a discrete set $G' = S' \cup B'$ of points (r_i, x_j) in G ,

$i = 1, 2, \dots, n$ and $j = 1, 2, \dots, m$, generating the nodes of our grid, with $x_1 = 0$, $x_m = L$, $r_1 = R_1$, and $r_n = R_2$, where the prime denotes the comparable discrete set.

Let

$$h_j = x_{j+1} - x_j, \quad j = 1, 2, \dots, m-1,$$

$$k_i = r_{i+1} - r_i, \quad i = 1, 2, \dots, n-1,$$

$$\hat{h}_j = h_j + h_{j-1}, \quad j = 2, 3, \dots, m-1,$$

$$\hat{k}_i = k_i + k_{i-1}, \quad i = 2, 3, \dots, n-1,$$

$$\bar{w}_j = \bar{w}(x_j), \quad w = u \text{ or } v, \quad j = 1, \dots, m,$$

$$w_{i,j} = w(r_i, x_j), \quad w = u \text{ or } v, \quad i = 1, 2, \dots, n; \\ j = 1, 2, \dots, m.$$

The finite difference approximations for the derivatives in Equations (2.3) (for unequal spacings) are

$$\left. \frac{\partial^2 w}{\partial x^2} \right|_{(r_i, x_j)} = 2 \left[\frac{h_j w_{i,j-1} - \hat{h}_j w_{i,j} + h_{j-1} w_{i,j+1}}{h_{j-1} h_j \hat{h}_j} \right],$$

$$\left. \frac{\partial^2 w}{\partial r^2} \right|_{(r_i, x_j)} = 2 \left[\frac{k_i w_{i-1,j} - \hat{k}_i w_{i,j} + k_{i-1} w_{i+1,j}}{k_{i-1} k_i \hat{k}_i} \right],$$

$$\left. \frac{\partial w}{\partial r} \right|_{(r_i, x_j)} = \frac{-k_i^2 w_{i-1,j} + (k_i^2 - k_{i-1}^2) w_{i,j} + k_{i-1}^2 w_{i+1,j}}{k_{i-1} k_i \hat{k}_i},$$

where $w = u$ or v .

For each point $(r_i, x_j) \in S'$, the Equations (2.3) then become

$$\begin{aligned}
 a_{i,j} u_{i,j} - (b_1 u_{i,j-1} + b_2 u_{i,j+1} + b_3 u_{i-1,j} + b_4 u_{i+1,j}) \\
 + c_1 \gamma(u_{i,j}, v_{i,j}) = 0, \\
 a_{i,j} v_{i,j} - (b_1 v_{i,j-1} + b_2 v_{i,j+1} + b_3 v_{i-1,j} + b_4 v_{i+1,j}) \\
 - c_2 \gamma(u_{i,j}, v_{i,j}) = 0,
 \end{aligned} \tag{3.1}$$

where

$$\begin{aligned}
 a_{i,j} = a(r_i, x_j) &= \frac{2}{h_{j-1} h_j} + \frac{4r_i - r_{i-1} - r_{i+1}}{r_i k_{i-1} k_i}, \\
 b_1 = b_1(x_j) &= \frac{2}{h_{j-1} h_j}, \\
 b_2 = b_2(x_j) &= \frac{2}{h_j h_j}, \\
 b_3 = b_3(r_i) &= \frac{3r_i - r_{i+1}}{r_i k_{i-1} k_i}, \\
 b_4 = b_4(r_i) &= \frac{3r_i - r_{i-1}}{r_i k_i k_i}, \\
 c_1 &= \frac{\rho W_u}{\eta_u}
 \end{aligned}$$

and

$$c_2 = \frac{\rho W_v}{D_v}.$$

We approximate the derivatives in Equations (2.4) by

$$\left. \frac{\partial w}{\partial r} \right| (r_i, x_j) \equiv \frac{w_{i,j} - w_{i-1,j}}{k_{i-1}}$$

and

$$\left. \frac{\partial w}{\partial x} \right| (r_i, x_j) \equiv \frac{w_{i,j} - w_{i,j-1}}{h_{j-1}},$$

where $w = u$ or v .

The boundary conditions in Equations (2.4) then become

$$\begin{aligned} w_{n,j} &= w_{n-1,j}, \quad j = 2, 3, \dots, m-1, \\ w_{i,1} &= w_{i,2}, \quad i = 2, 3, \dots, n-1, \\ w_{i,m} &= w_{i,m-1}, \quad i = 2, 3, \dots, n-1, \end{aligned} \tag{3.2}$$

where $w = u$ or v .

The derivatives in Equations (2.5), (2.6), (2.8), and (2.9) are approximated by

$$\begin{aligned} \left. \frac{\partial w}{\partial r} \right| (r_1, x_j) &\equiv \frac{-k_2(\hat{k}_2 + k_1)w_{1,j} + \hat{k}_2^2 w_{2,j} - k_1^2 w_{3,j}}{k_1 k_2 \hat{k}_2}, \\ \left. \frac{d\bar{w}}{dx} \right| x_j &\equiv \frac{\bar{w}_j - \bar{w}_{j-1}}{h_{j-1}}, \end{aligned}$$

where $w = u$ or v .

Then, for each point (r_i, x_j) in $B'_4 \cup B'_5$, the Equations (2.5), (2.6), (2.8), and (2.9), coupled in u and v , become

$$(R_1 Q + 2\ell(x_j)h_{j-1})\bar{u}_j - 2\ell(x_j)h_{j-1}u_{1,j} = R_1 Q\bar{u}_{j-1}, \quad (3.3)$$

$$\begin{aligned} k_1 \hat{k}_2 \ell(x_j) \bar{u}_j - [D_{u_j}(\hat{k}_2 + k_1) + k_1 \hat{k}_2 \ell(x_j)] u_{1,j} \\ = - \frac{D_{u_j}}{k_2} (\hat{k}_2^2 u_{2,j} - k_1^2 u_{3,j}), \end{aligned}$$

and

$$(R_1 Q + 2\ell(x_j)h_{j-1})\bar{v}_j - 2\ell(x_j)h_{j-1}v_{1,j} = R_1 Q\bar{v}_{j-1}, \quad (3.4)$$

$$\begin{aligned} k_1 \hat{k}_2 \ell(x_j) \bar{v}_j - [D_{v_j}(\hat{k}_2 + k_1) + k_1 \hat{k}_2 \ell(x_j)] v_{1,j} \\ = - \frac{D_{v_j}}{k_2} (\hat{k}_2^2 v_{2,j} - k_1^2 v_{3,j}). \end{aligned}$$

These equations furnish the values for $\bar{u}_j$, $\bar{v}_j$, $u_{1,j}$, and $v_{1,j}$, $j = 2, \dots, m-1$.

The general iterative scheme for this problem is as follows:

Step 0. Determine initial values for u and v .

Step 1. Fix $j = 2$.

Step 2. Calculate:

$$\alpha_1 = R_1 Q + 2\ell(x_j)h_{j-1},$$

$$\beta_1 = -2\ell(x_j)h_{j-1},$$

$$\xi_1 = R_1 Q\bar{u}_{j-1},$$

$$\alpha_2 = k_1 \hat{k}_2 \ell(x_j),$$

$$\beta_2 = -[D_{u_j}(\hat{k}_2 + k_1) + k_1 \hat{k}_2 \ell(x_j)],$$

$$\xi_2 = -\frac{D_{u_j}}{k_2} [\hat{k}_2^2 u_{2,j} - k_1^2 u_{3,j}].$$

Step 3. Calculate:

$$\bar{u}_j = \frac{\xi_1 \beta_2 - \xi_2 \beta_1}{\alpha_1 \beta_2 - \alpha_2 \beta_1},$$

$$u_{1,j} = \frac{\alpha_1 \xi_2 - \alpha_2 \xi_1}{\alpha_1 \beta_2 - \alpha_2 \beta_1}.$$

Step 4. Calculate:

$$\hat{\beta}_2 = -[D_{v_j}(\hat{k}_2 + k_1) + k_1 \hat{k}_2 \ell(x_j)],$$

$$\hat{\xi}_1 = R_1 Q \bar{v}_{j-1},$$

$$\hat{\xi}_2 = -\frac{D_{v_j}}{k_2} [\hat{k}_2^2 v_{2,j} - k_1^2 v_{3,j}].$$

Step 5. Calculate:

$$\bar{v}_j = \frac{\hat{\xi}_1 \hat{\beta}_2 - \hat{\xi}_2 \beta_1}{\alpha_1 \hat{\beta}_2 - \alpha_2 \beta_1},$$

$$v_{1,j} = \frac{\alpha_1 \hat{\xi}_2 - \alpha_2 \hat{\xi}_1}{\alpha_1 \hat{\beta}_2 - \alpha_2 \beta_1}.$$

Step 6. Calculate $u_{i,j}$ and $v_{i,j}$ for $i = 2, \dots, n-1$ using method Q, N or L (which are discussed later in this section).

Step 7. Do Steps 2-6 for $j = 3, \dots, m-1$.

Step 8. Calculate the new boundary values using Equations (3.2).

Step 9. Test for convergence.

The remaining portion of this section will be devoted to discussing methods Q, N and L referred to in Step 6. To simplify this discussion, let

$$\phi(w) = b_1 w_{i,j-1}^{(k)} + b_2 w_{i,j+1}^{(k-1)} + b_3 w_{i-1,j}^{(k)} + b_4 w_{i+1,j}^{(k-1)},$$

when k denotes the iteration number.

Method Q

In this method, we consider the first equation in (3.1), take the previous iterate for the value of $v_{i,j}$, treat the equation as a quadratic equation in $u_{i,j}$, and solve the resulting equation by the quadratic formula. We then consider the second equation in (3.1), use the newly calculated value for $u_{i,j}$, and solve the resulting quadratic equation in $v_{i,j}$ by the quadratic formula.

The equations for this method are written as follows:

$$a_{i,j} u_{i,j}^{(k)} - \phi(u) + c_1 \gamma(u_{i,j}^{(k)}, v_{i,j}^{(k-1)}) = 0, \quad (3.5)$$

$$a_{i,j} v_{i,j}^{(k)} - \phi(v) - c_2 \gamma(u_{i,j}^{(k)}, v_{i,j}^{(k)}) = 0. \quad (3.6)$$

Equation (3.5) can then be written as

$$\begin{aligned} a_{i,j} \hat{K}_3 (u_{i,j}^{(k)})^2 + [a_{i,j} (1 + \hat{K}_2 v_{i,j}^{(k-1)}) - \hat{K}_3 \phi(u) + \hat{K}_1 c_1] u_{i,j}^{(k)} \\ - (1 + \hat{K}_2 v_{i,j}^{(k-1)}) \phi(u) = 0, \end{aligned}$$

where

$$\hat{K}_1 = K_1 R_u^T, \quad \hat{K}_2 = K_2 R_v^T, \quad \text{and} \quad \hat{K}_3 = K_3 R_u^T.$$

Let

$$\hat{A} = a_{i,j} \hat{K}_3,$$

$$\hat{B} = a_{i,j} (1 + \hat{K}_2 v_{i,j}^{(k-1)}) - \hat{K}_3 \phi(u) + \hat{K}_1 c_1,$$

$$\hat{C} = (1 + \hat{K}_2 v_{i,j}^{(k-1)}) \phi(u).$$

If $\hat{B} < 0$, set

$$u_{i,j}^{(k)} = \frac{-\hat{B} + \sqrt{\hat{B}^2 + 4\hat{A}\hat{C}}}{2\hat{A}}.$$

If $\hat{B} = 0$, then

$$u_{i,j}^{(k)} = \frac{\sqrt{\hat{A}\hat{C}}}{\hat{A}}.$$

If $\hat{B} > 0$, then calculate

$$\hat{u} = \frac{-\hat{B} - \sqrt{\hat{B}^2 + 4\hat{A}\hat{C}}}{2\hat{A}}$$

and set

$$u_{i,j}^{(k)} = \frac{-\hat{C}}{\hat{A}\hat{u}}.$$

Similarly, Equation (3.6) can be written as

$$a_{i,j} \hat{K}_2 (v_{i,j}^{(k)})^2 + [a_{i,j} (1 + \hat{K}_3 u_{i,j}^{(k)}) - \hat{K}_2 \phi(v)] v_{i,j}^{(k)}$$

$$- [\phi(v) (1 + \hat{K}_3 u_{i,j}^{(k)}) + c_2 \hat{K}_1 u_{i,j}^{(k)}] = 0.$$

Let

$$\tilde{A} = a_{i,j} \hat{K}_2,$$

$$\tilde{B} = a_{i,j}(1 + \hat{K}_3 u_{i,j}^{(k)}) - \hat{K}_2 \phi(v)$$

$$\tilde{C} = (1 + \hat{K}_3 u_{i,j}^{(k)}) \phi(v) + c_2 \hat{K}_1 u_{i,j}^{(k)}.$$

If $\tilde{B} < 0$, set

$$v_{i,j}^{(k)} = \frac{-\tilde{B} + \sqrt{\tilde{B}^2 + 4\tilde{A}\tilde{C}}}{2\tilde{A}}.$$

If $\tilde{B} = 0$, set

$$v_{i,j}^{(k)} = \frac{\sqrt{\tilde{A}\tilde{C}}}{\tilde{A}}.$$

If $\tilde{B} > 0$, then calculate

$$\hat{v} = \frac{-\tilde{B} - \sqrt{\tilde{B}^2 + 4\tilde{A}\tilde{C}}}{2\tilde{A}},$$

and set

$$v_{i,j}^{(k)} = \frac{-\tilde{C}}{\tilde{A}\hat{v}}.$$

Method N

This method is what might be called a Generalized Newton [2] or a Newton-Gauss-Seidel-Overrelaxation Method. Here we consider the negative of the first equation in (3.1), take the previous iterate for the value of $v_{i,j}$, and treat the resulting equation as a function F of $u_{i,j}$. We obtain a new value of $u_{i,j}$ by subtracting from the present value of $u_{i,j}$ the product of a constant ω , $0 < \omega < 2$, and the quotient of $F(u_{i,j})$ and its derivative with respect to $u_{i,j}$. We then consider the negative of the second equation of (3.1), using the newly calculated value for $u_{i,j}$ and treat it as a function H of $v_{i,j}$. We obtain a new value of

$v_{i,j}$ by subtracting from the present value of $v_{i,j}$ the product of ω and the quotient of $H(v_{i,j})$ and its derivative with respect to $v_{i,j}$.

The equations for this method are written as follows:

$$u_{i,j}^{(k)} = u_{i,j}^{(k-1)} - \omega \frac{F(u_{i,j}^{(k-1)})}{\frac{\partial F}{\partial u_{i,j}}(u_{i,j}^{(k-1)})},$$

$$v_{i,j}^{(k)} = v_{i,j}^{(k-1)} - \omega \frac{H(v_{i,j}^{(k-1)})}{\frac{\partial H}{\partial v_{i,j}}(v_{i,j}^{(k-1)})},$$

where

$$F(u_{i,j}^{(k-1)}) = -a_{i,j} u_{i,j}^{(k-1)} + \phi(u) - c_1 \gamma(u_{i,j}^{(k-1)}, v_{i,j}^{(k-1)}) = 0,$$

and

$$H(v_{i,j}^{(k-1)}) = -a_{i,j} v_{i,j}^{(k-1)} + \phi(v) + c_2 \gamma(u_{i,j}^{(k)}, v_{i,j}^{(k-1)}) = 0.$$

Method L

In this method, we consider the first equation in (3.1), take the previous iterate for the value of $v_{i,j}$ and the previous iterate for the value of $u_{i,j}$ in the denominator of γ , and solve the resulting equation, which is linear in $u_{i,j}$, for the new value of $u_{i,j}$. We then consider the second equation in (3.1), take the newly calculated value of $u_{i,j}$, and the previous iterate for the value of $v_{i,j}$ in the denominator of γ , and solve the resulting linear equation in $v_{i,j}$ for the new value of $v_{i,j}$.

The equations for this method are written as follows:

$$u_{i,j}^{(k)} = \frac{\phi(u)}{a_{i,j} + f(u_{i,j}^{(k-1)})},$$

$$v_{i,j}^{(k)} = \frac{1}{a_{i,j}} [\phi(v) + c_2 \gamma(u_{i,j}^{(k)}, v_{i,j}^{(k-1)})],$$

where

$$f(u_{i,j}^{(k-1)}) = \frac{c_1 \hat{K}_1}{1 + \hat{K}_2 v_{i,j}^{(k-1)} + \hat{K}_3 u_{i,j}^{(k-1)}}.$$

4. Comparison of Numerical Methods

In Section 3 we developed three iterative methods of solution - methods Q, N and L. We shall now discuss and compare these three methods. Further, we shall discuss two other methods that might seem reasonable for such a problem.

For simplicity let us write our system of partial differential equations in the form

$$\begin{aligned} \nabla^2 u - \frac{c_1 u}{1 + c_2 v + c_3 u} &= 0, \\ \nabla^2 v + \frac{c_4 u}{1 + c_2 v + c_3 u} &= 0. \end{aligned} \tag{4.1}$$

For different "reasonable" cases, the functions c_1 , c_2 , c_3 and c_4 range from extremely small to very large numbers. In the "test" case described earlier, these functions take on quite small values. However, a good numerical method should not only solve this "test" case, but should adequately handle the full range of possibilities for the c_i 's.

All three methods solved our "test" case very well. On an IBM Model 360/75, methods L, N and Q took, respectively, 1.90, 2.43, and 3.19 minutes to converge.

Method L

For the "test" case, Method L was slightly better than Method N and approximately twice as fast as Method Q. Similarly, Method L was superior for cases with larger values of the c_i 's. Since Method L is so

easy to apply, is more efficient, and effectively handles the general case for different values of the c_i 's, we recommend it over all other methods discussed in this report.

Method N

Although we favor Method L, the Generalized Newton Method has much to recommend it. The algorithm is simple, and, for good initial values, can be expected to effectively solve this type of problem.

Method Q

Method Q works well for small values of the c_i 's. However, as these terms get larger, Method Q becomes less efficient. Furthermore, this method is too sensitive; to get accurate results, one must carry the coefficient of the first degree term in double precision. Although Method Q is satisfactory for certain cases, it is not recommended as the general method of solution for this type of problem.

Other Methods

When one first considers Equations (4.1), he tends to want to first linearize the non-linear terms in the finite difference equations by using all previous iterates for u and v in these terms. This method of attack is very good for small values of the c_i 's. However, as the c_i 's get larger and the non-linear terms become more influential, this method fails.

Another approach considered is that of using the quadratic equation of Method Q and linearizing it by replacing one factor of the

quadratic term by the previous iterate. This method suffers from the same difficulties as the method just above.

5. Miscellaneous

In this section we shall discuss two important concepts relating to this problem. These are overrelaxation and unequal spacings.

Overrelaxation

In those cases where the c_i 's were small, convergence was so rapid that overrelaxation was unnecessary. For the cases with large c_i 's, overrelaxation (and underrelaxation) did not appreciably improve convergence.

Unequal Spacings

In most physical problems of this type, the region of graphite nearest the coolant stream will be more critical and that farthest away of a lesser concern. Therefore, it behooves us, in general, to make the grid much finer near the coolant stream. The unequal spacings we used in our finite difference equations allowed us this flexibility without introducing any real difficulties.

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APPENDIX A

VOLUMETRIC AVERAGE REACTION RATE

At each point (r_i, x_j) of the grid, a reaction rate, $R_{i,j}$, is calculated from

$$R_{i,j} = \rho W \gamma(u_{i,j}, v_{i,j}).$$

This reaction rate can be used to obtain a volumetric average reaction rate, $\bar{R}$, for the graphite cylinder by

$$\bar{R} = \frac{\sum_{i,j=1}^{n-1, m-1} R_{i,j} V_{i,j}}{\sum_{i,j=1}^{n-1, m-1} V_{i,j}},$$

where

$$V_{i,j} = \pi k_i h_j (r_{i+1} + r_i).$$

APPENDIX B

THE COMPUTER CODE

Steamcar is a code, written in Fortran IV for the IBM 360/75, which solves the system of ordinary and non-linear partial differential equations given in Section 2, and utilizes the numerical techniques given in Section 3. The purpose of this section is to describe Steamcar by outlining:

- (1) the definitions of the variables used,
- (2) the logical flow of the code, and
- (3) the input to the code.

A Fortran listing of Steamcar is also included. Whenever possible, the definitions given to variables and routines in Steamcar will be related to the variables used previously in the report.

Definition of Variables in COMMON

The notation $A(I,J)$ indicates that A is an array and the value of A at the (I,J) position corresponds to the value at the point (r_i, x_j) in the discrete set G' defined in Section 3.

Blank common contains the following variables:

- $A(I,J)$: The water vapor concentration, $u(r_i, x_j)$, in the graphite.
- $B(I,J)$: The hydrogen concentration, $v(r_i, x_j)$, in the graphite.
- $ABAR(J)$: The water vapor concentration, $\bar{u}(x_j)$, in the coolant stream.

BBAR(J): The hydrogen concentration, $\bar{v}(x_j)$, in the coolant stream.

HFX(J): The film coefficient, $h(x_j)$.

The following are the labeled commons and the variables they contain:

(a) SLOW:

$\left. \begin{array}{l} C1(I,J) \\ C2(I,J) \\ C3(I,J) \end{array} \right\} :$ The temperature dependent functions K_1 , K_2 , and K_3 in (2.2).

DH20(I,J): The diffusion coefficient $D_u(r_i, x_j)$.

DH2(I,J): The diffusion coefficient $D_v(r_i, x_j)$.

(b) MESH:

NX: The number, m , of node points in the x -direction.

NR: The number, n , of node points in the r -direction.

DELX(J): The value h_j .

DELR(I): The value k_i .

RDST(I): The distance r_i .

DINTX(J): The value $\hat{h}_j$.

DINTR(J): The value $\hat{k}_i$.

(c) PARMS:

$\left. \begin{array}{l} R1 \\ R2 \\ GLENTH \end{array} \right\} :$ The graphite cylinder dimensions, R_1 , R_2 , and L .

$\left. \begin{array}{l} C10 \\ C20 \\ C30 \end{array} \right\} :$ The constants K_{01} , K_{02} , and K_{03} used in defining K_1 , K_2 , and K_3 .

$\left. \begin{array}{l} E1 \\ E2 \\ E3 \end{array} \right\} :$	The constants E_1 , E_2 , and E_3 used in defining K_1 , K_2 , and K_3 .
$\left. \begin{array}{l} RH20 \\ RH2 \end{array} \right\} :$	The constants R_u and R_v used in the definition of $\gamma(u,v)$.
RHO:	The density ρ of the graphite.
R:	The constant R in the definition of K_1 , K_2 , and K_3 .
$\left. \begin{array}{l} WTA \\ WTB \\ WTC \end{array} \right\} :$	The molecular weights W_u , W_v , and W .
UBARX:	The bulk average coolant velocity, Q .
$\left. \begin{array}{l} REN \\ SCN \\ DHE \end{array} \right\} :$	The constants N_{Re} , N_{SC} , and D_c used in the definition of $\ell(x_j)$.
PRESS:	The pressure, P .
$\left. \begin{array}{l} XKNUD \\ PSI \end{array} \right\} :$	The graphite constants K_0 and ϕ .

(d) LIMITS:

$\left. \begin{array}{l} NXDIM \\ NRDIM \end{array} \right\} :$	The maximum allowable I and J values.
MAXCT:	The maximum number of iterations the code is to compute.
NPRINT:	The values of the ABAR, A, BBAR, and B arrays are printed out every NPRINT iterations.
NRTEST:	The convergence tests are made every NRTEST iterations.

ACONV	}	The limits which determine convergence for A
BCONV		
NAME:		The identification of the case.
RELAX:		The over-relaxation constant, ω .

Logical Flow

When Steamcar terminates computation on a case, either because convergence with respect to the values of ACONV and BCONV is obtained or because the number of iterations computed exceeds MAXCT, it writes on tape the values of the arrays and parameters for the case. Thus the subroutine INPUTS, depending on the value of the input variable ISTART, either begins a new case from card input of the parameters or restarts a previously calculated case from tape input.

If ISTART = 0, the case parameters are read from cards, otherwise, the case is extended from tape.

The subroutine MSHSET sets up the discrete set of points (r_i, x_j) which define the grid to be used. There are two methods which may be used to determine these grid points.

- (1) The user first divides the graphite length into NSEGX segments and the graphite thickness, $(R2-R1)$, into NSEGR segments. For each axial segment, s , $s = 1, \dots, NSEGX$, he specifies the number, ND_s , of equal spaced grid intervals, each having length DEL_s , in which the segment is to be divided. Similarly, he specifies a ND and DEL for each radial segment.

(2) The user specifies NSEGX and NSEGR as the number of axial and radial grid intervals, and then specifies the values of DELX(J), J = 1, ..., NSEGX, and DELR(I), I = 1, ..., NSEGR. The restrictions that $NX \leq MXDIM$ and $NR \leq NRDIM$ must be met. In Method (1),

$$NX = 1 + ND_1 + ND_2 + \dots + ND_{NSEGX},$$

and in Method (2),

$$NX = NSEGX + 1.$$

In order that the sum of the DELX's equals GLENTH to machine accuracy, MSHSET calculates the DEL for the last axial segment in Method (1) and recalculates, if necessary, the DELX(NSEGX) in method (2). A similar statement can be made for the radial spacing parameters.

If the input variable IREAD = 0, MSHSET expects the user to define the grid using Method (1); if IREAD $\neq$ 0, MSHSET expects the user to define the grid using method (2).

The subroutine HSETUP calculates the film coefficient function HFX(J). The subroutine ESTIMT furnishes initial estimates for the water vapor and hydrogen concentration arrays, and is furnished by the user. The subroutine CDSET sets up the C1, C2, C3, DH20, and DH2 arrays and calls the function subprogram TEMP for the value of the temperature at each point. TEMP is furnished by the user.

The subroutine PRINT prints the case parameters and, depending on the value of the input variable ICODE, prints the grid spacing, HFX(J), and temperature dependent arrays.

ICODE = 0: No arrays are printed.

ICODE = 1: The grid spacing arrays and HFX(J) are printed.

ICODE = 2: The arrays printed with ICODE = 1 and the temperature dependent arrays are printed.

The subroutine SOLVER calls the routine which solves the system of equations. In the listing below, the routine LIEB2 is the method L discussed in Section 3. LIEB2 also handles the convergence tests, the calling of the output routine, and the calculation of the reaction rate and volumetric average.

The subroutine OUTPUT handles the output of the concentration and the reaction rate arrays. It writes the information needed to restart the case on tape, and returns control to the routine called by SOLVER. The subroutine ARR360 is an "array printer" routine.

The subroutines PGMMSK and ITIME are IBM 360 machine language routines. PGMMSK causes the computer system to allow underflows to occur, and ITIME is a timing routine.

Description of Card Input

	FORMAT	Variables read
Card A:	I1	ISTART
	A4	NAME
	3I5	MAXCT, NPRINT, NRTEST
	3F10.0	RELAX, ACONV, BCONV
	I1	ICODE

The remaining cards are needed if ISTART = 0.

Card B:	3F10.0	R1, R2, GLENTH
	3F10.0	WTA, WTB, WTC
	2F10.0	RHO, UBARX
Card C:	3F10.0	C10, C20, C30
	3F10.0	E1, E2, E3
	2F10.0	RH20, RH2
Card D:	4F10.0	R, REN, SCN, DHE
	3F10.0	PRESS, XKUND, PSI
Card E:	2F10.0	ABAR(1), BBAR(1)
Card F:	I1	IREAD
	4X,2I5	NSEGX, NSEGR

If IREAD = 0, the remaining cards are as follows:

Card G _s :	A1	"X"
s = 1, ..., NSEGX-1	I4	ND: The number of DELX's in the axial segment s.
	F10.8	DEL: The value of the ND DELX's in segment s.
Card G _{NSEGX} :	A1	"X"
	I4	ND: The number of DELX's in the last axial segment. (The DEL for the last segment is calculated.)
Card H _t :	A1	"R"
t = 1, ..., NSEGR-1	I4	ND: The number of DELR's in the radial segment t.

	F10.8	DEL: The value of the ND DELR's in segment t.
Card H _{NSEGR} :	A1	"R"
	I4	ND: The number of DELR's in the last radial segment. (The DEL for the last segment is calculated.)

If IREAD $\neq$ 0, the remaining cards are as follows (where NSEGX = NX-1,
NSEGR = NR-1):

Cards G:	8F10.8	DELX(J) (J = 1, ..., NSEGX).
Cards H:	8F10.8	DELR(I) (I = 1, ..., NSEGR).

Code Listing

The remaining portion of this section consists of a FORTRAN IV
listing of Steamcar.

```

C ***** STEAM-CAR *****
C *** MAIN CONTROL DECK ***
      CALL PGMSK(1,0,0,0)
      CALL INPUTS(ISTART,ICODE)
C *** ISTART= 0 MEANS THIS CASE ORIGINATES FROM CARD INPUT ONLY,
C      .GT.0 MEANS EXTENSION OF A CASE ON UNIT 9.
C      ISTART= -1 MEANS AN ERROR CONDITION IN THE INPUT OF UNIT 9.
      IF(ISTART)100,10,20
10  CALL MSHSET(ICK)
      IF(ICK.LT.0) GO TO 100
      CALL HSETUP
      CALL ESTIMT
      CALL CDSET
20  CALL PRINT(ICODE)
      CALL ITIME(ITM1)
      CALL SOLVER
100 CALL ITIME(ITM1,ITM2)
      XTM2=FLOAT(ITM2)/6000.
      WRITE(6,8000)XTM2
8000 FORMAT('1EXECUTION TOOK',F10.5,' MINS'/)
      RETURN
      END

      SUBROUTINE INPUTS(ISTART,ICODE)
C *** THIS ROUTINE READS THE CASE PARAMETERS EITHER FROM CARDS
C      (IF ISTART IS 0) OR FROM LOGICAL UNIT NO. 9 (IF ISTART IS NOT 0).
      COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
      COMMON/SLOW/C1(70,300),C2(70,300),C3(70,300),DH20(70,300),
1      DH2(70,300)
      COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
      COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,WTA,
1      WTB,UTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
      COMMON/LIMITS/NXDIM,NRDIM,MAXCT,NPRINT,NRTEST,ITERNO,ACONV,BCONV,
1      NAME,RELAX
      ITERNO=0
      NXDIM=300
      NRDIM=70
C *** INITIALIZE ARRAYS ***
      DO 10 J=1,NXDIM
      ABAR(J)=0.
      BBAR(J)=0.
      HFX(J)=0.
      DELX(J)=0.
      DINTX(J)=0.
      DO 10 I=1,NRDIM
      C1(I,J)=0.
      C2(I,J)=0.
      C3(I,J)=0.
      DH20(I,J)=0.
      DH2(I,J)=0.
      A(I,J)=0.
10  B(I,J)=0.
      DO 20 I=1,NRDIM
      DELR(I)=0.
      RDST(I)=0.
      DINTR(I)=0
20  CONTINUE

```

```

C      *** *** ***
      READ(5,8000) ISTART,NAME,MAXCT,NPRINT,NRTEST,RELAX,ACONV,BCONV,
1      ICODE
8000  FORMAT(I1,A4,3I5,3F10.0,I1)
      IF(ISTART.EQ.0) GO TO 40
      REWIND 9
      READ(9) NMCK,R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,
1      R, WTA, WTB, WTC, UBARX, REN, SCN, DHE, PRESS, XKNUD, PSI, ITERNO, NX,
2      NR
      IF(NAME.NE.NMCK) GO TO 30
      READ(9) (DELX(J),DINTX(J),ABAR(J),BBAR(J),HFX(J),J=1,NX),
1      (DELR(I),DINTR(I),RDST(I),I=1,NR)
      READ(9) ((A(I,J),B(I,J),C1(I,J),C2(I,J),C3(I,J),DH20(I,J),DH2(I,J),
1      J=1,NX),I=1,NR)
      REWIND 9
      RETURN
30  WRITE(6,8010) NAME,NMCK
8010  FORMAT('1INPUT NAME = ',A4,' AND TAPE NAME = ',A4,' DO NOT EQUAL'/
1'0END OF RUN')
      REWIND 9
      ISTART=-1
      RETURN
40  READ(5,8020) R1,R2,GLENTH,WTA,WTB,WTC,RHO,UBARX
8020  FORMAT(8F10.0)
      READ(5,8020) C10,C20,C30,E1,E2,E3,RH20,RH2
      READ(5,8020) R,REN,SCN,DHE,PRESS,XKNUD,PSI
      READ(5,8020) ABAR(1),BBAR(1)
C *** CONVERT C10, C20, AND C30 TO DYNE UNITS ***
      ATM=1.013E+6
      C10=C10/(60.*ATM)
      C20=C20/ATM
      C30=C30/ATM
      RETURN
      END

```

```

      SUBROUTINE MSHSET(ICK)
C *** THIS ROUTINE READS THE MESH SPACING PARAMETERS AND SETS UP THE
C      ARRAYS DELX,DELR,RDST,DINTX,DINTR.
      COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
      COMMON/PARMS/R1,R2,GLENTH,DUM1(20)
      COMMON/LIMITS/NXDIM,NRDIM,DUM2(8)
      DATA LCODEX/1HX/,LCODER/1HR/
      READ(5,8000) IREAD,NSEGX,NSEGR
8000  FORMAT(I1,4X,2I5)
C *** IREAD=0 IMPLIES SEGMENTATION INPUT WHERE...
C      NSEGX=NO. OF X DIRECTION SEGMENTS EACH WITH AN EQUAL DELTA X
C      NSEGR=NO. OF R DIRECTION SEGMENTS EACH WITH AN EQUAL DELTA R
C *** IREAD .NE. 0 IMPLIES ALL THE DELTAS ARE FURNISHED WHERE...
C      NSEGX=NO. OF DELTAS IN THE X-DIRECTION
C      NSEGR=NO. OF DELTAS IN THE R-DIRECTION
      ICK=0
      IF(IREAD.NE.0) GO TO 200
      NX=0
      XDST=0.
      DO 50 K=1,NSEGX
      READ(5,8010) LCODE,ND,DEL
8010  FORMAT(A1,I4,F10.8)

```

```

      IF(LCODE.NE.LCODEX) GO TO 500
      IF(K.NE.NSEGX) GO TO 10
      DEL=(GLENTH-XDST)/FLOAT(ND)
10   DO 20 N=1,ND
      J=NX+N
      DELX(J)=DEL
20   XDST=XDST+DEL
      NX=NX+ND
50   CONTINUE
C *** NOTE THAT DEL IS CALCULATED FOR THE LAST SEGMENT.
      NX=NX+1
C *** NX=NO. MESH POINTS IN THE X-DIRECTION...NOT THE NO. OF DELX(J).
      IF(NX.GT.NXDIM) GO TO 520
      IF(XDST.EQ.GLENTH) GO TO 60
      DELX(NX-1)=DELX(NX-1) + (GLENTH-XDST)
60   NR=0
      RDST(1)=R1
      DO 100 K=1,NSEGR
      READ(5,8010)LCODE,ND,DEL
      IF(LCODE.NE.LCODER) GO TO 510
      IF(K.NE.NSEGR) GO TO 70
      DEL=(R2-RDST(NR+1))/FLOAT(ND)
70   DO 80 N=1,ND
      I=NR+N
      DELR(I)=DEL
80   RDST(I+1)=RDST(I)+DEL
      NR=NR+ND
100  CONTINUE
C *** NOTE THAT DEL IS CALCULATED FOR THE LAST SEGMENT.
      NR=NR+1
C *** NR=NO. MESH POINTS IN THE R-DIRECTION.
      IF(NR.GT.NRDIM) GO TO 530
      IF(RDST(NR).EQ.R2) GO TO 110
      DELR(NR-1)=DELR(NR-1) + (R2-RDST(NR))
      RDST(NR)=R2
110  NNX=NX-1
      DO 120 J=2,NNX
120  DINTX(J)=DELX(J)+DELX(J-1)
      NNR=NR-1
      DO 130 I=2,NNR
130  DINTR(I)=DELR(I)+DELR(I-1)
      RETURN
200  RDST(1)=R1
      READ(5,8020)(DELX(J),J=1,NSEGX)
      READ(5,8020)(DELR(I),I=1,NSEGR)
8020 FORMAT(9F10.8)
      NX=NSEGX+1
      NR=NSEGR+1
      DO 210 I=2,NR
210  RDST(I)=RDST(I-1)+DELR(I-1)
      IF(RDST(NR).EQ.R2) GO TO 220
      WRITE(6,8030)NR,RDST(NR),DELR(NR-1)
8030 FORMAT('1RDST(',I2,')=',F10.7,' DOES NOT EQUAL R2. THE LAST DELR='
1,F10.7,' IS BEING CHANGED.')
      DELR(NR-1)=DELR(NR-1) + (R2-RDST(NR))
      RDST(NR)=R2
220  XDST=0.
      DO 230 J=1,NSEGX
230  XDST=XDST+DELX(J)

```

```

      IF(XDST.EQ.GLENTH) GO TO 110
      WRITE(6,9040)XDST,DELX(NSEGX)
8040  FORMAT('0XDST=',F10.7,' DOES NOT EQUAL GLENTH. THE LAST DELX=',
      1F10.7,' IS BEING CHANGED.')
      DELX(NSEGX)=DELX(NSEGX) + (GLENTH-XDST)
      GO TO 110
C *** ERROR ROUTINES ***
      500 WRITE(6,9000)NSEGX
      9000 FORMAT('1THERE ARE NOT THE',I3,' X SEGMENTS SPECIFIED.')
      GO TO 600
      510 WRITE(6,9010)NSEGR
      9010 FORMAT('1THERE ARE NOT THE',I3,' R SEGMENTS SPECIFIED.')
      GO TO 600
      520 WRITE(6,9020)NX,NXDIM
      9020 FORMAT('1NX=',I4,' IS TOO BIG FOR THIS PROGRAM WHERE MAX NX=',I4)
      GO TO 600
      530 WRITE(6,9030)NR,NRDIM
      9030 FORMAT('1NR=',I4,' IS TOO BIG FOR THIS PROGRAM WHERE MAX NR=',I4)
      GO TO 600
      600 WRITE(6,9100)
      9100 FORMAT('0END OF JOB')
      ICK=-1
      RETURN
      END

```

```

      SUBROUTINE HSETUP
C *** THIS ROUTINE CALCULATES THE FILM COEFFICIENT FUNCTION VALUES.
      COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
      COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
      COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,WTB,
      1 WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
      CST1=(DHE/((2.*R1))*(REN**.8)*(SCN**.33)
      H1=.029*(10.**.2)*CST1
      H11=.023*CST1
      XSTAR=(2.*R1)*(.029/.023)**5
      XCOMP=.2*R1
      XDST=0.
      DO 10 K1=1,NX
      K1X=K1
      IF(XDST.GT.XCOMP) GO TO 20
      HFX(K1)=H1
      XDST=XDST+DELX(K1)
10  CONTINUE
      GO TO 60
      20 DO 30 K2=K1X,NX
      K2X=K2
      IF(XDST.GE.XSTAR) GO TO 40
      HFX(K2)=.029*CST1*(((2.*R1)/XDST)**.2)
      XDST=XDST+DELX(K2)
      30 CONTINUE
      GO TO 60
      40 DO 50 K3=K2X,NX
      50 HFX(K3)=H11
      60 RETURN
      END

```



```

SUBROUTINE CDSET
C *** THIS ROUTINE CALCULATES THE VALUES FOR ...
C     THE TEMPERATURE DEPENDENT FUNCTIONS FOUND IN THE NON-LINEAR TERM,
C     THE DIFFUSION COEFFICIENTS.
COMMON/SLOW/C1(70,300),C2(70,300),C3(70,300),DH2G(70,300),
1     DH2(70,300)
COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,MTA,
1     WTB,WTB,WTB,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
CST1=C10*RH20
CST11=-E1/R
CST2=C20*RH2
CST22=-E2/R
CST3=C30*RH20
CST33=-E3/R
CST4=(7.317E-5)/XKNUD
CST5=(8.403E+3)*PRESS/PSI
CST6=(2.187E-4)/XKNUD
CST7=(1.449E+4)*PRESS/PSI
XDST=0.
DO 20 J=1,NX
DO 10 I=1,NR
T=TEMP(XDST,RDST(I))
C1(I,J)=CST1*T*EXP(CST11/T)
C2(I,J)=CST2*T*EXP(CST22/T)
C3(I,J)=CST3*T*EXP(CST33/T)
T1=SQRT(T)
T2=T**(-1.6722)
Z=CST6/T1 + CST7*T2
DH2G(I,J)=1./Z
Z=CST4/T1 + CST5*T2
10 DH2(I,J)=1./Z
XDST=XDST+DELX(J)
20 CONTINUE
WRITE(6,8000)
8000 FORMAT('CDSET CALCULATE COMPLETED...')
RETURN
END

```

```

FUNCTION TEMP(XDST,RDST)
C *** THIS FUNCTION SUBPROGRAM FURNISHES THE TEMPERATURE DISTRIBUTION
C     FUNCTION FOR THE CODE.
C     IT IS SUPPLIED BY THE USER.
COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,MTA,
1     WTB,WTB,WTB,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
TEMP=1723. + (111./GLENTH)*XDST + 111.*(RDST-R1)/(R2-R1)
RETURN
END

```

```

SUBROUTINE ESTIMT
C *** THIS ROUTINE FURNISHES INITIAL ESTIMATES (OTHER THAN ZERO SINCE
C     THE ARRAYS ARE ALWAYS INITIALIZED TO ZERO IN INPUTS).
C     IT MUST BE WRITTEN BY THE USER.
COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
COMMON/MESH/NX,NR,DUM1(810)

```

```

EST1=.1*ABAR(1)
MM=NX-1
DO 10 J=2,MM
  A(1,J)=EST
10 ABAR(J)=EST
RETURN
END

SUBROUTINE PRINT(ICODE)
C *** THIS ROUTINE PRINTS OUT THE BASIC PARAMETERS FOR THE CASE.
COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
COMMON/SLOW/C1(70,300),C2(70,300),C3(70,300),DH20(70,300),
1 DH2(70,300)
COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
COMMON/PARMS/R1,R2,GLENTN,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,WTB,
1 WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
COMMON/LIMITS/NXDIM,NRDIM,MAXCT,NPRINT,NRTEST,ITERNO,ACONV,BCONV,
1 NAME,RELAX
C **** ICODE=0 MEANS NO ARRAYS ARE PRINTED.
C ICODE=1 MEANS THE FOLLOWING ARRAYS ARE PRINTED ...
C DELX,DELR,RDST,DINTX,DINTR, AND HFX.
C ICODE=2 MEANS ALL ARRAYS ARE PRINTED.
WRITE(6,8000)NAME
8000 FORMAT('1GRAPHITE CASE ',A4,' WITH THE FOLLOWING FIXED PARAMETERS.
1...')
WRITE(6,8010)R1,R2,GLENTN,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,WTB,
1 WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
8010 FORMAT('0R1=',F10.5,' R2=',F10.5,' GLENTN=',F10.5,' C10=',E15.8,
1 ' C20=',E15.8,' C30=',E15.8/'CE1=',E15.8,' E2=',E15.8,' E3=',E15.8
2 ' RH20=',E15.8,' RH2=',E15.8,' RHO=',F10.5,' R=',E15.8/'OWTA=',
3 F10.5,' WTB=',F10.5,' WTC=',F10.5,' UBARX=',F10.3,' REN=',E15.8,
4 ' SCN=',E15.8,' DHE=',E15.8/'OPRESS=',F10.5,' XKNUD=',E15.8,
5 ' PSI=',E15.8)
WRITE(6,8020)NR,NX
8020 FORMAT('0THE FIXED GRAPHITE MESH DIMENSIONS ARE.../'0NO. OF ROWS=
1 ',I4,' NO. OF COLS=',I4)
WRITE(6,8030)MAXCT,NPRINT,ITERNO
8030 FORMAT('0THIS RUN IS DESIGNATED TO COMPLETE',I5,' ITERATIONS WITH
1 MESH PRINT OUTS EVERY ',I5,' ITERATIONS.'/'0THIS CASE HAS PREVIOUS
2 LY RUN ',I5,' ITERATIONS.')
WRITE(6,8035)RELAX,ACONV,BCONV,NRTEST
8035 FORMAT('0RELAX=',F10.8,' ACONV=',E15.7,' BCONV=',E15.7,' NRTEST=',
1 I4)
IF(ICODE.EQ.0) GO TO 100
WRITE(6,8040)NX
8040 FORMAT('1DELX(J),J=1 TO ',I3)
WRITE(6,8045)(DELX(J),J=1,NX)
8045 FORMAT(1P8E15.5)
WRITE(6,8050)NR
8050 FORMAT('1DELR(I),I=1 TO ',I2)
WRITE(6,8045)(DELR(I),I=1,NR)
WRITE(6,8060)NR
8060 FORMAT('0RDST(I),I=1 TO ',I2)
WRITE(6,8045)(RDST(I),I=1,NR)
WRITE(6,8070)NX
8070 FORMAT('1DINTX(J),J=1 TO ',I3)
WRITE(6,8045)(DINTX(J),J=1,NX)

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```

      WRITE(6,8080)NX
8080  FORMAT('1HFX(J),J=1 TO ',I3)
      WRITE(6,8045)(HFX(J),J=1,NX)
      WRITE(6,8090)NR
8090  FCRMAT('1DINTR(I),I=1 TO ',I2)
      WRITE(6,8045)(DINTR(I),I=1,NR)
      IF(ICODE.EQ.1) GO TO 100
      WRITE(6,9000)
9000  FORMAT('1')
      CALL ARR360(C1,NR,NX,NRDM,4H C1 )
      CALL ARR360(C2,NR,NX,NRDM,4H C2 )
      CALL ARR360(C3,NR,NX,NRDM,4H C3 )
      CALL ARR360(DH2O,NR,NX,NRDM,4HDH2O)
      CALL ARR360(DH2,NR,NX,NRDM,4H DH2)
100  RETURN
      END

      SUBROUTINE OUTPUT(KKK,ISWT)
      COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
      COMMON/SLDW/C1(70,300),C2(70,300),C3(70,300),DH2O(70,300),
1      DH2(70,300)
      COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
      COMMON/PARMS/R1,R2,GLENTN,C10,C20,C30,E1,E2,E3,RH2O,RH2,RHO,R,WTB,
1      WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
      COMMON/LIMITS/NXDIM,NRDM,MAXCT,NPRINT,NRTEST,ITERNO,ACONV,BCONV,
1      NAME,RELAX
      COMMON/MAX/ARMAX,BRMAX,KKKR
C *** ISWT=0 MEANS NPRINT TYPE OUTPUT.
C      =1 MEANS CASE CONVERGED.
C      =2 MEANS MAX. COUNT WAS EXCEEDED.
C      =3 MEANS PRINT GRAPHITE CORROSION RATE.
      IF(ISWT.EQ.3) GO TO 100
      ITOT1=KKK+ITERNO
      A(1,1)=A(1,2)
      B(1,1)=B(1,2)
      WRITE(6,8000)ITOT1
8000  FORMAT('1RESULTS AFTER',I5,' ITERATIONS...')
      WRITE(6,8010)(ABAR(J),J=1,NX)
8010  FORMAT('1OH2O CONCENTRATION IN THE GAS STREAM='/(1P8E15.5))
      CALL ARR360(A,NR,NX,NRDM,4H H2O)
      WRITE(6,8015)ARMAX,KKKR
8015  FORMAT('1OMAX. RESIDUE FOR THE MESH=',E15.8,' WHICH WAS CALCULATED
1  AT ITERATION ',I5)
      WRITE(6,8020)(BBAR(J),J=1,NX)
8020  FORMAT('1H2 CONCENTRATION IN THE GAS STREAM='/(1P8E15.5))
      CALL ARR360(B,NR,NX,NRDM,4H H2 )
      WRITE(6,8015)BRMAX,KKKR
      IF(ISWT.EQ.0) RETURN
C *** WRITE RE-START TAPE ***
      ITERNO=ITERNO + KKK
      REWIND 10
      WRITE(10)NAME,R1,R2,GLENTN,C10,C20,C30,E1,E2,E3,RH2O,
1      RH2,RHO,R,WTB,WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI,
2      ITERNO,NX,NR
      WRITE(10)(DELX(J),DINTX(J),ABAR(J),BBAR(J),HFX(J),J=1,NX),
1      (DELR(I),DINTR(I),RDST(I),I=1,NR)
      WRITE(10)((A(I,J),B(I,J),C1(I,J),C2(I,J),C3(I,J),DH2O(I,J),

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```

1          DH2(I,J),J=1,NX),I=1,NR)
END FILE 10
REWIND 10
IF(ISWT.EQ.2) GO TO 50
C *** CASE CONVERGED ***
WRITE(6,8030)
8030 FORMAT('0CASE CONVERGED...')
RETURN
50 WRITE(6,8035)
8035 FORMAT('0MAX. COUNT EXCEEDED...')
RETURN
100 WRITE(6,8040)
8040 FORMAT('1')
CALL ARR360(A,NR,NX,NRDM,4HGRAP)
RETURN
END

SUBROUTINE RESIDU
C CALCULATE THE RESIDUAL FOR EACH POINT IN BOTH THE H2O AND H2 MESH.
COMMON//A(70,300),B(70,300),ABAR(300),BBAR(300),HFX(300)
COMMON/SLOW/C1(70,300),C2(70,300),C3(70,300),DH20(70,300),
1          DH2(70,300)
COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RHO,R,WTB,
1          WTB,WTC,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
COMMON/LIMITS/NXDIM,NRDM,MAXCT,NPRINT,NRTEST,ITERNO,ACONV,BCONV,
1          NAME,RELAX
COMMON/ME SH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
COMMON/RESBAR/ABAR(300),BRBAR(300)
DO 10 J=1,NX
  ARBAR(J)=0.
  BRBAR(J)=0.
DO 10 I=1,NR
  C1(I,J)=(C1(I,J)*A(I,J))/(1.+C2(I,J)*B(I,J)+C3(I,J)*A(I,J))
  C2(I,J)=0.
10 C3(I,J)=0.
C *** C1(I,J) NOW CONTAINS THE NON-LINEAR EVALUATION FOR EACH POINT, AND
C C2(I,J) WILL BE USED FOR H2O RESIDUAL, C3(I,J) FOR H2 RESIDUAL.
NN=NR-1
MM=NX-1
CSTA=RHO*WTB
CSTB=RHO*WTB
CST1=UBARX*R1
CST2=DELR(1)*DINTR(2)
CST3=DELR(1)+DINTR(2)
CST4=(DELR(1)*DELR(1))/DELR(2)
CST5=(DINTR(2)*DINTR(2))/DELR(2)
DO 100 J=2,MM
  ALP1=CST1 + 2.*HFX(J)*DELX(J-1)
  BET1=-2.*HFX(J)*DELX(J-1)
  GAM1=CST1*ABAR(J-1)
  ALP2=CST2*HFX(J)
  BET2=-DH20(1,J)*CST3 - ALP2
  GAM2=DH20(1,J)*(CST4*A(3,J) - CST5*A(2,J))
  ARBAR(J)=ALP1*ABAR(J) + BET1*A(1,J) - GAM1
  C2(1,J)=ALP2*ABAR(J) + BET2*A(1,J) - GAM2
  GAM1=CST1*BBAR(J-1)
  GAM2=DH2(1,J)*(CST4*B(3,J) - CST5*B(2,J))

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BET2=-DH2(1,J)*CST3 - ALP2
BRBAR(J)=ALP1*BBAR(J) + BET1*B(1,J) - GAM1
C3(1,J)=ALP2*BBAR(J) + BET2*B(1,J) - GAM2
PX1=2./(DELX(J-1)*DELX(J))
PX2=2./(DELX(J-1)*DINTX(J))
PX3=2./(DELX(J)*DINTX(J))
DO 100 I=2,NN
PR12=(4.*RDST(I)-RDST(I+1)-RDST(I-1))/(RDST(I)*DELR(I-1)*DELR(I))
PR3=(2.*RDST(I)-DELR(I))/(RDST(I)*DELR(I-1)*DINTR(I))
PR4=(2.*RDST(I)+DELR(I-1))/(RDST(I)*DELR(I)*DINTR(I))
ALPIJ=PX1 + PR12
BETIJ=PX2*A(I,J-1) + PX3*A(I,J+1) + PR3*A(I-1,J) + PR4*A(I+1,J)
C2(I,J)=ALPIJ*A(I,J) - BETIJ + (CSTA/DH20(I,J))*C1(I,J)
BETIJ=PX2*B(I,J-1) + PX3*B(I,J+1) + PR3*B(I-1,J) + PR4*B(I+1,J)
C2(I,J)=ALPIJ*B(I,J) - BETIJ - (CSTB/DH2(I,J))*C1(I,J)
100 CONTINUE
WRITE(6,8000)ITERNO,NAME
8000 FORMAT('1RESIDUAL RESULTS AFTER',I5,' ITERATIONS FOR CASE ',A4)
WRITE(6,8010)(ARBAR(J),J=1,NX)
8010 FORMAT('OH2O RESIDUALS IN GAS STREAM='/(1P8E15.5))
CALL ARR360(C2,NR,NX,NRDM,4H H2O)
WRITE(6,8015)(BRBAR(J),J=1,NX)
8015 FORMAT('1H2 RESIDUALS IN GAS STREAM='/(1P8E15.5))
CALL ARR360(C3,NR,NX,NRDM,4H H2 )
RETURN
END

```

```

SUBROUTINE ARR360(B,NRR,NCC,LVV,NAME)
DIMENSION B(1)
DATA COLUMN/4HCOLM/
NR = NRR
NC = NCC
LV = LVV
DO 500 ML = 1,NC,8
MH = ML + 7
IF(NC.GE.MH)GO TO 200
MH=NC
200 MLM1 = (ML-1)*LV
MHM1 = (MH-1)*LV
DO 500 LI = 1,NR,50
NL = LI
NH = NL + 49
IF(NR.GE.NH)GO TO 400
NH=NR
400 WRITE(6,4)NAME
4 FORMAT(1H0,A4)
WRITE(6,1)(COLUMN,J,J=ML,MH)
1 FORMAT(4H0ROW,4X,8(3X,A4,I4,3X))
WRITE(6,3)
3 FORMAT(1H0)
DO 500 L = NL,NH
MML = MLM1 + L
MMH = MHM1 + L
WRITE(6,2)L,(B(J),J=MML,MMH,LV)
500 CONTINUE
2 FORMAT(1H ,I3,4X,1P8E14.5)
RETURN

```

END

SUBROUTINE SOLVER
CALL LIEB2
RETURN
END

```

SUBROUTINE LIEB2
COMMON//A(70,300),B(70,300),ABAR(300),PBAR(300),HFX(300)
COMMON/SLOW/C1(70,300),C2(70,300),C3(70,300),DH20(70,300),
1 DH2(70,300)
COMMON/MESH/NX,NR,DELX(300),DELR(70),RDST(70),DINTX(300),DINTR(70)
COMMON/PARMS/R1,R2,GLENTH,C10,C20,C30,E1,E2,E3,RH20,RH2,RH0,R,MTA,
1 WTB,WTB,UBARX,REN,SCN,DHE,PRESS,XKNUD,PSI
COMMON/LIMITS/NXDIM,NRDIM,MAXCT,NPRINT,NRTEST,ITERNO,ACONV,PCONV,
1 NAME,RELAX
COMMON/MAX/ARMAX,BRMAX,KKKR
C *** SET UP CONSTANTS ***
MM=NX-1
NN=NR-1
CST1=UBARX*R1
CST2=DELR(1)*DINTR(2)
CST3=DELR(1)+DINTR(2)
DELR2=DELR(1)*DELR(1)
DINTR2=DINTR(2)*DINTR(2)
CST4=DELR2/DELR(2)
CST5=DINTR2/DELR(2)
CSTA=RHO*MTA
CSTB=RHO*WTB
C ***
DO 1000 KKK=1,MAXCT
DO 100 J=2,MM
C *** CALCULATE ELEMENT J OF GAS STREAM AND OF ROW 1 OF THE GRAPHITE***
ALP1=CST1 + 2.*HFX(J)*DELX(J-1)
BET1=-2.*HFX(J)*DELX(J-1)
GAM1=CST1*ABAR(J-1)
ALP2=CST2*HFX(J)
BET2=-DH20(1,J)*CST3 - ALP2
GAM2=DH20(1,J)*(CST4*A(3,J) - CST5*A(2,J))
DENOM=ALP1*BET2 - ALP2*BET1
ABAR(J)=(GAM1*BET2 - GAM2*BET1)/DENOM
A(1,J)=(ALP1*GAM2 - ALP2*GAM1)/DENOM
BET2=-DH2(1,J)*CST3 - ALP2
DENOM=ALP1*BET2 - ALP2*BET1
GAM1=CST1*PBAR(J-1)
GAM2=DH2(I,J)*(CST4*B(3,J) - CST5*B(2,J))
PBAR(J)=(GAM1*BET2 - GAM2*BET1)/DENOM
B(1,J)=(ALP1*GAM2 - ALP2*GAM1)/DENOM
C *** - *** - ***
PX1=2./(DELX(J-1)*DELX(J))
PX2=2./(DELX(J-1)*DINTX(J))
PX3=2./(DELX(J)*DINTX(J))
C *** CALCULATE ELEMENT J IN THE GRAPHITE FOR EACH I , I=2,3,...,NM
DO 100 I=2,NM
ASAVE=A(I,J)

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BSAVE=B(I,J)
PR12=(4.*RDST(I)-RDST(I+1)-RDST(I-1))/(RDST(I)*DELR(I-1)*DELR(I))
PR3=(2.*RDST(I)-DELR(I))/(RDST(I)*DELR(I-1)*DINTR(I))
PR4=(2.*RDST(I)+DELR(I-1))/(RDST(I)*DELR(I)*DINTR(I))
ALPIJ=PX1 + PR12
BETIJ=PX2*A(I,J-1) + PX3*A(I,J+1) + PR3*A(I-1,J) + PR4*A(I+1,J)
C2B=1. + C2(I,J)*BSAVE
FCT=(CSTA*C1(I,J))/(DH20(I,J)*(C2B + C3(I,J)*ASAVE))
AVALUE=BETIJ/(ALPIJ + FCT)
A(I,J)=ASAVE + RELAX*(AVALUE - ASAVE)
BETIJ=PX2*B(I,J-1) + PX3*B(I,J+1) + PR3*B(I-1,J) + PR4*B(I+1,J)
GCT=(CSTB*C1(I,J)*A(I,J))/(DH2(I,J)*(C2B + C3(I,J)*A(I,J)))
BVALUE=(BETIJ + GCT)/ALPIJ
B(I,J)=BSAVE + RELAX*(BVALUE - BSAVE)
100 CONTINUE
C *** APPLY THE NO FLUX BOUNDARY CONDITIONS ***
DO 200 I=2,NN
  A(I,1)=A(I,2)
  B(I,1)=B(I,2)
  A(I,NX)=A(I,MM)
  B(I,NX)=B(I,MM)
200 CONTINUE
DO 250 J=2,MM
  A(NR,J)=A(NN,J)
  B(NR,J)=B(NN,J)
250 CONTINUE
C *** END OF ITERATION
ITERM=KKK
C *** TEST FOR CONVERGENCE EVERY NRTEST ITERATIONS ***
IF(MOD(ITERM,NRTEST).NE.0) GO TO 300
ARMAX=0.
BRMAX=0.
KKKR=ITERM
DO 275 J=2,MM
  PX1=2./(DELX(J-1)*DELX(J))
  PX2=2./(DELX(J-1)*DINTX(J))
  PX3=2./(DELX(J)*DINTX(J))
DO 275 I=2,NN
  PR12=(4.*RDST(I)-RDST(I+1)-RDST(I-1))/(RDST(I)*DELR(I-1)*DELR(I))
  PR3=(2.*RDST(I)-DELR(I))/(RDST(I)*DELR(I-1)*DINTR(I))
  PR4=(2.*RDST(I)+DELR(I-1))/(RDST(I)*DELR(I)*DINTR(I))
  FCT=(C1(I,J)*A(I,J))/(1.+C2(I,J)*B(I,J)+C3(I,J)*A(I,J))
  ALPIJ=PX1 + PR12
  BETA1=PX2*A(I,J-1) + PX3*A(I,J+1) + PR3*A(I-1,J) + PR4*A(I+1,J)
  BETA2=PX2*B(I,J-1) + PX3*B(I,J+1) + PR3*B(I-1,J) + PR4*B(I+1,J)
  RESA=ABS(ALPIJ*A(I,J) - BETA1 + (CSTA/DH20(I,J))*FCT)
  RESB=ABS(ALPIJ*B(I,J) - BETA2 - (CSTB/DH2(I,J))*FCT)
  IF(RESA.GT.ARMAX) ARMAX=RESA
  IF(RESB.GT.BRMAX) BRMAX=RESB
275 CONTINUE
C *** ARMAX IS NOW THE MAX. RESIDUE IN A(I,J) AND BRMAX SAME FOR B(I,J)
IF(ARMAX.GT.ACONV) GO TO 300
IF(BRMAX.GT.BCONV) GO TO 300
CALL OUTPUT(ITERM,1)
GO TO 1100
300 IF(KKK.EQ.MAXCT) GO TO 1000
IF(MOD(KKK,NPRINT).EQ.0) CALL OUTPUT(KKK,0)
1000 CONTINUE
CALL OUTPUT(MAXCT,2)

```

```
C *** CALCULATE RESIDUES ***
1100 CALL RESIDU
C *** UPON RETURN OF RESIDU, THE FOLLOWING ARRAYS HAVE NEW MEANINGS...
C   C1(I,J) CONTAINS THE NON-LINEAR TERM  $C1*A/(1.+C2*B+C3*A)$ 
C   C2(I,J) CONTAINS H2O RESIDUE (IE A(I,J) RESIDUE)
C   C3(I,J) CONTAINS H2 RESIDUE (IE B(I,J) RESIDUE) ***
C   CSTC=RHO*WTC
C *** CALCULATE GRAPHITE CORROSION RATE ***
C   DO 1300 I=1,NR
C     DO 1300 J=1,NX
C       A(I,J)=CSTC*C1(I,J)
1300 CONTINUE
C *** A(I,J) NOW CONTAINS CORROSION RATE ***
C   CALL OUTPUT(ITERM,3)
C *** CALCULATE VOLUMETRIC AVERAGE ***
C   ADEN=0.
C   ANUM=0.
C   DO 1410 I=1,NN
C     ROWRAT=0.
C     RMOD=DELR(I)*(RCST(I+1)+RDST(I))
C     ADEN=ADEN + (RMOD*GLENTH)
C     DO 1400 J=1,MM
1400 ROWRAT=ROWRAT + (DELX(J)*A(I,J))
C     ANUM=ANUM + (RMCD*ROWRAT)
1410 CONTINUE
C   AVE=ANUM/ADEN
C   VOL=(3.141593)*ADEN
C   WRITE(6,8010)AVE,VOL
8010 FORMAT('O AVERAGE=',E15.8,' WHERE VOLUME=',E15.8)
C   RETURN
C   END
```