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AN ANALYSIS OF THE METHODS UTILIZED IN OXIDE-3

J. Skalyo, Jr., L.G. Epel and C. Sastre

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HTGR SAFETY DIVISION

**DEPARTMENT OF NUCLEAR ENERGY BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973**

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DEPARTMENT OF NUCLEAR ENERGY
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UPTON, NEW YORK 11973**

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ABSTRACT

OXIDE-3 is an evolving code developed to analyze the transient response of certain state variables of a High Temperature Gas Cooled Reactor (HTGR) during an accident involving the inleakage of steam and/or air into the helium primary coolant system. Primary tasks of the code are to calculate the primary coolant constituents as a function of time, their resultant chemical interaction with the graphite fuel elements, and their possible egress into the containment building. The present report takes a critical look at certain aspects of the problem solving methods implemented in OXIDE-3 and gives estimates of the expected accuracy. Attendant to the latter finding, some of the calculated output may require careful interpretation since programmatic warnings are not given when an accuracy limitation is exceeded. The code has been used at BNL in an investigation to calculate the full power steady state impurity concentrations in the primary coolant system as a function of steam leak rate, steam graphite reaction rate, and the effective diffusion constant of steam in graphite. The results are in reasonable agreement with those obtained from the steady state oxidation code GOPTWO.

1. INTRODUCTION

The OXIDE-3¹ computer code has been written by the General Atomic Company (GA) to analyze the transient response of its prismatic element HTGR following an accidental inleakage of air and/or steam into the helium gas primary coolant stream. It is one of several codes utilized for purposes of design verification and for the safety assessment of the 2000, 3000, or 4000 Mwt power reactor. The present code has evolved from two earlier versions and is concerned with the release of fission products as well as graphite oxidation. Additionally, the time dependent heat and mass diffusion equations are solved for a realistic geometric representation of the prismatic element.

While a comprehensive view of the two earlier code versions is not available, the current version has been extensively described in a Licensing Topical Report (GA-LTR-7)^{1,2} submitted for the review and endorsement of the Nuclear Regulatory Commission Directorate of Licensing. The HTGR Safety Division at Brookhaven National Laboratory has also received a Fortran copy of OXIDE-3 for incorporation into the HTGR Safety Code Library. The modeling of the HTGR, the method of solving the model, and the physical/chemical data base are therefore available for the use of the Safety Division in its investigations.

The primary emphasis of the present report is an evaluation of the methods used in OXIDE-3 to solve the HTGR model. This evaluation will consist in part of a comparison of the exact results obtained for a one-dimensional problem with the approximate results obtained using OXIDE-3 methodology. This report also contains a comparison of results on primary coolant equilibrium compositions as obtained from OXIDE-3 and GOPTWO.³

These impurity concentrations in the coolant were calculated for various constant steam leak rates with the HTGR at full power. These latter results served as scoping data for the Safety Division's experimental work concerning the physical and chemical properties of all materials in the primary coolant system.

2. THE HTGR OXIDE-3 MODEL

The 3000 MWt nuclear power plant heats 3137 pounds of circulating helium gas per second at 725 psia from 640°F to 1370°F.⁴ The heat is removed by 6 steam generators emplaced in the multicavity Prestressed Concrete Reactor Vessel (PCRVR). The central cavity contains the nuclear core with gas mixing plena above and below the graphite elements. A purification system is designed to remove impurities from the coolant at a given rate; and PCRVR overpressure relief valves, which empty into the containment building, are located in the plena.

The salient features of the model are depicted in Figure 1. The 6 steam generators and the 3 Core Auxiliary Cooling Systems (CACS) are modeled as having zero volume; the temperature and amount of helium gas entering the upper plenum are input to the code in the form of tables. This input is accident dependent and is calculated from other codes; e.g. the TAP code.⁵ The purification system is also modeled as a zero volume system taking gas at a given rate from the upper plenum and returning purified helium at another temperature to the upper plenum. The upper plenum, lower plenum, and containment building are assumed to be uniformly mixed volumes, each having a homogeneous temperature and pressure.

The once-through steam generator has a feedwater pressure of 3300

psia and a superheater outlet pressure of 2515 psia; the helium circulators operate at a steam inlet pressure of 902 psia. Both are possible sources of H_2O ingress to the primary coolant system. The rate of ingress is accident dependent and calculated from other codes, e.g. the FLASH code.⁶ The ingress rate of the steam is input to OXIDE-3 in tabular form; while air ingress is either specified at some fixed rate and initiated when the PCRV pressure is less than the pressure in the containment building or it is calculated by a general flow equation for subsonic flow.⁷

The containment building is modeled in OXIDE-3 in a subroutine called BLDG. The latter appears to be a miniversion of the CONTEMP⁸ code in that the containment is modeled as 3 constructs whose main function is to dissipate heat during core depressurization accidents. The transfer of heat from the containment gases is necessary to preserve containment integrity during PCRV depressurization.

The graphite core of the reactor has been modeled into the calculation in great detail since it is only here that the chemical reactions take place and that fission products are released. Though also made of graphite, the radial reflector (both permanent and removable), the core support blocks, and the core support posts are neglected in the code. This may be justified on the basis that a relatively small (compared to the active core) exposed surface area is in contact with the coolant due to these components. This point will be amplified later in this report*.

*Although the surface area of these components is relatively small, the chemical reactivity of the graphite in some of these components can be relatively large.

The core itself is made up of many hexagonal fuel blocks each of which can generate a different amount of power. This power variation occurs both radially and axially in the core and is modeled by taking account of 200 different reference blocks. A radial cross section of the core indicates an element array that is nearly six-fold symmetric with regard to power and exposure history. The program therefore mandates a six-fold symmetry by modeling 1/6 of the core as illustrated in Figure 2; the radial cross section is comprised of 20 different fuel regions. An axial power distribution is permitted and is simulated with 10 different axial elements in a fuel column; all columns in the same fuel region are considered to be the same. The coolant channels in any fuel region are homogenized so that there is no distinction between channels in fuel element, control elements, etc. All fuel elements are modeled as isolated from one another except that thermal and material communication is permitted axially through the coolant channels. As a result, 200 separate calculations are done per programmed time step as the impurities in the coolant stream traverse the core.

A large portion of the fuel element has a regular disposition of fuel and coolant channels. Neglecting the edges of the blocks, this array is shown in Figure 3b and has hexagonal symmetry. The 200 calculations therefore need only to be done on the reduced unit cell shown in Figure 3a. This reduced unit cell is divided into 17 nodes as shown in Figure 4 and a finite difference, time dependent calculation is done for both mass and heat transfer between the nodes.

Each time step during execution of the program therefore involves material and heat balances for 3400 nodal volumes. The code, as received

from GA, generated an object code $\approx 151000_8$ words long that fit well into the 160000_8 word user-available fast memory of the BNL CDC-7600 computer; it is made up of several component subroutines which can be refined as needed or as permitted by advances in computational power.

3. CHEMICAL REACTIONS AND DIFFUSION LENGTHS

As stated earlier, in the code only the nuclear grade core elements made of H451 graphite react with the steam/air. The steam reaction with failed fuel particles is also considered in a calculation of noble gas fission product release. The effect of the metallic steam generators on the chemical balance of the gaseous impurities in the coolant stream are not considered.

The only three reactions considered in the OXIDE-3 code are:

The product gases H_2 and CO are considered inert within the OXIDE-3 code; CO_2 production is neglected. The hydrolysis of failed fuel kernels is calculated on the basis of Eq. (3). The value for X is 2 above 1740°F and increases (forming hydrates) with decreasing temperature; Y is dependent on the type of hydrocarbons produced.^{9,10}

A. Oxidation Reactions and Diffusion Coefficient

The steam-graphite reaction rate is of the Langmuir-Hinshelwood form,¹¹

$$R_{\text{st}} = \frac{K_1 P_{\text{st}} F_b F_c}{1 + K_2 P_{\text{H}}^n + K_3 P_{\text{st}}} \quad (4)$$

where

$$K_1 = 1.069 \times 10^{10} \exp (-40900/RT) \quad \%/hr\text{-}atm$$

$$K_2 = 1.66 \times 10^{-2} \exp (28600/RT) \quad atm^{-0.75}$$

$$K_3 = 5.31 \times 10^{-2} \exp (27500/RT) \quad atm^{-1}$$

$$n = 0.75$$

Here, R_{st} is the percent of graphite reacting per hour, P_{st} and P_H are partial pressures of steam and hydrogen in atm, F_b and F_c are reaction enhancement factors due to burnoff and the presence of the catalytic fission products Sr and Ba, and the K_i are temperature dependent Arrhenius coefficients (with T in $^{\circ}K$ and $R = 1.986 \text{ cal/mole } ^{\circ}K$). The reaction rate of the graphite in the fuel rod matrix is taken to be a factor 10 higher. The derivation of the equation parameters is discussed in GA-LTR-7¹ and by R. P. Wichner.¹²

The denominator of Eq. (4) shows the reaction is inhibited by the presence of either hydrogen or steam. It is of particular interest that the reaction rate tends to a constant at high partial pressures of steam, essentially leveling off at 0.1 atm; i.e.

$$R_{st} \approx \frac{K_1 F_b F_c}{K_3} \quad P_{st} > 0.1 \text{ atm.} \quad (5)$$

The supportive evidence for this functional form is from the work of Giberson and Walker¹³ taken on a different grade of graphite. The data were obtained in the range $3.5 \times 10^{-4} \text{ atm} < P_{st} < 2.5 \times 10^{-2} \text{ atm}$ with a temperature of $1545^{\circ}F$ and hydrogen partial pressure of 0.01 atm. The upper limit of P_{st} in these measurements must be compared with a pressure of 0.88 atm which occurs in an accident involving a guillotine break of a steam generator tube. (This accident is discussed in Reference 1).

The steam ingress accident discussed in GA-LTR-7 is followed by a reactor scram with subsequent cooling of the graphite core to the point where graphite reaction with steam is negligible after ≈ 200 seconds. The steam pressure at this time is 0.76 atm which indicates that the amount of reacted graphite is dependent almost totally on the unverified extrapolated portion of the R_{st} dependence on P_{st} . The amount of graphite oxidized in this accident is very small, but other transients with failure of immediate scram might give larger burnoffs that require greater accuracy than presently available with the oxidation data built into the code.

The oxygen-graphite reaction rate is:

$$R_{ox} = 2.8 \times 10^{10} \exp(-40000/RT) P_{ox} \quad (6)$$

where R_{ox} is the percent of graphite reacting per hour and P_{ox} is the oxygen partial pressure in atm.¹⁴ This latter reaction of oxygen with graphite could occur during an air ingress. The ingress would be into the PCRV through an accident-created opening and would occur following blowdown.

GA data on the fuel hydrolysis of uncoated UC_2 and ThC_2 particles makes possible the estimation of a reaction rate for fuel particles with broken coatings. The rate equation in percent per hour is:

$$R_f = 12.0 \exp(-1755/RT) (P_{st}/0.03)^{0.5} \quad (7)$$

where the order of the reaction, 0.5, is uncertain (data are available only for $P_{st} = 0.03$ atm).¹⁰

The diffusion coefficient for all gases in graphite except hydrogen is given by:

$$Z = 1.06 \times 10^{-6} \frac{T^{1.58}}{P} \quad (8)$$

where Z is in cm^2/sec , T is in $^{\circ}\text{K}$, and P is the total pressure in atm.¹⁵ The value for hydrogen is taken as a factor of 2 times the value found by using Eq. (8). This latter equation, in conjunction with the rate equations, can be used to define diffusion lengths for each of the reactions.

B. Diffusion Length in a Semi-Infinite Medium

The diffusion length, L , is a useful concept which derives from the steady state one-dimensional diffusion equation with concomitant reaction of the diffusing gas in a semi-infinite medium.¹⁶ The diffusion length is the distance into the semi-infinite medium in which gas concentration is reduced by a factor of e . When L is large compared to the distance between mesh points (shown in Figure 4), the finite difference approach will give quite accurate answers for the spatial dependence of the gas concentration; poor accuracy is expected when L is very small compared to the distance between mesh points.

The one-dimensional steady state diffusion equation for a reacting gas in a homogeneous, porous solid is:

$$Z \frac{d^2 C}{dx^2} - K C = 0 \quad (9)$$

where C is the undiluted gas concentration, Z is the effective diffusion coefficient given by Eq. (8), and K is a reaction rate constant obtained by modifying Eqs. (4), (6), and (7); e.g. for steam

$$K_{st} = \rho \frac{RT}{M} \frac{R_{st}}{P_{st}} \quad (10)$$

where ρ is the graphite density, M is the graphite molecular weight, and R is the universal gas constant.

The solution of Eq. (9) in a semi-infinite solid is:

$$C = C_0 \exp (-x/L) \quad (11)$$

where

$$L \equiv \sqrt{\frac{Z}{K}} \quad (12)$$

C. Computed Diffusion Length and OXIDE-3 Mesh Size

Values of L were calculated as a function of temperature and are shown in Figures 5 to 7 for the graphite-steam, graphite-oxygen, and fuel rod-steam reactions, respectively. The relevant mesh spacings (see Figure 4) to be compared are indicated on the figures; these are the widths of mesh volume 2 or mesh volume 3 for the first two reactions and the width of mesh volume 12 or 13 for the last reaction. The fuel rod reaction rate constant consisted of both a graphite-steam reaction (10X that of the graphite web-steam reaction rate) and a fuel hydrolysis reaction which was calculated assuming a 1.6% fuel failure. Figures 5 and 7 show the effect of three different concentrations of hydrogen and steam on the graphite oxidation reaction. The top curve in each figure is calculated using the peak steam concentration that occurs in the steam inleakage problem illustrated in Chapter 9 of GA-LTR-7 (guillotine break of steam generator tube followed by reactor scram). This occurs approximately 24 seconds into the transient while the core is still hot. The lower two curves are for equilibrium impurity concentrations in the primary coolant stream for constant steam leaks of 0.9 lb/hour and 0.09 lb/hour (upper and lower of the two curves, respectively).

It is apparent that any given mesh may give inaccurate answers if the temperature is high enough. The knee in the curve of Figure 7 which

occurs near 1200°F, is the boundary between the temperature at which fuel hydrolysis dominates and the temperature at which the graphite-steam reaction dominates. After a scram following an accident, fuel hydrolysis will continue to take place when the temperature falls below ≈1000°F. The high temperature part of the curves in Figure 7 are only slightly shifted from the curves of Figure 5. The temperature at which the mesh spacing would be inadequate in the fuel rod occurs when the web graphite near the coolant channel surface is getting most of the steam; hence, relatively little steam reaches the fuel rod and the attendant error due to the mesh size is of no consequence. At the low temperatures where the fuel hydrolysis dominates and the web graphite offers no protection, the mesh size in the fuel rod is more than adequate.

As seen from Figure 5, the temperature at which the mesh spacing for volume 3 of the unit cell is equal to the diffusion length depends on the accident scenario postulated. For the transient problem of GA-LTR-7 this temperature is about 2110°F while for the 0.9 lb/hour and 0.09 lb/hour constant steam leak rate problems the corresponding temperatures are 1690°F and 1570°F, respectively. Hence the mesh spacing is adequate for the transient problem in GA-LTR-7 (core temperatures in that scenario fall rapidly due to proper scram initiation and continuous cooling), but inadequate for the hotter fuel elements during the constant steam leak problems.

As with the steam-graphite reaction, significant rates of graphite-oxygen reaction occur only at the coolant channel surface. Thus in Figure 6 the mesh spacing corresponding to volumes 2 and 3 of the unit cell are shown, together with the diffusion lengths for the graphite-oxygen reaction

at 2 and 50 atmospheres helium pressure as a function of temperature. If an air ingress accident (following depressurization) is considered, the mesh spacing for volume 3, for example, is larger than the diffusion length at temperatures above 1520°F. Since a large portion of the core is expected to exceed this temperature following such an accident, the mesh spacing appears inadequate for such scenarios.

4. FINITE DIFFERENCE METHODS

The diffusion equation for heat transfer and the diffusion equation with reaction for the various gases of the primary coolant cannot be solved in closed form as a function of time and position for the geometry of the core. An implicit finite difference method¹⁷ is employed in OXIDE-3 to solve the differential equations for the two-dimensional geometry of Figure 4. The use of the implicit method allows a stable solution to be obtained when using a large time step; however, care must be exercised in that a stable solution need not necessarily be an accurate one.

The 10 axial layers of the core are solved sequentially; the various impurity gases which are added or subtracted from the coolant stream in a particular layer are accounted for and the appropriate coolant composition entering the next layer is established. The coolant composition at each layer serves as a boundary condition for the solution of the 17 node problem. While the individual calculations of the difference equations for the geometry of Figure 4 are stable, the procedure of sequentially solving the 10 different layers can give wildly oscillating and incorrect results for the partial pressures of the impurity gases in the upper and lower plena when too large a time step is used.

The magnitude of the time step is chosen by the program user in the form of input data for a particular problem and can be varied as a function of time. While an experienced programmer might be able to choose a proper time step to ensure problem accuracy, this is by no means assured. The oscillatory behavior of some output parameters of the code due to an overly large time step would probably be noticed; however, a slowly varying but increasingly inaccurate result would most likely go unnoticed. The dependence of the size of the error on the time step is a complicated subject. Some empirical results will be illustrated in Section 5 where a few sample problems, which were calculated using the OXIDE-3 code, are discussed.

A. Implicit and Explicit Techniques

The time dependent, one-dimensional diffusion equation with chemical depletion is given by Eq. (13). This differential equation can be cast into several finite difference forms (see Figure 8).

$$\frac{\partial C}{\partial t} = Z \frac{\partial^2 C}{\partial X^2} - K C \quad (13)$$

The fully explicit form of the equivalent finite difference equation is:

$$\frac{C_{i,n} - C_{i,n-1}}{t_n - t_{n-1}} = \frac{Z}{\Delta^2} (C_{i-1,n-1} - 2C_{i,n-1} + C_{i+1,n-1}) - K C_{i,n-1} \quad (14)$$

where Δ is the spacing, the first index is spatial, and the second index is temporal. The fully implicit form¹⁸ of Eq. (13) on the other hand is

$$\frac{C_{i,n} - C_{i,n-1}}{t_n - t_{n-1}} = \frac{Z}{\Delta^2} (C_{i-1,n} - 2C_{i,n} + C_{i+1,n}) - K C_{i,n} \quad (15)$$

Various combinations of Eqs. (14) and (15) are also possible in which the latter is multiplied by θ , where $0 \leq \theta \leq 1$ and combined with $(1-\theta)$

times the former. For different values of θ the various combinations lead to different accuracies and different conditions of stability, depending on several other choices available to the analyst. Some of these choices deal with

- (a) the nature and specification of the boundary conditions
- (b) the manner in which the nodal points are distributed
(e.g. starting on the boundary versus the interior of the conducting solid)
- (c) the geometry of the actual problem
- (d) the order of the dimensions (i.e. whether one-, two-, or three-dimensional)
- (e) the presence of lower order terms (such as the depletion terms in Eq. [13]).

These matters are quite complex and outside the scope of the present study.¹⁷ Suffice it to say that several techniques were studied and it was found that the method adopted in OXIDE-3, i.e. the fully implicit method, has many benefits. The error with $\theta=1$ is $O(\Delta t) + O(\Delta x)^2$ and the stability is guaranteed. A very popular alternative is the Crank-Nicholson method¹⁹ ($\theta=\frac{1}{2}$) which is also always stable and additionally has an error $O(\Delta t)^2 + O(\Delta x)^2$. However, this technique led to an oscillatory solution for certain combinations of choices of nodal point distribution and boundary conditions. In all of the following, the results discussed are based on the fully implicit mode of solution.

B. Errors Inherent in Finite Difference Techniques

The exact solution of Eq. (13) for the one-dimensional semi-infinite solid with the time independent boundary condition $C(0) = C_0$ and

with an initial zero mass concentration is:^{16,20}

$$\frac{C}{C_0} = \frac{1}{2} \exp(-x \sqrt{K/Z}) \operatorname{erfc}\left(\frac{x}{2\sqrt{Zt}} - \sqrt{Kt}\right) + \frac{1}{2} \exp(x \sqrt{K/Z}) \operatorname{erfc}\left(\frac{x}{2\sqrt{Zt}} + \sqrt{Kt}\right) \quad (15)$$

The solution was obtained assuming K and Z are spatially independent. For the purpose of investigating the accuracy of the finite difference method, this is acceptable since most interest derives when the temperature is high and thus the mass concentration of the steam or oxygen is limited to the vicinity of the coolant channel.

There are several comparisons relating to accuracy which can be made; however, it was decided to use the rate of graphite oxidation as the basis for such comparisons. For this purpose, the mass flux at the solid-gas interface is obtained from Eq. (16) as

$$R = -Z \left(\frac{\partial C}{\partial x} \right)_{x=0} = C_0 \sqrt{ZK} \left[\operatorname{erf} \sqrt{Kt} + \frac{e^{-Kt}}{\sqrt{\pi Kt}} \right] \quad (17)$$

The time constant for approach to equilibrium of Eq. (16) is on the order of $\tau = K^{-1}$ for values of x that are on the order of $\sqrt{Z/K}$ or less; the same time constant holds for R. For values of $t \gg \tau$, Eqs. (16) and (17) tend to the time independent solution of Eq. (13); i.e.

$$\frac{C}{C_0} \approx \exp(-\sqrt{K/Z} x) \quad (18)$$

and

$$R \approx C_0 \sqrt{ZK} \quad (19)$$

The values of τ for the graphite-oxygen reaction, for example, are 2.0×10^{-1} , 3.7×10^{-3} and 2.6×10^{-4} seconds at 1500° , 2000° , and 2500°F , respectively. Thus, for times greater than about a second, the time independent solutions, Eqs. (18) and (19), are suitable approximations

to use for concentration profiles and mass flux. (When $t = K^{-1}$ the difference between Eqs. [17] and [19] is only 5%).

A number of finite difference calculations were done and compared to the results of the exact solution (Eq. [19]). The results are quite general and are not particular to any given chemical reaction considered in OXIDE-3. In the following paragraphs, a particular application will be illustrated for the graphite-oxygen reaction, and additional general results will be given for varying the surface film mass transfer coefficient and for an alternative nodal placement.

1. Effect of Mesh Size

The semi-infinite solid was represented by 100 nodal points and the simulations were carried to times equal to 100τ using time steps of 0.1τ . Figure 9 shows the results of varying the mesh spacing Δ (made dimensionless by dividing by the diffusion length) for isothermal conditions through the solid. It is seen from this figure that the mass loss rate is increasingly underestimated by the finite difference method as Δ/L increases. When the mesh spacing is about as large as the diffusion length this underestimate amounts to roughly 10%.

The aforesaid calculations are general and it is desirable to particularize them to the OXIDE-3 reactions. The oxygen-graphite reaction is chosen for illustration since the complicating effects of inhibiting environments need not be considered; e.g. inhibition effects are included in the Langmuir-Hinshelwood rate equation for steam-graphite reaction.

The oxygen-graphite reactant length is shown in Figure 6 as a function of temperature. Since Z is inversely proportional to pressure, the two curves are illustrative of the two extremes that might be en-

countered; under depressurization conditions the initial blowdown reduces PCRV internal pressures to ~ 2 atmospheres. The widths of the mesh volumes 2 and 3 are 0.037 inch and 0.029 inch, respectively; these lengths are also marked on Figure 6. At 2 atmospheres, one has reached the condition of $\Delta = L$ at 1470°F giving an underestimation of burnoff of $\sim 10\%$. During the depressurization transient, a large fraction of the core is at considerably higher temperatures; errors greater than 10% should therefore be encountered for many of the fuel blocks.

The ratio of actual to finite difference method mass loss rates for the oxygen-graphite reaction is shown in Figure 10 as a function of temperature, pressure, and spatial widths of the surface nodal volume (these latter are fixed in OXIDE-3 as shown in Figure 4).

It is noted that a similar underestimation of graphite burn-off accrues to the steam-graphite reaction calculation also. The mesh spacing for the steam-graphite reaction should be adequate for transient studies with scram which give a quickly decreasing temperature for the core. It is, however, evident that any given mesh will give answers which depart from reality in an increasing manner as the temperature rises.

It is shown in Figure 6 that the L for the oxygen-graphite reaction is falling rapidly with temperature. It is difficult to choose a mesh arrangement without choosing a limit of acceptable error and thence an upper limit to the temperature of the transient. An alternative nodal placement which would overestimate burnoff is discussed in Part 3 of this subsection.

ii. Effect of Finite Mass Transfer Coefficient

The effect of considering a finite mass transfer coefficient has been investigated in a similar fashion. In such a situation the

boundary condition at the graphite-coolant interface becomes

$$-Z \left(\frac{\partial C}{\partial x} \right)_{x=0} = H [C_o - C(0)] \quad (20)$$

where H is the mass transfer coefficient, C_o is the free stream reactant concentration, and $C(0)$ is the reactant concentration in the solid at the interface. The mass flux for this boundary condition is

$$R(H) = \frac{H C_o \sqrt{ZK}}{H + \sqrt{ZK}} \quad (21)$$

In this comparison of the closed form solution with that obtained by finite difference, the mesh size was fixed at $\Delta = 4L$ and the dimensionless mass transfer coefficient, $H/\sqrt{ZK}$, was varied. The results of this comparison are shown in Figure 11. As seen from this figure, for values of $H/\sqrt{ZK}$ greater than about 20 a further increase in this parameter does not change the mass loss rate appreciably. For HTGR conditions this corresponds to coolant flow rates greater than ≈ 10 pounds/second. Thus, conclusions for the graphite-oxygen reaction drawn from Figure 10, which is based on an infinite mass transfer coefficient, are appropriate to any case for which OXIDE-3 should be used.

iii. Effect of Nodal Placement

Although the placement of nodal points illustrated in Figures 9 and 11 lead to underestimates of graphite burnoff, the opposite effect can be achieved by placing the first nodal point on the surface, rather than in the interior of the solid. This is shown in Figure 12, which is the counterpart of Figure 9 (infinite mass transfer coefficient). Similarly, in Figure 13, which is the counterpart of Figure 11, it is seen that the graphite burnoff is consistently overestimated. The OXIDE-3 code, however, does not have this option (of intentionally overestimating the

burnoff) available to the user.

5. OXIDE-3 CALCULATIONS

The OXIDE-3 code received from GA is the Univac 1108 version. It is written in Fortran V and was converted to run on the Brookhaven National Laboratory CDC 7600 by T. Wang of the Applied Mathematics Department at BNL. Since no user's manual exists, he has also supplied an input data deck description by analyzing the Fortran coding of the OXIDE-3 input. This description is given in Appendix A. Some of the input relates to the possible interruption of a problem due to exceeding computation time limits before the calculation is completed and saving relevant restart data on tape for subsequent calculation. Due to the higher calculational speed of the CDC 7600, interrupt/restart capabilities were not included in the BNL version (such coding is usually dependent upon facility restrictions particular to a given computing system).

An updated version of OXIDE-3 was obtained from GA in May, 1975 giving listings of an input data deck, the Fortran coding, and the results of the Univac 1108 execution of the problem. The Fortran was checked several times line by line and logic changes from the Fortran V in use on the Univac 1108 to the Fortran IV in use at BNL were verified. A comparison of the Univac 1108 results with the CDC 7600 results showed agreement to within expected roundoff errors; the roundoff is due to the Univac 1108 having a 36 bit word while the CDC 7600 has a 60 bit word.

Following verification of proper program execution by comparison with the GA output listing, several steady state problems were calculated. Although OXIDE-3 is primarily a transient code, the steady state results are valuable in that comparisons could be made with the steady state code,

GOPTWO. The steady state problems also were simpler physical situations which were more amenable to Fortran debugging and consistency checks. Some of the problems involved calculating the equilibrium impurity concentrations in the primary coolant stream resulting from various constant steam leak rates while the HTGR operates at full power. These impurity conditions in the primary coolant stream served as scoping data for the design of loop experiments which were under construction at BNL. Additional steady state problems were concerned with calculating the equilibrium contaminant concentrations as a function of the graphite-steam reaction rate and as a function of the diffusion constant of steam in graphite.

OXIDE-3 is written so that the time step for the calculation is fixed during input in each of six time regions extending over the entirety of the transient. This was not felt to be a feasible method for running OXIDE-3 in a calculation to equilibrium, which requires following a time history of 100k-200k seconds (the longest physical time constant in the problem is the purification process, 36k seconds). The program was therefore modified to include an internally calculated variable time step feature based on assuring the absence of numerical oscillations in the solution (Appendix B).

The calculations to steady state conditions which are described herein are directly related to the sample problem shown in Section 9 of GA-LTR-7 (GA-A12493)¹ for a 3000 MWt reactor; the input data deck for the latter is given as an example in Appendix A. The main differences are that in the steady state calculations the time step is automatically varied, the reactor is not scrammed, a constant steam leak rate is started at $t=0$, the helium cold-leg temperature is fixed at $T=640^{\circ}\text{F}$, and the helium

flow rate is fixed at 3066 lb/second.

A. Effect of Leak Rate, Reaction Rate, and Diffusion Coefficient
on Impurity Levels

In the first of three series of calculations the steam leak rate was fixed at 0.009, 0.09, and 0.9 lb/hour. For the case of $L = 0.09$ lb/hour (a value that results in 10 ppmv of total oxidants at equilibrium), the partial pressure of steam (psia) computed by OXIDE-3 in the upper and lower plena was found to be accurately represented for $0 < t < 200,000$ seconds by

$$P_{\text{upper}} = [3.50 - 2.29 \exp(-0.0072 t) - 1.17 \exp(-0.000025 t)] \times 10^{-4} \quad (22)$$

$$P_{\text{lower}} = [3.49 - 2.28 \exp(-0.0070 t) - 1.17 \exp(-0.000025 t)] \times 10^{-4} \quad (23)$$

where t is in seconds. These formulas result from nonlinear least squares fits to the numerically calculated steam concentration. It is evident that the upper and lower plena are subjected to the same steam partial pressure to within the standard deviation associated with the fits (the neglect of a pressure drop across the core is built into the code). The hydrogen and carbon monoxide partial pressures are given as a function of time by

$$P_{\text{H}} = [6.68 + 0.0682 \exp(-0.00138 t) - 6.75 \exp(-0.000016 t)] \times 10^{-3} \quad (24)$$

$$P_{\text{CO}} = [6.67 + 0.167 \exp(-0.00052 t) - 6.85 \exp(-0.000021 t)] \times 10^{-3} \quad (25)$$

where the partial pressures are in psia. A justification for the use of the sum of two exponential terms to fit the OXIDE-3 results is given in Appendix C.

The time-dependent concentrations for steam, hydrogen, carbon monoxide, and the $\text{CO}/\text{H}_2\text{O}$ ratio are illustrated in Figures 14-17, respectively,

for each of the three leak rates. Note that the scale multipliers apply to Figures 14-16 only. It is evident from these figures that there is no linear relationship between concentration and leak rate. For example, the dependence of the equilibrium partial pressure of steam on the leak rate is

$$P_{St} \text{ (psia)} \approx 0.0064 L^{1.18} \quad (26)$$

where L is in pounds per hour.

The second series of calculations varied the graphite-steam reaction rate while the steam ingress rate was held constant at 0.09 lb/hour. The reaction rate obtained from the Langmuir-Hinshelwood equation was multiplied by a factor, F, which had values of 100, 1, and 0.01 for this series. These results are shown in Figures 18-21 for steam, hydrogen, carbon monoxide, and the CO/H₂O ratio, respectively (note there are no scale multipliers on these curves). In the OXIDE-3 sample problem the graphite fuel rod reaction rate is multiplied by another factor of 10 (supplied as input). This factor was also used in this series. For the case where the graphite-steam reaction rate is multiplied by 0.01, it was apparent that steam could penetrate to the fuel rod and hydrolyze the broken fuel pellets (a Fortran error in the version received from GA allowed all the fuel to hydrolyze rather than the more appropriate ~1.6% broken fuel pellets).

In the third series of calculations the effective diffusion constant Z, where

$$Z = \left(\frac{\epsilon}{q}\right) D \quad (27)$$

was varied. The porosity-tortuosity factor $\frac{\epsilon}{q}$ is a property of the type of graphite and D is the free gas diffusion constant of the impurity gas in helium. In this study ϵ/q was varied from 10^{-3} to 10^{-2} (GA-LTR-7 suggests 10^{-2}) and the impurity concentrations were obtained for a fixed steam ingress of 0.09 lb/hour. The results of the OXIDE-3 calculations for three values of ϵ/q are shown in Figures 22 to 25 for steam, hydrogen, carbon monoxide, and CO/H₂O ratio, respectively.

All three series of equilibrium calculations have been fit to the double exponential form to predict the partial pressure of steam, hydrogen, or carbon monoxide; viz:

$$P = P_o - P_1 \exp(-\lambda_1 t) - P_2 \exp(-\lambda_2 t) \quad (28)$$

where P_1 is in mpsia and t is in seconds. The values of P_1 and λ_1 are shown in Tables 1-3 for variations in steam ingress rate, steam-graphite reaction rate, and diffusion rate, respectively.

B. Mass Conservation and OXIDE-3 Results

Excluding steam-fuel reactions, the chemical reaction equations incorporated in OXIDE-3 dictate that for every mole of steam reacted there must be one mole of carbon monoxide generated. If L is the steam ingress rate in moles/hour and K_p is the purification factor (hr^{-1}), then at equilibrium simple mass conservation demands that

$$L = K_p (M_{\text{St}} + M_{\text{CO}}) \quad (29)$$

where M is in moles of constituent (see Appendix C).

This relationship can be used to compare with the values of P_o given in Tables 1-3 (which were generated utilizing a purification factor

of 0.1 hr^{-1}). For example, for a steam ingress rate of 0.09 lb/hour (0.005 mole/hour) and a purification factor of 0.1 hr^{-1} , $M_{\text{St}} + M_{\text{CO}}$ is 0.05 mole .

This amount of contaminant in a helium inventory of 4991 moles , which is at a total pressure of 718.2 psia , is equivalent to a partial pressure of 7.19 mpsia . The equilibrium partial pressures for steam plus carbon monoxide found from Table 3 are 7.16 , 7.07 , and 7.02 mpsia for ϵ/q equal to 10^{-3} , 5×10^{-3} , and 10^{-2} , respectively. The agreement is excellent and the small discrepancy increases with increasing values of ϵ/q . Since the fuel hydrolysis reaction takes no account of any gas formation, the slight disagreement may be an indication that the amount of fuel hydrolysis increases as Z increases, as expected.

The sensitivity of agreement between Eq. (29) and the OXIDE-3 code to a variation in the steam-graphite reaction rate is found from Table 2 where values for $P_{\text{St}} + P_{\text{CO}}$ of 5.27 , 7.02 , and 7.24 mpsia are obtained at steady state for values of F equal to 0.01 , 1.0 , and 100.0 , respectively. The agreement for F values 1.0 and 100.0 is again excellent while the deviation found for $F = 0.01$ is once more attributed to the occurrence of fuel hydrolysis (the lower graphite reaction rate tends not to protect the fuel).

The results given in Table 1 for the equilibrium value of $P_{\text{St}} + P_{\text{CO}}$ for leak rates 0.009 , 0.09 , and 0.9 lb/hour are 0.710 , 7.02 , and 69.0 mpsia , respectively. The increasing discrepancy with the values computed with Eq. (29) as ingress rates increase can again be attributed to fuel hydrolysis. The tendency for the fuel to hydrolyze is thus noted to increase with higher diffusion, lower graphite reaction rate, and higher ingress rate.

C. Comparison with Example in GA-LTR-7

Two other transient problems have been calculated for code verification purposes. These are the problem examples given in the OXIDE-3 report GA-LTR-7¹ and in its associated Amendment I.² The first is a steam break accident with reactor scram and a total inleakage of 1626 pounds of steam, while the second involves an air ingress accident which follows the depressurization of the PCRV through a cold-leg penetration of 100 in². The input data for the first problem is given in the example of Appendix A. The air ingress for the second problem is assumed to occur at a fixed rate of 0.3 lb/second whenever the pressure in the PCRV is below the containment building pressure.

The steam break problem was run and gave excellent numerical agreement with the results illustrated in GA-LTR-7. The problem was then repeated using the automatic time stepping feature discussed in Appendix B and extended to obtain a history up to 200 ksec. The point of this latter calculation was to confirm an intuitive feeling that the code should show hydrolysis of a substantial fraction of the failed fuel and thence a release of noble gas activity. The problem is very similar to one discussed in GA-A13171²¹ that implies a noble gas activity release leveling off at $\sim 2 \times 10^5$ Ci near 1400 seconds. This leveling off is unexpected since the steam cannot be purged from the PCRV by the purification system until ~ 200 ksec and the reduction in core temperature due to reactor scram eliminates the steam-graphite gettering process, thus providing substantial water for fuel hydrolysis.

The long-time behavior for the steam, hydrogen, and carbon monoxide is shown in Figures 26-28, respectively, for the first problem.

The results are as expected in that the purification system eventually cleans the primary coolant stream. The steam-graphite reaction is very slow after 10 ksec due to the scram-induced reduction of the core temperature. The fraction of fuel hydrolyzed, as a function of time, is shown in Figure 29, indicating an asymptotic value of about 30%. This result was a first indication that a coding error existed in the OXIDE-3 version received at BNL since the average failed fuel fraction in the core was only 1.58%. The error was subsequently verified and corrected in the coding. Although the fraction of fuel hydrolyzed is printed as output, it is not used by the code in computing the noble gas release. The latter was calculated and reasonable agreement was obtained with Figure 5-10 in GA-A13171²¹ up to 1400 seconds, the limit of the calculation of Barsell and Perroomian. However, the current result does not concur with their statement which indicates a leveling off of release at this time at a value of 2×10^5 Ci. The current calculation results in a noble gas release of 3.3×10^6 Ci at 200 ksec. Since the noble gas inventory for the entire core is 1.065×10^9 Ci, this release represents 0.31% of core inventory ($\approx 20\%$ of the failed fuel fraction).

When the problem was run without the automatic time step option it was found that only ~ 1 mole of graphite was oxidized, 90% of this taking place in the first 150 seconds of the transient. The algorithm utilizing automatic time step selection resulted in about half as much graphite loss as when the time step in GA-LTR-7 was used. Since such a small amount of graphite is involved (compared to the 1626 pounds of steam that enters the core during the transient) the factor of two discrepancy cannot be resolved from any of the other data printed in the OXIDE-3 output.

D. Comparison with Example in Amendment 1

The problem in Amendment 1 (air ingress following depressurization) was run at BNL and substantial agreement with GA results was found. However, mass balances pointed to a Fortran coding error in the program. For example, the amount of oxygen that had entered the PCRV up to any time did not balance properly with the amount of CO produced plus unreacted oxygen. Also, there was a discrepancy between the number of moles of graphite oxidized and the number of moles of carbon monoxide produced. These inconsistencies were traced to a coding error in which the fact that 1 mole of oxygen results in the evolution of 2 moles of carbon monoxide was inadvertently disregarded.

The problem in Amendment 1 was run four times to ascertain the effects of the above error, the choice of time step, and the nodal point arrangement in the unit cell. Table 4 summarizes these results at 1500 seconds into the transient. Case I refers to the problem as computed in Amendment 1, Case II incorporates the correction for molar balancing, Case III is a repeat of Case II but with one-quarter the time step used previously, and Case IV is the same as Case III except that the mesh configuration shown in Figure 30 was utilized. This configuration was justified on the basis of independent heat and mass transfer calculations in the geometry of the unit cell which indicated that the transport problem is essentially one-dimensional near the coolant channel.^{22,23} Comparison of columns A and D in Table 4 indicates that correcting the Fortran error caused the discrepancy in oxygen balance to be reduced from 59% (Case I) to 33% (Case II). Reducing the time step (Case III) helped to lower this error to 14%. Rearranging the nodes did not serve to reduce the error any

further.

Note that when the time step is reduced (Case III) less air enters the PCRV (column A). This is due to the different PCRV pressure history achieved as the time step is made smaller.

It is also interesting to compare columns C and E in Table 4. The improvement obtained in balancing the carbon monoxide generated against the graphite burned in going from Case I to Case II, etc. parallels the experience on oxygen balances. However, even with a smaller time step, a 14% discrepancy remained in the balance and was never completely resolved.

E. Containment Building Gas Composition Following Depressurization

One of the accidents analyzed in GA-A13171 involving the possible generation of combustibles following depressurization of the PCRV is similar to the Amendment 1 problem discussed above. The result of the analysis in Amendment 1 indicated that the egressing gases would be comprised of a 3% CO in helium mixture 6900 seconds into the depressurization*. This is the value shown in Figure 31, taken from GA-A13171 (see the intersection of the solid line with the base of the triangle). The solid line indicates the possible compositions a bubble of gas egressing from the PCRV could assume as it became diluted with the containment building atmosphere of roughly 50% air - 50% helium. Even if the carbon monoxide concentration of the egressing gas were doubled, to compensate for the coding error discussed in Section D, the locus of mixtures would not enter the flammable region illustrated in Figure 31.

*At 10,000 seconds into the depressurization the egressing mixture is enriched to 4.1% carbon monoxide.

A variant of this depressurization-air ingress accident is one considered in the class 9 category. In this variation it is assumed that a steam generator tube breaks, concomitant with the depressurization, resulting in the ingress of 3179 pounds of steam. The hydrogen and carbon monoxide generated from the graphite-steam reaction are seen to reach ~25% before leaving the PCRV (see the intersection of the dashed line with the base of the triangle) according to GA-A13171, thus again skirting the flammable region. However, correction of the coding error, together with the use of a smaller time step, could bring the locus of mixtures possible from this scenario within the flammability region.

This is so without consideration of layering effects. If the hot helium leaving the PCRV were to layer at the top of the containment building, the air-helium mixture at the top of the PCRV would be richer in air than the 50% air - 50% helium mixture obtained by assuming complete mixing. In Figure 31 this effect is simulated by moving the point on the right leg of the triangle up toward the top vertex. The locus of combustible gas-containment gas mixtures would thus move more solidly through the flammable region for the combined steam break, air-ingress accident. Layering appears to require an inoperative containment air purification and cleanup system.

The concentration of egressing combustibles is dependent on the air ingress rate (air is ingressed during a time step only when the CV pressure is greater than the PCRV plenum pressure). Two methods of calculating air ingress are available to the user:

1. A constant rate of air ingress can be implemented in the input card deck (12th card set in Appendix A).

2. If the constant air ingress rate of the 12th card set is set to 0.0, then subsonic flow equations for an orifice are implemented within the code to calculate the rate with which the uniformly mixed CV atmosphere ingresses the PCR.V.

A comparison between ~~these two methods~~, for the problem in Amendment 1 and using various time steps is shown in Table 5 for the time points 500 and 1500 seconds into the transient. Method 1 uses a rate suggested in GASSAR⁴ and need not agree precisely with Method 2. The variability of the results illustrates their sensitivity to choice of time step in the OXIDE-3 algorithms.

6. COMPARISON WITH GOPTWO

The GOPTWO (Graphite Oxidation Program-2) code is a revised version of GOP, the latter code having been written by R. C. Giberson and G. L. Tingey at BNWL.³ Although there is no documentation on GOPTWO, the short description of GOP in Reference 3 and a report on its predecessor yield some insight into the physical problem that GOPTWO solves and the algorithms that it uses. These references together with a Fortran card deck supplied by W. C. Morgan made it possible to compare certain OXIDE-3 results with those generated by GOPTWO. Although there are many basic differences in the intent and uses of the GOPTWO code vis-a-vis the OXIDE-3 code, there is also a common area in which the two codes can be applied. Specifically, although GOPTWO considers several reactions between various gases and between gases and graphite, the only reaction common to both codes is the steam-graphite reaction. The input to the codes can be adjusted so that the diffusion constants, reaction rates, etc. are the same for both.

The other input to the two codes was made as internally consistent as the input formats allow. Where the modeling in the two codes is so different that completely different data are called for, every attempt was made to make the input compatible between the two. Even so, it was impossible to guarantee that each code was run precisely under the same conditions or with exactly the same geometry and values of variables. From an engineering point of view, however, the two codes were made to solve a very similar set of problems.

The problems addressed here concern steady state operation at full reactor power and they focus on the graphite-steam reaction assuming a constant steam ingress rate. This is exactly the series of problems considered in Section 5.A and the results of interest are the values of P_o given in Tables 1-3 (i.e. the steady state concentrations of the impurities). Thus, the same kind of parametric study was done utilizing the GOPTWO code as had been done with the OXIDE-3 code, varying the leak rate, reaction rate, and diffusion constant. The results of the comparison are summarized in Tables 6 and 7.

A. Nominal Case and Variations About Nominal

The nominal case ($F^* = 1$, $\epsilon/q = 0.01$, $L = 0.09$ lb/sec) resulted in good agreement (35% difference in steam concentration and 0.4% difference in carbon monoxide concentration) between the two codes. The 35% difference, it must be remembered, is between relatively small concentrations; the carbon monoxide concentrations, which agree quite well between the two codes, are at a level ~ 15 times as high as the steam

*F is the ratio of the steam-graphite reaction rate used in a particular run to the nominal value (see Eq. [4]) of this reaction rate.

concentrations. It is noteworthy that the larger discrepancies between computed steam concentrations occur when either the ingress rate is large, the diffusion coefficient is high, or the reaction rate is low. All three of these situations tend to allow more steam to reach the fuel stick. The OXIDE-3 code considers the fuel hydrolysis reaction whereas this is neglected in the GOPTWO code.

GOPTWO is a very fast running code for which equilibrium concentrations can be easily obtained while varying some parameters over a wide range. In particular, by holding the graphite-water reaction rate constant at the nominal value, the effect of diffusion coefficient and water ingress rate could be observed by varying these on both sides of their nominal values. The results of these calculations are shown in Figure 32. Similarly, holding the diffusion coefficient constant, allowed for an appreciation of the effect of varying the graphite-water reaction rate. These results are shown in Figure 33.

An interesting result of these calculations is that, except for roughly the last upper half decade of the steam ingress range, the effect of increasing (or decreasing) the graphite-steam reaction rate is the same as increasing (or decreasing) the diffusion coefficient of water in graphite. This result is consistent with the argument that the overall reaction rate should be proportional to the square root of the product of the volumetric reaction rate and the effective diffusion coefficient (see Eq. [19]). Thus, as shown by comparing Figure 32 with Figure 33, the equilibrium concentrations of water vapor and carbon monoxide are insensitive to which of the two parameters in Eq. (19) are varied.

B. Effect of Mass Transfer Coefficient

In the GOPTWO program the mass transfer coefficient in the coolant channels is assumed to be infinite, i.e. the concentration of steam in the free stream of the coolant channels is the same as in the pores of the graphite at the solid-gas interface. On the other hand, OXIDE-3 calculates a finite mass transfer coefficient and thus a discrepancy can exist between the two codes concerning graphite-steam reaction rates. To study the effect that the mass transfer coefficient might have on overall results, the GOPTWO code was modified as described in Appendix D.

Figure 34 shows the results of incorporating the effects of the mass transfer coefficient into GOPTWO. The ingress rate, diffusion coefficient, and graphite-steam reaction rate used in the calculation were the "nominal values;" i.e. 0.09 lb/hr, Eq. (8) and Eq. (4), respectively. It is evident that a mass transfer coefficient of about 1 cm/second is essentially equivalent to an infinite value at the particular operating conditions modeled in this example. Since the mass transfer coefficient at nominal HTGR flow and power conditions is about 10 cm/second, the assumption concerning an infinite value for this parameter, that the original GOPTWO was based on, is quite justified. Thus the differences between the OXIDE-3 and GOPTWO results at (or near) full flow conditions are not due to the different ways the two codes model film resistance.

7. SUMMARY

The OXIDE-3 code is operational on the Brookhaven CDC 7600 and can be used in the analysis of certain air or steam ingress accidents. The

code was validated using a GA listing of input, output, and Fortran coding. The code was run for several steady state problems involving constant steam ingress at full operating power. The results were compared with results for similar problems obtained from the GOPTWO code. Taking into consideration the basic differences between the two codes, the agreement was very good.

The program has been analyzed with respect to results obtained for a limited number of problems (e.g. steam ingress with and without scram, air and air/steam ingress following depressurization). This analysis has focused on the accuracy that can be expected from the method of solution used in OXIDE-3 and on the models themselves. The adequacy of the model and the accuracy of the solution depend strongly on the nature of the accident scenario under investigation and on the particular question that is being addressed. For example, the sample problem in GA-LTR-7 (steam ingress with scram) yields an inaccurate result with regard to the amount of core graphite that is oxidized. However, the total amount is insignificant and so the inaccuracy is inconsequential for that case.

In what follows, a number of weaknesses in the code are briefly summarized. The effect of these will depend on the particular accident being modeled and the questions that are being asked with respect to that scenario.

Additional Reactive Graphites

As mentioned in the Introduction, the existence of the core support blocks is not accounted for in the OXIDE-3 code. One error resulting from their omission pertains to the thermal inertia that these components represent and the effect that they would have during any temperature

transient. Perhaps more important, however, is the effect that these relatively active graphites can have on the primary coolant impurity level. Assuming that it is the graphite in the lower third of the active core that is hot enough to react appreciably with impurities and that at the higher temperatures the reaction takes place essentially at exposed surfaces, the core support blocks and support posts can have significant effects on impurity levels. Both the blocks and the posts have surfaces that are exposed to primary coolant that are roughly 1/45 and 1/30, respectively, that of the chemically reactive core. Thus, if the support block graphite (PGX, the most reactive nuclear graphite) had a material loss rate (proportional to $\sqrt{ZK}$) only 45 times the core graphite (H451), for example, its contribution to the impurity levels in the helium would be as significant as that due to the core. Some very preliminary data indicate that PGX may be two orders of magnitude more reactive (proportional to K) than H451.²⁴

Mesh Size and Spacing

In Section 4.B the errors introduced by the choice of mesh size and nodal point distribution were discussed. It is evident from the calculations presented there that the mesh spacing in OXIDE-3 can lead to significant errors when the graphite temperatures exceed normal operating temperatures. At high temperatures graphite oxidation occurs predominantly at the coolant passage surface and is essentially one-dimensional in nature. A one-dimensional, closely packed mesh spacing, as in Figure 30, would improve accuracy without adding nodal points. It would also be convenient to have the first nodal point either on the surface, or alternatively in the interior of the graphite, accessible as a user option. This would allow a choice between over or underestimating the graphite burnoff,

respectively, to be made during program execution.

Time Step

The appropriate time step to be used in OXIDE-3 is intimately linked to the particular problem being investigated. Although this aspect was not investigated exhaustively, several automatic time step setting devices were considered. In Appendix B, for example, an algorithm is described that automatically varies the time step during program execution in accordance with criteria on relative impurity levels in the upper and lower plena. This technique proved very satisfactory for a class of steam ingress calculations, yielding long term histories for moderate computer running times. The unsatisfactory variation in mass balance and air ingress upon the size of the time step has been illustrated in Section 5.D for the depressurization accident.

Flammability Analysis

OXIDE-3 has a rudimentary model to consider the possibility of a flammable mixture entering the CV from a depressurization of the PCRV. Scenarios in GA-A13171²¹ that seem to lead to near-flammable conditions (combined depressurization and massive steam ingress) should be recalculated in view of the factor of two error germane to graphite-oxygen balances and because even with this error rectified there remain mass balance discrepancies in the code. (The appropriate mass balances should be summarized in the printout of future versions of OXIDE-3). Although accidents leading to near-flammable conditions are in the "Class 9" category because of certain modeling assumptions in OXIDE-3 (e.g. complete mixing of egressing PCRV gases with CV atmosphere is assumed) certain sensitivity analyses seem in order. For example, the constant air ingress

rate of 0.3 pounds/second used in GA-A13171 should be varied over the history of the transient to ascertain whether or not it does indeed lead to the "worst" case.

Noble Gas Release

A coding error, that resulted in an overestimate in the amount of fuel hydrolyzed by a factor of ~ 100 , was corrected. The steam break (with scram) accident, calculated in GA-A13171, was carried out to 200 ksec and resulted in a noble gas release of 3.3 MCi. This is in contrast to a release of 0.2 MCi suggested in the former document. The larger value results from the fact that steam is not purged from the primary coolant until several "half lives" have passed and this in turn is controlled by the rate at which helium passes through the purification system. This computed value is also a result of certain modeling assumptions in OXIDE-3. For example, in the code the fraction of fuel particles that are failed is determined solely by irradiation time which is fixed during input; it is not a function of the temperature history evolved during the transient, as it realistically should be. Future versions of OXIDE-3 should include the relationship between temperature and failed fuel fraction, as well as improved correlations between fuel hydrolysis and the amount of noble gas released to the primary coolant.

8. ACKNOWLEDGEMENTS

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Table 1

Parameters for Equation (28) for Various Values of Leak Rate

$$(F = 1, \frac{\varepsilon}{q} = 10^{-2})$$

<u>Impurity</u>	<u>P₀</u>	<u>P₁</u>	<u>λ₁</u>	<u>P₂</u>	<u>λ₂</u>
A. L = 0.009 lb/hour					
Steam	0.0249	0.0200	8.6x10 ⁻⁴	0.0047	2.6x10 ⁻⁵
Hydrogen	0.685	-0.005	3.7x10 ⁻³	0.690	1.6x10 ⁻⁵
Carbon Monoxide	0.685	-0.013	8.2x10 ⁻⁴	0.699	2.1x10 ⁻⁵
B. L = 0.09 lb/hour					
Steam	0.349	0.228	7.0x10 ⁻⁴	0.117	2.5x10 ⁻⁵
Hydrogen	6.68	-0.07	1.4x10 ⁻³	6.75	1.6x10 ⁻⁵
Carbon Monoxide	6.67	-0.17	5.2x10 ⁻⁴	6.85	2.1x10 ⁻⁵
C. L = 0.9 lb/hour					
Steam	5.78	2.93	4.6x10 ⁻⁴	2.76	2.7x10 ⁻⁵
Hydrogen	63.1	-1.4	1.8x10 ⁻⁴	64.7	1.6x10 ⁻⁵
Carbon Monoxide	63.2	-2.5	2.9x10 ⁻⁴	65.8	2.1x10 ⁻⁵

Table 2

Parameters for Equation (28) for Various Values of Reaction Rate

$(L = 0.09 \text{ lb/hour}, \frac{\varepsilon}{q} = 10^{-2})$

<u>Impurity</u>	<u>P_o</u>	<u>P₁</u>	<u>λ_1</u>	<u>P₂</u>	<u>λ_2</u>
A. F = 0.01					
Steam	1.17	0.66	1.9×10^{-4}	0.49	3.3×10^{-5}
Hydrogen	4.07	-0.29	1.7×10^{-4}	4.37	1.9×10^{-5}
Carbon Monoxide	4.10	-0.51	1.5×10^{-4}	4.62	2.4×10^{-5}
B. F = 1.0					
Steam	0.349	0.228	7.0×10^{-4}	0.117	2.5×10^{-5}
Hydrogen	6.68	-0.07	1.4×10^{-3}	6.75	1.6×10^{-5}
Carbon Monoxide	6.67	-0.17	5.2×10^{-4}	6.85	2.1×10^{-5}
C. F = 100.0					
Steam	0.190	0.170	1.1×10^{-3}	0.019	3.2×10^{-5}
Hydrogen	7.05	-0.04	4.5×10^{-3}	7.09	1.6×10^{-5}
Carbon Monoxide	7.05	-0.12	8.9×10^{-4}	7.17	2.0×10^{-5}

Table 3

Parameters for Equation (28) for Various Values of Porosity/Tortuosity

(L = 0.09 lb/hour, F = 1)

Impurity	P_0	P_1	λ_1	P_2	λ_2
A. $\frac{\epsilon}{q} = 10^{-3}$					
Steam	1.77	1.46	1.2×10^{-4}	0.31	3.3×10^{-5}
Hydrogen	5.39	-1.43	1.2×10^{-4}	6.82	2.5×10^{-5}
Carbon Monoxide	5.39	-1.50	1.2×10^{-4}	6.89	2.6×10^{-5}
B. $\frac{\epsilon}{q} = 5 \times 10^{-3}$					
Steam	0.569	0.408	4.1×10^{-4}	0.157	2.9×10^{-5}
Hydrogen	6.50	-0.32	3.3×10^{-4}	6.83	2.1×10^{-5}
Carbon Monoxide	6.50	-0.39	3.4×10^{-4}	6.90	2.3×10^{-5}
C. $\frac{\epsilon}{q} = 10^{-2}$					
Steam	0.349	0.228	7.0×10^{-4}	0.117	2.5×10^{-5}
Hydrogen	6.68	-0.07	1.4×10^{-3}	6.75	1.6×10^{-5}
Carbon Monoxide	6.67	-0.17	5.2×10^{-4}	6.85	2.1×10^{-5}

Table 4

CO-O₂ Molar Account at t = 1500 Seconds

<u>Case</u>	<u>A</u>	<u>B</u>	<u>C</u>	<u>D</u>	<u>E</u>
I	2.88	0.43	1.50	1.18	4.54
II	2.88	0.43	3.01	1.94	4.54
III	2.53	0.45	3.47	2.18	4.04
IV	2.57	0.53	3.33	2.20	3.91

A is the moles of oxygen gas ingressed

B is the moles of unreacted oxygen in the PCRV and released

C is the moles of produced carbon monoxide in the PCRV and released

D is $(B + C/2)$ and should equal A

E is the moles of graphite burned and should equal C, also $B + E/2 = A$

Table 5

Total Air Ingress as a Function of Time Step at 500 and 1500 Seconds

<u>t = 500 sec</u>		<u>Time Step</u>		
		<u>1 sec</u>	<u>5 sec</u>	<u>20 sec</u>
Method 1 (rate = 0.3 lb/sec)		22 lb	79 lb	114 lb
Method 2		55 lb	1080 lb	5170 lb
<u>t = 1500 sec</u>		<u>Time Step</u>		
		<u>1 sec</u>	<u>5 sec</u>	<u>20 sec</u>
Method 1 (rate = 0.3 lb/sec)		270 lb	348 lb	396 lb
Method 2		613 lb	2927 lb	>5170 lb

Table 6

Comparison of GOPTWO and OXIDE-3 Results
Steady-State Water Concentration (psia)

<u>F</u>	<u>ϵ/q</u>	<u>L (lb/hr)</u>	<u>GOPTWO</u>	<u>OXIDE-3</u>	<u>% Difference</u>
1	10^{-2}	0.009	2.64 E-5	2.49 E-5	6
1	10^{-2}	0.09	5.34 E-4	3.49 E-4	35
1	10^{-2}	0.9	1.10 E-2	5.78 E-3	47
1	10^{-3}	0.09	1.45 E-3	1.77 E-3	-22
1	10^{-2}	0.09	5.34 E-4	3.49 E-4	35
1	10^{-1}	0.09	1.74 E-4	5.43 E-5	69
0.01	10^{-2}	0.09	3.18 E-3	1.17 E-3	63
1	10^{-2}	0.09	5.34 E-4	3.49 E-4	35
100	10^{-2}	0.09	*	1.90 E-4	*

*The GOPTWO code becomes unstable for certain combinations of reaction rate, diffusion coefficient, water ingress rate and initial estimates of impurity concentration.

Table 7

Comparison of GOPTWO and OXIDE-3 Results
Steady-State Carbon Monoxide Concentration (psia)

<u>F</u>	<u>ϵ/q</u>	<u>L (lb/hr)</u>	<u>GOPTWO</u>	<u>OXIDE-3</u>	<u>% Difference</u>
1	10^{-2}	0.009	6.97 E-4	6.85 E-4	1.7
1	10^{-2}	0.09	6.70 E-3	6.67 E-3	0.4
1	10^{-2}	0.9	6.13 E-2	6.32 E-2	3.1
1	10^{-3}	0.09	5.78 E-3	5.39 E-3	6.7
1	10^{-2}	0.09	6.70 E-3	6.67 E-3	0.4
1	10^{-1}	0.09	7.06 E-3	6.83 E-3	3.3
0.01	10^{-2}	0.09	4.05 E-3	4.10 E-3	1.2
1	10^{-2}	0.09	6.70 E-3	6.67 E-3	0.4
100	10^{-2}	0.09	*	7.05 E-3	*

*The GOPTWO code becomes unstable for certain combinations of reaction rate, diffusion coefficient, water ingress rate and initial estimates of impurity concentration.

Figure 1. HTGR model simulated by OXIDE-3.

Figure 2. Symmetry related slice of 3000 MWt core simulated in OXIDE-3 (sample data given in Appendix A).

(a) TRIANGULAR UNIT CELL

(b) TYPICAL COOLANT-MODERATOR-FUEL SECTION

Figure 3. A portion of a fuel element cross section. The reduced triangular unit cell modeled in OXIDE-3 is shown in (a). Its relation to the area immediately surrounding a coolant hole is shown in (b).

Figure 4. Finite difference model array of the reduced triangular unit cell modeled in OXIDE-3.

Figure 5. Reactant length versus temperature for the graphite-steam reaction. The upper curve is the peak concentration for steam during a guillotine steam tube break and the lower two curves are equilibrium concentrations occurring for constant steam leaks of 0.9 and 0.09 lb/hour.

Figure 6. Reactant length versus temperature for the graphite-oxygen reaction. The pressure dependence of the diffusion constant affects L as shown.

Figure 7. Reactant length versus temperature for the fuel rod-steam reaction. The high temperature portion of the curve is primarily a reaction with the graphite of the fuel rod (10X the rate used for the web graphite), and the leveled portion of the curves for $T < 1000^\circ\text{F}$ is an indication of the dominance of the failed fuel (1.6%) hydrolysis reaction.

Figure 8. One-dimensional finite difference analysis.

Figure 9. Finite difference calculational error as a function of mesh separation. The first node point is internal as in OXIDE-3.

Figure 10. The ratio of actual to finite difference mass loss rates for the oxygen-graphite reaction. The points relevant to OXIDE-3 are felt to be on the 2 atm curves at a finite difference spatial step of 0.037 and 0.029 inches for mesh volumes 2 and 3, respectively of Figure 4.

Figure 11. The effect of film coefficient, H, on a finite difference mass loss calculation for a fixed mesh separation, Δ . The first node point is internal as in OXIDE-3.

Figure 12. Finite difference calculational error as a function of mesh separation. The first node point is on the surface.

Figure 13. The effect of film coefficient, H , on a finite difference mass loss calculation for a fixed mesh separation, Δ . The first node point is on the surface.

Figure 14. Partial pressure of steam in the hot plenum as a function of time due to various step function leak rates L starting at $t=0$.

Figure 15. Partial pressure of hydrogen in the hot plenum as per Figure 14.

Figure 16. Partial pressure of carbon monoxide in the hot plenum as per Figure 14.

Figure 17. The ratio of the partial pressures of carbon monoxide and steam in the hot plenum as per Figure 14.

Figure 18. Partial pressure of steam in the hot plenum as a function of time due to a step function leak rate $L = 0.09$ lb/hour for various graphite-steam reaction rate multipliers, F .

Figure 19. Partial pressure of hydrogen in the hot plenum as per Figure 18.

Figure 20. Partial pressure of carbon monoxide in the hot plenum as per Figure 18.

Figure 21. The ratio of the partial pressures of carbon monoxide and steam in the hot plenum as per Figure 18.

Figure 22. Partial pressure of steam in the hot plenum as a function of time due to a step function leak rate $L = 0.09$ lb/hour for various gas-graphite diffusion factors, ϵ/q .

Figure 23. Partial pressure of hydrogen in the hot plenum as per Figure 22.

Figure 24. Partial pressure of carbon monoxide in the hot plenum as per Figure 22.

Figure 25. The ratio of the partial pressures of carbon monoxide and steam in the hot plenum as per Figure 22.

Figure 26. Partial pressure of steam in the hot plenum as a function of time due to a transient 1626 pound steam leak and resultant scram.

Figure 27. Partial pressure of hydrogen in the hot plenum as per Figure 26.

Figure 28. Partial pressure of carbon monoxide in the hot plenum as per Figure 26.

Figure 29. Fraction of UC₂ fuel inventory hydrolyzed as per Figure 26.

Figure 30. Revised OXIDE-3 symmetry element.

Figure 31. Flammability limits for helium, air, and fuel mixtures. Possible states of composition of a gas bubble emerging from the PCRV at 6900 seconds following depressurization are shown by the two paths, ——— only depressurization, - - - - - depressurization and steam leak.

Figure 32. Effect of graphite-steam diffusion coefficient on the equilibrium partial pressures of steam and carbon monoxide versus steam leak rate.

Figure 33. Effect of graphite-steam reaction rate multipliers on the equilibrium partial pressures of steam and carbon monoxide versus steam leak rate.

Figure 34. Effect of the mass transfer coefficient on the GOPTWO calculation of the partial pressures of carbon monoxide and steam for the nominal HTGR case.

Figure 35. Variation of the gas concentrations from the center of the coolant channel across the film barrier and into the graphite web.

APPENDIX A

OXIDE-3 Input Data Deck Description

These sheets give the basic information needed to set up input data for the program OXIDE-3. The data deck is arranged as follows:

First card set is a two-card set for run identification.

FORMAT: (12A6)

INPUT: TITLE(24)

FUNCTION: The characters punched in cards 1-72 of these two cards will printout at the top of the first output page for run identification.

Second card set is a one-card set for restart control.

FORMAT: (12I6)

INPUT: NTAPE, ISTART, NDUMP(6)

FUNCTION: NTAPE is an integer in columns 1-6. When NTAPE is greater than "1", the OXIDE-3 will continue the previous run (restart).

ISTART is an integer in columns 7-12. This integer indicates the time point for restart. If ISTART is less than the previous run time point, the restart run will be terminated.

NDUMP is a six-element array. This array is not used in OXIDE-3.

Third card set is a one-card set for run specification.

FORMAT: (I6, 2L6, I6)

INPUT: NCASE, TPUNCH, STDY, ISMAX

FUNCTION: NCASE is an integer in columns 1-6. NCASE is the case number of the run.

TPUNCH is a logical variable in columns 7-12. When TPUNCH is .TRUE., this means the segment temperature output punch deck is required at the end of the calculation; i.e., when the real time of the transient exceeds TFINAL or the computation time exceeds IWARN (both are input on card set 14). For TPUNCH set to .FALSE. there is no punch output.

STDY is a logical input in columns 13-18. When STDY is .TRUE. the program will calculate the steady state temperatures of the graphite and coolant by iterating through the code ISMAX times (card sets 25 and 26 can be entered as blank cards). A punch deck of graphite and coolant temperatures is produced. When STDY is .FALSE. the calculation starts immediately using the temperatures on card sets 25 and 26.

ISMAX is an integer in columns 19-24. It is the number of iterations through the core to obtain steady state temperatures when STDY is .TRUE. (usually 5-6 is sufficient).

Fourth card set is a one-card set for geometry organization.

FORMAT: (2I12, 3E12.6)

INPUT: NREG, NSEG, SEGLG1, SEGLG2, SEGLG3

FUNCTION: NREG is an integer in columns 1-12. NREG specifies the number of regions considered.

NSEG is an integer in columns 13-24. NSEG indicates in each core region there are "NSEG" core segment average temperatures in it; i.e., the number of blocks per column.

SEGLG1, the floating point number in columns 25-36, indicates the top reflector segment length in feet.

SEGLG2, the floating point number in columns 37-48, indicates the fuel segment length in feet.

SEGLG3, the floating point number in columns 49-60, indicates the bottom reflector segment length in feet.

Fifth card set is a one-card set. This punched card gives the number of columns in each core region.

FORMAT: (20F3.0)

INPUT: COL(1), COL(2), ..., COL(K). Where $K=NREG$
(see Fourth card set).

FUNCTION: COL(I), where $1 \leq I \leq NREG$, is the number of columns in region "I".

Sixth card set, one-card set, inputs the irradiation life time in core for each region.

FORMAT: (20F3.0)

INPUT: RADTIM(1), RADTIM(2), ..., RADTIM(K). Where $K=NREG$.

FUNCTION: RADTIM(I), where $1 \leq I \leq NREG$, indicates the irradiation life time in years in core for region "I".

Seventh card set is a one-card set for PCRV initial conditions.

FORMAT: (6E12.6)

INPUT: PRS(1), PRS(2), TMP(1), TMP(2), VOL(1), VOL(2)

FUNCTION: PRS(1) is the lower plenum pressure in psia.

PRS(2) is the upper plenum pressure in psia.

TMP(1) is the lower plenum temperature in °F.

TMP(2) is the upper plenum temperature in °F.

VOL(1) is the lower plenum volume in ft³.

VOL(2) is the upper plenum volume in ft³.

Eighth card set is a one-card set for core power and density parameters.

FORMAT: (6E12.6)

INPUT: POWER, CARDEN, CNOBLE, FUJ1, FUJ2, THEAT

FUNCTION: POWER is the core power in MW(t).

CARDEN is the carbon density in lb/ft³.

CNOBLE is the noble gas inventory per fuel element.

FUJ1 is a decay heat generation factor before THEAT.

FUJ2 is a decay heat generation factor after THEAT.

THEAT is the time for full insertion of the control rods
in seconds.

Ninth card set is a one-card set for core flow.

FORMAT: (6E12.6)

INPUT: HEFLOW, TCOEF, TMPREF, ENT, XKCH, EXIT

FUNCTION: HEFLOW is the normal coolant flow rate in lb/sec.

TCOEF is the non-bypass core flow factor.

ENT represents the pressure losses at the core inlet.
TMPREF is a factor used to determine temperature of the bypass helium entering the lower plenum.

XKCH represents the pressure losses at offset

blocks (channel loss).
EXIT represents the pressure losses at the core exit.

Tenth card set is a one-card set for the purification system.

FORMAT: (6E12.6)

INPUT: PURFLO, TMPHEP, SMPUG

FUNCTION: PURFLO is the purification flow rate in lb/hr.

TMPHEP is the return helium temperature in °F.

SMPUG is the steam purification capacity in pounds.

Eleventh card set is a two-card set for PCRV safety relief valve data.

FORMAT: (I12,5E12.6/6E12.6)

INPUT: IPUFF, OPSET, PVALVE, VALFRA, AORIF, APIPE, HDIA,
XLENT, COEFF, FACTOR, PRUPT

FUNCTION: IPUFF is the safety relief valve location.

OPSET is the flow trip pressure in psia.

PVALVE is the relief valve pressure in psia.

VALFRA is the relief valve close fraction.

AORIF is the orifice flow area in ft².

APIPE is the pipe flow area in ft².

HDIA is the hydraulic diameter of flow path in feet.

XLENT is the length of flow path in feet.

COEFF is the orifice discharge coefficient.

FACTOR is the friction (resistance) factor (velocity heads) of pipe flow area.

PRUPT is the rupture pressure in psia.

Twelfth card set is a one-card set for air ingress.

FORMAT: (6E12.6)

INPUT: AIRRAT, TMPAIR, AIRTOT

FUNCTION: AIRRAT is the air ingress rate in lb/sec.

TMPAIR is the air temperature in °F.

AIRTOT is the maximum air ingress in pounds.

Thirteenth card set is a two-card set for steam diffusion and reaction data input.

FORMAT: (6E12.6)

INPUT: BSTART, FUD1, FUD2, ZULU, XDIFFO, XDIFFH, XDIFFC

FUNCTION: BSTART is an initial burnoff ratio in percentage.

FUD1 is a reaction rate factor, F, for the graphite web.

FUD2 is the reaction rate factor, F, of the fuel rod.

ZULU is the gas-gas diffusion constant in cm²/sec
for steam in helium.

XDIFFO is the relative diffusion factor of oxygen to steam.
XDIFFH is the relative diffusion factor of hydrogen to steam.
XDIFFC is the relative diffusion factor of carbon monoxide to steam.

Fourteenth card set is a one-card set for time constants.

FORMAT: (2E12.3, I12)
INPUT: TFINAL, TSCRAM, IWARN
FUNCTION: TFINAL is a final time in seconds when the elapsed problem time (time point) equals TFINAL, the iteration process of OXIDE-3 stops and terminates the program run.
TSCRAM is a scram time in seconds.
IWARN is a warning time in seconds; i.e., warns of approaching computer calculation time limit.

Fifteenth card set is a one-card set for the magnitude of the core time steps in each time interval.

FORMAT: (6E6.2, 6I6)
INPUT: TSTEP(6), MAPRNT(6)
FUNCTION: TSTEP is a six-elements array. The input data of array TSTEP is the magnitude of the core time steps associated with each time interval.
MAPRNT is a six-element array. This array together with the warning time "IWARN" and the time of flammable gas burning within the containment building determines the map (nodal arrangement for symmetric triangle analysis) print frequency.

Sixteenth card set is a one-card set for the number of core time steps in time interval.

FORMAT: (12I6)
INPUT: NITER(6), NTIME(6)
FUNCTION: NITER is a six-elements array. The elements in this array indicate the number of core time steps to be performed with time interval TSTEP.
NTIME is a six-elements array. The elements in NTIME indicate the number of OXIDE subroutine iterations performed for each core subroutine iteration.

Seventeenth card set is a one-card set for the print frequencies of data.

FORMAT: (12I6)
INPUT: NCPRT(6), NSPRT(6)
FUNCTION: NCPRT is a six-elements array. Array NCPRT controls the normal output print frequencies.
NSPRT is a six-elements array. This array controls the distribution output print frequencies.

Eighteenth card set is a one-card set that inputs the plot frequencies.

FORMAT: (24I1, 8I6)
INPUT: IPLOT(24), NFPLLOT(6), IPC
FUNCTION: IPLOT is a 24-elements array. The elements in IPLOT are either zero or non-zero. The order of the non-zero elements determines the correspondent parameter to be plotted (cf. OXID.795-OXID.818). NFPLLOT is a six-elements array. Array NFPLLOT stores the information of interval plot frequencies.
IPC is an initial plot set up constant (always 0).

Nineteenth card set is a one-card set that inputs the optional print information.

FORMAT: (12I6)
INPUT: ISATZ(6)
FUNCTION: ISATZ(1) $\neq$ 0 indicates a core steam partial pressure MATRIX-(ATM) list is required.
ISATZ(2) $\neq$ 0 indicates a core oxygen partial pressure MATRIX-(ATM) list is required.
ISATZ(3) $\neq$ 0 indicates to list the graphite average temperature and coolant temperatures associated with the core regions respectively.
ISATZ(4) $>$ 0 prints out the steady state temperature distribution.
ISATZ(5) $\neq$ 0 prints out the distributions of cesium, strontium and barium in the nodes of carbon.
ISATZ(6) $\neq$ 0 lists the matrix of unoxidized fraction of the nodes of carbon.

Twentieth card set is a one-card set that inputs the optional map (of the nodal arrangement for symmetric triangle analysis) requested data.

FORMAT: (36I2)
INPUT: (MAPID(N), III(N), KKK(N), N=1,12). There are 12 groups of data. Each group contains three elements (MAPID(I), III(I), KKK(I)). The maximum combination of optional map requests in each run is 12.
FUNCTION: MAPID is a 12-elements array. According to the subscript, the element of MAPID belongs to the different optional groups, that is the MAPID(I) belongs to the Ith optional map request group.
MAPID(I) $>$ 0 means the plot of a basic analysis element of the nodal arrangement for symmetric triangle analysis is required. The commands are defined as follows:
MAPID(I)=1 indicates a temperature map is required.
MAPID(I)=2 indicates a map of partial pressure of steam is required.
MAPID(I)=3 indicates a map of partial pressure of oxygen is required.
MAPID(I)=4 indicates a map of partial pressure of hydrogen is required.
MAPID(I)=5 indicates a map of partial pressure of carbon monoxide is required.

III is a 12-elements array. The subscription (order) of the element in III indicates the element belongs to which optional map group. The constants of element in III indicates the section numbers which optional map requires; i.e., block position in the column.

KKK is a 12-elements array. The order of the elements tells the element belongs to which optional map group. The contents of the elements in KKK indicates the region that the optional map group is required to plot.

Twenty-first card set is a one-card set that inputs steam leak and helium specificational data.

FORMAT: (3I12, 3E12.6)

INPUT: NSTM, NTMP, NHEF, TMPSTM, STMTOT, STMEXP

FUNCTION: NSTM indicates how many elements of the steam leak table are input (maximum 50).

NTMP indicates the helium temperature table entries (maximum 50).

NHEF indicates the helium flow table entries (maximum 50).

TMPSTM is the steam temperature in °F.

STMTOT is the maximum steam ingress in pounds.

STMEXP is the steam leak delay time in seconds.

Twenty-second card set is a $\left[\frac{NSTM + 2}{3}\right]$ card set that inputs steam leak table where $\left[\frac{NSTM + 2}{3}\right]$ is a truncated integer.

FORMAT: (6E12.6)

INPUT: (XSTM(K), YSTM(K), K=1, NSTM)

FUNCTION: XSTM is a one-dimensional array with 50 or less elements. Array XSTM stores the time scale of steam leak rate.

YSTM is a one-dimensional array with 50 or less elements. Array YSTM stores the steam leak rate table with respect to XSTM. The units of steam leak rate is in lb/sec.

Twenty-third card set is a $\left[\frac{NTMP + 2}{3}\right]$ punch card set that inputs helium inlet temperature table, where $\left[\frac{NTMP + 2}{3}\right]$ is a truncated integer.

FORMAT: (6E12.6)

INPUT: (XTMP(K), YTMP(K), K=1, NTMP)

FUNCTION: XTMP and YTMP are one-dimensional arrays with 50 or less elements.

XTMP stores helium post trip time table in seconds.

YTMP stores helium temperature table in °F corresponding to the array XTMP.

Twenty-fourth card set, a $\left[\frac{NHEF + 2}{3}\right]$ punched card set, inputs the helium flow rate table, where $\left[\frac{NHEF + 2}{3}\right]$ is a truncated integer.

FORMAT: (6E12.6)

INPUT: (XHEF(K), YHEF(K), K=1, NHEF)

FUNCTION: XHEF and YHEF are one-dimensional arrays with 50 or less elements.

XHEF stores helium post trip time scale in seconds.
YHEF stores helium flow table in lb/sec corresponding to the array XHEF.

Data card set 25 to the card set 29 are core parameter distributions. The input data are as follows:

Twenty-fifth card set has $NREG * \left[\frac{NSEG + 5}{6} \right]$ (see fourth card set) punched cards. This card set inputs the initial segment temperature in °F.

FORMAT: (6E12.6)
INPUT: (SEGTMP(I,K), I=1, NSEG) for NREG subsets (K=1,NREG)
FUNCTION: SEGTMP is a two-dimensional array with NSEG*NREG elements matrix. The element SEGTMP(I,K) stores the initial segment temperature at the Ith segment in the Kth region.

Twenty-sixth card set has $NREG * \left[\frac{NSEG + 5}{6} \right]$ punched cards. This card set inputs the initial coolant temperatures in °F. The input format, input order and relations of segments to the regions are the same as card set 25.

Twenty-seventh card set has $\left[\frac{NSEG + 5}{6} \right]$ punch cards. This card set inputs axial power factors.

FORMAT: (6E12.6)
INPUT: (SEGPWR(I), I=1,NSEG)
FUNCTION: Array SEGPWR has 50 or less elements. This array stores the segment axial power factors.

Twenty-eighth card set has $\left[\frac{NREG + 5}{6} \right]$ punched cards. This card set gives the region power density factors.

FORMAT: (6E12.6)
INPUT: (REGPFR(K), K=1, NREG)
FUNCTION: REGPFR has 50 or less elements. REGPFR stores the region power density factors. The array REGPFR and array SEGPWR are the data to generate a matrix of local-to-average power factors for each core segment.

Twenty-ninth card set, the $\left[\frac{NREG + 5}{6} \right]$ punched card set, gives region orifice coefficients.

FORMAT: (6E12.6)
INPUT: (XKORIF(K), K=1, NREG)
FUNCTION: Array XKORIF is a one-dimensional array with 50 or less elements. This array is used to store core region coolant flow orifice pressure loss factors.

The following card sets pertain to the containment building data:

Thirtieth card set is a one-card set giving the building atmosphere data.

FORMAT: (6E12.6)
INPUT: BPRESS, BTEMP, BVOL, FLALIM, HUM

FUNCTION: BPRESS is the building atmosphere pressure in psia.
 BTEMP is the building atmosphere temperature in °F.
 BVOL is an atmosphere volume in ft³.
 FLALIM is a combustion limit factor (is not used in the program).
 HUM is a humidity in percentage (is not used in the program).

Thirty-first card set is a one-card set giving the data of environmental exchange.

FORMAT: (6E12.6)
 INPUT: BLK1, BLK2, TAIR
 FUNCTION: BLK1 is an air linear leak rate in %/day/psi.
 BLK2 is an air non-linear leak rate in %/day/psi.
 TAIR is an ambient temperature in °F.

Thirty-second card set is a one-card set giving optional building steam leak data.

FORMAT: (6E12.6)
 INPUT: STMLK, STMMAX, STMTMP, FWENTH
 FUNCTION: STMLK is steam inleakage rate in lb/sec.
 STMMAX is the maximum steam ingress in pounds.
 STMTMP is steam temperature in °F.
 FWENTH is steam enthalpy in Btu.

Thirty-third card set is a two-card set giving the heat sink data of sink 1 (building walls?) and sink 2 (PCRV walls?).

FORMAT: (6E12.6)
 INPUT: BSURF1, BMASS1, BCAP1, BHEIT1, THICK1, COND1,
 BSURF2, BMASS2, BCAP2, BHEIT2
 FUNCTION: BSURF1 is the surface area of sink 1 in ft².
 BMASS1 is the mass of sink 1 in pounds.
 BCAP1 is a heat capacity of sink 1 in Btu/lb-°F.
 BHEIT1 is the height of sink 1 in feet.
 THICK1 is the thickness of sink 1 in feet.
 COND1 is a material conductivity of sink 1 in Btu/hr-ft²-°F.
 BSURF2 is the surface area of sink 2 in ft².
 BMASS2 is the mass of sink 2 in pounds.
 BCAP2 is a heat capacity of sink 2 in Btu/lb-°F.
 BHEIT2 is the height of sink 2 in feet.

Thirty-fourth card set is a one-card set giving the heat sink data of sink 3 (steel component surfaces?)

FORMAT: (6E12.6)
 INPUT: BSURF3, BMASS3, BCAP3, BHEIT3
 FUNCTION: BSURF3 is the surface area of sink 3 in ft².
 BMASS3 is the mass of sink 3 in pounds.
 BCAP3 is a heat capacity of sink 3 in Btu/lb-°F.
 BHEIT3 is the height of sink 3 in feet.

Card Sets 1-24

0	0	0	0	0	0	0	0
3	F	F	40				

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Card Set 25

639.9994	967.4493	1102.2887	1243.1484	1364.1845	1437.7969
1524.5175	1566.1958	1547.7266	1414.8409		
639.9980	972.7329	1108.3692	1249.9185	1371.1437	1444.1281
1530.6135	1571.3980	1551.3153	1415.4346		
639.9987	1079.7382	1231.6889	1387.3855	1512.6800	1573.2831
1655.3069	1678.3038	1625.8218	1429.6453		
639.9978	984.7608	1122.0680	1265.0197	1386.4846	1457.8399
1543.6138	1582.1903	1558.2809	1415.4787		
639.9978	989.0647	1127.1431	1270.7953	1392.5711	1463.5822
1549.3141	1587.3080	1562.2130	1417.0653		
639.9981	993.1837	1131.8534	1276.0090	1397.8925	1468.3737
1553.8868	1591.1491	1564.7660	1417.2639		
639.9985	1088.6375	1241.9762	1398.8876	1524.5695	1584.2039
1665.9082	1687.4800	1632.3530	1431.2061		
639.9977	966.0064	1100.7814	1241.6308	1362.8170	1436.8110
1523.7841	1565.8941	1548.0271	1416.0757		
639.9977	975.3398	1111.8143	1254.2146	1376.1089	1449.3911
1536.3070	1577.1870	1556.7748	1419.7517		
639.9979	971.4460	1106.8657	1248.2221	1369.3723	1442.4796
1528.4952	1569.9716	1550.2547	1415.0919		
639.9988	1126.0425	1295.9753	1470.3943	1611.7768	1682.2830
1776.0727	1804.9522	1750.4093	1536.8531		
639.9983	1005.7188	1146.2932	1292.0972	1414.4454	1483.4564
1568.4314	1603.5927	1573.3985	1418.8152		
639.9985	977.6305	1113.9498	1256.0735	1377.3982	1449.7220
1535.9206	1575.8087	1554.1712	1415.4744		
639.9983	1011.1417	1152.5427	1299.0652	1421.6173	1489.9976
1574.7445	1609.0026	1577.1633	1419.5196		
639.9979	980.7939	1117.7789	1260.5313	1382.2139	1454.4191
1540.7092	1580.2904	1557.8831	1417.5359		
639.9973	957.0048	1090.7538	1230.8111	1352.1075	1427.6277
1515.4099	1559.4430	1544.6726	1418.0726		
639.9987	1054.4442	1202.2315	1354.2289	1478.1472	1541.2223
1623.8978	1650.6953	1605.5159	1423.3147		
639.9985	1190.6427	1383.0394	1580.5972	1741.1406	1822.0941
1929.2626	1963.4250	1903.5177	1664.0664		
639.9986	1092.5496	1250.5438	1412.6488	1543.7793	1608.5826
1695.1747	1721.0917	1669.1685	1468.9863		
639.9984	813.1428	873.5998	935.6865	985.4758	1008.8420
1040.7668	1048.5432	1025.6455	944.6388		

Card Set 26

639.9995	688.7328	786.1980	896.0953	1012.8956	1124.7110
1228.5757	1321.1119	1389.7699	1414.8440		
639.9993	688.7412	786.2764	896.2534	1013.1417	1125.0465
1228.9922	1321.6048	1390.3257	1415.4383		
639.9996	689.2078	788.4589	900.3857	1019.3917	1133.3966
1239.2644	1333.6548	1403.7870	1429.6472		
639.9993	688.6789	786.2084	896.1813	1013.0722	1124.9904
1228.9443	1321.5746	1390.3229	1415.4813		
639.9993	688.7601	786.4863	896.6815	1013.8107	1125.9604
1230.1281	1322.9512	1391.8463	1417.0681		
639.9994	688.7526	786.5004	896.7208	1013.8786	1126.0592
1230.2543	1323.1050	1392.0250	1417.2669		
639.9996	689.2795	788.7225	900.8667	1020.1065	1134.3396
1240.4178	1334.9996	1405.2795	1431.2080		
639.9993	688.8217	786.4443	896.5185	1013.5059	1125.4983
1229.5278	1322.2090	1390.9723	1416.0784		
639.9993	689.0083	787.0861	897.6751	1015.2142	1127.7426
1232.2673	1325.3961	1394.5007	1419.7549		
639.9993	688.7260	786.2189	896.1481	1012.9849	1124.8391
1228.7383	1321.3087	1389.9970	1415.0946		
639.9997	695.9376	808.6809	935.8222	1070.9982	1200.4797
1320.7230	1427.9168	1507.5422	1536.8553		
639.9995	688.7937	786.7271	897.1585	1014.5469	1126.9578
1231.3629	1324.4094	1393.4869	1418.8174		
639.9995	688.7169	786.2525	896.2310	1013.1236	1125.0368
1228.9884	1321.6106	1390.3447	1415.4772		
639.9995	688.8147	786.8327	897.3606	1014.8539	1127.3691
1231.8695	1325.0047	1394.1531	1419.5219		
639.9993	688.8340	786.6269	896.8960	1014.0989	1126.3113
1230.5402	1323.4113	1392.3323	1417.5391		
639.9991	689.0076	786.8919	897.2591	1014.5512	1126.8249
1231.1200	1324.0285	1392.9469	1418.0758		
639.9996	688.8871	787.3546	898.3951	1016.4509	1129.5331
1234.5490	1328.1688	1397.7128	1423.3168		
639.9996	703.8921	832.6429	977.8359	1132.1998	1280.0504
1417.3539	1539.7452	1630.6436	1664.0685		
639.9996	691.6908	795.8952	913.4069	1038.3473	1158.0297
1269.1722	1368.2586	1441.8699	1468.9885		
639.9996	658.9638	697.2368	740.3965	786.2901	830.2647
871.1028	907.5252	934.6070	944.6402		

Card Sets 27-34

0.0	0.932	1.070	1.190	1.220	1.10
1.05	0.877	0.569	0.0		
.8051	.8358	1.485	.9084	.9322	.9571
1.5402	.7947	.845	.8286	1.6	1.032
.8652	1.0646	.8812	.7387	1.3325	1.8
1.500	0.600				
54.54	49.65	6.93	39.82	37.29	34.665
5.563	56.58	48.93	50.715	8.48	27.99
45.37	25.52	43.51	68.215	11.52	8.303
8.303	8.303				
14.7	100.0		1.945E060.10	50.0	
	4.0E-030.0	80.0			
0.0	0.0	0.0	0.0		
	9.486E+04	5.0E+07	2.0E-01217.0	3.78	1.0
	2.9E+04	2.01E+06	2.0E-0148.0		
	4.1E+04	8.39E+05	11.0E-0235.0		

APPENDIX B

Implementation of Variable Time Step in OXIDE-3

OXIDE-3 allows the user to specify up to six time intervals, each with its user-selected time step, to cover the history of the transient being studied. Unfortunately, there is no guide, other than experience, for choosing appropriate time steps. The specific scenario under investigation, and especially the particular result of interest, will strongly affect the choice of time step. In general, short time steps will improve accuracy and prevent numerical instabilities but these advantages must be weighed against the resulting increase in computation time, particularly for long-term transients such as were of interest in many of the analyses presented here.

As a starting point in determining the appropriate sizes of time steps for the studies presented here, the sample problem in GA-LTR-7 was run repeatedly, with larger and larger time steps. As the time increment was increased one of the results of the OXIDE-3 computation noted was a growing discrepancy between the hydrogen concentrations in the upper and lower plena. This was followed by oscillations in the hydrogen concentration in both plena. This artifact is partly due to the algorithm used in the code.

After some experimentation, a procedure was coded into OXIDE-3 that automatically adjusts the time step during the course of the transient. This recipe, given below, is certainly not optional or unique; it simply proved utilitarian for the problems investigated during this review. After each time step the concentrations of hydrogen in the upper and lower plena were compared.

- . If the difference was less than 5% the time step was increased 10%.
- . If the difference was between 5% and 10% the time step was unaltered.
- . If the difference was greater than 10% the time step was decreased 20%.
- . The time step was limited to a maximum of 200 seconds.

There is an option in the code which allows the user to iterate through a time step sensitive subroutine (OXID3, dealing with the material balance in the upper and lower plena) more times than the CORE subroutine. However, this option is also user specified (16th card set of Appendix A).

APPENDIX C

Impurity Concentration in the Primary Circuit

In Section 5.A, where the OXIDE-3 computations were discussed, it was stated that calculated impurities in the coolant were fit by an expression such as Eq. (28). A justification for the use of this form is presented in this Appendix.

A very simple model considers two interconnected volumes - the coolant volume and the pore volume in the graphite (both web and fuel rod). The distinction between the web graphite and fuel graphite is thus lost and differences in reaction rate and hydrolysis effects cannot be properly accounted for in this model. This approach is validated by the numerical results of the ~~OXIDE-3 calculations~~ for steam concentration, which will be the focus of this analysis.

Let C be the concentration of steam, L the steam leak rate into the coolant volume, k_1 the coolant purification rate constant, k_2 the diffusion rate constant between the two volumes, and k_3 the reaction rate constant. Material balance equations can be formulated for the coolant volume and pore volume (subscripts c and p , respectively) as

$$\frac{dC_c}{dt} = L - k_1 C_c - k_2 (C_c - C_p) \quad (C-1)$$

$$\frac{dC_p}{dt} = k_2 (C_c - C_p) - k_3 C_p \quad (C-2)$$

Rewriting these two equations in operator notation results in

$$[D + (k_1 + k_2)] C_c - k_2 C_p = L \quad (C-1')$$

$$- k_2 C_c + [D + (k_2 + k_3)] C_p = 0 \quad (C-2')$$

The OXIDE-3 results refer to the steam concentration in the coolant volume; therefore C_p can be eliminated between these two, yielding a differential equation in C_c only. Operating on Eq. (C-1') with $[D + (k_2 + k_3)]$, then operating on Eq. (C-2') with k_2 , and then adding the two resulting expressions yields:

$$[D^2 + (k_1 + 2k_2 + k_3) D + (k_1 k_2 + k_1 k_3 + k_2 k_3)] C_c = (k_2 + k_3) L \quad (C-3)$$

The general solution of Eq. (C-3) is

$$C_c = A e^{m_1 t} + B e^{m_2 t} + \frac{(k_2 + k_3) L}{k_1 k_2 + k_1 k_3 + k_2 k_3} \quad (C-4)$$

where $m_{1,2}$ are the roots of the auxiliary equation

$$m^2 + (k_1 + 2k_2 + k_3) m + (k_1 k_2 + k_1 k_3 + k_2 k_3) = 0 \quad (C-5)$$

By solving Eq. (C-5) it is seen that both roots are always real and negative and thus the form of Eq. (28) is justified.

It is noted that in this two volume model the carbon monoxide and/or hydrogen concentrations can be included in the analysis. Denoting the carbon monoxide (or hydrogen) concentration by C' the two equations to supplement Eqs. (C-1) and (C-2) are

$$\frac{dC'_c}{dt} = -k_1 C'_c + k_4 (C'_p - C'_c) \quad (C-6)$$

$$\frac{dC'_p}{dt} = -k_4 (C'_p - C'_c) + k_3 C_p \quad (C-7)$$

where k_4 is the diffusion rate constant between the coolant volume and the pore volume for carbon monoxide/hydrogen.

In order to solve this set of equations it is necessary to know C_p , the steam concentration in the pore volume. This is obtained from Eqs. (C-1') and (C-2') by eliminating C_c between them. The result is

$$C_p = E e^{m_1 t} + F e^{m_2 t} + \frac{k_2 L}{k_1 k_2 + k_1 k_3 + k_2 k_3} \quad (C-8)$$

where E and F are constants related to A and B .

It is interesting to solve Eqs. (C-6) and (C-7) for the carbon monoxide/hydrogen concentration in the coolant volume; i.e. to obtain C'_c . To do this, eliminate C'_p between the two equations. Then, utilizing Eq. (C-8) the general solution for C'_c becomes

$$C'_c = R e^{n_1 t} + S e^{n_2 t} + G e^{m_1 t} + H e^{m_2 t} + \frac{k_2 k_3 L}{k_1 (k_1 k_2 + k_1 k_3 + k_2 k_3)} \quad (C-9)$$

where $n_{1,2}$ are the roots of the auxiliary equation

$$n^2 + (k_1 + 2k_4) n + k_1 k_4 = 0 \quad (C-10)$$

As was true for Eq. (C-5), it is seen that both roots are always real and negative. Also, in Eq. (C-9) G is related to E and H is related to F. The solution for the carbon monoxide/hydrogen in the coolant volume is thus seen to be the sum of four exponential terms plus a constant. However, the two exponential form found for the steam concentration proved also to yield an excellent fit to the OXIDE-3 results for these impurities and so the more complicated form was abandoned.

If the steady state concentrations of steam and carbon monoxide/hydrogen are added together (Eq. [C-4] and Eq. [C-9]) it is clear that their sum satisfied the conservation relation that is always true for the coolant volume during steady state, viz.

$$L = k_1 (C_c + C'_c) \quad (C-11)$$

This material balance equation simply states that at steady state the rate of steam ingress is equal to the purification rate of steam plus carbon monoxide (or hydrogen).

APPENDIX D

Implementation of Mass Transfer Coefficient in GOPTWO

The results depicted in Figure 34, showing the effects of varying the mass transfer coefficient in the HTGR coolant channels, were used to determine if any differences between OXIDE-3 calculations and GOPTWO calculations could be attributed to this parameter. In order to incorporate a finite mass transfer coefficient into GOPTWO, it was necessary to model the steam diffusion in cylindrical geometry and then code this model into the original GOPTWO program.

The change made in GOPTWO is based on a simple change in the stipulated boundary condition at the graphite-free stream interface. Instead of asserting that the water vapor concentration at the graphite surface is equal to that in the free stream, the net flux of water vapor through the boundary layer has been equated to the net flux at the graphite surface.

In the derivation below:

C	is the concentration of steam
K	is the volumetric reaction rate constant for graphite and steam
Z	is the diffusion coefficient of steam in graphite
I_0	is the modified Bessel Function of the first kind, zero order
I_1	is the modified Bessel Function of the first kind, first order
K_0	is the modified Bessel Function of the second kind, zero order
K_1	is the modified Bessel Function of the second kind, first order
$\kappa_1, \kappa_2, \kappa_3$	are dimensionless groupings of the modified Bessel Functions.

The diffusion equation (at steady state) is:

$$\frac{d^2C}{dr^2} + \frac{1}{r} - \frac{K}{Z} C = 0$$

and the boundary conditions are (see Figure 35):

$$\text{BC1: } \frac{dC}{dr} = 0 \text{ at } r = r_o$$

$$\text{BC2: } \beta(C_s - C_1) = -Z \frac{dC}{dr} \text{ at } r = r_1$$

where β is the mass transfer coefficient.

The diffusion equation in this case is a form of Bessel's differential equation and has the general solution:

$$C = A I_0 \left(\frac{r}{L} \right) + B K_0 \left(\frac{r}{L} \right)$$

where

$$L^2 = \frac{Z}{K}.$$

Making use of boundary condition 1 yields:

$$B = \kappa_1 A$$

where

$$\kappa_1 = \frac{I_1 \left(\frac{r_o}{L} \right)}{K_1 \left(\frac{r_o}{L} \right)}.$$

Applying boundary condition 2 results in:

$$A = \frac{\beta C_s}{\beta \kappa_2 - \frac{Z}{L} \kappa_3}$$

where

$$\kappa_2 = I_0 \left(\frac{r_i}{L} \right) + \kappa_1 K_0 \left(\frac{r_i}{L} \right)$$

and

$$\kappa_3 = I_1 \left(\frac{r_i}{L} \right) - \kappa_1 K_1 \left(\frac{r_i}{L} \right).$$

Having evaluated the two constants of integration, we now have the particular solution:

$$C = \frac{\beta C_s}{\beta \kappa_2 - \frac{Z}{L} \kappa_3} \left[I_0 \left(\frac{r}{L} \right) + \kappa_1 K_0 \left(\frac{r}{L} \right) \right].$$

Under the original GOPTWO modeling scheme the mass transfer coefficient was considered so large that the free stream concentration, C_g , existed at the surface of the graphite, $r = r_1$. The effect of the film is to lower the surface concentration (and all of the interior concentrations as well) to what the particular solution predicts. Thus, the reaction rates computed by GOPTWO must be multiplied by the ratio of the concentration that this equation predicts at $r = r_1$ to that which would be there with an infinite mass transfer coefficient, i.e., C_g . This ratio is

$$\Lambda = \frac{\beta \kappa_2}{\beta \kappa_2 - \frac{D}{L} \kappa_3}.$$

The above relationship yields, as it should, a value for this ratio between zero and unity, as the mass transfer coefficient increases from zero to infinity.