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SIMTRAN I—A Computer Code for the Simultaneous Calculation of Oxygen Distributions and Temperature Profiles in Zircaloy During Exposure to High-Temperature Oxidizing Environments

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METALS AND CERAMICS DIVISION

SIMTRAN I - A COMPUTER CODE FOR THE SIMULTANEOUS CALCULATION OF OXYGEN DISTRIBUTIONS AND TEMPERATURE PROFILES IN ZIRCALOY DURING EXPOSURE TO HIGH-TEMPERATURE OXIDIZING ENVIRONMENTS

S. Malang

NOVEMBER 1975

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FOREWORD

Postulated loss-of-coolant accidents (LOCA's) for light water reactors generally involve an excursion in temperature for parts of the reactor core in which the reaction of the Zircaloy fuel rods with the steam environment may become appreciable. The effects of the Zircaloy-steam reaction must be considered in the emergency core cooling system (ECCS) design because of their potential influence on both the thermal and mechanical behavior of the system. Thus, it is important to demonstrate a reliable method of evaluating and predicting quantitatively the extent of reaction during transient temperature exposures.

The Zirconium Metal-Water Oxidation Kinetics (ZWOK) program in the Metals and Ceramics Division of the Oak Ridge National Laboratory is generating kinetic data necessary for the above evaluation. An important part of this program is an investigation of the applicability of the models and mathematical treatments that can be used to describe the details of the reaction under transient temperature conditions. This is a complicated mathematical problem which can be handled satisfactorily only by computer techniques. While several analytical solutions and computer programs are available to examine simpler models of Zircaloy oxidation, the computer program, SIMTRAN I, described in this report, is a sophisticated calculation which yields a complete description of the oxygen distribution and temperature profiles for a variety of input or boundary conditions. The code is based on an ideal model which will eventually be tested by comparison of the theoretical and experimental results for a number of transient temperature excursions.

The code was written by Dr. Siegfried Malang, a visiting scientist on assignment to ORNL from Karlsruhe Nuclear Research Center. Since the editing and publication of this report has taken place since Dr. Malang's return to Germany, we apologize herewith - to Dr. Malang and to the readers - for any changes in meaning which have occurred as a result of the editing process. In addition, we would like to emphasize, as has been done in the body of the report, that while the program has survived numerous tests of its mechanical soundness, no serious testing has yet been accomplished that examines the individual or group accuracy of the input physical property, kinetic, or thermodynamic data for the Zircaloy-steam reaction. This aspect of the code's application will be reported at a later date when additional information to support a model verification will be available.

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ABSTRACT

SIMTRAN I is a Fortran IV computer program written for the IBM 360/91 system which solves SIMultaneously the TRANsport equations for both heat and mass flow for the one-dimensional, multiphase, moving-boundary, transient-temperature transport problem in a finite-geometry system defined by cylindrical coordinates. The code utilizes an ideal diffusion model which requires uniform layer growth of all phases and assumes the existence of thermodynamic equilibrium at all interfaces at all times. While SIMTRAN was constructed specifically for the consideration of oxidation phenomena during the reaction of Zircaloy fuel tubes with steam under high-temperature transient oxidation conditions, only minor changes are necessary to make it generally applicable to other materials and a number of oxidation, diffusion, and heat-transfer problems. A variety of boundary-condition options permit the mathematical simulation of a wide range of oxidation experiments.

The basic operational input to the code, which must include physical property, thermodynamic, and kinetic data over the desired temperature range, was selected from a variety of literature sources. Thus, while the results of the code yield acceptably accurate and self-consistent results in terms of the model and the mathematical operations, the user is cautioned to interpret the output results in terms of his confidence in his input information. The data presently incorporated into the code were assembled, at least in part, expediently and have not yet been subject to a critical evaluation either separately or as a whole (in terms of a model verification). Such information will be published at a later date.

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*On assignment to ORNL from Karlsruhe Nuclear Research Center, West Germany.

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1. INTRODUCTION

The cladding of nuclear fuel rods in water cooled reactors is the first barrier against the release of fission products. Its integrity is especially important in a postulated Loss of Coolant Accident (LOCA) since in this case the second barrier - the pressure vessel and the primary coolant cycle - is partly open to the reactor containment.

The cladding material in all water-cooled power reactors is Zircaloy. This alloy has a good corrosion resistance against water at normal operating temperature. During a LOCA, however, the cladding temperature may rise to high levels. At such temperatures, Zircaloy will react vigorously with steam, and the resulting exothermal reaction can influence significantly the temperature attained during such an event.

The amount of oxidation during a LOCA also has an important influence on the mechanical strength of the clad and therefore its integrity. While the total weight gain due to the oxidation is a rough measure of the change in mechanical strength, a complete examination of the oxidation phenomena is necessary for a more detailed analysis of the behavior of the clad.

In addition to the oxide layer, there are two different metallic phases which exist for partially oxidized Zircaloy, depending on the temperature and the oxygen concentration. Since the ductility of the material is strongly influenced by the oxygen concentration, the distribution of the oxygen is generally a more important variable than the total oxygen content. This distribution can be calculated by application of the basic laws of diffusion to the three different layers in an oxidizing specimen.

A computer code based on a finite difference analysis has been developed which can simultaneously solve the oxygen diffusion and heat conduction equations for a material consisting of up to three different layers. A wide range of arbitrary boundary conditions for oxidation and heat transfer on both surfaces of a specimen can be used. The code has been designed primarily for the investigation of Zircaloy oxidation. It can be used, however, for a variety of oxidation, diffusion and/or heat transfer problems in other materials.

2. PROBLEM DEFINITION

The oxidation of Zircaloy at temperatures above the α/β transition range involves the dissolution of oxygen into the metal as well as the growth of layers of oxide and oxygen-stabilized alpha. The particular case of the reaction of steam with a Zircaloy fuel tube during a typical hypothetical LOCA is a complicated example of this general sort of behavior.

As part of an effort to develop a predictive capability by which to describe the extent of the Zircaloy-steam reaction during non-normal or accident conditions, the computer program SIMTRAN I has been written. The basic assumption invoked in obtaining solutions to the mass-transport equations is that thermodynamic equilibrium is maintained at all boundaries, regardless of their rate of movement or the rate of temperature change. Supersaturation in all phases is permissible when arrived at by temperature changes, and must be dissipated by diffusion and uniform phase growth rather than by precipitation. The growth of all phases is assumed to take place uniformly, in the manner envisioned when applying the ideal diffusion equations. In addition, it is assumed that each transport equation is completely characterized by a single kinetic parameter, although this parameter is generally a function of the particular phase, the temperature, and the oxygen concentration.

SIMTRAN I utilizes finite difference techniques to solve, in cylindrical coordinates, the one-dimensional, multiphase, moving boundary diffusion problem in a tube wall of finite thickness. Physical property data, as well as kinetic and thermodynamic parameters serve as the basic input to the code which, on the basis of the ideal model, can then examine simultaneously both the heat and mass transport processes that occur during a given reaction. Both isothermal and transient temperature oxidation can be studied as well as oxidation in a particular reaction environment where self-heating of the specimen might take place. In addition, the high degree of flexibility in defining the boundary conditions in this program permits the modeling of a large number of useful reaction sequences.

3. MODEL, METHODS, AND ASSUMPTIONS

A finite difference approach is used for the calculation of both temperature profiles and oxygen distributions. The general finite difference methodology for diffusion in a system without moving boundaries is well known and will, therefore, be described only very briefly. More emphasis will be placed on the description of the specific method used here to deal with the problem of the moving boundaries.

3.1 General Method for the Calculation of Temperature Profiles and Oxygen Distributions

The method will be explained for a flat wall in order to keep the description as simple as possible. The code itself uses cylindrical coordinates.

The basic equations for one dimensional conduction and diffusion in a flat wall are

$$\frac{\partial T}{\partial \tau} = \alpha \cdot \frac{\partial^2 T}{\partial x^2} \tag{1}$$

$$\frac{\partial C}{\partial \tau} = D \cdot \frac{\partial^2 C}{\partial x^2} \tag{1a}$$

where

x [cm] = distance

τ [sec] = time

T [°C] = temperature

α $\left[\frac{cm^2}{sec}\right]$ = thermal diffusivity

C $\left[\frac{gram}{cm^3}\right]$ = concentration (i.e., oxygen in Zircaloy)

D $\left[\frac{cm^2}{sec}\right]$ = oxygen diffusion coefficient

The use of a finite difference method defines the wall as being divided into a number of nodes in which all the mass is assumed to be concentrated. These nodes are connected by "conductors" which "conduct" heat and oxygen. The differential equations (1) and (1a) are converted to the following difference equations:

$$\underbrace{\frac{T_n^* - T_n}{\Delta\tau}(\rho \cdot c \cdot v)_n}_{\text{change in stored heat}} = \underbrace{L_{t,n,n-1}(T_{n-1} - T_n) + L_{t,n,n+1}(T_{n+1} - T_n)}_{\text{net heat transport}} + \underbrace{q}_{\text{heat generation in node n}} \qquad (2)$$

$$\underbrace{\frac{C_n^* - C_n}{\Delta\tau} \cdot v_n}_{\text{change in oxygen content}} = \underbrace{L_{c,n,n-1}(C_{n-1} - C_n) + L_{c,n,n+1}(C_{n+1} - C_n)}_{\text{net diffusion}} \qquad (2a)$$

Equations (2) and (2a) show the heat and mass transport balances for the node n. T_n and C_n are the mean temperature and concentration values at the time τ; T_n^* and C_n^* are the corresponding values at the time $\tau + \Delta\tau$. The meaning of the other symbols is:

$\rho \left[\frac{\text{gram}}{\text{cm}^3}\right]$ = density

$c \left[\frac{\text{ws}}{\text{gram}^\circ\text{K}}\right]$ = specific heat

$v \left[\text{cm}^3\right]$ = volume

$L_t \left[\frac{\text{w}}{\text{K}}\right]$ = conductance, thermal conductor

$L_c \left[\frac{\text{cm}^3}{\text{sec}}\right]$ = conductance, oxygen 'conductor'

$q \left[\text{w}\right]$ = heat generated in node during $\Delta\tau$.

L_t and L_c can be determined with the equations

$$L_t = K \cdot \frac{A}{x} \tag{3}$$

$$L_c = D \cdot \frac{A}{x} \tag{3a}$$

where X [cm] is the distance between the two nodes and A the cross-sectional area [cm^2] of the conductor. K [$\frac{W}{cm \cdot K}$] is the thermal conductivity and D [$\frac{cm^2}{sec}$] is the oxygen diffusion coefficient. "A" is usually chosen to be 1 cm^2 for convenience. The equations (2) and (2a) have to be solved for each node. The sets of solutions comprise the temperature profiles and oxygen distributions as functions of time. Arbitrary boundary conditions as well as temperature dependent and concentration dependent material properties can be used with this method.

As part of the basis for the temperature calculation, it is assumed that a reaction heat (specified as 34330 $\frac{ws}{\text{gram oxygen}}$) is generated at the oxide-α interface. The heat which is necessary to split steam into O and H_2 at the gas-oxide interface must also be accounted for. The fraction of this energy supplied by the specimen is specified as an input.

3.2 Treatment of the Moving Boundaries

The basic assumption of the entire method is that the oxygen concentration on both sides of an interface between two phases is always the equilibrium concentration. Such an assumption is almost universal in isothermal, diffusion-controlled oxidation processes, but it is difficult to judge how accurate it is in transient temperature cases. Therefore, a particularly important check on the validity of the code will be its ability to predict the results of transient temperature oxidation experiments after the adjustment of the kinetic input parameters determined on the basis of the results of isothermal experiments. The treatment is presented without explicit consideration of density changes in the phases during oxidation. The method chosen to account for this effect is discussed in par. 3.7.

Two different methods are used for the treatment of the moving boundaries, depending upon the thicknesses of the oxide and alpha Zircaloy layers.

3.21 Oxide Layer Less Than 4 μm Thick

To avoid excessive computing time, the mesh sizes for the main diffusion calculations are chosen in such a way that the oxide layer must be at least 4 μm and the alpha layer at least 6 μm thick in order for the calculations to be made. To enable the code to describe the growth of very thin layers, a separate simplified method was developed that utilizes only two nodes in each of the oxide and alpha layers. This stipulation results in the assignment of linear concentration gradients to these thin growing layers. This method will be described with the help of Fig. 1 which shows the oxygen concentration profile near the surface. Only a few nodes in the beta layer are shown, but the code calculates over the entire wall.

The three oxygen fluxes, FLUX O, A, and B, are each kept constant during one time step $\Delta\tau$. The movement of the interfaces after each time step is calculated in the following way.

$$S_O^* - S_O = \frac{(\text{FLUX O} - \text{FLUX A}) \cdot \Delta\tau + S_O \cdot (\bar{C}_O - \bar{C}_A^*)}{\bar{C}_O^* - \bar{C}_A} \tag{4}$$

$$S_A^* - S_A = \frac{(\text{FLUX A} - \text{FLUX B}) \cdot \Delta\tau + S_A (\bar{C}_A - \bar{C}_A^*)}{\bar{C}_A^* - \bar{C}_B} \tag{5}$$

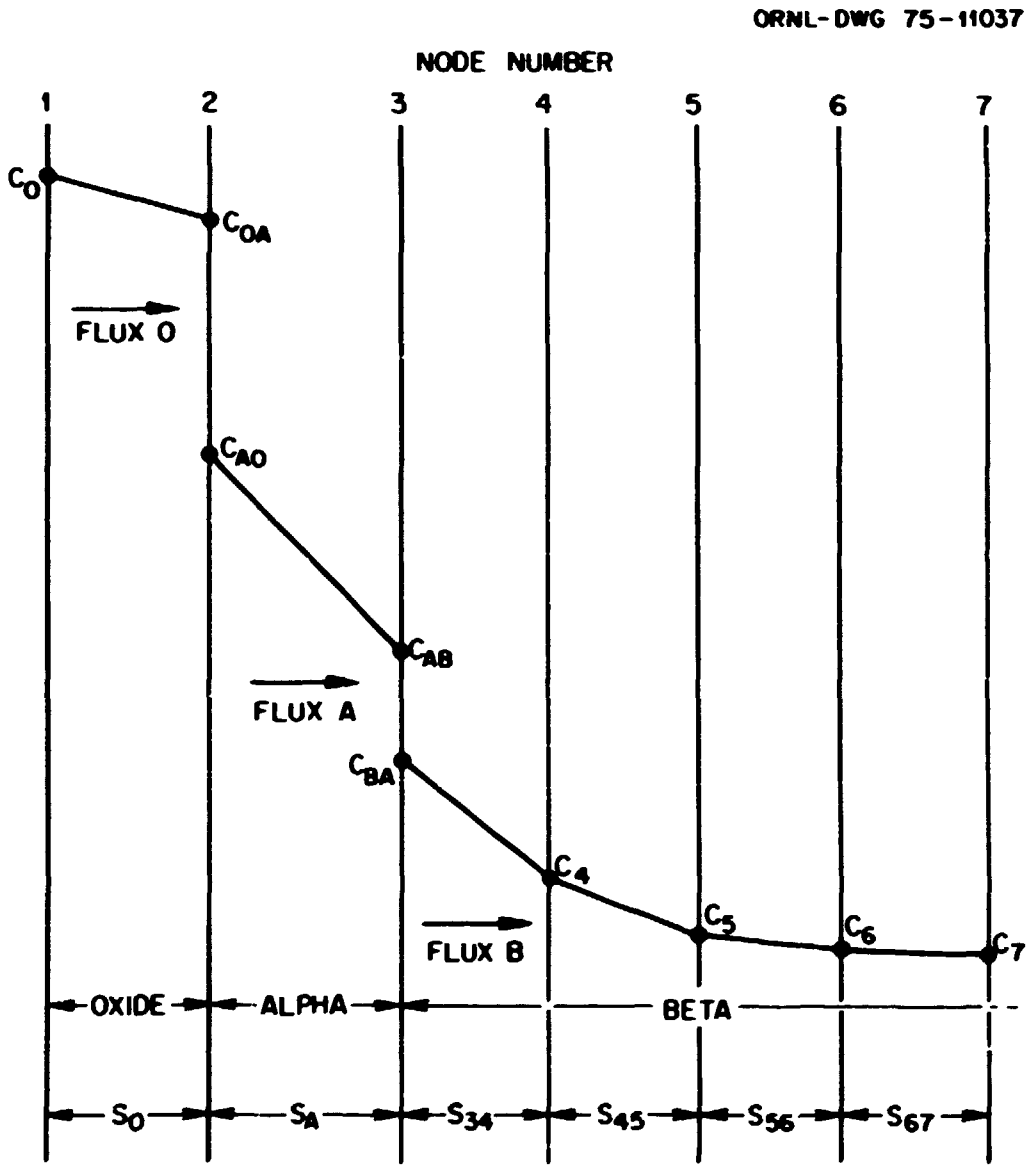


Fig. 1. Model for the treatment of moving boundaries for thin layers.

The meaning of the symbols is: (see Fig. 1)

$\Delta\tau$ [sec] time step

$$\text{FLUX O} = D_O \frac{C_O - C_{OA}}{S_O} \qquad (6)$$

$$\text{FLUX A} = D_A \frac{C_{AO} - C_{AB}}{S_A} \qquad (7)$$

$$\text{FLUX B} = D_B \frac{C_{BA} - C_4}{S_{34}} \qquad (8)$$

$\left[\frac{\text{gram}}{\text{cm}^2 \cdot \text{sec}}\right]$ oxygen fluxes

$\bar{C}_O = \frac{C_O + C_{OA}}{2}$	$\left[\frac{\text{gram}}{\text{cm}^3}\right]$	Average oxygen concentration in oxide.
$\bar{C}_A = \frac{C_{AO} + C_{AB}}{2}$	$\left[\frac{\text{gram}}{\text{cm}^3}\right]$	Average oxygen concentration in alpha-Zircaloy.
$\bar{C}_B = \frac{C_{BA} + C_4}{2}$	$\left[\frac{\text{gram}}{\text{cm}^3}\right]$	Average oxygen concentration in beta Zircaloy between nodes 3 and 4.
C_{OA}, C_{AO}, C_{AB}, C_{BA}, C_4	$\left[\frac{\text{gram}}{\text{cm}^3}\right]$	Concentrations at the various interfaces; see Fig. 1.
$\bar{C}_O^*, \bar{C}_A^*$	$\left[\frac{\text{gram}}{\text{cm}^3}\right]$	Concentrations after time step $\Delta\tau$. (Can be different from $\bar{C}_O, \bar{C}_A$ if temperature changed during time step.)
S_O, S_A	[cm]	Thicknesses of oxide and alpha layers at start of time step.
S_O^*, S_A^*	[cm]	Thicknesses of oxide and alpha layers at end of time step.

The concentration in the beta phase is calculated by using the general method described in section 3.1.

3.22 General Treatment of the Moving Boundaries

The concentration gradients and interface movement for oxide and alpha Zircaloy are computed by using the method described in section 3.21 for layer thicknesses up to 4 and 6 μm, respectively. For thicker layers, a different method is used which, in general, makes use of at least four nodes in each phase. These methods shall be described focusing on the profiles at the oxide/alpha interface as illustrated in Fig. 2.

The oxygen fluxes, FLUX OA and AO, and the concentrations are kept constant during the time step $\Delta\tau$. After this time step, the movement of the interface is calculated from the following equations:

$$S_{O1} \cdot \frac{C_{O1}+C_{OA}}{2} + S_{A1} \cdot \frac{C_{AO}+C_{A1}}{2} + (\text{FLUX OA} - \text{FLUX AO}) \cdot \Delta\tau$$

$$= S_{O1}^{*} \cdot \frac{C_{O1}^{*}+C_{OA}^{*}}{2} + S_{A1}^{*} \cdot \frac{C_{AO}^{*}+C_{A1}^{*}}{2} \qquad (9)$$

$$S_{O1} + S_{A1} = S_{O1}^{*} + S_{A1}^{*} \qquad (9a)$$

For a flat wall the oxygen fluxes would be:

$$\text{FLUX OA} = D_O \frac{C_{O1}-C_{OA}}{S_{O1}} \qquad (10)$$

$$\text{FLUX AO} = D_A \frac{C_{AO}-C_{A1}}{S_{A1}} \qquad (11)$$

The symbols are similar to those used in par. 3.21, with reference to Fig. 2. The code solves the equations (9) - (11) for cylindrical coordinates. The movement of the alpha-beta interface is treated in an identical manner.

The concentrations in the nodes inside the three layers are all calculated according to the methods outlined in section 3.1. The possible boundary conditions at the surfaces of the wall are described in the next section.

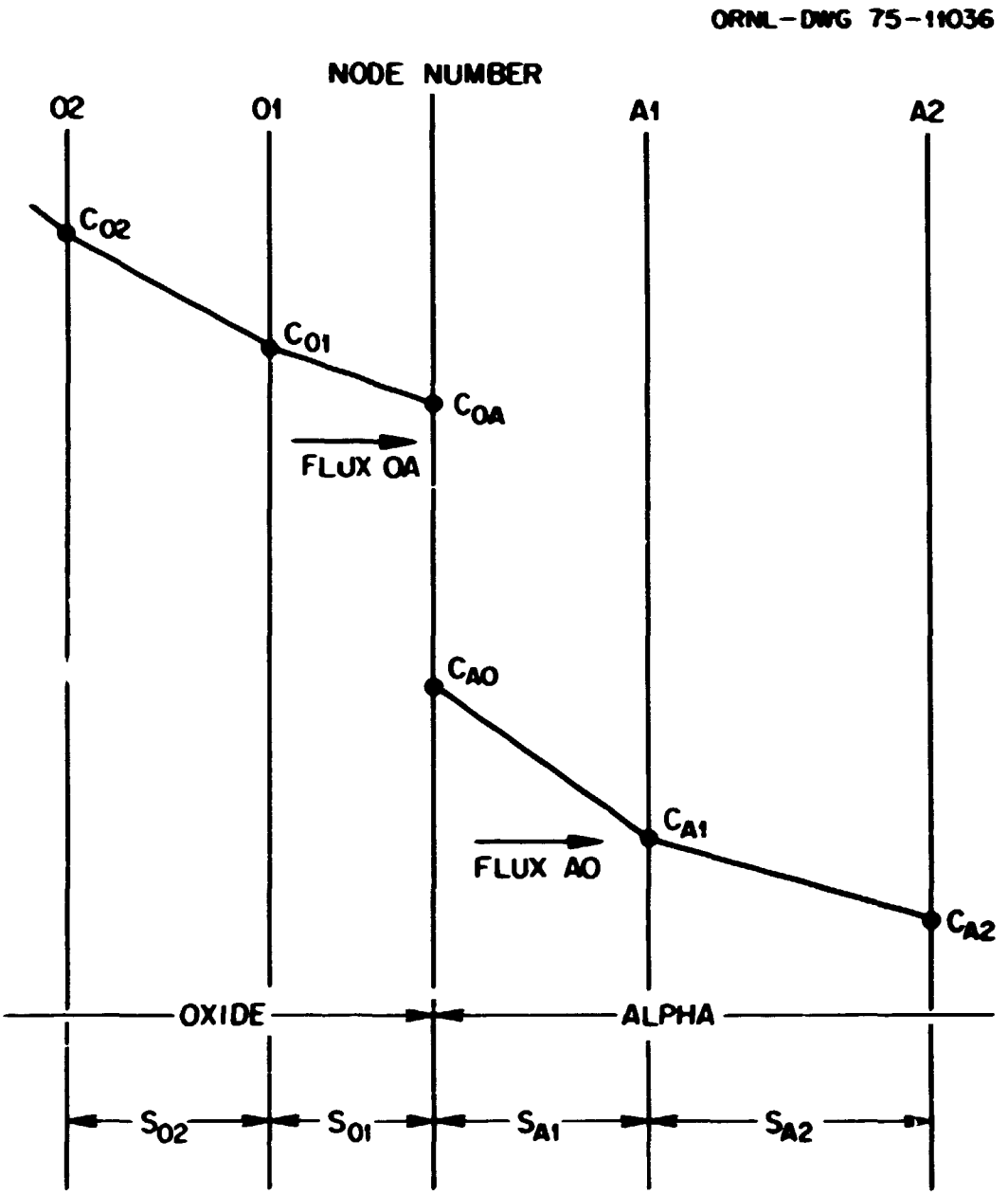


Fig. 2. Model for the general treatment of moving boundaries.

3.3 Boundary Conditions at the Two Surfaces of the Wall

The code allows for oxidation and/or heat transfer at the inner surface, at the outer surface, or at both surfaces of a hollow cylinder. All boundary conditions can be time dependent.

3.31 Boundary Conditions in Regard to Temperature Profile Calculations

Three kinds of heat transfer associated with each surface can be specified:

a) Convection, determined with h, T_{cool}

b) Radiation, determined with ϵ, T_{wall}

where T_{cool} is the temperature of the gas stream in contact with each surface; T_{wall} is the temperature of the surroundings with which the specimen exchanges heat by radiation; h is the convective heat transfer coefficient; and ϵ is the Stefan-Boltzmann constant.

c) Fixed heat flux (independent of specimen temperature or heat transfer by convection or radiation).

3.32 Boundary Conditions in Regard to Concentration Profile Calculations

An upper limit for the oxygen flux available to either surface can be specified. As long as the actual oxygen flux, determined by the diffusion constant and the concentration gradient, is smaller than this limit, stoichiometric oxide at the surface is assumed. Otherwise the concentration at the surface node is calculated with the equation:

$$C_1 = C_n + Q_{limit} \cdot (r_1 - r_n)/D \qquad (12)$$

where

$C_1 \left[\frac{gram}{cm^3}\right]$ = oxygen concentration at the surface.

$C_n \left[\frac{gram}{cm^3}\right]$ = oxygen concentration at the next node.

$r_1 - r_n \left[cm\right]$ = distance between the two nodes.

$Q_{limit} \left[\frac{gram}{cm^2 \cdot sec}\right]$ = upper limit for oxygen flux to the surface.

$D \left[\frac{cm^2}{sec}\right]$ = diffusion coefficient.

The purpose of the variable O_{limit} is to allow the effect of gas phase control of the oxidation rate, or "steam starvation," to be observed. In the present version of the code, O_{limit} is an input which can be time dependent. If this variable (for either side) is specified in the code as uniquely zero, then no oxidation takes place on that side. If intermittent oxidation (i.e. oxidation-annealing steps or tube-burst simulation) is desired, then the oxygen flux limit for the periods when no oxidation is taking place is given by some small number greater than zero, such as 1×10^{-2}.

3.4 Selection of Mesh Sizes

It can be shown that the stable time step for the integration (see section 3.5) is proportional to the square of the mesh size. Since the number of nodes increases linearly with decreasing mesh size, the computing time increases approximately with (1/mesh size)^3. Therefore, it is important that small mesh sizes be used only at the places and times when it is really necessary. For example, for temperature calculations a larger mesh size should be used in the metal than in the oxide since the thermal conductivity in the metal is much larger and, therefore, the temperature gradients much smaller.

Similarly for diffusion calculations, a larger mesh size can be used in the beta phase than in the alpha phase or the oxide. In addition, it would be desirable to keep the number of nodes in the oxide and alpha layer approximately constant, independent of the layer thickness. For all these reasons, up to seven different mesh sizes may be used to complete a typical calculation. This means that the mesh size can and will vary as a function of purpose (temperature or diffusion calculation), phase (oxide, alpha, or beta), and layer thickness (and, therefore, time). To determine the smallest mesh size, DR, the largest integer M for the equation

$$DR = \frac{\text{wall thickness}}{M-2} \geq 1 \ \mu m \qquad (13)$$

is calculated. This basic (minimum) mesh size is used for diffusion calculations in the thinnest oxide and alpha phases only. For other purposes, mesh sizes determined by multiplying DR by 2, 4, 8, 16, 32, or 64 are used. The particular mesh sizes for specific uses can be seen in Table 1. It should be mentioned, however, that the interfaces between the different phases do not have to be exactly at the location of a node but may be located between them.

For the selection of the mesh size for diffusion calculations, the following guidelines are used.

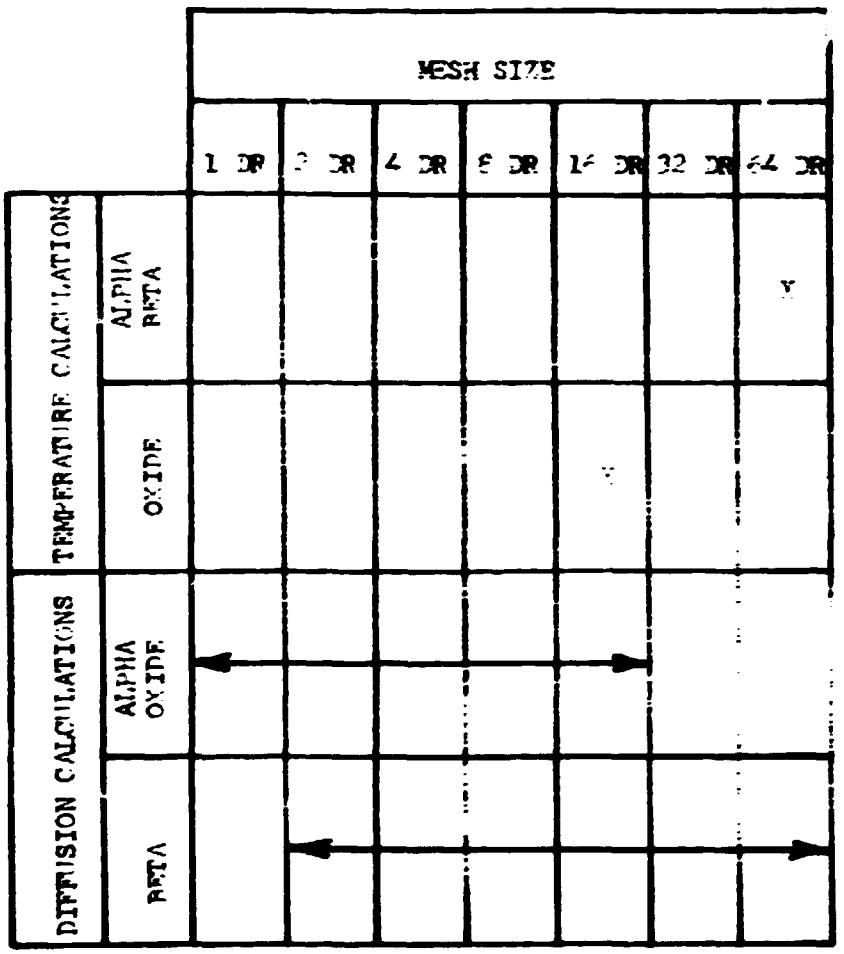
a) mesh size in alpha = mesh size in oxide
b) mesh size in beta = 2 x mesh size in alpha for the 10 meshes adjacent to the α/β interface, otherwise 64 DR.
c) oxide layer is divided into at least 2 meshes
d) alpha layer is divided into at least 3 meshes
e) not more than 8 meshes in alpha layer if this is not a contradiction to c), given condition a)
f) not more than 8 meshes in oxide layer if this is not a contradiction to d), given condition a).

Using these guidelines, the mesh sizes can increase or decrease during the computation, depending on which direction the interfaces are moving, in order to create a balance between accuracy and computing time.

3.5 Integration Method

In cases with fast temperature changes, the heat conduction equation (2) and the diffusion equation (2a) have to be solved simultaneously since the diffusion constants and equilibrium oxygen concentrations, especially, are strongly temperature dependent. The most simple method to do this is to use an explicit integration scheme. An explicit method, however, has the disadvantage of having a very small stable time step, which can lead to a very long computing time for many useful types of cases. To keep the option for the implementation of an implicit method open, the concentration and temperature integrations are performed in

Table 1. Mesh sizes utilized in computations



separate subroutines. An alternate integration scheme can, therefore, be added without too many problems. As a first approach, a compromise was made by using an explicit integration utilizing up to four different time steps.

The appropriate stability criteria are given by the equations:

$$\Delta\tau_a \leq \frac{(c \cdot \varrho \cdot v)_n}{\bar{\kappa}_{t,n,n-1} + \bar{\kappa}_{t,n,n+1}} \tag{14}$$

$$\Delta\tau_b \leq \frac{v_n}{\bar{\kappa}_{c,n,n-1} + \bar{\kappa}_{c,n,n+1}} \tag{14a}$$

where

$\Delta\tau_a$ = stable time step for the finite difference equation for the temperature calculations

$\Delta\tau_b$ = stable time step for the finite difference equation for the concentration calculations.

The meaning of the symbols is the same as in Eq. (2) and (2a).

In addition, use is made of $\Delta\tau_c$, a maximal time increment during which all boundaries and material properties for temperature calculations are kept constant, and $\Delta\tau_d$, a maximal time increment during which all boundaries and material properties for concentration calculations are kept constant.

Equations (14) and (14a) have to be applied to each node, and the smallest of the two stable time steps, $\Delta\tau_a$ and $\Delta\tau_b$, is used. It can be seen that $\Delta\tau_a$ and $\Delta\tau_b$ depend only on the mesh size and the values of the thermal conductivity or diffusion constant. If $\Delta\tau_a$ or $\Delta\tau_b$ is small, then this small step has to be used even for very slow transients to insure stability of the finite difference solutions. However, in this case it is practical to change the model so that the much larger time increments $\Delta\tau_c$ and $\Delta\tau_d$ can be used. Therefore, provisions are made in the code so that a number of $\Delta\tau_a$ (stable) steps can be performed between a single $\Delta\tau_c$ step; similar provisions are made for $\Delta\tau_b$ and $\Delta\tau_d$. The calculations which have to be repeated for each step $\Delta\tau_a$ and $\Delta\tau_b$ are kept as simple

as possible. The test runs showed that this approach together with the automatic time step control (see section 3.4) leads to a reasonable computing time for diffusion calculations for both high and low oxidation temperatures. Only if a detailed temperature calculation is desired for cases with low oxidation temperatures will the computing time be excessively long. A "lumped" (see par. 5.1) temperature calculation would be more appropriate for those cases. A rough rule of thumb for the computing time in reasonable cases is, for an IBM 370/168, that about 1.5 min is required for each 1000 Å movement of the Si/SiO2 interface. Due to the automatic time step control, the computing time is not highly dependent on oxidation temperature and layer thickness.

3.4 Time Step Control

The optimal time step for temperature and concentration calculations varies over a wide range. This is due to the strong temperature dependence of the material properties, especially the diffusion constants. In addition, the optimal time step depends on the mesh size which varies with layer thickness. Therefore, the time step may vary from 10^{-7} sec to a few seconds in a single experiment.

It would be very difficult if not impossible to find manually a satisfying compromise between precision and computing time. Therefore, an automatic time step control has been chosen. Using this feature, the user has only to specify the time step for printing out the results. The code uses the four different time steps mentioned in section 3.3 for calculation. There are different levels of control. The first level assures stable time steps for temperature and concentration calculations. These time steps are determined with Eq. (14) and (14a), and the values are never exceeded. They are used for the integration in the explicit method. The next level controls the time steps during which all boundary conditions and material properties are kept constant. These steps can be specified by the user, but they are checked by the code itself. The code calculates upper limits which are actually used if the step specified by the user is larger than the calculated upper limit or if the step size is not

specified at all. These upper limits are calculated so that the following conditions are not exceeded during the time step:

1. For the temperature profile calculations, the temperature at the wall surface does not change by more than 1°C.
2. For the concentration profile calculations,
   (a) the oxygen gain at one surface is limited to the amount which is necessary for the oxidation of $2 \cdot 10^{-6}$ cm Zircaloy to stoichiometric oxide;
   (b) the oxide - α interface shall not move more than $2 \cdot 10^{-4}$ cm; and
   (c) the γ/α interface shall not move more than $5 \cdot 10^{-6}$ cm.

The values specified above are not inputs to the code. A user, however, can change them easily if desired. They are only the result of a first approach and could be optimized later in a sensitivity analysis. It is not recommended, however, that the user generally attempt to specify the time steps as an input.

3.7 Volume Changes Associated with Oxidation

It is assumed that the entire volume increase associated with the oxidation of Zircaloy to Zircaloy oxide takes place in one dimension. In all the calculations, however, the properties of a fictive material are used instead of those of the "real" oxide in order to facilitate the keeping of the mathematical origin ($x = 0$) at the original wall surface. Only for the output of the program is the increase in wall thickness due to oxidation calculated. To determine the properties of this fictive material, the following conversion factor is calculated:

$$\text{FICFAC} = \frac{\text{DENZIR}}{\text{DENZRO} - \text{OSTOCH}} \qquad \left[\frac{\text{cm}^3 \text{ oxide}}{\text{cm}^3 \text{ metal}}\right] \text{ volume ratio} \qquad (15)$$

where

DENZIR $\left[\frac{\text{gram}}{\text{cm}^3}\right]$ = density of Zircaloy

DENZRO $\left[\frac{\text{gram}}{\text{cm}^3}\right]$ = density of ZrO_2

OSTOCH $\left[\frac{\text{gram}}{\text{cm}^3}\right]$ = oxygen density in stoichiometric ZrO_2

The conversions between the real values of the properties in the oxide and the fictive values (written with +) are:

$S^+ = S/FICFAC$	layer thickness
$D^+ = D/FICFAC^2$	diffusion constant
$C^+ = C \cdot FICFAC$	oxygen concentration
$(C_p \cdot \rho)^+ = C_p \cdot \rho_{ZrO_2} \cdot FICFAC$	heat capacity
$K^+ = K/FICFAC$	thermal conductivity

The volume change associated with the transition from β-Zircaloy to α is neglected as well as the small effect of oxygen concentration on the density in all the phases.

4. GENERAL FEATURES OF THE CODE

The features of the code development can be summarized as follows:

1. The code permits simultaneous determination of the temperature and oxygen profiles for a variety of typical oxidation experiments.

2. All material properties input to the program are located in separate subroutines so that changes can be made easily.

3. All physical, thermodynamic and kinetic variables are input to the program as temperature dependent functions.

4. Diffusion constants may be designated as concentration dependent, if desired.

5. It is possible to specify an upper limit for the oxygen flux into the wall, which permits the effects of gas-phase control of the kinetics to be examined.

6. Oxidation and heat transfer may occur at either or both free surfaces of the tube.

7. All boundary conditions may be time dependent.

8. Options are included for performing several simpler oxidation calculations such as total oxygen calculations based on the data of Baker-Just, Hobson, or Lemmon.

9. Options are provided whereby either a complete temperature profile may be calculated, or the temperature calculated on the basis of no temperature gradient (Lumped). The latter is useful when gradients are expected to be small, and it results in an appreciable saving in computation time.

Figure 3 shows the flow chart for the code. The general outline and the calling sequence for the subroutines are shown. In the following sections, the purpose of each subroutine is described briefly.

4.1 Main Program, SIMTRAN

This is a short and simple program which calls the different subroutines where the various computations are accomplished. In addition, the time step control and selection described in section 3.6 is performed here.

4.2 Subroutines INPUT and INDATA

These routines read all the input data and print them out. No elaborate calculations are made.

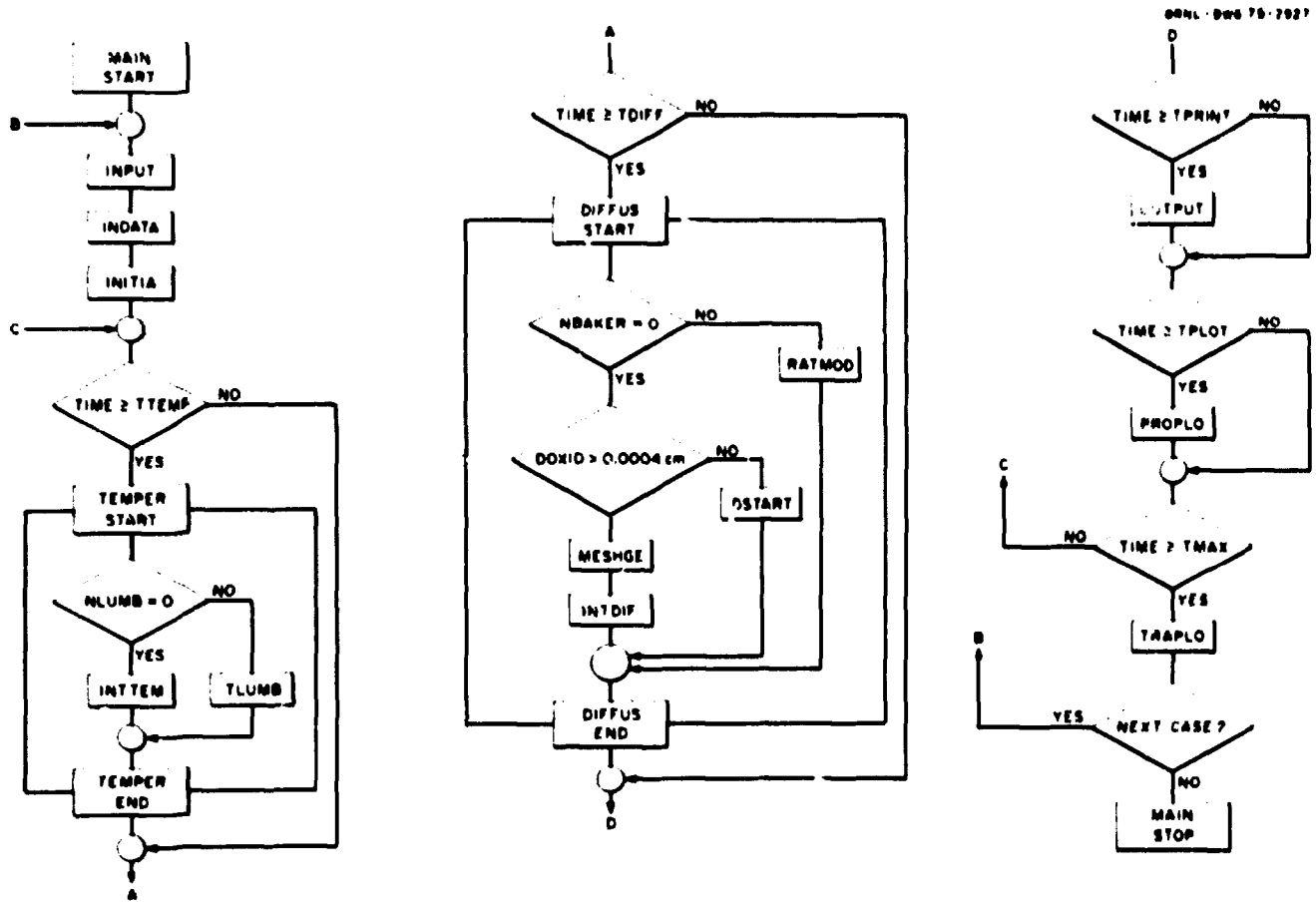


Fig. 3. Flow chart for SIMTRAN I

4.3 Subroutine INITIA

In this routine, initial values are assigned to a number of boundary condition variables.

4.4 Subroutines TEMPER, TLUMB, and INTTEM

In TEMPER, the temperature calculation is prepared. If the option for a lumped temperature calculation is used, the subroutine TLUMB is called and the temperature calculated there. The subroutine INTTEM is called for the calculation of the temperature distribution across the wall.

4.5 Subroutines DIFFUS, DSTART, MESHGE, INTDIF, and RATMOD

These are the largest and most complicated subroutines of the code. They calculate the oxygen distribution throughout the wall. The controlling routine is DIFFUS. Depending upon the layer thickness and other specified options, the other subroutines are called. DSTART performs the complete diffusion calculation for thin oxide and α layers. For thicker layers the calculation is prepared in DIFFUS and MESHGE, and the integrations to provide values of total oxygen uptake are performed in INTDIF. RATMOD is used for the total-oxygen calculations based on the Baker-Just, Hobson or Lemmon data. With these equations it is assumed that all the oxygen consumed forms stcichiometric ZrO_2.

4.6 Subroutines OUTPUT and PREPAR

OUTPUT prints out the results in specified time steps. It calls PREPAR to calculate the oxygen content in each phase and to prepare the variables for plotting.

4.7 Subroutines PROPLO and TRAPLO

PROPLO is a cathode ray tube (VIDEO) plotting routine which plots the oxygen profile in the wall in specified time steps. The time steps

are chosen as multiples of the output time step. The concentration can be plotted in two different scales which are selected by the user. With one scale the profiles in oxide, α- and β-Zircaloy are plotted; with the other, only the α and β profiles are plotted. The user can select one of them or both.

TRAPLO is a pen-and-ink (CALCOMP) plotting routine which plots up to 25 output variables as functions of time or square root of time. Both routines use the standard plotting package of the ORNL-computers which is described in Appendix A.

4.3 Functions for Material Properties

The code must contain a set of functions for the calculation of the material properties. No claim is made that the equations presently used for these functions are the best ones. They are rather considered to be reasonable values which may be used for testing purposes.

For every case, a table with the material properties in the range from 750°C to 1500°C (1382–2732°F) is calculated and printed with the subroutine MATMAP. The subroutines which furnish these data to the computational routines are:

1. INTFAC: Calculates equilibrium oxygen concentrations at all phase boundaries.
2. DIFCON: Calculates oxygen diffusion constants for all phases.
3. CONDUC: Calculates thermal conductivity for all phases.
4. SPEC: Calculates heat capacity (product of specific heat and density) for all phases. This subroutine is presently utilized to account for the heat of the α-β transformation by appropriately modifying the specific heat input.

The temperature application limit of these functions is presently arbitrarily restricted to a maximum of 1850°C (3362°F) (melting point of Zircaloy). A lower limit of 850°C (1562°F) is arbitrarily set in INTFAC for the solubility data calculations. Except for specific heat values,

these temperature limits are used for the calculation of the material properties, and arbitrary constant values are applied outside these limits. It should be realized, of course, that the oxidation model applied by the program is not valid outside the temperature range approximately 850-1500°C (1562-2732°F) in any event.

5. DESCRIPTION OF THE INPUT AND OUTPUT DATA

All input and output data are listed in Appendix B and C. In addition, three sample problems are given in Appendix D. Therefore, the description here is restricted to the use of the major options.

5.1 Temperature Calculations

The particular option for this calculation is specified with the variable NLUMB (card 4, field 1-10). There are three different options:

a) NLUMB = 0

The complete temperature distribution across the wall is calculated. This calculation increases the computing time considerably. In cases where the temperature gradients are expected to be small, options (b) or (c) can be substituted with little loss in definition.

b) NLUMB = 1

The entire wall is treated as one node only (referred to as a "lumped" calculation). The temperature is calculated as a function of heat transfer at the two surfaces and the heat generation associated with the oxidation. The nature of the heat transfer is specified in data cards 5 and 6. Every combination of oxidation, convective heat transfer, radiation, and fixed heat flux can be specified for each surface.

c) NLUMB = 2

With this option, the wall temperature is identical with the variable TSTEAM(1) (card 5, field 21-30). No heat transfer coefficients have to be specified. If TSTEAM (1) is zero, TSTEAM(2) (card 6, field 21-30) is used instead.

5.2 Concentration Calculations

The surface where oxidation occurs is specified with the variables HDIFF(1) and HDIFF(2) (card 5 and 6, field 1-10) which set the maximum oxygen flux available at each surface. If there is oxidation on one or both surfaces, the corresponding HDIFF has to be greater than zero. After oxidation has occurred on a given surface, HDIFF can then be made arbitrarily small (but not zero) for the remainder of the transient or for a part of it. Thus, intermittent oxidation - annealing steps can be considered.

If the oxygen distribution in the wall is to be calculated, the variable NBAKER (card 4, field 11-20) has to be zero. For:

a) NBAKER = 0,

the oxygen concentration profile is calculated as a function of time, starting with a constant concentration across the wall, given by CSTART (card 11, field 11-20).

b) NBAKER > 0,

only the total oxygen gain is calculated. It is assumed in this case that all the oxygen forms stoichiometric oxide. There are no provisions for limiting the oxygen supply. Specifically, for:

b1) NBAKER = 1, the Baker-Just equation is used.

b2) NBAKER = 2, the Hobson equation is used.

b3) NBAKER = 3, the Lemmon equation is used.

6. CONCLUSION AND OUTLOOK

A number of cases with a variety of boundary conditions have been considered with the code for testing purposes. Preliminary results have shown excellent mechanical operation and self-consistency in the calculations. Further testing and model verification is in progress.

So far, it has been shown that in nearly all practical cases, a lumped (single-node) temperature calculation is adequate; this leads to

a considerable saving in computer time compared to the more detailed temperature calculation. Generally, the maximum temperature difference in a specimen exceeds one to two degrees only in cases where comparatively thick oxide layers exist and where a large heat flux through the wall is specified by the experimental conditions.

No attempt has been made yet to select or to adjust the equations for the materials properties in order to get the best possible agreement between calculation and experiment. To aid in this purpose, a specialized version of the code will be developed which utilizes experimental data from isothermal oxidation rate measurements as input and selects by an optimization scheme the "best" diffusion constants and equilibrium concentrations for all three phases as functions of temperature. We consider such an optimization step to be of great importance, and all users of the code are strongly advised to keep this fact in mind. The various material parameters contained in the code were selected from a variety of literature sources, and at this time we can offer no assurances as to their correctness despite the fair agreement we have obtained between calculated and early experimental results. The final verification of SIMTRAN I awaits the completion of the experimental phase of our program, and not until that time will we be able to comment on the applicability of the code to the steam-Zircaloy reaction over a wide temperature range or on the validity of the material parameters presently incorporated in the code.

APPENDIX A

DESCRIPTION OF THE PLOTTING ROUTINES*

A1. Calcomp Pen and Ink Plotter Subroutines

The Calcomp tape transport accepts a seven-track magnetic tape written on the IBM/360 computers in a special format and uses data from this tape to drive the pen and ink plotters. The basic plotting package may be called by FORTRAN programs. A description of the subroutines and their calling sequences follows. The basic plotting package performs all necessary manipulations to generate the tape for plotting.

The package computes the incremental steps necessary to move the plotter from its current (X,Y) position to the (X,Y) position given in the calling sequence. The data generated are stored in an array and written onto magnetic tape each time the array is filled or when an end-of-graph call is given. Sequential graph addresses are generated for each graph written, and the graph address is displayed to the Calcomp operator as plotting progresses.

Subroutine PLOTS has two entry points. The first entry, PLOTS, is used to initialize the routine by transmitting parameters indicating the location of a storage area available to the routine and the length of the storage area. The second entry, PLOT, is used to convey coordinate data to be converted into incremental plotter commands.

Initialization Entry - CALL PLOTS (A, LENGTH)

A is the first location of a storage area which may be used by the routine for accumulating data to be written on tape. Normally, an array is set aside for this purpose.

LENGTH is an integer such that 47 ≤ LENGTH ≤ 8191 which specifies the number of consecutive four-byte locations beginning with location A available to the routine. If A is an array, then LENGTH is the dimension of the array. For plotting efficiency, the value of LENGTH should be

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*Taken from "Programmer's Notebook," Computer Science Division, Oak Ridge National Laboratory, Section 13, (June 1975).

between 3000 and 5000. The programmer must not use that portion of storage from location A through location A (LENGTH) at any time between the initialization of the package and the final use of the routine.

Plotting Entry - CALL PLOT (X,Y,I)

This call generates the necessary plotter commands to move the pen in the nearest approximation of a straight line from the current (X,Y) position to the (X,Y) given in the calling sequence. The arguments are as follows.

X is the abscissa in inches expressed in floating point.

Y is the ordinate in inches expressed in floating point.

I is an integer which specifies whether or not the pen is to contact the paper while moving to the new (X,Y) position. The sign of I specifies either a continuation of the current graph ($I \geq 0$) or an end-of-graph call ($I < 0$).

If $|I| \geq 3$, the pen will be lifted prior to execution of the movement to given (X,Y) position; if $|I| = 2$, the pen will be lowered and a straight line drawn to the given (X,Y) position; and if $|I| = 0$ or 1, the pen will not be altered. If $I < 0$, the command will be interpreted as an end-of-graph call, and following movement to the given (X,Y) position, the X reference point will be set to 0 to establish a new origin for the following graphs. Note also that $|I|$ will determine whether the pen is lifted on this final call for each graph. The end-of-graph call also causes any data remaining in the storage area to be written out and the sequential graph number to be incremented. PLOT keeps track of the current status of the pen so that redundant pen commands are not generated.

Subroutine SYMBOL. - This routine provides the programmer with the ability to draw alphanumeric characters. It may be used for labeling, annotation, data point plotting, legends, etc. It allows the programmer to choose the size of the characters and the orientation to suit himself. One hundred twenty-seven alphanumeric characters are available in the SYMBOL routine.

The calling sequences and arguments are given below.

Entry - SYMBOL. - Two functions are served by this entry point. Although the calling sequences are very similar, each will be described individually to avoid confusion. The normal entry is used for titles, identification, etc. The calling sequence is

CALL SYMBOL (X,Y,H,BCD,THETA,N),

where

X is the abscissa of the left edge of the first character to be drawn.

Y is the ordinate of the lower edge of the first character to be drawn.

H is the height, in inches, of the characters to be drawn and $H \geq 0.035$. Best results will be obtained if H is an integral multiple of 0.035; e.g., 0.035, 0.07, 0.105, 0.14 ... . The width of a character is four-sevenths of the height.

BCD specifies, in either of two forms, the alphanumeric characters to be drawn. The argument may (1) list the BCD characters; e.g., ..., 17HALPHANUMERIC DATA, ..., or (2) be the address of the first element of an array containing BCD characters; e.g., ..., BCDARY(1), ...

THETA is the angle, in degrees, expressed in floating point at which the characters are to be written. THETA is measured counter-clockwise from the positive X axis; hence for THETA = 0.0, the characters are drawn left to right parallel to the X axis. For THETA = 0.0, the sine and cosine are not computed, but for any other angle, SIN and COS are called. If a string of characters is to be drawn at an angle other than 0.0, the entire string is rotated with the (X,Y) given in the calling sequence as the pivot plant.

N is an integer which specifies the number of characters to be drawn.

If N > 1, spacing between the characters is accomplished automatically and is one-half the width of the characters.

The second function of this entry is to provide plotting of data points with the option of connecting consecutive data points with a straight line. The calling sequence is

CALL SYMBOL (X,Y,H,ICHAR,THETA,L),

where

X is the abscissa, in inches, of the center of the character.

Y is the ordinate, in inches, of the center of the character.

H is the height, in inches, of the character and H ≥ 0.02. Best results in this sequence will be obtained if H is an integral multiple of 0.02.

ICHAR is an integer which determines which symbol is to be plotted.

THETA is the angle of rotation as previously described.

L is a negative integer which indicates whether or not the points are to be connected with a straight line. If L = −1, the character will be plotted without a straight line being drawn from the previous (X,Y) position.

If L < −1, a straight line will be drawn from the previous (X,Y) to the given (X,Y) and the symbol will then be drawn. Note that L must be negative or the subroutine assumes a normal calling sequence as previously described. Only one character per entry is drawn in this calling sequence. At the completion of any of the centered symbols, the pen is at the (X,Y) position given in the calling sequence and the pen is DOWN.

Subroutine NUMBER. - This is a subroutine to convert a machine format number to its decimal equivalent and plot it according to a specified format. The calling sequence is

CALL NUMBER (S,Y,H,A,THETA,nHFORMAT),

where X,Y,H, and THETA are as described in the normal entry to subroutine SYMBOL. A is the name of the machine format number to be converted and

plotted. The type (integer or real) must conform to the FORMAT specified. nHFORMAT is a BCD argument which specifies the manner in which the number is to be converted and plotted. The nH portion of this argument is the normal FORTRAN method for transmitting BCD characters to a subroutine. The FORMAT portion is one of the four numeric format specifications I, E, F, or D. Examples of this argument are 5HE12.5, 4HF8.3, 2HI5, 5HD10.3. The FORMAT specification must not exceed six characters, and scale factors must not be used. The total field width must not exceed 99 characters. The numbers are converted by the standard library conversion routines and are right-adjusted in the field. This subroutine is designed primarily for annotation where a single number is involved.

A2. Subroutine CRT for the Cathode Ray Tube Plotter

Subroutine CRT writes the plot commands on a 9-track tape for the cathode ray tube plotter. The basic calling sequence is

CALL CRT (ARG1, ARG2, IARG3, MODE)

The action taken depends on the value of MODE. The possible actions are described in the following sections and summarized in Table A1.

It is convenient to think of this plotter as writing on a page with a normal plotting area of 11" x 17" plus a margin on each side of about 1". If the user does not specify his own origin and scaling factors, the subroutine CRT will set up an 11" x 17" coordinate system with origin at the lower left corner of the normal plotting area. A request to move the beam from position (0.,0.) to position (4.,0.) will then produce a horizontal line along the bottom of the normal plotting area. Whether or not this line will be visible depends on the beam intensity requested for this beam movement.

Table A1. Summary of modes in CRT(ARG1,ARG2,IARG3,MODE)

ARG1[1]	ARG2[1]	IARG3[2]	MODE[3]	ACTION
buffer name	buffer length (integer)	'your name$'	0	Initialization
position X,Y		beam intensity indicator IZ	1	Move the beam
			-1	Find present beam coordinates
position X,Y		see Table 3	2	Write block numbers or advance film or close tape file
dummy YDUM,YDUM		IBLOCK	-2	Find last block number
XORG	YORG	beam intensity offset IZORG	3	Change offset values
			-3	Find present offset values
XFACT	YFACT	dummy IDUM	4	Change scale factors
			-4	Find present scale factors
position X,Y		point intensity indicator IZ	5	Plot a point
position X,Y		beam intensity indicator IZ	6	Ignore limit switches and move beam
dummy YDUM,YDUM		IZSET	7	Change IZSET
			-7	Find present IZSET

1 ARG1 and ARG2 are floating-point numbers, REAL*4 or REAL*8 (except when MODE=0).
2 IARG3 is a 4-byte integer (except when MODE=0).
3 MODE is a 4-byte integer.

As this line is produced on the cathode ray tube it is also recorded by a 35 mm camera. The film is advanced to a new frame for each new plot. Later, the film is developed and sent to the user.

Subroutine CRT may be called by Fortran programs and is included in the standard Fortran library on disk.

MODE=0, Initialization

CALL CRT (BUFFER,NBUFF,'YOUR NAME$",0)

This is an initialization call and must precede all other calls to CRT. Normally it is done only once and normally the subroutine will ignore further initialization calls. However, it is possible to force the system to reinitialize by setting NBUFF < 0.

BUFFER is the symbolic name of an array that CRT may use as an output buffer.

|NBUFF| is the number of 4-byte words in the array that CRT may use. Normally, it is the DIMENSION of BUFFER. 3000 ≤ NBUFF ≤ 5000 is recommended.

'YOUR NAME$' Your name (12 characters or less) followed by a $, within apostrophes. This will be used to plot a special identification frame on the film strip.

MODE=1, Moving the Beam and Plotting Lines

CALL CRT (X,Y,IZ,1)

X,Y represents the position to which the beam will be moved from its present position. However, X and Y will be translated and scaled, as described below. X and Y must be floating-point numbers, either single or double precision, REAL*4 or REAL*8.

IZ indicates the intensity to be used, as described below.

All movements are made to positions defined by coordinates relative to an origin. The initial origin (0.,0.) is always in the lower left corner of the normal plotting area. However, by using a call with MODE=3, a translated origin (XORG,YORG) may be obtained, and subsequent plotting

will be relative to the new origin. Each movement is made in a straight line approximation from the present position to a new position (ABSC,ORD) calculated from the first two arguments (X,Y) of the call statement. The coordinates are translated and scaled as follows:

$$ABSC = (X+XORG) * XFACT$$

$$ORD = (Y+YORG) * YFACT$$

(ABSC,ORD) are the translated and scaled coordinates, in inches, relative to the lower left corner.

(X,Y) are the first two arguments given in the calling sequence and represent the new position in the user's coordinate system.

(XORG,YORG) is the present position of the origin relative to the lower left corner, in user's units. XORG and YORG are initially 0. but they may be changed by a call with MODE=3.

XFACT and YFACT are scaling factors for abscissa and ordinate values respectively. For a movement parallel to the X-axis, XFACT *(distance in user's units) = distance in inches. XFACT and YFACT are initially 1.0 but they may be changed by a call with MODE=4. If XFACT=YFACT=1.0, a line of length 1.0 will be 1.0 inches long on an 11" x 17" print. If X and Y values both range from 0. to 100. and if one wants a square picture, then appropriate scaling factors are XFACT=YFACT=0.11.

With the Model 835 plotter it is possible to have 30 different intensity levels. The beam intensity is calculated from the third argument (IZ) in the call statement. If the value of IZ is zero, the beam is turned off. If the value is 99, the routine uses a value IZSET stored in the subroutine. IZSET may be changed by a call to CRT with MODE=7.

If IZ is not 0 or 99, the true beam intensity IZTRUE is IZ offset by the value of IZORG.

IZTRUE = 0 if IZ = 0

IZTRUE = IZ+IZORG if IZ ≠ 0 and IZ ≠ 99

IZTRUE = IZSET+IZORG if IZ = 99

IZTRUE is the beam intensity request transmitted to the plotter.

IZ is the value specified by the argument in the call statement.

IZORG is a positive or negative intensity level offset. IZORG is initially 0 but may be changed by a call with MODE=3.

IZSET is a value stored for use when IZ=99. Initially, IZSET=16.

If IZTRUE is zero or negative, the beam will be turned off. If it is between 1 and 30, it is the intensity level used, and the beam will be turned on. If IZTRUE is greater than 30, the intensity used is [(IZTRUE+1) mod 32 − 1].

IZTRUE=16 is a typical intensity for plotting lines. Intensities less than 7 are scarcely visible. A shift of four intensity units corresponds roughly to a factor of two change in brightness.

A line plotted with MODE=1 may not cross from inside to outside the normal plotting area. See Figure A1 and MODE=6.

MODE= −1

CALL CRT (XWHERE,YWHERE,IZWHAT,-1)

This call is used to return the values of the present beam location and intensity.

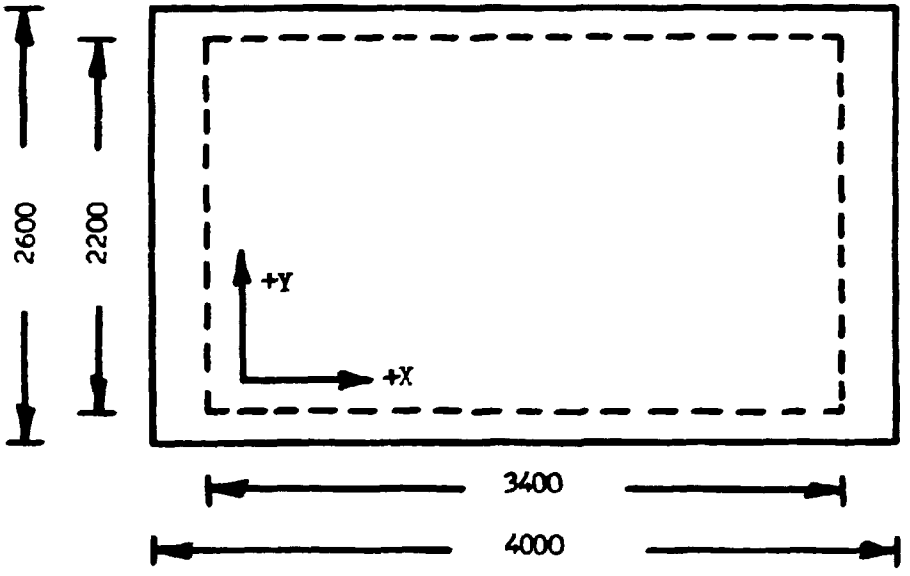
XWHERE, YWHERE — is the present beam position, in the user's coordinate system.

IZWHAT — is the present intensity level. This is the last positive non-zero value of IZTRUE used in plotting.

Table A2. Block numbers and film advance with CRT(X,Y,IB,2)

Value of IB	Block Number Produced	Film Advance and Reorigin	Output Tape File Closed
0	Next Sequential Number	Yes	No
1-999	IB	Yes	No
1000	Next Sequential Number	No	No
1001-1999	IB - 1000	No	No
9000	Next Sequential Number	Yes	Yes
9001-9999	IB - 9000	Yes	Yes

Figure A1. Plotting area available



MODE=2, Ending a Graph

CALL CRT (X,Y,IB,2)

This call is used to generate block numbers. A block number is a separator between two adjacent graphs or plots on the tape. It is possible for the operator of the Model 835 plotter to search the plot tape for a particular block number and plot the corresponding graph.

A block number may be written with or without advancing the film. If the film is advanced, the origin for the next plot will be the final value of (XORG,YORG) of the present plot. A move to (X,Y) will always be made whether or not the film is advanced. The beam will always be turned off when the move is made.

X,Y is the position to which the beam will be moved.

IB is a four digit decimal number with a value from 0 to 9999. The three least significant digits specify the block number to be written. If nonzero, a block number consisting of those three digits will be written; if zero, the next sequential block number (starting with 1) will be written. The most significant digit is used to control film advance and to close the output file. If the most significant digit is zero, the film will be advanced. If it is 9, the output tape file will be closed and no further plotting commands may be written during the execution of this source program. See also Table A2; ranges of IB not described in Table A2 should not be used.

MODE= -2

CALL CRT (XDUM,YDUM,IBLOCK,-2)

This routine is used to return the value of the last block number that was used.

XDUM, YDUM are not used at this time.

IBLOCK is the last block number.

MODE=3, Changing the Origin

CALL CRT (XORG, YORG, IZORG, 3)

This call sets the internal values of XORG, YORG, and IZORG. It is used to establish a translated origin for subsequent movements. IZORG functions as a beam intensity origin. These values are all initialized at 0. If any of these values are changed, all subsequent movements will be made with the specified translation until the values are again changed by another call with MODE=3.

XORG, YORG is the new position of the origin relative to the lower left corner of the normal plotting area.

IZORG is the value to be used for translation of beam intensity.

MODE= -3

CALL CRT (XORG, YORG, IZORG, -3)

This call is used to return the current origin and beam translation values in effect.

XORG, YORG are the positions of the present origin relative to the lower left corner.

IZORG is the present translation value for beam intensity.

MODE=4, Changing Scale Factors

CALL CRT (XFACT, YFACT, IDUM, 4)

The purpose of this call is to set scaling factors for the X and Y coordinates. Scaling of abscissa and ordinate values are completely independent. XFACT and YFACT are both initialized with a value of 1.0.

If XFACT=YFACT=1.0, a line of length 1.0 will be 1.0 inches long on an 11" x 17" print.

XFACT is the scaling factor for the abscissa.
YFACT is the scaling factor for the ordinate.
IDUM is not used at this time.

MODE=-4

CALL CRT (XFACT,YFACT,IDUM,-4)

This call returns the values of the scaling factors currently in use.

MODE=5, Plotting a Point

CALL CRT (XPOINT,YPOINT,IZ,5)

This call moves the beam to the position (XPOINT,YPOINT) with the beam off and, when the beam arrives at that position, turns the beam on. This produces a point at the intensity level indicated by IZ at the position (XPOINT,YPOINT).

XPOINT,YPOINT is the position where the point will be produced.
IZ indicates the intensity to be used, as for MODE=1.

As with MODE=1, the beam movement performed with MODE=5, may not cross from inside to outside the normal plotting area.

MODE=6, Plotting Outside the 11" x 17" Area

CALL CRT (X,Y,IZ,6)

This call is used to bypass the limit switches and to plot outside the normal 11" x 17" area. Because of distortion outside the normal plotting area, this call should be used only for labelling or plotting

which does not require the full accuracy of the system. The action is done as for MODE=1, except that if MODE=6 the beam is allowed to pass the limit switch boundaries.

MODE=7, Changing IZSET

CALL CRT (XDUM,YDUM,IZSET,7)

This call sets the internal parameter IZSET to any desired value.

XDUM,YDUM	are not used.
IZSET	This is the value of the intensity level to be used in calls with MODE=1, 5, or 6, and IZ=99, or in calls to CRTSYM. After translation, IZTRUE=IZSET+IZORG. IZSET is initialized at 16. If it is changed by this call, the new setting will remain in effect until changed again.

MODE= -7

CALL CRT (XDUM,YDUM,IZSET,-7)

This call returns the value stored in IZSET.

APPENDIX B

DESCRIPTION OF THE INPUT DATA

SIMTRAN I

Format for the Input Data Cards

Card No. (Format)	Field	Variable	Units	General Description
1 (20 A4)	1-80	NTITLE	-	Heading line for printed output and plots (only 1-60 used for plot title).
	1-10	R(1)	cm	outer radius of tube.
	11-20	WALL	cm	wall thickness (prior to oxidation).
	21-30	OLAYER(1)	cm	thickness of oxide layer at the outer surface. (Initial)
2 (6D10.9) (Initial geometry)	31-40	ALAYER(1)	cm	thickness of the alpha layer at the outer surface. (Initial)
	41-50	OLAYER(2)	cm	thickness of the oxide layer at the inner surface. (Initial)
	51-60	ALAYER(2)	cm	thickness at the alpha layer at the inner surface. (Initial)
	1-10	TMAX	sec	maximum time of experiment.
	11-20	DTTEMP	sec	max. time step for temperature calculation (if 0, then DTTEMP= DTPRIN will be set).
3 (4D10.9,4I10)	21-30	DTDIFF	sec	max. time step for diffusion calculation (if 0, then DTDIFF= DTPRIN will be set).
(Run conditions and output)	31-40	DTPRIN	sec	time step for printed output (can be function of time, then next variable > 0).
	41-50	NSTEP	-	number of changes in output time steps. (If > 0, then card 3A has to be supplied.)
	51-60	MPRINT	-	number of printed output steps between oxygen concentration - distance plots (not used if there are no plots of this type to be made).

Card No. (Format)	Field	Variable	Units	General Description
	61-70	NUMBER	-	identification number for first oxygen concentration-distance plot (if 0 then no plots of this type are made).
	71-80	NSCALE	-	NSCALE = 0 : Type A plots (y-axis:0 to $2\frac{gr}{cm^3}$) NSCALE = 1 : Type B plots (y-axis:0 to $0.5\frac{gr}{cm^3}$) NSCALE = 2 : Type A + Type B plots
3A (8D10.9) (card only if NSTEP >0)	K=1, NSTEP	TIMSTP(K)	sec	time at which change in output time step takes place.
		DTNEW(K)	sec	new output time step.
4 (2I10) (Type of calculation)	1-10	NLUMB	-	NLUMB = 0 : complete temperature distribution in wall is calculated. NLUMB = 1 : uniform wall temperature, but calculated as function of heat transfer and heat generation. NLUMB = 2 : uniform wall temperature, set equal to TSTEAM(1) or TSTEAM(2) if TSTEAM(1) = 0.
	11-20	NBAKER	-	NBAKER = 0 : oxygen distribution in wall is calculated. NBAKER = 1 : total oxygen calculation on basis of Baker-Just Eq. NBAKER = 2 : total oxygen calculation on basis of Hobson data. NBAKER = 3 : total oxygen calculation on basis of Lemmon Eq.

Card No. (Format)	Field	Variable	Units	General Description
5 (6D10.9) (Initial conditions at outer surface.)	1-10	HDIFF(1)	$\frac{gram}{cm^2 \cdot sec}$	upper limit for oxygen flux into the wall at the outer surface (if 0, then no oxidation at this surface).
	11-20	HCOOL(1)	$\frac{w}{cm^2 \cdot °C}$	convective heat transfer coefficient at the outer surface.
	21-30	TSTEAM(1)	°C	coolant temperature at the outer surface.
	31-40	ERADIA(1)	-	thermal emissivity at the outer surface.
	41-50	TWALL(1)	°C	temperature of surface to which outer surface is radiating.
	51-60	QFIXED(1)	$\frac{w}{cm^2}$	additional heat flux at outer surface (independent from HCOOL, TSTEAM, ERADIA, TWALL).
6 (6D10.9) (Initial conditions at inner surface.)				identical meaning as card 5 but for inner surface. (Either card 5 or card 6 can be empty if there is heat transfer and oxidation on one surface only.)
7 (6I10) (Time dependent functions, outer surface.)	1-10	NDIFIN(1)	-	number of oxygen flux limit-time pairs for outer surface (0 if constant).
	11-20	NCOEFF(1)		number of heat transfer coeff.-time pairs for outer surface (0 if constant).
	21-30	NTCOOL(1)		number of coolant temperature-time pairs for outer surface (0 if constant).
	31-40	NRADCO(1)		number of emissivity-time pairs for outer surface (0 if constant).
	41-50	NTWALL(1)		number of radiation temperature-time pairs for outer surface (0 if constant).
	51-60	NQFLUX(1)		number of heat flux-time pairs for outer surface (0 if constant).

Card No. (Format)	Field	Variable	Units	General Description
8 (6I10) (Time dependent functions, inner surface)				identical meaning as card 7 but for inner surface. Either card 7 or 8 or both cards can be empty if there are no time functions. For each of the variables in card 7 or card 8 that is greater than 0, a corresponding card 9A to 9F or 10A to 10F has to be supplied.
9A (8D10.9)	K=1,NDIFIN(1)	HDIFIN(1,K)	TIMDIF(1,K)	time functions for variables pertaining to outer surface.
9B (8D10.9)	K=1,NCOEFF(1)	HCOEFF(1,K)	TCOEFF(1,K)	omit if corresponding variable in card 7 is 0.
.....				separate card(s) for each function.
9F (8D10.9)	K=1,NQFLUX(1)	QFLUX(1,K)	TQFLUX(1,K)	up to 25 cards for each type of pair can be used.
10A				identical meaning as cards 9A to 9F, but for inner surface.
.....				
10F				
11 (3D10.9,40X I10)	1-10	TSTART	°C	initial temperature in wall.
	11-20	CSTART	gram/cm³	initial oxygen concentration in beta-phase.
	21-30	QSPLIT	$\frac{\text{wsec}}{\text{gram oxygen}}$	endothermic reaction heat for converting steam into oxygen and hydrogen, subtracted at the surface. (Full value is 15,650 wsec/gram O_2)
	31-70	EMPTY		
	71-80	MPLOT		number of graphs and/or tables, to be plotted using variables determined as functions of time. (If 0, omit cards 12 and 13.)

Card No. (Format)	Field	Variable	Units	General Description
	1-[illegible]	[illegible]	-	defined variable for [illegible] axis (see Table [illegible])
	11-[illegible]	[illegible]	units/in.	scale factor for [illegible] axis
1[illegible] (I1[illegible], F1[illegible], [illegible] I1[illegible], F1[illegible], [illegible] A[illegible]). (Omit if [illegible]: Repeat card 1[illegible] for each graph: [illegible])	[illegible]1-[illegible]	[illegible]	Units of variable for [illegible] axis	value of [illegible] at origin (empty, if [illegible])
	[illegible]1-[illegible]	[illegible]	-	number of Y-axis variables plotted as a function of single [illegible]-axis variable. NVAR[illegible]
	[illegible]1-[illegible]	[illegible]	-	Determines if variables are plotted and/or printed [illegible] = [illegible]: No plot; no print [illegible] 1: No plot; print [illegible] = 1[illegible]: Plot; no print [illegible] = 11: Plot; print
	[illegible]1-[illegible]	[illegible]	in.	Distance between [illegible] axis and paper border. (Generally, [illegible])
	[illegible]1-[illegible]	[illegible]	-	used to describe variable on [illegible]-axis
	1-[illegible]	[illegible]	-	defined variable for Y axis (see Table [illegible])
1[illegible] (I1[illegible], F1[illegible], [illegible] I1[illegible], [illegible] A[illegible]). (Repeat for each curve on graph: [illegible], NVAR)	11-[illegible]	[illegible]	Units/in.	scale factor for Y axis (1[illegible] in. max. for Y-axis)
	[illegible]1-[illegible]	[illegible]	Units of variable for [illegible] axis	value of Y at origin. (empty, if [illegible])
	1-[illegible]	[illegible]	-	[illegible] = [illegible]: Points only are plotted [illegible] 1: Points are connected with a line
	[illegible]1-[illegible]	[illegible]	-	used to describe variable on Y axis.

Table B1. Variables available for GRAPHICAL OUTPUT

(Defined variables 3-12 refer to outer surface of tube; variables 13-22 refer to inner surface of tube.)

NPLOTX NPLOTY	VARIABLE	UNITS
1	time	sec.
2	square-root of time	$(sec)^{1/2}$
3	steam (or coolant) temperature	°C
4	temp. of surface to which specimen is radiating	°C
5	surface temperature of specimen	°C
6	thickness of oxide layer	μm
7	thickness of alpha layer	μm
8	ξ-layer thickness (oxide + alpha)	μm
9	oxide/ξ ratio	-
10	oxygen gain	mg/cm^{2*}
11	square of oxygen gain	$(mg/cm^2)^{2*}$
12	square of ξ-layer thickness	$(\mu m)^2$
13-22	identical to 3-12 above, except that variable applies to inner surface of tube.	
23	total oxygen consumption	mg/cm^{2*}
24	avg. oxygen concentration in Beta phase	g/cm^3
25	F_w, beta layer thickness/orig. wall thickness	-

*area reference is outer surface.

APPENDIX C

DESCRIPTION OF THE OUTPUT DATA

In addition to the printing of the input data, (except for cards 3a, 9a-9f, 10a-10f, 12, and 13), and tables of values of the materials properties utilized for each run, the following variables are printed for each specified time step (where applicable, for both inner and outer tube surfaces):

TIME	[sec]	Oxidation time.
PLOT NO.	[–]	Identification number for oxygen concentration profile plots (0 if there are no plots of this type).
H.T.COEFF	$[\frac{W}{cm^2 \cdot K}]$	Convective heat transfer coefficient.
STEAM TEMP	[°C]	Steam temperature.
EMISSIVITY	[–]	Thermal emissivity.
RAD.WALL	[°C]	Temperature of surroundings with which radiation heat is exchanged.
SURFACE TEMP	[°C]	Surface temperature of Zircaloy.
OX/MET TEMP	[°C]	Temperature at the oxide/α interface.
FIX.HEATFLUX	$[\frac{W}{cm^2}]$	Fixed heat flux at the surface of the Zircaloy (in addition to convection and radiation).
CON.HEATFLUX	$[\frac{W}{cm^2}]$	Convective heat flux.
RAD.HEATFLUX	$[\frac{W}{cm^2}]$	Radiative heat flux.
QCON + QRAD	$[\frac{W}{cm^2}]$	Sum of radiative and convective heat fluxes.
O.FL.LIMIT	$[\frac{gram}{cm^2 \cdot sec}]$	Upper limit for oxygen flux; identical with HDIFF.
OXYGEN FLUX	$[\frac{mg}{cm^2 \cdot sec}]$	Actual (instantaneous) oxygen flux.
O.IN OXID	$[\frac{mg}{cm^2}]$	Oxygen content in oxide layer.
O.IN ALPHA	$[\frac{mg}{cm^2}]$	Oxygen content in α layer.

O.IN BETA	$[\frac{mg}{cm^2}]$	Oxygen content in remaining β layer.
OXYG.TOTAL*	$[\frac{mg}{cm^2}]$	Total oxygen content.
OXYG.GAIN*	$[\frac{mg}{cm^2}]$	Oxygen gain.
OXIDE LAYER	[μm]	Thickness of oxide layer.
ALPHA LAYER	[μm]	Thickness of α layer.
BETA LAYER	[μm]	Thickness of β layer.

If there is oxidation and/or heat transfer on both surfaces, the first line of the variables is for the outer surface, the second line for the inner surface. In each case, the variables O.IN OXIDE to OXYG.GAIN are calculated with the outer surface as reference area.

In addition, for each calculated node the following variables are printed out:

POINT NUMBER	[–]	Number of the node which indicates the position from the outer surface.
DISTANCE	[cm]	Distance of the node from the original outer surface. Since the volume of the oxide is larger than the volume of unoxidized Zircaloy, DISTANCE will be negative for some point(s) if oxidation occurs at the outer surface.
TEMPERATURE	[°C]	Temperature of the node.
CONCENTRATION	$[\frac{gram}{cm^3}]$	Oxygen concentration in the node.

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*Note: OXYG.TOTAL is determined by an integration of the oxygen concentration over the entire wall for each output time. OXYG.GAIN is determined by an integration of instantaneous flux over the time. The difference between the two variables can vary slightly from the value of the initial oxygen content (OXYG.TOTAL = 0) due to numerical inaccuracy.

APPENDIX D

EXAMPLE PROBLEMS

Three test cases have been selected as sample problems to illustrate the preparation of the input and to show typical output results.

Test Case 1. A Comparison of a SIMTRAN Result with an Analytical Solution

A simple nonmoving-boundary diffusion problem was chosen since there are no analytical solutions known for the problem of the two moving boundaries in a wall with a finite thickness. To enable a comparison to be made, the code was "degraded" by giving all three layers the same material properties. The properties of beta-Zircaloy were used for the basis material. The concentration at the "interfaces" was set arbitrarily at 75% and 25% of the equilibrium oxygen concentration. The initial and the boundary conditions for the problem were chosen as:

T = constant = 1400°C

at $\tau = 0$:

$C = 0.00649$ for $0 < x \leq \ell$

$C = C_{\beta/\alpha} = 0.068356$ for $x = 0$

at $x = 0$:

$C = C_{\beta/\alpha}$ for $0 \leq \tau \leq \tau_{max}$

at $x = \ell$:

$\frac{\partial C}{\partial x} = 0$ for $0 \leq \tau \leq \tau_{max}$

The analytical solution $C(x,\tau)$ is given by:

$$C = C_o + \left\{C_s - C_o\right\}\left\{1 - \frac{4}{\pi}\sum_{m=0}^{\infty}\frac{1}{2m+1}\sin\left[\frac{(2m+1)\pi x}{\ell}\right]\exp\left[-\frac{(2m+1)^2\pi^2 D_T}{\ell^2}\right]\right\} \quad (D1)$$

The results of Eq. (D1) are plotted in Fig. D1 for τ = 5, 15, and 60 sec. Also shown in this figure are a number of concentration values calculated with SIMTRAN. The agreement is seen to be quite good.

Table D1 shows the complete listing of the input data and the output for three selected times. The computing time for this problem was 27 sec on an IBM 360/91.

Test Case 2. Isothermal Reaction at 1000°C (1832°F), Two-Side Oxidation

This case simulates an ideal isothermal oxidation experiment at 1000°C (1832°F) with an oxidation time of 30 min. Figure D2 shows the thickness of the oxide and ζ (oxide plus alpha) layers as functions of time. Figures D3 and D4 show the concentration profiles across the wall after 30 minutes in two different scales. The input data and the output data for three selected times are listed in Table D2. The computing time was 13 sec.

Test Case 3. Burst Test of a Zircaloy Tube in Steam

This case represents an application of SIMTRAN to a simple tube-burst problem. In this problem, a Zircaloy tube is visualized as being heated by an internal electrical heater having a constant rate of temperature increase. The gap between tube and heater assumed to be filled with helium under pressure. The intention is to cut off the electrical power as soon as the tube bursts in order to measure the existing deformation. The test is assumed to be made in a steam environment. The question was: can the steam-Zircaloy reaction generate sufficient heat at higher temperatures so that the Zircaloy temperature would continue to rise even after the heater power was cut off?

The calculation has been made with no initial oxide layer which leads to the maximum reaction. Heat transfer to the steam has been neglected for simplicity, (although it could be considered if desired).

The Zircaloy temperature and the temperature of the heater surface are plotted vs time in Fig. D5. In the same figure the penetration of the α/β-interface into the wall is shown. Figure D6 shows the oxygen concentration in the α and β phases after 35 sec. Input and output are listed in Table D3. Computing time was 11 sec.

In order to show the difference between the lumped temperature calculation (NLUMB=1), where the entire wall is treated as a single node and the more detailed calculation (NLUMB=0), where the complete temperature profile in the wall is calculated, test case 3 was repeated as case 3A with NLUMB=0.* The output for three selected time steps for this latter case is printed in Table D4.

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*The computing time increased by a factor of 3.

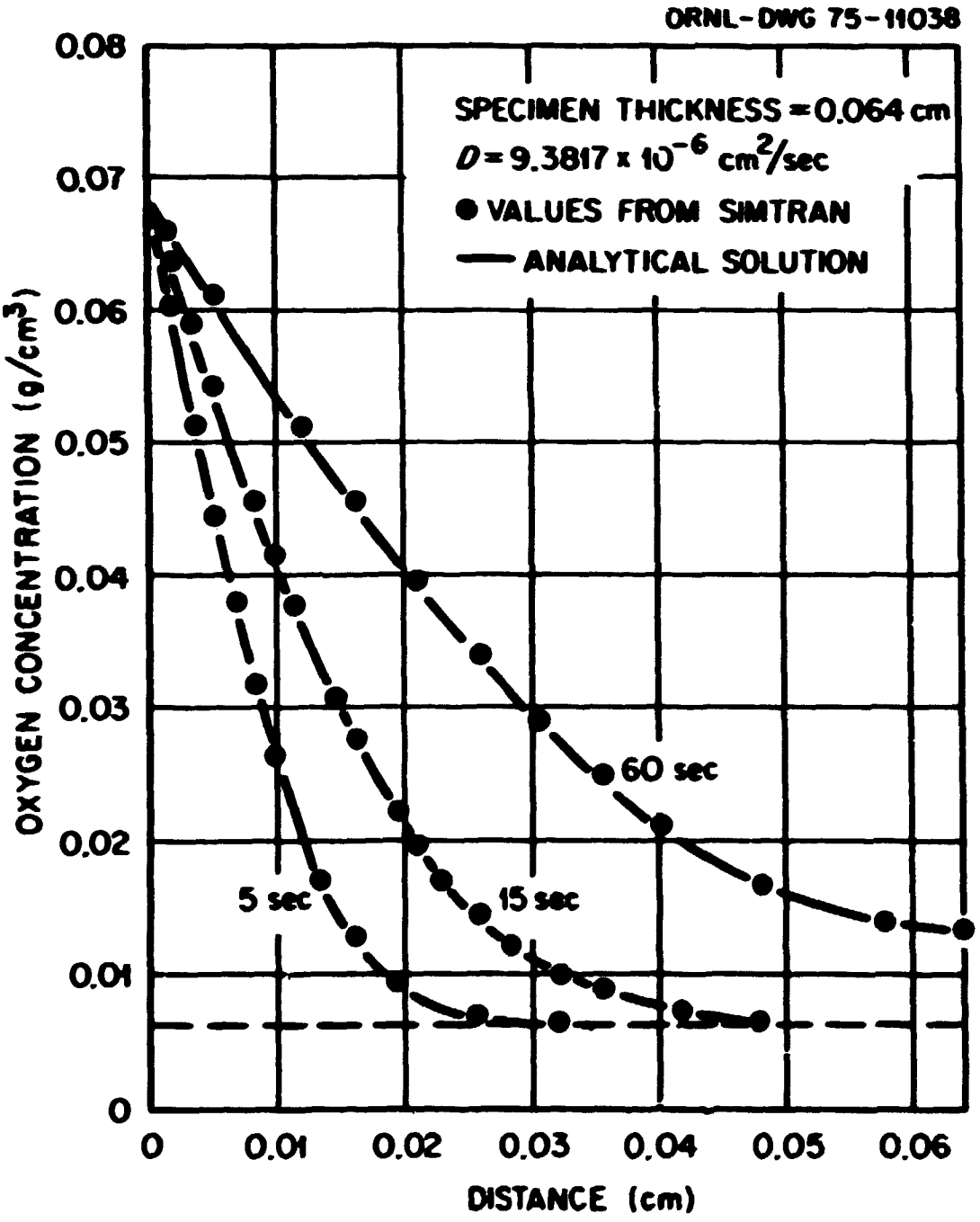

Fig. D1. Comparison of SIMTRAN result with analytical solution for single-phase, nonmoving-boundary case. Test Case 1.

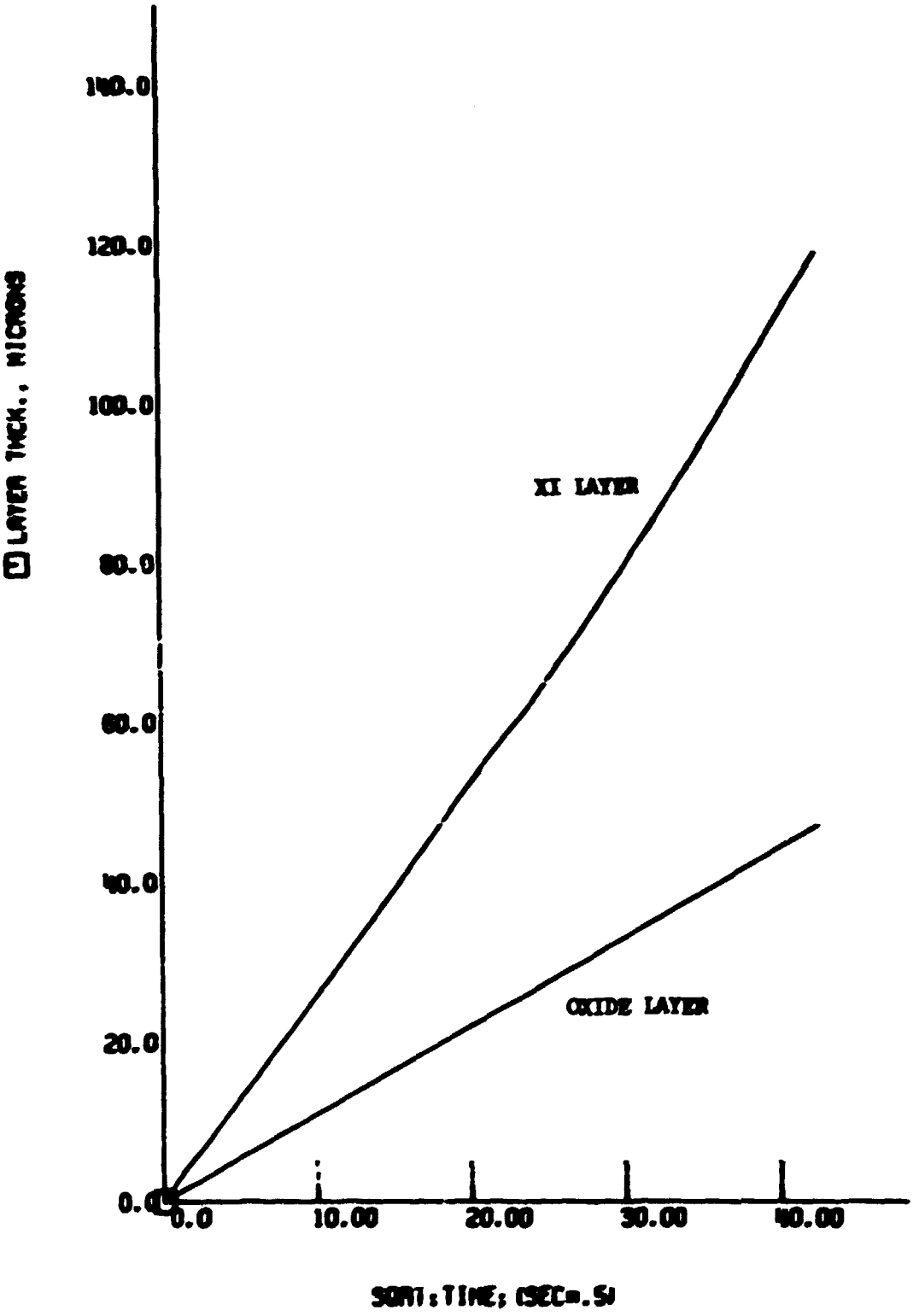

Fig. D2. Ideal isothermal oxidation curves. Test Case 2.

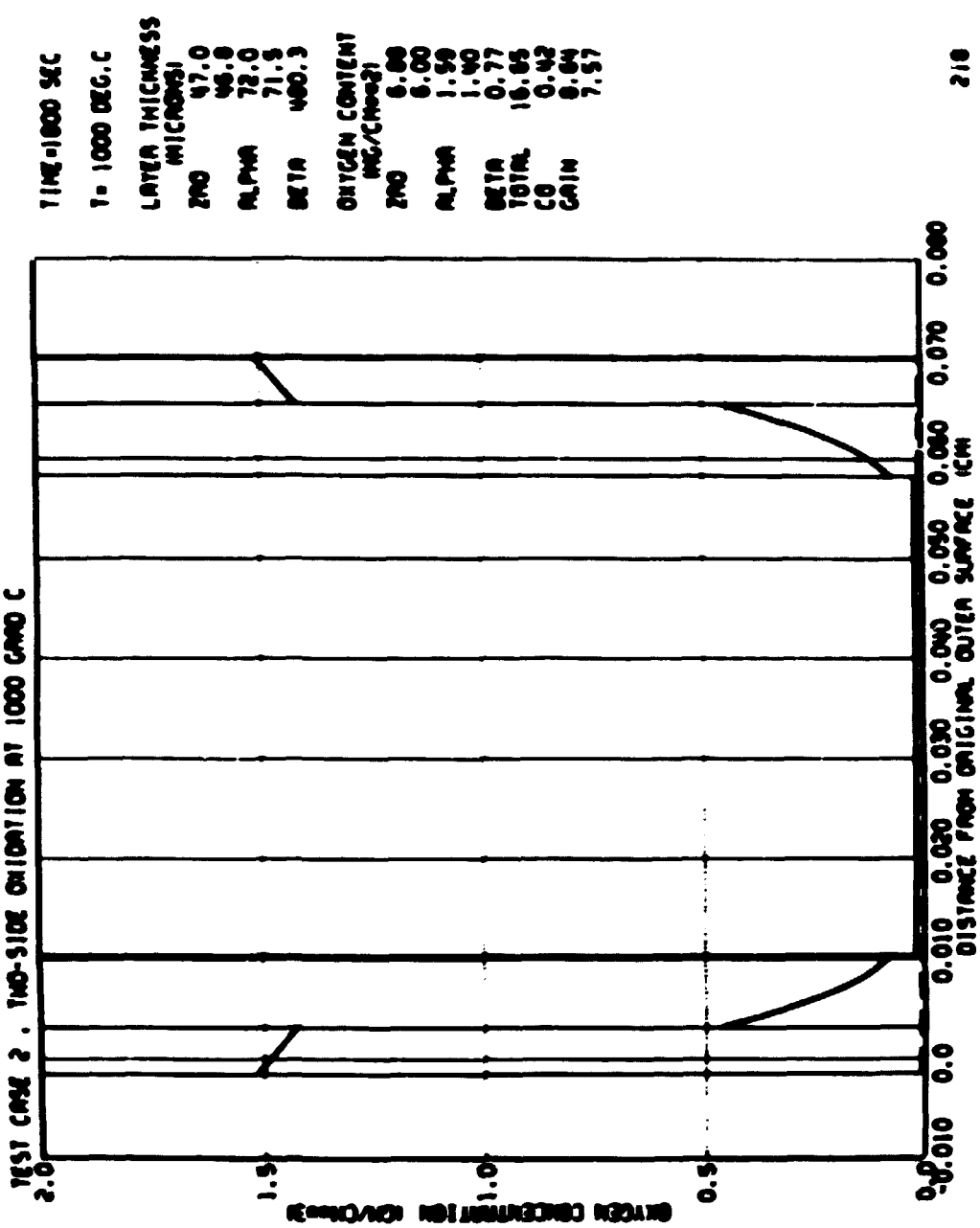

Fig. D3. Oxygen concentration in oxide, α- and β-Zircaloy. Test Case 2.

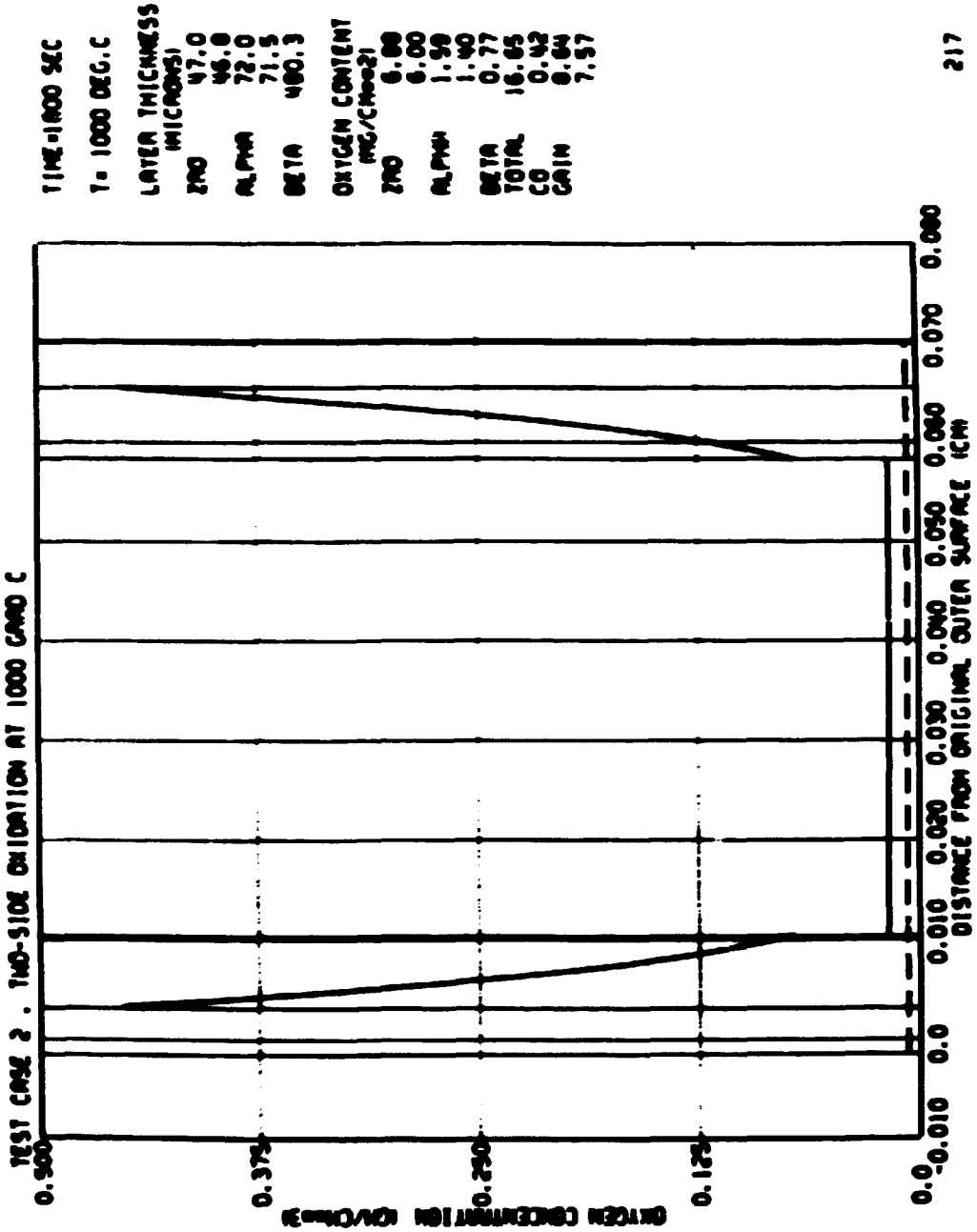

Fig. D4. Oxygen concentration in α- and β-Zircaloy. Test Case 2.

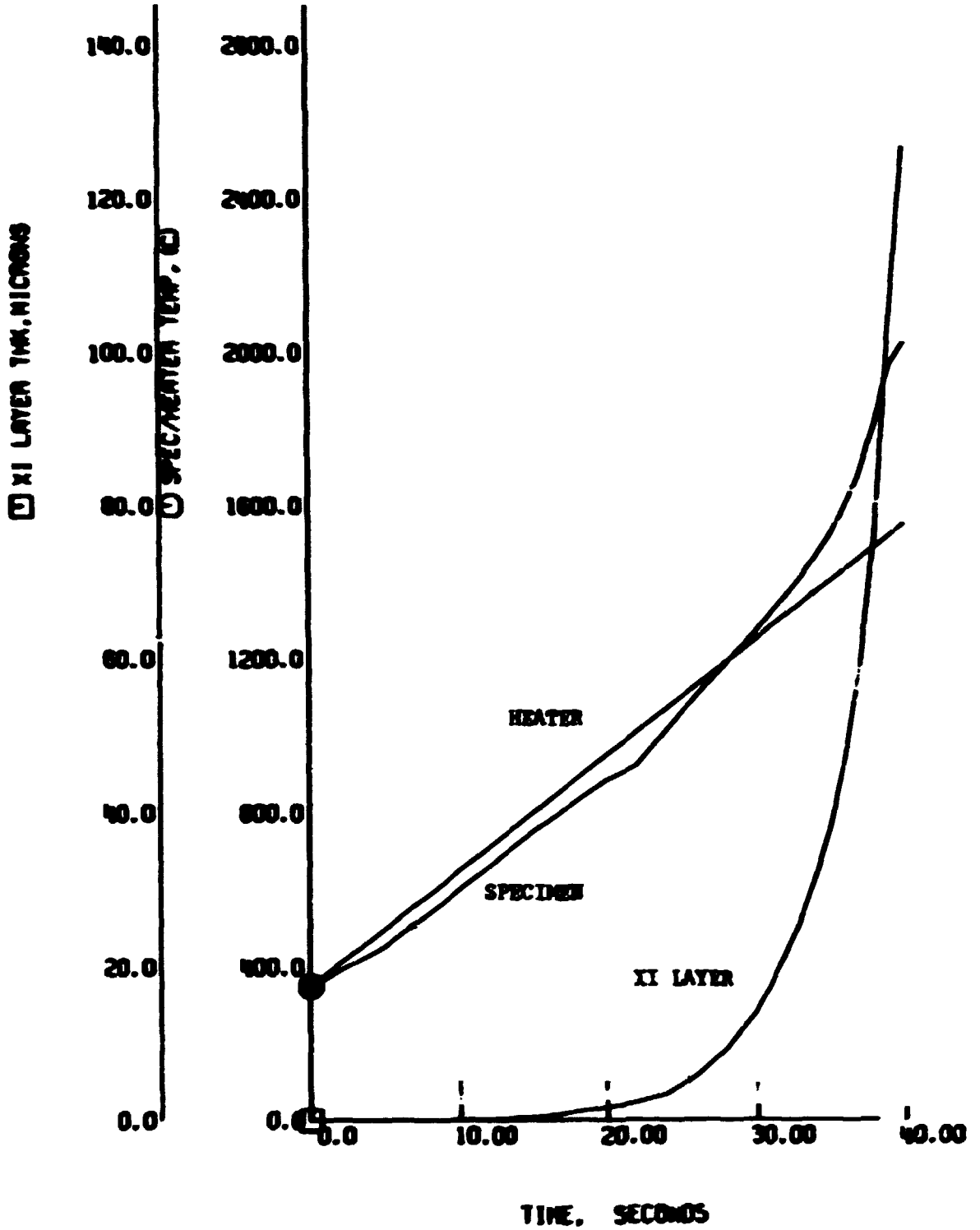

Fig. D5. Temperature and layer thickness variations. Test Case 3.

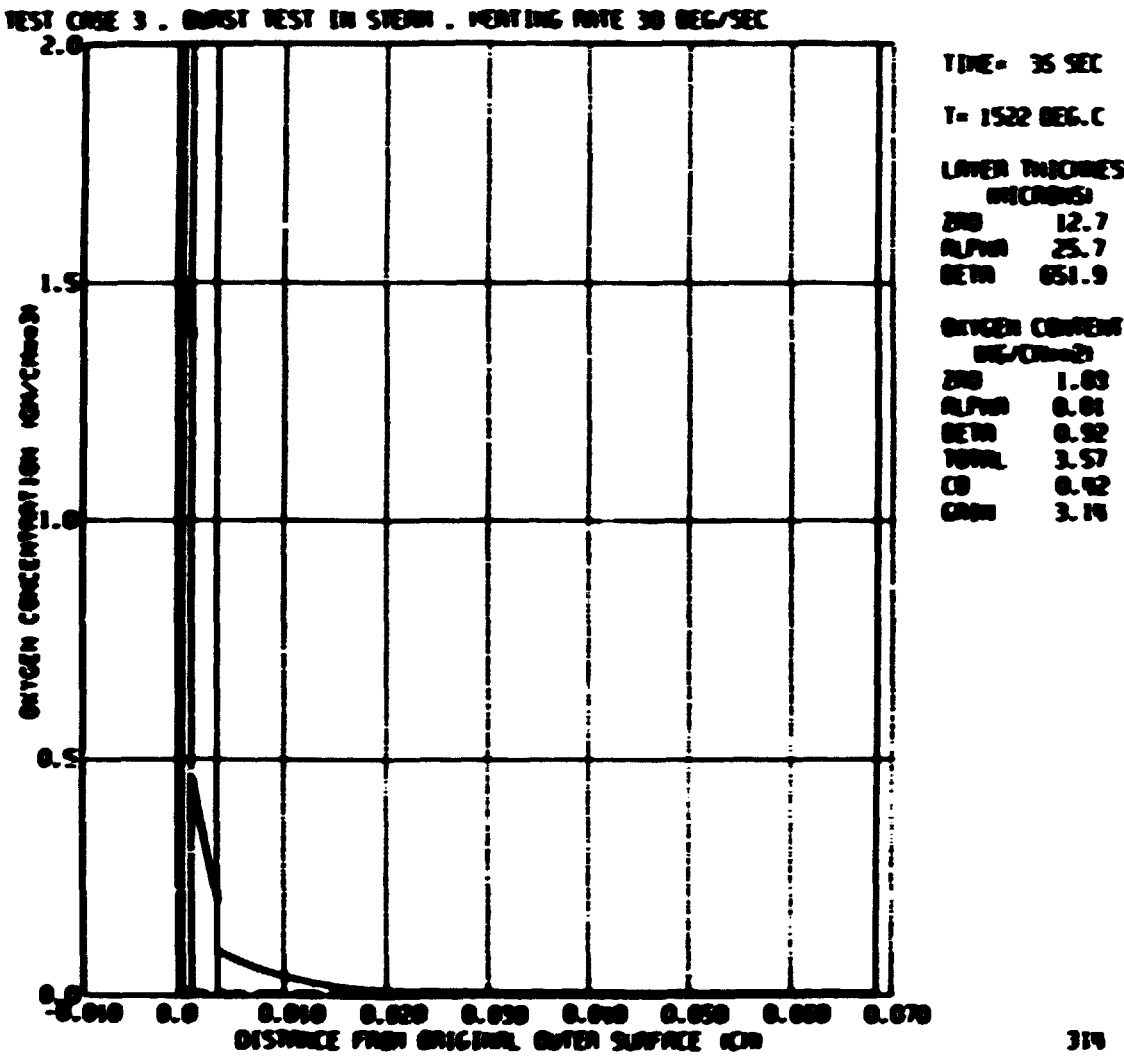

Fig. D6. Oxygen concentration in oxide, α- and β-Zircaloy. Test Case 3.

TABLE 14. SELECTED INPUT-OUTPUT FOR TEST CASE 1: SINGRAN-ANALYTICAL SOLUTION COMPARISON.

DOUT	WALL	DDIIO(1)	DALPA(1)	DDIIO(2)	DALPA(2)
100.00000	0.000000	0.0	0.0	0.0	0.0

TMAX	DTSTOP	DTDIFF	DTPRIN	NSTOP	NPRINT	NORDER	NSCALE
60.0000	0.0	0.0	0.1000	9	0	0	0

NLONG	NSHORT
20	0

DDIFF(1)	DCOOL(1)	TSTRAN(1)	DDASTA(1)	TWALL(1)	QFIXED(1)
10.0000	0.0	1000.0000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0

DDIFF2(1)	DCDIFF(1)	DTCOOL(1)	DDADCO(1)	DTWALL(1)	DQFLUX(1)
0	0	0	0	0	0
0	0	0	0	0	0

TSTART	CSTART	QSPLIT	NPLOT
1400.00	0.000000	0.0	0

• • • MATERIAL PROPERTIES • • •

METAL DENSITY = 8.490 OXID DENSITY = 5.020 GRAM/CM**3 REACTION HEAT = 26110.00 USEC/GRAM OXIDE

	EQUILIBRIUM CONCENTRATION (GRAM/CM**3)				DIFFUSION CONSTANT (CM**2/SEC)			TH.CONDUC.W/(CM*C)	SP.HEAT W*SEC/(GM.C)		
TEMP.(C)	STOCH.OX.	OX./AL.	AL./AL.	AL./BETA	BETA/AL.	OXID	ALPHA	BETA	OXID	METAL	OXID	METAL
750.00	0.01737	0.01303	0.01103	0.000230	0.000230	0.9200-07	0.9200-07	0.9200-07	0.02000	0.19377	0.61765	0.36530
800.00	0.01737	0.01303	0.01303	0.000230	0.000230	0.0100-07	0.0100-07	0.01[illegible]-07	0.02000	0.20754	0.62000	0.36530
850.00	0.01737	0.01303	0.01303	0.000230	0.000230	0.1070-06	0.1070-06	0.1070-06	0.02000	0.22127	0.62025	0.36530
900.00	0.01737	0.01303	0.01303	0.000230	0.000230	0.2520-06	0.2520-06	0.2520-06	0.02000	0.23502	0.62760	0.36530
950.00	0.01737	0.01303	0.01303	0.000230	0.000230	0.5100-06	0.5100-06	0.5100-06	0.02000	0.24877	0.63000	0.36530
1000.00	0.01737	0.01303	0.01303	0.000230	0.000230	0.9510-06	0.9510-06	0.9510-06	0.02000	0.26252	0.63230	0.36530
1050.00	0.02157	0.01618	0.01618	0.000139	0.000139	0.9950-06	0.9950-06	0.9950-06	0.02000	0.27627	0.63765	0.36530
1100.00	0.02637	0.01978	0.01978	0.000849	0.000849	0.1070-05	0.1070-05	0.1070-05	0.02000	0.29002	0.64100	0.36530
1150.00	0.03178	0.02383	0.02383	0.000706	0.000706	0.2110-05	0.2110-05	0.2110-05	0.02000	0.30377	0.64435	0.36530
1200.00	0.03782	0.02836	0.02836	0.000584	0.000584	0.3970-05	0.3970-05	0.3970-05	0.02000	0.31752	0.64770	0.36530
1250.00	0.04449	0.03337	0.03337	0.001112	0.001112	0.6070-05	0.6070-05	0.6070-05	0.02000	0.33127	0.65105	0.36530
1300.00	0.05181	0.03886	0.03886	0.001295	0.001295	0.9470-05	0.9470-05	0.9470-05	0.02000	0.34502	0.65440	0.36530
1350.00	0.05977	0.04483	0.04483	0.001494	0.001494	0.7220-05	0.7220-05	0.7220-05	0.02000	0.35877	0.65775	0.36530
1400.00	0.06836	0.05127	0.05127	0.001709	0.001709	0.9300-05	0.9300-05	0.9300-05	0.02000	0.37252	0.66110	0.36530
1450.00	0.07757	0.05818	0.05818	0.001939	0.001939	0.1200-04	0.1200-04	0.1200-04	0.02000	0.38627	0.66445	0.36530
1500.00	0.08741	0.06556	0.06556	0.002185	0.002185	0.1510-04	0.1510-04	0.1510-04	0.02000	0.40002	0.66780	0.36530
1550.00	0.09786	0.07339	0.07339	0.002446	0.002446	0.1890-04	0.1890-04	0.1890-04	0.02000	0.41377	0.67115	0.36530

• • • • TIME = 9.300 • • • •

PLOT # = 0

N.T.COEFF	STEAM TEMP	EMISSIVITY	GAS,WALL SURFACE TEMP	OIL/SOOT TEMP	PIL.HEATFLUX	CON.HEATFLUX	GAS.HEATFLUX	QCON+QRAD
0.0	1400.00000	0.0	0.0	1400.00000	1400.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1400.00000	1400.00000	0.0	0.0	0.0	0.0

O.PL.LIMIT	OXIDEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
10.0000	0.0078	0.2926	0.1104	0.1021	0.0997	0.0700	11.0077	96.0702	949.6231

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	17	14
DISTANCE =	0.0	0.00160	0.33134
TEMPERATURE =	1400.00	1400.00	1403.00
CONCENTRATION =	0.06036	0.06023	0.05127

OUTSIDE ALPHA LAYER

POINT NUMBER =	95	49	65	81	97	113	121
DISTANCE =	0.00170	0.00480	0.00804	0.01040	0.00960	0.01120	0.01304
TEMPERATURE =	1400.00	1400.00	1403.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION =	0.05127	0.04991	0.01002	0.01101	0.02019	0.02102	0.01709

BETA LAYER

POINT NUMBER =	131	141	191	275	257	290	321	341	345	417	449	481	513
DISTANCE =	0.01304	0.01440	0.21920	0.02240	0.02440	0.02480	0.01200	0.01520	0.01040	0.00160	0.00000	0.00000	0.05120
TEMPERATURE =	1400.00	1400.00	1403.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION =	0.01709	0.01306	0.03164	0.00706	0.00702	0.00644	0.00654	0.00649	0.00649	0.00649	0.00649	0.00649	

BETA LAYER

POINT NUMBER =	545	577	609	641
DISTANCE =	0.05040	0.05760	0.06000	0.06480
TEMPERATURE =	1400.00	1400.00	1403.00	1400.00
CONCENTRATION =	0.00649	0.00649	0.00649	0.00649

• • • • TIME = 14.300 • • • •

PLOT # = 0

N.T.COEFF	STEAM TEMP	EMISSIVITY	GAS,WALL SURFACE TEMP	OIL/SOOT TEMP	PIL.HEATFLUX	CON.HEATFLUX	GAS.HEATFLUX	QCON+QRAD
0.0	1400.00000	0.0	0.0	1400.00000	1400.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1400.00000	1400.00000	0.0	0.0	0.0	0.0

O.PL.LIMIT	OXIDEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
10.0000	0.0277	0.3524	0.1424	0.1525	1.2073	0.0240	59.0076	160.7904	911.1960

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	17	33	49	60
DISTANCE =	0.0	0.00160	0.01320	0.00480	0.00590
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION =	0.06036	0.06344	0.01007	0.01430	0.01127

OUTSIDE ALPHA LAYER

POINT NUMBER =	60	81	97	113	129	145	161	177	193	209	230	
DISTANCE =	0.00590	0.00800	0.00960	0.01120	0.01280	0.01440	0.01600	0.01760	0.01920	0.02080	0.02280	
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	
CONCENTRATION=	0.05127	0.04575	0.04163	0.03773	0.03408	0.03068	0.02756	0.02471	0.02215	0.01987	0.01709	

BETA LAYER

POINT NUMBER =	230	257	289	321	353	385	417	449	481	513	545	577	609
DISTANCE =	0.02288	0.02560	0.02880	0.03200	0.03520	0.03840	0.04160	0.04480	0.04800	0.05120	0.05440	0.05760	0.06080
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION=	0.01709	0.01461	0.01207	0.01018	0.00885	0.00795	0.00737	0.00700	0.00670	0.00665	0.00657	0.00654	0.00652

BETA LAYER

POINT NUMBER =	641
DISTANCE =	0.06400
TEMPERATURE =	1400.00
CONCENTRATION=	0.00651

* * * * TIME = 60.000 * * * * PLOT # = 0

N.T.COEFF	STEAM TEMP	EMISSIVITY	RAD.WALL	SURFACE TEMP	OX/MET TEMP	FIX.HEAT LOS	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	1400.00000	0.0	0.0	1400.00000	1400.00000	0.	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1400.00000	1400.00000	0.0	0.0	0.0	0.0

O.PL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
10.0000	0.0137	0.7099	1.1277	0.2386	2.0762	1.6508	110.8493	360.1670	160.9829

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	17	33	49	65	81	97	120
DISTANCE =	0.0	0.00160	0.00320	0.00480	0.00640	0.00800	0.00960	0.01189
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION=	0.06836	0.06601	0.06367	0.06134	0.05903	0.05674	0.05448	0.05127

OUTSIDE ALPHA LAYER

POINT NUMBER =	120	129	145	161	177	193	209	225	241	257	273	289	305
POINT NUMBER =	321	337	353	369	385	401	417	433	449	465	480		
DISTANCE =	0.01188	0.01280	0.01440	0.01600	0.01760	0.01920	0.02080	0.02240	0.02400	0.02560	0.02720	0.02880	0.03040
DISTANCE =	0.03200	0.03360	0.03520	0.03680	0.03840	0.04000	0.04160	0.04320	0.04480	0.04640	0.04798		
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00		
CONCENTRATION=	0.05127	0.04902	0.04787	0.04576	0.04370	0.04169	0.03973	0.03784	0.03601	0.03424	0.03254	0.03091	0.02935
CONCENTRATION=	0.02786	0.02645	0.02511	0.02384	0.02265	0.02153	0.02049	0.01952	0.01863	0.01781	0.01709		

BETA LAYER

POINT NUMBER =	480	513	545	577	609	641
DISTANCE =	0.04798	0.05120	0.05440	0.05760	0.06080	0.06400
TEMPERATURE =	1400.00	1400.00	1400.00	1400.00	1400.00	1400.00
CONCENTRATION=	0.01709	0.01593	0.01493	0.01422	0.01379	0.01365

TABLE D-1. SELECTED INPUT-OUTPUT FOR TEST CASE 3: TWO-SIDE ISOTHERMAL REACTION AT 1000 DEG. C.

DOUT	WALL	DOXID(1)	DALPA(1)	DOXID(2)	DALPA(2)
0.53200	0.06860	0.0	0.0	0.0	0.0

TMAX	DTTEMP	DTDIFF	DTPAIR	NSTEP	NPRINT	NUMBER	NSCALE
1000.0000	0.0	0.0	200.0000	0	1	201	2

NLSMO	NBARIER
2	0

NDIFF(K)	NCOOL(K)	TSTEAM(K)	NRADIA(K)	TWALL(K)	OPIXED(K)
1.3000	0.0	1000.0000	0.0	0.0	0.0
1.0000	0.0	0.0	0.0	0.0	0.0

NDIFIN(K)	NCOEFF(K)	NTCOOL(K)	NRADCO(K)	NTWALL(K)	NOFLUX(K)
0	0	0	0	0	0
0	0	0	0	0	0

TSTART	CSTART	OSPLIT	NPLOT
1000.00	0.000490	0.0	1

* * * MATERIAL PROPERTIES * * *

METAL DENSITY = 6.490 OXID DENSITY = 5.020 GRAM/CM**3 REACTION HEAT = 34330.00 WSEC/GRAM OXYGEN

	EQUILIBRIUM CONCENTRATION (GRAM/CM**3)				DIFFUSION CONSTANT (CM**2/SEC)				TH.CONDUC.W/(CM°C)		SP.HEAT W°SEC/(GR.C)	
TEMP.(C)	STOCH.OI.	OI./AL.	AL./OI.	AL./BETA	BETA/AL.	OXID	ALPHA	BETA	OXID	METAL	OXID	METAL
750.00	1.51400	1.44026	0.45365	0.00016	0.00391	0.4720-08	0.731D-10	0.429D-07	0.02000	0.19377	0.61755	0.36530
800.00	1.51400	1.43651	0.45365	0.00016	0.00391	0.1020-07	0.234D-09	0.610D-07	0.02000	0.20782	0.62090	0.36530
850.00	1.51400	1.43276	0.45365	0.00016	0.00391	0.206D-07	0.677D-09	0.147D-06	0.02000	0.22127	0.62425	0.36530
900.00	1.51400	1.42901	0.45365	0.03010	0.00840	0.391D-07	0.178D-08	0.252D-06	0.02000	0.23502	0.62760	1.02400
950.00	1.51400	1.42526	0.45365	0.05075	0.01289	0.704D-07	0.435D-08	0.410D-06	0.02000	0.24077	0.63095	0.36530
1000.00	1.51400	1.42151	0.45365	0.07010	0.01738	0.121D-06	0.989D-08	0.653D-06	0.02000	0.26253	0.63430	0.36530
1050.00	1.51400	1.41776	0.45365	0.08815	0.02187	0.200D-06	0.211D-07	0.995D-06	0.02000	0.27627	0.63765	0.36530
1100.00	1.51400	1.41401	0.45365	0.10491	0.02637	0.319D-06	0.427D-07	0.147D-05	0.02000	0.29002	0.64100	0.36530
1150.00	1.51400	1.41026	0.45365	0.12038	0.03178	0.492D-06	0.821D-07	0.211D-05	0.02000	0.30377	0.64435	0.36530
1200.00	1.51400	1.40651	0.45365	0.13454	0.03782	0.736D-06	0.151D-06	0.297D-05	0.02000	0.31752	0.64770	0.36530
1250.00	1.51400	1.40276	0.45365	0.14742	0.04449	0.107D-05	0.267D-06	0.407D-05	0.02000	0.33127	0.65105	0.36530
1300.00	1.51400	1.39901	0.45365	0.15899	0.05181	0.153D-05	0.455D-06	0.547D-05	0.02000	0.34502	0.65440	0.36530
1350.00	1.51400	1.39526	0.45365	0.16927	0.05977	0.213D-05	0.751D-06	0.723D-05	0.02000	0.35877	0.65775	0.36530
1400.00	1.51400	1.39151	0.45365	0.17826	0.06836	0.290D-05	0.120D-05	0.938D-05	0.02000	0.37252	0.66110	0.36530
1450.00	1.51400	1.38776	0.45365	0.18595	0.07757	0.389D-05	0.187D-05	0.120D-04	0.02000	0.38627	0.66445	0.36530
1500.00	1.51400	1.38401	0.45365	0.19238	0.08741	0.513D-05	0.285D-05	0.151D-04	0.02000	0.40002	0.66780	0.36530
1550.00	1.51400	1.38026	0.45365	0.19754	0.09785	0.666D-05	0.423D-05	0.189D-04	0.02000	0.41377	0.67115	0.36530

H.T.COEFF	SYRAM TEMP	EMISSIVITY	RAD.WALL	SURFACE TEMP	OX/MET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	1000.00000	0.0	0.0	1000.00000	1000.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1000.00000	1000.00000	0.0	0.0	0.0	0.0

O.FL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.0072	2.2044	0.4942	0.6242	5.8249	3.0706	15.5013	21.0281	623.3042
1.0000	0.0073	1.9907	0.4314	0.0	0.0	2.5111	15.5553	20.9291	0.0

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	5	9	11
DISTANCE =	-0.00052	0.00012	0.00077	0.00103
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	1.51400	1.47541	1.43711	1.42151

OUTSIDE ALPHA LAYER

POINT NUMBER =	11	13	17	21	25	30
DISTANCE =	0.00103	0.00129	0.00172	0.00214	0.00257	0.00314
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.45365	0.39096	0.29136	0.20850	0.14365	0.07010

BETA LAYER

POINT NUMBER =	30	41	49	57	65	73	81	89	97	105	113	129	193
DISTANCE =	0.00314	0.00429	0.00515	0.00600	0.00686	0.00772	0.00858	0.00943	0.01029	0.01115	0.01201	0.01372	0.02058
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.01738	0.01669	0.01618	0.01567	0.01518	0.01469	0.01422	0.01376	0.01331	0.01288	0.01246	0.01167	0.00920

BETA LAYER

POINT NUMBER =	257	321	385	449	513	529	537	545	553	561	569	577	585
DISTANCE =	0.02784	0.03430	0.04116	0.04802	0.05488	0.05660	0.05745	0.05831	0.05917	0.06003	0.06088	0.06174	0.06260
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.00785	0.00742	0.00780	0.00912	0.01156	0.01235	0.01277	0.01321	0.01366	0.01413	0.01461	0.01511	0.01562

BETA LAYER

POINT NUMBER =	593	601	612
DISTANCE =	0.06386	0.06431	0.06548
TEMPERATURE =	1000.00	1000.00	1000.00
CONCENTRATION=	0.01613	0.01666	0.01738

INSIDE ALPHA LAYER

POINT NUMBER =	612	617	621	625	629	631
DISTANCE =	0.06548	0.06603	0.06646	0.06689	0.06731	0.06757
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.07010	0.14226	0.20723	0.29029	0.39021	0.45365

INSIDE OXIDE LAYER

POINT NUMBER =	631	633	637	641
DISTANCE =	0.06757	0.06783	0.06848	0.06912
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	1.42151	1.43697	1.47531	1.51400

N.T.COEFF	STEAM TEMP	EMISSIVITY	RAD.WALL SURFACE TEMP	OI/MET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	1000.00000	0.0	0.0	1000.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1000.00000	0.0	0.0	0.0	0.0

O.FL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.0042	3.9575	0.8707	0.7591	9.7983	4.9925	27.0116	36.7961	576.8701
1.0000	0.0042	3.4496	0.7615	0.0	0.0	4.3632	26.9320	36.5432	0.0

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	9	18
DISTANCE =	-0.00091	0.00038	0.00179
TEMPERATURE =	1000.00	1000.00	1000.00
CONCENTRATION=	1.51400	1.46961	1.42151

OUTSIDE ALPHA LAYER

POINT NUMBER =	18	25	33	41	52
DISTANCE =	0.00179	0.00257	0.00343	0.00429	0.00547
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.45365	0.34759	0.24159	0.16212	0.07010

BETA LAYER

POINT NUMBER =	52	65	81	97	113	129	145	161	177	193	209	257	321
DISTANCE =	0.00547	0.00686	0.00858	0.01029	0.01201	0.01372	0.01544	0.01715	0.01887	0.02058	0.02230	0.02744	0.03430
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.01738	0.01699	0.01650	0.01603	0.01557	0.01512	0.01470	0.01430	0.01393	0.01359	0.01328	0.01257	0.01218

BETA LAYER

POINT NUMBER =	385	433	449	465	481	497	513	529	545	561	577	590
DISTANCE =	0.04116	0.04631	0.04802	0.04974	0.05145	0.05317	0.05488	0.05660	0.05831	0.06003	0.06174	0.06316
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.01251	0.01319	0.01349	0.01383	0.01420	0.01460	0.01503	0.01549	0.01596	0.01645	0.01696	0.01738

INSIDE ALPHA LAYER

POINT NUMBER =	590	601	609	617	624
DISTANCE =	0.06316	0.06431	0.06517	0.06603	0.06681
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.07010	0.15967	0.23924	0.34578	0.45365

INSIDE OXIDE LAYER

POINT NUMBER =	624	633	641
DISTANCE =	0.06681	0.06821	0.06951
TEMPERATURE =	1000.00	1000.00	1000.00
CONCENTRATION=	1.42151	1.46944	1.51400

R.T.COEFF	STEAM TEMP	EMISSIVITY	RAD.WALL	SURFACE TEMP	OX/NBE TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	1000.00000	0.0	0.0	1000.00000	1000.00000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1000.00000	1000.00000	0.0	0.0	0.0	0.0

O.FL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.0024	6.8833	1.5888	0.7709	16.6511	8.6370	67.0397	71.9781	480.3545
1.0000	0.0024	6.0037	1.4045	0.0	0.0	7.5694	66.8105	71.4995	0.0

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	9	17	25	30
DISTANCE =	-0.00158	-0.00029	0.00100	0.00229	0.00312
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	1.51400	1.48845	1.46296	1.43762	1.42151

OUTSIDE ALPHA LAYER

POINT NUMBER =	30	41	49	57	65	73	81	89	,7
DISTANCE =	0.00312	0.00429	0.00515	0.00600	0.00686	0.00772	0.00858	0.00943	0.01032
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.42151	0.36161	0.29740	0.24145	0.19357	0.15330	0.12016	0.09384	0.07010

BETA LAYER

POINT NUMBER =	97	113	129	145	161	177	193	209	225	241	257	321	385
DISTANCE =	0.01032	0.01201	0.01372	0.01544	0.01715	0.01887	0.02058	0.02230	0.02401	0.02573	0.02744	0.03436	0.04116
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.01730	0.01734	0.01730	0.01727	0.01723	0.01720	0.01717	0.01714	0.01712	0.01710	0.01708	0.01704	0.01707

BETA LAYER

POINT NUMBER =	401	417	433	449	465	481	497	513	529	545
DISTANCE =	0.04288	0.04459	0.04631	0.04802	0.04974	0.05145	0.05317	0.05488	0.05660	0.05834
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.01709	0.01711	0.01713	0.01716	0.01719	0.01723	0.01726	0.01730	0.01734	0.01738

INSIDE ALPHA LAYER

POINT NUMBER =	545	553	561	569	577	585	593	601	612
DISTANCE =	0.05834	0.05917	0.06003	0.06088	0.06174	0.06260	0.06346	0.06431	0.06549
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	0.07010	0.09200	0.11818	0.15112	0.19118	0.23888	0.29477	0.35926	0.45365

INSIDE OXIDE LAYER

POINT NUMBER =	612	617	625	633	641
DISTANCE =	0.06549	0.06630	0.06759	0.06888	0.07018
TEMPERATURE =	1000.00	1000.00	1000.00	1000.00	1000.00
CONCENTRATION=	1.42151	1.43719	1.46258	1.48822	1.51400

TABLE D3. SELECTED INPUT-OUTPUT FOR TEST CASE 7: SIMULATED BURST TEST OF ZIRCALOY TUBE IN STEAM.

ROUT	WALL	DOXID(1)	CALPA(1)	DOXID(2)	CALPA(2)
0.53200	0.06860	0.0	0.0	0.0	0.0

TMAX	DTTEMP	DTDIFF	DTPRIN	NSTEP	NPRINT	NUMBER	NSCALE
40.0000	0.0	0.0	5.0000	2	1	301	0

NLOOP	NBAKER
1	0

NDIFF(K)	NCOOL(K)	TSTEAM(K)	ERADIA(K)	TWALL(K)	QFIXED(K)
1.0000	0.0	0.0	0.0	0.0	0.0
0.0	0.1000	350.0000	0.0	0.0	0.0

NDIFIN(K)	NCOEFF(K)	NTCOOL(K)	NRADCO(K)	NTWALL(K)	NQFLUX(K)
0	0	0	0	0	0
0	0	2	0	0	0

TSTART	CSTART	QSPLIT	NPLOT
350.00	0.006430	0.0	1

* * * MATERIAL PROPERTIES * * *

METAL DENSITY = 6.490 OXID DENSITY = 5.820 GRAM/CM**3 REACTION HEAT = 34330.00 BTU/GRAM OXYGEN

	EQUILIBRIUM CONCENTRATION (GRAM/CM**3)					DIFFUSION CONSTANT (CM**2/SEC)			TH.CONDUC.W/(CM*C)		SP.HEAT W*SEC/(GM.C)	
TEMP.(C)	STOCH.OX.	OX./AL.	AL./OX.	AL./BETA	BETA/AL.	OXID	ALPHA	BETA	OXID	METAL	OXID	METAL
750.00	1.51400	1.44026	0.45365	0.00816	0.00391	0.6720-08	0.7310-10	0.4290-07	0.02000	0.19377	0.61755	0.36530
800.00	1.51400	1.43651	0.45365	0.00816	0.00391	0.1020-07	0.2140-09	0.8100-07	0.02000	0.20752	0.62090	0.36530
850.00	1.51400	1.43276	0.45365	0.00816	0.00391	0.2060-07	0.6770-09	0.1470-06	0.02000	0.22127	0.62425	0.36530
900.00	1.51400	1.42901	0.45365	0.03010	0.00840	0.3910-07	0.1780-08	0.2520-06	0.02000	0.23502	0.62760	1.02400
950.00	1.51400	1.42526	0.45365	0.05075	0.01289	0.7040-07	0.4150-08	0.4140-06	0.02000	0.24877	0.63095	0.36530
1000.00	1.51400	1.42151	0.45365	0.07010	0.01738	0.1210-06	0.9090-08	0.6530-06	0.02000	0.26252	0.63430	0.36530
1050.00	1.51400	1.41776	0.45365	0.08815	0.02187	0.2000-06	0.2110-07	0.9950-06	0.02000	0.27627	0.63765	0.36530
1100.00	1.51400	1.41401	0.45365	0.10491	0.02637	0.3190-06	0.4270-07	0.1470-05	0.02000	0.29002	0.64100	0.36530
1150.00	1.51400	1.41026	0.45365	0.12038	0.03178	0.4920-06	0.8210-07	0.2110-05	0.02000	0.30377	0.64435	0.36530
1200.00	1.51400	1.40651	0.45365	0.13458	0.03702	0.7360-06	0.1510-06	0.2970-05	0.02000	0.31752	0.64770	0.36530
1250.00	1.51400	1.40276	0.45365	0.14752	0.04049	0.1070-05	0.2670-06	0.4070-05	0.02000	0.33127	0.65105	0.36530
1300.00	1.51400	1.39901	0.45365	0.15899	0.05101	0.1530-05	0.4550-06	0.5470-05	0.02000	0.34502	0.65440	0.36530
1350.00	1.51400	1.39526	0.45365	0.16927	0.05977	0.2130-05	0.7510-06	0.7220-05	0.02000	0.35877	0.65775	0.36530
1400.00	1.51400	1.39151	0.45365	0.17826	0.06836	0.2900-05	0.1200-05	0.9380-05	0.02000	0.37252	0.66110	0.36530
1450.00	1.51400	1.38776	0.45365	0.18595	0.07757	0.3890-05	0.1870-05	0.1200-04	0.02000	0.38627	0.66445	0.36530
1500.00	1.51400	1.38401	0.45365	0.19234	0.08741	0.5130-05	0.2850-05	0.1510-04	0.02000	0.40002	0.66780	0.36530
1550.00	1.51400	1.38026	0.45365	0.19744	0.09705	0.6660-05	0.4230-05	0.1890-04	0.02000	0.41377	0.67115	0.36530

*** * * * TIME = 20.000 * * * *** **PLOT # = 308**

R.T.COEFF	STREAM TEMP	EMISSIVITY	RAD.WALL	SURFACE TEMP	OX/NET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	0.0	0.0	0.0	885.54677	885.54677	0.0	0.0	0.0	0.0
0.10000	949.86444	0.0	0.0	885.54677	885.54677	0.0	6.43177	0.0	6.43177

O.PL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.0293	0.1378	0.0191	0.0148	0.5717	0.1549	0.9361	0.0003	604.5706

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	2
DISTANCE =	-0.00003	0.00006
TEMPERATURE =	885.55	885.55
CONCENTRATION=	1.51400	1.43010

OUTSIDE ALPHA LAYER

POINT NUMBER =	2	2
DISTANCE =	0.00006	0.00018
TEMPERATURE =	885.55	885.55
CONCENTRATION=	0.45365	0.02309

BETA LAYER

POINT NUMBER =	2	5	7	9	11	13	15	17	19	21	65	129	193
DISTANCE =	0.00018	0.00063	0.00064	0.00086	0.00107	0.00129	0.00150	0.00172	0.00193	0.00214	0.00686	0.01372	0.02058
TEMPERATURE =	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55	885.55
CONCENTRATION=	0.00710	0.00633	0.00600	0.00587	0.00587	0.00593	0.00603	0.00613	0.00623	0.00630	0.00649	0.00649	0.00649

BETA LAYER

POINT NUMBER =	257	321	385	449	513	577	641
DISTANCE =	0.02764	0.03430	0.04114	0.04802	0.05488	0.06174	0.06860
TEMPERATURE =	885.55	885.55	885.55	885.55	885.55	885.55	885.55
CONCENTRATION=	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649

*** * * * TIME = 30.000 * * * *** **PLOT # = 309**

R.T.COEFF	STREAM TEMP	EMISSIVITY	RAD.WALL	SURFACE TEMP	OX/NET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	0.0	0.0	0.0	1269.57167	1269.57167	0.0	0.0	0.0	0.0
0.10000	1249.86772	0.0	0.0	1269.57167	1269.57167	0.0	-1.97040	0.0	-1.97040

O.PL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.2407	0.8429	0.2560	0.5388	1.8382	1.2180	5.7850	0.4911	674.6784

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	5
DISTANCE =	-0.00019	0.00038
TEMPERATURE =	1269.57	1269.57
CONCENTRATION=	1.51400	1.40129

OUTSIDE ALPHA LAYER

POINT NUMBER =	5	13
DISTANCE =	0.00038	0.00121
TEMPERATURE =	1269.57	1269.57
CONCENTRATION=	0.45365	0.15210

BETA LAYER

POINT NUMBER =	13	15	17	19	21	23	25	27	29	31	65	129	193
DISTANCE =	0.00123	0.00150	0.00172	0.00193	0.00214	0.00236	0.00257	0.00279	0.00300	0.00322	0.00604	0.01372	0.02050
TEMPERATURE =	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57
CONCENTRATION=	0.04728	0.04431	0.04236	0.04033	0.03838	0.03681	0.03472	0.03301	0.03130	0.02983	0.01911	0.00673	0.00649

BETA LAYER

POINT NUMBER =	257	321	385	449	513	577	641
DISTANCE =	0.02784	0.03430	0.04116	0.04802	0.05488	0.06174	0.06860
TEMPERATURE =	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57	1269.57
CONCENTRATION=	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649

* * * * TIME = 35.000 * * * * PLOT # = 314

N.T.COEFF	STEAM TEMP	EMISSIVITY	RAD.WALL SURFACE TEMP	OX/NET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	0.0	0.0	0.0	1522.17114	1522.17114	0.0	0.0	0.0	0.0
0.10000	1399.90080	0.0	0.0	1522.17114	1522.17114	0.0	-12.21903	0.0	-12.21903

O.PL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.6008	1.8314	0.8145	0.9221	3.5686	3.1410	12.6573	25.7024	651.8997

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	5	9
DISTANCE =	-0.00043	0.00022	0.00086
TEMPERATURE =	1522.17	1522.17	1522.17
CONCENTRATION=	1.51000	1.44665	1.38235

OUTSIDE ALPHA LAYER

POINT NUMBER =	9	13	17	21	25	29	33
DISTANCE =	0.00086	0.00129	0.00172	0.00214	0.00257	0.00300	0.00341
TEMPERATURE =	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17
CONCENTRATION=	0.45365	0.40417	0.35729	0.31260	0.27004	0.23048	0.19476

BETA LAYER

POINT NUMBER =	33	41	49	57	65	73	81	89	97	105	113	129	193
DISTANCE =	0.00341	0.00429	0.00515	0.00600	0.00686	0.00772	0.00858	0.00943	0.01029	0.01115	0.01201	0.01372	0.02058
TEMPERATURE =	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17
CONCENTRATION=	0.09197	0.08239	0.07347	0.06543	0.05826	0.05188	0.04621	0.04114	0.03660	0.03248	0.02878	0.02229	0.01652

BETA LAYER

POINT NUMBER =	257	321	385	449	513	577	641
DISTANCE =	0.02784	0.03430	0.04116	0.04802	0.05488	0.06174	0.06860
TEMPERATURE =	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17	1522.17
CONCENTRATION=	0.00736	0.00665	0.00652	0.00649	0.00649	0.00649	0.00649

TABLE D4. SELECTED INPUT-OUTPUT FOR TEST CASE 3A: BURST-TEST WITH TEMPERATURE PROFILE CALCULATION.

ROOT	WALL	BOXID(1)	BALPA(1)	BOXID(2)	BALPA(2)
0.53200	0.04666	0.0	0.0	0.0	0.0

TBAI	DTTEMP	DTDIFF	DTMAIN	NSTEP	NPRINT	MGRADE	NSCALE
35.0000	0.0	0.0	5.0000	2	1	401	0

NLOOP	NBANDS
0	0

NDIFF(K)	NCOOL(K)	TSTBAS(K)	BBADIA(K)	TWALL(K)	QFIXED(K)
1.0000	0.0	0.0	0.0	0.0	0.0
0.0	0.1000	350.0000	0.0	0.0	0.0

NDIFB(K)	NCOMPP(K)	NFCOOL(K)	NBADCO(K)	NTWALL(K)	NQFLUX(K)
0	0	0	0	0	0
0	0	2	0	0	0

TSTART	CSTART	QSPLIT	NPLOT
350.00	0.000490	0.0	0

• • • MATERIAL PROPERTIES • • •

METAL DENSITY = 6.490 OXID DENSITY = 5.020 GRAM/CM**3 REACTION HEAT = 34330.00 MJOC/GRAM OXYGEN

	EQUILIBRIUM CONCENTRATION (GRAM/CM**3)			DIFFUSION CONSTANT (CM**2/SEC)			TH.CONDUC.W/(CM°C)		SP.HEAT W°SEC/(GR.C)	
TEMP.(C)	STOCH.OI.	OI./AL.	AL./OI.	AL./BETA	BETA/AL.	OXID	ALPHA	BETA	OXID	METAL	OXID	METAL
750.00	1.51400	1.44026	0.45365	0.00016	0.00391	0.6720-08	0.7310-10	0.6290-07	0.02000	0.10377	0.61795	0.36530
800.00	1.51400	1.43651	0.45365	0.00016	0.00391	0.1020-07	0.2340-09	0.0100-07	0.02000	0.20752	0.62090	0.36530
850.00	1.51400	1.43276	0.45365	0.00016	0.00391	0.2060-07	0.4770-09	0.1070-06	0.02000	0.22127	0.62425	0.36530
900.00	1.51400	1.42901	0.45365	0.03010	0.00040	0.3910-07	0.1780-08	0.2520-06	0.02000	0.23502	0.62760	1.03400
950.00	1.51400	1.42526	0.45365	0.05075	0.01209	0.7040-07	0.4350-08	0.6140-06	0.02000	0.24877	0.63095	0.36530
1000.00	1.51400	1.42151	0.45365	0.07010	0.01738	0.1210-06	0.9890-08	0.6530-06	0.02000	0.26252	0.63430	0.36530
1050.00	1.51400	1.41776	0.45365	0.08815	0.02157	0.2000-06	0.2110-07	0.9950-06	0.02000	0.27627	0.63765	0.36530
1100.00	1.51400	1.41401	0.45365	0.10491	0.02637	0.3190-06	0.4270-07	0.1070-05	0.02000	0.29002	0.64100	0.36530
1150.00	1.51400	1.41026	0.45365	0.12038	0.03170	0.4920-06	0.8210-07	0.2110-05	0.02000	0.30377	0.64435	0.36530
1200.00	1.51400	1.40651	0.45365	0.13458	0.03782	0.7360-06	0.1510-06	0.2070-05	0.02000	0.31752	0.64770	0.36530
1250.00	1.51400	1.40276	0.45365	0.14752	0.04449	0.1070-05	0.2670-06	0.4070-05	0.02000	0.33127	0.65105	0.36530
1300.00	1.51400	1.39901	0.45365	0.15919	0.05181	0.1530-05	0.4550-06	0.5470-05	0.02000	0.34503	0.65440	0.36530
1350.00	1.51400	1.39526	0.45365	0.16927	0.05977	0.2130-05	0.7510-06	0.7230-05	0.02000	0.35877	0.65775	0.36530
1400.00	1.51400	1.39151	0.45365	0.17826	0.06836	0.2900-05	0.1200-05	0.9380-05	0.02000	0.37252	0.66110	0.36530
1450.00	1.51400	1.38776	0.45365	0.18595	0.07757	0.3890-05	0.1870-05	0.1200-04	0.02000	0.38627	0.66445	0.36530
1500.00	1.51400	1.38401	0.45365	0.19234	0.08741	0.5130-05	0.2850-05	0.1510-04	0.02000	0.40002	0.66780	0.36530
1550.00	1.51400	1.38026	0.45365	0.19744	0.09785	0.6660-05	0.4230-05	0.1890-04	0.02000	0.41377	0.67115	0.36530

```
 * * * * TIME =   20.000 * * * *                                                    PLOT # =      404

   H.T.COEFF   STEAM TEMP   EMISSIVITY     RAD.WALL SURFACE TEMP  OX/NET TEMP FIX.HEATFLUX CON.HEATFLUX RAD.HEATFLUX    QCON*GRAD
         0.0         0.0          0.0          0.0      884.99547    884.99769          0.0          0.0          0.0          0.0
     0.10000   949.27205          0.0          0.0      885.76602    885.76602          0.0      6.35060          0.0      6.35060

  O.PL.LIMIT   OXIGEN FLUX   C.IN OXIDE   O.IN ALPHA    O.IN BETA   OXYG.TOTAL    OXYG.GAIN  OXIDE LAYER  ALPHA LAYER   BETA LAYER
      1.0000        0.0293       0.1374       0.0190       0.0148       0.5712       0.1545       0.9335       0.7982     684.5025

OUTSIDE OXIDE LAYER
POINT NUMBER =         1         2
DISTANCE     =  -0.00003   0.00006
TEMPERATURE  =    885.00    885.00
CONCENTRATION=   1.51400   1.43014

OUTSIDE ALPHA LAYER

POINT NUMBER =         2         2
DISTANCE     =   0.00006   0.00014
TEMPERATURE  =    885.00    885.00
CONCENTRATION=   0.45365   0.02365

BETA LAYER

POINT NUMBER =         2         5         7         9        11        13        15        17        19        21        65       129       193
DISTANCE     =   0.00014   0.00043   0.00064   0.00086   0.00107   0.00129   0.00150   0.00172   0.00193   0.00214   0.00686   0.01372   0.02058
TEMPERATURE  =    885.00    885.00    885.00    884.99    884.99    884.99    884.99    884.99    884.99    884.99    884.98    884.98    885.00
CONCENTRATION=   0.00705   0.00631   0.00599   0.00587   0.00587   0.00593   0.00603   0.00614   0.00623   0.00631   0.00649   0.00649   0.00649

BETA LAYER

POINT NUMBER =       257       321       385       449       513       577       641
DISTANCE     =   0.02744   0.03430   0.04116   0.04802   0.05488   0.06174   0.06860
TEMPERATURE  =    885.04    885.11    885.19    885.30    885.43    885.59    885.77
CONCENTRATION=   0.00649   0.00649   0.00649   0.00649   0.00649   0.00649   0.00649


 * * * * TIME =   30.000 * * * *                                                    PLOT # =      409

   H.T.COEFF   STEAM TEMP   EMISSIVITY     RAD.WALL SURFACE TEMP  OX/NET TEMP FIX.HEATFLUX CON.HEATFLUX RAD.HEATFLUX    QCON*GRAD
         0.0         0.0          0.0          0.0     1270.80870   1270.82047          0.0          0.0          0.0          0.0
     0.10000  1249.72037          0.0          0.0     1269.77106   1269.77106          0.0     -2.00507          0.0     -2.00507

  O.PL.LIMIT   OXIGEN FLUX   C.IN OXIDE   O.IN ALPHA    O.IN BETA   OXYG.TOTAL    OXYG.GAIN  OXIDE LAYER  ALPHA LAYER   BETA LAYER
      1.0000        0.2429       0.8443       0.2578       0.5352       1.6373       1.2179       5.7946       0.9209     673.6344

OUTSIDE OXIDE LAYER

POINT NUMBER =         1         5
DISTANCE     =  -0.00020   0.00038
TEMPERATURE  =   1270.61   1270.62
CONCENTRATION=   1.51400   1.40120
```

OUTSIDE ALPHA LAYER

POINT NUMBER =	5	13
DISTANCE =	0.00038	0.00124
TEMPERATURE =	1270.82	1270.80
CONCENTRATION=	0.45365	0.15239

BETA LAYER

POINT NUMBER =	13	15	17	19	21	23	25	27	29	31	65	129	193
DISTANCE =	0.00124	0.00150	0.00172	0.00193	0.00214	0.00236	0.00257	0.00279	0.00300	0.00322	0.00686	0.01372	0.02058
TEMPERATURE =	1270.80	1270.79	1270.79	1270.78	1270.78	1270.77	1270.77	1270.76	1270.76	1270.75	1270.67	1270.52	1270.30
CONCENTRATION=	0.04746	0.04473	0.04259	0.04054	0.03858	0.03670	0.03490	0.03318	0.03155	0.02998	0.01316	0.00673	0.00649

BETA LAYER

POINT NUMBER =	257	321	385	449	513	577	641
DISTANCE =	0.02764	0.03430	0.04116	0.04802	0.05488	0.06174	0.06860
TEMPERATURE =	1270.25	1270.14	1270.04	1269.95	1269.88	1269.82	1269.77
CONCENTRATION=	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649	0.00649

* * * * TIME = 35.000 * * * * PLOT # = 414

B.T.COEFF	STEAM TEMP	EMISSIVITY	RAD.WALL SURFACE TEMP	OX/MET TEMP	FIX.HEATFLUX	CON.HEATFLUX	RAD.HEATFLUX	QCON+QRAD
0.0	0.0	0.0	0.0	1524.46213	1524.51070	0.0	0.0	0.0	0.0
0.10000	1399.89815	0.0	0.0	1521.79352	1521.79352	0.0	-12.18954	0.0	-12.18954

O.FL.LIMIT	OXIGEN FLUX	O.IN OXIDE	O.IN ALPHA	O.IN BETA	OXYG.TOTAL	OXYG.GAIN	OXIDE LAYER	ALPHA LAYER	BETA LAYER
1.0000	0.6037	1.8472	0.8261	0.9288	3.6021	3.1738	12.7677	26.0563	651.4726

OUTSIDE OXIDE LAYER

POINT NUMBER =	1	5	9
DISTANCE =	-0.00043	0.00022	0.00085
TEMPERATURE =	1524.46	1524.49	1524.51
CONCENTRATION=	1.91400	1.44714	1.38217

OUTSIDE ALPHA LAYER

POINT NUMBER =	9	13	17	21	25	29	33
DISTANCE =	0.00085	0.00124	0.00172	0.00218	0.00257	0.00300	0.00345
TEMPERATURE =	1524.51	1524.49	1524.47	1524.45	1524.43	1524.40	1524.38
CONCENTRATION=	0.45365	0.40568	0.35845	0.31518	0.27327	0.23430	0.19899

BETA LAYER

POINT NUMBER =	33	41	49	57	65	73	81	89	97	105	113	129	193
DISTANCE =	0.00345	0.00429	0.00515	0.00600	0.00686	0.00772	0.00858	0.00943	0.01029	0.01115	0.01201	0.01372	0.02058
TEMPERATURE =	1524.38	1524.34	1524.26	1524.17	1524.09	1524.04	1523.99	1523.94	1523.89	1523.84	1523.79	1523.69	1523.58
CONCENTRATION=	0.09263	0.08337	0.07448	0.06645	0.05923	0.05277	0.04700	0.04183	0.03719	0.03300	0.02921	0.02274	0.01060

BETA LAYER

POINT NUMBER =	257	321	385	449	513	577	641
DISTANCE =	0.02764	0.03430	0.04116	0.04802	0.05488	0.06174	0.06860
TEMPERATURE =	1523.28	1523.00	1522.73	1522.48	1522.23	1522.01	1521.79
CONCENTRATION=	0.00780	0.00666	0.00652	0.00649	0.00649	0.00649	0.00649

```
      C     SIMTRAN 1
ISN 0002    IMPLICIT REAL*8 (A-H,O-Z)
ISN 0003    REAL*8 PLO
ISN 0004    COMMON/RESULT/PLO(25,200),KPLOT,MPLOT
ISN 0005    COMMON/GEOMET/ R(1000),ROXID(2),RALFA(2),WALL,DOXID(2),DALFA(2),DR
ISN 0006    COMMON/TEMP  / T(1000),TOXID(2),TALFA(2),TSTART,TSTEAM(2),TWALL(2)
           1,TSURF(2)
ISN 0007    COMMON/TENTIN/ TCOOL(100,2),ZTCOOL(100,2),TWAD(100,2),ETWAD(100,2)
ISN 0008    COMMON/HEAT  / HVER(100)  ,HCOOL(2),FRADIA(2),HRATPL(2),QFINFD(2),
           1                 QSPLIT,HCAP(100)  ,HSTEAM(2),HRADIA(2)
           2                ,QSURF(2),QCON(2),QRAD(2),QRFACT(2)
ISN 0009    COMMON/HEADLN/ HTITLE(20)
ISN 0010    COMMON/CONCRW/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
           1               OXIGPL(2),NDIFF(2),CSTART,SALN(2)
           2,          OCAP(500),OVEP(500),ODTMAX(500)
           3,          COA(2),CAO(2),CAB(2),CBA(2)
           4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0011    COMMON/EXIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
           1,             NTEMP,NDIFF,NPRINT
ISN 0012    COMMON/MESH  /MGROSS,MPINE,MOXID(2),MOXI(2)
           1,             NLUMB,NSTART,NALFA(2)
ISN 0013    COMMON/MESHTP/MT(100),MTCOOL(2),MTWALL(2),MTCOOL(2),MTWALL(2),MGES
ISN 0014    COMMON/MESHCO/MC(500),MBAKEP,MGES,MOA(2),MAB(2)
           1,             MOA(2),MAO(2),MAB(2),MBA(2),INTOXI(2),INTB
           2,             MOA1,MAO1,MAB1,MBA1,MOXID1,MALFA1
           3,             MOA2,MAO2,MAB2,MBA2,MOXID2,MALFA2
ISN 0015    COMMON/MATPRO/ DENZIR,DENERO,OSTOCH,OXICON,DENRAT,FICFAC,OXHEAT
ISN 0016    COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
           1OALFA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
           2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0017    COMMON/HINPUT/ NDIFIN(100,2),TINDIF(100,2),HCOEFF(100,2),
           1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
           2               QFLUXI(100,2),TQFLUX(100,2),TINSTP(100),DTNEW(100),
           3               NDIFIN(2),NDIFIN(2),FQFLUX(2),NQFLUX(2),
           4               NCOEFF(2),NCOEFF(2),FRADCO(2),NRADCO(2),NSTEP
ISN 0018    COMMON/PLOVAR/OLINIT(2),CINIT,PLOTIN
ISN 0019    DIMENSION DOXOLD(2),DALOLD(2)
      C     DXO = MAX.MOVEMENT OF OXIDE/ALPHA INTERFACE DURING 1 TIME STEP
      C     DXA = MAX.MOVEMENT OF ALPHA/BETA  INTERFACE DURING 1 TIME STEP
      C     DTE = MAX.TEMPERATURE CHANGE DURING 1 TIME STEP
ISN 0020    DXO=2.D-6
ISN 0021    DXA=5.D-6
ISN 0022    DTE=1.
ISN 0023    DTE2=DTE/2.
ISN 0024   1 CALL INPUT
ISN 0025    IF(R(1).EQ.0.) GO TO 9999
      C     R(1)=0. IS SET IN INPUT IF THERE IS NO NEXT CASE
ISN 0027    CALL INDATA
      C     INDATA PRINTS ALL INPUT DATA
ISN 0029    NSTART=0
ISN 0029    CALL INITIA
ISN 0030    TTEMP=-1.D-10
ISN 0031    TDIFF=-1.D-10
ISN 0032    TPRINT=DTPRIN-1.D-10
ISN 0033    TPLOT=DTPRIN*DFLOAT(NPRINT)-1.D-10
ISN 0034    TMAX=TMAX-1.D-10
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```
ISN 0035            TEMMAX=DTTEMP
ISN 0036            DIFMAX=DTDIFF
ISN 0037            DXLIM=DXO  *DENSIN*DENRAT
ISN 0038            LSTEP=1
ISN 0039            DOXOLD(1)=DOXID(1)
ISN 0040            DOXOLD(2)=DOXID(2)
ISN 0041            DALOLD(1)=DALPA(1)
ISN 0042            DALOLD(2)=DALPA(2)
ISN 0043            DTOLD=DOXID(1)*DOXID(2)
ISN 0044            DTOLD2=DTOLD
ISN 0045            DTOLD3=DTOLD
ISN 0046            TEMOLD=T(1)
ISN 0047         10 DTMIN=TPRINT-TIME+1.D-10
                 C     TIME STEP CONTROL (UP TO LABEL 140)
                 C     DTDIFF = TIME STEP FOR DIFFUSION CALCULATION
                 C     DTTEMP = TIME STEP FOR TEMPERATURE CALCULATION
ISN 0048            DTDIFF=DIFMAX
ISN 0049            DTTEMP=TEMMAX
ISN 0050            DO 20 K=1,2
ISN 0051            IF(XDIFF(K).EQ.0.) GO TO 20
ISN 0053            DT=DXLIM/DXIGPL(K)
ISN 0054            IF(DT.GT.DTOLD ) DT=1.03*DTOLD
ISN 0056            IF(DT.LT.DTDIFF) DTDIFF=DT
ISN 0058            DO=DABS(DOXID(K)-DOXOLD(K))
ISN 0059            DA=DABS(DALPA(K)-DALOLD(K))
ISN 0060            IF(DO.GT.DXO) DTDIFF=DTOLD *DXO/DO
ISN 0062            IF(DA.GT.DXA) DTDIFF=DTOLD *DXA/DA
ISN 0064            DOXOLD(K)=DOXID(K)
ISN 0065            DALOLD(K)=DALPA(K)
ISN 0066         20 CONTINUE
ISN 0067            IF(DTDIFF.LT.DTMIN) DTMIN=DTDIFF
ISN 0069            IF(DTTEMP.LT.DTMIN) DTMIN=DTTEMP
ISN 0071            IF(NLOOP.EQ.2) GO TO 70
                 C     NLOOP=2 NO TEMPERATURE CALCULATION
ISN 0073            DELTA=DABS(T(1)-TEMOLD)
ISN 0074            IF(DELTA-DTE2) 50,50,60
ISN 0075         50 DTTEMP=DTMIN
ISN 0076            GO TO 140
ISN 0077         60 DTTEMP=DTOLD*DTE2/DELTA
ISN 0078            IF(DTTEMP.LT.DTMIN) DTMIN=DTTEMP
ISN 0080            GO TO 140
ISN 0081         70 IF(NTCOOL(1).GT.0) GO TO 80
                 C     NTCOOL(1) OR NTCOOL(2) GREATER THAN 0:
                 C     TEMPERATURE IS FUNCTION OF TIME
ISN 0083            DTTEMP=TMAX
ISN 0084            GO TO 100
ISN 0085         80 T(1)=TINPUN(NTCOOL(1),TCOOL,ZTCOOL,1,TIME)
ISN 0086            TNEW=TINPUN(NTCOOL(1),TCOOL,ZTCOOL,1,TPRINT)
ISN 0087            DELTA=DABS(T(1)-TNEW)
ISN 0088            IF(DELTA.GT.1.) GO TO 90
ISN 0090            DTTEMP=TPRINT-TIME
ISN 0091            GO TO 140
ISN 0092         90 DTTEMP=(TPRINT-TIME)/DELTA
ISN 0093            TTEMP=TIME
ISN 0094            GO TO 140
ISN 0095        100 IF(NTCOOL(2).EQ.0) GO TO 140
ISN 0097            T(NPINE)=TINPUN(NTCOOL(2),TCOOL,ZTCOOL,2,TIME)
ISN 0098            TNEW    =TINPUN(NTCOOL(2),TCOOL,ZTCOOL,2,TPRINT)
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ISN 0099            DELTA=DABS(T(NPINE)-TNEW)
ISN 0100            IF(DELTA.GT.1.) GO TO 120
ISN 0102            DTTEMP=TPRINT-TIME
ISN 0103            GO TO 140
ISN 0104      120   DTTEMP=(TPRINT-TIME)/DELTA
ISN 0105            TTEMP=TIME
ISN 0106      140   IF(DTMIN.LT.DTDIFF) DTDIFF=DTMIN
                C   END OF TIME STEP CONTROL
ISN 0109            IF(TIME.LT.TTEMP) GO TO 200
ISN 0110            DO 150 K=1,2
ISN 0111            IF(NTCOOL(K).GT.0)TSTEAM(K)=TIMFUN(NTCOOL(K),TCOOL ,TTCOOL,K,TIME)
ISN 0113            IF(NTWALL(K).GT.0)TWALL(K) =TIMFUN(NTWALL(K),TRAD  ,TTRAD ,K,TIME)
ISN 0115            IF(NCOEFF(K).GT.0)HCOOL(K) =TIMFUN(NCOEFF(K),HCOEFF,TCOEFF,K,TIME)
ISN 0117            IF(NRADCO(K).GT.0)ERADIA(K)=TIMFUN(NRADCO(K),HRADCO,TRADCO,K,TIME)
ISN 0119            IF(NQFLUX(K).GT.0)QFIXED(K)=TIMFUN(NQFLUX(K),QFLUXI,TQFLUX,K,TIME)
ISN 0121      150   CONTINUE
ISN 0122            TTNOLD=T(1)
ISN 0123            CALL TEMPER
                C   TEMPER CALCULATES TEMPERATURES IN WALL
ISN 0124            TTEMP=TTEMP+DTTEMP
ISN 0125      200   IF(TIME.LT.TDIFF) GO TO 300
ISN 0127            N1=NDIFF(1)
ISN 0128            N2=NDIFF(2)
ISN 0129            IF(NDIFIN(1).GT.0)NDIFF(1)=TIMFUN(NDIFIN(1),NDIFIN,TIMDIF,1,TIME)
ISN 0131            IF(NDIFIN(2).GT.0)NDIFF(2)=TIMFUN(NDIFIN(2),NDIFIN,TIMDIF,2,TIME)
ISN 0133            IF((NDIFF(1).LE.N1).AND.(NDIFF(2).LE.N2)) GO TO 220
ISN 0135            DTDIFF=1.D-7
ISN 0136            DTMIN =1.D-7
ISN 0137      220   CALL DIFFUS
                C   DIFFUS CALCULATES OXYGEN PROFIL IN WALL
ISN 0138            IF(TIME.GT.0.) GO TO 250
ISN 0140            CALL OUTPUT
ISN 0141            OBETAS=OTOTAL
ISN 0142      250   TDIFF=TDIFF+DTDIFF
ISN 0143      300   TIME=TIME+DTMIN
ISN 0144            DTDIFF=DTOLD3
ISN 0145            DTOLD3=DTOLD2
ISN 0146            DTOLD2=DTOLD
ISN 0147            DTOLD=DTMIN
ISN 0148            IF(TIME.LT.TPRINT) GO TO 10
ISN 0150            DTOLD =DTOLD3
ISN 0151            DTOLD2=DTOLD3
ISN 0152            CALL OUTPUT
                C   OXYGEN - AND TEMPERATURE PROFILE ARE PRINTED
ISN 0153            IF((LSTEP.GT.NSTEP).OR.(TIME.LT.TIMSTP(LSTEP)-.000001))GO TO 400
ISN 0155            DTPRIN=DTMIN(LSTEP)
                C   DTMIN (LSTEP) IS THE NEW OUTPUT TIME STEP
ISN 0156            LSTEP=LSTEP+1
ISN 0157      400   TPRINT=TPRINT+DTPRIN
ISN 0159            IF(TIME.LT.TPLOT) GO TO 10
ISN 0160            TPLOT=TPLOT+DTPRIN*DFLOAT(NPRINT)
ISN 0161            IF((NUMBER.EQ.0).OR.(NBAKER.GT.0)) GO TO 4010
ISN 0163            CINIT=CSTART
ISN 0164            PLOTIN=TIME
ISN 0165            OLIMIT(1)=NDIFF(1)
ISN 0166            OLIMIT(2)=NDIFF(2)
ISN 0167            STEMP=T(1)
                C   OXYGEN PROFILE IS PLOTED
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ISN 0168            CALL PROPLO
ISN 0169            NSCALE=NSCALE
ISN 0170            IF(NSCALE.NE.2) GO TO 3500
ISN 0172            NUMBER=NUMBER+1
ISN 0173            NSCALE=0
ISN 0174            CALL PROPLO
ISN 0175            NSCALE=2
ISN 0176         3500 NUMBER=NUMBER+1
ISN 0177         4000 IF(TIME.LT.TMAX) GO TO 10
ISN 0179            IF(NPLOT .GT.0) CALL TRAPLO
                 C      TRAPLO PLOTS UP TO 24 VARIABLES AS FUNCTIONS OF TIME OR SQUARE
                 C      ROOT OF TIME
ISN 0181            GO TO 1
ISN 0182         9999 IF(NUMBER.EQ.0) STOP
ISN 0184            NUMBER=-NUMBER
ISN 0185            CALL PROPLO
ISN 0186            STOP
ISN 0187            END
```

```
ISN 0002            SUBROUTINE INPUT
                C   ALL INPUT DATA ARE READ IN THIS SUBROUTINE
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*8 PLO
ISN 0005            COMMON/RESULT/PLO(25,200),MPLOT,MPLOT
ISN 0006            COMMON/GENNET/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DP
ISN 0007            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTRAN(2),TWALL(2)
                   1,TSTEP(2)
ISN 0008            COMMON/TENTIN/ TCOOL(100,2),ETCOOL(100,2),TRAD(100,2),ETRAD(100,2)
ISN 0009            COMMON/HEAT  / HVPP(100) ,HCOOL(2),FRADIA(2),HEATPL(2),QPIXED(2),
                   1                        QSPLIT,HCAP(100) ,HSTEAM(2),HRADIA(2)
                   2                ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0010            COMMON/HEADLN/ HTITLE(20)
ISN 0011            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1               OXIGPL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          QCAP(500),OVER(500),QDTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2),
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0012            COMMON/EXIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              HTEMP,HDIFF,HPRINT
ISN 0013            COMMON/MESH  /HGROSS,HFINE,ROXID(2),ROXT(2)
                   1,              HLUMB,HSTART,HALPA(2)
ISN 0014            COMMON/TESNTE/HT(100),HTCOOL(2),HTWALL(2),HTCOOL(2),HTWALL(2),HGRS
ISN 0015            COMMON/TESNCO/HC(500),HBAKER,HGRS,HOA(2),HAB(2)
                   1,              HOA(2),HAO(2),HAB(2),HBA(2),INTOXI(2),INTB
                   2,              HOA1,HAO1,HAB1,HBA1,HOXID1,HALPA1
                   3,              HOA2,HAO2,HAB2,HBA2,HOXID2,HALPA2
ISN 0016            COMMON/MATPRO/ DENSIR,DENSHO,OSTOCH,OXICON,DENRAT,FICFAC,OXHEAT
ISN 0017            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2H1,H2,H3,H4,H5,HUMBER,HSCALE
ISN 0018            COMMON/MINPUT/ HDIFIN(100,2),TIMDIF(100,2),HCOEPP(100,2),
                   1               TCOEPP(100,2),HRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TINSTP(100),DTHIN(100),
                   3               HDIFIN(2),HDIFIN(2),HQFLUX(2),HQFLUX(2),
                   4               HCOEPP(2),HCOEPP(2),HRADCO(2),HRADCO(2),HSTEP
ISN 0019            K=5
ISN 0020            READ(N,150,END 1001) (HTITLE(K),K=1,20)
ISN 0021          150 FORMAT(20A4)
ISN 0022            READ (N,200) R(1),WALL,OLAYER(1),ALAYER(1),OLAYER(2),ALAYER(2)
ISN 0023          200 FOR   (8D10.5)
ISN 0024            RE   (,250) TMAX,DTTEMP,DTDIFF,DTPRIN,HSTEP,HPRINT,HUMBER,HSCALE
ISN 0025          250 FORMAT(4D10.5,4I10)
ISN 0026            IF(NSTEP.GT.0) READ(N,200) (TINSTP(K),DTHIN(K),K=1,NSTEP)
ISN 0028            READ(N,400) WLUMB,NBAKER
ISN 0029            READ(N,300) (HDIFF(K),HCOOL(K),TSTRAN(K),FRADIA(K),TWALL(K),
                   1               QPIXED(K),K=1,2)
ISN 0030          300 FORMAT(6D10.5)
ISN 0031            READ(N,400) (HDIFIN(K),HCOEPP(K),HTCOOL(K),HRADCO(K),HTWALL(K),
                   1               HQFLUX(K),K=1,2)
ISN 0032          400 FORMAT(6I10)
ISN 0033            DO 100 K=1,2
ISN 0034            IF(HDIFIN(K).EQ.0) GO TO 20
ISN 0036            M=HDIFIN(K)
ISN 0037            READ(N,200) (HDIFIN(L,K),TIMDIF(L,K),L=1,M)
ISN 0038           20 IF(HCOEPP(K).EQ.0) GO TO 30
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ISN 0040            M=MCOEFF(K)
ISN 0041            READ(N,200)  (HCOEFF(L,K),TCOEFF(L,K),L=1,M)
ISN 0042         30 IF(NTCOOL(K).EQ.0) GO TO 40
ISN 0044            M=NTCOOL(K)
ISN 0045            READ(N,200)  (TCOOL(L,K),ZTCOOL(L,K),L=1,M)
ISN 0046         40 IF(NRADCO(K).EQ.0) GO TO 50
ISN 0048            M=NRADCO(K)
ISN 0049            READ(N,200)  (RRADCO(L,K),TRADCO(L,K),L=1,M)
ISN 0050         50 IF(NTWALL(K).EQ.0) GO TO 60
ISN 0052            M=NTWALL(K)
ISN 0053            READ(N,200)  (TTRAD(L,K),ZTRAD(L,K),L=1,M)
ISN 0054         60 IF(NQFLUX(K).EQ.0) GO TO 100
ISN 0056            M=NQFLUX(K)
ISN 0057            READ(N,200)  (QFLUXI(L,K),TQFLUX(L,K),L=1,M)
ISN 0058        100 CONTINUE
ISN 0059            READ(N,250)  TSTART,CSTART,QSPLIT,DUMMY,NDUMY1,NDUMY2,NDUMY3,NPLOT
ISN 0060            RETURN
ISN 0061       1001 R(1)=0.
ISN 0062            RETURN
ISN 0063            END
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ISN 0002            SUBROUTINE INDATA
                C   INDATA PRINTS ALL INPUT DATA
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*8 PLO
ISN 0005            COMMON/RESULT/PLO(25,200),KPLOT,NPLOT
ISN 0006            COMMON/GROMET/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DR
ISN 0007            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0008            COMMON/TEMTIM/ TCOOL(100,2),TTCOOL(100,2),TRAD(100,2),TTRAD(100,2)
ISN 0009            COMMON/HEAT  / HVER(100) ,HCOOL(2),EFACIA(2),HEATPL(2),QFIXED(2),
                   1                QSPLIT,HCAP(100) ,HSTEAM(2),HRADIA(2)
                   2              ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0010            COMMON/HEADLN/ HTITLE(20)
ISN 0011            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALSPT(2),CBETA(2),
                   1              OXIGPL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),ODTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0012            COMMON/EDIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,             HTEMP,HDIFF,HPRINT
ISN 0013            COMMON/MESH  /HGROSS,HPINF,HOXID(2),HOXI(2)
                   1,            HLUMB,HSTART,HALPA(2)
ISN 0014            COMMON/MESHTI/HT(100),HTCOOL(2),HTWALL(2),HTCOOL(2),HTWALL(2),HGRO
ISN 0015            COMMON/MESHCO/HC(500),HBAKER,HGRO,HCA(2),HAB(2)
                   1,             HOA(2),HAO(2),HAB(2),HBA(2),INTOXI(2),INTB
                   2,             HOA1,HAO1,HAB1,HBA1,HOXID1,HALPA1
                   3,             HOA2,HAO2,HAB2,HBA2,HOXID2,HALPA2
ISN 0016            COMMON/MATPRO/ DENSIR,DENZRO,OSTOCH,OXICON,DENRAT,VICPAC,OXHEAT
ISN 0017            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0018            COMMON/HINPUT/ HDIFIN(100,2),TIMDIF(100,2),HCOEFF(100,2),
                   1              TCOEFF(100,2),HRADCO(100,2),TRADCO(100,2),
                   2              QFLUXI(100,2),TQFLUX(100,2),TMSTP(100),DTNEW(100),
                   3              RDIFIN(2),HDIFIN(2),HQFLUX(2),TQFLUX(2),
                   4              HCOEFF(2),TCOEFF(2),HRADCO(2),TRADCO(2),HSTEP
ISN 0019            J=6
ISN 0020            WRITE(J,500) (HTITLE(K),K=1,20)
ISN 0021          500 FORMAT(1H1,25X,20A4//)
ISN 0022            WRITE(J,599)
ISN 0023          599 FORMAT(10HO      ROUT,10H       WALL,10H   DOXID(1),10H   DALPA(1),
                   110H   DOXID(2),10H   DALPA(2))
ISN 0024            WRITE(J,600) R(1),WALL,OLAYER(1),ALAYER(1),OLAYER(2),ALAYER(2)
ISN 0025          600 FORMAT(6F10.4)
ISN 0026            WRITE(J,650)
ISN 0027          650 FORMAT(10HO      TMAX,10H     DTTEMP,10H     DTDIFF,10H     DTPRIN,
                   1       10H     HSTEP,10H     HPRINT,10H     NUMBER,10H     NSCALE)
ISN 0028            WRITE(J,660) TMAX,DTTEMP,DTDIFF,DTPRIN,HSTEP,HPRINT,NUMBER,NSCALE
ISN 0029          660 FORMAT(6P10.6,4I10)
ISN 0030            WRITE(J,798)
ISN 0031          798 FORMAT(10HO     HLUMB,10H     HBAKER)
ISN 0032            WRITE(J,800) HLUMB,HBAKER
ISN 0033            WRITE(J,698)
ISN 0034          698 FORMAT(10HO HDIFF(K),10H   HCOOL(K),10H TSTEAM(K),10H ERADIA(K),
                   1       10H   TWALL(K),10H QFIXED(K))
ISN 0035            WRITE(J,700) (HDIFF(K),HCOOL(K),TSTEAM(K),ERADIA(K),
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     1                TWALL(K),QFIXED(K),K=1,2)
ISN 0036       700 FORMAT(6F10.4)
ISN 0037           WRITE(J,799)
ISN 0038       799 FORMAT(10HONDIFIN(K),10H NCOEFF(K),10H NTCOOL(K),
     1         10H NRADCO(K),10H NTWALL(K),10H NQFLUX(K))
ISN 0039           WRITE(J,800) (NDIFIN(K),NCOEFF(K),NTCOOL(K),NRADCO(K),NTWALL(K),
     1                 NQFLUX(K),K=1,2)
ISN 0040       800 FORMAT(6I10)
ISN 0041           WRITE(J,699)
ISN 0042       699 FORMAT(10HO    TSTART,10H    CSTART,10H    QSPLIT,45X,5HNPLOT)
ISN 0043           WRITE(J,750) TSTART,CSTART,QSPLIT,NPLOT
ISN 0044       750 FORMAT(F10.2,F10.6, F10.2, 40X,I10/////)
ISN 0045           RETURN
ISN 0046           END
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ISN 0002            SUBROUTINE MATMAP
                C   A TABLE WITH ALL MATERIAL PROPERTIES IS CALCULATED AND PRINTED
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/HEADLN/ HTITLE(20)
ISN 0005            COMMON/MATPRO/ DENZIR,DENZRO,OSTOCH,CXICON,DENRAT,FICFAC,OXHEAT
ISN 0006            J=6
ISN 0007            WRITE(J,10)
ISN 0008           10 FORMAT(1HO//47X, 35H  * * * MATERIAL PROPERTIES * * *     ,//)
ISN 0009            WRITE(J,20) DENZIR,DENZRO,OXHEAT
ISN 0010           20 FORMAT(1HO,15HMETAL DENSITY = ,F7.3,5X,14HOXID DENSITY = ,F7.3,5X,
                     1       10HGRAM/CM**3 ,10X,15HREACTION HEAT = ,F10.2,3X,
                     2       14HJSEC/GRAM OXYGEN     )
ISN 0011            WRITE(J,30)
ISN 0012           30 FORMAT(1HO/20X,40HEQUILIBRIUM CONCENTRATION  (GRAM/CM**3)    ,2X,
                     130HDIFFUSION CONSTANT (CM**2/SEC),1X,18HTH.CONDUC.W/(CM*C),1X,
                     220HSP.HEAT W*SEC/(GR.C) )
ISN 0013            WRITE(J,40)
ISN 0014           40 FORMAT(1HO,10H  TEMP.(C),10H STOCH.OX.,10H   OX./AL.,10H   AL./OX.
                     1,           10H  AL./BETA,10H  BETA/AL.,10H   OXID   ,10H   ALPHA
                     2,           10H   BETA   ,10H   OXID   ,10H   METAL  ,10H   OXID
                     3,           10H   METAL  )
ISN 0015            T=750.
ISN 0016            DO 100 L=1,17
ISN 0017            CALL INTPAC(T,COXAL,CALOX,1)
ISN 0018            CALL INTPAC(T,CALBE,CBEAL,2)
ISN 0019            DOX= DIFCON(T,T,OXICON,COXAL,1)*FICFAC**2
ISN 0020            COXAL=COXAL/FICFAC
ISN 0021            DAL= DIFCON(T,T,CALOX,CALBE,2)
ISN 0022            DBE= DIFCON(T,T,CBEAL,0.,3)
ISN 0023            THCOXO=CONDUC(T,T,1)*FICFAC
ISN 0024            THCOXM=CONDUC(T,T,2)
ISN 0025            SPHEOX=SPEC(T,1)/(FICFAC*DENZRO)
ISN 0026            SPHEME=SPEC(T,2)/DENZIR
ISN 0027            WRITE(J,50) T,OSTOCH,COXAL,CALOX,CALBE,CBEAL,DOX,DAL,DBE,
                     1           THCOXO,THCOXM,SPHEOX,SPHEME
ISN 0028           50 FORMAT(1H ,F10.2,5F10.5,3D10.3,4F10.5)
ISN 0029            T=T+50.
ISN 0030           100 CONTINUE
ISN 0031            WRITE(J,500) (HTITLE(K),K=1,20)
ISN 0032           500 FORMAT(1H1,25X,20A4//)
ISN 0033            RETURN
ISN 0034            END
```

```
ISN 0002            SUBROUTINE INITIA
                C   INITIA SETS THE INITIAL CONDITIONS
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 PLO
ISN 0005            COMMON/RESULT/PLO(25,200),KPLOT,NPLOT
ISN 0006            COMMON/GEONET/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DR
ISN 0007            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0008            COMMON/TEMTIM/ TCOOL(100,2),ITCOOL(100,2),TRAD(100,2),ITRAD(100,2)
ISN 0009            COMMON/HEAT  / HVER(100)  ,HCOOL(2),FRADIA(2),HEATFL(2),QFIXED(2),
                   1                        QSPLIT,NCAP(100)  ,NSTEAM(2),NRADIA
                   2                ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0010            COMMON/HEADLN/ HTITLE(20)
ISN 0011            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1              OXIGFL(2),NDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),ODTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0012            COMMON/TIME  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              NTEMP,NDIFF,NPRINT
ISN 0013            COMMON/MESH  /NGROSS,NPINE,NOXID(2),NOXI(2)
                   1,              NLUNG,NSTART,NALPA(2)
ISN 0014            COMMON/MESHTE/MT(100),MTCOOL(2),MTWALL(2),MTCOOL(2),MTWALL(2),NGPS
ISN 0015            COMMON/MESHCO/MC(500),NBAKER,NGES,NOA(2),NAB(2)
                   1,              NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                   2,              NOA1,NAO1,NAB1,NBA1,NOXI01,NALPA1
                   3,              NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0016            COMMON/MATPRO/ DENZIR,DENZRO,OSTOCM,OXICON,DENRAT,FICPAC,OXHEAT
ISN 0017            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2M1,M2,M3,M4,M5,NUMBER,NSCALE
ISN 0018            COMMON/MINPUT/ NDIFIN(100,2),TIMDIF(100,2),NCOEFF(100,2),
                   1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTMAX(100),
                   3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                   4               NCOEFF(2),NCOEFF(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0019            DENZIR=6.49
ISN 0020            DENZRO=5.82
ISN 0021            OSTOCM=1.514
ISN 0022            DENRAT=OSTOCM/(DENZRO-OSTOCM)
ISN 0023            FICPAC=DENZIR/(DENZRO-OSTOCM)
ISN 0024            OXICON=OSTOCM*FICPAC
ISN 0025            OXHEAT=34330.
ISN 0026            TIMP=0.
ISN 0027            KPLOT=0
ISN 0028            IF(DTTEMP.EQ.0.) DTTEMP=DTPRIN
ISN 0030            IF(DTDIFF.EQ.0.) DTDIFF=DTPRIN
ISN 0032            NGROSS=WALL/.0064
ISN 0033            NPINE=64*NGROSS
ISN 0034            KPINE=NPINE
ISN 0035            DR=WALL/KPINE
ISN 0036            NGROSS=NGROSS+1
ISN 0037            NPINE=NPINE+1
ISN 0038            T(1)=TSTART
ISN 0039            C(1)=CSTART
ISN 0040            DO 10 N=2,NPINE
```

```
ISN 0041            R(K)=R(K-1)-DR
ISN 0042            T(K)=TSTART
ISN 0043            C(K)=CSTART
ISN 0044         10 CONTINUE
ISN 0045            KDIFIN(1)=1
ISN 0046            KDIFIN(2)=1
ISN 0047            IF(NDIFIN(1).GT.0)HDIFF(1)=TIMFUN(KDIFIN(1),HDIFIN,TIMDIF,1,TIME)
ISN 0049            IF(NDIFIN(2).GT.0)HDIFF(2)=TIMFUN(KDIFIN(2),HDIFIN,TIMDIF,2,TIME)
ISN 0051            DO 20 K=1,2
ISN 0052            KTCOOL(K)=1
ISN 0053            KTWALL(K)=1
ISN 0054            KQ*LTX(K)=1
ISN 0055            KCOEFF(K)=1
ISN 0056            KRADCO(K)=1
ISN 0057            DOXID(K)=0.
ISN 0058            DALPA(K)=0.
ISN 0059            TSURF(K)=TSTART
ISN 0060            TOXID(K)=TSTART
ISN 0061            TALPA(K)=TSTART
ISN 0062            IF(OLAYER(K).EQ.0.)  OLAYER(K)=1.D-7*FICFAC
ISN 0064            IF(ALAYER(K).EQ.0.)  ALAYER(K)=1.D-7
ISN 0066            DOXID(K)=OLAYER(K)/FICFAC
ISN 0067            DALPA(K)=DOXID(K)+ALAYER(K)
ISN 0068            HOXID(K)=DOXID(K)/DR*.5
ISN 0069            HALPA(K)=DALPA(K)/DR*.5
ISN 0070            CALL INTFAC(TOXID(K),COA(K),CAO(K),1)
ISN 0071            CALL INTFAC(TALPA(K),CAB(K),CBA(K),2)
ISN 0072         20 CONTINUE
ISN 0073            ROXID(1)=R(1)-DOXID(1)
ISN 0074            ROXID(2)=R(NPINE)+DOXID(2)
ISN 0075            RALPA(1)=R(1)-DALPA(1)
ISN 0076            RALPA(2)=R(NPINE)+DALPA(2)
ISN 0077            DO 30 K=1,2
ISN 0078            DOXID(K)=0.
ISN 0079            DALPA(K)=0.
ISN 0080            QRADN(K)=0.
ISN 0081            QCON(K)=0.
ISN 0082            QRAD(K)=0.
ISN 0083            NOA(K)=0
ISN 0084            NAO(K)=0
ISN 0085            NAB(K)=0
ISN 0086            NBA(K)=0
ISN 0087            NOA(K)=2
ISN 0088            NAB(K)=2
ISN 0089            NBA1=1
ISN 0090            NBA2=NPINE
ISN 0091            KK=0
ISN 0092            KK=0
ISN 0093            QRIGPL(K)=0.
ISN 0094            GAIN(K)=0.
ISN 0095            HSTEAM(K)=0.
ISN 0096            HRADIA(K)=0.
ISN 0097            IF(NTCOOL(K).GT.0)TSTEAM(K)=TIMFUN(KTCOOL(K),TCOOL  ,ZTCOOL,K,TIME)
ISN 0099            IF(NTWALL(K).GT.0)TWALL(K)  =TIMFUN(KTWALL(K),TRAD  ,ZTRAD ,K,TIME)
ISN 0101            IF(NCOEFF(K).GT.0)HCOOL(K)  =TIMFUN(KCOEFF(K),HCOEFF,TCOEFF,K,TIME)
ISN 0103            IF(NRADCO(K).GT.0)ERADIA(K)=TIMFUN(KRADCO(K),HRADCO,TRADCO,K,TIME)
ISN 0105            IF(HCOOL(K).GT.0.)  QCON(K)=HCOOL(K)*(TSTEAM(K)-TSTART)
ISN 0107            IF(ERADIA(K).GT.0.)QRAD(K)=FRADIA(K)*5.778-12*
```

```
     1;(TWALL(K)+273.16)**4-(TSTART+273.16)**4)
ISH 0109          HEATPL(K)=QCON(K)+QRAD(K)
ISH 0110       30 CONTINUE
ISH 0111          IF((HDIFF(1).EQ.0.).OR.(NBAKER.GT.0))GO TO 40
ISH 0113          C(1)=OXICON
ISH 0114          SLOPE=(C(1)-CA(1))/DOXID(1)
ISH 0115          OXIGFL(1)=SLOPE*DIFCON(T(1),TOXID(1),C(1),COA(1),1)
ISH 0116          IF((DOXID(1).LT.6.*DR).OR.(DALPA(1)-DOXID(1).LT.6.*DR)) GO TO 40
ISH 0118          NN=NOXID(1)
ISH 0119          DO 31 L=2,NN
ISH 0120       31 C(L)=C(L-1)-SLOPE*DR
ISH 0121          NL=NN+2
ISH 0122          SLOPE=(CAO(1)-CAB(1))/(ROXID(1)-RALPA(1))
ISH 0123          C(NL)=CAO(1)-(ROXID(1)-R(NL))*SLOPE
ISH 0124          NN=NALPA(1)
ISH 0125          NL=NL+1
ISH 0126          DO 32 L=NL,NN
ISH 0127       32 C(L)=C(L-1)-SLOPE*DR
ISH 0128       40 IF((HDIFF(2).EQ.0.).OR.(NBAKER.GT.0))GO TO 50
ISH 0130          C(NPINE)=OXICON
ISH 0131          SLOPE=(C(NPINE)-COA(2))/DOXID(2)
ISH 0132          OXIGFL(2)=SLOPE*DIFCON(T(NPINE),TOXID(2),C(NPINE),COA(2),1)
ISH 0133          IF((DOXID(2).LT.6.*DR).OR.(DALPA(2)-DOXID(2).LT.6.*DR)) GO TO 50
ISH 0135          NN=NPINE-1
ISH 0136          NL=NPINE-NOXID(2)
ISH 0137          C(NL)=C(NPINE)-SLOPE*(R(NL)-R(NPINE))
ISH 0138          NL=NL+1
ISH 0139          DO 41 L=NL,NN
ISH 0140       41 C(L)=C(L-1)+SLOPE*DR
ISH 0141          NN=NPINE-NOXID(2)-1
ISH 0142          NL=NPINE-NALPA(2)
ISH 0143          SLOPE=(CAO(2)-CAB(2))/(RALPA(2)-ROXID(2))
ISH 0144          C(NN)=CAO(2)-(R(NN)-ROXID(2))*SLOPE
ISH 0145          C(NL)=CAO(2)-(R(NL)-ROXID(2))*SLOPE
ISH 0146          NN=NN-1
ISH 0147          NL=NL+1
ISH 0148          DO 42 L=NL,NN
ISH 0149       42 C(L)=C(L-1)+DR*SLOPE
ISH 0150       50 CALL MATMAP
ISH 0151          IF(NBAKER.GT.0) CALL BATMOD
ISH 0153          RETURN
ISH 0154          END
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ISN 0002            SUBROUTINE TEMPER
                C   TEMPER CALCULATES THE TEMPERATURES IN THE WALL
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/GEOMET/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DR
ISN 0005            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0006            COMMON/TEMTIM/ TCOOL(100,2),ZTCOOL(100,2),TRAD(100,2),ZTRAD(100,2)
ISN 0007            COMMON/HEAT  / HVER(100)  ,HCOOL(2),HRADIA(2),HEATPL(2),QFIXED(2),
                   1                        QSPLIT,HCAP(100)  ,HSTEAM(2),HRADIA(2)
                   2                  ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0008            COMMON/HEADLN/ HTITLE(20)
ISN 0009            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1                  OXIGPL(2),NDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),ODTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010            COMMON/TIME  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              TTEMP,NDIFF,NPRINT
ISN 0011            COMMON/MESH  /NGROSS,NFINE,NOXID(2),NOXI(2)
                   1,             NLUMB,NSTART,NALPA(2)
ISN 0012            COMMON/MESNTE/NT(100),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NGES
ISN 0013            COMMON/MESNCO/NC(500),NBAKER,NGES,NOA(2),NAB(2)
                   1,             NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                   2,             NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                   3,             NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0014            COMMON/MATPRO/ DENZIR,DENSRO,OSTOCH,OXICON,DENRAT,FICFAC,OXHEAT
ISN 0015            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016            COMMON/MINPUT/ NDIFIN(100,2),TIMDIF(100,2),NCOFFP(100,2),
                   1               TCOEFP(100,2),NRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTNEW(100),
                   3               KDIFIN(2),NDIFIN(2),KQFLUX(2),NQFLUX(2),
                   4               KCOEFP(2),NCOEFP(2),KRADCO(2),NRADCO(2),NSTEP
ISN 0017            DIMENSION NZIR1(2),NZIR2(2),TW(1000),  NOXI(2),NZIR(2)
ISN 0018            DIMENSION RSURF(2),TSURR(2)
ISN 0019            TSURF(1)=T(1)+273.15
ISN 0020            TSURR(2)=T(NFINE)+273.15
ISN 0021            NGES=NGROSS
ISN 0022            ROXID(1)=R(1)-DOXID(1)
ISN 0023            ROXID(2)=R(NFINE)+DOXID(2)
ISN 0024            RSURF(1)=R(1)
ISN 0025            RSURF(2)=R(NFINE)
ISN 0026            DO 10 K=1,2
ISN 0027            IF(NDIFF(K).EQ.0.) GO TO 5
ISN 0029            NOXID(K)=DOXID(K)/DR+.5
ISN 0030            NOXI(K)=NOXID(K)/16
ISN 0031            NGES=NGES+NOXID(K)/16-NOXID(K)/32+NOXID(K)/64
ISN 0032            IF(NLUMB.GT.0) NGES=1
ISN 0033          5 IF(NCOOL(K).GT.0.)  HSTEAM(K)=HCOOL(K)*RSURF(K)
ISN 0034            IF(ERADIA(K).EQ.0.) GO TO 10
ISN 0035            T2=TWALL(K)+273.15
ISN 0039            HRADIA(K)=ERADIA(K)*5.77E-12*(TSURR(K)+T2)*(TSURR(K)**2+T2**2)
                   1          *RSURF(K)
ISN 0040         10 CONTINUE
ISN 0041            NT(1)=1
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ISN 0042            NVEP(1)=NSTEAM(1)+NRADIA(1)
ISN 0043            NVEP(NGES+1)=NSTEAM(2)+NRADIA(2)
                C   TLOWB = 0:  TEMPERATURE PROFIL IS CALCULATED
                C   TLOWB = 1:  UNIFORM WALL TEMPERATURE IS CALCULATED
                C   TLOWB = 2:  WALL TEMPERATURE IS INPUT
ISN 0044            IF(NLOWB.EQ.0) GO TO 18
ISN 0046            CALL TLOWB
ISN 0047            GO TO 2000
ISN 0048         18 NT(NGES)=NPINE
ISN 0049            IF(NDIFF(1).GT.0.) GO TO 20
ISN 0051            NCAP(1)=32.*DR*R(17)*SPEC(T(1),2)
ISN 0052            NSOUT=2
ISN 0053            GO TO 100
ISN 0054         20 NOXI(1)=NOXI(1)+1
ISN 0055            IF(NOXI(1).GT.1) GO TO 30
ISN 0057            NEAN=(2+NOXID(1))/2
ISN 0058            NOXI(1)=R(NEAN      )/DOXID(1)*CONDUC(T(1),T(NOXID(1)+1),1)
ISN 0059            NEAN2=(NOXID(1)+34)/2
ISN 0060            NCAP(1)=R(NEAN)*DOXID(1)*SPEC(TOXID(1),1)
                   1       +R(NEAN2)*(ROXID(1)-R(33))*SPEC(TOXID(1),2)
ISN 0061            NT(2)=65
ISN 0062            NEAN2=(NOXID(1)+66)/2
ISN 0063            NSIR(1)=R(NEAN2)/(ROXID(1)-R(65))*CONDUC(TOXID(1),T(65),2)
ISN 0064            NVEP(2)=NSIP(1)*NOXI(1)/(NSIR(1)+NOXI(1))
ISN 0065            NCAP(2)=R(65)*64.*DR*SPEC(T(65),2)
ISN 0066            NSOUT=3
ISN 0067            GO TO 100
ISN 0068         30 NCAP(1)=8.*DR*R(5)*SPEC(T(1),1)
ISN 0069            NT(NOXI(1))=NOXID(1)+1
ISN 0070            T(NT(NOXI(1)))=TOXID(1)
ISN 0071            NOXOUT=NOXI(1)-1
ISN 0072            IF(NOXOUT.LT.2) GO TO 50
ISN 0074            DO 40 K=2,NOXOUT
ISN 0075            NT(K)=NT(K-1)+16
ISN 0076            NT=NT(K)
ISN 0077            NCAP(K)=16.*DR*R(NT)*SPEC(T(NT),1)
ISN 0078            NVEP(K)=R(NT-8)/(16.*DR)*CONDUC(T(NT),T(NT-16),1)
ISN 0079         40 CONTINUE
ISN 0080         50 NT(NOXI(1)+1)=(NT(NOXI(1)))+95)/64*64+1
ISN 0081            NEAN=(NT(NOXOUT)+NT(NOXI(1)))/2
ISN 0082            NVEP(NOXI(1))=R(NEAN)/(R(NT(NOXOUT))-ROXID(1))
                   1                *CONDUC(T(NT(NOXOUT)),TOXID(1),1)
ISN 0083            NEAN2=(NT(NOXI(1)+1)-32+NT(NOXI(1)))/2
ISN 0084            NEAN3=(NT(NOXOUT)+8+NT(NOXI(1)))/2
ISN 0085            NCAP(NOXI(1))=R(NEAN3)*(R(NT(NOXOUT)+8)-ROXID(1))+SPEC(TOXID(1),1)
                   1+R(NEAN2)*(ROXID(1)-R(NT(NOXI(1)+1)-32))*SPEC(TOXID(1),2)
ISN 0086            NEAN=(NT(NOXOUT)+16+NT(NOXI(1)))/2
ISN 0087            NOXI(1)=R(NEAN)/(R(NT(NOXOUT)+16)-ROXID(1))
                   1         *CONDUC(T(NT(NOXOUT)+16),TOXID,1)
ISN 0088            N1=NOXI(1)+1
ISN 0089            NT=NT(N1)
ISN 0090            NEAN2=(NT(NOXI(1))+NT)/2
ISN 0091            NVEP(N1)  =R(NEAN2)/(ROXID(1)-R(NT))*CONDUC(TOXID(1),T(NT),2)
ISN 0092            NCAP(N1)  =64.*DR*R(NT)*SPEC(T(N1),2)
ISN 0093            NSOUT=NOXI(1)+2
ISN 0094         100 IF(NDIFF(2).GT.0.) GO TO 120
ISN 0096            NCAP(NGES)=32.*DR*R(NPINE-16)*SPEC(T(NPINE),2)
ISN 0097            NVEP(NGES)=R(NPINE-16)/(64.*DR)*CONDUC(T(NPINE),T(NPINE-64),2)
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ISN 0098            NRIN=NGES-1
ISN 0099            GO TO 200
ISN 0100        120 NOXI(2)=NGES-NOXI(2)
ISN 0101            IF((NGES-NOXI(2)).GT.0) GO TO 130
ISN 0103            NEAN=(NPINE+NT(NOXI(2)))/2
ISN 0104            NOXI(2)=R(NEAN)/DOXID(2)*CONDUC(T(NPINE),T(NT(NOXI(2))),1)
ISN 0105            NEANS=(NPINE-64+NT(NOXI(2)))/2
ISN 0106            NRIP(2)    =R(NEANS)/(R(NPINE-64)-ROXID(2))
                   1             *CONDUC(T(NPINE-64),TOXID(2),2)
ISN 0107            NVER(NGES)=NOXI(2)*NRIR(2)/(NOXI(2)+NRIR(2))
ISN 0109            NEANS=(NPINE-32+NT(NOXI(2)))/2
ISN 0109            NCAP(NGES)=R(NEAN)*DOXID(2)*SPEC(TOXID(2),1)+R(NEANS)*
                   1                (R(NPINE-32)-ROXID(2))*SPEC(TOXID(2),2)
ISN 0110            NRIN=NGES-1
ISN 0111            GO TO 200
ISN 0112        130 NCAP(NGES)=8.*DR*R(NPINE-4)*SPEC(T(NPINE),1)
ISN 0113            NT(NOXI(2))=NPINE-NOXID(2)
ISN 0114            T(NT(NOXI(2)))=TOXID(2)
ISN 0115            NOXIN=NOXI(2)+2
ISN 0116            NOXUP=NGES-1
ISN 0117            IF(NOXIN.LE.NGES) NVER(NGES)=R(NPINE-8)/(16.*DR)
                   1*CONDUC(T(NPINE),T(NPINE-16),1)
ISN 0119            IF(NOXUP.LT.NOXIN) GO TO 150
ISN 0121            NT(NOXUP)=NPINE-16
ISN 0122            MAX=NT(NGES-1)
ISN 0123            DO 140 K=NOXIN,NOXUP
ISN 0124            NT(K)=MAX-16*(NOXUP-K)
ISN 0125            NT=NT(K)
ISN 0126            NCAP(K)=16.*DR*R(NT)*SPEC(T(NT),1)
ISN 0127            NVER(K)=R(NT-8)/(16.*DR)*CONDUC(T(NT),T(NT-16),1)
ISN 0128        140 CONTINUE
ISN 0129        150 N1=NOXI(2)+1
ISN 0130            NT(N1)=NPINE-NOXID(2)/16*16+16
ISN 0131            NEAN=(NT(N1)+NT(NOXI(2)))/2
ISN 0132            NVER(N1)=R(NEAN)/(ROXID(2)-R(NT(N1)))*CONDUC(TOXID(2),T(NT(N1)),1)
ISN 0133            IF(NOXIN.LE.NGES)
                   1NCAP(N1)=16.*DR*R(N1)*SPEC(T(NT(N1)),1)
ISN 0135            NEANO=(NT(N1)-16+NT(NOXI(2)))/2
ISN 0136            NOXI(2)=R(NEANO)/(ROXID(2)-R(NT(N1)-16))
                   1*CONDUC(TOXID(2),T(NT(N1)-16),1)
ISN 0137            N2=NOXI(2)-1
ISN 0138            NT(N2)=(NT(NOXI(2))-34)/64*64+1
ISN 0139            NEANS=(NT(N2)+NT(NOXI(2)))/2
ISN 0140            NVER(NOXI(2))=R(NEANS)/(R(NT(N2))-ROXID(2))
                   1                *CONDUC(T(NT(N2)),TOXID(2),2)
ISN 0141            R1=R(NT(N1)-8)
ISN 0142            R2=R(NT(N2)+32)
ISN 0143            NCAP(NOXI(2))=.5*((R2**2-ROXID(2)**2)*SPEC(TOXID(2),2)+
                   1                  (ROXID(2)**2-R1**2)*SPEC(TOXID(2),1))
ISN 0144            NRIN=N2
ISN 0145        200 DO 250 K=NFOUT,NRIN
ISN 0146            NT(K)=NT(K-1)+64
ISN 0147            NVER(K)=R(NT(K)-32)/(64.*DR)*CONDUC(T(NT(K-1)),T(NT(K)),2)
ISN 0148            NCAP(K)=64.*DR*R(NT(K))*SPEC(T(NT(K)),2)
ISN 0149        250 CONTINUE
ISN 0150            IF(NSTART.EQ.0) GO TO 2000
ISN 0152            DO 310 K=1,NGES
ISN 0153        310 QRFACT(K)=0.
```

```
ISN 0154            QSURF(1)=0.
ISN 0155            QSURF(2)=0.
ISN 0156            IF(QFIXED(1).GT.0.)QSURF(1)=QFIXED(1)*RSURF(1)
ISN 0158            IF(QFIXED(2).GT.0.)QSURF(2)=QFIXED(2)*RSURF(2)
ISN 0160            IF(NDIFF(1).EQ.0.)  GO TO 320
ISN 0162            OXI=OXIGFL(1)*R(1)
ISN 0163            QSURF(1)=QSURF(1)-QSPLIT*OXI
ISN 0164            QREACT(NOXI(1))=OXHEAT*OXI
ISN 0165            IF(NOXI(1).GT.1)  GO TO 320
ISN 0167            QREACT( 2)=HVER(2)*QREACT(1)/NOXI(1)
ISN 0168            QREACT(1)=QREACT(1)*HVER(2)/HZIR(1)
ISN 0169        320 IF(NDIFF(2).EQ.0.)  GO TO 400
ISN 0171            OXI=OXIGFL(2)*R(NPINE)
ISN 0172            QSURF(2)=QSURF(2)-QSPLIT*OXI
ISN 0173            QREACT(NOXI(2))=OXHEAT*OXI
ISN 0174            IF(NOXI(2).NE.NGES)  GO TO 400
ISN 0176            QREACT(NGES-1)=HVER(NGES)*QREACT(NGES)/NOXI(2)
ISN 0177            QREACT(NGES)=QREACT(NGES)*HVER(NGES)/HZIR(2)
ISN 0178        400 CALL INTTER
ISN 0179            TOXID(1)=T(1)
ISN 0180            TOXID(2)=T(NPINE)
ISN 0181            IF(NDIFF(1).EQ.0.)  GO TO 1200
ISN 0183            IF(NOXI(1).EQ.1)  GO TO 1110
ISN 0185            N0=NT(NOXI(1))
ISN 0186            N1=NT(NOXI(1)-1)
ISN 0187            T(N1+16)=T(N0)-HVER(NOXI(1))*(T(N0)-T(N1))/NOXI(1)
ISN 0188            TOXID(1)=T(N0)
ISN 0189            GO TO 1200
ISN 0190        1110 TOXID(1)=QREACT(1)/NOXI(1)+HVER(2)*(T(1)/HZIR(1)+T(65)/NOXI(1))
ISN 0191            T(17)=TOXID(1)
ISN 0192        1200 IF(NDIFF(2).EQ.0.)  GO TO 2000
ISN 0194            IF(NOXI(2).EQ.NGES)  GO TO 1210
ISN 0196            N0=NT(NOXI(2))
ISN 0197            N1=NT(NOXI(2)+1)
ISN 0198            T(N1-16)=T(N0)-HVER(NOXI(2)+1)*(T(N0)-T(N1))/NOXI(2)
ISN 0199            TOXID(2)=T(N0)
ISN 0200            GO TO 2000
ISN 0201        1210 TOXID(2)=QREACT(NGES)/NOXI(2)+HVER(NGES)*
                    1          (T(NPINE)/HZIR(2)+T(NPINE-64)/NOXI(2))
ISN 0202            T(NPINE-16)=TOXID(2)
ISN 0203        2000 IF(T(1).LT.2200.)  RETURN
ISN 0205            WRITE(6,3000)
ISN 0206        3000 FORMAT(1HO,*ONTEMPERATURE HIGHER  THAN 2200 DEG C
ISN 0207            CALL OUTPUT
ISN 0208            TIME=TMAX
ISN 0209            RETURN
ISN 0210            END
```

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ISN 0002            SUBROUTINE TLOWB
                C   TLOWB IS USED IF NLOWB=1 (UNIFORM TEMPERATURE) OR
                C   NLOW=2 (TEMPERATURE IS INPUT)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/GEONET/ R(1000),ROXID(2),RALPA(2),WALL,BOXID(2),BALPA(2),DR
ISN 0005            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0006            COMMON/TENTEN/ TCOOL(100,2),ETCOOL(100,2),TRAD(100,2),ETRAD(100,2)
ISN 0007            COMMON/HEAT  / HVEA(100)  ,HCOOL(2),ERADIA(2),HEATPL(2),QFIXED(2),
                   1                        QSPLIT,HCAP(100)  ,HSTEAM(2),HRADIA(2)
                   2                ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0008            COMMON/HEADLN/ HTITLE(20)
ISN 0009            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1               OXIGPL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),OUTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010            COMMON/EXIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              HTEMP,HDIFF,HPRINT
ISN 0011            COMMON/MESH  /MGROSS,MFINE,NOXID(2),MOXI(2)
                   1,            NLOWB,NSTART,NALPA(2)
ISN 0012            COMMON/MESHTE/HT(100),HTCOOL(2),HTWALL(2),HTCOOL(2),HTWALL(2),MGRS
ISN 0013            COMMON/MESHCO/MC(500),MBAKER,MGRS,MOA(2),MAB(2)
                   1,             MOA(2),MAO(2),MAB(2),MBA(2),TMTOXI(2),INTB
                   2,             MOA1,MAO1,MAB1,MBA1,NOXID1,NALPA1
                   3,             MOA2,MAO2,MAB2,MBA2,NOXID2,NALPA2
ISN 0014            COMMON/MATPRO/ DENZIR,DENZRO,OSTOCH,OXICON,DEKMAT,FICFAC,OXHEAT
ISN 0015            COMMON/PROFIL/ CO(500),K(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2M1,M2,M3,M4,M5,MNUMBER,MSCALE
ISN 0016            COMMON/MINPUT/ HDIFIN(100,2),TIMDIF(100,2),HCOEFF(100,2),
                   1               TCOEFF(100,2),HRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTNEW(100),
                   3               HDIFIN(2),HDIFIN(2),HQFLUX(2),HQFLUX(2),
                   4               HCOEFF(2),HCOEFF(2),HRADCO(2),HRADCO(2),HSTEP
ISN 0017            IF(NLOWB.EQ.1) GO TO 1
ISN 0019            T(1)=TSTEAM(1)
ISN 0020            IF(TSTEAM(1).EQ.0.) T(1)=TSTEAM(2)
ISN 0022            GO TO 2000
ISN 0023          1 QREACT(1)=0.
ISN 0024            IF(QFIXED(1).GT.0.) QREACT(1)=QFIXED(1)*R(1)
ISN 0026            IF(QFIXED(2).GT.0.) QREACT(1)=QFIXED(2)*R(MFINE)*QREACT(1)
ISN 0028            IF((HDIFF(1)*HDIFF(2)).EQ.0.) GO TO 11
ISN 0030            HCAP(1)=.5*(R(1)**2-ROXID(1)**2+ROXID(2)**2-R(MFINE)**2)*
                   1      SPEC(T(1),1)+(ROXID(1)**2-ROXID(2)**2)*SPEC(T(1),2))
ISN 0031            QREACT(1)=QREACT(1)+(QXHEAT-QSPLIT)*(QXIGPL(1)*R(1)+
                   1QXIGPL(2)*R(MFINE))
ISN 0032            GO TO 13
ISN 0033          11 IF(HDIFF(1).EQ.0) GO TO 12
ISN 0035            HCAP(1)=.5*(R(1)**2-ROXID(1)**2)*SPEC(T(1),1)+
                   1         (ROXID(1)**2-R(MFINE)**2)*SPEC(T(1),2))
ISN 0036            QREACT(1)=QREACT(1)+(QXHEAT-QSPLIT)*QXIGPL(1)*R(1)
ISN 0037            GO TO 13
ISN 0038          12 HCAP(1)=.5*(R(1)**2-ROXID(2)**2)*SPEC(T(1),2)+
                   1         (ROXID(2)**2-R(MFINE)**2)*SPEC(T(1),1))
ISN 0039            QREACT(1)=QREACT(1)+(QXHEAT-QSPLIT)*QXIGPL(2)*R(MFINE)
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ISN 0040          13 DTN=WCAP(1)/(WVER(1)*WVER(2))
ISN 0041             DTMAX(1)=DTN
ISN 0042             NMAX=DTTEMP/DTN+1.
ISN 0043             IF(DTN.GE.DTTEMP) NMAX=1
ISN 0045             XMAX=NMAX
ISN 0046             DTN=DTTEMP/XMAX
ISN 0047             IF(NSTART.EQ.0) GO TO 2000
ISN 0049             DELTAQ=QREACT(1)*HEATPL(1)*R(1)      *HEATPL(2)*R(NPINP)
ISN 0050             DO 10 N=1,NMAX
ISN 0051          10 T(1)=T(1)+DELTAQ*DTN/WCAP(1)
ISN 0052             DO 15 I=1,2
ISN 0053             QCON(I)=0.
ISN 0054             QRAD(I)=0.
ISN 0055             IF(WCOOL(I).GT.0.) QCON(I)=WCOOL(I)*(TSTEAM(I)-T(1))
ISN 0057             IF(ERADIA(I).GT.0.)
                    1QRAD(I)=ERADIA(I)*5.77E-12*((TWALL(I)+273.16)**4-(T(1)+273.16)**4)
ISN 0059             HEATPL(I)=QCON(I)+QRAD(I)
ISN 0060          15 CONTINUE
ISN 0061        2000 T(NPINP)=T(1)
ISN 0062             TSURF(1)=T(1)
ISN 0063             TSURF(2)=T(1)
ISN 0064             TOXID(1)=T(1)
ISN 0065             TOXID(2)=T(1)
ISN 0066             RETURN
ISN 0067             END
```

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ISN 0002            SUBROUTINE INTTEM
                C   IN THIS SUBROUTINE THE TEMPERATURE INTEGRATION IS PERFORMED
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/GEOMRT/ R(1000),ROXID(2),RALPA(2),RWALL,BOXID(2),BALPA(2),DR
ISN 0005            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0006            COMMON/TEMTIM/ TCOOL(100,2),ZTCOOL(100,2),TRAD(100,2),ZTRAD(100,2)
ISN 0007            COMMON/HEAT  / NVER(100)  ,NCOOL(2),NRADIA(2),NHEATPL(2),QPIXED(2),
                   1                        QSPLIT,NCAP(100)  ,NSTEAM(2),NRADIA(2)
                   2                 ,QSURF(2),QCOM(2),QRAD(2),QREACT(2)
ISN 0009            COMMON/HEADLN/ HTITLE(20)
ISN 0009            COMMON/CONCRN/ C(1000),COXID(2),COALI2),CALBET(2),CBETA(2),
                   1                 OXIGPL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),ODTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010            COMMON/TEIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,MTMAX(100)
                   1,             MTEMP,MDIFF,MPRINT
ISN 0011            COMMON/MESH  /MGROSS,MPINE,NOXID(2),NOXI(2)
                   1,             MLOAD,MSTART,MALPA(2)
ISN 0012            COMMON/MESNIE/MT(100),MTCOOL(2),MTWALL(2),MTCOOL(2),MTWALL(2),MGRS
ISN 0013            COMMON/MESHCO/MC(500),MBAKER,MGRS,MOA(2),MAB(2)
                   1,             MOA(2),MAO(2),MAB(2),MBA(2),INTOXI(2),INTB
                   2,             MOA1,MAO1,MAB1,MBA1,MOXID1,MALPA1
                   3,             MOA2,MAO2,MAB2,MBA2,MOXID2,MALPA2
ISN 0014            COMMON/MATPRO/ DENZIR,DENZPO,OSTOCH,OXICON,DENRAT,PICPAC,OXMEAT
ISN 0015            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016            COMMON/MINPUT/ NDIPIN(100,2),TIMDIV(100,2),NCOEPP(100,2),
                   1                 TCOEPP(100,2),NPADCO(100,2),TPADCO(100,2),
                   2                 QPLUXI(100,2),TQPLUX(100,2),TINSTP(100),DTMPN(100),
                   3                 NDIPIN(2),NDIPIN(2),NQPLUX(2),NQPLUX(2),
                   4                 NCOEPP(2),NCOEPP(2),NPADCO(2),NPADCO(2),NSTEP
ISN 0017            DIMENSION TN(1000)
ISN 0018            DTN=DTTEMP
ISN 0019            DO 300 L=1,NGRS
ISN 0020            DTMAX(L)=NCAP(L)/(NVER(L)+NVER(L+1))
ISN 0021            IF(DTMAX(L).LT.DTN)  DTN=DTMAX(L)
ISN 0023            LGRS=NGRS-1
ISN 0024          300 CONTINUE
                C   DTMAX(L) IS THE MAXIMUM STABLE TIME STEP FOR EACH NODE
ISN 0025            IF(DTN.NE.DTTEMP) GO TO 310
ISN 0027            NMAX=1
ISN 0028            GO TO 800
ISN 0029          310 NMAX=DTTEMP/DTN+1.
ISN 0030            XMAX=NMAX
ISN 0031            DTN=DTTEMP/XMAX
ISN 0032          800 DO 1000 N=1,NMAX
ISN 0033            IF((NSTEAM(1)+NRADIA(1)).GT.0.) GO TO 810
ISN 0035            TN(1)=T(1)+(NVER(2)*(T(NT(2))-T(1))+ QSURF(1)+QREACT(1))*
                   1DTN/NCAP(1)
ISN 0036            GO TO 850
ISN 0037          810 TN(1)=T(1)+(NSTEAM(1)*(TSTEAM(1)-T(1))+NRADIA(1)*(TWALL(1)-T(1))
                   1+NVER(2)*(T(NT(2))-T(1))+ QSURF(1)+QREACT(1))*DTN/NCAP(1)
ISN 0039          850 IF((NSTEAM(2)+NRADIA(2)).GT.0.) GO TO 860
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ISN 0040            TN(NPINE)=T(NPINE)+(NVER(NGES)*(T(NT(NGES-1))-T(NPINE))+ QSURF(2)+
                   1QREACT(NGES))*DTN/NCAP(NGES)
ISN 0041            GO TO 500
ISN 0042          460 TN(NPINE)=T(NPINE)+(NSTRAN(2)*(TSTRAN(2)-T(NPINE))+NRADIA(2)*
                   1(TWALL(2)-T(NPINE))+NVER(NGES)*(T(NT(NGES-1))-T(NPINE))
                   2+QREACT(NGES)+ QSURF(2))*DTN/NCAP(NGES)
ISN 0043          500 DO 550 N=2,LGES
ISN 0044            NTL=NT(N-1)
ISN 0045            NT =NT(N)
ISN 0046            NTP=NT(N+1)
ISN 0047            TN(NT)=T(NT)+(NVER(N)*(T(NTL)-T(NT))+NVER(N+1)*(T(NTP)-T(NT))
                   1+QREACT(N))*DTN/NCAP(N)
ISN 0048          550 CONTINUE
ISN 0049            DO 600 K=1,NGES
ISN 0050          600 T(NT(K))=TN(NT(K))
ISN 0051         1000 CONTINUE
ISN 0052            TSURF(1)=T(1)
ISN 0053            TSURF(2)=T(NPINE)
ISN 0054            DO 1100 I=1,2
ISN 0055            QCON(I)=0.
ISN 0056            QRAD(I)=0.
ISN 0057            IF(NCOOL(I).GT.0.)  QCON(I)=NCOOL(I)*(TSTRAN(I)-TSURF(I))
ISN 0059            IF(ERADIA(I).GT.0.)QRAD(I)=ERADIA(I)*5.77E-12*
                   1((TWALL(I)+273.16)**4-(TSURF(I)+273.16)**4)
ISN 0061            HEATPL(I)=QCON(I)+QRAD(I)
ISN 0062         1100 CONTINUE
ISN 0063            RETURN
ISN 0064            END
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ISN 0002          SUBROUTINE DIFFUS
                  C     THIS SUBROUTINE CONTROLS THE CALCULATION OF THE CONCENTRATION
                  C     PROFILE
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004          COMMON/MZONE*/ R(1000),ROXID(2),RALPA(2),WALL,BOXID(2),BALPA(2),DR
ISN 0005          COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TWTEAM(2),TWALL(2)
                 1,TSURF(2)
ISN 0006          COMMON/PRATIN/ TCOOL(100,2),RTCOOL(100,2),TRAD(100,2),RTRAD(100,2)
ISN 0007          COMMON/HEAT  / HVER(100) ,HCOOL(2),FRADTA(2),HFATPL(2),QPIXED(2),
                 1                      QSPLIT,HCAP(100) ,HSTEAM(2),HRADIA(2)
                 2                 ,QSURF(2),QCON(2),QRAD(2),QREAC*(2)
ISN 0008          COMMON/HEADLN/ HTITLE(20)
ISN 0009          COMMON*CONCEN/ C(1000),COXID(2),COXAL(2),CALDET(2),CBETA(2),
                 1              OXIGPL(2),NDIFF(2),CSTAR*,GAIN(2)
                 2          OCAP(500),OVER(500),ODT4AX(500)
                 3,         COA(2),CAO(2),CAB(2),CBA(2)
                 4,         OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAI   (2)
ISN 0010          COMMON/TEXT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRT ,DTMAX(100)
                 1,              RTEMP,NDIFF,NPPINT
ISN 0011          COMMON/MESH  /NGROSS,NPINP,NOXID(2),NOXI(2)
                 1,             NLOWP,NSTART,NALPA(2)
ISN 0012          COMMON/MESHTE/NT(150),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NURS
ISN 0013          COMMON/MESHCO/NC(500),NBAKER,NGES,NOA(2),NAB(2)
                 1,             NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                 2,             NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                 3,             NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0014          COMMON/RATPRO/ DENSIR,DENSMO,OSTOCH,OXICOF,DENRAT,PICPAC,OXHTAT
ISN 0015          COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,COXID(2),
                 1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                 2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016          COMMON/MINPUT/ NDIFIN(100,2),TIMDIF(100,2),NCOEFF(100,2),
                 1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                 2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTMAX(100),
                 3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                 4               NCOEFF(2),NCOEFF(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0017          DIMENSION CN(1000),STOROA(2),STORAB(2)
ISN 0018          IF(NBAKER.EQ.0) GO TO 1
                  C     NBAKER = 0;  DETAILED DIFFUSION CALCULATION
                  C     NBAKER = 1;  BAKER-JUST-EQUATION
                  C     NBAKER = 2;  HOBSON - EQUATION
                  C     NBAKER = 3;  LENNON - EQUATION
ISN 0020          CALL RATMOD
ISN 0021          NSTART=3
ISN 0022          RETURN
ISN 0023        1 IF(NDIFF(1).EQ.0.) GO TO 3
ISN 0024          IF((DOXID(1).LT.4.*DR).OR.(DALPA(1)-DOXID(1).LT.4.*DR)) GO TO 5
ISN 0025        3 IF(NDIFF(2).EQ.0.) GO TO 50
ISN 0026          IF((DOXID(2).LT.4.*DR).OR.(DALPA(2)-DOXID(2).LT.4.*DR)) GO TO 5
ISN 0027          GO TO 50
ISN 0028        5 DO 10 N=1,2
ISN 0029          IF(NDIFF(N).EQ.0.) GO TO 10
ISN 0030          IF(NSTART.NE.1) GO TO 7
ISN 0031          IF((DOXID(N).GE.2.*DR).AND.(DALPA(N)-DOXID(N).GT.3.*DR)) GO TO 10
ISN 0032        7 CALL DSTART
ISN 0033          NSTART=2
ISN 0034          RETURN
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ISN 0042          10 CONTINUE
ISN 0043          50 CALL MESHGE
                  C     MESHGE DETERMINES MESH SIZE AND INTERPOLATES IF THERE IS A CHANGE
                  C     IN MESH SIZE
ISN 0044                NC(1)=1
ISN 0045                NGRS=1
ISN 0046                IF(NDIFF(1).EQ.0.) GO TO 100
ISN 0048                INT=INTOXI(1)
ISN 0049                NL=1+INT
ISN 0050                XINT=INT
ISN 0051                XDP=XINT*DP
ISN 0052                XDP2=XDP*0.5
ISN 0053                OCAP(1)=(R(1)-0.25*XDP)*XDP2
ISN 0054                IF(NLONG) 203,203,201
ISN 0055          201 DO 202 L=NL,NOA1,INT
ISN 0056          202 T(L)=T(1)
ISN 0057                GO TO 210
ISN 0058          203 IF(INT.EQ.16) GO TO 210
ISN 0060                IF(NOXI(1).GT.1) GO TO 205
ISN 0062                SLOPE=(T(1)-TOXID(1))/(R(1)-ROXID(1))
ISN 0063                DO 204 L=NL,NOA1,INT
ISN 0064          204 T(L)=T(L-INT)-XDP*SLOPE
ISN 0065                GO TO 210
ISN 0066          205 NN=NOXI(1)-1
ISN 0067                IC=1
ISN 0068                DO 207 N=1,NN
ISN 0069                SLOPE=(T(NT(N))-T(NT(N+1)))/(R(NT(N))-R(NT(N+1)))
ISN 0070                DO 206 L=INT,16,INT
ISN 0071                TA=T(IC)
ISN 0072                IC=IC+L
ISN 0073          206 T(IC)=TA-XDP*SLOPE
ISN 0074          207 CONTINUE
ISN 0075                IF(NOA1+INT).GE.NT(NN)) GO TO 210
ISN 0077                NN1=NOA1-INT
ISN 0078                DO 208 L=IC,NN1,INT
ISN 0079          208 T(IC+INT)=T(IC)-XDP*SLOPE
ISN 0080          210 CONTINUE
ISN 0081                NA=1
ISN 0082                NN=NOA(1)
ISN 0083                DO 220 L=INT,NN,INT
ISN 0084                N=NA+INT
ISN 0085                NGRS=NGRS+1
ISN 0086                NC(NGRS)=N
ISN 0087                OCAP(NGRS)=R(N)*XDP
ISN 0088                OVFP(NGRS)=(R(N)-XDP2)/XDP*DIFCON(T(N),T(NA),C(N),C(NA),1)
ISN 0089                NA=N
ISN 0090          220 CONTINUE
ISN 0091                OCAP(NGRS)=.5*OCAP(NGRS)
ISN 0092                NGRS=NGRS+1
ISN 0093                NA=NOA1
ISN 0094                RNRAN=.5*(R(NA)+ROXID(1))
ISN 0095                RDIFF=R(NA)-ROXID(1)
ISN 0096                OVFP(NGRS)=RNRAN/RDIFF*DIFCON(TOXID(1),T(NA),COA(1),C(NA),1)
ISN 0097                NOA(1)=NGRS
ISN 0098                NC(NGRS)=NOXID+1
ISN 0099                OCAPOA(1)=RNRAN*RDIFF
ISN 0100                NL=NA+1
ISN 0101                NN=NA+1
```

```
      IF(NLTND)233,233,231
  231 DO 232 L=NL,NN,INT
  232 T(L)=T(1)
      TALPA(1)=T(1)
      GO TO 240
  233 NTH=NT(NOXI(1)+1)
      NTH1=NTH+60
      SLOPE=(TOXIP(1)-T(NTH))/(ROXIP(1)-R(NTH))
      NMAX=NTH
      T(NL) = TOXIP(1)-(ROXIP(1)-R(NL   ))*SLOPE
      IF(NN.LT.NTH) NMAX=NN
      TA=T(NL)
      NL=NL+INT
  234 DO 235 L=NL,NMAX,INT
      T(L)=TA-XDP*SLOPE
      TA=T(L)
  235 CONTINUE
      IF(NMAX.EQ.NN) GO TO 239
      NTH=NTH1
      NTH1=NTH+60
      NMAX=NTH1
      SLOPE=(T(NTH)-T(NTH1))/(R(NTH)-R(NTH1))
      NL=NMAX+INT
      IF(NN.LT.NTH1)NMAX=NN
      GO TO 234
  239 N2=NA01
      N1=N2-INT
      TALPA(1)=T(N2)+(T(N2)-T(N1))/(R(N1)-R(N2))*(R(N2)-RALPA(1))
  240 NOPS=NOPS+1
      NL=NA01
      NC(NOPS)=NL
      RMEAN=.50*(ROXID(1)+R(NL))
      RDIFF=ROXIP(1)-R(NL)
      NA=NL
      OVER(NOPS)=RMEAN/RDIFF*DIFCON(T(NL),TOXIP(1),C(NL),CAC(1),2)
      OCAPAO(1)=RMEAN*RDIFF
      OCAP(NOA(1))=OCAPAO(1)*OCAPOA(1)
      OCAP(NOPS)=.50*R(NL)*XDR
      NL=NL+INT
      DO 250 L=NL,NN,INT
      NOPS=NOPS+1
      N = NA+INT
      OVER(NOPS)=(R(N)-XDR2)/XDR*DIFCON(T(N),T(NA),C(N),C(NA),2)
      NC(NOPS)=N
      NA=N
      OCAP(NOPS)=R(N)*XDR
  250 CONTINUE
      OCAP(NOPS)=.50*OCAP(NOPS)
      NOPS=NOPS+1
      RMEAN=.50*(R(NN)+RALPA(1))
      RDIFF=R(NN)-RALPA(1)
      OVER(NOPS)=RMEAN/RDIFF*DIFCON(TALPA(1),T(NN) CAP(1),C(NN),2)
      OCAPAB(1)=RMEAN*RDIFF
      NAB(1)=NOPS
      NC(NOPS)=NALPA1
      IF(NBA2-NBA1.LT.INTB) GO TO 301
      IF(NLTND)255,255,256
  256 T(NBA1   )=T(1)
```

```
ISN 0164            GO TO 256
ISN 0165        255 N1=(RC(NGRS)-1)/64*64+1
ISN 0166            N2=N1+64
ISN 0167            IF(N2.GT.NPINE) N2=N1-64
ISN 0168            IF(N1.LT.NOXID(1)) GO TO 258
ISN 0171            SLOPE=(T(N1)-T(N2))/(R(N1)-R(N2))
ISN 0172            T(NBA1   )=T(N1)-(R(N1)-R(NBA1))*SLOPE
ISN 0173            GO TO 256
ISN 0174        258 SLOPE=(TOXID(1)-T(N2))/(ROXID(1)-R(N2))
ISN 0175            T(NBA1)=TOXID(1)-(ROXID(1)-R(NBA1))*SLOPE
ISN 0176        256 NGRS=NGRS+1
ISN 0177            RC(NGRS)=NBA1
ISN 0178            RNEAN=.5*(RALPA(1)+R(NBA1   ))
ISN 0179            RDIFF=RALPA(1)-R(NBA1   )
ISN 0180            OVER(NGRS)=RNEAN/RDIFF**DIFCON(TALPA(1),T(NBA1   ),CBA(1),C(NBA1   ),
                   1)
ISN 0181            OCAPBA(1)=RNEAN*RDIFF
ISN 0182            OCAP(NAB(1))=OCAPBA(1)*OCAPAB(1)
ISN 0183            OCAP(NGRS)=(R(NBA1   )+RDIF)*IBR
ISN 0184        300 NBSUM=NBA2-NBA1
ISN 0185            IF(NBSUM.GT.INTB) GO TO 300
ISN 0187        301 IF(NDIFF(1)*NDIFF(2).GT.0.) GO TO 320
ISN 0189            IF(NDIFF(1).EQ.0.) GO TO 310
ISN 0191            NBA1=(NALPA1+NPINE)/2
ISN 0192            C(NBA1)=0.5*(CBA(1)+C(NPINE))
ISN 0193            T(NBA1)=0.5*(TALPA(1)+T(NPIFF))
ISN 0194            NGRS=NAB(1)+1
ISN 0195            RC(NGRS)=NBA1
ISN 0196            RNEAN=0.5*(RALPA(1)+R(NBA1))
ISN 0197            RDIFF=RALPA(1)-R(NBA1)
ISN 0198            OVER(NGRS)=RNEAN/RDIFF**DIFCON(TALPA(1),T(NBA1),CBA(1),C(NBA1),1)
ISN 0199            OCAPBA(1)=RNEAN*RDIFF
ISN 0200            OCAP(NAB(1))=OCAPBA(1)*OCAPAB(1)
ISN 0201            RNEAN=0.5*(R(NBA1)+R(NPINE))
ISN 0202            RDIFF=R(NBA1)-R(NPINE)
ISN 0203            OCAP(NGRS)=0.5*RNEAN*RDIFF
ISN 0204            NGRS=NGRS+1
ISN 0205            RC(NGRS)=NPINE
ISN 0206            OVER(NGRS)=RNEAN/RDIFF**DIFCON(T(NBA1),T(NPINE),C(NBA1),C(NPINE),1)
ISN 0207            OCAP(NGRS)=OCAP(NGRS-1)
ISN 0208            GO TO 1000
ISN 0209        310 NBA2=(NALPA2+1)/2
ISN 0210            C(NBA2)=0.5*(CBA(2)+C(1))
ISN 0211            IF(NLOWB)315,315,312
ISN 0212        312 T(NBA2)=T(1)
ISN 0213            TALPA(2)=T(1)
ISN 0214            GO TO 318
ISN 0215        315 SLOPE=(T(1)-T(60))/(R(1)-R(60))
ISN 0216            T(NBA2)=T(1)-(R(1)-R(NBA2))*SLOPE
ISN 0217            TALPA(2)=T(1)-(R(1)-RALPA(2))*SLOPE
ISN 0218        318 NGPS=2
ISN 0219            RC(2)=NBA2
ISN 0220            RNEAN=0.5*(R(1)+R(NBA2))
ISN 0221            RDIFF=R(1)-R(NBA2)
ISN 0222            OCAP(1)=0.5*RNEAN*RDIFF
ISN 0223            OVER(2)=RNEAN/RDIFF**DIFCON(T(1),T(NBA2),C(1),C(NBA2),1)
ISN 0224            OCAP(2)=OCAP(1)
ISN 0225            RNEAN=0.5*(R(NBA2)+RALPA(2))
```

```
      RDIFF=R(NDA2)-RALPA(2)
      OVER(1)=RMEAN/RDIFF*DIFCON(T(NDA2),TALPA(2),C(NDA2),CBA(2),1)
      NGRS=1
      NAB(2)=1
      NC(1)=NALPA2
      OCAPBA(2)=RMEAN*RDIFF
      GO TO 510
  320 NDIFF=(NALPA2-NALPA1)/3
      NDA1=NALPA1+NDIFF
      NDA2=NALPA2-NDIFF
      IF(NLOWM) 330,330,325
  325 TALPA(2)=T(1)
      T(NDA1)=T(1)
      T(NDA2)=T(1)
      GO TO 335
  330 NL=(NALPA2-1)/60*60+1
      NH=NL+60
      IF(NH.GT.NFINP) NH=NL-60
      SLOPE=(T(NL)-T(NH))/(R(NL)-R(NH))
      TALPA(2)=T(NL)-(R(NL)-RALPA(2))*SLOPE
      T(NDA1) =T(NL)-(R(NL)-R(NDA1)) *SLOPE
      T(NDA2) =T(NL)-(R(NL)-R(NDA2)) *SLOPE
  335 C(NDA1)=(CBA(1)+CBA(2))*0.5
      C(NDA2)=C(NDA1)
      NGRS=NAB(1)+1
      NC(NGRS)=NDA1
      RMEAN=0.50*(RALPA(1)+R(NDA1))
      RDIFF=RALPA(1)-R(NDA1)
      OVER(NGRS)=RMEAN/RDIFF*DIFCON(TALPA(1),T(NDA1),CBA(1),C(NDA1),1)
      OCAPBA(1)=RMEAN*RDIFF
      OCAP(NAB(1))=OCAPB (1)+OCAPAB(1)
      RMEAN=0.50*(R(NDA1)+R(NDA2))
      RDIFF=R(NDA1)-R(NDA2)
      OCAP(NGRS)=0.5*RMEAN*RDIFF
      NGRS=NGRS+1
      NC(NGRS)=NDA2
      OVER(NGRS)=RMEAN/RDIFF*DIFCON(T(NDA1),T(NDA2),C(NDA1),C(NDA2),1)
      OCAP(NGRS)=OCAP(NGRS-1)
      NGRS=NGRS+1
      NC(NGRS)=NALPA2
      NAB(2)=NGRS
      RMEAN=0.50*(R(NDA2)+RALPA(2))
      RDIFF=R(NDA2)-RALPA(2)
      OVER(NGRS)=RMEAN/RDIFF*DIFCON(T(NDA2),TALPA(2),C(NDA2),CBA(2),1)
      OCAPBA(2)=RMEAN*RDIFF
      GO TO 510
  180 IF(NDIFF(1).GT.0.) GO TO 190
      XINT=INTB
      XDP=XINT*DR
      XDR2=.5*XDP
      OVER(1)=0.
      NMAX=NDA2-5*INTB
      IF(NMAX.LE.69) GO TO 185
      OCAP(1)=R(17)*32.*DR
      NL=1
      GO TO 180
  185 OCAP(1)=0.
      IF(NMAX.LT.INTB+1) NMAX=INTB+1
```

```
ISN 0288            NP=1
ISN 0289            NL=65
ISN 0290            GO TO 400
ISN 0291          390 NL=NBA1*INTB
ISN 0292            NN=NL*8*INTB
ISN 0293            NA=NN
ISN 0294            IF(NBSNN.LE.30*INTB) NN=NL+NBSNN-INTB
ISN 0296            NP=NN*INTB-1
ISN 0297            IF((NA.EQ.NN).AND.(NP/64*64.NE.NP))
                   1C(NN*INTB)=2.*C(NN)-C(NN-INTB)
ISN 0299            NINT=INTB
ISN 0300            NDR=NINT*DR
ISN 0301            NDR2=.5*NDR
ISN 0302            IF(NL-NB)393,393,391
ISN 0303          391 DO 392 L=NL,NN,INTB
ISN 0304          392 T(L)=T(1)
ISN 0305            GO TO 360
ISN 0306          393 N1=(NL-1)/64*64+1
ISN 0307            TA=T(NBA1  )
ISN 0308          394 N2=N1+64
ISN 0309            NMAX=N2
ISN 0310            IF(N2.GT.NPINB) N2=N1-64
ISN 0312            IF(N1.LT.NONIB1) GO TO 356
ISN 0314            SLOPE=(T(N1)-T(N2))/(R(N1)-R(N2))
ISN 0315            GO TO 358
ISN 0316          356 SLOPE=(TONIB(1)-T(N2))/(RONIB(1)-R(N2))
ISN 0317          358 IF(NN.LT.NMAX) NMAX=NN
ISN 0318            DO 359 L=NL,NMAX,INTB
ISN 0320            T(L)=TA-NDR*SLOPE*2.
ISN 0321            TA=T(L)
ISN 0322          359 CONTINUE
ISN 0323            IF(NMAX.EQ.NN) GO TO 360
ISN 0325            NL=NMAX+INTB
ISN 0326            N1=N1+64
ISN 0327            GO TO 394
ISN 0328          360 TA=NBA1
ISN 0329            NL=NA+INTB
ISN 0330            DO 370 L=NL,NN,INTB
ISN 0331            NGES=NGES+1
ISN 0332            NC(NGES)=L
ISN 0333            OVER(NGES)=(R(L)-NDR2)/NDR*DIPCON(T(NA),T(L),C(NA),C(L),1)
ISN 0334            OCAP(NGES)=R(L)*NDR
ISN 0335            NA=L
ISN 0336          370 CONTINUE
ISN 0337            NMAX=NBA2
ISN 0338            OCAP(NGES)=.5*OCAP(NGES)
ISN 0339            IF(NN.EQ.NMAX) GO TO 500
ISN 0341            IF(NDIFF(2).NE.0.) NMAX=NMAX-8*INTB
ISN 0343            NL=(NN-2*INTB)/64*64+65
ISN 0344            NP=NN
ISN 0345            NN=(NMAX-1-INTB)/64*64+1
ISN 0346            IF(NL.GT.NMAX) GO TO 400
ISN 0348            IF(NL-NB.EQ.0) GO TO 175
ISN 0350            DO 171 L=N1,NN,64
ISN 0351          171 T(L)=T(1)
ISN 0352          175 RMEAN=.5*(R(NP)+R(NL))
ISN 0353            RDIFF=R(NP)-R(NL)
ISN 0354            OCAP2=.5*(R(NP)**2-RMEAN**2)
```

```
ISN 0355          OCAP(NOBS)=OCAP(NOBS)+OCAP2
ISN 0356          NOBS=NOBS+1
ISN 0357          NC(NOBS)=NL
ISN 0358          OVER(NOBS)=RMEAN/RDIFF*DIFCON(T(NP),T(NL),C(NP),C(NL),1)
ISN 0359          OCAP(NOBS)=.50*(RMEAN**2-R(NL)**2)
ISN 0360          IF(NL.EQ.NPTWP) GO TO 1000
ISN 0362          OCAP(NOBS)=OCAP(NOBS)+R(NL+16)*32.*DR
ISN 0363      300 NA=NL
ISN 0364          NL=NL+64
ISN 0365          IF(NL.LT.NMAX) GO TO 385
ISN 0367          IF((NDIFF(2).GT.0.).OR.(NL.GT.NMAX))   GO TO 390
ISN 0369      385 NOBS=NOBS+1
ISN 0370          NC(NOBS)=NL
ISN 0371          OVER(NOBS)=R(NL-32)/(64.*DR)*DIFCON(T(NL),T(NA),C(NL),C(NA),1)
ISN 0372          OCAP(NOBS)=R(NL)*64.*DR
ISN 0373          IF(NLMNP.GT.0) T(NL)=T(1)
ISN 0375          GO TO 300
ISN 0376      390 OCAP(NOBS)=0.5*OCAP(NOBS)
ISN 0377          NP=NL-64
ISN 0378      400 IF(NDIFF(2).EQ.0.) GO TO 1000
ISN 0380          NP=NMAX-INTP-1
ISN 0381          IF((NMAX.GT.INTP+1).AND.(NP/64*64.NE.NP))
                 1C(NMAX-INTP)=2.*C(NMAX)-C(NMAX+INTP)
ISN 0383          IF(NLUMP)413,413,411
ISN 0384      411 T(NMAX)=T(1)
ISN 0385          GO TO 430
ISN 0386      413 IF(NL-NOXID2)415,415,420
ISN 0387      415 SLOPE=(T(NL-64)-T(NL))/(R(NL-64)-R(NL))
ISN 0388          GO TO 425
ISN 0389      420 SLOPE=(T(NL-64)-TOXID(2))/(R(NL-64)-ROXID(2))
ISN 0390      425 T(NMAX)=T(NP)-SLOPE*(R(NP)-R(NMAX))
ISN 0391      430 RDIFF=R(NP)-R(NMAX)
ISN 0392          RMEAN=.50*(R(NP)+R(NMAX))
ISN 0393          OCAP(NOBS)=OCAP(NOBS)+.50*(R(NP)**2-RMEAN**2)
ISN 0394          NOBS=NOBS+1
ISN 0395          NC(NOBS)=NMAX
ISN 0396          OVER(NOBS)=RMEAN/RDIFF*DIFCON(T(NP),T(NMAX),C(NP),C(NMAX),1)
ISN 0397          OCAP(NOBS)=.50*(RMEAN**2-R(NMAX+INTP/2)**2)
ISN 0398          NSTN=NMAX+INTP
ISN 0399          IF(NLUMP)431,433,431
ISN 0400      431 DO 432 L=NSTN,NDA2
ISN 0401      432 T(L)=T(1)
ISN 0402          NN=NDA2
ISN 0403          GO TO 440
ISN 0404      433 IF(NL.LT.NMIN) GO TO 450
ISN 0406      435 NN=NDA2
ISN 0407          IF(NL.LT.NDA2) NN=NL
ISN 0409          DO 440 L=NSTN,NN,INTP
ISN 0410      440 T(L)=T(L-INTP)-SLOPE*XDR
ISN 0411          IF(NN.EQ.NDA2) GO TO 490
ISN 0413          NSTN=NN+INTP
ISN 0414      450 NA=NL
ISN 04            NL=NL+64
ISN 04            IF(NL-NOXID2)455,455,460
ISN 0417      455 SLOPE=(T(NA)-T(NL))/(R(NA)-R(NL))
ISN 04            GO TO 435
ISN 0419      460 SLOPE=(T(NA)-TOXID(2))/(R(NA)-ROXID(2))
ISN 0             GO TO 435
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IBM 0421        480 NA=NMAX
IBM 0422            NL=NMAX-INTD
IBM 0423            DO 490 L=NL,NN,INTD
IBM 0424            NOBS=NOBS+1
IBM 0425            NC(NOBS)=L
IBM 0426            OVER(NOBS)=(R(L)-XDR2)/XDR*DIPCON(T(NA),T(L),C(NA),C(L),1)
IBM 0427            OCAP(NOBS)=A(L)*XDR
IBM 0428            NA=L
IBM 0429        490 CONTINUE
IBM 0430            OCAP(NOBS)=0.5*OCAP(NOBS)
IBM 0431        500 IF(NDIFF(2).EQ.0.) GO TO 1000
IBM 0432            TALPA(2)=T(1)
IBM 0433            RMEAN=.5*(R(NDA2)+RALPA(2))
IBM 0434            RDIFF=R(NDA2)-RALPA(2)
IBM 0435            IF(NLONG.EQ.0) TALPA(2)=T(NDA2)-SLOPE*RDIFF
IBM 0436            NOBS=NOBS+1
IBM 0437            NAD(2)=NOBS
IBM 0438            NC(NOBS)=NALPA2
IBM 0439            OVER(NOBS)=RMEAN/RDIFF*DIPCON(T(NDA2),TALPA(2),C(NDA2),CBA(2),1)
IBM 0440            OCAPBA(2)=RMEAN*RDIFF
IBM 0441        510 INT=INTOKI(2)
IBM 0442            IINT=INT
IBM 0443            XDR=DR*IINT
IBM 0444            XDR2=.5*XDR
IBM 0445            IF(NLONG)513,513,511
IBM 0446        511 DO 512 L=NAD2  ,NPINB,INT
IBM 0447        512 T(L)=T(1)
IBM 0448            GO TO 590
IBM 0449        513 NA=(NALPA2-1)/64*64+1
IBM 0450            NL=NA+64
IBM 0451            IF(NL-NOKIB2)515,515,520
IBM 0452        515 SLOPE=(T(NA)-T(NL))/(R(NA)-R(NL))
IBM 0453            GO TO 525
IBM 0454        520 SLOPE=(T(NA)-TOKIB(2))/(R(NA)-ROKIB(2))
IBM 0455        525 T(NAD2)=TALPA(2)-SLOPE*(RALPA(2)-R(NAD2))
IBM 0456        530 NOBS=NOBS+1
IBM 0457            NC(NOBS)=NA2
IBM 0458            RMEAN=.5*(RALPA(2)+R(NAD2))
IBM 0459            RDIFF=RALPA(2)-R(NAD2)
IBM 0460            OVER(NOBS)=RMEAN/RDIFF*DIPCON(TALPA(2),T(NAD2),CAB(2),C(NA82),2)
IBM 0461            OCAP(NOBS)=XDR2*R(NAD2)
IBM 0462            OCAPAB(2)=RMEAN*RDIFF
IBM 0463            OCAP(NAB(2))=OCAPAB(2)+OCAPBA(2)
IBM 0464            NMIN=NAD2+INT
IBM 0465            IF(NLONG)537,537,535
IBM 0466        535 DO 536 L=NMIN,NA82,INT
IBM 0467        536 T(L)=T(1)
IBM 0468            GO TO 600
IBM 0469        537 NN=NA82
IBM 0470        540 NL=NA+64
IBM 0471            IF(NL-NOKIB2)545,545,550
IBM 0472        545 SLOPE=(T(NA)-T(NL))/(R(NA)-R(NL))
IBM 0473            GO TO 555
IBM 0474        550 SLOPE=(T(NA)-TOKIB(2))/(R(NA)-ROKIB(2))
IBM 0475        555 NN=NA82
IBM 0476            IF(NL.LT.NA82) NN=NL
IBM 0477            DO 560 L=NMIN,NN,INT
IBM 0478        560 T(L)=T(L-INT)-SLOPE*XDR
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ISN 0482            IF(NN.EQ.NAO2) GO TO 600
ISN 0483            NA=NA+68
ISN 0484            NNIN=NN+INT
ISN 0485            GO TO 640
ISN 0486        600 NA=NAB2
ISN 0487            NNIN=NAB2+INT
ISN 0488            DO 610 L=NNIN,NAO2,INT
ISN 0489            NGP =NGPS+1
ISN 0490            NC(NGPS)=L
ISN 0491            OVFP(NGPS)=(P(L)+XDP2)/XDP*DIPCON(T(NA),T(L),C(NA),C(L),J)
ISN 0492            OCAP(NGPS)=P(L)*XDR
ISN 0493            NA=NA+INT
ISN 0494        610 CONTINUE
ISN 0495            OCAP(NGPS)=.5*OCAP(NGPS)
ISN 0496            PMEAN=.5*(P(NAO2)+POXID(2))
ISN 0497            RDIFF=P(NAO2)-POXID(2)
ISN 0498            NGPS=NGPS+1
ISN 0499            NOA(2)=NGPS
ISN 0500            NC(NGPS)=NOXID2
ISN 0501            OCAPAO(2)=PMEAN*RDIFF
ISN 0502            OVFP(NGPS)=PMEAN/RDIFF*DIPCON(T(NAO2),TOXID(2),C(NAO2),CAO(2),2)
ISN 0503            PMEAN=.5*(POXID(2)+P(NOA2))
ISN 0504            RDIFF=POXID(2)-P(NOA2)
ISN 0505            OCAPOA(2)=PMEAN*RDIFF
ISN 0506            OCAP(NOA(2))=OCAPAO(2)+OCAPOA(2)
ISN 0507            IF(NLOWB)623,623,621
ISN 0508        621 DO 622 L=NOA2,NPINR,INT
ISN 0509        622 T(L)=T(1)
ISN 0510            GO TO 630
ISN 0511        623 NNN=(NOXYD2-1)/16*16+17
ISN 0512            IF(NNN.GT.NPINR) NNN=NPINR
ISN 0513            SLOPE=(TOXID(2)-T(NNN))/(POXID(2)-P(NNN))
ISN 0514            T(NOA2)=TOXID(2)-SLOPE*RDIFF
ISN 0515        630 NGPS=NGPS+1
ISN 0516            NC(NGPS)=NOA2
ISN 0517            OVFP(NGPS)=PMEAN/RDIFF*DIPCON(TOXID(2),T(NOA2),COA(2),C(NOA2),1)
ISN 0518            OCAP(NGPS)=XDR2*P(NOA2)
ISN 0519            IF((NLOWB.GT.0).OR.(INT.EQ.16)) GO TO 700
ISN 0520            NNIN=NOA2+INT
ISN 0521        635 NN=NPINR
ISN 0522            IF(NNN.LT.NN) NN=NPINR
ISN 0523            DO 640 L=NNIN,NN,INT
ISN 0524        640 T(L)=T(L-INT)-SLOPE*XDR
ISN 0525            IF(NN.EQ.NPINR) GO TO 700
ISN 0526            NNL=NNN
ISN 0527            NNN=NNL+16
ISN 0528            NNIN=NN+INT
ISN 0529            GO TO 635
ISN 0530        700 NA=NOA2
ISN 0531            NL=NA+INT
ISN 0532            DO 720 L=NL,NPINR,INT
ISN 0533            NGPS=NGPS+1
ISN 0534            NC(NGPS)=L
ISN 0535            OVFP(NGPS)=(P(L)+XDR2)/XDR*DIPCON(T(NA),T(L),C(NA),C(L),1)
ISN 0536            OCAP(NGPS)=P(L)*XDR
ISN 0537            NA=L
ISN 0538        720 CONTINUE
ISN 0539            OCAP(NGPS)=.5*OCAP(NGPS)
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ISN 0545      1000 IF((RALPA(1)-PALPA(2)).LT.4.*DR) GO TO 6000
ISN 0547           IF(NDIFF(1).EQ.0.) GO TO 1310
ISN 0549           STOROA(1)=.5*(C(NOA1  )+COA(1))*OCAPOA(1)+
                  1           .5*(C(NAO1  )+CAO(1))*OCAPAO(1)
ISN 0550           STORAB(1)=.5*(C(NAB1  )+CAB(1))*OCAPAB(1)+
                  1           .5*(C(NBA1  )+CBA(1))*OCAPBA(1)
ISN 0551           STOROA(1)=STOROA(1)+(OVER(NOA(1))*(C(NOA1  )-COA(1))
                  1           -OVER(NOA(1)+1)*(CAO(1)-C(NAO1  )))*DTDIFF
ISN 0552           STORAB(1)=STORAB(1)+(OVER(NAB(1))*(C(NAB1  )-CAB(1))
                  1           -OVER(NAB(1)+1)*(CBA(1)-C(NBA1  )))*DTDIFF
ISN 0553           C(NC(NOA(1)))=COA(1)
ISN 0554           C(NC(NAB(1)))=CBA(1)
ISN 0555      1310 IF(NDIFF(2).EQ.0.) GO TO 1315
ISN 0557           STOROA(2)=.5*(C(NOA2  )+COA(2))*OCAPOA(2)+
                  1           .5*(C(NAO2  )+CAO(2))*OCAPAO(2)
ISN 0558           STORAB(2)=.5*(C(NAB2  )+CAB(2))*OCAPAB(2)+
                  1           .5*(C(NBA2  )+CBA(2))*OCAPBA(2)
ISN 0559           STOROA(2)=STOROA(2)-(OVER(NOA(2))*(CAO(2)-C(NAO2))
                  1           -OVER(NOA(2)+1)*(C(NOA2)-COA(2)))*DTDIFF
ISN 0560           STORAB(2)=STORAB(2)-(OVER(NAB(2))*(CBA(2)-C(NBA2))
                  1           -OVER(NAB(2)+1)*(C(NAB2)-CAB(2)))*DTDIFF
ISN 0561           C(NC(NAB(2)))=CBA(2)
ISN 0562           C(NC(NOA(2)))=COA(2)
ISN 0563      1315 IF(NSTART.NE.1) GO TO 5000
ISN 0565           CALL INTDIF
                C  IN THIS SUBROUTINE THE CONCENTRATION INTEGRATION IS PERFORMED
ISN 0566           IF(NDIFF(1).EQ.0.) GO TO 2100
ISN 0568           CALL INTFAC(TOXID(1),COA(1),CAO(1),1)
ISN 0569           OCAPAO(1)=(OCAP(NOA(1))*(C(NOA1  )+COA(1))-2.*STOROA(1))/
                  1(C(NOA1  )+COA(1)-C(NAO1  )-CAO(1))
ISN 0570           OCAPOA(1)=OCAP(NOA(1))-OCAPAO(1)
ISN 0571           CALL INTFAC(TALPA(1),CAB(1),CBA(1),2)
ISN 0572           OCAPBA(1)=(OCAP(NAB(1))*(C(NAB1  )+CAB(1))-2.*STORAB(1))/
                  1(C(NAB1  )+CAB(1)-C(NBA1  )-CBA(1))
ISN 0573           IF((OCAPBA(1).GT.0.).AND.(OCAPBA(1).LT.OCAP(NAB(1)))) GO TO 1400
ISN 0575           CALL OUTPUT
ISN 0576           OCAPBA(1)=0.5*OCAP(NAB(1))
ISN 0577           WRITE(6,1399)
ISN 0578      1399 FORMAT(1H ,3GWALPHA/BETA INTERFACE FIXED              )
ISN 0579      1400 OCAPAB(1)=OCAP(NAB(1))-OCAPBA(1)
ISN 0580           ROXID(1)=R(NAO1)+2.*OCAPAO(1)/(ROXID(1)+R(NAO1))
ISN 0581           RALPA(1)=R(NBA1)+2.*OCAPBA(1)/(RALPA(1)+R(NBA1))
ISN 0582           DOXID(1)=R(1)-ROXID(1)
ISN 0583           DALPA(1)=R(1)-PALPA(1)
ISN 0584           GAIN(1)=GAIN(1)+OXIGPL(1)*DTDIFF
ISN 0585           OXIGPL(1)=OVER(2)*(C(1)-C(NC(2)))/R(1)
ISN 0586           IF(OXIGPL(1).LE.0.) OXIGPL(1)=NDIFF(1)
ISN 0588      2100 IF(NDIFF(2).EQ.0.) GO TO 2500
ISN 0590           CALL INTFAC(TOXID(2),COA(2),CAO(2),1)
ISN 0591           OCAPAO(2)=(OCAP(NOA(2))*(C(NOA2  )+COA(2))-2.*STOROA(2))/
                  1(C(NOA2  )+COA(2)-C(NAO2  )-CAO(2))
ISN 0592           OCAPOA(2)=OCAP(NOA(2))-OCAPAO(2)
ISN 0593           CALL INTFAC(TALPA(2),CAB(2),CBA(2),2)
ISN 0594           OCAPBA(2)=(OCAP(NAB(2))*(C(NAB2  )+CAB(2))-2.*STORAB(2))/
                  1(C(NAB2  )+CAB(2)-C(NBA2  )-CBA(2))
ISN 0595           IF((OCAPBA(2).GT.0.).AND.(OCAPBA(2).LT.OCAP(NAB(2)))) GO TO 2400
ISN 0597           OCAPBA(2)=0.5*OCAP(NAB(2))
ISN 0598           WRITE(6,1399)
```

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ISN 0599      2400 OCAPAB(2)=OCAP(NAB(2))-OCAPBA(2)
ISN 0600           ROXID(2)=R(NAO2)-2.*OCAPAO(2)/(ROXID(2)+R(NAO2))
ISN 0601           RALPA(2)=R(NBA2)-2.*OCAPBA(2)/(RALPA(2)+R(NBA2))
ISN 0602           DOXID(2)=ROXID(2)-R(NPINE)
ISN 0603           DALPA(2)=RALPA(2)-R(NPINE)
ISN 0604           GAIN(2)=GAIN(2)+OXIGPL(2)*DTDIFF
ISN 0605           OXIGPL(2)=OVEP(NGES)*(C(NPINE)-C(NC(NGES-1)))/P(NPINE)
ISN 0606           IF(OXIGPL(2).LE.0.)  OXIGPL(2)=HDIFF(2)
ISN 0608      2500 CONTINUE
ISN 0609      5000 NSTART=1
ISN 0610           RETURN
ISN 0611      6000 WRITE(6,6001)
ISN 0612      6001 FORMAT(1HO,40HBETA-ZIRCALOY LESS THAN .0005 CM THICK    )
ISN 0613           CALL OUTPUT
ISN 0614           TIME=TMAX
ISN 0615           RETURN
ISN 0616           END
```

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ISN 0002            SUBROUTINE DSTART
                C   DSTART PERFORMS THE CONCENTRATION CALCULATION IF OXIDE OR ALPHA
                C   LAYER ARE THIN
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/GEOMET/ R(1000),ROXID(2),RALPA(2),RWALL,DOXID(2),DALPA(2),DR
ISN 0005            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0006            COMMON/TEMTIM/ TCOOL(100,2),STCOOL(100,2),TRAD(100,2),STRAD(100,2)
ISN 0007            COMMON/HEAT  / HVER(100) ,HCOOL(2),HRADIA(2),HEATFL(2),QFIXED(2),
                   1                       QSPLIT,HCAP(100)  ,HSTEAM(2),HRADIA(2)
                   2                  ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0008            COMMON/HEADLN/ HTITLE(20)
ISN 0009            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1              OXIGFL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),ODTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010            COMMON/TIME  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              NTEMP,NDIFF,NPRINT
ISN 0011            COMMON/MESH  /NGROSS,NPINE,NOXID(2),NOXI(2)
                   1,             NLOWB,NSTART,NALPA(2)
ISN 0012            COMMON/MESHTE/NT(100),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NGES
ISN 0013            COMMON/MESHCO/NC(500),NBAKER,NGES,NOA(2),NAB(2)
                   1,              NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                   2,              NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                   3,              NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0014            COMMON/MATPRO/ DENSIR,DENSNO,OSTOCH,OXICON,DENRAT,PICFAC,OXHEAT
ISN 0015            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),CBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016            COMMON/MINPUT/ NDIFIN(100,2),TINDIF(100,2),NCOEFF(100,2),
                   1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TINSTP(100),DTMIN(100),
                   3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                   4               NCOEFF(2),NCOEFF(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0017            DIMENSION CN(1000),STOROA(2),STORAB(2)
                   1,DALOLD(2),ALPAFL(2),BETAFL(2),COXOLD(2),CALOLD(2),CBEOLD(2)
ISN 0018            IF(NSTART.NE.2) GO TO 5500
ISN 0020          1 NGES=NGROSS
ISN 0021            DO 21 K=1,2
ISN 0022            IF(NDIFF(K).EQ.0.) GO TO 21
ISN 0024            OSURF=C(1)
ISN 0025            IF(K.EQ.2)  OSURF=C(NPINE)
ISN 0027            CBET=C(NP1)
ISN 0028            IF(K.EQ.2)  CBET=C(NP2)
ISN 0030            COXOLD(K)=0.5*(OSURF+COA(K))
ISN 0031            CBEOLD(K)=0.5*(CBET+CBA(K))
ISN 0032            CALOLD(K)=0.5*(CAO(K)+CAB(K))
ISN 0033            DALOLD(K)=DALPA(K)-DOXID(K)
ISN 0034            CALL INTPAC(TOXID(K),COA(K),CAO(K),1)
ISN 0035            CALL INTPAC(TOXID(K),CAB(K),CBA(K),2)
ISN 0036            IF(COXOLD(K).LT.COA(K))  COXOLD(K)=0.5*(COA(K)+OXICON)
ISN 0038            IF(CALOLD(K).LT.CAB(K))  CALOLD(K)=0.5*(CAB(K)+CAO(K))
ISN 0040            IF(K.EQ.2)  GO TO 2
ISN 0042            T1=T(1)
ISN 0043            C(1)=OXICON
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ISN 0044            GO TO 3
ISN 0045          2 T1=T(NPINB)
ISN 0046            C(NPINB)=OXICON
ISN 0047          3 DIFOXI  =DIFCON(T1,TOXID(K),OXICON,COA(K),1)
ISN 0048            OXIGFL(K)=(OXICON-COA(K))/DOXID(K)*DIFOXI
ISN 0049            IF(OXIGFL(K).LE.NDIFF(K)) GO TO 11
ISN 0051            OXIGFL(K)=NDIFF(K)
ISN 0052            IF(K.EQ.1)  C(1)=COA(1)+OXIGFL(1)*DOXID(1)/DIFOXI
ISN 0054            IF(K.EQ.2)  C(NPINB)=COA(2)+OXIGFL(2)*DOXID(2)/DIFOXI
ISN 0056         11 ALPAFL(K)=DIFCON(TOXID(K),TOXID(K),CAO(K),CAB(K),2)
                   1          *(CAO(K)-CAB(K))/(DALPA(K)-DOXID(K))
ISN 0057            BETAFL(K)=0.
ISN 0058            DELRAD=2.*DR
ISN 0059            DIFBET=DIFCON(TOXID(K),TOXID(K),CBA(K),CSTART,3)
ISN 0060            IF(NDIFF(1)*NDIFF(2).EQ.0.) GO TO 5
ISN 0062            IF(K.EQ.2)  GO TO 12
ISN 0064            R1=DALPA(1)/DR
ISN 0065            NB=(R1+1)/2**2+7
ISN 0066            NP1=NB-4
ISN 0067            R2=DALPA(2)/DR
ISN 0068            NO=NPINB-(R2+1)/2**2-6
ISN 0069            NP2=NO+4
ISN 0070            GO TO 9
ISN 0071          5 IF(NDIFF(1).EQ.0.)  GO TO 7
ISN 0073            R1=DALPA(1)/DR
ISN 0074            NB=(R1+1)/2**2+7
ISN 0075            NP1=NB-4
ISN 0076            NO=NPINB-2
ISN 0077            NP2=NPINB
ISN 0078            GO TO 9
ISN 0079          7 R2=DALPA(2)/DR
ISN 0080            NO=NPINB-(R2+1)/2**2-6
ISN 0081            NP2=NO+4
ISN 0082            NP=3
ISN 0083            NP1=1
ISN 0084          9 IF(NP.GT.NO) GO TO 6000
ISN 0086            IF(K.EQ.2)  GO TO 12
ISN 0088            RDIF1=RALPA(1)-R(NP1)
ISN 0089            DTNA=RDIF1*DELRAD*(DR+RDIF1)/((RDIF1+DELRAD)*DIFBET)
ISN 0090            DTN1=DTNA
ISN 0091            DIFB1=DIFBET
ISN 0092            IF(NDIFF(2)) 15,15,405
ISN 0093         12 RDIF2=R(NP2)-RALPA(2)
ISN 0094            DTNA=RDIF2*DELRAD*(DR+RDIF2)/((RDIF2+DELRAD)*DIFBET)
ISN 0095            IF(NDIFF(1).EQ.0.)  GO TO 15
ISN 0097            IF(DIFBET.LT.DIFB1)  DIFBET=DIFB1
ISN 0099            IF(DTNA.GT.DTN1)  DTNA=DTN1
ISN 0101         15 DTN=0.5*DELRAD**2/DIFBET
ISN 0102            IF(DTNA.LT.DTN)  DTN=DTNA
ISN 0104            DTN=0.9*DTN
ISN 0105            XMAX=DTDIFF/DTN+1.
ISN 0106            XMAX=XMAX
ISN 0107            DTN=DTDIFF/XMAX
ISN 0108            FACTOR=DTN*DIFBET/DELRAD**2
ISN 0109        405 IF(((DALPA(K)-DOXID(K)).GT.1.00001D-7).AND.(DOXID(K).GT.1.D-7))
                   1GO TO 430
ISN 0111            IF((DOXID(K).LE.1.D-7).AND.(ALPAFL(K).GT.OXIGFL(K)))
                   1ALPAFL(K)=OXIGFL(K)
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ISN 0113            IF((ALPA(K)-DOXID(K)).GT.1.000001D-7) GO TO 430
ISN 0114            IF(K-1) 410,410,420
ISN 0116          410 CBAN1 =ALPAPL(1)*RDIF1/DIFBET+C(NP1)
ISN 0117            IF(CBAN1.GT.CBA(1)) GO TO 415
ISN 0119            CBA(1)=CBAN1
ISN 0120            RPL1=ALPAPL(1)
ISN 0121          415 CBEOLD(1)=CBEOLD(1)+CBA(1)-CALOLD(1)
ISN 0122            CAB(1)=CBA(1)
ISN 0123            CAO(1)=CAB(1)
ISN 0124            CALOLD(1)=CAO(1)
ISN 0125            GO TO 430
ISN 0126          420 CBAN2 =ALPAPL(2)*RDIF2/DIFBET+C(NP2)
ISN 0127            IF(CBAN2.GT.CBA(2)) GO TO 425
ISN 0129            CBA(2)=CBAN2
ISN 0130            RPL2=ALPAPL(2)
ISN 0131          425 CBEOLD(2)=CBEOLD(2)+CBA(2)-CALOLD(2)
ISN 0132            CAB(2)=CBA(2)
ISN 0133            CAO(2)=CAB(2)
ISN 0134            CALOLD(2)=CAO(2)
ISN 0135          430 IF(DOXID(K).GT.1.D-7) GO TO 490
ISN 0137            IF(K-1) 440,440,450
ISN 0138          440 COA(1)=CAO(1)*PICFAC
ISN 0139            C(1)=COA(1)
ISN 0140            COXOLD(1)=COA(1)
ISN 0141            GO TO 490
ISN 0142          450 COA(2)=CAO(2)*PICFAC
ISN 0143            C(NPINE)=COA(2)
ISN 0144            COXOLD(2)=COA(2)
ISN 0145          490 IF((K.EQ.1).AND.(NDIFF(2).GT.0.)) GO TO 21
ISN 0147            NL=NO-2
ISN 0148            NN=NO+2
ISN 0149            DO 20 K=1,KMAX
ISN 0150            DO 16 L=NO,NO,2
ISN 0151           16 CN(L)=C(L)+FACTOR*(C(L+2)+C(L-2)-2.*C(L))
ISN 0152            IF(NDIFF(1).EQ.0.) GO TO 17
ISN 0154            IF(CBA(1).NE.CBAN1)
                   1BPL1=DIFBET*(CBA(1)-C(NP1))/RDIF1
ISN 0156            BETAPL(1)=BETAPL(1)+BPL1
ISN 0157            CN(NP1)=C(NP1)+(BPL1+DIFBET*(C(NL)-C(NP1))/DELRAD)*DTH
                   1        /(0.5*RDIF1+0.75*DR)
ISN 0158            CN(NL)=C(NL)+(C(NL+2)+C(NL-2)-2.*C(NL))*DTH*DIFBET
                   1       /(1.125*DELRAD**2)
ISN 0159            IF(NDIFF(2).EQ.0.) CN(NPINE)=C(NPINE)+2.*FACTOR*
                   1(C(NPINE-2)-C(NPINE))
ISN 0161            IF(K.EQ.1) GO TO 18
ISN 0163           17 IF(CBA(2).NE.CBAN2)
                   1BPL2=DIFBET*(CBA(2)-C(NP2))/RDIF2
ISN 0165            BETAPL(2)=BETAPL(2)+BPL2
ISN 0166            CN(NP2)=C(NP2)+(BPL2+DIFBET*(C(NN)-C(NP2))/DELRAD)*DTH
                   1        /(0.5*RDIF2+0.75*DR)
ISN 0167            CN(NN)=C(NN)+(C(NN+2)+C(NN-2)-2.*C(NN))*DTH*DIFBET
                   1       /(1.125*DELRAD**2)
ISN 0168            IF(NDIFF(1).EQ.0.) CN(1)=C(1)+2.*FACTOR*(C(3)-C(1))
ISN 0170            DO 19 L=NP1,NP2
ISN 0171           19 C(L)=CN(L)
ISN 0172           20 CONTINUE
ISN 0173            IF(NDIFF(1).GT.0.) BETAPL(1)=BETAPL(1)/KMAX
ISN 0175            IF(NDIFF(2).GT.0.) BETAPL(2)=BETAPL(2)/KMAX
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ISN 0177         21 CONTINUE
ISN 0178            DO 35 K=1,2
ISN 0179            IF(NDIFF(K).EQ.0.) GO TO 35
ISN 0181            DSTORO =(OXIGPL(K)-ALPAPL(K))*DTDIFF
ISN 0182            OSURF=C(1)
ISN 0183            IF(K.EQ.2) OSURF=C(NPINE)
ISN 0185            CMEAN=0.5* (OSURF+COA(K))
ISN 0186            DOXID(K)=DOXID(K)+(DSTORO+DOXID(K)*(CAOLD(K)-CMEAN))
                   1          /(CMEAN-CAOLD(K))
ISN 0187            IF(DOXID(K).LT.1.00)1D-7)DOXID(K)=1.D-7
ISN 0189            NOXYD=DOXID(K)/DR
ISN 0190            NOXID(K)=DOXID(K)/DR+.5
ISN 0191            DSTORA = (ALPAPL(K)-BETAPL(K))*DTDIFF
ISN 0192            CMEAN=0.5*(CAO(K)+CAB(K))
ISN 0193            DALPA(K)=DALPA(K)+(DSTORA+DALOLD(K)*(CALOLD(K)-CMEAN))
                   1          /(CMEAN-CBBOLD(K))
ISN 0194            IF(DALPA(K).LT.(DOXID(K)+1.0001D-7))DALPA(K)=DOXID(K)+1.D-7
ISN 0196            NALPR=DALPA(K)/DR
ISN 0197            NALPA(K)=DALPA(K)/DR+.5
ISN 0198            IF(K.EQ.2) GO TO 25
ISN 0200            NOXID(1)=R(1)-DOXID(1)
ISN 0201            NALPA(1)=R(1)-DALPA(1)
ISN 0202            NGRS=NGRS+11
ISN 0203            NOA(1)=2
ISN 0204            NC(2)=NOXID(1)+1
ISN 0205            NAB(1)=3
ISN 0206            NC(3)=NALPA(1)+1
ISN 0207            IF((NOXID(1).LT.6.*DR).OR.(DALPA(1)-DOXID(1).LT.6.*DR)) GO TO 30
ISN 0209            NL=2
ISN 0210            NN=NOXYD+1
ISN 0211            CDIFF=(C(1)-COA(1))/DOXID(1)*DR
ISN 0212            DO 22 L=NL,NN
ISN 0213         22 C(L)=C(L-1)-CDIFF
ISN 0214            NL=NN+1
ISN 0215            SLOPE=(CAO(1)-CAB(1))/(DALPA(1)-DOXID(1))
ISN 0216         24 C(NL)=CAO(1)-SLOPE*(NOXID(1)-R(NL))
ISN 0217            NL=NL+1
ISN 0218            IF(NL.LE.NALPR+1) GO TO 24
ISN 0220            GO TO 30
ISN 0221         25 NOXID(2)=R(NPINE)+DOXID(2)
ISN 0222            NALPA(2)=R(NPINE)+DALPA(2)
ISN 0223            NGRS=NGRS+11
ISN 0224            NOA(2)=NGRS-1
ISN 0225            NC(NOA(2))=NPINE-NOXID(2)
ISN 0226            NAB(2)=NGRS-2
ISN 0227            NC(NAB(2))=NPINE-NALPA(2)
ISN 0228            IF((NOXID(2).LT.6.*DR).OR.(DALPA(2)-DOXID(2).LT.6.*DR)) GO TO 30
ISN 0230            NL=NPINE-NOXYD
ISN 0231            NN=NPINE-1
ISN 0232            SLOPE=(C(NPINE)-COA(2))/DOXID(2)
ISN 0233            C(NL)=C(NPINE)-SLOPE*(R(NL)-R(NPINE))
ISN 0234            CDIFF=SLOPE*DR
ISN 0235            NL=NL+1
ISN 0236            DO 26 L=NL,NN
ISN 0237         26 C(L)=C(L-1)+CDIFF
ISN 0238            NN=NL-2
ISN 0239            NL=NPINE-NALPR
ISN 0240            SLOPE=(CAO(2)-CAB(2))/(DALPA(2)-DOXID(2))
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ISN 0281            C(NN)=CAO(2)-(R(NN)-ROXID(2))*SLOPE
ISN 0282            C(NL)=CAO(2)-(R(NL)-ROXID(2))*SLOPE
ISN 0283            NN=NN-1
ISN 0284            NL=NL+1
ISN 0285            CDIFF=SLOPE*DP
ISN 0286            DO 27 L=NL,NN
ISN 0287         27 C(L)=C(L-1)+CDIFF
ISN 0288         30 GAIN(K)=GAIN(K)+OXIGPL(K)*DMDIFF
ISN 0289         35 CONTINUE
ISN 0290            NC(NGES)=NPINE
ISN 0291            MAX=NGES-12
ISN 0292            IF(NDIFF(1).GT.0.) GO TO 37
ISN 0293            DO 36 N=2,MAX
ISN 0294            NC(N)=NC(N-1)+64
ISN 0295            IF(NC(N).GT.NP2-10) NC(N)=NC(N-1)
ISN 0296            IF(NLOWB.GT.0) T(NC(N))=T(1)
ISN 0297         36 CONTINUE
ISN 0298            GO TO 45
ISN 0299         37 NALPH=DALPA(1)/DR
ISN 0300            NPH=(NALPH+1)/2*2+3
ISN 0301            IF(NPH-NP1) 237,337,137
ISN 0302        137 NL=NP1+2
ISN 0303            SLOPE=(C(NP1)-C(NL))/(R(NP1)-R(NL))
ISN 0304            C(NPH)=C(NP1)-(R(NP1)-R(NPH))*SLOPE
ISN 0305            NP1=NPH
ISN 0306            GO TO 337
ISN 0307        237 SLOPE=(CBA(1)-C(NP1))/(RALPA(1)-R(NP1))
ISN 0308            C(NPH)=C(NP1)+(R(NPH)-R(NP1))*SLOPE
ISN 0309            NP1=NPH
ISN 0310        337 NC(4)=NP1
ISN 0311            DO 38 N=5,12
ISN 0312            NC(N)=NC(N-1)+2
ISN 0313            IF(NC(N).GT.NP2) NC(N)=NP2
ISN 0314         38 CONTINUE
ISN 0315            NC(13)=(NC(12)+63)/64*64+1
ISN 0316            IF(NDIFF(2)) 138,138,139
ISN 0317        138 MAX=NGES
ISN 0318            NPO=NPINE
ISN 0319            GO TO 140
ISN 0320        139 NPO=NP2-10
ISN 0321        140 DO 39 N=14,MAX
ISN 0322            NC(N)=NC(N-1)+64
ISN 0323            IF(NC(N).GT.NPO) NC(N)=NC(N-1)
ISN 0324         39 CONTINUE
ISN 0325            IF(NLOWB)42,42,40
ISN 0326         40 DO 41 N=2,MAX
ISN 0327         41 T(NC(N))=T(1)
ISN 0328            DALPA(1)=T(1)
ISN 0329            GO TO 44
ISN 0330         42 SLOPE=(TOXID(1)-T(65))/(ROXID(1)-R(65))
ISN 0331            TALPA(1)=TOXID(1)-SLOPE*(ROXID(1)-DALPA(1))
ISN 0332            DO 43 N=4,12
ISN 0333         43 T(NC(N))=TOXID(1)-SLOPE*(ROXID(1)-R(NC(N)))
ISN 0334         44 IF(NDIFF(2).EQ.0.) GO TO 5000
ISN 0335         45 NALPH=DALPA(2)/DR
ISN 0336            NPH=NPINE-(NALPH+1)/2*2-2
ISN 0337            IF(NP2-NPH) 185,385,185
ISN 0338        185 NH=NP2-2
```

```
ISN 0305            SLOPE=(C(NP2)-C(NN))/(R(NN)-R(NP2))
ISN 0306            C(NPN)=C(NP2)-(R(NPN)-R(NP2))*SLOPE
ISN 0307            NP2=NPN
ISN 0308            GO TO 345
ISN 0309        245 SLOPE=(CBA(2)-C(NP2))/(R(NP2)-RALPA(2))
ISN 0310            C(NPN)=C(NP2)+(R(NP2)-R(NPN))*SLOPE
ISN 0311            NP2=NPN
ISN 0312        345 NC(NGES-3)=NP2
ISN 0313            NC(NGES-11)=NC(NGES-3)-16
ISN 0314            NL=NGES-10
ISN 0315            NN=NGES-4
ISN 0316            DO 47 N=NL,NN
ISN 0317            NC(N)=NC(N-1)+2
ISN 0318            IF(NC(N-1).LT.NP1) NC(N-1)=NP'
ISN 0320         47 CONTINUE
ISN 0321            IF(NC(NGES-11).LE.NPINE-64) NC(NGES-12)=NC(NGES-11)-2
ISN 0323            NL=NGES-11
ISN 0324            NN=NGES-3
ISN 0325            IF(NL@NN) 53,53,51
ISN 0326         51 DO 52 N=NL,NN
ISN 0327         52 T(NC(N))=T(1)
ISN 0328            TALPA(2)=T(1)
ISN 0329            GO TO 5000
ISN 0330         53 NP=NPINE-64
ISN 0331            SLOPE=(T(NP       )-TOXID(2))/(R(NP       )-ROXID(2))
ISN 0332            DO 49 N=NL,NN
ISN 0333         49 T(NC(N))=T(NP)-SLOPE*(R(NP)-R(NC(N)))
ISN 0334            TALPA(2)=T(NP)-SLOPE*(R(NP)-RALPA(2))
ISN 0335       5000 RETURN
ISN 0336       5500 IF(TIME.EQ.0.) GO TO 6000
ISN 0338            NLG=1
ISN 0339            NNG=NGES
ISN 0340            IF(NDIFF(1).GT.0.) NLG=NAB(1)+10
ISN 0342            IF(NDIFF(2).GT.0.) NNG=NAB(2)-10
ISN 0344       5600 NL=NC(NLG)
ISN 0345            NN=NC(NLG+1)
ISN 0346            CDIFF=2.*DR*(C(NL)-C(NN))/(R(NL)-R(NN))
ISN 0347            NL=NL+2
ISN 0348            NN=NN-2
ISN 0349            IF(NL.GT.NN) GO TO 5800
ISN 0351            DO 5700 N=NL,NN,2
ISN 0352       5700 C(N)=C(N-2)-CDIFF
ISN 0353       5800 NLG=NLG+1
ISN 0354            IF(NLG.LT.NNG) GO TO 5600
ISN 0356            BOXID(1)=BOXID(1)/DR
ISN 0357            BOXID(2)=BOXID(2)/DR
ISN 0358            BALPA(1)=BALPA(1)/DR
ISN 0359            BALPA(2)=BALPA(2)/DR
ISN 0360       6000 NGES=NGROSS
ISN 0361            NLG=2
ISN 0362            NC(1)=1
ISN 0363            DO 6100 L=1,NPINE,2
ISN 0364       6100 CW(L)=C(L)
ISN 0365            IF(NDIFF(1).EQ.0.) GO TO 6500
ISN 0367            NGES=NGES+11
ISN 0368            NOA(1)=2
ISN 0369            NAB(1)=1
ISN 0370            NC(2)=1+BOXID(1)
```

```
ISN 0371          NC(3)=1+NALPA(1)
ISN 0372          NALPH=DALPA(1)/DP
ISN 0373          NC(4)=(NALPH+1)/2*2+3
ISN 0374          NP1=NC(4)
ISN 0375          NC(13)=65
ISN 0376          DO 6800 N=5,12
ISN 0377    6800  NC(N)=NC(N-1)+2
ISN 0378          NLG=16
ISN 0379          NHG=NGES
ISN 0380    6500  IF(NDIFF(2).EQ.0.) GO TO 7150
ISN 0382          NGES=NGES+11
ISN 0383          NOA(2)=NGES-1
ISN 0384          NAB(2)=NGES-2
ISN 0385          NC(NGES)=NFINE
ISN 0386          NC(NOA(2))=NFINE-NOXID(2)
ISN 0387          NC(NAB(2))=NFINE-NALPA(2)
ISN 0388          NALPH=DALPA(2)/DA
ISN 0389          NC(NGES-3)=NFINE-(NALPH+1)/2*2-2
ISN 0390          NP1=1
ISN 0391          NP2=NC(NGES-3)
ISN 0392          NL=NGES-10
ISN 0393          NC(NL-1)=NC(NGES-3)-16
ISN 0394          NH=NGES-4
ISN 0395          NHG=NGES-12
ISN 0396    7000  DO 7100 N=NL,NH
ISN 0397    7100  NC(N)=NC(N-1)+2
ISN 0398    7150  DO 7200 N=NLG,NHG
ISN 0399    7200  NC(N)=NC(N-1)+64
ISN 0400          IF(NSTART.NE.2) GO TO 1
ISN 0402          CALL OUTPUT
ISN 0403          TIME=TMAX
ISN 0404          RETURN
ISN 0405          END
```

```
ISN 0002            SUBROUTINE RATMOD
                C   RATMOD IS USED FOR NBAKER > 0 AND CALCULATES THICKNESS OF OXIDE
                C   LAYER WITH ONE OF THE RATE EQUATIONS
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*8 LBRNOR
ISN 0005            COMMON/GROWRT/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DR
ISN 0006            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0007            COMMON/TEMTIM/ TCOOL(100,2),TTCOOL(100,2),TRAD(100,2),TTRAD(100,2)
ISN 0008            COMMON/MBAT  / NVER(100)  ,NCOOL(2),FRADIA(2),NRATPL(2),QPINFO(2),
                   1                          QSPLIT,NCAP(10C)  ,NSTEAM(2),NRADIA(2)
                   2                ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0009            COMMON/MBABLK/ MTITLE(20)
ISN 0010            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1               OXIGPL(2),NDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),OMTMAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0011            COMMON/MBIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,              NTEMP,NDIFF,NPRINT
ISN 0012            COMMON/MESH  /NGROSS,NPINE,NOXID(2),NOXI(2)
                   1,              WLENG,WSTART,WALPA(2)
ISN 0013            COMMON/MESHTB/MT(100),MTCOOL(2),MTWALL(2),MTCOOL(2),MTWALL(2),NGRS
ISN 0014            COMMON/MESHCO/MC(500),NBAKER,NGRS,NOA(2),NAB(2)
                   1,              NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                   2,              NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                   3,              NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0015            COMMON/MATPRO/ DENSIB,DENSID,OSTOCH,OXICON,DENRAT,PICFAC,OXNRAT
ISN 0016            COMMON/PROPIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0017            COMMON/MINPUT/ NDIFIN(100,2),TIMDIF(100,2),NCORPP(100,2),
                   1               TCOEPP(100,2),NRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTNEW(100),
                   3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                   4               NCOEPP(2),NCOEPP(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0018            REFRAD=R(1)
ISN 0019            IF(NDIFF(1).EQ.0.) REFRAD=R(NPINE)
ISN 0021            DO 100 N=1,2
ISN 0022            IF(NDIFF(N).EQ.0.) GO TO 100
ISN 0024            FLUX=OXIGPL(N)
ISN 0025            TK=T(1)+273.16
ISN 0026            IF(WLENG.EQ.0) TK=.5*(TSURF(N)+TOXID(N))
ISN 0028            IF(TK.GT.2073.16) TK=2073.16
ISN 0030            GO TO (1,2,3,20),NBAKER
ISN 0031          1 BARYN=0.5*33.3*EXP(-45500./(1.987*TK))*DENRAT**2
ISN 0032            DOXDT=BARYN/DOXID(N)
ISN 0033            GO TO 90
ISN 0034          2 RBSON=.155311*EXP(-39291./(1.987*TK))
ISN 0035            DOXDT=RBSON/DOXID(N)
ISN 0036            GO TO 90
ISN 0037          3 LBNNOR=.8286T5*EXP(-34000./(1.987*TK))
ISN 0038            DOXDT=LBNNOR/DOXID(N)
ISN 0039            GO TO 90
ISN 0040         20 DALDT=0.3538*EXP(-41054./(1.987*TK))/DALPA(N)
ISN 0041            IF(NSTART.GT.0)
```

```
                  1DALPA(K)=DALPA(K)+DALDT*DTDIFF
ISN 0048             GO TO 2
ISN 0049          50 DXIGFL(K)=DOXDT/(DENAIR*DENRAT)
ISN 0045             IF(NSTART.EQ.0) GO TO 100
ISN 0047             DOXID(K)=DOXID(K)+DXIGFL(K)*DTDIFF/(OXICON-CSTAR*)
ISN 0048             GAIN(K)=GAIN(K)+PLOX*DTDIFF*R(K)/REYRAD
ISN 0049          100 CONTINUE
ISN 0050             ROXID(1)=R(1)-DOXID(1)
ISN 0051             ROXID(2)=R(NPINE)+DOXID(2)
ISN 0052             BLAYER=CALL-DOXID(1)-DOXID(2)
ISN 0053             IF(BLAYER) 500,500,200
ISN 0054          200 IF(NLOOP.NE.0) RETURN
ISN 0056             IF(BLAYER.GT.120.*DR) RETURN
ISN 0058             IF((NDIFF(2)*NDIFF(1).EQ.0.).AND.(BLAYER.GT.32.*DR)) RETURN
ISN 0060             NLOOP=1
ISN 0061             RETURN
ISN 0062          500 TIME=TMAX
ISN 0063             RETURN
ISN 0064             END
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ISN 0002            SUBROUTINE RESMSH
                C   RESMSH DETERMINES MESH SIZE AND INTERPOLATES IF THERE IS A CHANGE
                C   IN MESH SIZE
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/GROWTH/ R(1000),ROXID(2),RALPA(2),WALL,DOXID(2),DALPA(2),DR
ISN 0005            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTPAR(2),TWALL(2)
                   1,TSURF(2)
ISN 0006            COMMON/TWINS/ TCOOL(100,2),ETCOOL(100,2),TPAD(100,2),ETPAD(100,2)
ISN 0007            COMMON/BEAT  / WVER(100)  ,WCOOL(2),ERADIA(2),WRATPL(2),QFIXED(2),
                   1                          QSPLIT,WCAP(100)  ,WSTRAN(2),WPADTA(2)
                   2             ,QSURF(2),QCLAD(2),QRAD(2),QREACT(2)
ISN 0008            COMMON/TRANSM/ TITLE(20)
ISN 0009            COMMON/CONCIN/ C(1000),COXID(2),CONAL(2),CALBET(2),CBETA(2),
                   1               OXIGEN(2),WDIFF(2),CSTART,GAIN(2)
                   2.          OCAP(500),OVER(500),OBTMAX(500)
                   3.          COA(2),CAO(2),CAB(2),CBA(2)
                   4.          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010            COMMON/EXIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,             NTEMP,NDIFF,NPRINT
ISN 0011            COMMON/MESH  /NGROSS,NFINE,NOXID(2),NOX(2)
                   1,            XLOWB,XSTART,XALPA(2)
ISN 0012            COMMON/MESHTB/NT(100),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NGRS
ISN 0013            COMMON/MESHCO/NC(500),NBANDP,NGES,NOA(2),NAB(2)
                   1,             NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTR
                   2,             NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                   3,             NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0014            COMMON/MATPRO/ DENSIR,DENSPO,OSTOCN,CRICON,DENRAT,PICFAC,DXMFAT
ISN 0015            COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016            COMMON/MINPUT/ NDIFIN(100,2),TINDIF(100,2),NCOEFF(100,2),
                   1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                   2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTMIN(100),
                   3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                   4               NCOEFF(2),NCOEFF(2),NPADCO(2),NRADCO(2),NSTEP
ISN 0017            DO 190 K=1,2
ISN 0018            IF(NDIFF(K).EQ.0.) GO TO 190
ISN 0020            IF(NSTART.EQ.1) INT=INTOXI(K)
ISN 0022            NOXID(K)=ROXID(K)/DR+.5
ISN 0023            NALPA(K)=RALPA(K)/DR+.5
ISN 0024            JALPA=NALPA(K)-NOXID(K)
ISN 0025            IF(JALPA/2.GT.NOXID(K)) JALPA=NOXID(K)*2+1
ISN 0027            IF(JALPA.GT.0) GO TO 60
ISN 0029            INTOXI(K)=1
ISN 0030            NOA(K)=NOXID(K)-1
ISN 0031            NAO(K)=NOXID(K)+1
ISN 0032            NAB(K)=NALPA(K)-1
ISN 0033            NBA(K)=(NALPA(K)/2+1)*2
ISN 0034            GO TO 100
ISN 0035         60 IF(JALPA.GT.16) GO TO 70
ISN 0037            INTOXI(K)=2
ISN 0038            NOA(K)=(NOXID(K)-1)/2*2
ISN 0039            NAO(K)=(NOXID(K)+2)/2*2
ISN 0040            NAB(K)=(NALPA(K)-1)/2*2
ISN 0041            NBA(K)=(NALPA(K)+5)/4*4
ISN 0042            GO TO 100
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ISN 0043          70 IF(JALPA.GT.32) GO TO 80
ISN 0045             INTOXI(K)=8
ISN 0046             NOA(K)=(NOXID(K)-2)/8+8
ISN 0047             NAO(K)=(NOXID(K)+5)/8+8
ISN 0048             NAB(K)=(NALPA(K)-2)/8+8
ISN 0049             NBA(K)=(NALPA(K)+11)/8+8
ISN 0050             GO TO 100
ISN 0051          80 IF(JALPA.GT.64) GO TO 90
ISN 0053             INTOXI(K)=8
ISN 0054             NOA(K)=(NOXID(K)-4)/8+8
ISN 0055             NAO(K)=(NOXID(K)+11)/8+8
ISN 0056             NAB(K)=(NALPA(K)-4)/8+8
ISN 0057             NBA(K)=(NALPA(K)+23)/16+16
ISN 0059             GO TO 100
ISN 0059          90 INTOXI(K)=16
ISN 0060             NOA(K)=(NOXID(K)-8)/16+16
ISN 0061             NAO(K)=(NOXID(K)+23)/16+16
ISN 0062             NAB(K)=(NALPA(K)-8)/16+16
ISN 0063             NBA(K)=(NALPA(K)+47)/32+32
ISN 0064         100 IF((NDIFF(1)*NDIFF(2).GT.0.).AND.(K.EQ.2)) GO TO 101
ISN 0066             INTB=2*INTOXI(K)
ISN 0067             GO TO 104
ISN 0068         101 IF(INTOXI(2).LT.INTOXI(1)) INTB=2*INTOXI(2)
ISN 0070         104 IF(NSTART.NE.1) GO TO 190
ISN 0072             IF(INTOXI(K)-INT) 600,190,500
ISN 0073         500 IF((NBA2-NBA1).LE.(40*INT)) GO TO 190
ISN 0075             IF(NDIFF(1).EQ.0.) GO TO 550
ISN 0077             NL=NBA1+16*INT
ISN 0078             NN=(NL-1+64)/64+64+1
ISN 0079             LN=NFINS
ISN 0080             IF(NDIFF(2).GT.0.) LN=NBA2-16*INT
ISN 0082             IF(NN.GT.LN) NN=LN
ISN 0084             SLOPE=(C(NL)-C(NN))/(R(NL)-R(NN))
ISN 0085             NL=(NL-1+INTB)/INTB+INTB+1
ISN 0086             IF(NL.EQ.NL) NL=NL+INTB
ISN 0088         505 NN=NN-INTB
ISN 0089             DO 510 L=NL,NN,INTB
ISN 0090         510 C(L)=C(NL)-SLOPE*(R(NL)-R(L))
ISN 0091             IF(NN+INTB.EQ.LN) GO TO 190
ISN 0093             NL=NN+INTB
ISN 0094         520 NN=NL+64
ISN 0095             IF(NN.GT.LN) NN=LN
ISN 0097             SLOPE=(C(NL)-C(NN))/(R(NL)-R(NN))
ISN 0098             NL=NL+INTB
ISN 0099             GO TO 505
ISN 0100         550 LN=NBA2-16*INT
ISN 0101             LL=NBA2-16*INTB
ISN 0102             NL=(LL-1)/64+64+1
ISN 0103             IF(NL.LT.1) NL=1
ISN 0105             GO TO 520
ISN 0106         600 INT=INTOXI(K)
ISN 0107             INT2=INT/2
ISN 0108             IF(K.EQ.2) GO TO 150
ISN 0110             IF(INT.GT.1) GO TO 105
ISN 0112             NL=2
ISN 0113             NN=NC(NOA(1)-1)-1
ISN 0114             DO 102 L=NL,NN,2
ISN 0115         102 C(L)=0.5*(C(L-1)+C(L+1))
```

```
ISN 0116            NL=NC(NOA(1)+1)+1
ISN 0117            NN=NC(NAB(1)-1)-1
ISN 0118            DO 103 L=NL,NN,2
ISN 0119        103 C(L)=0.5*(C(L-1)+C(L+1))
ISN 0120            GO TO 130
ISN 0121        105 NN=NC(NOA(1)-1)-INT
ISN 0122            DO 110 L= 1,NN,INT
ISN 0123        110 C(L+INT2)=0.5*(C(L)+C(L+INT))
ISN 0124            NL=NC(NOA(1)+1)
ISN 0125            NN=NC(NAB(1)-1)-INT
ISN 0126            DO 120 L=NL,NN,INT
ISN 0127        120 C(L+INT2)=0.5*(C(L)+C(L+INT))
ISN 0128        130 IF(NDIPP(2).GT.0.) GO TO 190
ISN 0130            NL=NC(NAB(1)+1)
ISN 0131            NN=NPTNE-INTB
ISN 0132            GO TO 159
ISN 0133        150 IF(NDIPP(1).GT.0.) GO TO 151
ISN 0135            NL=1
ISN 0136            GO TO 155
ISN 0137        151 NL=NC(NAB(1)+1)
ISN 0138        155 NN=NC(NAB(2)-1)-INTB
ISN 0139        159 DO 160 L=NL,NN,INTB
ISN 0140        160 C(L+INT )=0.5*(C(L)+C(L+INTB))
ISN 0141            IF(N.EQ.1) GO TO 190
ISN 0143            IF(INT.GT.1) GO TO 165
ISN 0145            NL=NC(NAB(2)+1)+1
ISN 0146            NN=NC(NOA(2)-1)-1
ISN 0147            DO 162 L=NL,NN,2
ISN 0148        162 C(L)=0.5*(C(L-1)+C(L+1))
ISN 0149            NL=NC(NOA(2)+1)+1
ISN 0150            NN=NPTNE-1
ISN 0151            DO 163 L=NL,NN,2
ISN 0153        163 C(L)=0.5*(C(L-1)+C(L+1))
ISN 0153            GO TO 190
ISN 0154        165 NL=NC(NAB(2)+1)
ISN 0155            NN=NC(NOA(2)-1)-INT
ISN 0156            DO 170 L=NL,NN,INT
ISN 0157        170 C(L+INT2)=0.5*(C(L)+C(L+INT))
ISN 0159            NL=NC(NOA(2)+1)
ISN 0159            NN=NPTNT-INT
ISN 0160            DO 180 L=NL,NN,INT
ISN 0161        180 C(L+INT2)=0.5*(C(L)+C(L+INT))
ISN 0162        190 CONTINUE
ISN 0163            IF(NDIPP(1).EQ.0.) GO TO 300
ISN 0165            IF(NSTART.NE.1) GO TO 200
ISN 0167            INTPOL=INTOXI(1)
ISN 0168            IF(INTPOL.GT.1) INTPOL=INTPOL/2
ISN 0170            NP=NOA1
ISN 0171            NA=NP+INTPOL
ISN 0172        210 IF(R(NA).LT.ROXID(1)) GO TO 220
ISN 0174            C(NA)=C(NP)-(R(NP)-R(NA))*(C(NP)-COA(1))/(R(NP)-ROXID(1))
ISN 0175            NA=NA+INTPOL
ISN 0176            GO TO 210
ISN 0177        220 NP=NAO1
ISN 0178            NA=NP-INTPOL
ISN 0179        230 IF(R(NA).GT.ROXID(1)) GO TO 200
ISN 0181            C(NA)=CAO(1)-(ROXID(1)-R(NA))*(CAO(1)-C(NP))/(ROXID(1)-R(NP))
ISN 0182            NA=NA-INTPOL
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ISN 0187          GO TO 250
ISN 0188       240 NP=NAB1
ISN 0189          NA=NP+INTPOL
ISN 0190       250 IF(R(NA).LT.RALPA(1)) GO TO 260
ISN 0191          C(NA)=C(NP)-(R(NP)-R(NA))*(C(NP)-CAB(1))/(R(NP)-RALPA(1))
ISN 0192          NA=NA+INTPOL
ISN 0193          GO TO 250
ISN 0194       260 NP=NBA1
ISN 0195          NA=NP-INTOXI(1)
ISN 0196       270 IF(R(NA).GT.RALPA(1)) GO TO 280
ISN 0197          C(NA)=CBA(1)-(RALPA(1)-R(NA))*(CBA(1)-C(NP))/(RALPA(1)-R(NP))
ISN 0198          NA=NA-INTOXI(1)
ISN 0199          GO TO 270
ISN 0200       280 NOXID1=NOXID(1)+1
ISN 0201          NALPA1=NALPA(1)+1
ISN 0202          NOA1=NOA(1)+1
ISN 0203          NAO1=NAO(1)+1
ISN 0204          NAB1=NAB(1)+1
ISN 0205          NBA1=NBA(1)+1
ISN 0206          IF(NOIPP(2).EQ.0.) GO TO 400
ISN 0207       300 IF(NSTART.NE.1) GO TO 380
ISN 0208          INTPOL=INTOXI(2)
ISN 0209          IF(INTPOL.GT.1) INTPOL=INTPOL/2
ISN 0210          NP=NOA2
ISN 0211          NA=NP-INTPOL
ISN 0212       310 IF(R(NA).GT.ROXID(2)) GO TO 320
ISN 0213          C(NA)=C(NP)-(R(NA)-R(NP))*(C(NP)-COA(2))/(ROXID(2)-R(NP))
ISN 0214          NA=NA-INTPOL
ISN 0215          GO TO 310
ISN 0216       320 NP=NAO2
ISN 0217          NA=NP+INTPOL
ISN 0218       330 IF(R(NA).LT.ROXID(2)) GO TO 340
ISN 0219          C(NA)=CAO(2)+(R(NA)-ROXID(2))*(CAO(2)-C(NP))/(ROXID(2)-R(NP))
ISN 0220          NA=NA+INTPOL
ISN 0221          GO TO 330
ISN 0222       340 NP=NAB2
ISN 0223          NA=NP-INTPOL
ISN 0224       350 IF(R(NA).GT.RALPA(2)) GO TO 360
ISN 0225          C(NA)=C(NP)-(R(NA)-R(NP))*(C(NP)-CAB(2))/(RALPA(2)-R(NP))
ISN 0226          NA=NA-INTPOL
ISN 0227          GO TO 350
ISN 0228       360 NP=NBA2
ISN 0229          NA=NP+INTOXI(2)
ISN 0230       370 IF(R(NA).LT.RALPA(2)) GO TO 380
ISN 0231          C(NA)=CBA(1)+(R(NA)-RALPA(2))*(CBA(2)-C(NP))/(RALPA(2)-R(NP))
ISN 0232          NA=NA+INTOXI(2)
ISN 0233          GO TO 370
ISN 0234       380 NOXID2=NPINP-NOXID(2)
ISN 0235          NALPA2=NPINP-NALPA(2)
ISN 0236          NOA2=NPINP-NOA(2)
ISN 0237          NAO2=NPINP-NAO(2)
ISN 0238          NAB2=NPINP-NAB(2)
ISN 0239          NBA2=NPINP-NBA(2)
ISN 0240       400 RETURN
ISN 0241          END
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ISN 0002          SUBROUTINE INTDIF
                C     IN INTDIF THE CONCENTRATIONS INTEGRATION IS PERFORMED
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004          COMMON/ZEONET/ R(1000),ROXID(2),RALPA(2),RALL,DOXID(2),DALPA(2),DR
ISN 0005          COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                 1,TSURF(2)
ISN 0006          COMMON/TEMTIM/ TCOOL(100,2),ZTCOOL(100,2),TRAD(100,2),ZTRAD(100,2)
ISN 0007          COMMON/HEAT  / NVER(100) ,NCOOL(2),ZRADIA(2),NHATPL(2),QFIXED(2),
                 1                        QSPLIT,NCAP(100) ,NSTEAM(2),NRADIA(2)
                 2                 ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0008          COMMON/HEADLN/ HTITLE(20)
ISN 0009          COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALDET(2),CBETA(2),
                 1               OXIGPL(2),NDIFF(2),CSTART,GAIN(2)
                 2,          OCAP(500),OVER(500),ODTMAX(500)
                 3,          COA(2),CAO(2),CAB(2),CBA(2)
                 4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010          COMMON/EXIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                 1,              NTEMP,NDIFF,NPRINT
ISN 0011          COMMON/MESH  /NGROSS,NPINE,NOXID(2),NOXI(2)
                 1,              NLOWB,NSTART,NALPA(2)
ISN 0012          COMMON/MESHTE/NT(100),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NGRS
ISN 0013          COMMON/MESHCO/NC(500),NBARER,NGRS,NOA(2),NAB(2)
                 1,              NOA(2),NAO(2),NAB(2),NBA(2),INTOXI(2),INTB
                 2,              NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                 3,              NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0014          COMMON/MATPRO/ DENZIR,DENZBO,OSTOCH,OXICON,DENPAT,FICFAC,OXHEAT
ISN 0015          COMMON/PROFIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OOXID(2),
                1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016          COMMON/MINPUT/ NDIFIN(100,2),TIMDIF(100,2),NCOEFF(100,2),
                 1               TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                 2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTNEW(100),
                 3               NDIFIN(2),NDIFIN(2),NQFLUX(2),NQFLUX(2),
                 4               NCOEFF(2),NCOEFF(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0017          DIMENSION CN(1000)
ISN 0018          DTN=DTDIFF
ISN 0019          IF(NDIFF(1).GT.0.) GO TO 1100
ISN 0021          NL=1
ISN 0022          OVER(1)=0.
ISN 0023          GO TO 1200
ISN 0024     1100 NL=2
ISN 0025          NN=NOA(1)-1
ISN 0026     1110 DO 1150 L=NL,NN
ISN 0027          ODTMAX(L)=OCAP(L)/(OVER(L)+OVER(L+1))
ISN 0028          IF(ODTMAX(L).LT.DTN) DTN=ODTMAX(L)
ISN 0030     1150 CONTINUE
ISN 0031          IF(NL.GT.2) GO TO 1160
ISN 0033          NL=NOA(1)+1
ISN 0034          NN=NAB(1)-1
ISN 0035          GO TO 1110
ISN 0036     1160 NL=NAB(1)+1
ISN 0037          IF(NDIFF(2).GT.0.) GO TO 1200
ISN 0039          IF(NN.EQ.NGRS)    GO TO 1300
ISN 0041          OVER(NGRS+1)=0.
ISN 0042          NN=NGRS
ISN 0043          GO TO 1110
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ISN 0044      1200 NN=NAB(2)-1
ISN 0045      1210 DO 1250 L=NL,NN
ISN 0046           OBTMAX(L)=OCAP(L)/(OVER(L)*OVER(L+1))
ISN 0047           IF(OBTMAX(L).LT.DTM) DTM=OBTMAX(L)
ISN 0049      1250 CONTINUE
ISN 0050           IF(NN.EQ.NGES-1) GO TO 1300
ISN 0052           IF(NN.EQ.NOA(2)-1) GO TO 1260
ISN 0054           NL=NAB(2)+1
ISN 0055           NN=NOA(2)-1
ISN 0056           GO TO 1210
ISN 0057      1260 NL=NOA(2)+1
ISN 0058           NN=NGES-1
ISN 0059           GO TO 1210
ISN 0060      1300 IF(DTM.NE.DTDIFF) GO TO 1320
ISN 0062           NMAX=1
ISN 0063           GO TO 1350
ISN 0064      1320 DTM=0.9*DTM
ISN 0065           NMAX=DTDIFF/DTM+1.
ISN 0066           XMAX=NMAX
ISN 0067           DTM=DTDIFF/XMAX
ISN 0068           IF(DTM.GT.0.     ) GO TO 1350
ISN 0070           WRITE(6,1234)
ISN 0071      1234 FORMAT(1HO,30HTIME STEP 0                              )
ISN 0072           WRITE(6,5151) NOA(1),NAB(1),NAB(2),NOA(2),NOA1,NAO1,NAB1,NBA1,
                  1   NBA2,NAB2,NAO2,NOA2,NGES,  (C(L),L=1,NGES)
ISN 0073      5151 FORMAT(1H ,20F5)
ISN 0074           WRITE(6,5252) (OVER(L),L=1,NGES),(OCAP(L),L=1,NGES),(C(NC(L)),L=1
                  1,NGES),(OBTMAX(L),L=1,NGES)
ISN 0075      5252 FORMAT(1H ,10D13.5)
ISN 0076           TMAX=TIME
ISN 0077           BR=BRN
ISN 0078      1350 IF(NDIFF(1).EQ.0.) GO TO 1370
ISN 0080           C(1)=C(NC(2))+NDIFF(1)*R(1)/OVER(2)
ISN 0081           IF(C(1).GT.OXICON) C(1)=OXICON
ISN 0083           OXIGPL(1)=(C(1)-C(NC(2)))*OVER(2)/P(1)
ISN 0084           OA1=(C(NOA1)-COA(1))*OVER(NOA(1))
ISN 0085           AO1=(CAO(1)-C(NAO1))*OVER(NOA(1)+1)
ISN 0086           AB1=(C(NAB1)-CAB(1))*OVER(NAB(1))
ISN 0087           BA1=(CBA(1)-C(NBA1))*OVER(NAB(1)+1)
ISN 0088      1370 IF(NDIFF(2).EQ.0.) GO TO 1390
ISN 0090           C(NPINE)=C(NC(NN))+NDIFF(2)*R(NPINE)/OVER(NGES)
ISN 0091           IF(C(NPINE).GT.OXICON) C(NPINE)=OXICON
ISN 0093           OXIGPL(2)=(C(NPINE)-C(NC(NGES-1)))*OVER(NGES)/R(NPINE)
ISN 0094           OA2=(C(NOA2)-COA(2))*OVER(NOA(2)+1)
ISN 0095           AO2=(CAO(2)-C(NAO2))*OVER(NOA(2))
ISN 0096           AB2=(C(NAB2)-CAB(2))*OVER(NAB(2)+1)
ISN 0097           BA2=(CBA(2)-C(NBA2))*OVER(NAB(2))
ISN 0098      1390 DO 2000 N=1,NMAX
ISN 0099           IF(NDIFF(1).GT.0.) GO TO 1400
ISN 0101           NL=2
ISN 0102           CN(1)=C(1)+OVER(2)*(C(NC(2))-C(1))*DTM/OCAP(1)
ISN 0103           GO TO 1500
ISN 0104      1400 NL=2
ISN 0105           NN=NOA(1)-2
ISN 0106           CN(NOA1)=C(NOA1)+(OVER(NOA(1)-1)*(C(NC(NOA(1)-2))-C(NOA1))-C(1)
                  1      *DTM/OCAP(NOA(1)-1)
ISN 0107      1410 IF(NL.GT.NN) GO TO 1450
ISN 0109           DO 1450 L=NL,NN
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ISN 0110            N=NC(L)
ISN 0111            CN(N)=C(N)+(OVER(L)*(C(NC(L-1))-C(N))
                   1          +OVER(L+1)*(C(NC(L+1))-C(N)))*DTN/OCAP(L)
ISN 0112         1450 CONTINUE
ISN 0113            IF(NL.GT.2) GO TO 1460
ISN 0114            NL=NOA(1)+2
ISN 0115            NN=NAB(1)-2
ISN 0116            CN(NAO1)=C(NAO1)+(AO1-OVER(NOA(1)+2)*(C(NAO1)-C(NC(NOA(1)+2))))
                   1          *DTN/OCAP(NOA(1)+1)
ISN 0117            CN(NAB1)=C(NAB1)+(OVER(NAB(1)-1)*(C(NC(NAB(1)-2))-C(NAB1))-AB1)
                   1          *DTN/OCAP(NAB(1)-1)
ISN 0118            GO TO 1410
ISN 0119         1460 NL=NAB(1)+2
ISN 0120            CN(NBA1)=C(NBA1)+(BA1-OVER(NAB(1)+2)*(C(NB.1)-C(NC(NAB(1)+2))))
                   1          *DTN/OCAP(NAB(1)+1)
ISN 0121            IF(NDIFF(2).GT.0.) GO TO 1500
ISN 0122            IF(NN.EQ.NOBS) GO TO 1600
ISN 0123            NN=NOBS
ISN 0124            OVER(NOBS+1)=0.
ISN 0125            NC(NOBS+1)=1
ISN 0126            GO TO 1410
ISN 0127         1500 NN=NAB(2)-2
ISN 0128            CN(NBA2)=C(NBA2)+(BA2-OVER(NAB(2)-1)*(C(NBA2)-C(NC(NAB(2)-2))))
                   1          *DTN/OCAP(NAB(2)-1)
ISN 0129         1510 IF(NL.GT.NN) GO TO 1555
ISN 0130            DO 1550 L=NL,NN
ISN 0131            N=NC(L)
ISN 0132            CN(N)=C(N)+(OVER(L)*(C(NC(L-1))-C(N))
                   1          +OVER(L+1)*(C(NC(L+1))-C(N)))*DTN/OCAP(L)
ISN 0133         1550 CONTINUE
ISN 0134         1555 IF(NN.EQ.NOBS-1) GO TO 1600
ISN 0135            IF(NN.EQ.NOA(2)-2) GO TO 1560
ISN 0136            NL=NAB(2)+2
ISN 0137            NN=NOA(2)-2
ISN 0138            CN(NAB2)=C(NAB2)+(OVER(NAB(2)+2)*(C(NC(NAB(2)+2))-C(NAB2))-AB2)
                   1          *DTN/OCAP(NAB(2)+1)
ISN 0139            CN(NAO2)=C(NAO2)+(AO2-OVER(NOA(2)-1)*(C(NAO2)-C(NC(NOA(2)-2))))
                   1          *DTN/OCAP(NOA(2)-1)
ISN 0140            GO TO 1510
ISN 0141         1560 NL=NOA(2)+2
ISN 0142            NN=NOBS-1
ISN 0143            CN(NOA2)=C(NOA2)+(OVER(NOA(2)+2)*(C(NC(NOA(2)+2))-C(NOA2))-OA2,
                   1          *DTN/OCAP(NOA(2)+1)
ISN 0144            GO TO 1510
ISN 0145         1600 NL=1
ISN 0146            NN=NOBS
ISN 0147            IF(NDIFF(1).NE.0.) NL=2
ISN 0148            IF(NDIFF(2).NE.0.) NN=NOBS-1
ISN 0149            DO 1700 L=NL,NN
ISN 0150            N=NC(L)
ISN 0151            C(N)=CN(N)
ISN 0152         1700 CONTINUE
ISN 0153         2000 CONTINUE
ISN 0154            RETURN
ISN 0155            END
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ISN 0002            SUBROUTINE OUTPUT
                C   OUTPUT PRINTS THE RESULTS IN SPECIFIED TIME STEPS
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 PLO
ISN 0005            COMMON/RESULT/PLO(25,200),NPLOT,MPLOT
ISN 0006            COMMON/GROWTH/ R(1000),ROXID(2),RALPA(2),RALL,DOXID(2),DALPA(2),DR
ISN 0007            COMMON/TEMP  / T(1000),TOXID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                   1,TSURF(2)
ISN 0008            COMMON/TEMTIM/ TCOOL(100,2),STCOOL(100,2),TRAD(100,2),STRAD(100,2)
ISN 0009            COMMON/HEAT  / HVER(100) ,HCOOL(2),ERADIA(2),HFATPL(2),QPIPED(2),
                   1                        QSPLIT,HCAP(100) ,HSTEAM(2),HRADIA(2)
                   2                ,QSURF(2),QCON(2),QRAD(2),QREACT(2)
ISN 0010            COMMON/HEADLN/ HTITLE(20)
ISN 0011            COMMON/CONCEN/ C(1000),COXID(2),COXAL(2),CALBET(2),CBETA(2),
                   1              QSIGPL(2),HDIFF(2),CSTART,GAIN(2)
                   2,          OCAP(500),OVER(500),OBETAX(500)
                   3,          COA(2),CAO(2),CAB(2),CBA(2)
                   4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0012            COMMON/...T  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                   1,             NTEMP,NDIFF,NPRINT
ISN 0013            COMMON/MESH  /NGROSS,NPINE,NOXID(2),NOXT(2)
                   1,             NLOWB,NSTART,NALPA(2)
ISN 0014            COMMON/NBSNTE/NT(100),NTCOOL(2),NTWALL(2),NTCOOL(2),NTWALL(2),NOES
ISN 0015            COMMON/NBSNCO/NC(500),NBANER,NOPS,NOA(2),NAB(2)
                   1,             NOA(2),NAO(2),NAB(2),NBA(2),INTOXT(2),TNTB
                   2,             NOA1,NAO1,NAB1,NBA1,NOXID1,NALPA1
                   3,             NOA2,NAO2,NAB2,NBA2,NOXID2,NALPA2
ISN 0016            COMMON/MATRNO/ DENSIA,DENSBO,OSTOCH,OSTCON,DENRAT,PICPAC,CONRAT
ISN 0017            COMMON/PROPIL/ CO(500),X(500),OLAYER(2),ALAYER(2),BLAYER,OGXID(2),
                   1OALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                   2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0018            COMMON/MINPUT/ NDIFIN(100,2),TINDIF(100,2),NCOEFF(100,2),
                   1              TCOEFF(100,2),NRADCO(100,2),TRADCO(100,2),
                   2              QPLUXI(100,2),TQPLUX(100,2),TTHETP(100),DTHETH(100),
                   3              NDIFIN(2),NDIFIN(2),NQPIDX(2),NQPLUX(2),
                   4              NCOEFF(2),NCOEFF(2),NRADCO(2),NRADCO(2),NSTEP
ISN 0019            CALL PREPAR
                C   THIS SUBROUTINE PREPARES THE RESULTS FOR PRINTING AND PLOTTING
ISN 0020            J=6
ISN 0021            WRITE(J,55) TIME,NUMBER
ISN 0022         55 FORMAT(1HO///// 17H    * * * * TIME = F9.3,4H * * * *,80X,
                   1       8HPLOT # = I9)
ISN 0023            WRITE(J,59)
ISN 0024         59 FORMAT(1HO// 5X,9HN.T.COEFF ,3X,10HSTEAM TEMP ,3X,10HPRESSIVITY ,
                   1       5X,8HRAD.WALL,3X,12HSURFACE TEMP ,2X,11HOX/RET TEMP ,3X,
                   2       12HPIN.HEATPLUX ,3X,12HCON.HFATPLUX, 3X,12HRAD.HFATPLUX ,
                   3       6X,9HQCON+QRAD )
ISN 0025            DO 62 M=1,2
ISN 0026            WRITE(J,60) HCOOL(M),TSTEAM(M),ERADIA(M),TWALL(M),TSURF(M),
                   1           TOXID(M),QPIPED(M),QCON(M),QRAD(M),HFATPL(M)
ISN 0027         60 FORMAT(1H ,10F13.5)
ISN 0028         62 CONTINUE
ISN 0029            WRITE(J,65)
ISN 0030         65 FORMAT(1HO,13H  O.PL.LIMIT ,2X,11HOXIDEN PLUX,3X,10HO.IN ORDER ,
                   1       3X,10HO.IN ALPHA ,6X,9HO.IN BETA ,3X,10HOXYG.TOTAL ,
                   2                          8X,9HOXYG.GAIN,
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     3       2X,11HOXIDE LAYER ,2X,11HALPHA LAYER ,1X,10HBETA LAYER    )
ISN 0031           NZ=0
ISN 0032           DO 75 N=1,2
ISN 0033           IF(NDIFF(N).EQ.0.) GO TO 75
ISN 0035           OXIGP=OXIDPL(N)*1000.
ISN 0036           NDIFFN=NDIFF(N)
ISN 0037           IF(N2) 66,66,67
ISN 0038        66 OBET=OBETA
ISN 0039           OTOT=OTOTAL
ISN 0040           BLAY=BLAYER
ISN 0041           GO TO 69
ISN 0042        67 OBET=0.
ISN 0043           OTOT=0.
ISN 0044           BLAY=0.
ISN 0045        69 WRITE(J,70) NDIFFN,OXIGP      ,OOXID(N),OALPA(N),OBET,OTOT,
                  1           OBAIN(N),OLAYER(N),BLAYER(N),BLAY
ISN 0046           N2=1
ISN 0047        70 FORMAT(1H ,10F13.4)
ISN 0048        75 CONTINUE
ISN 0049           IF((NLONG.GT.0).OR.(NBANDS.EQ.0)) GO TO 1000
ISN 0051           NA=-12
ISN 0052           NZ=0
ISN 0053        50 NA=NA+13
ISN 0054           NB=NZ+13
ISN 0055           IF(NZ.GT.NGRID) NB=NGRID
ISN 0057           WRITE(J,300) (XT(N),N=NA,NB)
ISN 0058       300 FORMAT(1H0,14HPOINT NUMBER =,13I9)
ISN 0059           WRITE(J,600) (X(XT(N)),N=NA,NB)
ISN 0060       600 FORMAT(1H ,14HDISTANCE     =,13F9.5)
ISN 0061           WRITE(J,400) (T(XT(N)),N=NA,NB)
ISN 0062       400 FORMAT(1H ,14HTEMPERATURE  =,13F9.2)
ISN 0063           IF(NB.LT.NGRID) GO TO 50
ISN 0065      1000 IF(NBANDS.GT.0) GO TO 5000
ISN 0067           IF(NDIFF(1).GT.0.) GO TO 1200
ISN 0069           NL=-12
ISN 0070           NN=0
ISN 0071           NAX=NAB(2)
ISN 0072           WRITE(J,6500)
ISN 0073      6500 FORMAT(1H0,10HBETA LAYER  )
ISN 0074      1100 NL=NL+13
ISN 0075           NN=NN+13
ISN 0076           IF(NN.GE.NAX) GO TO 2000
ISN 0078           IF(NAX-NN.EQ.1) NN=NN-1
ISN 0080           WRITE(J,300) (NC(N),N=NL,NN)
ISN 0081           WRITE(J,600) (X(N),N=NL,NN)
ISN 0082           WRITE(J,400) (T(NC(N)),N=NL,NN)
ISN 0083           WRITE(J,650) (CO(N),N=NL,NN)
ISN 0084           NL=NN-12
ISN 0085           GO TO 1100
ISN 0086      1200 NN=NOA(1)-1
ISN 0087           WRITE(J,2500)
ISN 0088      2500 FORMAT(1H0,20HOUTSIDE OXIDE LAYER   )
ISN 0089           WRITE(J,300) (NC(N),N=1,NN),NC(NOA(1))
ISN 0090           WRITE(J,600) (X(N),N=1,NN)
ISN 0091           WRITE(J,400) (T(NC(N)),N=1,NN),TOXID(1)
ISN 0092           WRITE(J,650) (CO(N),N=1,NN)
ISN 0093       650 FORMAT(1H ,14HCONCENTRATION=,13F9.5)
ISN 0094           NL=NOA(1)+1
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ISN 0095          WRITE(J,3000)
ISN 0096      3000 FORMAT(140,20HOUTSIDE ALPHA LAYER   )
ISN 0097          NA=N1+1
ISN 0098          IF(NL.LT.NAB(1)) GO TO 1210
ISN 0100          WRITE(J,300) NC(NOA(1)),NC(NAB(1))
ISN 0101          WRITE(J,600) X(NA),X(N2)
ISN 0102          WRITE(J,600) TOMIB(1),TALPA(1)
ISN 0103          WRITE(J,650) CO(NA),CO(N2)
ISN 0104          GO TO 1260
ISN 0105      1210 NN=NAB(1)-1
ISN 0106          WRITE(J,300) NC(NOA(1)),(NC(K),K=NL,NN),NC(NAB(1))
ISN 0107          WRITE(J,600) (X(K),K=NA,N2)
ISN 0108          WRITE(J,600) TOMIB(1),(T(NC(K)),K=NL,NN),TALPA(1)
ISN 0109          WRITE(J,650) (CO(K),K=NA,N2)
ISN 0110      1260 NL=NAB(1)+1
ISN 0111          NOP=NL+11
ISN 0112          NA=N2+1
ISN 0113          NE=NA+12
ISN 0114          MAX=1000
ISN 0115          IF(NDIFF(2).EQ.0.) GO TO 1300
ISN 0117          MAX=NAB(2)
ISN 0118          IF(NOP.GE.MAX) GO TO 1500
ISN 0120      1300 IF(NOP.GT.NGES) NOP=NGES
ISN 0122          IF(NE.GT.N3) NE=N3
ISN 0124          WRITE(J,6500)
ISN 0125          WRITE(J,300) NC(NAB(1)),(NC(K),K=NL,NOP)
ISN 0126          WRITE(J,600) (X(K),K=NA,NE)
ISN 0127          WRITE(J,600) TALPA(1),(T(NC(K)),K=NL,NOP)
ISN 0128          WRITE(J,650) (CO(K),K=NA,NE)
ISN 0129          IF(NOP.EQ.NGES) GO TO 5000
ISN 0131      1400 NL=NOP+1
ISN 0132          NOP=NL+12
ISN 0133          NA=NE+1
ISN 0134          NE=NA+12
ISN 0135          IF(NOP.GE.MAX) GO TO 2000
ISN 0137          IF(NOP.GT.NGES) NOP=NGES
ISN 0139          IF(NE.GT.N3) NE=N3
ISN 0141          WRITE(J,6500)
ISN 0142          WRITE(J,300) (NC(K),K=NL,NOP)
ISN 0143          WRITE(J,600) (X(K),K=NA,NE)
ISN 0144          WRITE(J,600) (T(NC(K)),K=NL,NOP)
ISN 0145          WRITE(J,650) (CO(K),K=NA,NE)
ISN 0146          IF(NOP.EQ.NGES) GO TO 5000
ISN 0148          GO TO 1400
ISN 0149      1500 NL=NAB(1)+1
ISN 0150          NN=NAB(2)-1
ISN 0151          NA=N2+1
ISN 0152          WRITE(J,6500)
ISN 0153          WRITE(J,300) NC(NAB(1)),(NC(K),K=NL,NN),NC(NAB(2))
ISN 0154          WRITE(J,600) (X(K),K=NA,NE)
ISN 0155          WRITE(J,600) TALPA(1),(T(NC(K)),K=NL,NN),TALPA(2)
ISN 0156          WRITE(J,650) (CO(K),K=NA,N3)
ISN 0157          GO TO 3200
ISN 0158      2000 NN=MAX-1
ISN 0159          IF(NDIFF(1)) 2050,2050,2100
ISN 0160      2050 NA=NL
ISN 0161          NE=N1
ISN 0162          GO TO 2150
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ISN 0163      2100 N2=N3
ISN 0164      2150 WRITE(J,4500)
ISN 0165           WRITE(J,900) (NC(K),K=NL,NN),NC(NAB(2))
ISN 0166           WRITE(J,400) (X(K),K=NA,NE)
ISN 0167           WRITE(J,400) (T(NC(K)),K=NL,NN),TALPA(2)
ISN 0168           WRITE(J,450) (CO(K),K=NA,NE)
ISN 0169      2200 NL=NAB(2)+1
ISN 0170           IF(NDIPP(1)) 2002,2002,2003
ISN 0171      2002 NA=N1+1
ISN 0172           NE=N2
ISN 0173           GO TO 2005
ISN 0174      2003 NA=N3+1
ISN 0175           NE=N4
ISN 0176      2005 WRITE(J,4000)
ISN 0177      4000 FORMAT(1H0,20HINSIDE ALPHA LAYER     )
ISN 0178           IF(NL.LT.NOA(2)) GO TO 2210
ISN 0180           WRITE(J,900) NC(NAB(2)),NC(NOA(2))
ISN 0181           WRITE(J,400) X(NA),X(NE)
ISN 0182           WRITE(J,400) TALPA(2),TOXID(2)
ISN 0183           WRITE(J,450) CO(NA),CO(NE)
ISN 0184           GO TO 2222
ISN 0185      2210 NN=NOA(2)-1
ISN 0186           WRITE(J,900) NC(NAB(2)),(NC(K),K=NL,NN),NC(NOA(2))
ISN 0187           WRITE(J,400) (X(K),K=NA,NE)
ISN 0188           WRITE(J,400) TALPA(2),(T(NC(K)),K=NL,NN),TOXID(2)
ISN 0189           WRITE(J,450) (CO(K),K=NA,NE)
ISN 0190      2222 NL=NOA(2)+1
ISN 0191           IF(NDIPP(1)) 2250,2250,2260
ISN 0192      2250 NA=N2+1
ISN 0193           NE=N3
ISN 0194           GO TO 2300
ISN 0195      2260 NA=N4+1
ISN 0196           NE=N5
ISN 0197      2300 WRITE(J,3500)
ISN 0198      3500 FORMAT(1H0,20HINSIDE OXIDE LAYER     )
ISN 0199           WRITE(J,900) NC(NOA(2)),(NC(K),K=NL,NGTS)
ISN 0200           WRITE(J,400) (X(K),K=NA,NE)
ISN 0201           WRITE(J,400) TOXID(2),(T(NC(K)),K=NL,NGTS)
ISN 0202           WRITE(J,450) (CO(K),K=NA,NE)
ISN 0203      4000 IF(NPLOT.EQ.0) RETURN
                C     NPLOT > 0;  PLOTS OF VARIABLES AS FUNCTION OF TIME HAVE TO BE MADE
ISN 0205           NPLOT=NPLOT+1
ISN 0204           PLO(10,NPLOT)=0.
ISN 0207           PLO(20,NPLOT)=0.
ISN 0208           PLO( 1,NPLOT)=SNGL(TIME)
ISN 0209           PLO( 2,NPLOT)=SQRT(PLO(1,NPLOT))
ISN 0210           PLO( 3,NPLOT)=SNGL(TSTEAN(1))
ISN 0211           PLO(13,NPLOT)=SNGL(TSTEAN(2))
ISN 0212           PLO(14,NPLOT)=SNGL(TWALL(2))
ISN 0213           PLO(15,NPLOT)=SNGL(TSURF(2))
ISN 0214           PLO( 4,NPLOT)=SNGL(TWALL(1))
ISN 0215           PLO( 5,NPLOT)=SNGL(TSURF(1))
ISN 0216           PLO( 6,NPLOT)=SNGL(QLAYER(1))
ISN 0217           PLO( 7,NPLOT)=SNGL(ALAYER(1))
ISN 0218           PLO( 8,NPLOT)=PLO( 6,NPLOT)+PLO( 7,NPLOT)
ISN 0219           PLO( 9,NPLOT)=PLO( 6,NPLOT)/PLO( 8,NPLOT)
ISN 0220           PLO(10,NPLOT)=SNGL(QGAIN(1))
ISN 0221           PLO(11,NPLOT)=PLO( 8,NPLOT)**2
```

```
ISN 0222            PLO(12,KPLOT)=PLO(10,KPLOT)**2
ISN 0223            PLO(16,KPLOT)=SNGL(OLAYER(2))
ISN 0224            PLO(17,KPLOT)=SNGL(ALAYER(2))
ISN 0225            PLO(18,KPLOT)=PLO(16,KPLOT)*PLO(17,KPLOT)
ISN 0226            PLO(19,KPLOT)=PLO(16,KPLOT)/PLO(18,KPLOT)
ISN 0227            PLO(20,KPLOT)=SNGL(OMAIN(2))
ISN 0228            PLO(21,KPLOT)=PLO(18,KPLOT)**2
ISN 0229            PLO(22,KPLOT)=PLO(20,KPLOT)**2
ISN 0230            PLO(23,KPLOT)=PLO(20,KPLOT)*PLO(10,KPLOT)
ISN 0231            CDAVRG=.001*OBETA/(BALPA(1)**2-PALPA(2)**2)*2.*R(1)
ISN 0232            PLO(24,KPLOT)=CDAVRG
ISN 0233            PSUBW=0.0001*BLAYER/WALL
ISN 0234            PLO(25,KPLOT)=PSUBW
ISN 0235            RETURN
ISN 0236            END
```

```
ISN 0002          SUBROUTINE PREPAR
                C     THE RESULTS ARE PREPARED FOR PRINTING AND PLOTING
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004          COMMON/UBOUND/ B(1000),BOUID(2),BALPA(2),WALL,BOUID(2),DALPA(2),DR
ISN 0005          COMMON/TEMP  / T(1000),TOUID(2),TALPA(2),TSTART,TSTEAM(2),TWALL(2)
                 1,TSURF(2)
ISN 0006          COMMON/TEMTIM/ TCOOL(100,2),ITCOOL(100,2),TRAD(100,2),ITRAD(100,2)
ISN 0007          COMMON/HEAT  / HVER(100)  ,HCOOL(2),HRADIA(2),HEATPL(2),QPIPED(2),
                 1                          QSPLIT,HCAP(100)  ,HSTEAM(2),HRADIA(2)
                 2              ,QSURF(2),QCOND(2),QRAD(2),QREACT(2)
ISN 0008          COMMON/HEADLN/ HTITLE(20)
ISN 0009          COMMON/CONCEN/ C(1000),COUID(2),COEAL(2),CALDET(2),CBETA(2),
                 1               OXIGPL(2),HDIFF(2),CSTART,GAIN(2)
                 2,          OCAP(500),OVER(500),OBTMAX(500)
                 3,          COA(2),CAO(2),CAB(2),CBA(2)
                 4,          OCAPOA(2),OCAPAO(2),OCAPAB(2),OCAPBA(2)
ISN 0010          COMMON/UNIT  / TIME,TMAX,DTTEMP,DTDIFF,DTPRIN,DTMAX(100)
                 1,              HTEMP,HDIFF,HPRINT
ISN 0011          COMMON/MESH  /MGROSS,MPINE,MOUID(2),MOUI(2)
                 1,             MLOWS,MSTART,MALPA(2)
ISN 0012          COMMON/MESPTR/MT(100),MTCOOL(2),MTWALL(2),MTCOOL(2),MTWALL(2),MGRS
ISN 0013          COMMON/MESHCO/MC(500),MBANDR,MGRS,MOA(2),MAB(2)
                 1,              MOA(2),MAO(2),MAB(2),MBA(2),IMTOXI(2),IMTB
                 2,              MOA1,MAO1,MAB1,MBA1,MOXID1,MALPA1
                 3,              MOA2,MAO2,MAB2,MBA2,MOXID2,MALPA2
ISN 0014          COMMON/HATPRO/ DENSIB,DENSBO,OSTOCH,OHTCON,DENHAT,PICFAC,OMHEAT
ISN 0015          COMMON/PROFIL/ CO(500),H(500),OLAYER(2),ALAYER(2),BLAYER,OCHID(2),
                10ALPA(2),OGAIN(2),OBETA,OTOTAL,OBETAS,STEMP,
                2N1,N2,N3,N4,N5,NUMBER,NSCALE
ISN 0016          COMMON/MINPUT/ HDIFIN(100,2),TIMDIF(100,2),HCOEFF(100,2),
                 1               TCOEFF(100,2),HRADCO(100,2),TRADCO(100,2),
                 2               QFLUXI(100,2),TQFLUX(100,2),TIMSTP(100),DTMAX(100),
                 3               HDIFIN(2),HDIFIN(2),HQFLUX(2),HQFLUX(2),
                 4               HCOEFF(2),HCOEFF(2),HRADCO(2),HRADCO(2),HSTEP
ISN 0017          HEFRAD=H(1)
ISN 0018          IF(HDIFF(1).EQ.0.) HEFRAD=H(MPINE)
ISN 0020          IF(HRADER.GT.0) GO TO 50
ISN 0022          IF(HSTART.EQ.1) GO TO 5
ISN 0024          IF(HDIFF(1).GT.0.)GO TO 1
ISN 0026          OBETA=C(1)*DH*H(1)
ISN 0027          HL=3
ISN 0028          GO TO 2
ISN 0029        1 OOXID(1)=.5*(C(1)+COA(1))*BOUID(1)
                 1          +.5*(B(1)+BOXID(1))/HEFRAD
ISN 0030          OALPA(1)=.5*(CAO(1)+CAB(1))*(BALPA(1)-BOUID(1))
                 1          +.5*(BALPA(1)+BOXID(1))/HEFRAD
ISN 0031          HL=MC(4)+2
ISN 0032          HDIFF=BALPA(1)-H(MC(4))
ISN 0033          HHEAN=.5*(BALPA(1)+H(MC(4)))
ISN 0034          OBETA=.5*(CBA(1)+C(MC(4)))*HDIFF*HHEAN
                 1       +(0.75*C(MC(4))+0.25*C(HL))*DH*H(HL-1)
ISN 0035          IF(HDIFF(2).GT.0.) GO TO 3
ISN 0037          OBETA=OBETA+C(MPINE)*DH*H(MPINE)
ISN 0038          HH=MPINE-2
ISN 0039          GO TO 3
ISN 0040        2 HH=MC(MGRS-4)
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```
ISN 0041            OOXID(2)=.5*(C(NPINB)+COA(2))*DOXID(2)
                   1            *(R(NPINB)+.5*DOXID(2))/REFRAD
ISN 0042            OALFA(2)=.5*(CAO(2)+CAB(2))*(DALFA(2)-DOXID(2))
                   1            *.5*(DALFA(2)+DOXID(2))/REFRAD
ISN 0043            RDIFF=R(NC(NGES-3))-RALFA(2)
ISN 0044            RMEAN=.5*(R(NC(NGES-3))+RALFA(2))
ISN 0045            OBETA=OBETA+.5*(CBA(2)+C(NC(NGES-3)))*RDIFF*RMEAN
                   1         +(0.75*C(NN+2)+0.25*C(NN))*DR*R(NN+1)
ISN 0046          3 DO 4 N=NL,NN,2
ISN 0047          4 OBETA=OBETA+2.*DR*C(N)*R(N)
ISN 0048            GO TO 15
ISN 0049          5 IF(NDIFF(1).GT.0.) GO TO 6
ISN 0051            NLBETA=1
ISN 0052            OBETA=0.
ISN 0053            GO TO 10
ISN 0054          6 OOXID(1)=.5*(C(NOA1)+COA(1))*OCAPOA(1)
ISN 0055            NL=1
ISN 0056            NN=NOA(1)-1
ISN 0057            DO 7 N=NL,NN
ISN 0058          7 OOXID(1)=OOXID(1)+OCAP(N)*C(NC(N))
ISN 0059            OOXID(1)=OOXID(1)/REFRAD
ISN 0060            OALFA(1)=.5*(C(NAO1)+CAO(1))*OCAPAO(1)+
                   1            .5*(C(NAB1)+CAB(1))*OCAPAB(1)
ISN 0061            NL=NOA(1)+1
ISN 0062            NN=NAB(1)-1
ISN 0063            DO 8 N=NL,NN
ISN 0064          8 OALFA(1)=OALFA(1)+OCAP(N)*C(NC(N))
ISN 0065            OALFA(1)=OALFA(1)/REFRAD
ISN 0066            NLBETA=NAB(1)+2
ISN 0067            NNBETA=NGES
ISN 0068            OBETA=0.5*(CBA(1)+C(NBA1))*OCAPBA(1)
                   1         +OCAP(NAB(1)+1)*(0.75*C(NBA1)+0.25*C(NC(NAB(1)+2)))
ISN 0069            IF(NDIFF(2).EQ.0.) GO TO 13
ISN 0071         10 OOXID(2)=.5*(C(NOA2)+COA(2))*OCAPOA(2)
ISN 0072            NL=NOA(2)+1
ISN 0073            NN=NGES
ISN 0074            DO 11 N=NL,NN
ISN 0075         11 OOXID(2)=OOXID(2)+OCAP(N)*C(NC(N))
ISN 0076            OOXID(2)=OOXID(2)/REFRAD
ISN 0077            OALFA(2)=.5*(C(NAO2)+CAO(2))*OCAPAO(2)+
                   1            .5*(C(NAB2)+CAB(2))*OCAPAB(2)
ISN 0078            NL=NAB(2)+1
ISN 0079            NN=NOA(2)-1
ISN 0080            DO 12 N=NL,NN
ISN 0081         12 OALFA(2)=OALFA(2)+OCAP(N)*C(NC(N))
ISN 0082            OALFA(2)=OALFA(2)/REFRAD
ISN 0083            NNBETA=NAB(2)-2
ISN 0084            OBETA=0.5*(CBA(2)+C(NBA2))*OCAPBA(2)+OBETA
                   1         +OCAP(NAB(2)-1)*(0.75*C(NBA2)+0.25*C(NC(NAB(2)-2)))
ISN 0085         13 DO 14 N=NLBETA,NNBETA
ISN 0086         14 OBETA=OBETA+OCAP(N)*C(NC(N))
ISN 0087         15 OBETA=OBETA/REFRAD
ISN 0088            OTOTAL=0.
ISN 0089            IF(NDIFF(1).GT.0.) GO TO 25
ISN 0091            BLAYER=R(1)-RALFA(2)
ISN 0092            XOUT=R(1)
ISN 0093            NN=NAB(2)-1
ISN 0094            DO 18 N=1,NN
```

```
ISN 0095            M=MC(N)
ISN 0096            CO(N)=C(M)
ISN 0097         18 X(N)=XOUT-X(M)
ISN 0098            N1=NAB(2)
ISN 0099            X(N1)=BLAYER
ISN 0100            CO(N1)=CBA(2)
ISN 0101            X(N1+1)=BLAYER
ISN 0102            CO(N1+1)=CAB(2)
ISN 0103            NL=NAB(2)+1
ISN 0104            NN=NOA(2)-1
ISN 0105            DO 19 N=NL,NN
ISN 0106            M=MC(N)
ISN 0107            CO(N+1)=C(M)
ISN 0108         19 X(N+1)=XOUT-R(M)
ISN 0109            N2=NOA(2)+1
ISN 0110            CO(N2)=CAO(2)
ISN 0111            X(N2)=BOUT-BOXID(2)
ISN 0112            ALAYER(2)=BALFA(2)-BOXID(2)
ISN 0113            X(N2+1)=X(N2)
ISN 0114            CO(N2+1)=COA(2)/PICPAC
ISN 0115            NL=NOA(2)+1
ISN 0116            NN=NGES
ISN 0117            N3=NGES+2
ISN 0118            XOUT=R(1)+BOXID(2)*(PICPAC-1)
ISN 0119            DO 20 N=NL,NN
ISN 0120            M=MC(N)
ISN 0121            CO(N+2)=C(M)/PICPAC
ISN 0122         20 X(N+2)=XOUT-R(M)*PICPAC
ISN 0123            OLAYER(2)=BOXID(2)*PICPAC
ISN 0124            OTOTAL=OOXID(2)+OALFA(2)+OBETA
ISN 0125            OGAIN(2)=GAIN(2)
ISN 0126            GO TO 60
ISN 0127         25 NN=NOA(1)-1
ISN 0128            OLAYER(1)=BOXID(1)*PICPAC
ISN 0129            XOUT=R(1)+BOXID(1)*(PICPAC-1.)
ISN 0130            DO 26 N=1,NN
ISN 0131            M=MC(N)
ISN 0132            CO(N)=C(M)/PICPAC
ISN 0133         26 X(N)=XOUT-R(M)*PICPAC
ISN 0134            N1=NOA(1)
ISN 0135            X(N1)=BOXID(1)
ISN 0136            CO(N1)=COA(1)/PICPAC
ISN 0137            X(N1+1)=BOXID(1)
ISN 0138            CO(N1+1)=CAO(1)
ISN 0139            ALAYER(1)=BOXID(1)-BALFA(1)
ISN 0140            BLAYER=BALFA(1)-R(NPINS)
ISN 0141            XOUT=R(1)
ISN 0142            NL=NOA(1)+1
ISN 0143            NN=NAB(1)-1
ISN 0144            DO 27 N=NL,NN
ISN 0145            M=MC(N)
ISN 0146            CO(N+1)=C(M)
ISN 0147         27 X(N+1)=XOUT-R(M)
ISN 0148            N2=NAB(1)+1
ISN 0149            X(N2)=BALFA(1)
ISN 0150            CO(N2)=CAB(1)
ISN 0151            X(N2+1)=X(N2)
ISN 0152            CO(N2+1)=CBA(1)
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```
ISN 0153            NL=NAB(1)+1
ISN 0154            IF(NDIPP(2)) 28,28,29
ISN 0155         28 N3=NGES+2
ISN 0156            NN=NGES
ISN 0157            GO TO 30
ISN 0158         29 N3=NAB(2)+2
ISN 0159            NN=NAB(2)-1
ISN 0160            X(N3)=R(1)-RALPA(2)
ISN 0161            BLAYER=RALPA(1)-RALPA(2)
ISN 0162            CO(N3)=CBA(2)
ISN 0163         30 DO 31 N=NL,NN
ISN 0164            N=NC(N)
ISN 0165            CO(N+2)=C(N)
ISN 0166         31 X(N+2)=R(1)-R(N)
ISN 0167            OTOTAL=OOXID(1)+OALPA(1)+OBETA
ISN 0168            OGAIN(1)=GAIN(1)
ISN 0169            IF(NDIPP(2).EQ.0.) GO TO 40
ISN 0170            X(N3+1)=X(N3)
ISN 0171            CO(N3+1)=CAB(2)
ISN 0172            N4=NOA(2)+3
ISN 0173            NL=NAB(2)+1
ISN 0174            NN=NOA(2)-1
ISN 0175            DO 33 N=NL,NN
ISN 0176            N=NC(N)
ISN 0177            X(N+3)=R(1)-R(N)
ISN 0178         33 CO(N+3)=C(N)
ISN 0179            X(N4)=R(1)-ROXID(2)
ISN 0180            CO(N4)=CAO(2)
ISN 0181            X(N4+1)=X(N4)
ISN 0182            CO(N4+1)=COA(2)/PICPAC
ISN 0183            XOUT=R(1)+ROXID(2)*(PICPAC-1)
ISN 0184            NL=NOA(2)+1
ISN 0185            NN=NGES
ISN 0186            N5=NGES+4
ISN 0187            DO 34 N=NL,NN
ISN 0188            N=NC(N)
ISN 0189            X(N+4)=XOUT-R(N)*PICPAC
ISN 0190         34 CO(N+4)=C(N)/PICPAC
ISN 0191            ALAYER(2)=PALPA(2)-ROXID(2)
ISN 0192            OLAYER(2)=ROXID(2)*PICPAC
ISN 0193            OTOTAL=OTOTAL+OALPA(2)+OOXID(2)
ISN 0194            OGAIN(2)=GAIN(2)*R(NPINE)/R(1)
ISN 0195         40 CONTINUE
ISN 0196            GO TO 200
ISN 0197         50 OBETA=0.5*(ROXID(1)**2-ROXID(2)**2)*CSTART/REFRAD
ISN 0198            BLAYER=ROXID(1)-ROXID(2)
ISN 0199            ALAYER(1)=0.
ISN 0200            ALAYER(2)=0.
ISN 0201            OTOTAL=OBETA
ISN 0202            IF(NDIPP(1).EQ.0.) GO TO 100
ISN 0203            OOXID(1)=.5*(R(1)**2-ROXID(1)**2)*OXICON/REFRAD
ISN 0204            OTOTAL=OBETA+OOXID(1)
ISN 0205            OGAIN(1)=GAIN(1)
ISN 0206            OLAYER(1)=ROXID(1)*PICPAC
ISN 0207            IF(NDIPP(2).EQ.0.) GO TO 200
ISN 0208        100 OOXID(2)=.5*(ROXID(2)**2-R(NPINE)**2)*OXICON/REFRAD
ISN 0209            OTOTAL=OTOTAL+OOXID(2)
ISN 0210            OGAIN(2)=GAIN(2)
```

```
ISN 0214          OLAYER(2)=DOXID(2)*FICFAC
ISN 0215      200 DO 300 K=1,2
ISN 0216          IF(HDIFF(K).EQ.0.) GO TO 300
ISN 0218          OLAYER(K)=OLAYER(K)*10000.
ISN 0219          ALAYER(K)=ALAYER(K)*10000.
ISN 0220          OOXID(K)=OOXID(K)*1000.
ISN 0221          OALFA(K)=OALFA(K)*1000.
ISN 0222          OGAIN(K)=OGAIN(K)*1000.
ISN 0223      300 CONTINUE
ISN 0224          BLAYER=BLAYER*10000.
ISN 0225          OBETA=OBETA*1000.
ISN 0226          OTOTAL=OTOTAL*1000.
ISN 0227          IF(NSTART.EQ.0) OBETAS=OTOTAL
ISN 0229          RETURN
ISN 0230          END
```

```
ISN 0002          FUNCTION TIMFUN(I,F,Z,K,TIME)
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004          DIMENSION F(100,2),Z(100,2)
ISN 0005          IF(Z(1,K).NE.0.) GO TO 5
ISN 0007        1 IF(Z(I,K).GT.TIME) GO TO 2
ISN 0009          I=I+1
ISN 0010          GO TO 1
ISN 0011        2 IF(Z(I-1,K).LE.TIME) GO TO 3
ISN 0013          I=I-1
ISN 0014          GO TO 2
ISN 0015        3 U=(TIME-Z(I-1,K))/(Z(I,K)-Z(I-1,K))
ISN 0016          TIMFUN=F(I-1,K)+U*(F(I,K)-F(I-1,K))
ISN 0017          RETURN
ISN 0018        5 WRITE(6,10) K
ISN 0019       10 FORMAT(1H0,50HFIRST TIME IN FUNCTION-TIME-PAIRS FOR SURFACE NR   ,
                 1I3,19H  NOT EQUAL 0.     )
ISN 0020          WRITE(6,20)
ISN 0021       20 FORMAT(1H ,10HFUNCTION =    )
ISN 0022          WRITE(6,30) (F(L,K),L=1,10)
ISN 0023       30 FORMAT(1H ,10X,10D12.4)
ISN 0024          WRITE(6,40)
ISN 0025       40 FORMAT(1H ,10HTIME     =        )
ISN 0026          WRITE(6,30) (Z(L,K),L=1,10)
ISN 0027          TIME=1.D6
ISN 0028          RETURN
ISN 0029          END
```

```
ISN 0002            FUNCTION DIFCON(T1,T2,C1,C2,K)
                C   DIFFUSION CONSTANT ( CM**2/SEC)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/MATPRO/ DENZIR,DENZRO,OSTOCN,OXICON,DENRAT,FICFAC
ISN 0005            TN=0.5*(T1+T2)+273.16
ISN 0006            IF(TN.GT.2125.) TN=2125.
ISN 0008            R=1.987
ISN 0009            RTN=R*TN
ISN 0010            CN=.5*(C1+C2)
ISN 0011            GO TO (1,2,3),K
ISN 0012          1 DIFCON=0.0711*DEXP(-33600./RTN)
ISN 0013            DIFCON=DIFCON/FICFAC**2
                C   DIFCON=FICFAC**2 * DIF.CONST.OF ZRO2
ISN 0014            RETURN
ISN 0015          2 DIFCON=5.2000*DEXP(-50800./RTN)
                C   DIFCON = DIF.CONST.OF ALPHA ZIRCALOY
ISN 0016            RETURN
ISN 0017          3 DIFCON=0.0453*DEXP(-28200./RTN)
                C   DIFCON = DIF.CONST.OF BETA  ZIRCALOY
ISN 0018            RETURN
ISN 0019            END
```

```
ISN 0002            SUBROUTINE INTPAC(T,CH,CL,K)
                C   EQUILBRIUM CONCENTRATION AT THE INTERFACES (GRAM OXYGEN/CM**3)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/MATPRO/ DENSIR,DENSMO,OSTOCH,OXICON,DENRAT,PICPAC
ISN 0005            TK=T+273.16
ISN 0006            IF(TK.GT.2125.) TK=2125.
ISN 0007            GO TO (1,2),K
ISN 0008          1 CH=1.517-7.5D-5*TK
ISN 0010            CH=CH*PICPAC
                C   CH/PICPAC = CONCENTRATION AT OXIDE/ALPHA INTERFACE
ISN 0011            CL=0.0699*DENSIR
                C   CL = CONCENTRATION AT ALPHA/OXIDE INTERFACE
ISN 0012            RETURN
ISN 0013          2 IF(TK.LT.1123.16) TK=1123.16
ISN 0014            CH=(-0.127302+TK*1.5931D-4-TK**2*3.6618D-8)*DENSIR
                C   CH = CONCENTRATION AT ALPHA/BETA  INTERFACE
ISN 0016            IF(TK-1273.16) 3,3,4
ISN 0017          3 CL=(-0.0149344+1.3833D-5*TK)*DENSIR
                C   CL = CONCENTRATION AT BETA/ALPHA  INTERFACE
ISN 0018            RETURN
ISN 0019          4 CL=0.828263*DEXP(-14495.2/(1.987*TK))*DENSIR
                C   CL = CONCENTRATION AT BETA/ALPHA  INTERFACE
ISN 0020            RETURN
ISN 0021            END
```

```
ISN 0002            FUNCTION SPEC(T,K)
                C   VOL.SPEC.HEAT (MSEC/(CM**3*C))
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/MATPRO/ DENZIR,DENH2O,OSTOCM,OXICON,DENMAT,FICFAC
ISN 0005            TK=T+273.16
ISN 0006            IF(TK.GT.2125.) TK=2125.
ISN 0008            GO TO (1,2),K
ISN 0009          1 SPEC=0.549+TK*6.7D-5
ISN 0010            SPFC=SPEC*DENH2O*FICFAC
                C   SPEC./FICFAC = SPEC.HEAT OF ZRO2
ISN 0011            RETURN
ISN 0012          2 IF(TK-1000.) 3,3,4
ISN 0013          3 SPEC=.2409+1.68D-4*TK-4.36D-8*TK**2
                C   SPEC = SPEC.HEAT OF ZIRCALOY
ISN 0014            GO TO 5
ISN 0015          4 SPEC=.3653
ISN 0016            IF((TK.GT.1123.16).AND.(TK.LT.1223.16))
                   1SPEC=.3653+0.6595*DSIN(3.14159*(TK-1123.16)/100.)
ISN 0018          5 SPEC=SPEC*DENZIR
                C   SPEC = SPEC.HEAT OF ZIRCALOY
ISN 0019            RETURN
ISN 0020            END
```

```
ISN 0002            FUNCTION CONDUC(T1,T2,K)
                C   THERMAL CONDUCTIVITY (W/(CM*C))
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            COMMON/MATPRO/ DENZIR,DENZRO,OXTOCH,CRICON,DENPAT,PICPAC
ISN 0005            TK=.5*(T1+T2)+273.16
ISN 0006            IF(TK.GT.2125.) TK=2125.
ISN 0008            GO TO (1,2),K
ISN 0009          1 CONDUC=0.02
ISN 0010            CONDUC=CONPAC/PICPAC
                C   CONDUC*PICPAC = CONDUCT.OF ZRO2
ISN 0011            RETURN
ISN 0012          2 CONDUC=-0.0076+TK**2.75D-6
                C   CONDUC = CONDUCT.OF ZIRCALOY
ISN 0013            RETURN
ISN 0014            END
```

```
ISN 0002            SUBROUTINE TRAPLO
                C   INPUT DATA FOR PLOTS OF VARIABLES AS FUNCTIONS OF TIME ARE READ
                C   AND THE PLOTTING ROUTINE DATPLO IS CALLED
ISN 0003            COMMON/RESULT/PLO(25,200),KPLOT,NPLOT
ISN 0004            COMMON/DATAP/CD(5,200),DYN(4),DYS(4),DXN,DXS,HA(20),NPTT(4)
ISN 0005            COMMON/HEADLR/ HTITLE(20)
ISN 0006            DIMENSION NPLOTT(4)
ISN 0007            DO 75 K=1,KPLOT
ISN 0008            READ(5,500) NPLOTX,DXN,DXS,NVAR,IPLOT,Y00,(HTITLE(K),K=16,20)
ISN 0009          500 FORMAT(I10,2E10.4,2I10,E10.4,5A8)
ISN 0010            KA=1
ISN 0011            KE=5
ISN 0012            DO 10 L=1,NVAR
ISN 0013            READ(5,600)  NPLOTT(L),DYN(L),DYS(L),NPTT(L),(HA(K),K=KA,KE)
ISN 0014          600 FORMAT(I10,2E10.4,I10,20X,5A4)
ISN 0015            KA=KE+1
ISN 0016            KE=KA+4
ISN 0017           10 CONTINUE
ISN 0018            DO 50 I=1,KPLOT
ISN 0019            CD(5,I)=PLO(NPLOTX,I)
ISN 0020            DO 50 L=1,NVAR
ISN 0021            CD(L,I)=PLO(NPLOTT(L),I)
ISN 0022           50 CONTINUE
ISN 0023            IP(((IPLOT/2)*2).EQ.IPLOT) GO TO 71
ISN 0025            NHEAD=5*NVAR
ISN 0026            WRITE(6,700) (HTITLE(K),K=1,20),(HA(K),K=1,NHEAD)
ISN 0027          700 FORMAT(1H1,10X,20A4/1H0,9X,6HABSCISSA,8X,20A4)
ISN 0028            DO 70 I=1,KPLOT
ISN 0029            WRITE(6,800) CD(5,I),(CD(L,I),L=1,NVAR)
ISN 0030          800 FORMAT(1H ,5E20.5)
ISN 0031           70 CONTINUE
ISN 0032           71 IP(((((IPLOT/10)/2)*2).NE.(IPLOT/10))
                  1CALL DATPLO(Y00,NVAR,KPLOT,HTITLE)
ISN 0034           75 CONTINUE
ISN 0035            RETURN
ISN 0036            END
```

```
ISN 0002            SUBROUTINE DATPLO(Y00,NVAR,NT,NTITLE)
ISN 0003            COMMON/DATAP/CD(5,200),DYN(5),DYZ(5),DXN,DXZ,NA(20),NPTY(5)
ISN 0004            DIMENSION PLT(3000),NTITLE(20),IS(5)
ISN 0005            DATA IS/0,1,2,3/
                C   ROUTINE TO PLOT UP TO 5 VARIABLES
                C   SCALE VARIABLES IN ARRAY CD
                C   DYN -  UNITS PER INCH
                C   DYZ -  VALUE AT GRAPH 0
ISN 0006            DO 50 L=1,NVAR
ISN 0007            SF=1.0/DYN(L)
ISN 0008            DO 50 I=1,NT
ISN 0009         50 CD(L,I) = SF*(CD(L,I)-DYZ(L))
ISN 0010            SF=1.0/DXN
ISN 0011            DO 51 I=1,NT
ISN 0012         51 CD(5,I) = SF*(CD(5,I)-DXZ)
                C     PLOT SET UP
ISN 0013            SS = 0.14
ISN 0014            SN = 0.1
ISN 0015            X0 = 0.0
ISN 0016            YB = Y00 + 0.0
ISN 0017            YT = Y00 + 10.0
ISN 0018            CALL PLOTS(PLT,3000)
                C
                C   PLOT HEADER
ISN 0019            CALL SYMBOL(X0,2.0,0.105,20HR F PANEL RUN P 4500,90.0,20)
ISN 0020            X = X0 + 1.0
ISN 0021            CALL SYMBOL(X,2.0,0.105,NTITLE(1),90.0,80)
ISN 0022            X0 = X0 + 2.0
                C   LABEL PLOTS
                C
ISN 0023            DO 630 L=1,NVAR
ISN 0024            IF(L.EQ.1) GO TO 101
ISN 0025            DO 100 K=2,L
ISN 0026            IF((DYN(L).EQ.DYN(K-1)).AND.(DYZ(L).EQ.DYZ(K-1))) GO TO 630
ISN 0029         100 CONTINUE
ISN 0030         101 CONTINUE
ISN 0031            X = X0 + 0.08
ISN 0032            Y = Y00 + 4.0
ISN 0033            CALL SYMBOL(X,Y,SS,IS(L),90.0,-1)
ISN 0034            LN = 50L - 6
ISN 0035            Y = Y + 0.15
ISN 0036            X = X + 0.05
ISN 0037            CALL SYMBOL(X,Y,SN,NA(LN),90.0,20)
                C   LABEL SCALE
ISN 0038            X = X0 + 0.2
ISN 0039            Y = Y00 - 0.05
ISN 0040            YY = DYZ(L)
ISN 0041            DO 635 I=1,11
ISN 0042            CALL NUMBER(X,Y,SN,YY,0.0,6H(F9.1))
ISN 0043            Y = Y + 1.0
ISN 0044         635 YY = YY + DYN(L)
                C   DRAW VERTICAL LINE
ISN 0045            X = X0 + 1.0
ISN 0046            CALL PLOT(X,YB,3)
ISN 0047            CALL PLOT(X,YT,2)
ISN 0048         630 X0 = X
```

```
ISN 0049            XV = DXX
ISN 0050            YB = Y00-0.15
ISN 0051            XT = X0-0.2
ISN 0052            XMIN = X0
ISN 0053            XMAX=XMIN
ISN 0054            CALL NUMBER(XT,YB,SN,XV,0.0,6H(F7.2))
                C   DETERMINE PLOT CONDITIONS FOR 200 PTS PER SECTION
ISN 0055            IOV=0
ISN 0056            ISTART = 1
ISN 0057            ISTOP = 50
ISN 0058          640 IF(ISTOP.GT.NT) ISTOP=NT
ISN 0059            DO 650 L=1,NCAR
ISN 0060            DO 650 I=ISTART,ISTOP
ISN 0061            X = CD(5,I) + X0
ISN 0062            IF(X.GT.XMAX) XMAX=X
ISN 0063            Y=CD(L,I)+Y00
ISN 0064            IF(Y.LT.0.0.OR.Y.GT.YY)    GO TO 651
ISN 0065            IF(I.EQ.ISTART) GO TO 652
ISN 0066            IF(IOV.EQ.1) GO TO 652
ISN 0067            IF(NPTY(L).EQ.0) CALL PLOT(X,Y,3)
ISN 0068            CALL PLOT(X,Y,2)
ISN 0069            GO TO 650
ISN 0070          651 IOV=1
ISN 0071            GO TO 650
ISN 0072          652 IOV=0
ISN 0073            CALL PLOT(X,Y,3)
ISN 0074            CALL SYMBOL(X,Y,SS,IS(L),0.0,-2)
ISN 0075            CALL PLOT(X,Y,2)
ISN 0076          650 CONTINUE
ISN 0077            ISTART=ISTOP
ISN 0078            IF(ISTART.GE.NT) GO TO 700
ISN 0079            ISTOP=ISTOP+50
ISN 0080            GO TO 640
ISN 0081          700 XSTOP=XMAX-XMIN
ISN 0082            NSTOP=IPIX(XSTOP)+1
ISN 0083            X=X0
ISN 0084            YC=YB+0.25
ISN 0085            DO 660 I=1,NSTOP
ISN 0086            X=X+1.0
ISN 0087            XV=XV+DXX
ISN 0088            XT=XT+1.0
ISN 0089            CALL PLOT(X,YC,3)
ISN 0090            CALL PLOT(X,YB,2)
ISN 0091            CALL PLOT(X,YB,3)
ISN 0092          660 CALL NUMBER(XT,YB,SN,XV,0.0,6H(F7.2))
ISN 0100            CALL PLOT(X0,YB,3)
ISN 0101            CALL PLOT(XT,YB,2)
ISN 0102            X=X+3.0
ISN 0103            CALL PLOT(X,0.0,-3)
ISN 0104            RETURN
ISN 0105            END
```

```
ISN 0002          SUBROUTINE PROPLO
                C ** PROGRAM TO CRT PLOT DATA FOR PROGRAM SIMTRAN 1, 01-14-75
                C ** AUTHOR: OR NNSS, UCNC CSD ONNL, PO BOX X, OAK RIDGE, TN. 37830
                C
                C ** VARIABLES REQUIRED ARE IN COMMON, PARABOLIC INTERPOLATION IS
                C    DONE BETWEEN ELEMENTS (C(L),L=1,N1),(C(N),N=N1,N2),(C(N),N=N2,N3)
                C    FOR GRAPH TYPE 1, PLUS (C(L),L=N3,N4) AND (C(N),N=N4,N5) FOR
                C    GRAPH TYPE 2 DEPENDING ON NDIFF(1)*NDIFF(2)=0.0 OR >0.0.
                C ** X-AXIS SCALE: IF X(N1)-X(1).GE.0.05CM, 1 INCH = 0.005 CM, TYPE 1,
                C                  OR X(N5)-X(1).GE.0.05CM, 1 INCH = 0.005 CM, TYPE 2.
                C       SIMILARLY, IF X(N3)-X(1).LT.0.05CM, 1 INCH = 0.0025CM, TYPE 1,
                C                  OR X(N5)-X(1).LT.0.05CM, 1 INCH = 0.0025CM, TYPE 2.
                C       START AND END X-AXIS WITH DIVISION .LT. X(1) AND .GT. X(N1) OR
                C          X(N5).
                C ** Y-AXIS SCALE: SAME FOR BOTH GRAPHS, 1 INCH = 0.2 GM/CM**3, IN 0.4
                C                  GM/CM**3 DIVISIONS, STARTING WITH 0.
                C                  NEW FEATURE: NSCALE = 1, EXPAND Y-RANGE TO 0.0-0.4
                C                  INSTEAD OF 0.0-2.0 FOR NSCALE = 0.
                C ** LINE INTENSITIES: INCREASE FROM NPEN LINES TO LINES FOR X(N)'S TO
                C       X,Y-AXIS TO CURVES OF C VS. X.
                C ** N VALUES ARE DETERMINED FROM NDIFF(1).GT.0, NN = N = 1, TYPE1 PLOT,
                C                                 OR NDIFF(2).GT.0, NN = N = 2, TYPE1 PLOT,
                C                                 AND N1 = N2 = 1 OR N1 = N2 = 2
                C       FOR TYPE2, NN = N = 1 OR 2, N1 = 1 AND N2 = 2.
                C
ISN 0003          IMPLICIT REAL*8 (A-H,O-Z)
                C
                C    C = CONC., X = DIST., OLAYER & ALAYER ARE THICKN.; OXID & ALPA ARE
                C       OXYGEN CONTENT; BETA,TOTAL ARE SAME; BETAR IS CO; GAIN IS GAIN.
                C    ADD BLAYER = THICKNESS AND NSCALE = Y-AXIS SCALE FACTOR.
                C
ISN 0004          COMMON/PLOVAR/NDIFF(2),CSTART,TIME
ISN 0005          COMMON/HEADLN/HTITL(20)
ISN 0006          COMMON/PROPIL/C(500),X(500),OLAYER(2),ALAYER(2),BLAYER
                1,OXID(2),ALPA(2),GAIN(2),BETA,TOTAL,BETAR,TEMP
                2,          N1,N2,N3,N4,N5,NUMPLT,NSCALE
                C
ISN 0007          DIMENSION IPLTA(4000),NS(5)
                C
                C    INL,INS,INTA,ICYN ARE BEAM INTENSITIES FOR NPEN LINES, X()'S,
                C      X,Y-AXES AND C VS. X.
ISN 0008          DATA IPLTP/0/,NBUF/4000/,INL,INS,INTA,ICYN/11,15,17,19/
ISN 0009          DATA NIP/10/
                C    NIP IS NO. OF INTERPOLATED PTS. BETWEEN DATA PTS.
                C
                C    INITIALIZE CRT PLOTTER 1ST TIME ONLY
ISN 0010          IF( IPLTP.NE.1 ) GO TO 5
ISN 0012          CALL CRT( IPLTA,NBUF,'OVRUSS 4500NS',0 )
ISN 0013          IEPP = 0
ISN 0014          IPLTP = 1
ISN 0015        5 CONTINUE
                C
                C    CHECK NUMPLT-- IF NEG. THIS IS FINAL PLOT, SET INTEGER END PLOT
                C       FLG IEPP = 9000 AND NUMPLT TO POS. VALUE.
ISN 0016          IF( NUMPLT.LT.0 ) IEPP = 9000
ISN 0018          IF( NUMPLT.LT.0 ) NUMPLT = - NUMPLT
```

```
C
C     SET NS(1), ETC. TO N1, ETC.
ISN 0020          NS(1) = N1
ISN 0021          NS(2) = N2
ISN 0022          NS(3) = N3
ISN 0023          NS(4) = N4
ISN 0024          NS(5) = N5
C
C     INITIALIZE Y-AXIS (OXYGEN CONCEN.) VALUES.
C     INITIALIZE Y-MAX VALUE FOR NSCALE.GT.0, YUL = 0.5 INSTEAD OF 2.0
C ** CHANGE Y-AXIS LIMIT TO 5.0 IN. MAX. 02-03-75
C ** MAKE Y-AXIS HEIGHT = 9.0 INCHES, 02-28-75.
ISN 0025          NY = 5
ISN 0026          Y0 = 0.0
ISN 0027          YOFF = 0.0
ISN 0028          YLIN = 9.0
ISN 0029          YREF = 0.0
ISN 0030          YLL = 0.0
ISN 0031          YUL = 2.0
ISN 0032          IF( NSCALE.GT.0 ) YUL = 0.5
ISN 0033          YDIV = YUL/(NY-1)
ISN 0034          YFACT = YUL/YLIN
ISN 0035          YSCAL = 1.0/YFACT
ISN 0036          DDY = YDIV/YFACT
C
C     FOR TYPE1, SET K1 = K2 = KK = 1 OR 2
C     SET NN = NS(3) FOR TYPE 1, OR TO NS(4) FOR TYPE 2 GRAPHS.
C     FOR TYPE1, NC = 3, FOR NO. OF CURVES.
C     IF ( NDIFF(1)*NDIFF(2).EQ.0 FOR TYPE1'S, .GT.0 FOR TYPE2'S.
ISN 0037          IF( NDIFF(1)*NDIFF(2).GT.0.0 ) GO TO 20
ISN 0038          IF( NDIFF(1).GT.0.0 ) KK = 1
ISN 0039          IF( NDIFF(2).GT.0.0 ) KK = 2
ISN 0040          K1 = KK
ISN 0041          K2 = KK
ISN 0042          NN = MINO( NS(3),100 )
ISN 0043          NC = 3
ISN 0044          IF( NDIFF(1)*NDIFF(2).EQ.0.0 ) GO TO 25
C
C     PREPARE FOR TYPE2 GRAPHS
C     FOR TYPE2, NC = 5, FOR NO. OF CURVES.
ISN 0045       20 CONTINUE
ISN 0046          K1 = 1
ISN 0047          K2 = 2
ISN 0048          KK = K1 + K2
ISN 0049          NN = MINO( NS(5),100 )
ISN 0050          NC = 5
C
C     ESTABLISH FACTORS FOR X-AXIS: XDIV,XFACT,XLL,XUL,XLIN,NX,XSCAL,XOFF
C ** CHANGE XFACT TO REDUCE X-AXIS LENGTH BY HALF.
C        XFACT WAS 0.005 AND 0.0025 RESPECTIVELY.
ISN 0051       25 CONTINUE
ISN 0052          X0 = 0.0
ISN 0053          XDIV = 0.01
ISN 0054          IF( X(NN)-X(1).GE.0.05 ) XFACT = 0.010
ISN 0055          IF( X(NN)-X(1).LT.0.05 ) XFACT = 0.005
ISN 0056          IF( XFACT.EQ.0.005 ) XDIV = 0.005
ISN 0057          XLL = IDINT( X(1)/XDIV ) * XDIV - XDIV
ISN 0058          XUL = IDINT( X(NN)/XDIV ) * XDIV + XDIV
```

```
ISN 0067            XLIN = ( XUL-XLL )/XFACT
ISN 0068            NX =     ((XUL-XLL)/XDIV) + 1
ISN 0069            XSCAL = 1.0/XFACT
ISN 0070            XOFF  = XLL  * XSCAL
ISN 0071            DDX = XDIV/XFACT
                    C
                    C    MOVE GRAPH ORIGIN FROM (0.0,0.0) TO (0.5,0.5)
                    C ** MAKE GRAPH ORIGIN AT YO = 1.0 INSTEAD OF 0.5, 02-28-79.
ISN 0072            CALL CRT( 0.5,1.0,0,3 )
                    C
                    C    DRAW Y-AXIS VALUES, HEADING
                    C    FOR NSCALE = 0, DO Y-RANGE 0.0-2.0 W/FMT F3.1, = 1 DO 0.000-0.500
                    C       W/FMT F5.3.
ISN 0073            YY = 0.0
ISN 0074            YY = -DDY
ISN 0075            YLAB = -YDIV
ISN 0076            HGTY = 0.15
ISN 0077            WDTHY = 0.12
ISN 0078            DO 30 I = 1,NY
ISN 0079            YY = YY + DDY
ISN 0080            YLAB = YLAB + YDIV
ISN 0081            IF(NSCALE.EQ.0)CALL CRTNUM(XY-0.41,YY-0.07,HGTY,YLAB,0,'(F3.1)')
ISN 0082            IF(NSCALE.GT.0)CALL CRTNUM(XY-0.65,YY-0.07,HGTY,YLAB,0,'(F5.3)')
                    C
                    C    DRAW HORIZONTAL MESH LINES TOWARD THE RIGHT
ISN 0083            IF( I.EQ.1 ) GO TO 32
ISN 0084            XG = XY
ISN 0085            YG = YY
ISN 0086            CALL CRT( XG,YG,0,1 )
ISN 0087            XG = XLIN
ISN 0088            CALL CRT( XG,YG,IVL,1 )
ISN 0089            XG = XY
ISN 0090            CALL CRT( XG,YG,0,1 )
ISN 0091         32 CONTINUE
ISN 0092            IF( I.NE.NY/2 ) GO TO 30
ISN 0093            IF( NSCALE.EQ.0 ) XN = XY - 0.46
ISN 0094            IF( NSCALE.GT.0 ) XN = XY - 0.70
ISN 0095            YN = (YLIN - 31.0*WDTHY) * 0.5
ISN 0096            CALL CRTSYM( XN,YN,HGTY,'OXYGEN CONCENTRATION (GM/CM**3) ',90.0,31)
ISN 0097         30 CONTINUE
                    C
                    C    DRAW HEADING ACROSS TOP FROM HTITL(20) IN COMMON
ISN 0098            XT = (XLIN - 80.0*WDTHY) * 0.5
ISN 0099            YT = YLIN + 0.15
ISN 0100            CALL CRTSYM( XT,YT,HGTY,HTITL(1),0.0,80 )
                    C
                    C    DRAW TOP AXIS BACK TO LEFT, THEN DOWN TO ORIGIN.
ISN 0101            CALL CRT( XLIN,YLIN,0,1 )
ISN 0102            CALL CRT( XO,YLIN,IXYA,1)
ISN 0103            CALL CRT( XO,YO,IXYA,1)
ISN 0104            CALL CRT( XO,YO,0,1 )
                    C
                    C    DRAW X-AXIS VALUES, HEADING ALONG BOTTOM
ISN 0105            XX = -DDX
ISN 0106            YX = YO - 0.25
ISN 0107            HGTX = 0.15
ISN 0108            XLAB =  XLL - XDIV
ISN 0109            WDTHX = 0.12
```

```
ISN 0116            DO 40 I = 1,NX
ISN 0117            XX = XX + DDX
ISN 0118            XLAB = XLAB + XDIV
ISN 0119            CALL CRTMSN( XX-0.36,YX,HGTX,XLAB,0.0,'(F6.3)' )
                C
                C     DRAW VERTICAL MESH LINES UP AT EACH X-AXIS DIV., TOWARD THE RIGHT
ISN 0120            IF( I.EQ.1 ) GO TO 42
ISN 0122            XV = XX
ISN 0123            YV = Y0
ISN 0124            CALL CRT( XV,YV,0,1 )
ISN 0125            YV = YLIN
ISN 0126            CALL CRT( XV,YV,IWL,1 )
ISN 0127            YV = Y0
ISN 0128            CALL CRT( XV,YV,0,1 )
ISN 0129         42 CONTINUE
ISN 0130            IF( I.NE.NX/2 ) GO TO 40
ISN 0132            XM = (XLIN - 41.0*WDTHX) * 0.5
ISN 0133            YM = Y0 - 0.50
ISN 0134            CALL CRTSYM(XM,YM,HGTX,'DISTANCE FROM ORIGINAL OUTER SURFACE (CM)'
                   1,0.0,41 )
ISN 0135         40 CONTINUE
                C
                C     DRAW X-AXIS FROM RIGHT BACK TO ORIGIN.
ISN 0136            CALL CRT( XLIN,Y0,0,1 )
ISN 0137            CALL CRT( X0,Y0,IXYA,1 )
ISN 0138            CALL CRT( X0,Y0,0,1 )
                C
                C     DRAW VERTICAL X(1),--,X(NN) FROM LEFT TO RIGHT, NS(1),(NN) = N1,NN
                C        FOR TYPE1 OR 2, NL = NC + 1 = 4 OR 6 VERTICAL LINES
                C     XOFF IS DISTANCE (IN.) XLL IS OFFSET FROM 0,0, NEG. OR POS.
ISN 0139            NL = NC + 1
ISN 0140            DO 50 L = 1,NL
ISN 0141            NV = 1
ISN 0142            IF( L.GT.1 ) NV = NS(L-1)
ISN 0144            XV = X(NV) * XSCAL - XOFF
ISN 0145            YV = Y0
ISN 0146            CALL CRT( XV,YV,0,1 )
ISN 0147            YV = YLIN
ISN 0148            CALL CRT( XV,YV,IXS,1 )
ISN 0149            YV = Y0
ISN 0150            CALL CRT( XV,YV,0,1 )
ISN 0151         50 CONTINUE
                C
                C     PREPARE TO PLOT C VS. X, DO 3 OR 5 CURVES, NN = NS(3) OR NS(5)
                C     NA IS 1ST INDEX AND IS RESET TO VALUE OF 2ND INDEX FOR NEXT CURVE.
                C ** FOR NSCALE > 0, Y-AXIS RANGE = 0.0 - 0.5, OMIT ANY C VALUES > 0.5
                C ** NDIP, TO INTERPOLATE BETWEEN DATA POINTS, 01-30-75.
ISN 0152            NNIP = NIP
ISN 0153            NN1 = NIP-1
ISN 0154            NA = 1
ISN 0155            DO 60 I = 1,NC
ISN 0156            IND1 = 1
ISN 0157            NB = NS(I)
ISN 0158            NP = NB-NA+1
ISN 0159            NAP1 = NA+1
ISN 0160            DO 65 N = NAP1,NB
ISN 0161            NN1 = N-1
ISN 0162            XP = X(NN1)*XSCAL - XOFF
```

```
ISN 0163            YP = C(NN1)*YSCAL - YOFF
ISN 0164            IF( YP.GT.YLIM ) GO TO 65
                C     POSITION BEAM AT 1ST POINT OF EACH CURVE.
ISN 0166            CALL CRT( XP,YP,0,1 )
ISN 0167            IF( NP.LE.2 ) GO TO 64
ISN 0169            IND1 = IND1+1
ISN 0170            DX = (X(N)-X(NN1))/FNIP
ISN 0171            XI = X(NN1)
ISN 0172            DO 63 N = 1,NN1
ISN 0173            XI = XI + DX
ISN 0174            YI = YLAG( XI,X(NA),C(NA),IND1,3,NP,IFX )
ISN 0175            XP = XI*XSCAL - XOFF
ISN 0176            YP = YI*YSCAL - YOFF
ISN 0177            IF( YP.GT.YLIM ) GO TO 63
ISN 0179            CALL CRT( XP,YP,ICVX,1 )
ISN 0180         63 CONTINUE
ISN 0181         64 CONTINUE
ISN 0182            XP = X(N)*XSCAL - XOFF
ISN 0183            YP = C(N)*YSCAL - YOFF
ISN 0184            IF( YP.GT.YLIM ) GO TO 65
ISN 0186            CALL CRT( XP,YP,ICVX,1 )
ISN 0187         65 CONTINUE
ISN 0188            IF( L.LT.NC ) NA = NB + 1
ISN 0190         60 CONTINUE
                C     RESET NA TO NB + 1 FOR NEXT CURVE EXCEPT AFTER LAST CURVE.
                C
                C     ADD CSTART VS X(1),---,X(NN) IN DASHED LINE FROM X(1) TO X(NN).
ISN 0191            X1 = X(1)*XSCAL - XOFF
ISN 0192            XN = X(NN)*XSCAL - XOFF
ISN 0193            Y1 = CSTART*YSCAL - YOFF
ISN 0194            DXL = 0.25
ISN 0195            DXB = 0.125
ISN 0196            CALL CRT( X1,Y1,0,1 )
ISN 0197         67 X1 = DMIN1( X1+DXL,XN )
ISN 0198            CALL CRT( X1,Y1,ICVX,1 )
ISN 0199            X1 = DMIN1( X1+DXB,XN )
ISN 0200            CALL CRT( X1,Y1,0,1 )
ISN 0201            IF( X1.LT.XN ) GO TO 67
                C
                C     DRAW LEGEND AT RIGHT END OF GRAPH
                C       FOR TYPE1, K = 1 OR 2, DEPENDING ON NDIFF(1) OR (2)>0, K1=K2=K.
                C       FOR TYPE2, K = 2 FOR DRAWING ARRAY VALUES, K1 = 1, K2 = 2.
                C     DRAW LEGEND FROM TOP DOWNWARD, LINE 1 = TIME
ISN 0203            XX = XLIM + 0.5
ISN 0204            YY = YLIM - 0.25 *
ISN 0205            DY = 0.25
ISN 0206            YP = XX
ISN 0207            YR = YY
ISN 0208            CALL CRTSYM( XR,YR,HGTX,'TIME=' ,0.0,6 )
ISN 0209            XR = XR + 5.0*WDTHX
ISN 0210            ITIM = TIME+0.5
ISN 0211            CALL CRTNUM( XR,YR,HGTX,ITIM,0,0,'(I4)' )
ISN 0212            XR = XR + 4.0*WDTHX
ISN 0213            CALL CRTSYM( XR,YR,HGTX,' SEC',0.0,4 )
                C
                C     DRAW LINE 2 = TEMP, RESET X, DECREASE Y BY DY
                C ** MAKE MORE SPACE BETWEEN TIME AND T = TEMP, 02-28-79.
ISN 0214            XP = XX
```

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ISN 0215            YR = YR - 2.0*DY
ISN 0216            CALL CRTSYN( XR,YR,NGTX,'T= ',0.0,3 )
ISN 0217            XR = XR + 3.0*WDTHX
ISN 0218            ITMP = TEMP
ISN 0219            CALL CRTNUM( XR,YR,NGTX,ITMP,0.0,'(I4)' )
ISN 0220            XR = XR + 4.0*WDTHX
ISN 0221            CALL CRTSYN( XR,YR,NGTX,' DEG.C',0.0,6 )
                C
                C     DRAW LINES 3,4 LAYER THICKNESS AND (MICRONS)
                C ** MAKE MORE SPACE BETWEEN T = TEMP AND LAYER THICKNESS, 02-26-75.
ISN 0222            XR = XX
ISN 0223            YR = YR - 2.0*DY
ISN 0224            CALL CRTSYN( XR,YR,NGTX,'LAYER THICKNESS',0.0,15 )
ISN 0225            YR = YR - DY
ISN 0226            CALL CRTSYN( XR,YR,NGTX,'   (MICRONS)',0.0,12 )
                C
                C     DRAW LINES 5 - 8 FROM OLAYER, ALAYER ARRAYS, N1,N2 = 1,2,IF TYPE 2.
ISN 0227            XR = XX
ISN 0228            YR = YR - DY
ISN 0229            CALL CRTSYN( XR,YR,NGTX,'ZRO ',0.0,4 )
ISN 0230            XR = XR + 4.0*WDTHX
ISN 0231            DO 70 K = N1,N2
ISN 0232            CALL CRTNUM( XR,YR,NGTX,OLAYER(K),0.0,'(F9.1)' )
ISN 0233            YR = YR - DY
ISN 0234         70 CONTINUE
                C
ISN 0235            XR = XX
ISN 0236            CALL CRTSYN( XR,YR,NGTX,'ALPHA ',0.0,6 )
ISN 0237            XR = XR + 6.0*WDTHX
ISN 0238            DO 75 K = N1,N2
ISN 0239            CALL CRTNUM( XR,YR,NGTX,ALAYER(K),0.0,'(F7.1)' )
ISN 0240            YR = YR - DY
ISN 0241         75 CONTINUE
                C
                C     DRAW LINE 9A FOR BETA FROM BLAYER, ADDED 01-22-75.
ISN 0242            XR = XX
ISN 0243            CALL CRTSYN( XR,YR,NGTX,'BETA ',0.0,5 )
ISN 0244            XR = XR + 5.0*WDTHX
ISN 0245            CALL CRTNUM( XR,YR,NGTX,BLAYER,0.0,'(F8.1)' )
                C
                C     DRAW LINES 9,10, OXYGEN CONTENT & (MG/CM**2)
                C ** MAKE MORE SPACE BETWEEN BETA AND OXYGEN CONTENT, 02-26-75.
ISN 0246            XR = XX
ISN 0247            YR = YR - 2.0*DY
ISN 0248            CALL CRTSYN( XR,YR,NGTX,'OXYGEN CONTENT',0.0,14 )
ISN 0249            YR = YR - DY
ISN 0250            CALL CRTSYN( XR,YR,NGTX,'  (MG/CM**2)',0.0,12 )
                C
                C     DRAW LINE(S) 11,(12), FROM OXID(1),(2) AS ZRO(1),(2)
ISN 0251            XR = XX
ISN 0252            YR = YR - DY
ISN 0253            CALL CRTSYN( XR,YR,NGTX,'ZRO ',0.0,4 )
ISN 0254            XR = XR + 4.0*WDTHX
ISN 0255            DO 80 K = N1,N2
ISN 0256            CALL CRTNUM( XR,YR,NGTX,OXID(K),0.0,'(F9.2)' )
ISN 0257            YR = YR - DY
ISN 0258         80 CONTINUE
                C
```

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C     DRAW LINE(S) 13,(14) FROM ALPA(1),(2) AS ALPHA(1),(2)
ISN 0259            XR = XX
ISN 0260            CALL CRTSYM( XR,YR,HGTX,'ALPHA ',0.0,6 )
ISN 0261            XR = XR + 6.0*WDTHX
ISN 0262            DO 85 K = K1,K2
ISN 0263            CALL CRTNUM( XR,YR,HGTX,ALPA(K),0.0,'(F7.2)' )
ISN 0264            YR = YR - DY
ISN 0265         85 CONTINUE
C
C     DRAW LINE 15 FOR BETA
ISN 0266            XR = XX
ISN 0267            CALL CRTSYM( XR,YR,HGTX,'BETA ',0.0,5 )
ISN 0268            XR = XR + 5.0*WDTHX
ISN 0269            CALL CRTNUM( XR,YR,HGTX,BETA,0.0,'(F8.2)' )
C
C     DRAW LINE 16 FROM TOTAL
ISN 0270            XR = XX
ISN 0271            YR = YR - DY
ISN 0272            CALL CRTSYM( XR,YR,HGTX,'TOTAL ',0.0,6 )
ISN 0273            XR = XR + 6.0*WDTHX
ISN 0274            CALL CRTNUM( XR,YR,HGTX,TOTAL,0.0,'(F7.2)' )
C
C     DRAW LINE 17 FROM BETAS AS CO
ISN 0275            XR = XX
ISN 0276            YR = YR - DY
ISN 0277            CALL CRTSYM( XR,YR,HGTX,'CO ',0.0,3 )
ISN 0278            XR = XR + 3.0*WDTHX
ISN 0279            CALL CRTNUM( XR,YR,HGTX,BETAS,0.0,'(F10.2)' )
C
C     DRAW LINE 18 FROM GAIN
C ** DRAW GAIN(K) VALUE(S), 02-24-75.
ISN 0280            XR = XX
ISN 0281            YR = YR - DY
ISN 0282            CALL CRTSYM( XR,YR,HGTX,'GAIN ',0.0,5 )
ISN 0283            XR = XR + 5.0*WDTHX
ISN 0284            DO 90 K = K1,K2
ISN 0285            CALL CRTNUM( XR,YR,HGTX,GAIN(K),0.0,'(F8.2)' )
ISN 0286         90 YR = YR - DY
C
C     DRAW PLOT NUMBER FROM NUMPLT
C        NUMBER LOOKS LIKE-- 012275001 (I9 FORMAT)
C ** DRAW NUMPLT AT LOWER RIGHT, SAME LEVEL AS X-AXIS HEADING, 02-24-75.
ISN 0287            XPN = XX + 6.0*WDTHX
ISN 0288            YPN = Y0 - 0.5
ISN 0289            CALL CRTNUM( XPN,YPN,HGTX,NUMPLT,0.0,'(I9)' )
C
C     TERMINATE EACH GRAPH, ADVANCE FILM
C ** CHECK INTEGER END PLOT FLAG IEPP-- IF = 9000, THIS IS FINAL PLOT.
ISN 0290            XNU = 0.0
ISN 0291            YNU = 0.0
ISN 0292            CALL CRT( XNU,YNU,IEPP,2 )
C
ISN 0293            RETURN
ISN 0294            END
```

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