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COSIM—A Finite-Difference Computer Model to Predict Ternary Concentration Profiles Associated With Oxidation and Interdiffusion of Overlay-Coated Substrates

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August 2000

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Summary

A finite-difference computer program (COSIM) has been written which models the one-dimensional, diffusional transport associated with high-temperature oxidation and interdiffusion of overlay-coated substrates. The program predicts concentration profiles for up to three elements in the coating and substrate after various oxidation exposures. Surface recession due to solute loss is also predicted. Ternary cross terms and concentration-dependent diffusion coefficients are taken into account. The program also incorporates a previously-developed oxide growth and spalling model to simulate either isothermal or cyclic oxidation exposures. In addition to predicting concentration profiles after various oxidation exposures, the program can also be used to predict coating life based on a concentration dependent failure criterion (e.g., surface solute content drops to 2 percent). The computer code, written in an extension of FORTRAN 77, employs numerous subroutines to make the program flexible and easily modifiable to other coating oxidation problems.

Introduction

Many blades and vanes in gas turbine engines are coated with an aluminide or overlay coating to impart additional oxidation and corrosion protection to the component. These coatings provide protection by the selective oxidation of Al to form a compact and adherent Al_2O_3 scale. Under isothermal conditions, the Al_2O_3 scale thickens at a parabolic rate (scale thickness proportional to the square root of time). Diffusional transport within the coating supplies Al to the growing oxide scale at a rate consistent with the parabolic growth of the scale. Although Al is continually consumed from the coating, the rate is acceptably low such that the coating typically contains sufficient Al to easily provide protection during isothermal oxidation conditions. Although land-based turbines often operate in a nearly isothermal mode for long periods, aero gas turbines undergo thermal cycling with each flight. This thermal cycling, primarily to ambient temperatures when the engine is shut down, can cause cracking and partial spalling of the protective Al_2O_3 scale. This spallation generally occurs randomly across flat component surfaces but is higher at edges and corners. The spalling may occur to the metal surface but more commonly occurs only in the outer layers of the oxide scale. However, loss of the oxide is not catastrophic since selective oxidation of Al continues when the component again reaches high temperatures such that the damaged scale will “heal” and continue to grow. Whenever scale spallation occurs due to thermal cycling during oxidation (i.e., cyclic oxidation), the oxide scale on the surface will, on average, be thinner than a scale grown isothermally for equivalent hot exposure times. Since the rate of scale growth is inversely proportional to the scale thickness, a consequence of this thinner oxide scale is that the average rate of Al consumption is greater during cyclic oxidation accompanied by scale spallation than during isothermal oxidation. Hence, Al is depleted from the coating at a higher rate during cyclic oxidation, the exact rate
depending on the growth rate of the alumina scale and the amount of oxide spalling. This paper will focus specifically on degradation of MCrAlY overlay coatings, where M stands for either Ni, Co or Fe. These coatings are often used on components in marine environments where hot corrosion protection is required, and in military applications where higher temperatures are often encountered.

In addition to oxidative attack, overlay coatings are further degraded by interdiffusion with the substrate. Since the coating is, by nature, higher in Al content than the substrate, Al diffuses from the coating into the substrate and generally becomes unavailable to support the growth of the protective alumina scale. Likewise, the Cr concentration

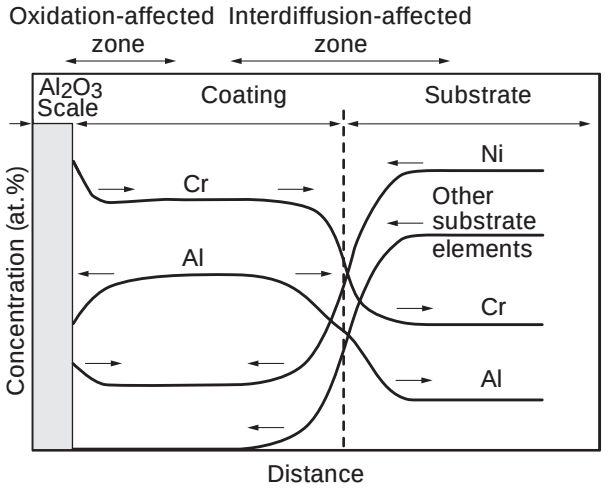

Figure 1.—Schematic concentration profiles after oxidation exposure. Arrows indicate direction of atomic transport.

in the coating is also typically greater than that in the substrate resulting in the diffusion of Cr from the coating into the substrate. In contrast, Ni and other elements in the substrate diffuse into the coating. Although the Y in the alloy strongly affects adherence of the Al_2O_3 scale during cyclic oxidation, it is at such low concentration in the coating (e.g., <0.2 at%) that dilution by interdiffusion with the substrate is generally not considered. Schematic concentration profiles in the coating and substrate after a short exposure in an oxidizing environment are shown in figure 1. When a coating is substantially depleted of Al during cyclic oxidation, it can no longer supply sufficient Al to reheal the protective scale. Less protective oxides, such as NiO , FeO or CoO, can form signaling the end of the protective life of the coating. A critical Al content in the coating can be defined to indicate the useful life of the coating. This critical Al content could indicate the time at which less-protective oxides form on the surface, or an earlier time at which the coating could be stripped from the component and a new coating applied. Modeling the Al transport in the coating and substrate during cyclic oxidation allows the coating life to be predicted. The purpose of the present work was to develop a one-dimensional ternary diffusion model to predict the concentration profiles associated with the oxidation and interdiffusion of coated superalloys undergoing cyclic oxidation. This model, given the name COSIM for Coating Oxidation and Substrate Interdiffusion Model, employs finite-difference techniques embodied in a FORTRAN computer program to provide numerical solutions to the appropriate diffusion equations. The computer code employs numerous subroutines to make the program flexible and easily modifiable to other coating oxidation problems. Although the computer program and discussion below are primarily in terms of a NiCrAl coating on a Ni-based substrate, other elements could be substituted for the Al and Cr.

Ternary Diffusion Equations

Because of the low Y content, MCrAlY overlay coatings can be approximated as ternary alloys with Al and Cr in a matrix of either Ni, Co or Fe. Ternary diffusion equations can be employed to simulate the Al and Cr transport associated with coating oxidation and coating/substrate interdiffusion. The choice of simulating Cr rather than Ni diffusion is inconsequential. In the ternary system, the concentration of the third component, being a dependent variable, is always determined by difference (i.e., $C_{Ni} = 100 - C_{Al} - C_{Cr}$). Since most superalloys are complex multicomponent, multiphase alloys, fully accounting for diffusional interactions of the various superalloy components, as well as that of Y in the coating, on the Al and Cr transport is beyond current capabilities. Hence, these potential interactions, other than those encountered in the ternary system, are ignored. In addition, NiCrAlY and CoCrAlY overlay coatings generally consist of two phases, a high-Al NiAl or CoAl β phase embedded in a Ni or Co solid solution γ phase. This β phase is depleted as Al is consumed as oxide and as Al diffuses into the substrate. It has previously been shown that this β phase is often completely dissolved well before the useful life of the coating has been reached (ref. 1). It was also shown in this same reference that good agreement was achieved between measured

and predicted concentration profiles in the coating at extended times after the β phase had been dissolved by assuming a single-phase coating for the entire oxidation exposure. Hence, in the current model development, the two-phase coating will be represented as a single phase.

Fick's laws describing diffusion in a ternary alloy are:

$$J_j = -D_{j,j}\frac{\partial C_j}{\partial X} - D_{j,k}\frac{\partial C_k}{\partial X} \quad j,k = \mathrm{Al,Cr}\,* \qquad \text{1st Law} \qquad (1)$$

and

$$\frac{\partial C_j}{\partial t} = \frac{\partial\left(D_{j,j}\left(\frac{\partial C_j}{\partial X}\right)\right)}{\partial X} + \frac{\partial\left(D_{j,k}\left(\frac{\partial C_k}{\partial X}\right)\right)}{\partial X} \quad j,k = \mathrm{Al,Cr} \qquad \text{2nd Law} \qquad (2)$$

where J_j and C_j refer to the flux and concentration of component j, $D_{j,j}$ and $D_{j,k}$ refer to the four ternary interdiffusion coefficients, or diffusivities, and X and t refer to distance and time, respectively. The first term on the right hand side (RHS) of equation (2) can be rewritten as:

$$\frac{\partial\left(D_{j,j}\left(\frac{\partial C_j}{\partial X}\right)\right)}{\partial X} = D_{j,j}\frac{\partial^2 C_j}{\partial X^2} + \frac{\partial D_{j,j}}{\partial X}\frac{\partial C_j}{\partial X} \quad j,k = \mathrm{Al,Cr} \qquad (3a)$$

Equation (3a) can be further expanded as:

$$\frac{\partial\left(D_{j,j}\left(\frac{\partial C_j}{\partial X}\right)\right)}{\partial X} = D_{j,j}\frac{\partial^2 C_j}{\partial X^2} + \left(\frac{\partial D_{j,j}}{\partial C_j}\frac{\partial C_j}{\partial X} + \frac{\partial D_{j,j}}{\partial C_k}\frac{\partial C_k}{\partial X}\right)\frac{\partial C_j}{\partial X} \quad j,k = \mathrm{Al,Cr} \qquad (3b)$$

A similar equation exists for the second term on the RHS of equation (2), namely:

$$\frac{\partial\left(D_{j,k}\left(\frac{\partial C_k}{\partial X}\right)\right)}{\partial X} = D_{j,k}\frac{\partial^2 C_k}{\partial X^2} + \left(\frac{\partial D_{j,k}}{\partial C_j}\frac{\partial C_j}{\partial X} + \frac{\partial D_{j,k}}{\partial C_k}\frac{\partial C_k}{\partial X}\right)\frac{\partial C_k}{\partial X} \quad j,k = \mathrm{Al,Cr} \qquad (3c)$$

Substituting equation (3b) and (3c) into the two terms on the right hand side of equation (2) yields:

$$\frac{\partial C_j}{\partial t} = D_{j,j}\frac{\partial^2 C_j}{\partial X^2} + \left(\frac{\partial D_{j,j}}{\partial C_j}\frac{\partial C_j}{\partial X} + \frac{\partial D_{j,j}}{\partial C_k}\frac{\partial C_k}{\partial X}\right)\frac{\partial C_j}{\partial X} + D_{j,k}\frac{\partial^2 C_k}{\partial X^2} + \left(\frac{\partial D_{j,k}}{\partial C_j}\frac{\partial C_j}{\partial X} + \frac{\partial D_{j,k}}{\partial C_k}\frac{\partial C_k}{\partial X}\right)\frac{\partial C_k}{\partial X} \quad j,k = \mathrm{Al,Cr} \qquad (4)$$

Initially, transport associated with oxidation and the interdiffusion of the coating and substrate may be viewed as independent problems. Hence, at short times, coating/substrate interdiffusion can be treated as interdiffusion between two semi-infinite materials at a location centered around the coating/substrate interface. Similarly, oxidation of the coating can be treated as oxidation of a semi-infinite material affecting only a thin region below the surface of the coating. These two regions, the "inner" diffusion zone resulting from coating/substrate interdiffusion and the

*The notation j, k = Al, Cr refers to the two conditions where j = Al, k = Cr or j = Cr, k = Al.

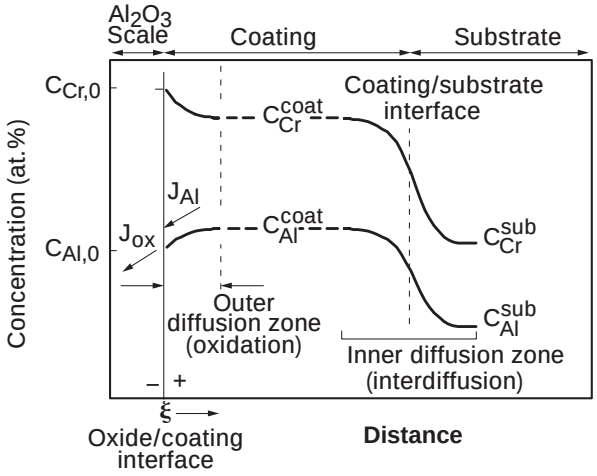

Figure 2.—Schematic concentration profiles after a short oxidation exposure.

"outer" diffusion zone resulting from transport associated with oxidation, are shown schematically in figure 2. At longer times, the two diffusion zones will overlap and diffusion associated with the two regions must be considered together. A solution to Fick's second law (eq. (2)), whether analytical or numerical, requires initial and boundary conditions. The boundary condition at the oxide/coating interface is discussed in the following paragraphs whereas the initial conditions and other boundary conditions used by the COSIM model are discussed in a later section.

For isothermal oxidation, the boundary condition at the oxide/coating interface, given as the rate of Al consumption, is well defined and decreases uniformly with time (the time dependence of the rate is inversely proportionate to the square root of time). However, for cyclic oxidation, the rate of Al consumption can vary in a nonuniform manner as the thickness of the oxide scale increases during the high temperature exposure but decreases on cooling as spallation occurs (ref. 2). In the present diffusion model, a separate model simulating oxide growth and spallation during cyclic oxidation has been adopted to provide the oxide/coating boundary condition. This oxide growth and spalling model (ref. 3), designated COSP by the authors, predicts the rate of Al consumption during each cycle by continuously tracking the thickness of the oxide scale, accounting for growth during high-temperature exposures, and partial oxide loss on cooling. This rate of Al consumption (J_{ox}) predicted by COSP is used as the boundary condition for the diffusion model. Hence, the supply of Al within the coating to the oxide/coating interface must equal J_{ox}. However, since Al is consumed from the coating, the coating surface recedes due to the loss of matter. This recession (ξ) is given as (ref. 4):

$$\xi = -V_{Al} J_{ox} t \tag{5}$$

where V_{Al} is the partial molar volume of Al in the coating and J_{ox} is the rate of Al consumption discussed above (which is also the flux of Al entering the oxide). J_{ox} can also be considered as the Al flux to the left of the moving oxide/metal interface in figure 2, or the Al flux *away from* the interface. Similarly, J_{Al} is the flux in the metallic coating *towards* the interface. Because of the interface motion, J_{ox} is greater than J_{Al} according to the relationship:

$$J_{ox}\Big|_{X=\xi^-} = \alpha \;\; J_{Al}\Big|_{X=\xi^+} \tag{6}$$

where ξ^- and ξ^+ refer to the left hand side and right hand side of the oxide/coating interface, respectively, as shown in figure 2. The parameter *a* in equation (6) is given as:

$$a = {}^{1}\!\Big/\!\left(1 - V_{Al} * C_{Al,0}\right) \tag{7}$$

where $C_{Al,0}$ is the Al concentration in the coating at the oxide/coating interface (fig. 2). Obviously, for the hypothetical case for $V_{Al} = 0$ (the Al atoms in the coating have no volume), $a = 1$, the Al flux to the interface, J_{Al}, becomes equal to the Al flux away from the interface, J_{ox}, and the interface is stationary. The partial molar volume for Al was assumed independent of concentration due to a lack of available data for most alloy systems of interest (e.g., the γ, Ni solid solution phase in NiCrAl alloys).

Hence, the boundary condition for Al at the oxide/coating interface is given by equation (6) whereby the rate of Al consumption due to oxide formation, predicted by the COSP oxide model, J_{ox}, is equated to the supply, or flux, of Al to the interface within the coating, J_{Al}, while taking into account the motion of the interface through the parameter a. The rate of Al transport within the coating to the oxide/coating interface (i.e., the Al flux, J_{Al}) is given by equation (1), stated as:

$$J_{Al}\big|_{X=\xi^+} = -D_{Al,Al}\frac{\partial C_{Al}}{\partial X} - D_{Al,Cr}\frac{\partial C_{Cr}}{\partial X} \tag{8}$$

Although no Cr is assumed to enter the Al_2O_3 scale, the surface recession requires the diffusion of Cr and Ni away from the oxide/coating interface into the coating. The boundary condition for Cr is:

$$J_{Cr}\big|_{X=\xi^+} = -D_{Cr,Al}\frac{\partial C_{Al}}{\partial X} - D_{Cr,Cr}\frac{\partial C_{Cr}}{\partial X} = C_{Cr,0}\frac{d\xi}{dt} \tag{9}$$

where J_{Cr} is the flux of Cr in the coating away from the interface and $C_{Cr,0}$ is the Cr concentration in the coating at this interface (fig. 2). In the computer program, the calculations for COSP have been contained in a subroutine to facilitate the incorporation of other oxide growth and spalling models (e.g., ref. 5).

Finite-Difference (F-D) Method

The initial step in the F-D technique is to establish a grid of equispaced nodes across the region of the material over which diffusion will occur (i.e., the diffusion zone). Each node has a specific concentration associated with it. Fick's laws (eqs. (1) and (4)) are replaced with F-D equivalents based on small differences in concentration, ΔC, distance, ΔX, and time, Δt. A solution yielding the concentration profile at some time t is derived by solving the appropriate F-D equivalents for small time increments (Δt) in an iterative manner. These iterations, or time steps, are continued until the Δt increments sum to the desired time t. A portion of a diffusion zone at time t and the new concentrations at time $t + \Delta t$ is shown schematically in figure 3 (ref. 6). Because of the typically large number of repetitive and tedious calculations made each iteration, F-D solutions are ideally handled by a computer.

The F-D equivalents to Fick's laws are based on Taylor series expansions (refs. 7 and 8). The F-D equivalent of Fick's 2nd law (eq. (4)) can be given by either an explicit or implicit representation. The explicit form was used throughout this work. F-D expressions for both first and second order partial derivatives for concentration with respect to distance, given on the right hand side of equation (4), were given by first central difference equations, stated as:

$$\frac{\partial C_j}{\partial X} = \frac{-C^i_{j,n+1} - C^i_{j,n-1}}{2\Delta X} \tag{10}$$

$$\frac{\partial^2 C_j}{\partial X^2} = \frac{-C^i_{j,n+1} - 2C^i_{j,n} + C^i_{j,n-1}}{(\Delta X)^2} \tag{11}$$

where j refers to either Al or Cr, n refers to the node number and the superscript i refers to the current iteration at time t. These equations apply to all nodes n where nodes $n - 1$ and $n + 1$ exist. A first forward difference expression was used for $\partial C/\partial t$ in the left hand side of equation (4), given as:

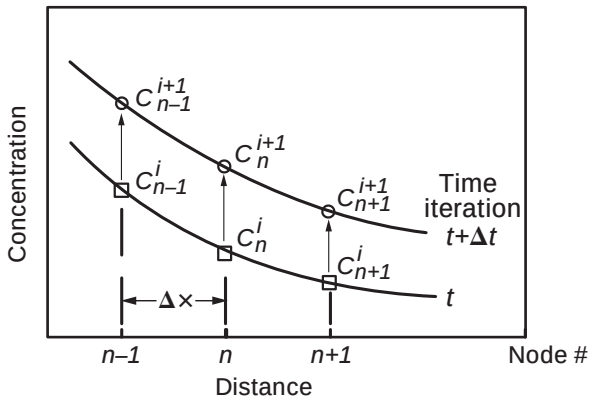

Figure 3.—Schematic diffusion zone for time t (squares) and time t+Δt (circles). The concentration subscript refers to the node number and the superscript refers to the time iteration.

$$\frac{\partial C_j}{\partial t} = \frac{C^{i+1}_{j,n} - C^{i}_{j,n}}{\Delta t} \qquad j = \mathrm{Al, Cr} \tag{12}$$

where the superscript $i + 1$ refers to the next iteration at time $t + \Delta t$. The time increment Δt for the explicit F-D method is limited by a stability criterion typically given as:

$$D_{\max} \frac{\Delta t}{(\Delta X)^2} \le 0.25 \tag{13}$$

where D_{max} is the appropriate diffusion coefficient which is discussed in a later section. Although Δt is initially very small, the grid expansion scheme described below allows the time increment each iteration to increase, generally allowing long term simulation of oxidation with a reasonable number of program iterations.

The last terms in equation (4) to be discussed are the eight derivatives of the diffusion coefficients ($\partial D/\partial C$). Obviously, the concentration dependence of the four ternary diffusivities is required to evaluate this expression. The concentration dependence of the diffusivities is input to the computer program in polynomial form. The computer program determines an abbreviated polynomial expression for each derivative using the polynomial coefficients. If some, or all of the ternary diffusivities are concentration independent, or if the concentration dependence is not known and cannot be input to the program, the value of the appropriate derivatives is zero. Hence, each of the terms on the right hand side of equation (4) have known values at time t and can be evaluated. Since Δt is determined from the stability criterion in equation (13) and values for $C^{i}_{j,n}$ are known, values for $C^{i+1}_{j,n}$ from the left hand side of equation 4 for the new time ($t + \Delta t$) can be calculated.

For the boundary condition at the oxide/coating interface (eqs. (8) and (9)), no node exists in the oxide (i.e., no $n - 1$ node exists, where n is located at the interface) so that the central difference formulas in equations (10) and (11) cannot be used. Consequently, concentration gradients ($\partial C_j/\partial X$) at the interface were determined using second order forward difference equations. Hence, the F-D equivalent for the Al concentration gradient in both equations (8) and (9) at the interface was given as:

$$\left.\frac{\partial C_{Al}}{\partial X}\right|_{X=\xi^+} = \frac{-C^{i}_{Al,2} + 4C^{i}_{Al,1} - 3C^{i}_{Al,0}}{2\Delta X} \tag{14}$$

where the second subscript number refers to the node which is numbered sequentially from zero at the interface and the superscript refers to the current iteration at time t (i.e., $C^{i}_{Al,0}$ is the Al concentration in the coating at the oxide/coating interface, $X = \xi^+$ shown in fig 2). A similar expression was used for the Cr gradient. The diffusivities for

equations (8) and (9) were evaluated for the Al and Cr concentrations in the coating at the oxide/coating interface (i.e., $C_{Al,0}$,$C_{Cr,0}$). Substituting equation (14) into equations (8) and (9) together with equations (5) to (7) are sufficient to yield the interface concentrations $C^i_{Al,0}$,$C^i_{Cr,0}$.

COSIM Computer Program

The COSIM program initially establishes separate diffusion zones for interdiffusion and oxidation. Typically, these diffusion zones are set to be very narrow (i.e., 0.1 μm) but are allowed to expand with increasing interdiffusion. When the diffusion zones eventually overlap within the coating, the two separate zones are combined and the simulation continues with a single zone across the coating and into the substrate. This approach allows the use of a reasonable number of nodes in a zone yet with a fine node spacing during the early times when the concentration gradients are steep. For greater accuracy, all variables used in the iterative calculations were defined as double precision. All input to the COSIM program is through the READ11 subroutine, discussed in a following section.

The starting width of the outer and inner zones, *DXCOAT* and *DXSUB*, and the number of nodes in each zone, *NCOAT* and *NSUB*, respectively, are parameters input to the program. The spacing between nodes, *DELX1* for the outer zone and *DELX2* for the inner zone (i.e., ΔX in the F-D equations), is equal to the width of the zone divided by the number of nodes minus one (i.e., *NCOAT-1* and *NSUB-1,* the minus one since both zones are bounded by nodes). The concentrations associated with each node for both diffusion zones are stored in arrays labeled 'Al' and 'Cr'. In the outer diffusion zone, the nodes are numbered sequentially starting with zero at the oxide/coating interface through *NCOATH* (equal to *NCOAT-1)*. The *NSUB* nodes in the inner diffusion zone are numbered from *NSUBL* (low) to *NSUBH* (high) with *NSUBL* starting at a value of *NCOAT+2*. Central difference equations, such as equations (10) and (11), cannot operate on the endpoints of a zone since concentrations at nodes $n + 1$ and $n - 1$ are required. Although forward and backward difference expressions can be used at these locations, a common technique is to add ancillary nodes to the zone to allow the continued use of central difference equations. Hence, an additional ancillary node was added to the inner end of the outer diffusion zone and an ancillary node was added to each end of the inner diffusion zone (*NSUBL-1* and *NSUBH+1*). The ancillary nodes maintain assigned constant concentration values. The node numbering scheme is schematically shown in figure 4 for *NCOAT*=7 (e.g., 7 nodes numbered 0 to 6) and *NSUB*=11 (e.g., 11 nodes numbered 9 to 19). The ancillary node for the outer diffusion zone is shown as node 7 and the ancillary nodes for the inner diffusion zone are shown as nodes 8 and 20. As shown, different values for *DXCOAT* or *DXSUB*, or for *NCOAT* or *NSUB,* may result in different values for *DELX1* or *DELX2*.

Initial Conditions

Initially, each of the nodes in the outer zone are assigned the concentration of the coating. The ancillary node (node 7 in fig. 4) maintains this coating concentration until the inner and outer diffusion zones overlap. These initial concentrations for the outer zone are shown in figure 4. An error function solution was used to assign the coating and substrate compositions to the nodes in order to provide a smooth transition between the coating and substrate compositions. The *NSUBL* to *NSUBH* nodes in the inner zone are assigned concentrations as:

$$C_j = C_j^{coat} + \left(C_j^{sub} - C_j^{coat}\right) * \frac{1}{2}\left(1 + erf\left(X_{\mathrm{mod}}\right)\right) \qquad j = \mathrm{Al}, \mathrm{Cr} \tag{15}$$

where C_j^{coat}, C_j^{sub} refer to the initial concentration of the coating and substrate, respectively and X_{mod} is a modified distance parameter ranging from ±2 across the diffusion zone of width *DXCOAT*. This range in X_{mod} produces a smooth concentration gradient with end compositions within 0.5 percent of C_j^{coat}, C_j^{sub}. The coating composition was assigned to the ancillary node at *NSUBL*-1 (node 8 in fig. 4) and the substrate composition was assigned to the ancillary node at *NSUBH*+1 (node 20 in fig 4). Again, these ancillary nodes maintain these assigned concentrations until the diffusion zones overlap (i.e., the ancillary nodes are not operated upon by Fick's 2nd law, as discussed below). The initial concentrations for the inner diffusion zone are also shown in figure 4.

Use of the error function solution to assign initial concentration values does not have a significant effect on later concentration values because of the small initial diffusion zone width and the small initial time increments. A value

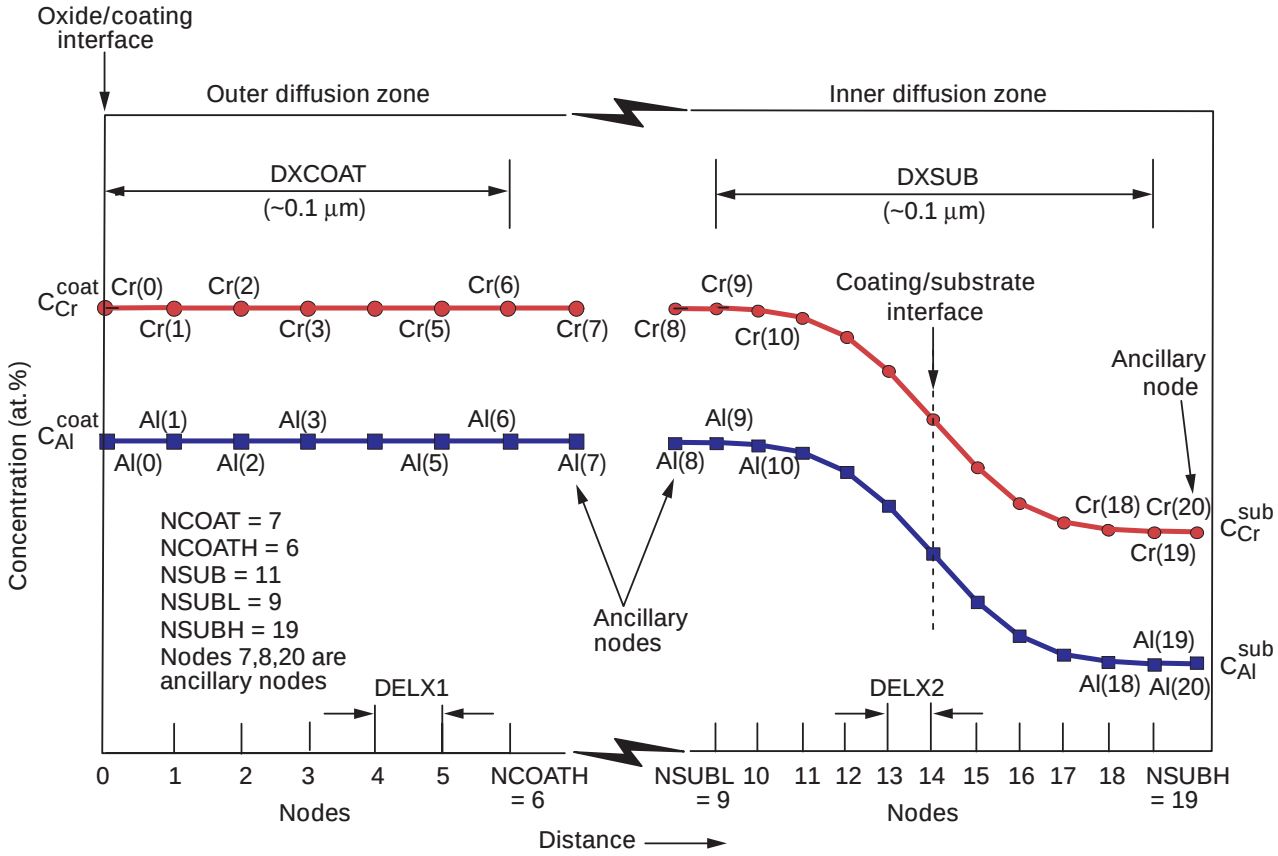

Figure 4.—Schematic of initial concentration profiles before oxidation exposure for NCOAT = 7 and NSUB = 11.

on the order of 0.1 μm was typically used for the initial diffusion zone width, *DXSUB*. Typically, 30 to 40 nodes are assigned to the zone so that the node spacing (ΔX) is 0.0025 to 0.003 μm. Substituting this latter value into equation 13 and using a typical value of 10^{-10} cm^2/s for D_{max} yields a time increment Δt of only 0.000225 sec. Hence, hundreds to thousands of iterations will typically be performed before the first minute of simulated exposure time allowing ample iterations for the starting concentrations to adjust to satisfy Fick's 2nd law (eqs. (2) to (4)).

Fortunately, when diffusion begins to affect the concentration at the ends of the zones, either at node *NCOATH*, *NSUBL* or *NSUBH*, the node spacings are allowed to expand (as shown in the following section) so that larger time increments can be used each iteration. Since the outer and inner zones may have different node spacings, the program determines the maximum diffusion coefficient (D_{max} in eq. (13)) for either the coating or substrate composition and uses the smaller of the two node spacings to determine the smallest time increment, *DELT* (i.e., Δt in the F-D equations), according to equation (13).

Surface Recession, Flexible Zones and Semi-Infinite Boundary Conditions

The COSIM model utilizes a flexible grid technique to account for surface recession and to simulate the semi-infinite boundary conditions. As the outer surface recedes due to Al loss, the entire outer zone is shifted and the concentrations at each node are adjusted. The technique used to accomplish this shift and adjustment is referred to as a "Murray-Landis" (M-L) transformation (ref. 9). This transformation shifts the nodes an amount proportional to their position from the moving boundary ($X = \xi$) to maintain a uniform node spacing. The semi-infinite boundary condition for the outer diffusion zone can be stated as:

$$C_i\big|_{x=\infty} = C_i^{coat} \qquad i = Al, Cr.$$

This boundary condition is approximated by increasing the zone width whenever diffusion "significantly changes" the concentration at the node *NCOATH*. Each iteration, the concentration at this node is changed slightly in accordance with Fick's 2nd law (eq. (4)). A "significant change" used in the COSIM program was taken as 0.005 at%. Varying this value from 0.002 to 0.008 at% changed the number of iterations required to reach a fixed time but had no significant effect on the predicted concentration profiles at short or long times (i.e., 1 and 1000 hr using the sample input data given in Appendix A). Hence, whenever the concentration of node *NCOATH* (either Al or Cr) varied from the coating composition by 0.005 at%, the zone width was expanded by *DELX1* and all node positions and concentrations were adjusted according to the M-L transformation. To further illustrate this operation, Al loss at the surface (node 0) and operation of Fick's 2nd law (eq. (4)) will eventually cause the initial Al profile in the outer diffusion zone (fig. 4) to appear as shown schematically by the solid squares in figure 5. Eventually, the Al concentration at node 6 will decrease to a value 0.005 at% below the concentration of the coating, C_{Al}^{coat}. During this iteration, the total zone width, *DXCOAT*, will be increased by an amount equal to the node spacing such that:

$$DXCOAT' = DXCOAT + DELX1 \tag{16}$$

The number of nodes remains constant but the new node spacing is given as:

$$DELX1' = DXCOAT'/(NCOAT - 1) \tag{17}$$

The node positions are shifted proportionately such that node 6 is shifted inward by *DELX*1 while node 0 at the surface ($X = \xi$) undergoes no shift (fig. 5). The concentrations at each node are shifted in a similar manner with node 6' taking the old position of the ancillary node 7 and being reassigned the concentration of the coating, C_i^{coat} (the concentration previously held by the ancillary node 7 at the same position). The ancillary node maintains the coating composition at the new position.

The semi-infinite boundary conditions at either end of the inner diffusion zone are simulated in a like fashion. Hence, as diffusion changes the concentrations at nodes *NSUBL* or *NSUBH* in the inner diffusion zone by 0.005 at%, the zone width is expanded by the node spacing, *DELX*2 and the node positions and concentrations are adjusted according to the M-L transformation. The expansion occurs at the end of the zone where the concentration change occurred such that the inner diffusion zone expands either into the coating or into the substrate for changes at node *NSUBL* or *NSUBH*, respectively. The ancillary nodes (*NSUBL*-1 and *NSUBH*+1) maintain the substrate composition and are repositioned at the ends of the zones with the new node spacing. Whenever the zones are expanded or contracted, a new time increment *DELT,* is calculated according to equation (13). As discussed above, the smaller of the

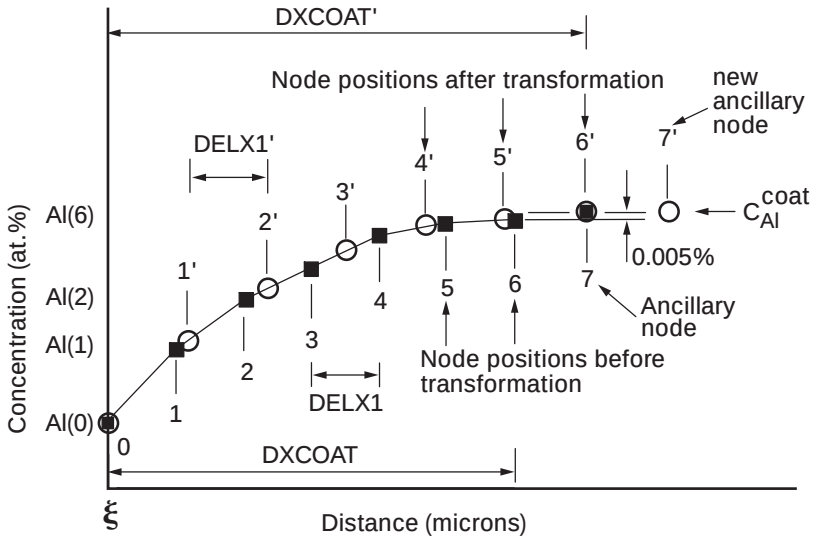

Figure 5. Schematic Al concentration profile in the outer diffusion zone before and after the M-L transformation.

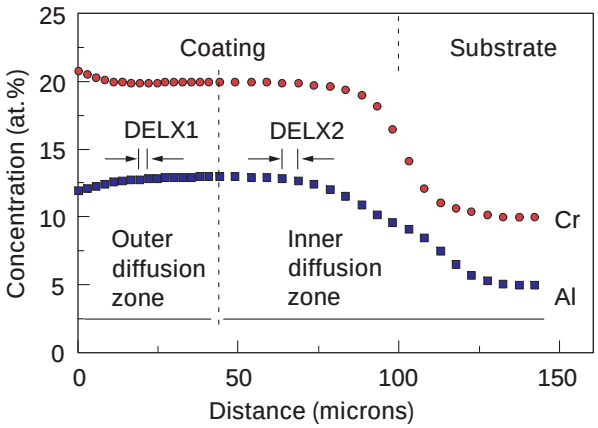

Figure 6.—(a) Al and Cr concentration profiles at the time (time = 1.34 hrs) when the inner and outer diffusion zones overlap. Input data for run given in Appendix A. (Alternate nodes hidden for clarity.)

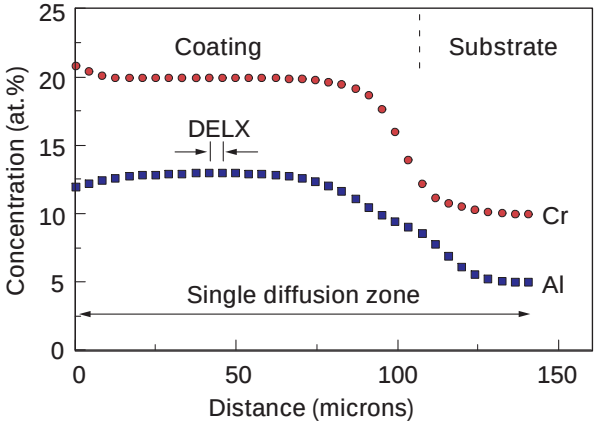

Figure 6.—(b) Al and Cr concentration profiles at the time = 1.34 hrs following the spline operation. Input data for run given in Appendix A. (Alternate nodes hidden for clarity.)

time increments calculated for the outer and inner diffusion zones is always used. Because of the concentration dependence of the diffusivities, one end of the inner diffusion zone may expand more than the other over the course of several thousand iterations. Although the inner and outer zones may appear very different with different widths, different numbers of nodes and different node spacings, both zones always operate with the same time increment such that the total exposure time for both the inner and outer diffusion zones is always identical.

The expansion of the inner and outer zones will eventually result in their impingement, or overlap, within the coating. From this time onward, the two diffusion problems, oxidation and coating/substrate interdiffusion, become coupled and can no longer be operated independently. At the time that the diffusion zones overlap, the COSIM model sums the current width of the inner and outer zones and redefines a single zone of equal width. Equidistant node spacings are also calculated using the combined number of nodes from the two zones (i.e., *NCOAT+NSUB*). The COSIM model then fits a natural cubic spline curve (refs. 10 and 11) through the concentration profiles from both zones and generates a single profile through the coating and into the substrate for both Al and Cr at each of the new node positions. Figure 6(a) shows predicted Al and Cr concentration profiles in the coating and substrate at the time (time = 1.34 hr) when the two diffusion zones overlap. The width of the inner diffusion zone is significantly larger with a larger number of nodes and a larger node spacing than that for the outer diffusion zone. Figure 6(b) shows the same data after the spline interpolation. Note that the nodes are equally spaced across the entire diffusion zone. The spline subroutines are based on equations and code given in reference 11. Following the combination of the two diffusion zones, the COSIM model continues to simulate Al transport to the surface and interdiffusion of the coating and substrate. Both boundary conditions, at the oxide/coating interface and in the substrate remain as before the combination. Loss of Al continues to cause surface recession and a shrinking of the zone while diffusion in the substrate continues to result in zone expansion. Within the program, the transition from two zones to one is reflected in the value of the parameter *ZONE*. The value of *ZONE* changes from two to one after the diffusion zones are combined and the program operates on the single diffusion zone thereafter. Parameters are redefined so that the new, single diffusion zone utilizes parameters associated with the outer diffusion zone (e.g., *DELX1*, *DELT1*, etc.) The model continues to simulate increasing oxidation exposure with each iteration of time. The program can print out concentration data at intermediate times (e.g., 50, 100, 500, 1000, 5000 hr) or at some predetermined failure condition (e.g., $C_{Al,0}$ = 0 or 5 at%). Figure 7 shows predicted concentration profiles after 1, 100 and 1000 hr. Diffusivities for the current examples were taken from reference 12. The value for the partial molar volume of Al was taken from reference 13.

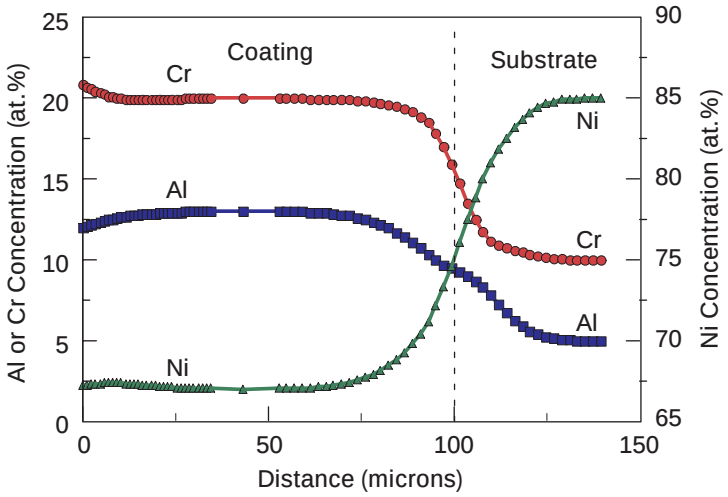

Figure 7.—(a) Al, Cr and Ni concentration profiles at time = 1.0 hr using the input data given in Appendix A.

Occasionally, oscillations in the values of the Al concentration at the oxide/coating interface, *AL(0)*, will occur the first few cycles. These oscillations can cause the computed value for the *AL(0)* to become negative or to exceed 100 at%. It has also been observed that a very high initial flux from the COSP oxide growth and spalling model can also cause the computed value for *AL(0)* to be negative for hundreds of cycles. To protect against this physical impossibility, the program limits the values of *AL(0)* to be between 0 and 100 at% (i.e., negative values are set equal to zero and values >100 are set equal to 100). The consequence of these limits is that equation (6) is not satisfied during these iterations. However, monitoring the computed values for *AL(0)* typically show convergence to acceptable values at relatively short times (i.e., less than one hour when unreasonably high values for K_p were used with the example input data given in Appendix A). Since these early oscillations could falsely trigger the test for *AL(0)* less than a critical Al concentration (i.e., *AL(0)* ≤ *CRITAL)* this test is not initiated in the program during the first two hours of oxidation exposure. No problems have been encountered using test cases using various values for *CRITAL,* including zero.

Certain constraints on the time increment used each iteration (*DELT*) are desirable when simulating certain oxidation conditions. For instance, a value for *DELT* much <1 hr might be desirable during cyclic oxidation with 1 hr cycles. In this case, a value of *DELT* of one or 5 min might be desired so that several iterations during oxide growth can be performed between periods of oxide spallation each cycle. In contrast, for isothermal oxidation for long periods, it might be preferable to have no constraint on the values for *DELT* in order to minimize the number of iterations to reach a solution. To provide this flexibility, a maximum value for *DELT* (*MAXDT*) may be input to the program. The default condition within the program is that no constraint be made on *DELT* beyond that given in equation (13).

Fortran version

The COSIM program was initially compiled and executed on mainframe computers and later revised for execution on a desktop PC. The current version of the program has been compiled with ANSI FORTRAN95. Very few extensions from the ANSI FORTRAN77 standard were used. These extensions consist of the use of the NAMELIST command, used for ease in reading and writing to files, and extended length variable names exceeding 6 characters and containing special characters which were used for better clarity in the description of the variables.

Description of Program Elements

Main Program

The main program defines all common blocks, initializes parameters, calls subroutines to define and initialize both zones and directs program flow. The basic iterations are performed in the main program calling the FSL (Fick's Second Law) subroutine to calculate new concentrations, and JEXT (COSP oxide spalling model) subroutine to provide the boundary condition for the oxide/coating interface. In addition, the main program also checks the end point nodes (*NCOATH, NSUBL* and *NSUBH*) to determine when the diffusion zones need to be expanded and calls the M_L (Murray-Landis) subroutine to shift nodes and concentrations as needed. Checks are also made within the main program for overlap of diffusion zones, whether the maximum number of iterations has been exceeded, and whether a time has been reached at which output is desired. As an option, the program also checks whether the surface Al concentration (*AL(0)*) has decreased below a critical value (*CRITAL*). Output may consist of writing concentration profiles at a specific time (e.g., 100 and 500 hrs) with appropriate headers and documentation to unit 6 (see Appendix B). This output is appropriate for printing. At the same time that concentration profiles are written to unit 6, the concentration data is written to unit 14 with minimal headers and without further documentation (see Appendix C). The data written to unit 14 is useful for reading into a graphing program to plot concentration/distance profiles. As a further option, select data (time (hrs), surface concentrations AL(0), CR(0), rate of Al consumption and total weight of Al consumed) are written to unit 15 on a more frequent time interval (see Appendix D). The data written to unit 15 is useful for plotting and viewing the time dependence of certain important variables. Examples of the data written to unit 15 are shown in figures 8(a) to (c). Subroutines and parameters are discussed below. An alphabetical list of all program variables is given in Appendix E. Flow charts for the main program and subroutines are given in Appendix F.

Subroutine READ11

The READ11 subroutine reads three descriptive character strings of 80 characters each. These character strings may contain any alphanumeric data and can be used to describe the conditions of the particular run. The names of the character string variables are: *SAMPLE*, *TITLE1* and *TITLE2*. All other data required by the program are entered via three NAMELIST statements, *INPUT*, *OX_INP*, and *INP15*. All data are read from unit 11. The file assigned in the subroutine to unit 11 is "COSIM.INP". Descriptions of the named input variables are given below. Parameters described as optional may be removed from the COSIM.INP file (i.e., *CRITAL = X* may be removed) or the parameter may remain in the file with the default value given below (i.e., *CRITAL* = –1.0 indicates to the program no test for a critical Al concentration). An example set of input data are given in Appendix A.

Parameters and definitions read in through the INPUT namelist are:

ALCOAT	Al concentration in the coating (at%)
CRCOAT	Cr concentration in the coating (at%)
ALSUB	Al concentration in the substrate (at%)
CRSUB	Cr concentration in the substrate (at%)
MW_AL	Molecular weight of Al (gm/mole)
MW_CR	Molecular weight of Cr (gm/mole)
MW_NI	Molecular weight of Ni (gm/mole)
DENSITY	Density of the coating (gm/cm^3)
VBAR	Partial molar volume of Al in the coating (cm^3/mole)
THICK	Coating thickness (μm)
TEMP	Oxidation temperature (numeric)
TMAX	Time(s) at which output is desired (hr) (e.g., 100, 500, 2000)
NCOAT	Number of nodes in the "outer" coating diffusion zone
NSUB	Number of nodes in the "inner" coating/substrate diffusion zone
DXCOAT	Initial width of the outer diffusion zone (μm)
DXSUB	Initial width of the inner diffusion zone (μm)

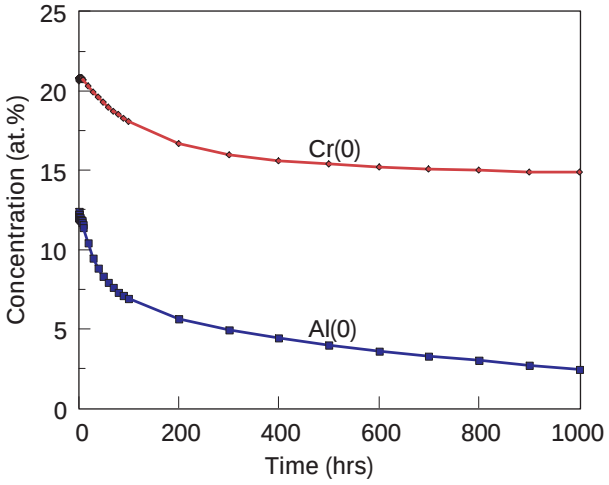

Figure 8.—(a) Time dependence of Al and Cr concentrations at the surface (Al(0) and Cr(0)) from data written to unit 15 (File OUT15) for the input data given in Appendix A.

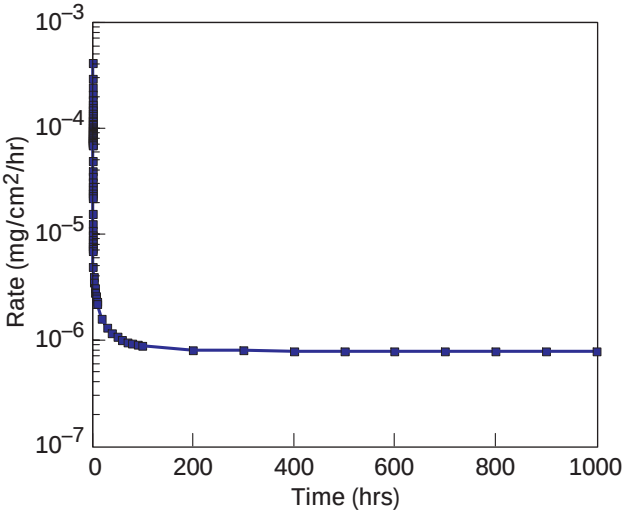

Figure 8.—(b) Time dependence of WMDOT (rate of Al consumption) from data written to unit 15 (File OUT15) for the input data given in Appendix A.

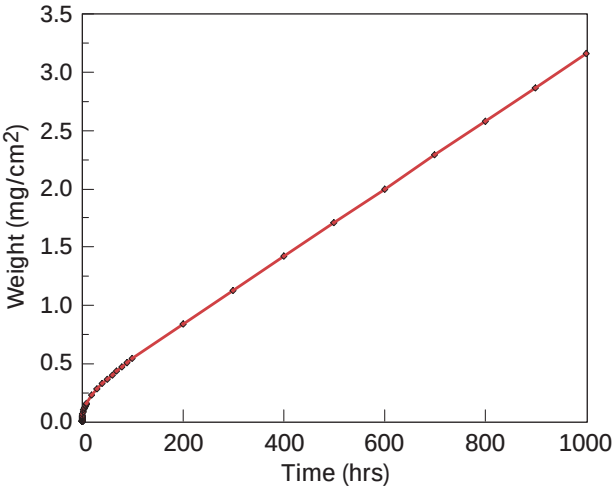

Figure 8.—(c) Time dependence of WMINT (weight of Al consumed) from data written to unit 15 (File OUT15) for the input data given in Appendix A.

MAXLOOP Maximum number of iterations (*ILOOP*) allowed. Can be used to halt and print data after a specific number of iterations, or to protect against infinite looping. Parameter is optional. (Default is 1,000,000)

MAXDT Maximum desired time increment per iteration (*DELT*), (min). Parameter is optional. (Default is no limit on *DELT* which is set in the program as *MAXDT* = –1.0.)

CRITAL Critical surface Al concentration. When *AL(0)* decreases to *CRITAL*, program calls subroutine WRT6F, then stops. Parameter is optional. (Default is no test for a critical surface Al concentration which is set in the program as *CRITAL* = –1.0.)

Parameters and definitions read in through the OX_INP namelist are:

MODEL Designates parabolic (*MODEL* = 1) or power law oxide growth kinetics (*MODEL* = 2) (see *AGROW* below)

KP Parabolic oxide growth parameter (used with *MODEL* = 1) due to weight of oxygen in the oxide (i.e., not weight of oxide). Units of $mg^2/cm^4/hr$.

AGROW Power law oxide growth parameter (used with *MODEL* =2) with units of mg/cm^2, defined as:

$$\Delta W = AGROW * time^{BGROW}$$

where time is given in hours.

BGROW Power law oxide growth parameter (unitless) as defined above.

A0 The ratio of the weight of Al in the oxide to the weight of oxygen in the oxide (Unitless) (e.g., A0 = 1.1242 for Al_2O_3).

TCYCLE The hot cycle duration for each thermal cycle, in hours.

QO The spall parameter for the COSP spalling model (ref. 3)

ETA Additional spall parameter for the COSP spalling model (ref. 3)

Five parameters are used to define each of the four ternary diffusion coefficients. These parameters are read in through the *D_COEF* namelist. The parameters are:

A110, A111, A112, A113, A114, A115
A120, A121, A122, A123, A124, A125
A210, A211, A212, A213, A214, A215
A220, A221, A222, A223, A224, A225

The parameters are defined in the equations:

$D_{AlAl}(C_{Al},C_{Cr})=[A110+(A111*C_{Al})+(A112*C_{Cr})+(A113*C_{Al}^2)+(A114*C_{Cr}^2)]*A115$
$D_{AlCr}(C_{Al},C_{Cr})=[A120+(A121*C_{Al})+(A122*C_{Cr})+(A123*C_{Al}^2)+(A124*C_{Cr}^2)]*A125$
$D_{CrAl}(C_{Al},C_{Cr})=[A210+(A211*C_{Al})+(A212*C_{Cr})+(A213*C_{Al}^2)+(A214*C_{Cr}^2)]*A215$
$D_{CrCr}(C_{Al},C_{Cr})=[A220+(A221*C_{Al})+(A222*C_{Cr})+(A223*C_{Al}^2)+(A224*C_{Cr}^2)]*A225$

Parameters and definitions read in through the *INP15* namelist are:

IO15 I/O switch for printing specific output to unit 15. When set to 1, the program prints specific data at predetermined intervals every 0.01, 0.1, 1.0, 10.0, hrs. Parameter is optional. (Default option is no printing to unit 15 which is set in the program as *IO15* = 0.

Subroutine WRT6

Subroutine to write out all input data to unit 6 with descriptive format statements. The file assigned in the subroutine to unit 6 is "OUT6". Sample output printed by WRT6 is given in Appendix B.

Subroutine WRT6F

Subroutine to write out current status. Simulated exposure time, surface recession, current zone widths and node spacings, weight of Al consumed and concentration profile data is written to unit 6 (file "OUT6"). Sample output printed by WRT6F after 1, 100 and 1000 cycles is given in Appendix B. For convenience in plotting the concentration profiles, node positions from the original surface in microns (i.e., *DIST*), Al and Cr, and Ni concentrations in at% and Time (hrs) are also printed to unit 14 (file "OUT14). Example output from file OUT14 is shown in Appendix C.

Subroutine WRT12

Subroutine which writes intermediate concentration/distance data for both diffusion zones to unit 12 at the time when the two diffusion profiles first overlap. The data is written sequentially as "Distance, C_{Al}, C_{Cr}." Unit 12 is assigned in the subroutine to file "OUT12." After the data for both diffusion zones are written to unit 12, the file is repositioned to the first record (rewind unit = 12) to prepare the file to be read by the SPLINE subroutine. The SPLINE subroutine is called, reads the data in OUT12 and fits a single smooth curve to the concentration/distance

data. The SPLINE subroutine rewrites the new concentration/distance data over the old data in file OUT12. The WRT12 subroutine then reads the new concentration/distance data from file OUT12. The new data for the single diffusion zone is reassigned in terms of the outer diffusion zone (i.e., the new zone width is assigned to *DXCOAT*, the new node spacing to *delx1*, and the innermost concentrations (*ALCOAT*, *CRCOAT*) are assigned the values *ALSUB*, *CRSUB*.

Subroutine WRT15

Subroutine which writes out specific data at regular intervals to unit 15 when *IO15* = 1. The data written to unit 15 are: time(hrs), surface concentrations *AL*(*0*) and *CR*(*0*), the rate of Al consumption *WMDOT*, and the total Al consumption *WMINT*. The data are written in increasing intervals of 0.01, 0.1, 1.0, 10, 100 hrs. Unit 15 is assigned in the MAIN program to file "OUT15". The subroutine is useful for tracking the time dependence of specific parameters. Sample output printed by WRT15 is given in Appendix D.

Subroutine MAXOUT

Subroutine called when *MAXLOOP* iterations are exceeded in MAIN program. Message is printed to unit 6 as well as current time *TIME* and time increments *DELT1*, *DELT2*. Subroutine WRT6F is called.

Subroutine CRITSB

Subroutine called when surface Al concentration *AL(0)* decreases below *CRITAL* (for *CRITAL* $\geq$ *0.0* specified in COSIM.INP. Message is printed to unit 6 as well as current time value for *CRITAL*. Subroutine WRT6F is called.

Subroutine OX_INIT

Subroutine to initialize variables for *COSP* oxide growth and spalling model. For *MODEL* = 1 (parabolic oxide growth), *KP* is redefined in terms of *AGROW* and *BGROW*.

Subroutine UNITS

Subroutine to convert units to a consistent set used throughout the program. Parameters converted are:

VBAR	Molar volume of Al from cm^3/mole to $(at\%)^{-1}$
DXCOAT	Microns to cm
DXSUB	Microns to cm
THICK	Microns to cm
DENSITY	g/cm^3 to mg/cm^3
ALWCOAT	Al concentration of the coating from at% to wt% (used in converting *WMDOT*, rate of Al consumption in mg/cm^2/hr predicted by COSP oxide spalling model to at%cm/s used in COSIM
TMAX(I)	All times in hrs converted to sec.
MAXDT	Time in minutes converted to sec.

Subroutine INIT1

Subroutine to set the initial concentration profile for the outer (oxidation) and inner (coating/substrate interdiffusion) diffusion zones. Concentrations for outer diffusion zone, nodes 0 to *NCOAT*, and inner diffusion zone, nodes *NSUBL*-1 to *NSUBH*+1 are assigned initial values as discussed above. Subroutine calls the Function DERF to generate an error function solution for the inner diffusion zone.

Subroutine DERF(*X*)

Function which returns the error function for parameter *X*.

Subroutine D_C(*Alx,Crx*)

Subroutine which returns values of the four interdiffusion coefficients and derivatives at the concentration *Alx,Crx*. Since the concentration dependence of the diffusivities for γ NiCrAl alloys is known in polynomial form (ref. 12), derivatives with respect to concentration (i.e., $\partial D/\partial C$, see eq. (4)) are calculated and evaluated at the specific concentration *Alx,Crx*.

Subroutine JEXT

Subroutine version of the COSP oxide growth and spalling program (ref. 3). Subroutine returns values for the rate of Al consumption, *WMDOT* for the outer boundary condition. Subroutine tracks oxide growth each iteration for time increment *DELT*, the total weight of Al consumed *TOTWM*, and the amount of oxide spall each thermal cycle.

Subroutine M_L(*N1,N2,DELX,DX,AN*)

Subroutine to shift concentrations when a zone is expanded or contracted. Al and Cr concentrations are shifted as explained in the text.

N1 the node number where the maximum shift in node spacing occurs
N2 the node number where the minimum shift in node spacing occurs
DELX the node spacing
DX the amount the zone is to be shifted (negative to the left, positive to the right)
AN the number of nodes in the zone

Subroutine FSL(*N1,N2,DELX,DELT*)

Subroutine to perform Fick's second law calculations on the indicated nodes according to equation (4).

N1 the minimum node number upon which to operate
N2 the maximum node number upon which to operate
DELX the current node spacing
DELT the current time increment

Subroutines SPLINE(*M*), CUBIC, EVALUAT

Subroutines to read concentration/distance data for both inner and outer diffusion zones from unit 12, fit to a single smooth curve using natural splines, and redetermine concentrations at equal node spacings (ref. 10)

M number of nodes in the new zone (equal to *NCOAT+NSUB*)

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13. J.A. Nesbitt, NASA TM 83738, Cleveland, OH, 1984.

Appendix A

Unit 11 Data Input to the Program (File: COSIM.INP)

```
COSIM (Thick=100um, Kp=0.002, Qo=0.008, 1100C) 1/28/98
Coating: Ni-20Cr-13Al   Substrate: Ni-10.0Cr-5.0Al
1100C DIFFUSION DATA FROM: MET. TRANS.,18A,(1987) p2075 (TABLE V).
 &INPUT
  ALCOAT=13.0, CRCOAT=20.0,
  ALSUB=5.0,  CRSUB=10.0,
  MW_AL=26.98, MW_CR=52.0, MW_NI=58.71,
  DENSITY= 7.754,
  THICK=100.0, TEMP=1100.0,
  TMAX(1)=1.0,
  TMAX(2)=100.0,
  TMAX(3)=1000.0,
  NCOAT=30, NSUB=40,
  DXCOAT=0.1, DXSUB=0.1,
  VBAR=7.1,
  MAXLOOP=100000,
  MAXDT=1.0,
  CRITAL=-1.0,
  /
 &OX_INP
  MODEL=1,
  KP=0.002,
  AGROW=0.0, BGROW=0.0, A0=1.1242,
  TCYCLE=1.0, QO=0.008, ETA=1.0,
  /
 &INP15
  IO15=1,
  /
 &D_COEF
  A110=1.229,  A111=0.0731,  A112=-0.0083, A113=0.0101,
               A114=0.00016, A115= 1.0D-10,
  A120=0.0116, A121=0.0923,  A122=-0.0010, A123=0.00016,
               A124=0.000017,A125= 1.0D-10,
  A210=0.0766, A211=-0.0153, A212= 0.0837, A213=0.00062,
               A214=-0.0015, A215= 1.0D-10,
  A220=0.783,  A221=-0.0123, A222= 0.0247, A223=0.00096,
               A224=-0.00057,A225= 1.0D-10,
  /
```

Appendix B

Output to Unit 6 (File: OUT6)

```
COSIM (Thick=100um, Kp=0.002, Qo=0.008, 1100C) 1/28/98
 Coating: Ni-20Cr-13Al   Substrate: Ni-10.0Cr-5.0Al
 1100C DIFFUSION DATA FROM: MET. TRANS.,18A,(1987) p2075 (TABLE V).

     TEMPERATURE = 1100.0

     OUTPUT TIMES (HRS) =      1.0
                             100.0
                            1000.0

     AL, CR COATING COMPOSITION   (at%) = 13.00   20.00
     AL, CR SUBSTRATE COMPOSITION (at%) =  5.00   10.00

     MOLECULAR WEIGHT: AL, CR, NI = 26.98   52.00   58.71
     COATING DENSITY (g/cm^3)    =  7.75
     COATING THICKNESS (MICRONS) = 100.00
     INITIAL # OF NODES IN COATING   =  30
     INITIAL # OF NODES IN SUBSTRATE =  40
     INITIAL DIFFUSION ZONE WIDTH IN COATING   (MICRONS) =   .10
     INITIAL DIFFUSION ZONE WIDTH IN SUBSTRATE (MICRONS) =   .10
     PARTIAL MOLAR VOLUME OF AL = 7.100
     MAXIMUM ITERATIONS ALLOWED =  100000
     MAXIMUM DELT (MINUTES) =   1.0

     OXIDE GROWTH MODEL IS   1
     KP (MODEL=1) =   .002000
     A (MODEL=2)  =   .000000
     B (MODEL=2)  =   .000000
     A0 RATIO     =  1.124200
     TCYCLE       =  1.000000
     QO SPALLING PARAMETER    =   .008000
     ETA SPALLING PARAMETER =  1.000000

     DIFFUSION COEFFICIENT PARAMETERS
               0         1         2         3         4         5
      A11=  .123E+01  .731E-01 -.830E-02  .101E-01  .160E-03   .10E-09
      A12=  .116E-01  .923E-01 -.100E-02  .160E-03  .170E-04   .10E-09
      A21=  .766E-01 -.153E-01  .837E-01  .620E-03 -.150E-02   .10E-09
      A22=  .783E+00 -.123E-01  .247E-01  .960E-03 -.570E-03   .10E-09

     DATA IS WRITTEN TO FILE OUT15



    TIME (HRS)=    1.00
    DELT (SEC)=    7.41
    ITERATIONS=   6306

    SURFACE RECESSION (MICRONS)=    .13
    TOTAL WEIGHT OF AL CONSUMED AS OXIDE (WMINT)=      .05 (MG/CM^2)
```

Node #	Distance (microns)	Al	Cr	Ni
		at.%		
0	.1	11.96	20.84	67.19
1	1.3	12.06	20.70	67.24
2	2.5	12.16	20.56	67.28
3	3.7	12.25	20.43	67.31
4	4.9	12.34	20.32	67.34
5	6.1	12.42	20.22	67.36
6	7.2	12.49	20.14	67.37
7	8.4	12.55	20.08	67.38
8	9.6	12.60	20.03	67.37
9	10.8	12.65	19.99	67.36
10	12.0	12.69	19.97	67.34
11	13.2	12.73	19.95	67.32
12	14.3	12.76	19.95	67.29
13	15.5	12.79	19.94	67.27
14	16.7	12.81	19.95	67.24
15	17.9	12.84	19.95	67.22
16	19.1	12.86	19.95	67.19
17	20.3	12.87	19.96	67.17
18	21.4	12.89	19.96	67.15
19	22.6	12.91	19.97	67.13
20	23.8	12.92	19.97	67.11
21	25.0	12.93	19.98	67.09
22	26.2	12.94	19.98	67.08
23	27.4	12.95	19.98	67.06
24	28.6	12.96	19.99	67.05
25	29.7	12.97	19.99	67.04
26	30.9	12.98	19.99	67.03
27	32.1	12.98	19.99	67.02
28	33.3	12.99	20.00	67.01
29	34.5	13.00	20.00	67.01
32	51.4	13.00	20.00	67.00
33	53.6	12.99	20.00	67.01
34	55.8	12.99	20.00	67.02
35	58.1	12.98	19.99	67.03
36	60.3	12.96	19.99	67.05
37	62.5	12.94	19.98	67.08
38	64.7	12.91	19.97	67.11
39	66.9	12.87	19.96	67.17
40	69.1	12.82	19.94	67.24
41	71.3	12.75	19.91	67.34
42	73.5	12.65	19.88	67.47
43	75.7	12.54	19.84	67.63
44	78.0	12.39	19.78	67.83
45	80.2	12.21	19.71	68.09
46	82.4	11.98	19.62	68.40
47	84.6	11.72	19.51	68.77
48	86.8	11.41	19.36	69.23
49	89.0	11.05	19.17	69.77
50	91.2	10.67	18.89	70.44
51	93.4	10.28	18.45	71.27
52	95.6	9.92	17.78	72.30
53	97.9	9.63	16.82	73.56

54	100.1	9.38	15.62	75.00
55	102.3	9.16	14.32	76.52
56	104.5	8.90	13.10	78.00
57	106.7	8.55	12.11	79.35
58	108.9	8.08	11.42	80.50
59	111.1	7.54	11.01	81.46
60	113.3	6.97	10.78	82.25
61	115.6	6.44	10.64	82.93
62	117.8	5.99	10.51	83.50
63	120.0	5.65	10.38	83.97
64	122.2	5.41	10.25	84.34
65	124.4	5.24	10.15	84.61
66	126.6	5.13	10.08	84.78
67	128.8	5.07	10.04	84.89
68	131.0	5.03	10.02	84.95
69	133.2	5.01	10.01	84.98
70	135.5	5.00	10.00	84.99
71	137.7	5.00	10.00	85.00

SPLINE CALLED AT LOOP 6434

TIME (HRS)= 100.01
DELT (SEC)= 60.00
ITERATIONS= 12719

SURFACE RECESSION (MICRONS)= 1.42
TOTAL WEIGHT OF AL CONSUMED AS OXIDE (WMINT)= .54 (MG/CM^2)

Node #	Distance (microns)	Al (at.%)	Cr (at.%)	Ni (at.%)
0	1.4	6.89	18.09	75.03
1	7.9	6.99	17.95	75.07
2	14.4	7.08	17.79	75.13
3	20.9	7.17	17.62	75.21
4	27.5	7.26	17.43	75.31
5	34.0	7.34	17.23	75.44
6	40.5	7.41	17.01	75.58
7	47.0	7.48	16.79	75.74
8	53.5	7.54	16.55	75.92
9	60.0	7.59	16.30	76.11
10	66.5	7.64	16.04	76.32
11	73.0	7.69	15.77	76.55
12	79.5	7.73	15.49	76.78
13	86.0	7.76	15.21	77.03
14	92.6	7.78	14.93	77.29
15	99.1	7.80	14.64	77.56
16	105.6	7.81	14.36	77.83
17	112.1	7.82	14.08	78.11
18	118.6	7.81	13.80	78.39
19	125.1	7.80	13.53	78.67
20	131.6	7.78	13.27	78.95

21	138.1	7.75	13.02	79.23
22	144.6	7.72	12.78	79.51
23	151.1	7.67	12.55	79.78
24	157.7	7.62	12.34	80.05
25	164.2	7.56	12.14	80.31
26	170.7	7.49	11.95	80.57
27	177.2	7.41	11.78	80.81
28	183.7	7.32	11.62	81.06
29	190.2	7.23	11.48	81.29
30	196.7	7.14	11.35	81.51
31	203.2	7.04	11.23	81.73
32	209.7	6.94	11.12	81.94
33	216.3	6.83	11.03	82.14
34	222.8	6.73	10.94	82.33
35	229.3	6.62	10.86	82.52
36	235.8	6.51	10.79	82.69
37	242.3	6.41	10.73	82.86
38	248.8	6.31	10.67	83.02
39	255.3	6.21	10.62	83.18
40	261.8	6.11	10.57	83.33
41	268.3	6.01	10.52	83.47
42	274.8	5.93	10.48	83.60
43	281.4	5.84	10.44	83.72
44	287.9	5.76	10.40	83.84
45	294.4	5.69	10.36	83.95
46	300.9	5.62	10.33	84.05
47	307.4	5.55	10.30	84.15
48	313.9	5.49	10.27	84.24
49	320.4	5.44	10.24	84.32
50	326.9	5.38	10.22	84.40
51	333.4	5.34	10.19	84.47
52	339.9	5.30	10.17	84.53
53	346.5	5.26	10.15	84.59
54	353.0	5.22	10.13	84.64
55	359.5	5.19	10.11	84.69
56	366.0	5.17	10.10	84.73
57	372.5	5.14	10.08	84.77
58	379.0	5.12	10.07	84.81
59	385.5	5.10	10.06	84.84
60	392.0	5.09	10.05	84.86
61	398.5	5.07	10.04	84.89
62	405.0	5.06	10.03	84.91
63	411.6	5.05	10.03	84.93
64	418.1	5.04	10.02	84.94
65	424.6	5.03	10.02	84.95
66	431.1	5.02	10.01	84.97
67	437.6	5.01	10.01	84.98
68	444.1	5.01	10.01	84.99
69	450.6	5.00	10.00	84.99

TIME (HRS)= 1000.01
DELT (SEC)= 60.00
ITERATIONS= 66719

SURFACE RECESSION (MICRONS)= 8.32
TOTAL WEIGHT OF AL CONSUMED AS OXIDE (WMINT)= 3.16 (MG/CM^2)

Node #	Distance (microns)	Al (at.%)	Cr (at.%)	Ni (at.%)
0	8.3	2.48	14.88	82.64
1	24.1	2.75	14.57	82.67
2	39.8	3.01	14.28	82.71
3	55.6	3.25	14.01	82.75
4	71.3	3.47	13.75	82.78
5	87.1	3.68	13.50	82.82
6	102.8	3.87	13.27	82.86
7	118.6	4.05	13.05	82.90
8	134.3	4.21	12.85	82.94
9	150.1	4.37	12.65	82.98
10	165.8	4.51	12.47	83.02
11	181.6	4.64	12.29	83.07
12	197.3	4.76	12.13	83.11
13	213.1	4.87	11.97	83.16
14	228.8	4.97	11.83	83.21
15	244.6	5.05	11.69	83.26
16	260.3	5.13	11.56	83.31
17	276.1	5.21	11.44	83.36
18	291.8	5.27	11.33	83.41
19	307.6	5.32	11.22	83.46
20	323.3	5.37	11.12	83.51
21	339.1	5.41	11.03	83.56
22	354.8	5.45	10.95	83.60
23	370.6	5.47	10.87	83.65
24	386.3	5.50	10.80	83.70
25	402.1	5.51	10.74	83.75
26	417.8	5.52	10.68	83.80
27	433.6	5.53	10.62	83.84
28	449.3	5.54	10.57	83.89
29	465.0	5.53	10.53	83.94
30	480.8	5.53	10.49	83.98
31	496.5	5.52	10.45	84.02
32	512.3	5.51	10.42	84.07
33	528.0	5.50	10.39	84.11
34	543.8	5.49	10.36	84.15
35	559.5	5.47	10.33	84.19
36	575.3	5.46	10.31	84.23
37	591.0	5.44	10.29	84.27
38	606.8	5.42	10.27	84.31
39	622.5	5.40	10.25	84.35
40	638.3	5.38	10.24	84.39
41	654.0	5.36	10.22	84.42
42	669.8	5.34	10.20	84.46
43	685.5	5.32	10.19	84.49
44	701.3	5.30	10.18	84.52
45	717.0	5.28	10.17	84.56

46	732.8	5.26	10.15	84.59
47	748.5	5.24	10.14	84.62
48	764.3	5.22	10.13	84.64
49	780.0	5.21	10.12	84.67
50	795.8	5.19	10.11	84.70
51	811.5	5.17	10.10	84.72
52	827.3	5.16	10.09	84.75
53	843.0	5.14	10.09	84.77
54	858.8	5.13	10.08	84.79
55	874.5	5.12	10.07	84.81
56	890.3	5.11	10.06	84.83
57	906.0	5.09	10.06	84.85
58	921.8	5.08	10.05	84.87
59	937.5	5.07	10.04	84.88
60	953.3	5.06	10.04	84.90
61	969.0	5.05	10.03	84.91
62	984.8	5.05	10.03	84.92
63	1000.5	5.04	10.02	84.94
64	1016.3	5.03	10.02	84.95
65	1032.0	5.03	10.02	84.96
66	1047.8	5.02	10.01	84.97
67	1063.5	5.01	10.01	84.98
68	1079.3	5.01	10.01	84.98
69	1095.0	5.00	10.00	84.99

Appendix C

Output to Unit 14 (File: OUT14)

```
COSIM (Thick=100um, Kp=0.002, Qo=0.008, 1100C) 1/28/98
 Coating: Ni-20Cr-13Al   Substrate: Ni-10.0Cr-5.0Al
 1100C DIFFUSION DATA FROM: MET. TRANS.,18A,(1987) p2075 (TABLE V).
      DIST(UM)     AL         CR         NI      TIME(HR)
         .13      11.96      20.84      67.19       1.00
        1.32      12.06      20.70      67.24       1.00
        2.50      12.16      20.56      67.28       1.00
        3.69      12.25      20.43      67.31       1.00
        4.87      12.34      20.32      67.34       1.00
        6.05      12.42      20.22      67.36       1.00
        7.24      12.49      20.14      67.37       1.00
        8.42      12.55      20.08      67.38       1.00
        9.61      12.60      20.03      67.37       1.00
       10.79      12.65      19.99      67.36       1.00
       11.98      12.69      19.97      67.34       1.00
       13.16      12.73      19.95      67.32       1.00
       14.34      12.76      19.95      67.29       1.00
       15.53      12.79      19.94      67.27       1.00
       16.71      12.81      19.95      67.24       1.00
       17.90      12.84      19.95      67.22       1.00
       19.08      12.86      19.95      67.19       1.00
       20.27      12.87      19.96      67.17       1.00
       21.45      12.89      19.96      67.15       1.00
       22.63      12.91      19.97      67.13       1.00
       23.82      12.92      19.97      67.11       1.00
       25.00      12.93      19.98      67.09       1.00
       26.19      12.94      19.98      67.08       1.00
       27.37      12.95      19.98      67.06       1.00
       28.56      12.96      19.99      67.05       1.00
       29.74      12.97      19.99      67.04       1.00
       30.92      12.98      19.99      67.03       1.00
       32.11      12.98      19.99      67.02       1.00
       33.29      12.99      20.00      67.01       1.00
       34.48      13.00      20.00      67.01       1.00
       51.42      13.00      20.00      67.00       1.00
       53.63      12.99      20.00      67.01       1.00
       55.84      12.99      20.00      67.02       1.00
       58.05      12.98      19.99      67.03       1.00
       60.26      12.96      19.99      67.05       1.00
       62.48      12.94      19.98      67.08       1.00
       64.69      12.91      19.97      67.11       1.00
       66.90      12.87      19.96      67.17       1.00
       69.11      12.82      19.94      67.24       1.00
       71.32      12.75      19.91      67.34       1.00
       73.53      12.65      19.88      67.47       1.00
       75.74      12.54      19.84      67.63       1.00
       77.96      12.39      19.78      67.83       1.00
       80.17      12.21      19.71      68.09       1.00
       82.38      11.98      19.62      68.40       1.00
       84.59      11.72      19.51      68.77       1.00
       86.80      11.41      19.36      69.23       1.00
```

89.01	11.05	19.17	69.77	1.00
91.23	10.67	18.89	70.44	1.00
93.44	10.28	18.45	71.27	1.00
95.65	9.92	17.78	72.30	1.00
97.86	9.63	16.82	73.56	1.00
100.07	9.38	15.62	75.00	1.00
102.28	9.16	14.32	76.52	1.00
104.50	8.90	13.10	78.00	1.00
106.71	8.55	12.11	79.35	1.00
108.92	8.08	11.42	80.50	1.00
111.13	7.54	11.01	81.46	1.00
113.34	6.97	10.78	82.25	1.00
115.55	6.44	10.64	82.93	1.00
117.76	5.99	10.51	83.50	1.00
119.98	5.65	10.38	83.97	1.00
122.19	5.41	10.25	84.34	1.00
124.40	5.24	10.15	84.61	1.00
126.61	5.13	10.08	84.78	1.00
128.82	5.07	10.04	84.89	1.00
131.03	5.03	10.02	84.95	1.00
133.25	5.01	10.01	84.98	1.00
135.46	5.00	10.00	84.99	1.00
137.67	5.00	10.00	85.00	1.00

DIST(UM)	AL	CR	NI	TIME(HR)
1.42	6.89	18.09	75.03	100.01
7.93	6.99	17.95	75.07	100.01
14.44	7.08	17.79	75.13	100.01
20.95	7.17	17.62	75.21	100.01
27.46	7.26	17.43	75.31	100.01
33.97	7.34	17.23	75.44	100.01
40.48	7.41	17.01	75.58	100.01
46.99	7.48	16.79	75.74	100.01
53.50	7.54	16.55	75.92	100.01
60.01	7.59	16.30	76.11	100.01
66.52	7.64	16.04	76.32	100.01
73.03	7.69	15.77	76.55	100.01
79.54	7.73	15.49	76.78	100.01
86.05	7.76	15.21	77.03	100.01
92.56	7.78	14.93	77.29	100.01
99.07	7.80	14.64	77.56	100.01
105.58	7.81	14.36	77.83	100.01
112.09	7.82	14.08	78.11	100.01
118.60	7.81	13.80	78.39	100.01
125.11	7.80	13.53	78.67	100.01
131.62	7.78	13.27	78.95	100.01
138.13	7.75	13.02	79.23	100.01
144.64	7.72	12.78	79.51	100.01
151.15	7.67	12.55	79.78	100.01
157.66	7.62	12.34	80.05	100.01
164.17	7.56	12.14	80.31	100.01
170.68	7.49	11.95	80.57	100.01
177.19	7.41	11.78	80.81	100.01
183.70	7.32	11.62	81.06	100.01
190.21	7.23	11.48	81.29	100.01
196.72	7.14	11.35	81.51	100.01

203.23	7.04	11.23	81.73	100.01
209.74	6.94	11.12	81.94	100.01
216.25	6.83	11.03	82.14	100.01
222.76	6.73	10.94	82.33	100.01
229.27	6.62	10.86	82.52	100.01
235.78	6.51	10.79	82.69	100.01
242.29	6.41	10.73	82.86	100.01
248.80	6.31	10.67	83.02	100.01
255.31	6.21	10.62	83.18	100.01
261.82	6.11	10.57	83.33	100.01
268.33	6.01	10.52	83.47	100.01
274.84	5.93	10.48	83.60	100.01
281.35	5.84	10.44	83.72	100.01
287.86	5.76	10.40	83.84	100.01
294.37	5.69	10.36	83.95	100.01
300.88	5.62	10.33	84.05	100.01
307.39	5.55	10.30	84.15	100.01
313.90	5.49	10.27	84.24	100.01
320.41	5.44	10.24	84.32	100.01
326.92	5.38	10.22	84.40	100.01
333.43	5.34	10.19	84.47	100.01
339.94	5.30	10.17	84.53	100.01
346.45	5.26	10.15	84.59	100.01
352.96	5.22	10.13	84.64	100.01
359.47	5.19	10.11	84.69	100.01
365.98	5.17	10.10	84.73	100.01
372.49	5.14	10.08	84.77	100.01
379.00	5.12	10.07	84.81	100.01
385.51	5.10	10.06	84.84	100.01
392.02	5.09	10.05	84.86	100.01
398.53	5.07	10.04	84.89	100.01
405.04	5.06	10.03	84.91	100.01
411.55	5.05	10.03	84.93	100.01
418.06	5.04	10.02	84.94	100.01
424.57	5.03	10.02	84.95	100.01
431.08	5.02	10.01	84.97	100.01
437.59	5.01	10.01	84.98	100.01
444.10	5.01	10.01	84.99	100.01
450.61	5.00	10.00	84.99	100.01

DIST(UM)	AL	CR	NI	TIME(HR)
8.32	2.48	14.88	82.64	1000.01
24.07	2.75	14.57	82.67	1000.01
39.82	3.01	14.28	82.71	1000.01
55.56	3.25	14.01	82.75	1000.01
71.31	3.47	13.75	82.78	1000.01
87.06	3.68	13.50	82.82	1000.01
102.81	3.87	13.27	82.86	1000.01
118.56	4.05	13.05	82.90	1000.01
134.31	4.21	12.85	82.94	1000.01
150.06	4.37	12.65	82.98	1000.01
165.81	4.51	12.47	83.02	1000.01
181.56	4.64	12.29	83.07	1000.01
197.31	4.76	12.13	83.11	1000.01
213.06	4.87	11.97	83.16	1000.01
228.81	4.97	11.83	83.21	1000.01

244.56	5.05	11.69	83.26	1000.01
260.31	5.13	11.56	83.31	1000.01
276.06	5.21	11.44	83.36	1000.01
291.81	5.27	11.33	83.41	1000.01
307.56	5.32	11.22	83.46	1000.01
323.31	5.37	11.12	83.51	1000.01
339.05	5.41	11.03	83.56	1000.01
354.80	5.45	10.95	83.60	1000.01
370.55	5.47	10.87	83.65	1000.01
386.30	5.50	10.80	83.70	1000.01
402.05	5.51	10.74	83.75	1000.01
417.80	5.52	10.68	83.80	1000.01
433.55	5.53	10.62	83.84	1000.01
449.30	5.54	10.57	83.89	1000.01
465.05	5.53	10.53	83.94	1000.01
480.80	5.53	10.49	83.98	1000.01
496.55	5.52	10.45	84.02	1000.01
512.30	5.51	10.42	84.07	1000.01
528.05	5.50	10.39	84.11	1000.01
543.80	5.49	10.36	84.15	1000.01
559.55	5.47	10.33	84.19	1000.01
575.30	5.46	10.31	84.23	1000.01
591.05	5.44	10.29	84.27	1000.01
606.79	5.42	10.27	84.31	1000.01
622.54	5.40	10.25	84.35	1000.01
638.29	5.38	10.24	84.39	1000.01
654.04	5.36	10.22	84.42	1000.01
669.79	5.34	10.20	84.46	1000.01
685.54	5.32	10.19	84.49	1000.01
701.29	5.30	10.18	84.52	1000.01
717.04	5.28	10.17	84.56	1000.01
732.79	5.26	10.15	84.59	1000.01
748.54	5.24	10.14	84.62	1000.01
764.29	5.22	10.13	84.64	1000.01
780.04	5.21	10.12	84.67	1000.01
795.79	5.19	10.11	84.70	1000.01
811.54	5.17	10.10	84.72	1000.01
827.29	5.16	10.09	84.75	1000.01
843.04	5.14	10.09	84.77	1000.01
858.79	5.13	10.08	84.79	1000.01
874.53	5.12	10.07	84.81	1000.01
890.28	5.11	10.06	84.83	1000.01
906.03	5.09	10.06	84.85	1000.01
921.78	5.08	10.05	84.87	1000.01
937.53	5.07	10.04	84.88	1000.01
953.28	5.06	10.04	84.90	1000.01
969.03	5.05	10.03	84.91	1000.01
984.78	5.05	10.03	84.92	1000.01
1000.53	5.04	10.02	84.94	1000.01
1016.28	5.03	10.02	84.95	1000.01
1032.03	5.03	10.02	84.96	1000.01
1047.78	5.02	10.01	84.97	1000.01
1063.53	5.01	10.01	84.98	1000.01
1079.28	5.01	10.01	84.98	1000.01
1095.03	5.00	10.00	84.99	1000.01

Appendix D

Output to Unit 15 (File: OUT15)

TIME(HRS)	AL(0)	CR(0)	WMDOT	WMINT
.278E-03	.124E+02	.206E+02	.419E-03	.833E-03
.556E-03	.122E+02	.207E+02	.296E-03	.118E-02
.833E-03	.122E+02	.207E+02	.242E-03	.145E-02
.111E-02	.122E+02	.207E+02	.209E-03	.167E-02
.139E-02	.121E+02	.208E+02	.187E-03	.187E-02
.167E-02	.121E+02	.208E+02	.171E-03	.205E-02
.195E-02	.121E+02	.208E+02	.158E-03	.221E-02
.223E-02	.121E+02	.208E+02	.148E-03	.237E-02
.250E-02	.121E+02	.208E+02	.140E-03	.251E-02
.278E-02	.121E+02	.208E+02	.133E-03	.265E-02
.306E-02	.121E+02	.208E+02	.126E-03	.277E-02
.334E-02	.121E+02	.208E+02	.121E-03	.290E-02
.361E-02	.121E+02	.208E+02	.116E-03	.302E-02
.389E-02	.121E+02	.208E+02	.112E-03	.313E-02
.417E-02	.121E+02	.208E+02	.108E-03	.324E-02
.445E-02	.121E+02	.208E+02	.105E-03	.335E-02
.473E-02	.121E+02	.208E+02	.102E-03	.345E-02
.500E-02	.121E+02	.208E+02	.987E-04	.355E-02
.528E-02	.120E+02	.208E+02	.961E-04	.365E-02
.556E-02	.120E+02	.208E+02	.937E-04	.374E-02
.583E-02	.120E+02	.208E+02	.915E-04	.384E-02
.612E-02	.120E+02	.208E+02	.893E-04	.393E-02
.640E-02	.120E+02	.208E+02	.873E-04	.402E-02
.668E-02	.120E+02	.208E+02	.855E-04	.410E-02
.695E-02	.120E+02	.208E+02	.838E-04	.419E-02
.722E-02	.120E+02	.208E+02	.822E-04	.427E-02
.751E-02	.120E+02	.208E+02	.806E-04	.435E-02
.778E-02	.120E+02	.208E+02	.792E-04	.443E-02
.806E-02	.120E+02	.208E+02	.778E-04	.451E-02
.834E-02	.120E+02	.208E+02	.765E-04	.459E-02
.862E-02	.120E+02	.208E+02	.752E-04	.466E-02
.890E-02	.120E+02	.208E+02	.741E-04	.474E-02
.917E-02	.120E+02	.208E+02	.729E-04	.481E-02
.945E-02	.120E+02	.208E+02	.719E-04	.488E-02
.972E-02	.120E+02	.208E+02	.708E-04	.495E-02
.100E-01	.120E+02	.208E+02	.698E-04	.503E-02
.200E-01	.120E+02	.208E+02	.494E-04	.711E-02
.300E-01	.120E+02	.208E+02	.403E-04	.871E-02
.400E-01	.120E+02	.208E+02	.349E-04	.101E-01
.500E-01	.120E+02	.208E+02	.312E-04	.112E-01
.601E-01	.120E+02	.208E+02	.285E-04	.123E-01
.701E-01	.120E+02	.208E+02	.264E-04	.133E-01
.801E-01	.120E+02	.208E+02	.247E-04	.142E-01
.900E-01	.120E+02	.208E+02	.233E-04	.151E-01
.100E+00	.120E+02	.208E+02	.221E-04	.159E-01
.200E+00	.120E+02	.208E+02	.156E-04	.225E-01
.301E+00	.120E+02	.208E+02	.127E-04	.276E-01
.400E+00	.120E+02	.208E+02	.110E-04	.318E-01
.500E+00	.120E+02	.208E+02	.988E-05	.356E-01
.601E+00	.120E+02	.208E+02	.901E-05	.390E-01

.700E+00	.120E+02	.208E+02	.835E-05	.421E-01
.802E+00	.120E+02	.208E+02	.780E-05	.450E-01
.901E+00	.120E+02	.208E+02	.736E-05	.477E-01
.100E+01	.120E+02	.208E+02	.698E-05	.503E-01
.200E+01	.120E+02	.208E+02	.494E-05	.712E-01
.301E+01	.120E+02	.208E+02	.403E-05	.872E-01
.401E+01	.119E+02	.208E+02	.350E-05	.101E+00
.501E+01	.119E+02	.208E+02	.313E-05	.113E+00
.600E+01	.118E+02	.208E+02	.286E-05	.123E+00
.701E+01	.118E+02	.208E+02	.265E-05	.133E+00
.801E+01	.117E+02	.207E+02	.248E-05	.142E+00
.901E+01	.116E+02	.207E+02	.234E-05	.151E+00
.100E+02	.114E+02	.207E+02	.223E-05	.159E+00
.200E+02	.104E+02	.203E+02	.160E-05	.226E+00
.300E+02	.949E+01	.199E+02	.134E-05	.279E+00
.400E+02	.883E+01	.196E+02	.118E-05	.324E+00
.500E+02	.833E+01	.193E+02	.109E-05	.365E+00
.600E+02	.793E+01	.190E+02	.102E-05	.403E+00
.700E+02	.760E+01	.187E+02	.972E-06	.439E+00
.800E+02	.733E+01	.185E+02	.936E-06	.473E+00
.900E+02	.709E+01	.183E+02	.908E-06	.506E+00
.100E+03	.689E+01	.181E+02	.887E-06	.539E+00
.200E+03	.564E+01	.167E+02	.813E-06	.841E+00
.300E+03	.493E+01	.160E+02	.803E-06	.113E+01
.400E+03	.441E+01	.156E+02	.802E-06	.142E+01
.500E+03	.398E+01	.154E+02	.802E-06	.171E+01
.600E+03	.362E+01	.152E+02	.802E-06	.200E+01
.700E+03	.329E+01	.151E+02	.802E-06	.229E+01
.800E+03	.300E+01	.150E+02	.802E-06	.258E+01
.900E+03	.273E+01	.149E+02	.802E-06	.287E+01
.100E+04	.248E+01	.149E+02	.802E-06	.316E+01

Appendix E

Variables used within the program, arranged alphabetically*:

Name	Description
	For the following 20 parameters A_{ijk} for diffusion coefficients, see description for READ11 subroutine in paper.
A110, A111,	A112, A113, A114, A115 Parameters for $D_{}$.
A120, A121,	A122, A123, A124, A125 Parameters for D^{AlAl}.
A210, A211,	A212, A213, A214, A215 Parameters for D^{AlCr}.
A220, A221,	A222, A223, A224, A225 Parameters for D^{CrAl}_{GrCr}.
A0	Parameter relating weight of metal in oxide to weight of oxygen
A	Local interim variable**
AB	Local interim variable
A(6)	Local array used in Function DERF to calculate error function
ADIST	Array containing equally spaced node distance positions after spline fit
AGROW	Parameter for power law oxide growth model (see see description for READ11 subroutine in paper.)
AJ	Single precision equivalent to index counter J
AL	Array containing current Al concentrations for all nodes (time=t)
AL2	Array containing new Al concentrations for all nodes (time=$t+\Delta t$)
ALX	Subroutine arguments for D_C representing Al concentration
ALCOAT	Al concentration of coating, in atomic percent
ALPHA	Parameter relating flux towards and away from moving interface (see Eq. 7)
ALSP	Array containing Al concentrations after spline interpolation
ALSUB	Al concentration of substrate, in atomic percent
ALWCOAT	Coating concentration in weight percent
ALY	Array containing spline parameters for Al (used in SPLINE subroutine)
AM	Real variable equivalent to M (used in SPLINE subroutine)
AN	Argument in Subroutine M_L giving the number of nodes in the diffusion zone
ANCOAT	Number of nodes in coating
ANSUB	Number of nodes in inner diffusion zone (coating/substrate interdiffusion)
ARG1	Interim variable used to produce correct shift to concentrations to concentrations in Subroutine M_L
ASUBL	Lowest node number in inner (substrate) diffusion zone (ncoat+2) (see NSUBL)
AX2	Interim variable used to determine distance coordinates for inner diffusion zone when printing to units 6, 12 and 14 (for ZONE=2)
B	Interim variable
B0	Parameter to convert weight of oxygen in scale to total weight of oxide (metal+oxygen). B0=A0+1.0
BAC	Local interim variable used to calculate error function in FUNCTION DERF
BGROW	Parameter for power law oxide growth model (see description for READ11 subroutine in paper.)
C	Local interim variable
CD	Local interim variable
CR	Array containing current Cr concentrations for all nodes
CR2	Array containing new Cr concentrations for all nodes (time=$t+\Delta t$)
CRITAL	Critical surface Al concentration (at.%)

CRSP	Array containing Cr concentrations after spline interpolation
CRX	Subroutine arguments for D_C representing Cr concentration
CRCOAT	Cr concentration of coating, in atomic percent
CRSUB	Cr concentration of substrate, in atomic percent
D	Local interim variable
D11	Main diffusion coefficient for Al (D^{AlAl}_{Al})
D12	Cross term diffusion coefficient for Al (D^{AlCr}_{Al})
D21	Cross term diffusion coefficient for Cr (D^{CrAl}_{Cr})
D22	Main diffusion coefficient for Cr (D^{CrCr}_{Cr})
D2ALDX	Second order Al concentration derivative (i.e., d^2C_{Al}/dX^2)
D2CRDX	Second order Cr concentration derivative (i.e., $d^2C_{Cr}^{Al}/dX^2$)
DAL	Interim local variable
DALDX	Al concentration gradient (i.e., dC_{Al}/dX)
DCR	Interim local variable
DCRDX	Cr concentration gradient (i.e., dC_{Cr}/dX)
DD111	Derivative of D (D11) diffusion coefficient wrt Al
DD112	Derivative of D^{AlAl} (D11) diffusion coefficient wrt Cr
DD121	Derivative of D^{AlAl} (D12) diffusion coefficient wrt Al
DD122	Derivative of D^{AlCr} (D12) diffusion coefficient wrt Cr
DD211	Derivative of D^{AlCr} (D21) diffusion coefficient wrt Al
DD212	Derivative of D^{CrAl} (D21) diffusion coefficient wrt Cr
DD221	Derivative of D^{CrAl} (D22) diffusion coefficient wrt Al
DD222	Derivative of D^{CrCr} (D22) diffusion coefficient wrt Cr
DELT	Time increment used each iteration
DELT1	Time interval for outer diffusion zone based on Eq. 13
DELT2	Time interval for inner diffusion zone based on Eq. 13
DELX	Argument in subroutines M_L and FSL representing node spacing
DELX1	node spacing in outer diffusion zone (calculated)
DELX2	node spacing in inner diffusion zone (calculated)
DELXI1	Surface recession in time Delt
DELXMN	Minimum node spacing between Delx1 and Delx2
DEL_X	Interim distance variable used in defining the initial concentration profile for the inner diffusion zone DENOM Interim variable used in the calculation of the weight percent of Al in the coating
DENSITY	Density of the coating (gm/cm^3)
DF	Array used to "weight" spline representation (used in SPLINE subroutine)
DIST	Array containing node distance positions before spline fit
DIST1	Width of outer diffusion zone measured from the original surface to node *ncoat*
DIST2	Width of inner diffusion zone from coating/substrate interface to node nsubl-1 (i.e., the width of the inner diffusion zone extending into the coating) Used with DIST2 and THICK to determine when the diffusion zones overlap in the coating
DIST_SP	Interim distance array containing node positions after spline interpolation
DMAX	Maximum diffusion coefficient used to calculate minimum Delt
DXCOAT	Initial width of the outer diffusion zone (microns)
DX	Argument in Subroutine M_L indicating the amount the zone is to be shifted
DXSUB	Initial width of the inner diffusion zone (microns)
ERFC	Complimentary error function calculated in FUNCTION DERF
ETA	Parameter used in COSP oxide spalling program (Ref 3)

HALF	Distance variable indicating the midpoint of the overlapping diffusion zones, used when printing to unit 12 (ZONE=2) in preparation for SPLINE curve fit
I	Local index counter
IC	Parameter used in SPLINE subroutine
ILOOP	Loop iteration counter
INT	Index for DO loop in Subroutine M_L (values of 1 or -1)
IO15	Flag indicating output to file15 desired
ITIME	Integer counter for times stored in array TMAX
J	Local index counter
JAL	Al flux in coating
JOX	Al flux in the oxide at the oxide/caoting interface
KP	Parabolic oxide growth constant due to weight of oxygen on surface
M	SPLINE subroutine argument equal to NCOAT+NSUB
MASSFACT	Factor to convert units for rate of al consumption (mg/cm^2/sec) to units compatible with Al flux in program(at%al*cm/sec)
MAXDT	Maximum time increment per iteration (minutes)
MAXLOOP	Maximum iterations allowed before stopping the program
MODEL	Parameter indicating oxide growth model
MW_AL	Molecular weight of Al
MW_CR	Molecular weight of Cr
MW_NI	Molecular weight of Ni
N	Local index counter
N1	Argument in subroutines M_L and FSL indicating node numbers
N2	Argument in subroutines M_L and FSL indicating node numbers
NCOAT	Number of nodes in the outer diffusion zone
NCOATH	Highest node number in outer (coating) diffusion zone (ncoat-1)
NICOAT	Ni concentration in the coating (at.%)
NN	local index counter
NSUB	number of nodes in the inner diffusion zone
NSUBH	Highest node number in inner (substrate) diffusion zone (nsubl+nsub-1)
NSUBL	Lowest node number in inner (substrate) diffusion zone (ncoat+2)
QO	Spalling parameter used in COSP oxide spalling program (Ref 3)
RATIO	Interim variable used to produce correct shift to concentrations to concentrations in Subroutine M_L
SAL	Single precision variable for AL
SAMPLE	80 character run id (1 of 3, for documentation only)
SCR	Single precision variable for CR
SDELT	Single precision variable for DELT
SDELT1	Single precision variable for DELT1
SDELT2	Single precision variable for DELT2
SDIST	Single precision variable for DIST
SHR	Single precision variable for HR
SNI	Single precision variable for NI
STIME	Single precision variable for TIME
SWMDOT	Single precision variable for WMDOT
SWMINT	Single precision variable for WMINT
SXI1	Single precision variable for XI1
T1	Interim time variable used in COSP oxide spalling model (Ref 3)
T2	Interim time variable used in COSP oxide spalling model (Ref 3)
T15	Intermediate time counter; time between writing to File15
TCYCLE	Thermal cycle duration used in COSP oxide spalling program (Ref 3)

TEFF	"Effective" time based on current oxide thickness used in COSP oxide spalling model (Ref 3)
TEMP	Oxidation temperature (C) (for documentation only)
THICK	Thickness of the coating (microns)
TIME	Simulated total oxidation time (TIME=TIME+DELT)
TIME15	Time intervals between writing to File15
TITLE1	80 character run id (2 of 3, for documentation only)
TITLE2	80 character run id (3 of 3, for documentation only)
TMAX	Array containing times for output to File6
TMID	Intermediate time variable used in COSP oxide spalling model (Ref 3)
TOTWM	Total weight of metal consumed predicted by COSP oxide spalling program (Ref 3)
TOTWO	Total weight of oxygen in the oxide (Ref 3)
TOTWR	Total weight of oxide retained on surface, predicted by COSP oxide spalling program (Ref 3)
TSUM	Intermediate time counter giving elapsed time between thermal cycles (sec)
VBAR	Partial molar volume of Al in coating (cm^3/mole)
WM	Weight of metal (Al) in oxide used in COSP oxide spalling model (Ref 3)
WMDOT	Rate of metal consumption predicted by COSP oxide spalling program (Ref 3)
WMINT	Total accumulated weight of metal consumption (mg/cm^2)
WO	Weight of oxygen in oxide used in COSP oxide spalling model (Ref 3)
WO1	Weight of oxygen in oxide at time T1 used in COSP oxide spalling model (Ref 3)
WO2	Weight of oxygen in oxide at time T2 used in COSP oxide spalling model (Ref 3)
WR	Weight of oxide retained on surface used in COSP oxide spalling model (Ref 3)
WS	Weight of oxide spall following a thermal cycle used in COSP oxide spalling model (Ref 3)
X	Interim distance variable used in printing node positions
XI1	Position of outer surface (i.e., amount of surface recession, cm)
YCR	Array containing spline parameters for Cr (used in SPLINE subroutine)
ZONE	Indicator for number of diffusion zones (zone=2 for inner and outer diffusion zones, zone=1 after SPLINE subroutine creating single combined diffusion zone)

* Variables associated with Spline subroutines EVALUAT and CUBIC are not included. See Ref 11.

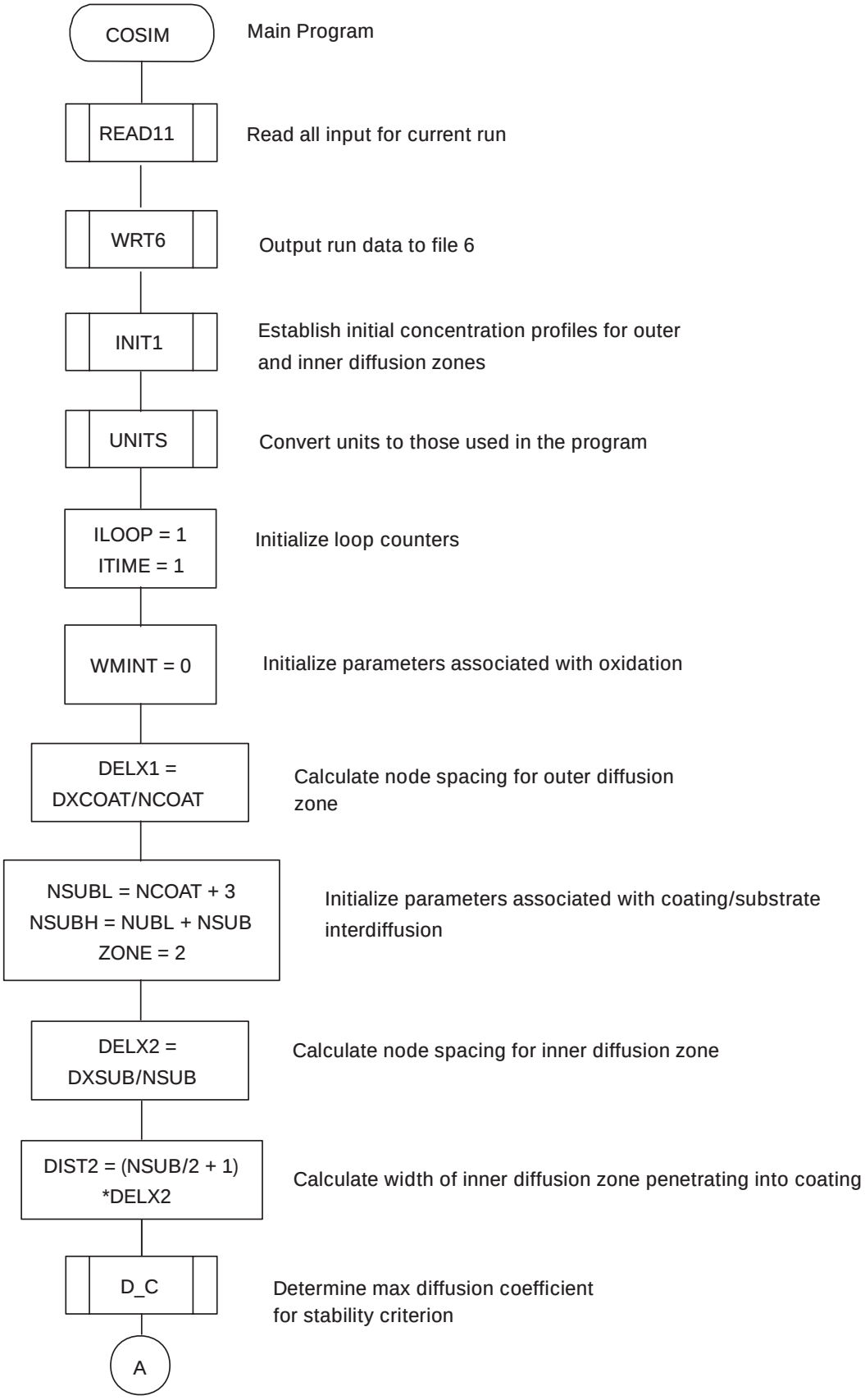
** Local interim variables are used in intermediate steps in an algebraic equation, such as:

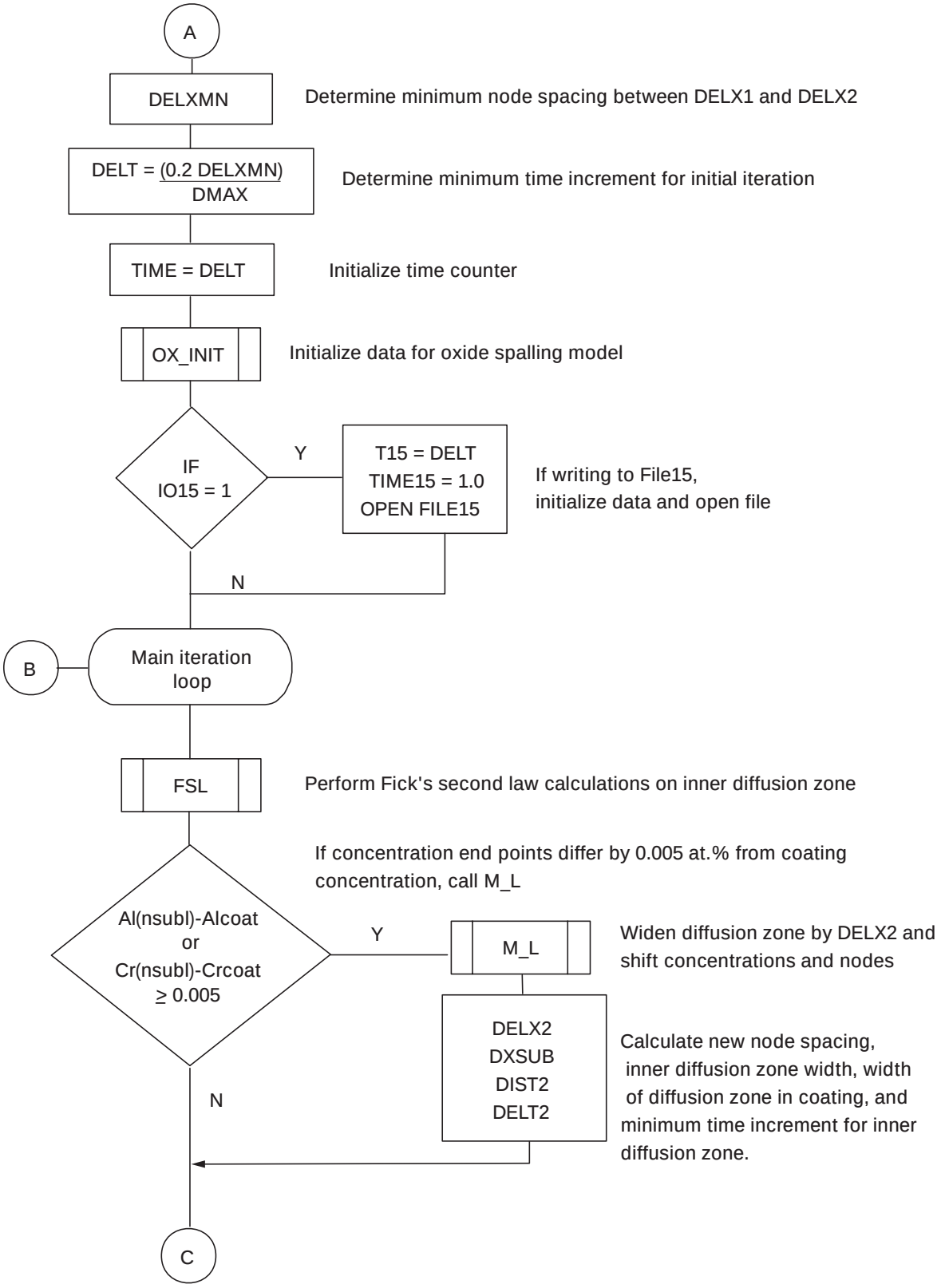
```
A=DD111*DALDX+DD112*DCRDX
B=DD121*DALDX+DD122*DCRDX
AB=A*DALDX+D11*D2ALDX+B*DCRDX+D12*D2CRDX
AL2(J)=AL(J)+DELT*AB
```

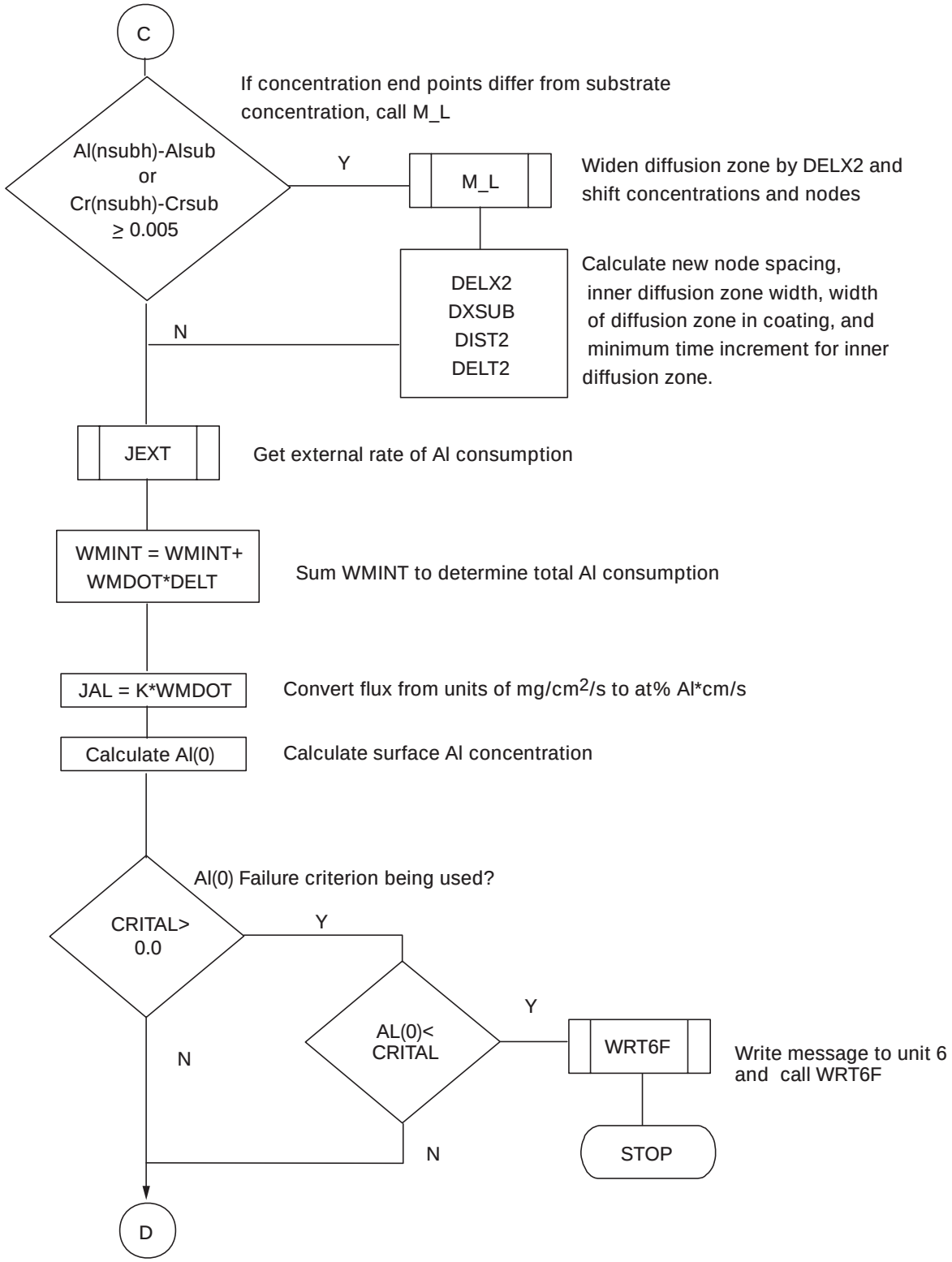
where the calculations for A, B, and AB are intermediate steps toward calculating the new Al concentration AL2(J).

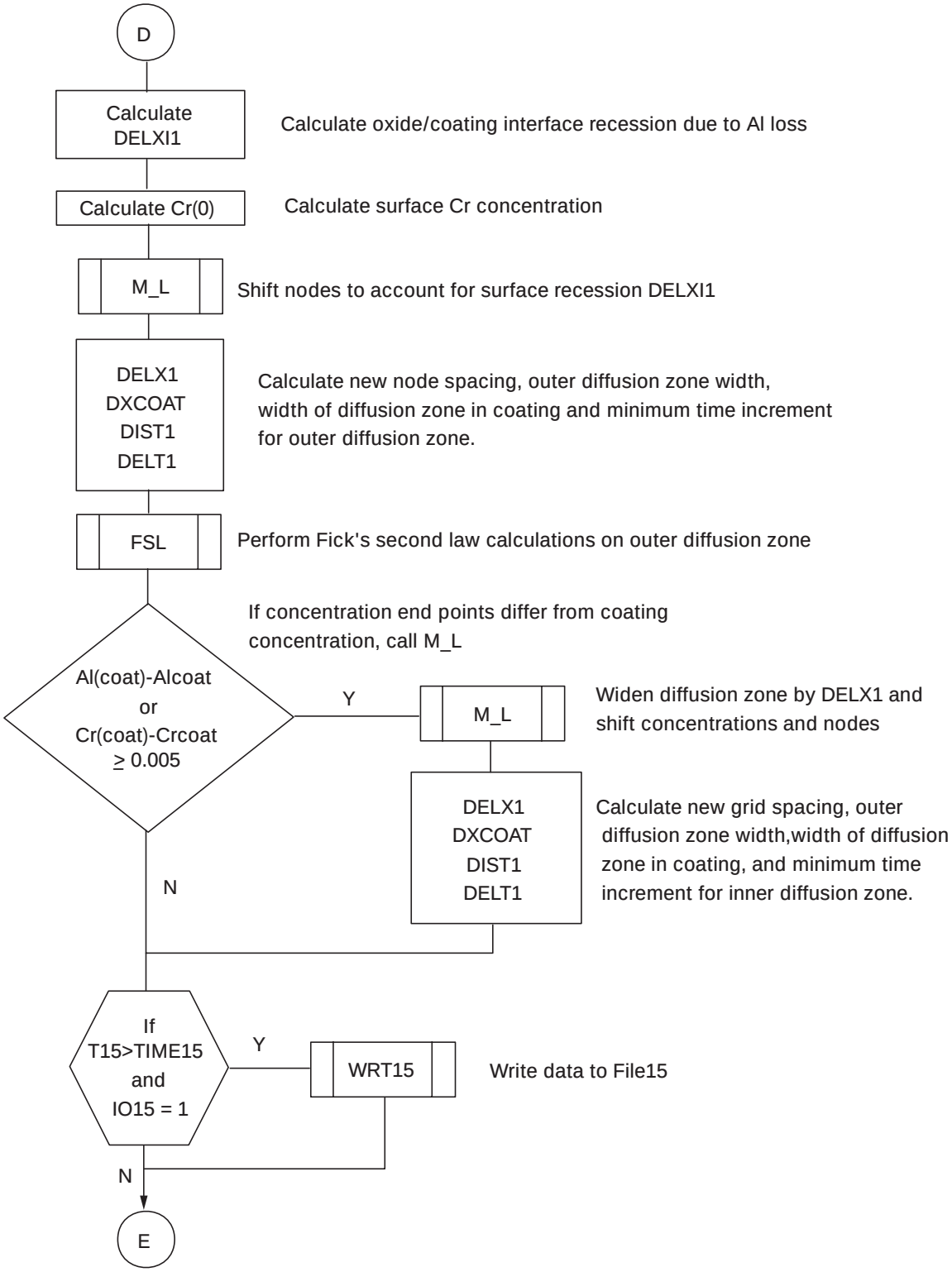
Appendix F

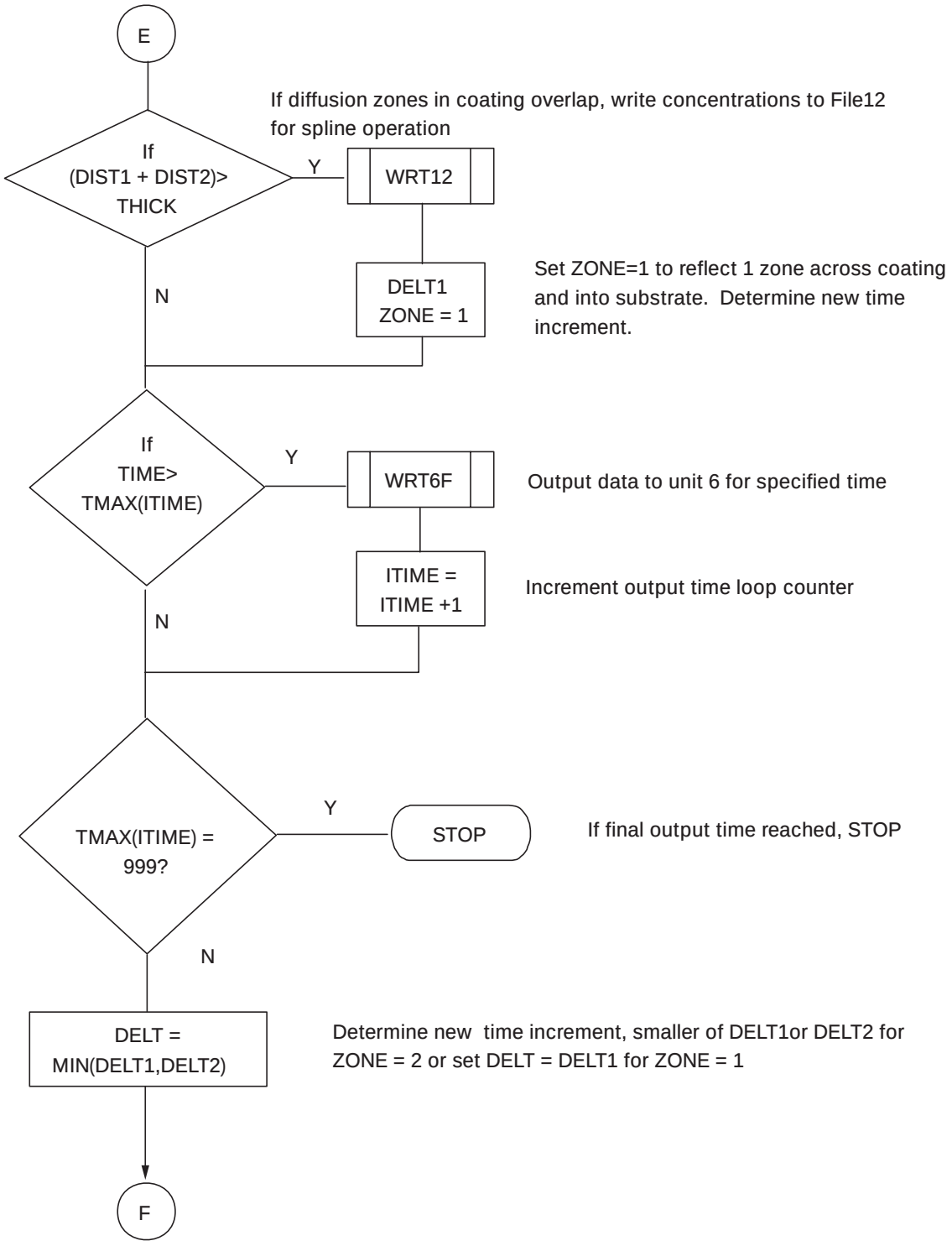
Flow charts.

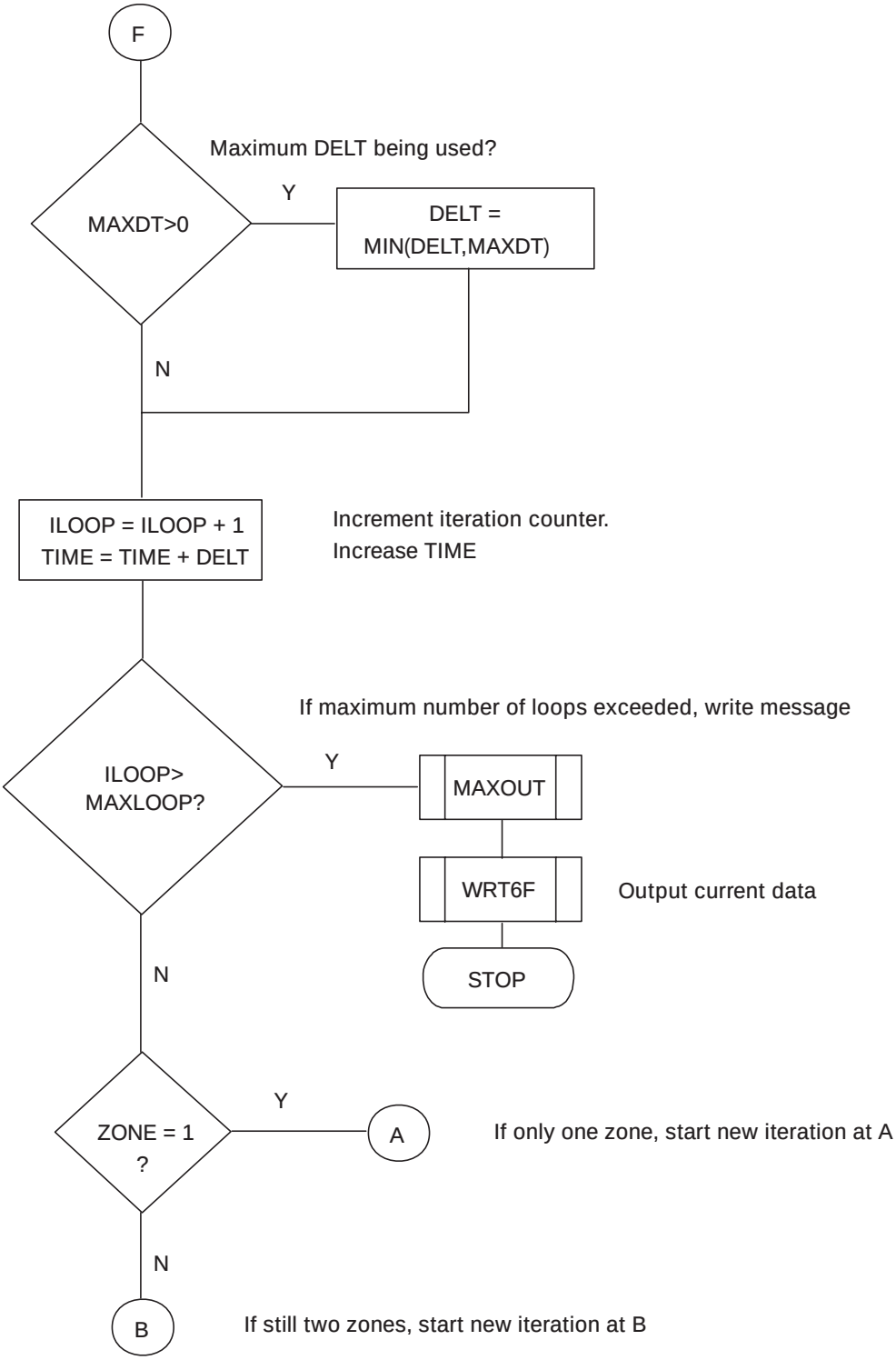


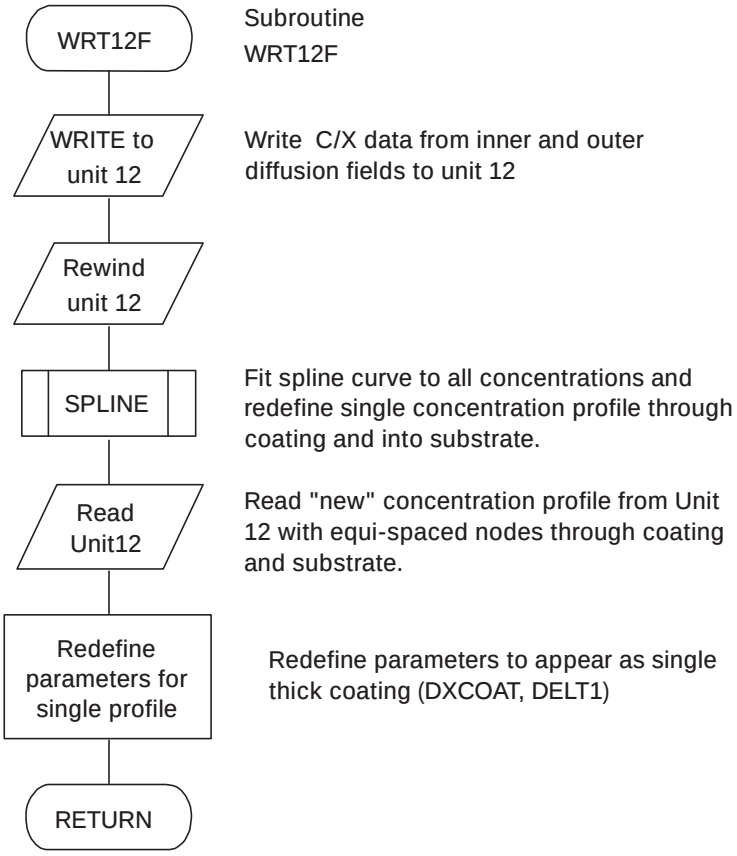

A
DELXMN
Determine minimum node spacing between DELX1 and DELX2
DELT = (0.2 DELXMN) / DMAX
Determine minimum time increment for initial iteration
TIME = DELT
Initialize time counter
OX_INIT
Initialize data for oxide spalling model
IF IO15 = 1
Y
T15 = DELT
TIME15 = 1.0
OPEN FILE15
If writing to File15, initialize data and open file
N
B
Main iteration loop
FSL
Perform Fick's second law calculations on inner diffusion zone
If concentration end points differ by 0.005 at.% from coating concentration, call M_L
Al(nsubl)-Alcoat or Cr(nsubl)-Crcoat ≥ 0.005
Y
M_L
Widen diffusion zone by DELX2 and shift concentrations and nodes
DELX2
DXSUB
DIST2
DELT2
Calculate new node spacing, inner diffusion zone width, width of diffusion zone in coating, and minimum time increment for inner diffusion zone.
N
C

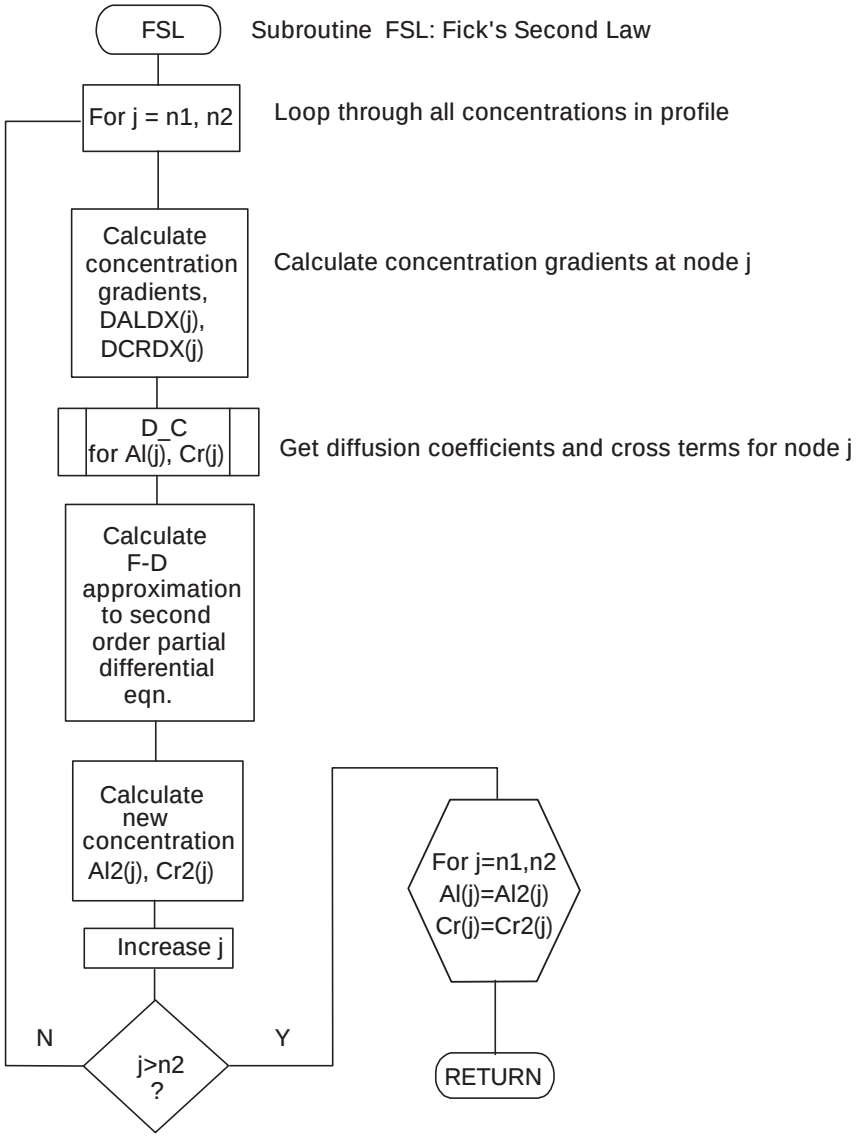

C
If concentration end points differ from substrate concentration, call M_L
Al(nsubh)-Alsub or Cr(nsubh)-Crsub ≥ 0.005
Y
M_L
Widen diffusion zone by DELX2 and shift concentrations and nodes
DELX2
DXSUB
DIST2
DELT2
Calculate new node spacing, inner diffusion zone width, width of diffusion zone in coating, and minimum time increment for inner diffusion zone.
N
JEXT
Get external rate of Al consumption
WMINT = WMINT+ WMDOT*DELT
Sum WMINT to determine total Al consumption
JAL = K*WMDOT
Convert flux from units of mg/cm2/s to at% Al*cm/s
Calculate Al(0)
Calculate surface Al concentration
Al(0) Failure criterion being used?
CRITAL> 0.0
Y
AL(0)< CRITAL
Y
WRT6F
Write message to unit 6 and call WRT6F
N
N
STOP
D

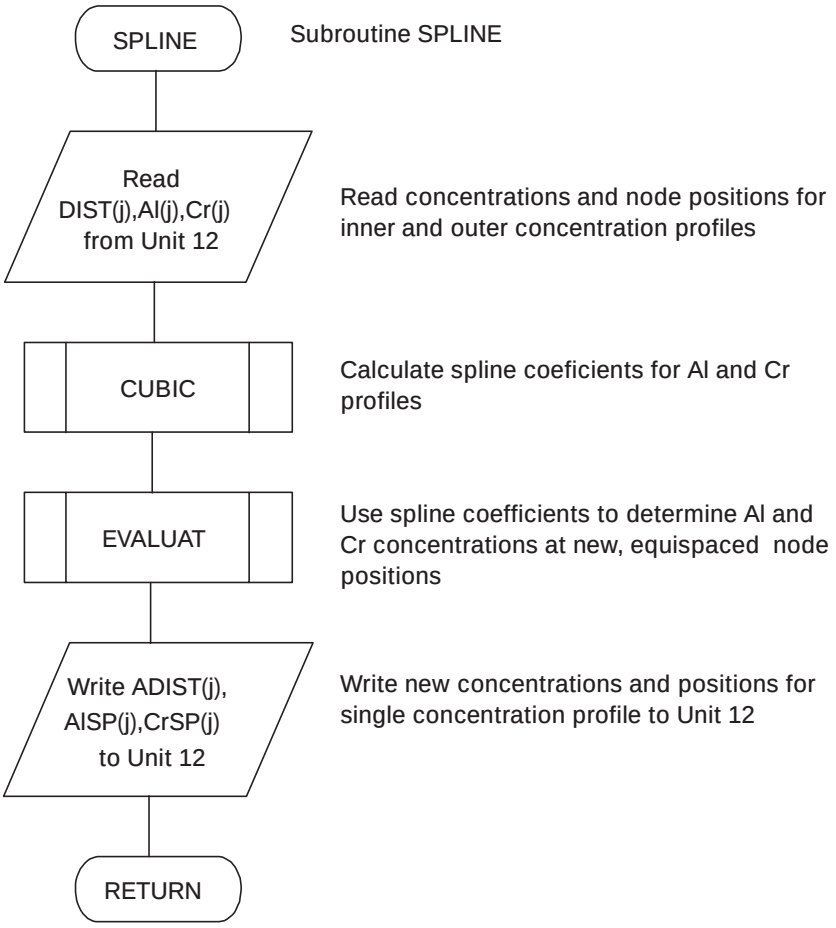

D
Calculate DELXI1
Calculate oxide/coating interface recession due to Al loss
Calculate Cr(0)
Calculate surface Cr concentration
M_L
Shift nodes to account for surface recession DELXI1
DELX1
DXCOAT
DIST1
DELT1
Calculate new node spacing, outer diffusion zone width, width of diffusion zone in coating and minimum time increment for outer diffusion zone.
FSL
Perform Fick's second law calculations on outer diffusion zone
If concentration end points differ from coating concentration, call M_L
Al(coat)-Alcoat or Cr(coat)-Crcoat ≥ 0.005
Y
M_L
Widen diffusion zone by DELX1 and shift concentrations and nodes
DELX1
DXCOAT
DIST1
DELT1
Calculate new grid spacing, outer diffusion zone width,width of diffusion zone in coating, and minimum time increment for inner diffusion zone.
N
If T15>TIME15 and IO15 = 1
Y
WRT15
Write data to File15
N
E


E
If diffusion zones in coating overlap, write concentrations to File12 for spline operation
If (DIST1 + DIST2)> THICK
Y
WRT12
N
DELT1 ZONE = 1
Set ZONE=1 to reflect 1 zone across coating and into substrate. Determine new time increment.
If TIME> TMAX(ITIME)
Y
WRT6F
Output data to unit 6 for specified time
ITIME = ITIME +1
Increment output time loop counter
N
TMAX(ITIME) = 999?
Y
STOP
If final output time reached, STOP
N
DELT = MIN(DELT1,DELT2)
Determine new time increment, smaller of DELT1or DELT2 for ZONE = 2 or set DELT = DELT1 for ZONE = 1
F


F
Maximum DELT being used?
MAXDT>0
Y
DELT =
MIN(DELT,MAXDT)
N
ILOOP = ILOOP + 1
TIME = TIME + DELT
Increment iteration counter.
Increase TIME
If maximum number of loops exceeded, write message
ILOOP>
MAXLOOP?
Y
MAXOUT
WRT6F
Output current data
STOP
N
ZONE = 1
?
Y
A
If only one zone, start new iteration at A
N
B
If still two zones, start new iteration at B


WRT12F
Subroutine
WRT12F
WRITE to
unit 12
Write C/X data from inner and outer
diffusion fields to unit 12
Rewind
unit 12
SPLINE
Fit spline curve to all concentrations and
redefine single concentration profile through
coating and into substrate.
Read
Unit12
Read "new" concentration profile from Unit
12 with equi-spaced nodes through coating
and substrate.
Redefine
parameters for
single profile
Redefine parameters to appear as single
thick coating (DXCOAT, DELT1)
RETURN


FSL
Subroutine FSL: Fick's Second Law
For j = n1, n2
Loop through all concentrations in profile
Calculate concentration gradients, DALDX(j), DCRDX(j)
Calculate concentration gradients at node j
D_C for Al(j), Cr(j)
Get diffusion coefficients and cross terms for node j
Calculate F-D approximation to second order partial differential eqn.
Calculate new concentration Al2(j), Cr2(j)
Increase j
N
j>n2 ?
Y
For j=n1,n2 Al(j)=Al2(j) Cr(j)=Cr2(j)
RETURN


SPLINE
Subroutine SPLINE
Read
DIST(j),Al(j),Cr(j)
from Unit 12
Read concentrations and node positions for inner and outer concentration profiles
CUBIC
Calculate spline coeficients for Al and Cr profiles
EVALUAT
Use spline coefficients to determine Al and Cr concentrations at new, equispaced node positions
Write ADIST(j),
AlSP(j),CrSP(j)
to Unit 12
Write new concentrations and positions for single concentration profile to Unit 12
RETURN

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13. ABSTRACT ***(Maximum 200 words)***

A finite-difference computer program (COSIM) has been written which models the one-dimensional, diffusional transport associated with high-temperature oxidation and interdiffusion of overlay-coated substrates. The program predicts concentration profiles for up to three elements in the coating and substrate after various oxidation exposures. Surface recession due to solute loss is also predicted. Ternary cross terms and concentration-dependent diffusion coefficients are taken into account. The program also incorporates a previously-developed oxide growth and spalling model to simulate either isothermal or cyclic oxidation exposures. In addition to predicting concentration profiles after various oxidation exposures, the program can also be used to predict coating life based on a concentration dependent failure criterion (e.g., surface solute content drops to 2%). The computer code, written in an extension of FORTRAN 77, employs numerous subroutines to make the program flexible and easily modifiable to other coating oxidation problems.

14. SUBJECT TERMS

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