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AN APPROXIMATE CLOSED FORM
SOLUTION TO THE FISSION PRODUCT DIFFUSION
EQUATION IN ONE-DIMENSIONAL SLAB GEOMETRY

by

Peter D. Smith

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1. INTRODUCTION AND SUMMARY

The mass transport of metallic fission products within an HTGR core is generally assumed to be governed by diffusion¹ and a partial differential equation that describes this process has been derived by Appel and Roos.² The equation is non-linear because the diffusion coefficients are functions of the mass concentration. In addition, the coefficients of the equation vary in an arbitrary manner with temperature and time. For these two reasons the equation has generally been solved using an iterative, finite-difference solution technique. This is the basis of the FIPER I, FIPER X, FIPER Q and FIPER II computer programs.^{3,4,5} The finite difference solution method is accurate and consistent with all the assumptions. Unfortunately, it is also quite slow, and it is not suited to core survey and parametric study applications.

In order to calculate the fission product release from an entire HTGR core it is necessary to account for a complicated spatial and time-dependent temperature field. It might be thought that one could simply perform a few representative calculations with the exact FIPER method and then use an interpolation procedure to extend these calculations to the entire HTGR core. This is not the case. The spatial distribution of temperature is quite complex, and the release is highly non-linear with temperature and strongly dependent on the temperature history. Therefore, an accurate full-core calculation cannot be done without performing many detailed local calculations in a relatively fine spatial grid. Even if calculations were performed using the relatively coarse mesh of one point per hexagonal fuel element, it would be necessary to include about 4000 spatial points in the model for an 1160 MW HTGR. Thus, it is of paramount importance to have a calculational method that is relatively efficient.

With this fact as a motivation, the FIPER S model^{6,7,8,9,10} was developed to rapidly calculate release from the HTGR core. The concept in FIPER S is to calculate the release using a closed-form solution of a somewhat simplified differential equation. The original FIPER S did this, but some of the conservative simplifications were too severe. The differential equation was solved using incorrect boundary conditions, mass was not conserved in the model, and a number of important effects were not taken into account. In order to remedy these deficiencies a new model has been devised and a new computer code called TRAFIC¹¹ (Transport of Fission products in the Core) has been written.

The TRAFIC code calculates metallic fission product release from an HTGR fuel block or from a small sub-section of an HTGR fuel block. The calculational model is the smallest unit of symmetry in the core, namely, a typical 30-60-90 triangular "web" as shown below.

In TRAFIC the diffusion process is modeled separately in three sub-regions: the fuel rod, the graphite web, and the coolant boundary layer. These regions are coupled through non-linear adsorption/vapor pressure boundary conditions. The fuel rod region is modeled in axisymmetric geometry and the graphite web region is modeled in slab geometry. The "equivalent slab" is defined as one which has the same resistance to a given concentration

difference. This is determined by means of a two-dimensional heat conduction analysis. A typical equivalent slab is shown below along with the concentration and mass flux boundary conditions.

In this report we are concerned with only one part (albeit an important part) of the new TRAFIC model. This part consists of a method to calculate the transient diffusion response in a one-dimensional slab geometry. This model is used to represent the diffusion process in the graphite moderator. It is being presented here as a separate report because the derivations are quite complicated.

The new model presented here includes the following effects not present in the original FIPER S model.

1. Correct boundary conditions.
2. Conservation of mass.
3. Radioactive decay.
4. Thermal diffusion.
5. Mixed species interaction on the coolant hole boundary.

The solution procedure is as follows. First a simplified differential equation having constant coefficients is derived. This equation is then solved in closed form with constant, time-independent boundary conditions. Assuming a known concentration, C_o , on the left hand boundary and a known "effective mas flux," $J_L L/D$, on the right hand boundary, a general solution is obtained. The solution is then evaluated to determine the two unknown boundary conditions: the concentration, C_L , on the right and the effective mass flux, $J_o L/D$, on the left. The general form of these solutions is expressed by the non-dimensional relationships

$$C_L(\rho) = G_1(\beta, \gamma, \rho) C_o + G_2(\beta, \gamma, \rho) J_L \cdot \frac{L}{D(t)} ,$$

and
$$J_o(\rho) \cdot \frac{L}{D(t)} = H_1(\beta, \gamma, \rho) C_o + H_2(\beta, \gamma, \rho) J_L \cdot \frac{L}{D(t)} ,$$

where

β and γ are constant coefficients,

ρ is a non-dimensional reduced time variable, and

$L/D(t)$ is a known function of time.

The functions G_1 , G_2 , H_1 , H_2 are non-dimensional and they can be evaluated numerically in advance.

The final time-dependent solutions can be obtained by a numerical application of Duhamel's superposition principle. This principle, when applied to the above solution functions, gives

$$C_L(\rho) = \int_0^\rho G_1(\rho-\rho') \frac{d}{d\rho'} (C_o) d\rho' + \int_0^\rho G_2(\rho-\rho') \frac{d}{d\rho'} \left(J_L \frac{L}{D} \right) d\rho'$$

$$J_o(\rho) = \int_0^\rho H_1(\rho-\rho') \frac{d}{d\rho'} \left(\frac{C_o D}{L} \right) d\rho' + \int_0^\rho H_2(\rho-\rho') \frac{d}{d\rho'} (J_L) d\rho' .$$

The evaluation of the above Duhamel integrals is accomplished most accurately, and with the least computational effort, through an integration by parts. The first step is to integrate the solution functions in closed-form. Then the final result is obtained by a numerical manipulation of the integrated functions. The solution technique also involves separating the solution into a transient and a steady-state part, with the objective of limiting the extent of the numerical integration to only the most recent parts of the history, where the transient solution is still active.

In the final application, the boundary condition J_L depends on C_L and the boundary condition C_0 depends on J_0 . A consistent solution can be obtained by an iterative procedure that does not involve further solution evaluations.

2. SIMPLIFICATION OF THE DIFFERENTIAL EQUATION

A general diffusion equation applicable to fission product transport in a single-species system is²

$$\frac{\partial}{\partial t} [C(\vec{x}, t)] = S(\vec{x}, t) - \lambda C(\vec{x}, t) - \text{Div } \vec{J}(\vec{x}, t) \quad . \quad (1)$$

$$\text{storage} = \text{source} - \text{decay} - \text{leakage}$$

For the usual case of a diffusion process controlled by both concentration and thermal gradients, the mass flux $\vec{J}$ is given by^{2,12,13}

$$\vec{J}(\vec{x}, t) = - D(T) \left[\vec{\text{grad}} C(\vec{x}, t) + \frac{C(\vec{x}, t) Q}{BRT^2} \vec{\text{grad}} T \right] , \quad (2)$$

where T , the temperature, is an arbitrary function of spatial position and time and Q , B , and R are fixed constants.

In the TRAFIC application, where speed of solution is the governing factor, we make several simplifications in order to arrive at a closed form solution. In particular, the following simplifications are needed:

1. The equation is reduced to one-dimensional slab geometry.
2. The equation is reduced to an equation with constant coefficients so that the general case of time-varying boundary conditions can later be treated using Duhamel's superposition principle.

Expressed in one-dimensional geometry, Eqs. (1) and (2) reduce to

$$\frac{\partial}{\partial t} C(x,t) = S(x,t) - \lambda C(x,t) - \frac{\partial}{\partial x} J(x,t) \quad , \quad (3)$$

$$J(x,t) = - D(T) \left[\frac{\partial}{\partial x} C(x,t) + \frac{C(x,t)Q}{BRT^2} \left(\frac{\partial T}{\partial x} \right) \right] \quad . \quad (4)$$

In order to solve the above equations we need to specify boundary conditions and initial conditions. The derivation shall be temporarily restricted to the case of constant, time-independent boundary conditions. Further, the assumption is made that the two known boundary values are (1) the concentration on the left-hand surface,

$$C(0,t) = C_o \quad , \quad (5)$$

and (2) the mass flux on the right-hand surface,

$$J(L,t) = J_L \quad . \quad (6)$$

These boundary conditions constitute just one of the four possible combinations, (C_o, C_L) , (J_o, J_L) , (C_o, J_L) , and (J_o, C_L) . The reason for the above choice is based partly on the physics of the problem and partly on the mathematical consequences of the choice, facts which shall be discussed in more depth in Section 4.

The initial conditions are given by

$$C(x,t) = 0 \quad \left[t \leq 0 \right] \quad . \quad (7)$$

We now make several simplifications that will reduce the differential equations (3) and (4) to a single second order equation having constant coefficients. First, it is assumed that the temperature difference across the slab is small compared with the temperature itself. Then

$$T(x,t) \approx \bar{T}(t) \quad . \quad (8)$$

Next it is assumed that the temperature field across the slab is linear (as it would be in a quasi-steady thermal state), which gives

$$\frac{\partial T}{\partial x}(x,t) \approx \frac{\Delta T(t)}{L} \quad . \quad (9)$$

With these approximations, which appear to be reasonable in the present application, one can eliminate the spatial dependence of the coefficients. Defining

$$\alpha(t) = \frac{D(\bar{T}) Q \Delta T(t)}{B \bar{T}(t)^2 L} \quad , \quad (10)$$

Eqs. (3) and (4) then combine to give the simpler form

$$\frac{\partial C}{\partial t} = D(t) \frac{\partial^2 C}{\partial x^2} + \alpha(t) \frac{\partial C}{\partial x} - \lambda C + S \quad . \quad (11)$$

It is further noted that in the slab portion of the model, which represents the graphite moderator, the source term S is zero. This is because all the fission products are born in the fuel rod, which is treated by another model. Equation (11) then reduces to

$$\frac{\partial C}{\partial t} = D(t) \frac{\partial^2 C}{\partial x^2} + \alpha(t) \frac{\partial C}{\partial x} - \lambda C \quad . \quad (12)$$

The above equation can be further simplified by non-dimensionalizing it. Multiplying all terms by the common factor

$$\frac{L^2}{D(t)} ,$$

we have

$$\frac{L^2}{D(t)} \frac{\partial C}{\partial t} = \frac{L^2}{D(t)} \frac{\partial^2 C}{\partial x^2} + \frac{L^2 \alpha(t)}{D(t)} \frac{\partial C}{\partial x} - \frac{\lambda L^2}{D(t)} C . \quad (13)$$

Then define

$$\xi = \frac{x}{L} \text{ (non-dimensional } x) , \text{ and} \quad (14)$$

$$\rho(t) = \int_0^t \frac{D(\tau)}{L^2} d\tau \text{ (effective time)} . \quad (15)$$

Further, note that

$$\frac{d\rho}{dt} = \frac{D(t)}{L^2} , \quad (16)$$

and

$$\frac{\partial}{\partial \rho} = \frac{L^2}{D(t)} \frac{\partial}{\partial t} . \quad (17)$$

Substituting (14) and (17) into (13) then gives

$$\frac{\partial}{\partial \rho} C(\xi, \rho) = \frac{\partial^2 C}{\partial \xi^2} + \beta \frac{\partial C}{\partial \xi} - \gamma C , \quad (18)$$

where

$$\beta = \frac{L \alpha(t)}{D(t)} = \frac{Q \Delta T(t)}{BRT(t)^2} , \quad (19)$$

and

$$\gamma = \frac{\lambda L^2}{D(t)} . \quad (20)$$

Equation (18) is a reasonably rigorous equation for the diffusion process, including the effects of thermal diffusion in the β term and radioactive decay in the γ term. One difficulty is that the coefficients β and γ are arbitrarily time-dependent, which means that a closed-form solution is impossible. This problem can be avoided by making the crude (but necessary) assumption that the β and γ coefficients are constant. This is true for a problem where the temperatures do not vary with time.

In the case of an HTGR, the temperatures do vary with time, but not by an extreme amount. Regardless of this, it is necessary to choose by a rational procedure some effective, constant values for β and γ . One might, for example, use the time average values

$$\bar{\beta} = \frac{1}{t_{\max}} \int_0^{t_{\max}} \beta(t) dt , \quad (21)$$

and

$$\bar{\gamma} = \frac{1}{t_{\max}} \int_0^{t_{\max}} \gamma(t) dt . \quad (22)$$

Many other weighted means are theoretically possible. In any case, the assumption is now made that effective constant values for β and γ can somehow be chosen. The basic rationale behind this assumption is that previously the thermal diffusion and radioactive decay effects were being completely ignored in FIPER S. It is presumably better to treat these effects in an approximate way than to ignore them altogether.

3. GENERAL SOLUTION

The object now is to solve a second-order partial differential equation with constant coefficients,

$$\frac{\partial}{\partial \rho} C(\xi, \rho) = \frac{\partial^2 C}{\partial \xi^2} + \beta \frac{\partial C}{\partial \xi} - \gamma C \quad , \quad (23)$$

where β and γ are constants,

and ξ and ρ are the independent variables.

The general solution can be found by means of the separation of variables technique. Assume that

$$C(\xi, \rho) = F(\rho) \cdot G(\xi) \quad . \quad (24)$$

Substituting (24) back into (23) gives

$$\dot{F}G = FG'' + \beta FG' - \gamma FG \quad . \quad (25)$$

Dividing each term by FG then gives

$$\frac{\dot{F}}{F} = \frac{G''}{G} + \beta \frac{G'}{G} - \gamma \quad . \quad (26)$$

The only way that the two sides of (26) can be equal (since they are functions of different independent variables) is for them to both equal the same constant number. Further, in order to ensure a real solution with a stable time dependency, that number must be real and negative. Thus,

$$\frac{\dot{\bar{F}}}{\bar{F}} = - \frac{\omega^2}{2} , \quad \text{Note: This is a bar, not a minus sign.} \quad (27)$$

and

$$\frac{G''}{G} + \beta \frac{G'}{G} - \gamma = - \omega^2 . \quad (28)$$

Multiplying Eq. (27) by $\bar{F}$ gives the ordinary differential equation

$$\dot{\bar{F}} + \omega^2 \bar{F} = 0 , \quad (29)$$

which has the general solution

$$\bar{F} = e^{-\omega^2 \rho} . \quad (30)$$

Multiplying Eq. (28) by G gives the ordinary differential equation

$$G'' + \beta G' + (\omega^2 - \gamma) G = 0 . \quad (31)$$

For a trial solution let

$$G(\xi) = e^{\lambda \xi} . \quad (32)$$

Substituting (32) into (31) gives

$$\left[\lambda^2 + \beta \lambda + (\omega^2 - \gamma) \right] e^{\lambda \xi} = 0 . \quad (33)$$

Since $e^{\lambda \xi} \neq 0$ for finite λ , Eq. (33) can be true only if

$$\lambda^2 + \beta \lambda + (\omega^2 - \gamma) = 0 , \quad (34)$$

which implies that

$$\lambda = -\frac{\beta}{2} \pm \sqrt{\frac{\beta^2}{4} + \gamma - \omega^2} . \quad (35)$$

We now define a useful variable

$$\theta^2 \equiv \frac{\beta^2}{4} + \gamma , \quad (36)$$

from which (35) becomes

$$\lambda = -\frac{\beta}{2} \pm \sqrt{\theta^2 - \omega^2} . \quad (37)$$

Either alternative for λ in (37) gives a valid solution for $G(\xi)$ in Eq. (32). Further, since Eq. (31) is linear, any linear combination of solutions is also a solution. Thus, the general solution of (31) is

$$G(\xi) = e^{\frac{-\beta\xi}{2}} \left(Ae^{\xi\sqrt{\theta^2 - \omega^2}} + Be^{-\xi\sqrt{\theta^2 - \omega^2}} \right) . \quad (38)$$

At this point we make some observations about the parameters in (38).

1. ω^2 is arbitrary, real, and non-negative.
 2. β is real.
 3. γ is real and non-negative.
 4. θ^2 is real and non-negative.
- $\therefore \sqrt{\theta^2 - \omega^2}$ is real or imaginary, but not complex.

We now form the combined solution by substituting (30) and (38) into (24). Thus, one solution to (23) is given by

$$C(\xi, \rho) = e^{-\frac{\beta \xi}{2}} e^{-\bar{\omega}^2 \rho} \left(A e^{\xi \sqrt{\theta^2 - \bar{\omega}^2}} + B e^{-\xi \sqrt{\theta^2 - \bar{\omega}^2}} \right) . \quad (39)$$

This is a valid solution for all A, B, and $\bar{\omega}$ and every possible combination thereof. Furthermore, since the differential equation (23) is linear, a linear combination of solutions is also a solution. Thus, another valid solution to (23) is

$$C(\xi, \rho) = e^{-\frac{\beta \xi}{2}} \sum_{i=0}^{\infty} e^{-\bar{\omega}_i^2 \rho} \left(A_i e^{\xi \sqrt{\theta^2 - \bar{\omega}_i^2}} + B_i e^{-\xi \sqrt{\theta^2 - \bar{\omega}_i^2}} \right) . \quad (40)$$

It is noted that the $\bar{\omega}^2$ are still arbitrary. In particular $\bar{\omega}^2=0$ is one possibility. Inspection of (40) will show that the particular case of $\bar{\omega}^2=0$ gives a steady-state solution (independent of ρ). All other choices of $\bar{\omega}^2>0$ give an exponentially decaying transient solution. For ease of physical interpretation and application of boundary conditions, it will be convenient at this stage to separate the solution into a steady and a transient part. Thus, we let

$$C(\xi, \rho) = C_S(\xi) + C_T(\xi, \rho) . \quad (41)$$

The steady term is the zero'th term in the summation (40), for which we arbitrarily assign $\bar{\omega}_0 = 0$, i.e.,

$$C_S(\xi) = e^{-\frac{\beta \xi}{2}} \left(A_0 e^{\theta \xi} + B_0 e^{-\theta \xi} \right) . \quad (42)$$

Then, the transient solution is

$$C_T(\xi, \rho) = e^{-\frac{\beta\xi}{2}} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \left(A_i e^{\xi \sqrt{\theta^2 - \omega_i^2}} + B_i e^{-\xi \sqrt{\theta^2 - \omega_i^2}} \right). \quad (43)$$

We now note that it is possible to put (43) in a more convenient form. Since ω_i is arbitrary at this stage we can equally well substitute another arbitrary constant defined by

$$j\omega_i = \sqrt{\theta^2 - \omega_i^2} \quad [j = \sqrt{-1}], \quad (44)$$

$$\therefore \omega_i^2 = \theta^2 + \omega_i^2. \quad (45)$$

Substituting (44) and (45) into (43), we have

$$C_T(\xi, \rho) = e^{-\frac{\beta\xi}{2}} e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \left(A_i e^{j\omega_i \xi} + B_i e^{-j\omega_i \xi} \right), \quad (46)$$

which is equivalent to the expression

$$C_T(\xi, \rho) = e^{-\frac{\beta\xi}{2}} e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \left(A_i \cos \omega_i \xi + B_i \sin \omega_i \xi \right). \quad (47)$$

The motivation for transforming (43) to the Fourier series form of (47) is that most of the roots ω_i are real, as will be shown later. This gives the resulting expansion more intuitive appeal, although either form is mathematically correct.

In summary, combination of (41) and (47) now gives the complete general solution

$$C(\xi, \rho) = e^{\frac{-\beta \xi}{2}} \left[A_0 e^{\theta \xi} + B_0 e^{-\theta \xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \left(A_i \cos \omega_i \xi + B_i \sin \omega_i \xi \right) \right] . \quad (48)$$

It is noted once again that the A_i , B_i , and ω_i are at present still arbitrary. A_i and B_i must be real for real ω_i and complex for imaginary ω_i . The actual values of the A_i , B_i , and ω_i parameters will be determined in the following sections.

4. BOUNDARY CONDITIONS

In order to complete the differential equation solution, it is necessary to eliminate some of the arbitrary constants in (48) by the use of auxiliary constraint equations which define the conditions on the boundary for all time and the conditions on the interior at time zero. The present section is concerned only with the boundary conditions. The initial conditions are treated in Section 6.

The boundary conditions to our problem are in actuality both time-dependent and non-linear. On each of the two slab surfaces, left and right, they take the general form

$$C_i(t) = C_i(J_i(t)) \quad ,$$

or

$$J_i(t) = J_i(C_i(t)) \quad .$$

Boundary conditions such as these are awkward if not impossible to treat analytically. The problem is simplified in two stages. The first stage is to assume that the boundary conditions are constant, independent of time. The time-dependency of the actual boundary conditions can be treated later by the Duhamel superposition principle. The second stage is to linearize the boundary conditions by assuming that two of the four interrelated quantities,

C_o = left hand concentration,
 J_o = left hand mass flux,
 C_L = right hand concentration, and
 J_L = right hand mass flux,

are known. With this assumption a solution can be readily obtained. It is then possible to solve for the two remaining boundary values by means of two linear equations, for example,

$$C_L = A_1 + A_2 C_o + A_3 J_L ,$$

and

$$J_o = B_1 + B_2 C_o + B_3 J_L .$$

These two equations can then be used as the basis of an iterative solution to satisfy the non-linear boundary conditions in a consistent matter. This point will be clarified in Section 8. For the present, let us simply assume that it is necessary to fix two of the four boundary values.

We next address ourselves to the question of which two to fix. The answer to this is not immediately obvious. The choice rests on some mathematical subtleties related to singularities in the solution functions. Without going into exhaustive detail, it is noted that the easiest choice, insofar as the algebra of the solution is concerned, is to pick the two concentrations, C_o and C_L , as given and to solve for the fluxes, J_o and J_L . The result is

$$J_o = f_1(\rho) C_o + f_2(\rho) C_L ,$$

and

$$J_L = g_1(\rho) C_o + g_2(\rho) C_L .$$

Unfortunately, both the f_1 and the g_2 functions are singular at $\rho=0$, a fact that causes numerical complications and accuracy problems. The results are particularly bad for g_2 , because the J_L term is of primary interest in calculating the release of fission products into the coolant stream. The singularity due to g_2 is eliminated by assuming that J_L rather than C_L is the given boundary condition on the coolant side.

One might then ask why we cannot similarly eliminate the singularity due to f_1 . The reason for this is that while this can, indeed, be done for the present slab solution, the result is that a second and more troublesome singularity is thereby introduced into the fuel rod portion of the composite TRAFIC model.

In view of the above factors, the known boundary conditions for this problem are assumed to be the concentration C_o on the left side of the slab and the mass flux J_L on the right side, as shown below.

We consider first the concentration boundary condition. By transforming to the new time variable, ρ , Eq. (5) becomes

$$C(\xi, \rho) \Big|_{\xi=0} = C_o \quad . \quad (49)$$

Evaluating (48) at $\xi=0$, we then have

$$C(0, \rho) = A_o + B_o + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} A_i = C_o \quad . \quad (50)$$

Since each term in the transient portion is a decaying function of time and since the boundary condition (49) is constant with time, Eq. (50) can be satisfied only if

$$A_o + B_o = C_o , \quad (51)$$

$$\text{and} \quad A_i = 0 \quad \left\{ \text{all } i \right\} \quad (52)$$

In view of (52), the new general solution is

$$C(\xi, \rho) = e^{-\frac{\beta \xi}{2}} \left[A_o e^{\theta \xi} + B_o e^{-\theta \xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \sin \omega_i \xi \right] . \quad (53)$$

Next, we consider the flux boundary condition on the right side,

$$J(\xi, \rho) \Big|_{\xi=1} = J_L . \quad (54)$$

The algebra is made easier by first non-dimensionalizing Eq. (4). Multiplying all terms by L/D , we arrive at the following equation:

$$\frac{J(\xi, \rho)L}{D(t)} = - \frac{\partial C(\xi, \rho)}{\partial \xi} - \beta C(\xi, \rho) . \quad (55)$$

The boundary condition (54) is then

$$\left[\frac{\partial C(\xi, \rho)}{\partial \xi} + \beta C(\xi, \rho) \right]_{\xi=1} = - \frac{J_L L}{D(t)} . \quad (56)$$

Differentiating (53) with respect to ξ , we obtain

$$\begin{aligned} \frac{\partial C}{\partial \xi} = & -\frac{\beta}{2} e^{-\frac{\beta \xi}{2}} \left[A_o e^{\theta \xi} + B_o e^{-\theta \xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \sin \omega_i \xi \right] \\ & + e^{-\frac{\beta \xi}{2}} \left[\theta A_o e^{\theta \xi} - \theta B_o e^{-\theta \xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \omega_i B_i \cos \omega_i \xi \right] . \quad (57) \end{aligned}$$

Combining (57) and (53) in Eq. (55) then gives

$$\begin{aligned} \frac{J(\xi, \rho) L}{D(t)} = & -\frac{\beta}{2} e^{-\frac{\beta \xi}{2}} \left[A_o e^{\theta \xi} + B_o e^{-\theta \xi} \right. \\ & \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \sin \omega_i \xi \right] \\ & - e^{-\frac{\beta \xi}{2}} \left[\theta A_o e^{\theta \xi} - \theta B_o e^{-\theta \xi} \right. \\ & \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \omega_i B_i \cos \omega_i \xi \right] . \quad (58) \end{aligned}$$

The boundary condition (56) is expressed by evaluating (58) at $\xi=1$, which gives

$$\begin{aligned} \frac{\beta}{2} e^{-\beta/2} \left[A_o e^{\theta} + B_o e^{-\theta} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \sin \omega_i \right] \\ + e^{-\beta/2} \left[\theta A_o e^{\theta} - \theta B_o e^{-\theta} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \omega_i \cos \omega_i \right] = -\frac{J_L L}{D(t)} . \quad (59) \end{aligned}$$

Examination of (59) will show that a time-dependent diffusion constant, $D(t)$, is lumped in the same term as the mass flux, J_L . If the flux J_L were in actuality constant with time, the presence of this time-dependent factor in Eq. (59) would have the effect of creating a time-varying boundary condition. The only way we can ever have a truly steady-state solution, independent of ρ , is to require that the quantity,

$$\frac{J_L L}{D(t)} \quad (\text{an effective mass flux}) \quad ,$$

be independent of time. It might appear that this is a restrictive and physically meaningless assumption. This does not matter, however, because the ultimate objective in this analysis is to perform the calculations with a time-varying boundary condition using the Duhamel superposition principle. Bearing this in mind, we can for the present assume that the term $J_L L/D(t)$ is independent of ρ . The actual time-dependency will be treated later in the superposition process.

Having made the above assumption, we can immediately separate Eq. (59) into a steady-state and a transient part. The steady-state part has the constant boundary condition and the transient part has a homogeneous boundary condition, i.e.,

$$\frac{\beta}{2} e^{-\beta/2} \left[A_o e^{\theta} + B_o e^{-\theta} \right] + e^{-\beta/2} \left[\theta A_o e^{\theta} - \theta B_o e^{-\theta} \right] = - \frac{J_L L}{D(t)} \quad , \quad (60)$$

and
$$e^{-\beta/2} e^{-\theta^2 \rho} \left[\frac{\beta}{2} \sum e^{-\omega_i^2 \rho} B_i \sin \omega_i + \sum e^{-\omega_i^2 \rho} \omega_i B_i \cos \omega_i \right] = 0 \quad . \quad (61)$$

Equation (60) can be reorganized to the following form

$$A_o \left(\theta + \frac{\beta}{2} \right) e^{\theta} - B_o \left(\theta - \frac{\beta}{2} \right) e^{-\theta} = e^{+\frac{\beta}{2}} \left(- \frac{J_L L}{D(t)} \right) . \quad (62)$$

Defining $Q_A = \left(\theta - \frac{\beta}{2} \right) e^{-\theta} , \quad (63)$

$$Q_B = \left(\theta + \frac{\beta}{2} \right) e^{+\theta} , \quad (64)$$

and $P(t) = e^{\beta/2} \frac{L}{D(t)} , \quad (65)$

Eq. (62) can be written

$$A_o Q_B - B_o Q_A = - J_L P(t) . \quad (66)$$

We can now combine Eqs. (51) and (66) to solve for the constants A_o and B_o .

$$A_o Q_A + B_o Q_A = C_o Q_A$$

$$A_o Q_B - B_o Q_A = -J_L P(t)$$

$$\therefore A_o = \frac{C_o Q_A - J_L P(t)}{Q_A + Q_B} , \quad (67)$$

and $B_o = \frac{C_o Q_B + J_L P(t)}{Q_A + Q_B} . \quad (68)$

Equation (61) can now be manipulated to give a requirement on the values of ω_i . Rearranging terms, Eq. (61) can be written

$$e^{-\frac{\beta}{2}} e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \left(\frac{\beta}{2} \sin \omega_i + \omega_i \cos \omega_i \right) = 0 \quad . \quad (69)$$

Since the B_i are not all zero, except in a trivial solution, Eq. (69) can be satisfied only if

$$\frac{\beta}{2} \sin \omega_i + \omega_i \cos \omega_i = 0 \quad , \quad (70)$$

or
$$\tan \omega_i = -\frac{2}{\beta} \omega_i \quad . \quad (71)$$

Solutions to (71) define a sequence of ω_i . These are the only possible values which satisfy the imposed flux boundary condition.

Given the boundary conditions (49) and (54), we have thus determined A_0 , B_0 , and the fact that all A_i are zero. We have also defined a sequence of admissible ω_i . All that remains is to determine the constants B_i . This is done in Section 6 by proving that the functions $\sin \omega_i \xi$ are an orthogonal set and by using standard Fourier series techniques to calculate the B_i coefficients.

5. ROOTS OF THE CHARACTERISTIC EQUATION

All solutions of the form derived thus far (see Eq. (53)) which satisfy the boundary conditions must also satisfy the characteristic equation.

$$\tan \omega_i = - \frac{2}{\beta} \omega_i \quad [i=1, \infty] \quad (72)$$

Through previous arguments (see p. 13 and Eq. (44)) we know that the ω_i must be either real or imaginary, but that they cannot be complex.

5.1 Real Roots

The real roots of (72) can be shown graphically by plotting the two functions

$$f_1(\omega) = \tan \omega$$

and

$$f_2(\omega) = - \frac{2}{\beta} \omega$$

on the same graph and noting where they intersect. As an example, two cases are shown on the next page — one with positive β and one with negative β .

Note that the root $\omega = 0$ is one possible solution in both cases. A superficial examination of this zero root would seem to indicate that the eigenfunction corresponding to this root is trivial because $\sin(0x) = 0$. A more careful theoretical investigation, however, will show that the zero root is trivial for all but the very special case of $\beta = -2$. For this peculiar case the eigenfunction $B_1 \sin \omega_1 x$ approaches a finite limiting value of $B_1 x$. For all other values of β , the eigenfunction is truly

Real Roots

zero. This fact is easily shown by substituting the condition $\omega = 0$ back into the original differential equation. The proof shall not be given here.

Note also that for every root $\omega_i > 0$ there is a matching root $\omega = -\omega_i$. Negative roots, however, do not provide independent eigenfunctions because

$$\sin \omega_i = -\sin(-\omega_i) \quad .$$

We could include these terms in our series expansion, but the net result would not be affected. It is easier to restrict the series to non-negative roots only.

It is worthy of mention that for the case $\beta = 0$, that is, when there is no thermal diffusion, the roots of (72) reduce to

$$\omega_i = \frac{(2i-1)\pi}{2} \quad . \quad [\beta=0] \quad (73)$$

This is the sequence typically experienced in thermal conduction problems, which obey a similar differential equation. In the present case, however, the thermal diffusion term distorts the eigenfunctions.

5.2 Imaginary Roots

Now let us consider the possibility that there may be some imaginary roots. If this is the case, then the imaginary roots can be expressed as

$$\omega_i = j\omega_i^* \quad , \quad (74)$$

where ω_i^* is the real magnitude of the root.

Substituting (74) into (72), we see that the imaginary roots, if any, must satisfy the equation

$$\tan(j \omega_1^*) = -\frac{2}{\beta} j \omega_1^* . \quad (75)$$

It can be shown, however, that

$$\tan(j \omega_1^*) = j \tanh \omega_1^* , \quad (76)$$

so Eq. (75) becomes

$$\tanh(\omega_1^*) = -\frac{2}{\beta} \omega_1^* . \quad (77)$$

Since the functions and the arguments in (77) are real, we can now find the roots graphically as before. This is shown below.

In this case it is seen that there is, at most, only one non-zero imaginary root. The negative root, as before, is not independent.

It is noted that

$$\left. \frac{d}{d\omega} \tanh(\omega) \right|_{\omega=0} = 1 , \quad (78)$$

and

$$\left. \frac{d}{d\omega} \tan(\omega) \right|_{\omega=0} = 1 . \quad (79)$$

In view of Eq. (78), an imaginary root exists only for β within the range

$$\beta < -2 . \quad (80)$$

Furthermore, in view of Eq. (79), a real root in the first quadrant ($\omega < \pi/2$) exists only for the range

$$-2 < \beta < 0 . \quad (81)$$

It is seen that as β approaches -2 from above, the real root in the first quadrant disappears. As β approaches -2 from below, the imaginary root disappears. The behavior at the limit $\beta = -2$ is discussed in the following section.

5.3 Transition Through $\beta = -2$

In the sketch on the following page, the functions $\tan \omega$ and $\tanh \omega$ are plotted on the same graph.

As β swings past -2 from above, the first real root ω_1 disappears to zero and reappears again immediately as an imaginary root. Plotted as a function of β , the root ω_1 has the appearance shown below.

The cusp at $\beta = -2$ is of particular interest. At this point the two real roots ω_1 and $-\omega_1$ collapse onto the existing trivial root ($\omega=0$) forming a triple zero root. As we have previously mentioned, this particular zero root is not trivial. For the case $\beta = -2$ it can be shown that the eigenfunction $B_1 \sin \omega_1 x$ approaches a limiting value of $B_1 x$. This is discussed further in Section 10.

5.4 Calculation of the Roots

The roots ω_1 shown graphically in the previous sections can be calculated numerically by means of Newton's method. Careful attention to detail must be paid in this, particularly in the area of choosing an appropriate first guess for the iterative procedure. With a little care, however, one can easily arrive at an algorithm to compute an infinite sequence of roots, ω_1 for any value of β . The details of this shall not be given in this report.

6. INITIAL CONDITIONS

Returning to the problem at hand, the general solution to the differential Eq. (23) has been shown to be

$$C(\xi, \rho) = e^{\frac{-\beta\xi}{2}} \left[A_0 e^{\theta\xi} + B_0 e^{-\theta\xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} B_i \sin \omega_i \xi \right] . \quad (82)$$

β and θ are constants, dependent on the two independent coefficients of the differential equation. A_0 , B_0 , and the ω_i have been determined from the boundary conditions (see Section 4). All that remains to complete the solution are the constants B_i . These are determined from the initial conditions.

The appropriate initial condition is

$$C(\xi, \rho) \Big|_{\rho=0} = 0 . \quad (83)$$

Evaluating (82) at $\rho=0$, then, we have

$$C(\xi, 0) = e^{-\beta/2} \left[A_0 e^{\theta\xi} + B_0 e^{-\theta\xi} + \sum_{i=1}^{\infty} B_i \sin \omega_i \xi \right] = 0 . \quad (84)$$

Since $e^{-\beta/2}$ is non-zero, the only way to satisfy (84) is to require that

$$\sum_{i=1}^{\infty} B_i \sin \omega_i \xi = -A_0 e^{\theta \xi} - B_0 e^{-\theta \xi} . \quad (85)$$

In other words, the transient solution at $\rho=0$ must be equal and opposite the steady-state solution at $\rho=\infty$.

Equation (85) resembles the familiar Fourier series expansion. The only difference is that the ω_i are not even multiples of $\pi/2$. Nevertheless, it will be proven that the functions $\sin \omega_i \xi$ are indeed orthogonal. In anticipation of this result, we use the classical method to evaluate the coefficients B_i .

The first step is to multiply both sides of (85) by a single one of the orthogonal functions, say, $\sin \omega_j \xi$. This gives

$$\sum_{i=1}^{\infty} B_i \sin \omega_i \xi \sin \omega_j \xi = f(\xi) \sin \omega_j \xi , \quad (86)$$

where
$$f(\xi) = -A_0 e^{\theta \xi} - B_0 e^{-\theta \xi} . \quad (87)$$

Next we integrate both sides between the boundary limits of ξ , i.e., from zero to one:

$$\sum_{i=1}^{\infty} B_i \int_0^1 \sin \omega_i \xi \sin \omega_j \xi d\xi = \int_0^1 f(\xi) \sin \omega_j \xi d\xi . \quad (88)$$

It will be proven in Section 6.1 that the $\sin \omega_j \xi$ functions are an orthogonal set, that is

$$\int_0^1 \sin \omega_i \xi \sin \omega_j \xi \, d\xi = 0 \quad , \quad i \neq j \quad , \quad (89)$$

and

$$\int_0^1 \sin^2 \omega_j \xi \, d\xi = g(\omega_j) \quad , \quad i = j \quad . \quad (90)$$

In view of (89), all terms in the summation of Eq. (88) are zero except one, namely, the term for which $i=j$. Eq. (88) then reduces to

$$B_j \int_0^1 \sin^2 \omega_j \xi \, d\xi = \int_0^1 f(\xi) \sin \omega_j \xi \, d\xi \quad . \quad (91)$$

Thus,

$$B_j(\omega_j) = \frac{\int_0^1 f(\xi) \sin \omega_j \xi \, d\xi}{\int_0^1 \sin^2 \omega_j \xi \, d\xi} \quad . \quad (92)$$

The proof of orthogonality and the evaluation of the integrals will be done in the following sections.

6.1 Proof of Orthogonality

We wish to prove that

$$\int_0^1 \sin \omega_i \xi \sin \omega_j \xi \, d\xi = 0 \quad [i \neq j] \quad . \quad (93)$$

First make the substitution

$$\sin a \sin b = \frac{1}{2} \cos(a-b) - \frac{1}{2} \cos(a+b) \quad . \quad (94)$$

Thus

$$\begin{aligned} \int_0^1 \sin \omega_i \xi \sin \omega_j \xi \, d\xi &= \frac{1}{2} \int_0^1 \cos(\omega_i - \omega_j) \xi \, d\xi \\ &\quad - \frac{1}{2} \int_0^1 \cos(\omega_i + \omega_j) \xi \, d\xi \quad . \end{aligned} \quad (95)$$

Noting that

$$\int \cos ax \, dx = \frac{1}{a} \sin ax \quad , \quad (96)$$

evaluation of (95) and slight rearrangement of terms gives

$$\begin{aligned} &\int_0^1 \sin \omega_i \xi \sin \omega_j \xi \, d\xi \quad [\omega_i \neq \omega_j] \\ &= \frac{(\omega_i + \omega_j) \sin(\omega_i - \omega_j) - (\omega_i - \omega_j) \sin(\omega_i + \omega_j)}{2(\omega_i^2 - \omega_j^2)} \\ &= \frac{\omega_j \sin \omega_i \cos \omega_j - \omega_i \sin \omega_j \cos \omega_i}{\omega_i^2 - \omega_j^2} \quad . \end{aligned} \quad (97)$$

Now, the ω 's themselves are defined as being the roots of the equation

$$\tan \omega = -\frac{2}{\beta} \omega . \quad (98)$$

From the above we obtain

$$\frac{\tan \omega_i}{\omega_i} = \frac{\tan \omega_j}{\omega_j} = -\frac{2}{\beta} . \quad (99)$$

Rearranging terms in (99) then gives

$$\omega_j \sin \omega_i \cos \omega_j = \omega_i \sin \omega_j \cos \omega_i . \quad (100)$$

Comparing (100) with the numerator of Eq. (97), it is apparent that, for the above definition of ω ,

$$\int_0^1 \sin \omega_i \xi \sin \omega_j \xi \, d\xi = 0 , \quad (101)$$

whenever $i \neq j$. It can be shown that the above results are equally valid when one or both of the roots ω is imaginary.

For the case $i=j$, the integral can be evaluated using standard integral tables. The result is

$$\int_0^1 \sin^2 \omega_i \xi \, d\xi = \frac{2\omega_i - \sin 2\omega_i}{4\omega_i} . \quad (102)$$

6.2 Evaluation of the B_i Coefficients

The coefficients B_i in Eq. (82) are determined by substituting (102) and (87) into (92). Thus, we obtain

$$B_i = \frac{4\omega_i}{2\omega_i - \sin 2\omega_i} \int_0^1 f(\xi) \sin \omega_i \xi \, d\xi, \quad (103)$$

where
$$f(\xi) = -A_o e^{\theta \xi} - B_o e^{-\theta \xi}.$$

Evaluation of the integral using standard integration tables gives

$$B_i = \left(\frac{-4\omega_i}{2\omega_i - \sin 2\omega_i} \right) \left\{ \left[\frac{A_o e^{\theta \xi} (\theta \sin \omega_i \xi - \omega_i \cos \omega_i \xi)}{\theta^2 + \omega_i^2} \right]_{\xi=0}^1 + \left[\frac{B_o e^{-\xi \theta} (-\theta \sin \omega_i \xi - \omega_i \cos \omega_i \xi)}{\theta^2 + \omega_i^2} \right]_{\xi=0}^1 \right\}. \quad (104)$$

The above equation is simplified by evaluating the expression at the limits, by substituting Eq. (70) to eliminate the $\omega \cos \omega$, and by collecting terms. The result is

$$B_i = \frac{-4\omega_i}{(2\omega_i - \sin 2\omega_i)(\theta^2 + \omega_i^2)} \left\{ A_o \left[\left(\theta + \frac{\beta}{2} \right) e^{\theta} \sin \omega_i + \omega_i \right] + B_o \left[-\left(\theta - \frac{\beta}{2} \right) e^{-\theta} \sin \omega_i + \omega_i \right] \right\}. \quad (105)$$

The same results are also valid for imaginary ω . We assume that

$$\omega_1 = j \omega^* , \quad (106)$$

where ω^* is real. It can be shown, then, that

$$\sin(\omega_1) = j \sinh(\omega^*) . \quad (107)$$

Substituting (106) and (107) into (105) we obtain

$$\begin{aligned} B_1^I = & \frac{-4j\omega^*}{(2j\omega^* - j \sinh 2\omega^*)(\theta^2 - \omega^{*2})} \\ & \times \left\{ A_o \left[\left(\theta + \frac{\beta}{2} \right) e^\theta j \sinh \omega^* + j \omega^* \right] \right. \\ & \left. + B_o \left[- \left(\theta - \frac{\beta}{2} \right) e^{-\theta} j \sinh \omega^* + j \omega^* \right] \right\} . \quad (108) \end{aligned}$$

Factoring out the common j terms, Eq. (108) becomes

$$\begin{aligned} B_1^I = & \frac{-4j\omega^*}{(2\omega^* - \sinh 2\omega^*)(\theta^2 - \omega^{*2})} \\ & \times \left\{ A_o \left[\left(\theta + \frac{\beta}{2} \right) e^\theta \sinh \omega^* + \omega^* \right] \right. \\ & \left. + B_o \left[- \left(\theta - \frac{\beta}{2} \right) e^{-\theta} \sinh \omega^* + \omega^* \right] \right\} . \quad (109) \end{aligned}$$

It is seen that B_1^I is imaginary. This is to be expected, because the complete term in the series is

$$\begin{aligned}
 B_1^I \sin(\omega_1 \xi) &= B_1^I j \sinh(\omega^* \xi) \\
 &= \frac{4\omega^* \sinh \omega^* \xi}{(2\omega^* - \sinh 2\omega^*)(\theta^2 - \omega^{*2})} \\
 &\times \left\{ A_o \left[\left(\theta + \frac{\beta}{2} \right) e^{\theta} \sinh \omega^* + \omega^* \right] \right. \\
 &\quad \left. + B_o \left[- \left(\theta - \frac{\beta}{2} \right) e^{-\theta} \sinh \omega^* + \omega^* \right] \right\} . \quad (110)
 \end{aligned}$$

Thus, the total contribution of this term to the series expansion is real.

7. SOLUTION AS A LINEAR COMBINATION OF BOUNDARY VALUES

The solution presented in the previous sections is not in the most convenient form for a practical application. This is because the boundary values, C_0 and J_L , are deeply entwined in the algebra of evaluating the various coefficients. By rearranging terms and simplifying the algebra, however, it is possible to extract the boundary values and express the solution as a linear combination of two non-dimensional functions,

$$C(\xi, \rho) = F_1(\beta, \gamma, \xi, \rho) C_0 + F_2(\beta, \gamma, \xi, \rho) J_L \frac{L}{D(t)} . \quad (111)$$

This has two advantages. First, the functions F_1 and F_2 do not depend on the boundary conditions, and they can be evaluated in advance. Second, the form of Eq. (111) is precisely the form we need in order to obtain a solution with time-varying boundary conditions using Duhamel's superposition principle.

As a motivation for what follows, it is noted that

1. The coefficients A_0 and B_0 are each linear combinations of C_0 and J_L (see Eqs. (67), (68)).
2. The coefficients B_i are each linear combinations of A_0 and B_0 (see (105)).
3. The complete solution (Eq. (82)) is a linear combination of A_0 , B_0 , and all the B_i .

As a consequence of the above, the complete solution must be a linear combination of C_0 and J_L .

7.1 Simplifying the Algebra

First, referring to Eq. (105), we define

$$S(\omega, \xi) = \frac{-4\omega \sin \omega \xi}{(2\omega - \sin 2\omega)(\theta^2 + \omega^2)} . \quad (112)$$

A corresponding definition for the single imaginary root is then, from Eq. (110),

$$S^*(\omega^*, \xi) = \frac{+4\omega^* \sinh \omega^* \xi}{(2\omega^* - \sinh 2\omega^*)(\theta^2 - \omega^{*2})} . \quad (113)$$

Next we define

$$T_A(\omega) = \left[\left(\theta + \frac{\beta}{2} \right) e^{\theta} \sin \omega + \omega \right] , \quad (114)$$

and

$$T_B(\omega) = \left[-\left(\theta - \frac{\beta}{2} \right) e^{-\theta} \sin \omega + \omega \right] . \quad (115)$$

Substituting (63) into (114) and (64) into (115) we have the further simplification that

$$T_A(\omega) = Q_B \sin \omega + \omega , \quad (116)$$

and

$$T_B(\omega) = -Q_A \sin \omega + \omega . \quad (117)$$

Comparing (105) and (110), it is seen that analogous quantities for the imaginary root are

$$T_A^*(\omega^*) = Q_B \sinh \omega^* + \omega^* , \quad (118)$$

$$T_B^*(\omega^*) = -Q_A \sinh \omega^* + \omega^* . \quad (119)$$

Substituting (112), (116) and (117) into (105) then gives

$$B_1 \sin \omega_1 \xi = S(\omega_1, \xi) \left[A_0 T_A(\omega_1) + B_0 T_B(\omega_1) \right] . \quad (120)$$

A corresponding expression for the single imaginary root is then, from Eq. (110),

$$B_1^I \sin(j \omega_1^* \xi) = S^*(\omega_1^*, \xi) \left[A_0^* T_A^*(\omega_1^*) + B_0^* T_B^*(\omega_1^*) \right] . \quad (121)$$

It is seen in comparing (120) and (121) that the imaginary and real roots both result in the same algebraic form. So long as we remember to use the appropriate starred expressions when required, we can proceed from here by dropping the distinction entirely.

Next, we substitute Eq. (120) into (82) to obtain the general solution

$$C(\xi, \rho) = e^{\frac{-\beta \xi}{2}} \left\{ A_0 e^{\theta \xi} + B_0 e^{-\theta \xi} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_1^2 \rho} S(\omega_1, \xi) \left[A_0 T_A(\omega_1) + B_0 T_B(\omega_1) \right] \right\} . \quad (122)$$

We now make use of Eqs. (67) and (68) which, to repeat, are

$$A_0 = \frac{C_0 Q_A - J_L P(t)}{Q_A + Q_B} , \quad (67)$$

and

$$B_0 = \frac{C_0 Q_B + J_L P(t)}{Q_A + Q_B} . \quad (68)$$

Substituting (67) and (68) into (122) we obtain

$$C(\xi, \rho) = \frac{e^{-\frac{\beta\xi}{2}}}{Q_A + Q_B} \left\{ \left(C_o Q_A - J_L P(t) \right) e^{\theta\xi} + \left(C_o Q_B + J_L P(t) \right) e^{-\theta\xi} \right. \\ \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} S(\omega_i, \xi) \cdot \left[\left(C_o Q_A - J_L P(t) \right) T_A(\omega_i) + \left(C_o Q_B + J_L P(t) \right) T_B(\omega_i) \right] \right\} . \quad (123)$$

Next we rearrange (123) into two separate functions, one proportional to C_o and one proportional to J_L . In the latter case, it is noted that the most convenient expression is in terms of the non-dimensional quantity

$$\frac{J_L L}{D(t)} = J_L P(t) e^{-\frac{\beta}{2}} .$$

The final form of the concentration solution is then

$$C(\xi, \rho) = F_1(\beta, \gamma, \xi, \rho) C_o + F_2(\beta, \gamma, \xi, \rho) \frac{J_L L}{D(t)} , \quad (124)$$

where

$$F_1(\beta, \gamma, \xi, \rho) = \frac{e^{-\frac{\beta\xi}{2}}}{Q_A + Q_B} \left\{ Q_A e^{\theta\xi} + Q_B e^{-\theta\xi} \right. \\ \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} S(\omega_i, \xi) \left[Q_A T_A(\omega_i) + Q_B T_B(\omega_i) \right] \right\} . \quad (125)$$

and

$$F_2(\beta, \gamma, \xi, \rho) = \frac{-e^{-\frac{\beta\xi}{2}} e^{\frac{\beta}{2}}}{Q_A + Q_B} \left\{ e^{\theta\xi} - e^{-\theta\xi} \right. \\ \left. + e^{-\theta^2\rho} \sum_{i=1}^{\infty} e^{-\omega_i^2\rho} S(\omega_i, \xi) \left[T_A(\omega_i) - T_B(\omega_i) \right] \right\} . \quad (126)$$

Now we can again use expressions (116) and (117) to simplify these expressions. We have

$$Q_A T_A + Q_B T_B = (Q_A + Q_B) \omega \quad (127)$$

$$\text{and} \quad T_A - T_B = (Q_A + Q_B) \sin \omega . \quad (128)$$

Substituting (127) and (128) into (125) and (126), we see that the $(Q_A + Q_B)$ factor cancels in the transient terms, giving

$$F_1(\beta, \gamma, \xi, \rho) = e^{-\frac{\beta\xi}{2}} \left\{ \frac{Q_A e^{\theta\xi} + Q_B e^{-\theta\xi}}{Q_A + Q_B} \right. \\ \left. + e^{-\theta^2\rho} \sum_{i=1}^{\infty} e^{-\omega_i^2\rho} \omega_i S(\omega_i, \xi) \right\} , \quad \text{and} \quad (129)$$

$$F_2(\beta, \gamma, \xi, \rho) = -e^{-\frac{\beta\xi}{2}} e^{\frac{\beta}{2}} \left\{ \frac{e^{\theta\xi} - e^{-\theta\xi}}{Q_A + Q_B} \right. \\ \left. + e^{-\theta^2\rho} \sum_{i=1}^{\infty} e^{-\omega_i^2\rho} \sin \omega_i S(\omega_i, \xi) \right\} . \quad (130)$$

It is seen that when the above solutions are evaluated there will be many terms in common, simplifying the computation.

8. EVALUATION OF UNKNOWN BOUNDARY VALUES

We are given as known boundary conditions the concentration, C_o , on the left hand side of the slab and the mass flux, J_L , on the right hand side of the slab. For a complete solution of the diffusion problem we wish to know the concentration C_L on the right hand side and the mass flux J_o on the left hand side. The internal profiles of concentration do not matter for calculating fission product release. Thus, we wish to find

$$C_L(\rho) = C(\xi, \rho) |_{\xi=1} \quad (131)$$

and

$$J_o(\rho) = \frac{-D(t)}{L} \left[\frac{\partial C(\xi, \rho)}{\partial \xi} + \beta C(\xi, \rho) \right]_{\xi=0} \quad (132)$$

8.1 Calculation of Concentration on Right Hand Boundary

Evaluating Eqs. (129) and (130) on the right hand boundary ($\xi=1$), we have

$$C_L(\rho) = G_1(\beta, \gamma, \rho) C_o + G_2(\beta, \gamma, \rho) J_L \frac{L}{D(t)} \quad , \quad (133)$$

where

$$G_1(\beta, \gamma, \rho) = e^{-\frac{\beta}{2}} \left\{ \frac{Q_A e^{\theta} + Q_B e^{-\theta}}{Q_A + Q_B} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \omega_i S(\omega_i, 1) \right\} \quad , \quad (134)$$

and

$$G_2(\beta, \gamma, \rho) = - \left\{ \frac{e^\theta - e^{-\theta}}{Q_A + Q_B} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \sin \omega_i S(\omega_i, 1) \right\} . \quad (135)$$

8.2 Calculation of the Flux on the Left Hand Boundary

From Eq. (132) we have

$$\frac{J_o(\rho) L}{D(t)} = \left[- \frac{\partial C(\xi, \rho)}{\partial \xi} - \beta C(\xi, \rho) \right]_{\xi=0} . \quad (136)$$

Substituting expression (124) into (136) we have

$$\frac{J_o(\rho) L}{D(t)} = H_1(\beta, \gamma, \rho) C_o + H_2(\beta, \gamma, \rho) \frac{J_L L}{D(t)} , \quad (137)$$

where
$$H_1(\beta, \gamma, \rho) = - \beta - \frac{\partial}{\partial \xi} F_1(\beta, \gamma, \xi, \rho) \Big|_{\xi=0} , \quad (138)$$

and
$$H_2(\beta, \gamma, \rho) = - \frac{\partial}{\partial \xi} F_2(\beta, \gamma, \xi, \rho) \Big|_{\xi=0} . \quad (139)$$

We shall now evaluate the above partial derivatives. Differentiating (129) with respect to ξ ,

$$\begin{aligned} \frac{\partial F_1}{\partial \xi} = & - \frac{\beta}{2} F_1(\beta, \gamma, \xi, \rho) + e^{\frac{-\beta \xi}{2}} \left\{ \frac{\theta Q_A e^{\theta \xi} - \theta Q_B e^{-\theta \xi}}{Q_A + Q_B} \right. \\ & \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \omega_i \frac{\partial}{\partial \xi} S(\omega_i, \xi) \right\} . \end{aligned} \quad (140)$$

Differentiating (130) with respect to ξ ,

$$\begin{aligned} \frac{\partial F_2}{\partial \xi} = & -\frac{\beta}{2} F_2(\beta, \gamma, \xi, \rho) - e^{\frac{-\beta \xi}{2}} e^{\frac{\beta}{2}} \left\{ \frac{\theta e^{\theta \xi} + \theta e^{-\theta \xi}}{Q_A + Q_B} \right. \\ & \left. + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \sin \omega_i \frac{\partial}{\partial \xi} S(\omega_i, \xi) \right\}. \end{aligned} \quad (141)$$

Equations (140) and (141) both contain the factor $\partial/\partial \xi S(\omega_i, \xi)$. Differentiating Eq. (112) we thus define

$$C(\omega_i, \xi) = \frac{\partial}{\partial \xi} S(\omega_i, \xi) = \frac{-4\omega_i^2 \cos \omega_i \xi}{(2\omega_i - \sin 2\omega_i)(\theta^2 + \omega_i^2)}. \quad (142)$$

Similarly, for the imaginary root we differentiate (113) to obtain

$$C^*(\omega^*, \xi) = \frac{+4\omega^{*2} \cosh \omega^* \xi}{(2\omega^* - \sinh 2\omega^*)(\theta^2 - \omega^{*2})}. \quad (143)$$

As with previous analogous quantities, these two functions will be indistinguishable in future algebraic manipulations, but we must remember to use the appropriate expression when the root is imaginary.

Evaluating the above derivatives at $\xi=0$ and substituting the resulting expressions into Eqs. (138) and (139), we have

$$H_1(\beta, \gamma, \rho) = -\frac{\beta}{2} - \left\{ \frac{\theta(Q_A - Q_B)}{Q_A + Q_B} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \omega_i C(\omega_i, 0) \right\}, \quad (144)$$

and

$$H_2(\beta, \gamma, \rho) = e^{\frac{\beta}{2}} \left\{ \frac{2\theta}{Q_A + Q_B} + e^{-\theta^2 \rho} \sum_{i=1}^{\infty} e^{-\omega_i^2 \rho} \sin \omega_i C(\omega_i, \theta) \right\}, \quad (145)$$

where, by setting $\cos(\theta)=1$ in Eq. (142),

$$C(\omega, \theta) = \frac{-4\omega^2}{(2\omega - \sin 2\omega)(\theta^2 + \omega^2)},$$

with a similar equation for the imaginary root. This completes the solutions for the case of boundary conditions that are constant with time.

9. SOLUTION WITH TIME VARYING BOUNDARY CONDITIONS

The solutions derived in the previous sections take the following general form

$$C_L(\rho) = G_1(\beta, \gamma, \rho) C_O + G_2(\beta, \gamma, \rho) \frac{J_L L}{D}, \quad (146)$$

and

$$J_O(\rho) = H_1(\beta, \gamma, \rho) \frac{C_O D}{L} + H_2(\beta, \gamma, \rho) J_L. \quad (147)$$

These equations have been derived under the assumption that the boundary conditions are constant with time. When the boundary conditions vary with time, the solution can be obtained by the Duhamel superposition principle. This principle, derived in Section 9.4, depends on the fact that the differential equation is linear and on the fact that the initial conditions are zero. These conditions are both satisfied in the present problem.

9.1 Normal Application of Duhamel's Theorem

In considering a problem with only one solution quantity and one-time-dependent boundary condition, Duhamel's theorem (see Section 9.4) takes the form

$$C(\rho) = \int_0^{\rho} F(\rho - \rho') \frac{d}{d\rho'} C_O(\rho') d\rho'.$$

In the present case we have two solutions, a concentration and a flux. These, in turn, are functions of two boundary conditions, also a concentration and a flux. Duhamel's theorem is easily extended in this case to give

$$C_L(\rho) = \int_0^\rho G_1(\beta, \gamma, \rho - \rho') \frac{d}{d\rho'} C_o(\rho') d\rho' + \int_0^\rho G_2(\beta, \gamma, \rho - \rho') \frac{d}{d\rho'} \left(\frac{J_L}{D} \right) d\rho' , \quad (148)$$

and

$$J_o(\rho) = \int_0^\rho H_1(\beta, \gamma, \rho - \rho') \frac{d}{d\rho'} \left(\frac{C_o}{L} \right) d\rho' + \int_0^\rho H_2(\beta, \gamma, \rho - \rho') \frac{d}{d\rho'} J_L(\rho') d\rho' . \quad (149)$$

The most obvious approach to this solution is to evaluate the above integrals numerically using the trapezoidal rule. The result is

$$C_L(\rho_n) = \sum_{i=1}^{n-1} \frac{1}{2} \left[G_1(\rho_n - \rho_i) + G_1(\rho_n - \rho_{i+1}) \right] (C_{o_{i+1}} - C_{o_i}) + \sum_{i=1}^{n-1} \frac{1}{2} \left[G_2(\rho_n - \rho_i) + G_2(\rho_n - \rho_{i+1}) \right] \left[\left(\frac{J_L}{D} \right)_{i+1} - \left(\frac{J_L}{D} \right)_i \right], \quad (150)$$

and

$$\begin{aligned}
 J_L(\rho_n) = & \sum_{i=1}^{n-1} \frac{1}{2} \left[H_1(\rho_n - \rho_i) + H_1(\rho_n - \rho_{i+1}) \right] \left[\left(\frac{C_o D}{L} \right)_{i+1} - \left(\frac{C_o D}{L} \right)_i \right] \\
 & + \sum_{i=1}^{n-1} \frac{1}{2} \left[H_2(\rho_n - \rho_i) + H_2(\rho_n - \rho_{i+1}) \right] \left(J_{L_{i+1}} - J_{L_i} \right) . \quad (151)
 \end{aligned}$$

The above method has two disadvantages. First, the H_1 function is singular (equal to infinity) at $\rho_n - \rho_{i+1} = 0$. The integral of the function, however, is finite. Thus, using the trapezoidal rule in this range gives absurd results. A second disadvantage is that the entire sum must be evaluated at each time step, even though the transient response to much of the past history may have completely dissipated.

These disadvantages are circumvented by derivations given in the following pages. The first problem, that of the singularity in H_1 and the accuracy of the integration, is solved by evaluating the integrals explicitly rather than by using the trapezoidal rule. The second problem, that of excessive computation time, is solved by separating the solution into a steady-state and a transient part. The transient part goes to zero in time, limiting the effective memory and making it possible to evaluate the summation with a limited number of terms.

9.2 Improvement of the Duhamel Integration

In deriving the trapezoidal rule of (150) and (151) it was tacitly assumed that the entire integrand could be well-approximated as a piecewise linear function. This is an overly restrictive assumption. It is more accurate to assume that only the applied boundary condition

is piecewise linear, but that the solution function itself is free to take on its actual values. Thus,

$$\int_{\rho_i}^{\rho_i + \Delta\rho} F(\rho - \rho') \frac{d C_o}{d \rho'} d \rho' \approx \frac{\Delta C_o}{\Delta\rho} \int_{\rho_i}^{\rho_i + \Delta\rho} F(\rho - \rho') d \rho' .$$

Applying this principle to all terms of (148) and (149) we obtain

$$\begin{aligned} C_L(\rho_n) = & \sum_{i=1}^{n-1} \left(\frac{C_{o_{i+1}} - C_{o_i}}{\rho_{i+1} - \rho_i} \right) \int_{\rho_i}^{\rho_{i+1}} G_1(\rho_n - \rho) d\rho \\ & + \sum_{i=1}^{n-1} \left[\frac{\left(\frac{J_L L}{D} \right)_{i+1} - \left(\frac{J_L L}{D} \right)_i}{\rho_{i+1} - \rho_i} \right] \int_{\rho_i}^{\rho_{i+1}} G_2(\rho_n - \rho) d\rho , \quad (152) \end{aligned}$$

and

$$\begin{aligned} J_o(\rho_n) = & \sum_{i=1}^{n-1} \left[\frac{\left(\frac{C_o D}{L} \right)_{i+1} - \left(\frac{C_o D}{L} \right)_i}{\rho_{i+1} - \rho_i} \right] \int_{\rho_i}^{\rho_{i+1}} H_1(\rho_n - \rho) d\rho \\ & + \sum_{i=1}^{n-1} \left(\frac{J_{L_{i+1}} - J_{L_i}}{\rho_{i+1} - \rho_i} \right) \int_{\rho_i}^{\rho_{i+1}} H_2(\rho_n - \rho) d\rho . \quad (153) \end{aligned}$$

The above integrals, being functions of ρ alone, can be evaluated in advance by simply integrating the expressions for the solution functions. The integrated functions, rather than the original solution functions, then form the basis for the analysis.

We shall now consider the details of integrating the solution functions. A typical integral in (152) or (153) takes the form

$$\int_{\rho_i}^{\rho_{i+1}} F(\rho_n - \rho) d\rho \quad .$$

The integration is accomplished by a change of variable. We define

$$U = \rho_n - \rho$$

$$\rho = \rho_n - U$$

$$d\rho = -dU$$

then

$$\int_{\rho_i}^{\rho_{i+1}} F(\rho_n - \rho) d\rho = \int_{\rho_n - \rho_{i+1}}^{\rho_n - \rho_i} F(U) dU$$

or

$$\int_{\rho_i}^{\rho_{i+1}} F(\rho_n - \rho) d\rho = FI(\rho_n - \rho_i) - FI(\rho_n - \rho_{i+1}) \quad , \quad (154)$$

where

$$FI(\rho) = \int F(\rho) d\rho \quad (155)$$

is the indefinite integral of the solution function. Next, for reasons that will be apparent later, we separate the solution function F into a steady-state and a transient part. Thus

$$F(\rho) = F_S + F_T(\rho) \quad (156)$$

and

$$\begin{aligned} \text{FI}(\rho) &= \int F_S \, d\rho + \int F_T(\rho) \, d\rho \\ &\equiv F_S \cdot \rho + \text{FI}_T(\rho) \quad . \end{aligned} \quad (157)$$

Substituting (157) into (154), the value of the definite integral is given by

$$\begin{aligned} \int_{\rho_i}^{\rho_{i+1}} F(\rho_n - \rho) \, d\rho &= F_S \cdot (\rho_{i+1} - \rho_i) \\ &+ \text{FI}_T(\rho_n - \rho_i) - \text{FI}_T(\rho_n - \rho_{i+1}) \quad . \end{aligned} \quad (158)$$

In order for the above method to succeed it is necessary, of course, for our basic solution functions to be explicitly integrated. The feasibility of the integration is established below.

The original solution functions G_1 and G_2 are shown in Eqs. (134) and (135), and the solution functions H_1 and H_2 are shown in Eqs. (144) and (145). It can be seen that each one of these functions takes the following general form:

$$F(\rho) = F_S + K \sum_{i=1}^{\infty} g(\omega_i) e^{-(\theta^2 + \omega_i^2)\rho} \quad . \quad (159)$$

The indefinite integral of the function (159) is then

$$\text{FI}(\rho) = F_S \cdot \rho + K \sum_{i=1}^{\infty} \frac{-g(\omega_i)}{(\theta^2 + \omega_i^2)} e^{-(\theta^2 + \omega_i^2)\rho} \quad . \quad (160)$$

The net effect of the integration is to multiply the steady-state solution by ρ and to divide each term of the transient solution series by $-(\theta^2 + \omega_1^2)$. It is apparent that, since the ω_1^2 are increasing in size throughout the summation, this infinite series will converge faster than did the series for the original solution function.

Having established the feasibility for the integration, we now substitute formula (158) into the first term on the right of Eq. (152), giving as a typical solution:

$$C_{L_1}(\rho_n) = \sum_{i=1}^{n-1} \left(\frac{C_{o_{i+1}} - C_{o_i}}{\rho_{i+1} - \rho_i} \right) \left[G_{S_1}(\rho_{i+1} - \rho_i) + G_{I_{T_1}}(\rho_n - \rho_i) - G_{I_{T_1}}(\rho_n - \rho_{i+1}) \right] . \quad (161)$$

It is noted that the integration, to be correct, must proceed from time $t=0^-$ and must consider the jump in concentration C_o (if any) at time zero. With complete generality we may consider this jump to be the "zero'th" term in the above summation, which is written separately below as

$$\frac{C_{o_1} - C_{o_0}}{\delta} \left[G_{S_1} \cdot \delta + G_{I_{T_1}}(\rho_n - 0) - G_{I_{T_1}}(\rho_n - \delta) \right]$$

or, since $C_{o_0} = 0$ by definition,

$$C_{o_1} \left[G_{S_1} + \frac{\partial}{\partial \rho} G_{I_{T_1}}(\rho_n) \right] = C_{o_1} \left[G_{S_1} + G_{T_1}(\rho_n) \right] .$$

It is seen that the ρ dependency of the steady-state term cancels. Thus, Eq. (161), including the jump term, becomes

$$C_{L_1}(\rho_n) = G_{S_1} C_{o_n} + \underbrace{G_{T_1}(\rho_n) \cdot C_{o_1}}_{\text{jump term}} + \sum_{i=1}^{n-1} \frac{GI_{T_1}(\rho_n - \rho_i) - GI_{T_1}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} (C_{o_{i+1}} - C_{o_i}) \quad (162)$$

In the actual TRAFIC application C_{o_1} is always zero, so the jump term (underlined above) is unnecessary. Now it is noted that, near the end of the summation in (162), the arguments of the GI_T function approach zero. For arguments in this range, the transient solution is still active and the terms have significance. Near the beginning of the summation, however, the arguments $\rho_n - \rho_i$ may be quite large. It is also noted that the transient solution always approaches zero for large ρ , which implies that its integral approaches a horizontal asymptote, as shown below.

This being the case, the derivative $\Delta GI/\Delta \rho$ approaches zero as ρ becomes large. In view of this fact, many of the terms at the beginning of the series (162) may be insignificant. The trick, then, is to sum the series backwards, discontinuing the summation whenever the transient terms become insignificant. The resulting formula is

$$C_{L_1}(\rho_n) = G_{S_1} C_{o_n} + \underline{G_{T_1}(\rho_n) \cdot C_{o_1}} + \sum_{i=n-1}^{i_{\min}} \frac{GI_{T_1}(\rho_n - \rho_i) - GI_{T_1}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} (C_{o_{i+1}} - C_{o_i}). \quad (163)$$

Similar expressions exist for the second term in (152) and both terms in (153). The complete solution expressions are then

$$C_L(\rho_n) = G_{S_1} C_{o_n} + \underline{G_{T_1}(\rho_n) \cdot C_{o_1}} + G_{S_2} \left(\frac{J_L L}{D} \right)_n + \underline{G_{T_2}(\rho_n) \cdot \left(\frac{J_L L}{D} \right)_1} + \sum_{i=n-1}^{i_{\min 1}} \frac{GI_{T_1}(\rho_n - \rho_i) - GI_{T_1}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} (C_{o_{i+1}} - C_{o_i}) + \sum_{i=n-1}^{i_{\min 2}} \frac{GI_{T_2}(\rho_n - \rho_i) - GI_{T_2}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} \left[\left(\frac{J_L L}{D} \right)_{i+1} - \left(\frac{J_L L}{D} \right)_i \right], \quad (164)$$

and

$$\begin{aligned}
J_o(\rho_n) = & \underline{H_{S_1} \left(\frac{C_o D}{L} \right)_n} + \underline{H_{T_1}(\rho_n) \left(\frac{C_o D}{L} \right)_1} + H_{S_2} J_{L_n} + \underline{H_{T_2}(\rho_n) J_{L_1}} \\
& + \sum_{i=n-1}^{i_{\min}^3} \frac{HI_{T_1}(\rho_n - \rho_i) - HI_{T_1}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} \left[\left(\frac{C_o D}{L} \right)_{i+1} - \left(\frac{C_o D}{L} \right)_i \right] \\
& + \sum_{i=n-1}^{i_{\min}^4} \frac{HI_{T_2}(\rho_n - \rho_i) - HI_{T_2}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} \left(J_{L_{i+1}} - J_{L_i} \right) . \tag{165}
\end{aligned}$$

Once again, it is noted that the jump terms underlined above are not needed in TRAFIC. Thus, only the integrated transient functions GI_T and HI_T need be stored in the code.

9.3 Iteration for Unknown Boundary Values

In the numerical evaluation of the above solutions there is one further difficulty we have not heretofore discussed. This is the fact that the two boundary conditions C_o and J_L are not known at time point n . The reason for this is that they are implicit functions of the unknown solution quantities J_o and C_L , respectively. That is,

$$C_{o_n} = C(J_{o_n}) \quad , \quad \text{and} \tag{166}$$

$$J_{L_n} = J(C_{L_n}) \quad . \tag{167}$$

The reason for this behavior is related to the physics of the HTGR application. The left hand concentration, C_o , depends on the history of mass flux, J_o , out of the fuel rod. The right hand flux, J_L , depends on a non-linear evaporation condition that relates the mass transfer into a coolant stream to the boundary concentration, C_L , adjacent to the stream. The details of these relationships need not concern us for the present. We need only to assume that the functions (166) and (167) can somehow be computed by means of a computer algorithm.

In view of the non-linear, unknown boundary conditions, one way to solve the problem is to separate the known from the unknown quantities and solve the resulting system of equations by iteration. Thus, Eq. (164) becomes

$$C_{L_n} = A_1 + A_2 \left(C_o \right)_n + A_3 \left(\frac{J_L L}{D} \right)_n, \quad (168)$$

where

$$\begin{aligned} A_1 = & G_{T_1}(\rho_n) \cdot C_{o_1} + G_{T_2}(\rho_n) \left(\frac{J_L L}{D} \right)_1 \quad \left[\begin{array}{c} \text{jump} \\ \text{terms} \end{array} \right] \\ & + \sum_{i=n-2}^{i_{\min 1}} \frac{G_{I_{T_1}}(\rho_n - \rho_i) - G_{I_{T_1}}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} (C_{o_{i+1}} - C_{o_i}) \\ & + \sum_{i=n-2}^{i_{\min 2}} \frac{G_{I_{T_2}}(\rho_n - \rho_i) - G_{I_{T_2}}(\rho_n - \rho_{i+1})}{\rho_{i+1} - \rho_i} \left[\left(\frac{J_L L}{D} \right)_{i+1} - \left(\frac{J_L L}{D} \right)_i \right] \\ & - \left[\frac{G_{I_{T_1}}(\rho_n - \rho_{n-1}) - G_{I_{T_1}}(o)}{\rho_n - \rho_{n-1}} \right] C_{o_{n-1}} \\ & - \left[\frac{G_{I_{T_2}}(\rho_n - \rho_{n-1}) - G_{I_{T_2}}(o)}{\rho_n - \rho_{n-1}} \right] \left(\frac{J_L L}{D} \right)_{n-1}, \quad (169) \end{aligned}$$

and where

$$A_2 = \frac{GI_{T_1}(\rho_n - \rho_{n-1}) - GI_{T_1}(0)}{\rho_n - \rho_{n-1}} + G_{S_1} , \quad (170)$$

$$A_3 = \frac{GI_{T_2}(\rho_n - \rho_{n-1}) - GI_{T_2}(0)}{\rho_n - \rho_{n-1}} + G_{S_2} . \quad (171)$$

A similar expression holds for Eq. (165), where we obtain

$$J_{O_n} = B_1 + B_2 \left(\frac{C_O}{L} \right)_n + B_3 \left(J_L \right)_n . \quad (172)$$

These B coefficients are similar in form to the A coefficients given by (169) through (171). All the coefficients A_i and B_i in Eqs. (168) and (172) are known. The remaining four boundary condition quantities are unknown. Two of the unknowns can be eliminated, however, by substituting Eqs. (166) and (167) into Eqs. (168) and (172). Thus, we are left with two non-linear equations in two unknowns:

$$C_{L_n} = A_1 + A_2 C \left(J_{O_n} \right) + A_3 \left(\frac{L}{D} \right)_n J \left(C_{L_n} \right) , \quad (173)$$

$$J_{O_n} = B_1 + B_2 \left(\frac{D}{L} \right)_n C \left(J_{O_n} \right) + B_3 J \left(C_{L_n} \right) . \quad (174)$$

These two non-linear equations can be solved by an iterative procedure.

9.4 Proof of Duhamel's Superposition Principle

The general form of Duhamel's theorem is as follows. We are given a linear partial differential equation,

$$\mathcal{L}(C) = 0 .$$

Assume that we know the solution of this differential equation for the case of (1) zero initial conditions, and (2) a known, constant boundary condition which is expressed abstractly as

$$\phi(x,y,z,\lambda) \tag{175}$$

and which is applied at time λ . The solution function then has the general form

$$C(x,y,z,t) = F(x,y,z,\lambda,t-\lambda) . \tag{176}$$

The single parameter λ in (176) designates the choice, among an infinite number of possible solutions F , of that particular solution corresponding to the given boundary condition (175). The $t-\lambda$ argument is simply a shift in time origin to account for the fact that the solutions F are usually derived with $t=0$ as the time at which the boundary condition is applied.

Now, if the boundary condition (175) is a continuous function of λ instead of being constant, the total solution can be obtained by a superposition of partial solutions of form (176). The superposition is accomplished incrementally by applying one boundary condition and then, after a short time, removing it and replacing it by another, as shown schematically below.

For the boundary condition history shown above, the solution would then be

$$\begin{array}{c}
 \text{Apply new} \quad \downarrow \quad \quad \quad \downarrow \quad \text{Remove it} \\
 \text{B.C.} \\
 C(\vec{x}, t) = F(\vec{x}, \lambda_1, t - \lambda_1) - F(\vec{x}, \lambda_1, t - \lambda_2) \\
 \\
 + F(\vec{x}, \lambda_2, t - \lambda_2) - F(\vec{x}, \lambda_2, t - \lambda_3) \\
 \\
 + F(\vec{x}, \lambda_3, t - \lambda_3) - F(\vec{x}, \lambda_3, t - \lambda_4) \\
 \vdots \\
 \text{etc.}
 \end{array} \tag{177}$$

The above superposition is always valid provided that the differential equation is linear and provided that each partial solution function was derived with zero initial conditions (otherwise the initial conditions would add, which is incorrect).

Each pair of terms in (177) can be replaced by a differential. First we collect terms and multiply numerator and denominator by $\Delta\lambda = \lambda_2 - \lambda_1$:

$$\frac{F[\vec{x}, \lambda_1, (t - \lambda_1)] - F[\vec{x}, \lambda_1, (t - \lambda_1) - (\lambda_2 - \lambda_1)] (\lambda_2 - \lambda_1)}{(\lambda_2 - \lambda_1)} .$$

Then, taking the limit as $\Delta\lambda$ approaches zero,

$$\lim_{\Delta\lambda \rightarrow 0} \frac{F(\vec{x}, \lambda, t - \lambda) - F(\vec{x}, \lambda, t - \lambda - \Delta\lambda)}{\Delta\lambda} \Delta\lambda = \frac{\partial F}{\partial t} d\lambda . \tag{178}$$

Thus, in the limit, Eq. (177) becomes

$$C(\vec{x}, t) = \int_0^t \frac{\partial}{\partial t} F(\vec{x}, \lambda, t-\lambda) d\lambda . \quad (179)$$

This is the general form of Duhamel's theorem. This form, however, is not particularly useful in the present analysis. By employing a simplified description of the solution function it is possible to rearrange (179) and obtain a form that is more useful in calculations.

The solution functions we are considering in the present analysis all take the form

$$F(\vec{x}, \lambda, t-\lambda) = C_o(\lambda) F_1(\vec{x}, t-\lambda) . \quad (180)$$

With this simplification, we note that

$$\frac{\partial}{\partial t} F(\vec{x}, \lambda, t-\lambda) = - C_o(\lambda) \frac{\partial}{\partial \lambda} F_1(\vec{x}, t-\lambda) . \quad (181)$$

Substituting (181) into (179) and integrating by parts, we obtain

$$\begin{aligned} C(\vec{x}, t) &= F_1(\vec{x}, t) C_o(0) - F_1(\vec{x}, 0) C_o(t) \\ &+ \int_0^t F_1(\vec{x}, t-\lambda) \frac{d}{d\lambda} C_o(\lambda) d\lambda . \end{aligned} \quad (182)$$

The first two terms in (182) are zero due to the initial conditions.* Thus, the final form of Duhamel's theorem applicable to our problem is

$$C(\vec{x}, t) = \int_0^t F_1(\vec{x}, t-\lambda) \frac{d}{d\lambda} C_o(\lambda) d\lambda . \quad (183)$$

It is noted that this equation could have been derived directly by assuming that the superposition was accomplished in the manner shown schematically below.

This form of superposition only works for the restrictive solution function described by Eq. (180), and the general derivation is of more interest mathematically.

*Note: By dropping the first two terms we imply that if there is a jump in boundary conditions at time zero the integral must be evaluated from time 0^- in order to account for it.

10. LIMITING SOLUTIONS FOR $\beta = -2$

As was discussed in Section 5.3, the case of $\beta = -2$ is of special interest because the previously neglected zero root suddenly and instantaneously becomes non-trivial. It might be of interest to note that, historically, this fact was discovered not by a theoretical analysis but by a numerical study. It was found in an early solution attempt, in which the root $\omega_1 = 0$ was ignored, that the solution was discontinuous at $\beta = -2$. The solution at $\beta = -2.000$ was radically different from the solution at $\beta = -1.999$. The discontinuity was then removed by finding the limiting value of the expression

$$\lim_{\substack{\omega \rightarrow 0 \\ \beta \rightarrow -2}} B_1 \sin \omega_1 \xi = B_1 \xi$$

which was, indeed, finite. It was subsequently determined by a proper theoretical analysis¹⁴ that this special linear eigenfunction could be obtained from first principles. The eigenfunction is guaranteed to be orthogonal by Sturm-Liouville theory, and the coefficient B_1 can be found by integration in the normal manner. Rather than go through this added complication, however, we shall simply present here the limiting solution, which is easily derived from the typical solution. The results are the same.

Only the first term in the series expansion has any unusual properties at $\beta = -2$. We shall now consider the series expansions of our four solution functions G_1 , G_2 , H_1 , and H_2 separately. First, from Eq. (129), we wish to find a limiting value for the expression

$$L_1 = \lim_{\substack{\omega \rightarrow 0 \\ \beta \rightarrow -2}} \left[e^{-\omega^2 \rho} \omega S(\omega, \xi) \right] . \quad (184)$$

An immediate observation is that

$$\lim_{\omega \rightarrow 0} e^{-\omega^2 \rho} = 1 . \quad (185)$$

So Eq. (184) becomes, after substituting (112),

$$L_1 = \lim_{\omega \rightarrow 0} \left[\frac{-4 \omega^2 \sin \omega \xi}{(2\omega - \sin 2\omega)(\theta^2 + \omega^2)} \right] . \quad (186)$$

We further note that

$$\lim_{\omega \rightarrow 0} \sin \omega \xi = \omega \xi , \quad (187)$$

$$\text{and} \quad \lim_{\omega \rightarrow 0} (\theta^2 + \omega^2) = \theta^2 , \quad (188)$$

whereupon Eq. (186) becomes

$$L_1 = \lim_{\omega \rightarrow 0} \left[\frac{-4 \omega^3 \xi}{(2\omega - \sin 2\omega)\theta^2} \right] . \quad (189)$$

Direct evaluation of (189) gives $0/0$, which is undefined. We must apply L'Hospital's rule, which states that

$$\text{if} \quad \lim_{x \rightarrow x_0} f(x) = 0, \quad \text{and}$$

$$\text{if} \quad \lim_{x \rightarrow x_0} g(x) = 0,$$

$$\text{then} \quad \lim_{x \rightarrow 0} \frac{f(x)}{g(x)} = \frac{f'(x)}{g'(x)}. \quad (190)$$

When both derivatives are zero, of course, repeated application with higher order derivatives continues until a definite limit is achieved. We now apply (190) to the expression (189) three times in succession.

	Numerator		Denominator	
	Expression	Limit ($\omega=0$)	Expression	Limit ($\omega=0$)
$f(\omega)$	$-4\omega^3\xi$	0	$(2\omega - \sin 2\omega)\theta^2$	0
$f'(\omega)$	$-12\omega^2\xi$	0	$(2 - 2\cos 2\omega)\theta^2$	0
$f''(\omega)$	$-24\omega\xi$	0	$(4\sin 2\omega)\theta^2$	0
$f'''(\omega)$	-24ξ	-24ξ	$(8\cos 2\omega)\theta^2$	$8\theta^2$

The limiting value of the expression is therefore

$$L_1 = \frac{-24\xi}{8\theta^2} = \frac{-3\xi}{\theta^2}. \quad (191)$$

Thus, in evaluating the series expansion of Eq. (129), we simply use

$$\lim_{\beta \rightarrow -2} \left[\omega_1 S(\omega_1, \xi) \right] = \frac{-3\xi}{\theta^2} . \quad (192)$$

In a similar manner, as a result of Eq. (187), the series expansion of Eq. (130) uses the same limiting expression, i.e.,

$$\lim_{\beta \rightarrow -2} \left[\sin \omega_1 S(\omega_1, \xi) \right] = \frac{-3\xi}{\theta^2} . \quad (193)$$

We now turn to the solution for the boundary flux J_0 . In view of Eq. (144) we wish to find a limiting value for the expression

$$L_2 = \lim_{\omega \rightarrow 0} \lim_{\beta \rightarrow -2} \left[e^{-\omega^2 \rho} \omega C(\omega, \xi) \right] . \quad (194)$$

Substituting Eqs. (185) and (142) into (194) we get

$$L_2 = \lim_{\omega \rightarrow 0} \left[\frac{-4 \omega^3 \cos \omega \xi}{(2\omega - \sin 2\omega)(\theta^2 + \omega^2)} \right] . \quad (195)$$

Of course

$$\lim_{\omega \rightarrow 0} (\cos \omega \xi) = 1 ,$$

so expression (195) has the same limit as expression (189), with the exception that ξ is replaced by 1. Thus,

$$\lim_{\beta \rightarrow -2} \left[\omega_1 \mathcal{C}(\omega_1, \xi) \right] = \lim_{\beta \rightarrow -2} \left[\sin \omega_1 \mathcal{C}(\omega_1, \xi) \right] = \frac{-3}{\theta^2} . \quad (196)$$

The limit (196), when substituted into either of Eqs. (144) and (145), will give the limiting value of the flux solution.

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