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The Time-Dependent Solution to Interstitial Diffusion in a Temperature Gradient

los alamos
scientific laboratory

of the University of California

LOS ALAMOS, NEW MEXICO 87544

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by

Clarence E. Lee
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ABSTRACT

This report demonstrates the feasibility of the simultaneous determination of the chemical interdiffusion coefficient and the effective heat of transport of interstitial compounds, such as refractory carbides and hydrides. A mathematical model is constructed, based on the thermodynamics of irreversible processes, which represents the time-dependent interstitial diffusion process in a temperature gradient. This model is then linearized and solved analytically. The analytical solution of this model is compared to a numerical difference solution method of attacking the original problem.

Conclusions derived from this study are as follows. (1) The linearized analytical solution agrees with the numerical difference solution to 1% in most cases and 3% in the worst case. (2) The sensitivity of the analytical solution to parameter variations is sufficient for least-squares evaluations of experiments. (3) The analytical solution method is comparably superior to the numerical difference solution method in terms of accuracy and speed (50 times faster) when applied to experimental data.

I. INTRODUCTION

An understanding of the fundamental properties of high-temperature materials is requisite to the systematic development of nuclear rocket engines.¹ This report demonstrates the feasibility of simultaneously determining two such properties, the chemical interdiffusion coefficient and the effective heat of transport, of refractory carbides. These parameters are basic for understanding the mass transport processes that occur under the extreme temperature gradients and corrosive conditions present in engines during operation.

The problem is investigated by applying the theory of the thermodynamics of irreversible processes. Considering the characteristics of the thermal diffusion process and the restrictions necessary to achieve reliable experimental data, a mathematical model is developed that, when solved, yields these transport properties. An analytical solution

of the equations is shown by the calculation of processes on zirconium hydride with known parameters.

II. STATEMENT OF THE PROBLEM AND DERIVATION OF THE THERMAL DIFFUSION EQUATION

Using the thermodynamics of irreversible processes and the Onsager reciprocity theorem,^{2,3} a set of equations is obtained from the laws governing matter transport that expresses the fluxes, J_i , as linear combinations of the forces, X_k .

$$J_i = \sum_{k=1}^n L_{ik} X_k \quad \text{for } i = 1, 2, \dots, n. \quad (1)$$

The fluxes may refer to the flow of matter, heat, electricity, etc., or to the formation of a constituent by chemical reaction. The forces may be temperature differences, electromotive force, a chemical potential difference, or the like. The theory was originally applied to matter transport in gases

and liquids.² Recently, however, Howard and Lidiard³ reviewed the applicability of the theory to crystalline solids. The basic difference is that in applying the theory to solids the fluxes are referred to the local crystal lattice, whereas in gases and liquids the fluxes are referred to the center of mass of the system. Howard and Lidiard discuss the transformation of the fluxes and forces from the center-of-mass system to the local crystal-lattice reference system such that the matrix of L coefficients is symmetric (Onsager's theorem).

$$L_{ik} = L_{ki}. \quad (2)$$

Considering this constraint, vacancy fluxes must be specified in addition to material fluxes. Heitkamp⁴ extended the above analysis for mass transport in a binary compound to include vacancy mechanisms for both component sublattices, which resulted in an equation specifying the flux of A atoms (in a binary compound of A and B atoms) relative to a fixed reference system,

$$J_a^R = - \left(c_a D_b + c_b D_a \right) \nabla c_a - \frac{c_a c_b}{RT^2} \frac{D_a (Q_a^* - a_{H_{vf}}) - D_b (Q_b^* - b_{H_{vf}})}{\left(\frac{\partial \ln a}{\partial \ln c_a} \right)_T} \nabla T. \quad (3)$$

This equation is the starting point for this investigation. The concentration variables c_a and c_b are expressed as mole fractions of the components a and b, respectively. The quantities Q_a^* , $a_{H_{vf}}$, Q_b^* , and $b_{H_{vf}}$ are the heats of transport and the formation enthalpy (kcal/mole) of the A and B components. In the formulation of Eq. (3), it was assumed that the vacancies were at thermal equilibrium and that their concentration was relatively small. The activity of component A, a_a , is defined relative to the standard state of the element A, i.e.,

$$\mu_a = \mu_a^0 + RT \ln(a_a) \quad (4)$$

where μ is the thermodynamic potential, R is the gas constant (cal/mole-°K), and T is the absolute temperature (°K). The intrinsic diffusion coefficients of the components in the binary compound are

D_a and D_b , which are related to the L_{ik} coefficients as

$$D_a = RT \left(L_{aa}/c_a - L_{ab}/c_b \right) \left(\frac{\partial \ln a}{\partial \ln c_a} \right)_T, \quad (5a)$$

$$D_b = RT \left(L_{bb}/c_b - L_{ba}/c_a \right) \left(\frac{\partial \ln a}{\partial \ln c_a} \right)_T, \quad (5b)$$

and

$$L_{ab} = L_{ba}. \quad (6)$$

The first term of Eq. (3) is the chemical interdiffusion coefficient, $\tilde{D}$,³ where

$$\tilde{D} = c_a D_b + c_b D_a. \quad (7)$$

A survey of some of the refractory carbides significant to nuclear rocket technology indicates the intrinsic diffusion coefficient of the metal to be much smaller than that of the carbon. For example: Resnick and Seigle⁵ found $D_{Ta}/D_C = 1.3 \cdot 10^{-2}$ in TaC at 2500°C; Lee and Barret⁶ found $D_U/D_C = 2 \times 10^{-3}$, assuming that $D_U/D_C = D_U^*/D_C^*$ (Darken's relationship for the intrinsic and self-diffusion coefficients³ in UC), and Gel'd and Liubimov⁷ found $D_{Nb}/D_C = 4 \times 10^{-2}$ at 2000°C. Further, the relative nonmobility of the metal in comparison to carbon has been observed to be small in layer-growth experiments on the carbides of TiC,⁸ ZrC,⁹ HfC,⁸ V₂C and VC,¹⁰ Nb₂C and NbC,¹¹ Ta₂C and TaC¹², and the carbides of Cr, Mo and W.¹³

Using $D_b/D_a \ll 1$, and factoring $\tilde{D}$ out of Eq. (3), one obtains the flux equation

$$J = \tilde{D} \left[\vec{\nabla} c_a + \frac{(Q_a^* - a_{H_{vf}})}{\left(\frac{\partial \ln a}{\partial \ln c_a} \right)_T} \frac{c_a}{RT} \vec{\nabla} T \right], \quad (8)$$

where c_a is the concentration of the more mobile component. Equation (8) is equivalent to Howard and Lidiard's³ flux equation for interstitial solutes in metals.

Flux equations of the form of Eq. (8) have been used to infer the effective heat of transport,

$$Q_{\text{eff}}^* = (Q_a^* - a_{H_{vf}}) / \left(\frac{\partial \ln a_a}{\partial \ln c_a} \right)_T, \quad (9)$$

from steady-state experiments. In this type of experiment, as performed in the past, parallel-faced binary sample of thickness l was subjected to a linear temperature gradient. The sample was isolated from its environment such that there was zero matter flux across the surface of the specimen. When the steady state was reached, Eq. (8) would imply

$$\frac{dc}{dx} + \frac{Q_{\text{eff}}^*}{RT^2} \frac{dT}{dx} c = 0. \quad (10)$$

Assuming Q_{eff}^* to be independent of c and $T(x)$, Eq. (10) can be integrated to yield

$$\ln c = \text{const.} + Q_{\text{eff}}^*/RT. \quad (11)$$

Note that a plot of $\ln c$ vs $1/T$ would yield Q_{eff}^* , since $\frac{d \ln c}{d(1/T)} = Q_{\text{eff}}^*$. However, it is apparent from Eq. (11) that if the magnitude of Q_{eff}^* is large,

the composition range from the hot to the cold surface could be very large. For refractory carbides, available activity data¹⁴ indicate that the quantity

$\left(\frac{\partial \ln a_a}{\partial \ln c_a} \right)_T$ may vary by several orders of

magnitude across the homogeneity range for compounds such as UC, NbC, and ZrC. The quantity

$(Q_{\text{eff}}^* - a_{H_{vf}})$ may also vary with composition. Thus

there is a possible composition variation in Q_{eff}^* as inferred in Eq. (9). A plot of $\ln c$ vs $1/T$ need not follow the linear relationship implied by Eq. (11).

If the sample is maintained at temperature for short times, so that concentration perturbations from the initial state are small, then Q_{eff}^* may be assumed to be approximately constant and to represent some average value characteristic of the initial homogeneous concentration and the average temperature range. This is also true for the chemical diffusion coefficient $\tilde{D}$. Applying the continuity equation to Eq. (8), a relationship is obtained in

which the concentration is a function of time and position

$$\frac{\partial c}{\partial t} = -\vec{\nabla} \cdot \mathbf{J} = \vec{\nabla} \cdot \left[\tilde{D} \left(\vec{\nabla} c + \frac{Q_{\text{eff}}^*}{RT^2} c \vec{\nabla} T \right) \right]. \quad (12)$$

To summarize, the arguments leading to Eq. (12) and additional assumptions required for solution are given below.

(1) The application of the thermodynamics of irreversible processes and the Onsager reciprocity theorem is useful as a fundamental description of mass transport in crystalline solids. A reasonable amount of information exists concerning the equilibrium thermodynamics of refractory carbide systems; however, there is a paucity of information regarding the atomic mechanism of mass transport under the influence of a temperature gradient in these compounds. The advantage of this application is that the description of the processes requires a knowledge of equilibrium thermodynamics rather than of atomic mechanisms.

(2) Although vacancy mechanism is operative on the sublattices, the total vacancy concentration is small and at thermal equilibrium.

(3) The intrinsic diffusion coefficient of one component is much larger than the other.

($D_M/D_1 \ll 1$.) This effect is observed in refractory carbides as well as in certain impurity atoms (i.e., H, C, O, and N) in the refractory metals (i.e., Ti, Zr, Nb, Ta, etc.).¹⁵ Consequently, there is a large class of compounds for which Eq. (12) is applicable as a model of mass transport processes.

(4) The matter flux and the temperature flux are unidirectional. The experimental temperature variation should be restricted to linear to admit the analytic solution of Eq. (12) for the one-dimensional case (assuming that the diffusion processes are independent of the crystallographic axes of the compound). Experimentally, this can be approximated by fabricating samples from a randomly oriented, small-grained, polycrystalline material of near theoretical crystal density. However, these requirements are difficult to achieve.

(5) The sample is isolated from its environment--to effect zero matter transport across its surface. The validity of this boundary condition for solution of Eq. (12) can be determined

postexperimentally by comparing the final average concentration to the initial uniform concentration.

(6) Time at temperature is short enough that the concentration perturbations from the initial state are small. Consequently, one may assume that $\tilde{D}$ and Q_{eff}^* are independent of concentration to first order. $\tilde{D}$ has the usual temperature dependence¹⁶

$$\tilde{D} = \tilde{D}_0 \exp(-\tilde{Q}/RT), \quad (13)$$

where $\tilde{D}_0$ is the pre-exponential factor (cm^2/sec) and $\tilde{Q}$ is the isothermal heat of diffusion (cal/mole). Additionally, Q_{eff}^* is assumed independent of temperature, and the temperature variation between the hot and cold ends of the sample must therefore be kept reasonably small.

Applying assumptions (1) through (6), Eq. (12) becomes

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[\tilde{D} \left(\frac{\partial c}{\partial x} + \frac{Q^*}{RT(x)^2} \frac{\partial T}{\partial x} c \right) \right] \quad (14)$$

with boundary conditions

$$c(x, t) = c_0 = \text{constant} \quad 0 \leq x \leq \ell \quad \text{at } t = 0, \quad (15)$$

and

$$J(x, t) = -\tilde{D} \left(\frac{\partial c}{\partial x} + \frac{Q^*}{RT(x)^2} \frac{\partial T}{\partial x} c \right) = 0$$

$$x = 0, \ell \text{ for } t > 0,$$

where

$$T(x) = T_h - kx \quad 0 \leq x \leq \ell$$

and

$$k = (T_h - T_c)/\ell.$$

For notational convenience, let $Q^* = Q_{\text{eff}}^*$.

Solution of Eqs. (14) through (16) implies a functional relationship of the form

$$c = F(c_0, T_h, T_c, \tilde{D}_0, \tilde{Q}, Q^*, x, \ell, t), \quad (17)$$

where c_0 is the initial homogeneous concentration, T_h and T_c are the hot and cold surface temperatures, x is the distance (cm) from the hot surface, ℓ is the sample thickness, and t is the time (sec) at temperature.

In principle, $\tilde{D}_0$, $\tilde{Q}$, and Q^* can be determined from an analysis of a concentration vs $T(x)$ curve because all other quantities are known. Thus the values determined for $\tilde{D}_0$ and $\tilde{Q}$ would depend on c_0 , Q^* , and the average temperature. The concentration dependence of $\tilde{D}_0$ and $\tilde{Q}$ could now be determined. Additionally, the temperature and concentration dependence of Q^* of a binary compound could be determined by making a sequence of thermal diffusion experiments for short times at a number of different initial concentrations and varying temperature ranges.

III. ANALYTICAL SOLUTION TO THE THERMAL DIFFUSION PROBLEM

Introducing the new function $u(x, t)$, defined as

$$u(x, t) = c(x, t) \exp[-Q^*/RT(x)], \quad (18)$$

makes Eqs. (14) and (15) become

$$\exp[Q^*/RT(x)] \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[\tilde{D}_0 \exp[-\tilde{Q} - Q^*/RT(x)] \frac{\partial u}{\partial x} \right], \quad (19)$$

with boundary conditions

$$u(x, 0) = c_0 \exp[-Q^*/RT(x)] \text{ for } 0 \leq x \leq \ell \text{ at } t = 0, \quad (20a)$$

and

$$\frac{\partial u}{\partial x} = 0 \quad \text{at } x = 0, \ell \quad \text{for } t > 0. \quad (20b)$$

Sawatzky and Vogt¹⁷ have treated the problem defined by Eqs. (18) through (20b) using the assumption that the quantity $\tilde{D}_0 \exp[-\tilde{Q}/RT(x)]/T^4(x)$ was approximately constant over the temperature range of interest. In their work this quantity varied by about 30%. For the temperature ranges of interest here, this quantity would vary about 200 to 300%; consequently, a different form of the transformation variable must be chosen.

One choice is the transformation defined by

$$\ln w = T_h/T(x). \quad (21)$$

Applying Eq. (21) to Eqs. (18) and (19) and using Eq. (16) results in

$$w^{Q^*/RT_h} \frac{\partial u}{\partial t} = \left(\frac{k}{T_h} \right)^2 \left[\ln(w) \right]^2 w \frac{\partial}{\partial w} \left\{ \tilde{D}_0 w^{-\tilde{Q}-Q^*/RT_h} \left[\ln(w) \right]^2 w \frac{\partial u}{\partial w} \right\}, \quad (22)$$

with boundary conditions

$$u(w, t) = c_0 w^{-Q^*/RT_h}, \quad (23a)$$

$$e = w_1 \leq w \leq w_2 = e^{T_h/T_c} \text{ at } t = 0,$$

and

$$\frac{\partial u}{\partial w} = 0, \text{ at } w = w_1, w_2 \text{ for } t > 0. \quad (23b)$$

Equation (22) requires that some approximations be made [as in Ref. (17)] before an analytic solution can be obtained.

The experimental conditions are such (assumption 6) that the ratio T_h/T_c is expected to be in the range

$$1 < T_h/T_c < 2. \quad (24)$$

Here it is interesting to examine the Taylor's series expansion of $\ln w$ about $w_1 (= e)$, namely,

$$\ln w = \frac{w}{w_1} - \left(\frac{w}{w_1} - 1 \right)^2 / 2! + \dots \quad (25)$$

Provided the ratio T_h/T_c is not too large, a reasonable approximation to $\ln w$ can be made by using only the first term of Eq. (25),

$$\ln w \approx w/e. \quad (26)$$

Comparative values and the percentage of error for this approximation are presented in Table I for the extreme case $w = w_2$.

If $T_h/T_c < 1.1$, Eq. (25) is quite reasonable as an approximation in that the error introduced is smaller than that already present in the concentration measurements (typically ≈ 2 to 3%). Sawatzky and Vogt's¹⁷ data correspond to $T_h/T_c \approx 1.3$.

Applying Eq. (26) to Eqs. (23) and (24) results in

$$w^{(3-Q^*/RT_h)} \frac{\partial u}{\partial \tau} = \frac{\partial}{\partial w} \left[w^{3-(\tilde{Q}-Q^*)/RT_h} \frac{\partial u}{\partial w} \right], \quad (27)$$

with boundary conditions

$$u(w, \tau) = c_0 w^{-Q^*/RT_h} \text{ for } w_1 \leq w \leq w_2 \text{ at } \tau = 0,$$

and

$$\frac{\partial u}{\partial w} = 0 \text{ at } w = w_1, w_2, \text{ for } \tau > 0, \quad (28)$$

where the new time variable τ is defined by

$$\tau = \tilde{D}_0 \left(\frac{k}{T_h} \right)^2 \frac{t}{e^4}. \quad (29)$$

A solution to Eq. (27) is now sought as an eigenfunction expansion of the form

$$u(w, \tau) = A_0 + \sum_{m=1}^{\infty} A_m e^{-\gamma_m^2 \tau} \psi_m(w), \quad (30)$$

where the A_m are a set of expansion coefficients (to be determined) and the $\psi_m(w)$ satisfies the ordinary differential equation

TABLE I

COMPARISON OF EXACT AND APPROXIMATE EXPRESSIONS FOR $\ln w_2$ vs T_h/T_c

$\ln w_2 = T_h/T_c$	$w_2/e = e^{T_h/T_c - 1}$	% Error = $10^2 \left(\frac{w_2/e}{\ln w_2} - 1 \right)$
1.01	1.01005	0.005
1.05	1.05127	0.12
1.1	1.10517	0.47
1.15	1.16183	1.03
1.2	1.22140	1.78
1.3	1.34986	3.86
1.4	1.49182	6.56
1.5	1.64872	9.91
2.0	2.718282	35.91

$$\frac{d}{dw} \left[w^{3-(\tilde{Q}-Q^*)/RT_h} \frac{d\psi_m}{dw} \right] + \gamma_m^2 w^{-(3-Q^*/RT_h)} \psi_m = 0, \quad (31)$$

subject to boundary condition

$$\frac{d\psi_m}{dw} = 0 \quad \text{at } w = w_1, w_2. \quad (32)$$

Equation (31) may be transformed into Bessel's equation

$$\frac{d^2\phi_m}{dr^2} + \frac{1}{r} \frac{d\phi_m}{dr} + (\lambda_m^2 - v^2/r^2)\phi_m = 0, \quad (33)$$

and the boundary condition, Eq. (32), becomes

$$r \frac{d\phi_m}{dr} + v\phi_m = 0 \quad \text{at } r = r_1, r_2 \quad (34)$$

using the transformation

$$w = r^\alpha \quad \text{and} \quad \psi_m = r^\beta \phi_m. \quad (35)$$

Substituting Eq. (35) into Eqs. (31) and (32), and comparing the result with Eqs. (33) and (34), the coefficients α, β and λ_m are given by

$$\alpha = 2 / \left(\frac{Q}{RT_h} - 4 \right),$$

$$\beta = v = \left(\frac{\tilde{Q} - Q^*}{RT_h} - 2 \right) / \left(\frac{\tilde{Q}}{RT_h} - 4 \right), \quad (36)$$

and

$$\lambda_m = 2\gamma_m / \left(\tilde{Q}/RT_h - 4 \right).$$

The general solution of Eq. (33) is of the form $\left[m = m(v) \right]$

$$\phi_m(\lambda_m r) = C_m J_v(\lambda_m r) + D_m Y_v(\lambda_m r), \quad (37)$$

where J_v and Y_v are the cylindrical Bessel functions of the first and second kind, respectively, and v is nonintegral. Equation (34) is used to determine the coefficients in Eq. (37) with the result that

$$\begin{aligned} \phi_m(\lambda_m r) &= N_m \left[Y_{v-1}(\lambda_m r_1) J_v(\lambda_m r) - J_{v-1}(\lambda_m r_1) Y_v(\lambda_m r) \right] \\ &= N_m u_v(\lambda_m r), \end{aligned} \quad (38)$$

where the normalization constants, N_m , are yet to be determined. The λ_m are found from the real positive roots $Z_m(v, \rho)$ of

$$Y_{v-1}(Z_m) J_{v-1}(\rho Z_m) - J_{v-1}(Z_m) Y_{v-1}(\rho Z_m) = 0, \quad (39)$$

where

$$Z_m = \lambda_m r_1,$$

and

$$\rho = \frac{r_2}{r_1} > 1.$$

The method for determining the roots, Z_m , is given in Appendix A.

The normalization constants, N_m , are readily determined by using the fact that the $\phi_m(\lambda_m r)$ form a complete orthonormal set of functions,

$$\begin{aligned} &\int_{r_1}^{r_2} r \phi_m(\lambda_m r) \phi_n(\lambda_n r) dr \\ &= N_m N_n \int_{r_1}^{r_2} r u_v(\lambda_m r) u_v(\lambda_n r) dr = \delta_{n,m}, \end{aligned} \quad (41)$$

where the Kroencker delta, $\delta_{n,m}$, is defined as

$$\delta_{n,m} = \begin{cases} 0 & \text{if } n \neq m \\ 1 & \text{if } n = m \end{cases}. \quad (42)$$

Using the result¹⁸

$$\int_{r_1}^{r_2} r u_v^2(\lambda_m r) dr = \frac{2}{\lambda_m^2 \pi^2} \left[\frac{J_{v-1}^2(\lambda_m r_1) - J_{v-1}^2(\lambda_m r_2)}{J_{v-1}^2(\lambda_m r_2)} \right] \quad (43)$$

along with Eq. (41), the normalization constants, N_m , are determined as

$$N_m = \frac{\lambda_m \pi}{\sqrt{2}} \left[\frac{J_{\nu-1}^2(\lambda_m r_2)}{J_{\nu-1}^2(\lambda_m r_1) - J_{\nu-1}^2(\lambda_m r_2)} \right]^{1/2} . \quad (44)$$

The expansion coefficients A_m are determined next. For $m = 0$ note that when $t = \infty$, Eq. (30) reduces to the form shown in Eq. (18), namely,

$$u(w, \infty) = A_0 = c(x, \infty) \exp[-Q^*/RT(x)] . \quad (45)$$

Equation (45) corresponds to the steady-state solution and is equivalent to Eq. (11). Because no matter passes through the sample surface, A_0 can be evaluated from

$$c_0 = A_0 \int_0^l e^{Q^*/RT(x)} dx / \int_0^l dx . \quad (46)$$

Setting $y = l/T(x)$, Eq. (46) may be written as

$$A_0 = c_0 \int_{1/T_h}^{1/T_c} dy/y^2 / \int_{1/T_h}^{1/T_c} \frac{e^{\frac{Q^*}{R}y}}{y^2} dy , \quad (47)$$

for which the solution for $Q^* < 0$ is

$$\frac{1}{A_0} = \begin{cases} \frac{T_c \exp\left(-\left|\frac{Q^*}{RT_c}\right|\right) \left[\left|\frac{Q^*}{RT_c}\right| \exp\left(\left|\frac{Q^*}{RT_c}\right|\right) E_1\left(\left|\frac{Q^*}{RT_c}\right|\right) - 1 \right]}{c_0(T_h - T_c)} \\ - \frac{T_h \exp\left(-\left|\frac{Q^*}{RT_h}\right|\right) \left[\left|\frac{Q^*}{RT_h}\right| \exp\left(\left|\frac{Q^*}{RT_h}\right|\right) E_1\left(\left|\frac{Q^*}{RT_h}\right|\right) - 1 \right]}{c_0(T_h - T_c)} \end{cases} , \quad (48)$$

and, if $Q^* > 0$,

$$\frac{1}{A_0} = \begin{cases} \frac{T_c \exp\left(\left|\frac{Q^*}{RT_c}\right|\right) \left[\left|\frac{Q^*}{RT_c}\right| \exp\left(-\left|\frac{Q^*}{RT_c}\right|\right) Ei\left(\left|\frac{Q^*}{RT_c}\right|\right) - 1 \right]}{c_0(T_h - T_c)} \\ - \frac{T_h \exp\left(\left|\frac{Q^*}{RT_h}\right|\right) \left[\left|\frac{Q^*}{RT_h}\right| \exp\left(-\left|\frac{Q^*}{RT_h}\right|\right) Ei\left(\left|\frac{Q^*}{RT_h}\right|\right) - 1 \right]}{c_0(T_h - T_c)} \end{cases} , \quad (49)$$

and, if $Q^* = 0$, $A_0 = c_0$. The exponential integrals $E_1(z)$ and $Ei(z)$ are defined by¹⁹

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t} dt, \quad \text{Re}(z) > 0 ,$$

and

$$Ei(z) = \int_{-\infty}^z \frac{e^t}{t} dt .$$

(50)

The technique used for computing $E_1(z)$ and $Ei(z)$ is given in Appendix B.

The expansion coefficients A_m ($m \neq 0$) are readily determined by transforming Eq. (30) into the (r, ϕ_m) space at $t = 0$, namely,

$$[u(w, 0) - A_0] r^{-\nu} = \sum_{m=1}^{\infty} A_m N_m u_{\nu}(\lambda_m r) , \quad (51)$$

or, using Eqs. (28), (35), and (36),

$$c_0 r^{\nu-2(1+\alpha)} - A_0 r^{-\nu} = \sum_{m=1}^{\infty} A_m N_m u_{\nu}(\lambda_m r) . \quad (52)$$

Multiplying Eq. (52) by $r N_n u_{\nu}(\lambda_n r)$ and applying Eq. (41),

$$A_m = c_0 N_m \int_{r_1}^{r_2} \left[r^{\nu-2(1+\alpha)} - \frac{A_0}{c_0} r^{-\nu+1} \right] u_{\nu}(\lambda_m r) dr . \quad (53)$$

The integral in Eq. (52) is determined in Appendix C with the results that for small arguments $(x_{1,m} = \lambda_m r_1 < 12)$,

$$A_m = \frac{c_o N_m}{\lambda_m \nu - 2\nu_o + 1} \left\{ \frac{4}{\pi} (\nu - \nu_o) x_1^{\nu - 2\nu_o - 1} \left[\left(\frac{x_2}{x_1} \right)^{\nu - 2\nu_o - 1} \frac{J_{\nu-1}(x_1)}{J_{\nu-1}(x_2)} - 1 \right] + \left[Y_{\nu-1}(x_1) - \cot \nu \pi J_{\nu-1}(x_1) \right] \left[S_{\nu, \nu_o}^{(1)}(x_2) - S_{\nu, \nu_o}^{(1)}(x_1) \right] + \frac{J_{\nu-1}(x_1)}{\sin \nu \pi} \left[S_{\nu, \nu_o}^{(2)}(x_2) - S_{\nu, \nu_o}^{(2)}(x_1) \right] \right\}, \quad (54)$$

and for large arguments ($x_{1,m} > 12$) we have the asymptotic form given by

$$A_m = \frac{4}{\pi} \frac{c_o N_m}{\lambda_m \nu - 2\nu_o + 1} x_1^{\nu - 2\nu_o - 1} T_{\nu, \nu_o}(x_1) \left[\left(\frac{x_2}{x_1} \right)^{\nu - 2\nu_o - 1} \frac{J_{\nu-1}(x_1)}{J_{\nu-1}(x_2)} \frac{T_{\nu, \nu_o}^N(x_2)}{T_{\nu, \nu_o}^N(x_1)} - 1 \right], \quad (55)$$

where $\nu_o \equiv 1 + x$ corresponds to ν for zero heat of transport ($Q^* = 0$). The functions $S_{\nu, \nu_o}^{(1)}(x)$, $S_{\nu, \nu_o}^{(2)}(x)$, and $T_{\nu, \nu_o}^N(x)$ defined in Eqs. (C.13) and (C. 21), are given by

Noting that from Eqs. (36) and (40)

$$\gamma_m = \frac{z_m}{2} \left(\frac{\tilde{Q}}{RT_h} - 4 \right) e^{-\frac{1}{2} \left(\frac{\tilde{Q}}{RT_h} - 4 \right)}, \quad (57)$$

$$S_{\nu, \nu_o}^{(1)}(x) = x^{\nu - 2\nu_o + 1} \left(\frac{1}{2} x \right)^{\nu + 1} \sum_{k=0}^{\infty} \frac{(-)^k \left(\frac{1}{2} x \right)^{2k}}{k! \Gamma(\nu + k + 1) \Gamma(\nu - \nu_o + k + 1)},$$

the time constant $(1/\gamma_m^2)$ in Eq. (30) becomes

$$S_{\nu, \nu_o}^{(2)}(x) = x^{\nu - 2\nu_o - 1} \left(\frac{1}{2} x \right)^{-\nu + 1} \sum_{k=0}^{\infty} \frac{(-)^k \left(\frac{1}{2} x \right)^{2k}}{k! \Gamma(-\nu + k + 1) \Gamma(k - \nu_o)}, \quad \frac{1}{t_m} = \gamma_m^2 = \tilde{D}_o \left(\frac{k}{T_h} \right)^2 \left(\frac{\tilde{Q}}{2RT_h} - 2 \right)^2 e^{-\tilde{Q}/RT_h} z_m^2. \quad (58)$$

and

$$T_{\nu, \nu_o}^N(x) = \sum_{p=0}^N \frac{(\nu - \nu_o - p)}{x^{2p}} \prod_{k=0}^{p-1} \left[\nu^2 - (\nu - 2\nu_o - 2k)^2 \right]. \quad (56)$$

The solution to Eqs. (14) through (16) then becomes

$$\frac{c(x, t)}{c_o} = e^{Q^*/RT(x)} \left[A_o - e^{\frac{\tilde{Q} - Q^*}{2RT_h} \left(\frac{T_h}{T(x)} - 1 \right)} \sum_{m=1}^{\infty} e^{-t/t_m} A_m N_m u_{\nu}(\lambda_m r) \right], \quad (59)$$

where

$$r = \exp \left[\left(\frac{\tilde{Q}}{2RT_h} - 2 \right) \left(\frac{T_h}{T(x)} - 1 \right) \right] \quad (60)$$

The terms A_o , A_m , N_m , Z_m , and $u_v(\lambda_m r)$ are given by Eqs. (48) and (49), (54) and (55), (44), (39) and (40), and (38), respectively.

From the analytic solution exhibited in Eq. (59) for this type of experiment, performed over extended periods of time, obviously the resulting concentration dependence upon the parameters Q^* , $\tilde{Q}$, and $\tilde{D}_o$ is primarily upon Q^* , inasmuch as the exponential time factor depletes any variation in $\tilde{Q}$ and $\tilde{D}_o$ into insignificance. For experiments performed over short periods of time (hours) this will not necessarily be the case, and an accurate analysis of the parameters Q^* , $\tilde{Q}$, and $\tilde{D}_o$ may be attempted provided the accuracy of the concentration determination is high enough.

IV. COMPARISON CALCULATIONS AND CONCLUSIONS

Calculations were performed on the CDC-6600 to anticipate their feasibility, accuracy, and speed for the design and analysis of planned experiments. We constructed a numerical difference equation solution to Eq. (14) for comparison purposes. The derivation and FORTRAN code are discussed in Appendix D. The analytical solution of Eq. (14) was also programmed. The FORTRAN code is listed in Appendix E.

All comparisons were made using Sawatzky and Vogt's⁽¹⁷⁾ parameters for ZrH (Table II) to determine the relative accuracy of the analytical solution and a refined numerical scheme.

TABLE II

ZrH PARAMETERS

$$\begin{aligned} Q^* &= 6,061 \text{ kcal/mole} \\ |\tilde{Q}| &= 8,306 \text{ kcal/mole} \\ D_o &= 2.17 \times 10^{-3} \text{ cm}^2/\text{sec} \end{aligned}$$

The numerical scheme showed no significant changes on further refinement of mesh and time increments for 100 mesh points at $\Delta t < 10$ sec (provided $(D\Delta t/(\Delta x)^2) < 0.5$).

Comparison runs were made for 1-, 5-, 10-, 24-, 48-, and 100-h time periods. The solutions are shown in Fig. 1. The relative comparison of the analytical to the numerical solution is given in Fig. 2.

Figure 2 shows that at the hot end of the sample, for all times, the solutions agree to within 1%; at the cold end a total variation of 3% occurs over the range of 100 h. In addition, at the cold end and after 10 h, the solutions agree to within 1%. This is somewhat better than was anticipated from the initial estimates given in Table I, which anticipated a 5% error.

Fig. 1. Solution to the numerical difference equations for various diffusion times (h) as a function of temperature (T).

Fig. 2. Percentage comparison of the analytical to numerical solution for various diffusion times (h) as a function of temperature (T).

The computation time for the analytical solution depends linearly upon the number of spatial points to be evaluated and only slightly on the diffusion time of the run. The computation time for the numerical difference equation depends linearly upon both the diffusion time of the run and the large number of spatial points that must be evaluated. Figure 3 illustrates the CDC-6600 central processor (CP) time vs diffusion time comparisons for the numerical difference equation solutions. The analytical solution required less than 10 sec for complete evaluation of all points in any given instance.

For experimental evaluations, comparisons, and evaluation of parameter adjustments, the numerical difference solution always requires a small mesh size (for accuracy) and computation (satisfying the stability criteria) out to the diffusion time. Conversely, the analytical solution needs to be evaluated only at the diffusion time and at the measured data points.

For example, for a typical 24-h run with 25 measured data points, the analytical solution would be at least 50 times faster than the numerical difference equation solution. For a 48-h run this factor would be 128. For parametric adjustments to

determine the best fit to the data this factor could cause serious delay, therefore, the analytical solution is always preferred.

In examining the sensitivity of the solution to deviations of the parameters Q^* , $\tilde{Q}$, D_0 , the summed squared deviation of the reference concentration, $C_R(i)$ is constructed and computed at mesh point i , and the analytical solution $C_p(i)$ is evaluated at mesh point i with parameters p . The reference concentration is calculated with the parameters of Table II.

Figures 4, 5, and 6 show that for 1-, 5-, and 10-h diffusion times the method can readily resolve individual parameter deviations (the other two being held fixed) of 5, 10, and 20%. A nominal least-squares search procedure should have no particular difficulty achieving convergence. It is interesting to note that the overall sensitivity of the parameters is approximately evident as $D_0 : Q^* : \tilde{Q} \approx 1:2:10$. The nonlinearity of the solution dependence on the parameter $\tilde{Q}$ is reflected in the asymmetry of that variation.

A full investigation of the squared deviation for the three parameters at 5, 10, and 20% parameter deviations is given in Table III. When plotted,

Fig. 3. Central processor (CDC-6600) time required for the numerical difference solution as a function of diffusion time (h) of the problem.

Fig. 4. Squared deviation of numerical and analytical solution vs fractional deviation of reference parameters for 1-h diffusion time.

Fig. 5. Squared deviation of numerical and analytical solution vs fractional deviation of reference parameters for 5-h diffusion time.

Fig. 6. Squared deviation of numerical and analytical solution vs fractional deviation of reference parameters for 10-h diffusion time.

these data exhibit the same characteristics as seen in Figs. 4 through 6.

From these results we conclude that the analytical solution is feasible, accurate, and rapid.

Further, it is sensitive enough to parameter variations to warrant its use in planning experiments and for the data analysis of subsequent concentration measurements for determining the parameters D_0 , Q^* , and $\tilde{Q}$.

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TABLE III

SQUARED DEVIATIONS FROM REFERENCE CONCENTRATION,

$$\sum_{i=1}^{100} |c_R(i) - c_p(i)|^2, \text{ AT 1 HOUR.}$$

REFERENCE PARAMETERS: $D_0 = 2.17 \times 10^{-3}$, $|\tilde{Q}| = 8,306$, $Q^* = 6,061$

D_0	$\tilde{Q}$	Q^*	$\sum_{i=1}^{100} c_R(i) - c_p(i) ^2$		
			$\delta = 0.05$	$\delta = 0.10$	$\delta = 0.20$
D_0	$\tilde{Q}$	Q^*	0	0	0
$D_0 + \delta D_0$	$\tilde{Q}$	Q^*	4.92×10^{-5}	1.94×10^{-4}	7.56×10^{-4}
$D_0 - \delta D_0$	$\tilde{Q}$	Q^*	5.06×10^{-5}	2.06×10^{-4}	8.50×10^{-4}
D_0	$\tilde{Q} + \delta \tilde{Q}$	Q^*	1.45×10^{-3}	4.68×10^{-3}	1.26×10^{-2}
D_0	$\tilde{Q} - \delta \tilde{Q}$	Q^*	2.26×10^{-3}	1.14×10^{-2}	7.56×10^{-2}
D_0	$\tilde{Q}$	$Q^* + \delta Q^*$	8.73×10^{-5}	3.49×10^{-4}	1.39×10^{-3}
D_0	$\tilde{Q}$	$Q^* - \delta Q^*$	8.74×10^{-5}	3.50×10^{-4}	1.40×10^{-3}
$D_0 + \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	Q^*	1.05×10^{-3}	3.54×10^{-3}	1.02×10^{-2}
$D_0 - \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	Q^*	1.91×10^{-3}	6.03×10^{-3}	1.55×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	Q^*	3.15×10^{-3}	1.65×10^{-2}	1.16×10^{-1}
$D_0 - \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	Q^*	1.50×10^{-3}	7.23×10^{-3}	4.23×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q}$	$Q^* + \delta Q^*$	2.69×10^{-4}	1.11×10^{-3}	4.74×10^{-3}
$D_0 - \delta D_0$	$\tilde{Q}$	$Q^* + \delta Q^*$	1.27×10^{-5}	4.59×10^{-5}	1.58×10^{-4}
$D_0 + \delta D_0$	$\tilde{Q}$	$Q^* - \delta Q^*$	1.61×10^{-5}	7.23×10^{-5}	3.66×10^{-4}
$D_0 - \delta D_0$	$\tilde{Q}$	$Q^* - \delta Q^*$	2.51×10^{-4}	9.70×10^{-4}	3.60×10^{-4}
D_0	$\tilde{Q} + \delta \tilde{Q}$	$Q^* + \delta Q^*$	9.81×10^{-4}	3.34×10^{-3}	9.73×10^{-3}
D_0	$\tilde{Q} - \delta \tilde{Q}$	$Q^* + \delta Q^*$	3.42×10^{-3}	1.80×10^{-2}	1.31×10^{-1}
D_0	$\tilde{Q} + \delta \tilde{Q}$	$Q^* - \delta Q^*$	2.03×10^{-3}	6.34×10^{-3}	1.60×10^{-2}
D_0	$\tilde{Q} - \delta \tilde{Q}$	$Q^* - \delta Q^*$	1.36×10^{-3}	6.45×10^{-3}	3.62×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	$Q^* + \delta Q^*$	6.52×10^{-4}	2.32×10^{-3}	7.29×10^{-3}
$D_0 - \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	$Q^* + \delta Q^*$	1.39×10^{-3}	4.59×10^{-3}	1.27×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	$Q^* + \delta Q^*$	4.56×10^{-3}	2.49×10^{-2}	1.93×10^{-1}
$D_0 - \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	$Q^* + \delta Q^*$	2.43×10^{-3}	1.22×10^{-2}	7.71×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	$Q^* - \delta Q^*$	1.57×10^{-3}	5.11×10^{-3}	1.38×10^{-2}
$D_0 - \delta D_0$	$\tilde{Q} + \delta \tilde{Q}$	$Q^* - \delta Q^*$	2.55×10^{-3}	7.75×10^{-3}	1.86×10^{-2}
$D_0 + \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	$Q^* - \delta Q^*$	2.04×10^{-3}	9.91×10^{-3}	3.90×10^{-2}
$D_0 - \delta D_0$	$\tilde{Q} - \delta \tilde{Q}$	$Q^* - \delta Q^*$	8.22×10^{-4}	3.68×10^{-3}	1.81×10^{-2}

APPENDIX A
DETERMINATION OF THE ROOTS Z_m

The root equation, Eq. (39), may be written as

$$f_\mu(Z_m, \rho) = Y_\mu(Z_m)J_\mu(\rho Z_m) - J_\mu(Z_m)Y_\mu(\rho Z_m) = 0, \quad (\text{A.1})$$

where $\mu = \nu - 1$, $\rho = r_2/r_1 > 1$, and $Z_m = \lambda_m r_1$ in the notation of Eq. (40).

The function $f_\mu(z, \rho)$ with ρ fixed has the property that after the first root, for which $f_\mu(Z_1, \rho) = 0$, it is an oscillatory function of Z . The roots of $f_\mu(Z_m, \rho)$ are real, positive, and ordered,²⁰

$$0 < Z_1 < \dots < Z_{m-1} < Z_m < Z_{m+1} < \dots \quad (\text{A.2})$$

For $Z_{m-1} > 12$, we may use McMahon's²⁰ asymptotic estimate of the root position, namely,

$$Z_m \approx \frac{m\pi}{\rho-1} \left[\frac{1}{1 + \frac{4\nu^2 - 1}{8\rho(\frac{m\pi}{\rho-1})^2}} \right] \quad (\text{A.3})$$

The next root, Z_m ($m = 1, 2, 3, \dots$), if the asymptotic condition is not satisfied, can be determined readily by examining $f_\mu(Z)$ from Z_{m-1} (for $m = 1$, $Z_0 \approx 0$) until the next sign change of $f_\mu(Z)$ occurs. At that point one has determined a neighborhood (the size of which depends upon the step size when examining $f_\mu(Z)$ of the root Z_m).

Once in the neighborhood of Z_m , Newton's method provides a useful convergent iterative procedure for a more exact determination of the root Z_m . For, making a Taylor's series expansion of $f_\mu(Z)$ about Z_m , we have

$$f_\mu(Z_m) = f_\mu(Z) - (Z - Z_m) \left. \frac{\partial f_\mu(Z')}{\partial Z'} \right|_{Z=Z'_m} + \dots \quad (\text{A.4})$$

But, by Eq. (A.1),

$$f_\mu(Z_m) = 0, \quad (\text{A.5})$$

and solving Eq. (A.4) for Z_m yields

$$Z_m \approx Z - \frac{f_\mu(Z)}{\left. \frac{\partial f_\mu(Z')}{\partial Z'} \right|_{Z=Z'}} \quad , \quad (\text{A.6})$$

$Z = Z'$

where

$$f_\mu(Z) = Y_\mu(Z)J_\mu(\rho Z) - J_\mu(Z)Y_\mu(\rho Z) \quad , \quad (\text{A.7})$$

$$\frac{\partial f_\mu(Z)}{\partial Z} = \frac{2\mu}{Z} f_\mu(Z) + g_\mu(Z) + \rho h_\mu(Z) \quad ,$$

and

$$g_\mu(Z) = J_{\mu+1}(Z)Y_\mu(\rho Z) - Y_{\mu+1}(Z)J_\mu(\rho Z) \quad ,$$

and

$$h_\mu(Z) = J_\mu(Z)Y_{\mu+1}(\rho Z) - Y_\mu(Z)J_{\mu+1}(\rho Z) \quad . \quad (\text{A.8})$$

Because at $f_\mu(Z)|_{Z=Z_m} = 0$, we have $\frac{\partial f_\mu(Z)}{\partial Z}|_{Z=Z_m} \neq 0$, and the procedure is nonsingular in its convergence. The direction of approach towards Z_m provides the estimate, Z , in the neighborhood of Z_m as indicated in Fig. A.1.

Fig. A-1. Graph of $f_\mu(Z)$.

Four possible cases that are labeled on Fig. A.1

can occur. Denoting f' by $\frac{\partial f_{\mu}(Z')}{\partial Z'}|_{Z'=Z}$, we see that the correction terms are as follows:

$$\begin{aligned} (1) \quad f < 0, f' > 0: \quad Z_m &\cong Z + |f/f'|, \\ (2) \quad f > 0, f' > 0: \quad Z_m &\cong Z - |f/f'|, \\ (3) \quad f > 0, f' < 0: \quad Z_m &\cong Z + |f/f'|, \\ (4) \quad f < 0, f' < 0: \quad Z_m &\cong Z - |f/f'|. \end{aligned} \quad (A.9)$$

The iterative procedure then consists of replacing Z by the result of Eq. (A.9) and repeating the

process. Whenever $|f_{\mu}(Z, \rho)| < 10^{-11}$, the iterative procedure is terminated.

The determination of the next root, $(m+1)$, is terminated whenever

$$e^{-t/t_m} < 10^{-8}, \quad (A.10)$$

where t is the time interval over which the experiment was performed, and t_m is defined by Eq. (58) as

$$\frac{1}{t_m} = \gamma_m^2 = \left(\frac{k}{T_h}\right)^2 \left(\frac{\tilde{Q}}{2RT_h} - 2\right)^2 \tilde{D}_0 e^{-\tilde{Q}/RT_h} Z_m^2. \quad (A.11)$$

APPENDIX B EXPONENTIAL INTEGRAL EVALUATION

We consider here the numerical evaluation of the exponential integrals¹⁹

$$Ei(x) = \int_{-\infty}^x \frac{e^t}{t} dt \quad (B.1)$$

and

$$E_1(x) = \int_x^{\infty} \frac{e^{-t}}{t} dt. \quad (B.2)$$

The series representations of Eqs. (B.1) and (B.2) are given by¹⁹

$$Ei(x) = \gamma + \ln x + \sum_{n=1}^{\infty} \frac{x^n}{nn!}, \quad x > 0 \quad (B.3)$$

and

$$E_1(x) = -\gamma - \ln x - \sum_{n=1}^{\infty} \frac{(-x)^n}{nn!}, \quad |\arg x| < \pi, \quad (B.4)$$

where $\gamma = 0.57721\ 56649\dots$ is Euler's constant.

Equation (B.3) for $Ei(x)$ may be evaluated by the method of continued fractions²¹ where the n 'th convergent corresponds exactly to the first n terms of the series by the following procedure. Let S denote $Ei(x)$. In MADCAP-MANIC notation²² the

evaluation procedure is given by

```
(... T = X; S = T
for k = 2, 3, ..., infinity
T = X * T * (1-k)/k
S = S + T
if |T/S| < Eps: exit from loop
S = \gamma + \ln X + S ...)
```

In words the above procedure indicates the following: Initialize T to be X and S to be T . Then for $k = 2, 3, \dots$, until the convergence criteria are satisfied (namely, $|T/S| < Eps$), evaluate the iterative contributions to S (in the indented region of the procedure). When the series is converged, add the contributions $\gamma + \ln x$ to the series, the result being $Ei(x)$.

Equation (B.4) may be evaluated by the continued fraction²¹

$$E_1(x) = e^{-x} \left(\frac{1}{x+} \frac{1}{1+} \frac{1}{x+} \frac{2}{1+} \frac{2}{x+} \dots \right). \quad (B.5)$$

However, the series in Eq. (B.4) is obviously oscillatory, and it is therefore more convenient to use the condensed form of Eq. (B.5) wherein the n 'th convergent corresponds to $2n$ terms of Eq. (B.5) and converges monotonically. The general procedure for condensation of a continued fraction is described in Khovanskii.²¹ A procedure for evaluation is as follows. Let S denote $E_1(x)$. Then the evaluation procedure is given by

```
(... q = X + 1; T = 1/q; S = T
```

for $k = 2, 3, \dots$, infinity
 $a = -(k-1)^2$; $b = X + 1 + 2(k-1)$
 $T = T/[1 + q(b/a)]$
 $q = b + a/q$
 $S = S + T$
 if $|T/S| < \text{Eps}$: exit from loop
 $S = e^{-X} S$...)

Typically, the convergence criteria, Eps, that we

used was about 10^{-10} , which gives ten or more significant figures to the result over the range of interest. In this application, if the variable X had been small ($X \ll 1$), it would have proved more efficient to utilize the series representation for $E_1(x)$ for those small values because of the $\ln x$ contribution to the continued fraction.

APPENDIX C

DETERMINATION OF THE EXPANSION COEFFICIENTS A_m

From Eq. (53), the expansion coefficients A_m are determined from

$$A_m = c_0 N_m \int_{r_1}^{r_2} \left[r^{v-2(1+\alpha)+1} - \frac{A_0}{C_0} r^{-v+1} \right] u_v(\lambda_m r) dr, \quad (C.1)$$

where $u_v(\lambda_m r)$

$$= Y_{v-1}(\lambda_m r_1) J_v(\lambda_m r) - J_{v-1}(\lambda_m r_1) Y_v(\lambda_m r), \quad (C.2)$$

Therefore, we need to examine integrals of the form

$$\int_{x_1}^{x_2} x^{v+1} u_v(x) dx, \quad (C.3)$$

where $x_i = \lambda_m r_i$, $i = 1, 2$.

We note that the term in Eq. (C.1) with coefficient A_0 vanishes identically. This follows immediately from

$$\begin{aligned} & \int_{x_1}^{x_2} x^{-v+1} u_v(x) dx \\ &= x^{-v+1} \left[Y_{v-1}(x_1) J_v(x) - J_{v-1}(x_1) Y_v(x) \right] \Big|_{x_1}^{x_2} = 0, \end{aligned} \quad (C.4)$$

because the lower limit vanishes identically and the upper limit is just the root equation, Eq. (38):

$$Y_{v-1}(x_1) J_v(x_2) - J_{v-1}(x_1) Y_v(x_2) = 0. \quad (C.5)$$

We define

$$v_0 = v(Q^* = 0) < 1 + \alpha, \quad (C.6)$$

as corresponding to zero heat of transport ($Q^* = 0$). Then using Eqs. (C.5) and (C.6), makes Eq. (C.1) become

$$A_m = \frac{c_0 N_m}{\lambda_m} \int_{x_1}^{x_2} x^{v-2v_0+1} u_v(x) dx. \quad (C.7)$$

We are interested in both small and large arguments (x_1, x_2), and in making the solutions join smoothly. For small arguments, one could substitute the ascending series representations for J_v and Y_v into u_v and then integrate term by term. This result would lose numerical significance in computation for large enough arguments. For large arguments, the asymptotic representations could be used but would result in a cumbersome doubly-infinite series.

Instead we use the Bessel differential equation,

$$\frac{d}{dx} \left(x \frac{du_v}{dx} \right) + \left(\lambda_m^2 x - \frac{v^2}{x} \right) u_v = 0, \quad (C.8)$$

in Eq. (C.7),

$$A_m = \frac{c_0 N_m}{\lambda_m} \int_{x_1}^{x_2} x^{v-2v_0} \left[\frac{v^2 u_v(x)}{x} - \frac{d}{dx} \left(x \frac{du_v}{dx} \right) \right] dx, \quad (C.9)$$

then integrate by parts and use the boundary condition,

$$x \frac{du_v(x)}{dx} + v u_v(x) = 0 \quad \text{at } x = x_1, x_2, \quad (C.10)$$

to obtain

$$A_m = \frac{c_{0N_m}}{\lambda_m} \left\{ \begin{aligned} & -(\nu - \nu_0) x^{v-2\nu_0} u_v(x) \Big|_{x_1}^{x_2} \\ & + \left[\nu^2 - (\nu - 2\nu_0)^2 \right] \int_{x_1}^{x_2} x^{v-2\nu_0-1} u_v(x) dx \end{aligned} \right. \quad (C.11)$$

For small arguments ($x < 12$) we use

$$J_\nu(x) = \left(\frac{1}{2}x\right)^\nu \sum_{k=0}^{\infty} \frac{(-)^k \left(\frac{1}{2}x\right)^{2k}}{k! \Gamma(\nu+k+1)} \quad (C.12)$$

and

$$Y_\nu(x) = \frac{J_\nu(x) \cos \nu \pi - J_{-\nu}(x)}{\sin \nu \pi}$$

to write $u_v(x)$ as

$$u_v(x) = \left[Y_{\nu-1}(x_1) - \cot \nu \pi J_{\nu-1}(x_1) \right] J_\nu(x) + \frac{J_{\nu-1}(x)}{\sin \nu \pi} J_{-\nu}(x) \quad (C.13)$$

Substituting Eq. (C.13) into the integral in Eq. (C.11) and using Eq. (C.12), we obtain

$$\int_{x_1}^{x_2} x^{v-2\nu_0+1} u_v(x) dx = \left[Y_{\nu-1}(x_1) \right.$$

$$\left. - \cot \nu \pi J_{\nu-1}(x_1) \right] S_{\nu, \nu_0}^{(1)}(x) \Big|_{x_1}^{x_2} + \frac{J_{\nu-1}(x_1)}{\sin \nu \pi} S_{\nu, \nu_0}^{(2)}(x) \Big|_{x_1}^{x_2}, \quad (C.14)$$

where

$$S_{\nu, \nu_0}^{(1)}(x) = x^{v-2\nu_0+1} \left(\frac{1}{2}x\right)^{\nu+1} \sum_{k=0}^{\infty} \frac{(-)^k \left(\frac{1}{2}x\right)^{2k}}{k! \Gamma(\nu+k+1) (\nu - \nu_0 + k + 1)}, \quad (C.15)$$

$$S_{\nu, \nu_0}^{(2)}(x) = x^{v-2\nu_0-1} \left(\frac{1}{2}x\right)^{-\nu+1} \sum_{k=0}^{\infty} \frac{(-)^k \left(\frac{1}{2}x\right)^{2k}}{k! \Gamma(-\nu+k+1) (k - \nu_0)}.$$

Using the root equation Eq. (C.5) and the Wronskian

$$W \{ J_\nu(x), Y_\nu(x) \} = \frac{2}{\pi x}, \quad (C.16)$$

we easily verify that

$$u_v(x_1) = 2/\pi x_1$$

and

$$u_v(x_2) = 2/\pi x_2 \frac{J_{\nu-1}(x_1)}{J_{\nu-1}(x_2)}. \quad (C.17)$$

Substituting Eqs. (C.14) and (C.17) into Eq. (C.11), we obtain for the small-argument solution the result

$$A_m = \frac{c_{0N_m}}{\lambda_m} \left\{ \begin{aligned} & \frac{4}{\pi} (\nu - \nu_0) x_1^{v-2\nu_0-1} \left[\left(\frac{x_2}{x_1} \right)^{v-2\nu_0-1} \frac{J_{\nu-1}(x_1)}{J_{\nu-1}(x_2)} - 1 \right] \\ & + \left[Y_{\nu-1}(x_1) - \cot \nu \pi J_{\nu-1}(x_1) \right] \left[S_{\nu, \nu_0}^{(1)}(x_2) - S_{\nu, \nu_0}^{(1)}(x_1) \right] \\ & + \frac{J_{\nu-1}(x_1)}{\sin \nu \pi} \left[S_{\nu, \nu_0}^{(2)}(x_2) - S_{\nu, \nu_0}^{(2)}(x_1) \right] \end{aligned} \right. \quad (C.18)$$

where $S_{\nu, \nu_0}^{(k)}(x)$ is defined by Eq. (C.15). For large arguments we proceed as follows. We define the integral

$$\int_{x_1}^{x_2} x^{\nu-2\nu_0+1} u_{\nu}(x) dx = g_{\nu-2\nu_0+1, \nu}(x_1, x_2) \quad ; \quad (C.19)$$

then Eq. (C.11) is equivalent to the recursion relation

$$g_{n, m}(x_1, x_2) = (n + m - 1) x^{n-1} u_m(x) \Big|_{x_1}^{x_2} + \left[m^2 - (n - 1)^2 \right] g_{n-2, m}(x_1, x_2) \quad , \quad (C.20)$$

with $n = \nu - 2\nu_0 + 1$ and $m = \nu$. From Eq. (C.20), we may develop an asymptotic expression for $g_{n, m}(x_1, x_2)$. Iterating Eq. (C. 20) N times yields

$$g_{n, m}(x_1, x_2) = \left\{ \sum_{p=0}^N \frac{n+m-2p-1}{x^{2p+1}} \prod_{k=0}^{p-1} \left[m^2 - (n-2k-1)^2 \right] x^n u_m(x) \Big|_{x_1}^{x_2} + \prod_{p=1}^N \left[m^2 - (n-2p-1)^2 \right] g_{n-2p-2, m}(x_1, x_2) \right\} \quad . \quad (C.21)$$

Equation (C.21) represents an asymptotic expansion of $g_{n, m}(x_1, x_2)$ in terms of $x^k u_m(x)$ at the end points, if we neglect the term involving $g_{n-2p-2, \nu}(x_1, x_2)$. This neglect is justified because $u_{\nu}(x)$ is oscillatory and bounded in the interval (x_1, x_2) and the contribution from $g_{n-2p-2, \nu}(x_1, x_2)$ is less than the last term in the series expression involving $u_{\nu}(x)$.

Thus, for $n = \nu - 2\nu_0 + 1$ and $m = \nu$, Eq. (C.21) takes the asymptotic form

$$g_{\nu-2\nu_0+1, \nu}(x_1, x_2) \cong 2x^{\nu-2\nu_0} u_{\nu}(x) T_{\nu, \nu_0}^N(x) \Big|_{x_1}^{x_2} \quad , \quad (C.22)$$

where

$$T_{\nu, \nu_0}^N(x_1, x_2) = \sum_{p=0}^N \frac{(\nu-\nu_0-p)}{x^{2p}} \prod_{k=0}^{p-1} \left[\nu^2 - (\nu - 2\nu_0 - 2k)^2 \right] \quad . \quad (C.23)$$

Substituting Eq. (34) into Eq. (C.11), we obtain

$$A_m = 2 \frac{c_0 N_m}{\nu-2\nu_0+2} x^{\nu-2\nu_0} u_{\nu}(x) T_{\nu, \nu_0}^N(x) \Big|_{x_1}^{x_2} \quad . \quad (C.24)$$

Using Eq. (C.17), the large-argument solution becomes

$$A_m = \frac{4}{\pi} \frac{c_0 N_m}{\nu-2\nu_0+1} x_1^{\nu-2\nu_0-1} T_{\nu, \nu_0}^N(x_1) \left[\left(\frac{x_2}{x_1} \right)^{\nu-2\nu_0-1} \frac{J_{\nu-1}(x_1)}{J_{\nu-1} x_2} \frac{T_{\nu, \nu_0}^N(x_2)}{T_{\nu, \nu_0}^N(x_1)} - 1 \right] \quad , \quad (C.25)$$

where T_{ν, ν_0}^N is determined by Eq. (C.23). We note that for $N = 0$, $T_{\nu, \nu_0}^0(x) = (\nu - \nu_0)$ and Eq. (C.25) reproduces the first term of Eq. (C.20) exactly, which term is the dominant portion of the solution for the expansion coefficients A_m .

APPENDIX D

DERIVATION OF THE NUMERICAL DIFFERENCE SOLUTION AND FORTRAN PROGRAM (FINC)

Differentiating Eq. (14), one obtains the expression

$$\frac{dC}{dt} = D_o e^{-\tilde{Q}/RT} \left[\frac{d^2 C}{dx^2} + \frac{Q^*}{RT} \frac{1}{T} \frac{dT}{dx} \left(\frac{dC}{dx} - \frac{2}{T} \frac{dT}{dx} C \right) + \frac{\tilde{Q}}{RT} \frac{1}{T} \frac{dT}{dx} \left(\frac{dC}{dx} + \frac{Q^*}{RT} \frac{1}{T} \frac{dT}{dx} C \right) \right] \quad (D.1)$$

Assuming that we know the values of the concentration, C_m , of a function $C(x)$ at regular intervals $x = m\epsilon$, $m = \dots 1, 2, \dots$, of its argument and that the temperature gradient (Eq. 16) may be represented by

$$\frac{dT}{dx} = -k = -\frac{\Delta T}{\epsilon} \quad ,$$

which may be transformed into the finite difference equation

$$\frac{dC}{dt} = \frac{D_o e^{-\tilde{Q}/RT}}{\epsilon^2} \left[\delta^2 C_m - \frac{Q^*}{RT} \frac{\Delta T}{T} \left(\delta^1 C_m + 2 \frac{\Delta T}{T} C_m \right) - \frac{\tilde{Q}}{RT} \frac{\Delta T}{T} \left(\delta^1 C_m - \frac{Q^*}{RT} \frac{\Delta T}{T} C_m \right) \right] \quad (D.2)$$

Choosing a notation for the finite difference equations that are symmetrical about m , we define first and second differences by

$$\delta^1 C_m = \frac{1}{2} (C_{m+1} - C_{m-1}) \quad (D.3)$$

and

$$\delta^2 C_m = C_{m+1} - 2C_m + C_{m-1} \quad (D.4)$$

To replace the time derivative, $\frac{\partial C}{\partial t}$, by a difference, we choose an interval of time τ and write $C_{m,n}$ for $C(m\epsilon, n\tau)$. The time derivative becomes

$$\left(\frac{dC_m}{dt} \right)_{t=n\tau} = \frac{C_{m,n+1} - C_{m,n}}{\tau} \quad (D.5)$$

The finite difference equation finally becomes

$$C_{m,n+1} = C_{m,n+M} \left[\delta^2 C_m - \frac{Q^*}{RT} \frac{\Delta T}{T} \left(\delta^1 C_m + 2 \frac{\Delta T}{T} C_m \right) - \frac{\tilde{Q}}{RT} \frac{\Delta T}{T} \left(\delta^1 C_m - \frac{Q^*}{RT} \frac{\Delta T}{T} C_m \right) \right] \quad (D.6)$$

where $M = \frac{\tau}{\epsilon} D_o e^{-\tilde{Q}/RT}$ is the modulus. Experience has shown that calculations based on Eq. (D.6) are stable for values of $M < 0.5$. The values of T are taken at the midpoint of each interval, i.e. at $x = n + 1/2$. Note that, consequently, the modulus is also a function of m .

Equation (D.6) is applicable over the thickness of the sample. In the program FINC, the thickness has been divided into 100 increments. The increment next to the hot surface (T_H) is defined as $m = 2$ and the increment next to the cold surface is defined as $m = 101$. The incremental step in time, τ , is taken as 10 sec.

The boundary conditions given by Eq. (15) enter as follows. For $n\tau = 0$, the concentration C_m ($m = 2, 101$) is constant and equal to the initial specified value. For $n\tau \geq 0$, the boundary condition at the hot and cold surfaces is given by

$$\delta C_m^1 = \frac{Q^*}{RT} \frac{\Delta T}{T} C_m \quad , \quad (D.7)$$

which takes the form

$$C_1 = C_3 - 2 \frac{Q^*}{RT} \cdot \frac{\Delta T}{T} C_2 \quad (D.8)$$

at the hot surface and

$$C_{102} = C_{100} - 2 \frac{Q^*}{RT} \frac{\Delta T}{T} C_{101} \quad (D.9)$$

at the cold surface.

The elements of the above derivation are contained in the following FORTRAN program (FINC).

	SUBROUTINE FINE	A	1
	DIMENSION T(105), T1(105), T2(105), T3(105), CN(105), C1(105), C2(105), CN1(105), D(105), CONC(105)	A	2
	COMMON /A2/ TH,TA,DO,OD,QT,TI,GRAD,CI	A	3
	COMMON /A4/ CONC,CN1,T	A	4
	TC=TA	A	5
	DX=.01*(TH-TC)/GRAD	A	6
	AM=10./DX**2	A	7
	DT=.01*(TH-TC)	A	8
	DC 10 I=2,101	A	9
	T1(I)=DT/T(I)	A	10
	T2(I)=DT/(1.9872*T(I)**2)	A	11
	T3(I)=QT*T2(I)	A	12
	CN(I)=CI	A	13
	D(I)=DO*EXP(-QD/(1.9872*T(I)))	A	14
10	CONTINUE	A	15
	CN(I)=CN(I)-2.*T3(I)*CN(I)	A	16
	CN(102)=CN(100)+2.*T3(101)*CN(101)	A	17
	DC 20 I=2,101	A	18
	J=I-1	A	19
	K=I+1	A	20
	C1(I)=.5*(CN(K)-CN(J))	A	21
	C2(I)=CN(K)-2.*CN(I)+CN(J)	A	22
20	CONTINUE	A	23
	ITF=IFIX(TI*360.)	A	24
	DC 60 KK=1,ITF	A	25
	DC 30 I=2,101	A	26
	CN1(I)=CN(I)+AM*D(I)*(C2(I)-T3(I)*(C1(I)+2.*T1(I)*CN(I))-QD*T2(I)*	A	27
	1(C1(I)-T3(I)*CN(I)))	A	28
30	CONTINUE	A	29
	DC 40 I=2,101	A	30
	CN(I)=CN1(I)	A	31
40	CONTINUE	A	32
	CN(I)=CN(I)-2.*T3(I)*CN(I)	A	33
	CN(102)=CN(100)+2.*T3(101)*CN(101)	A	34
	DC 50 I=2,101	A	35
	J=I-1	A	36
	K=I+1	A	37
	C1(I)=.5*(CN(K)-CN(J))	A	38
	C2(I)=CN(K)-2.*CN(I)+CN(J)	A	39
50	CONTINUE	A	40
60	CONTINUE	A	41
	RETURN	A	42
	END	A	43
		A	44

The input parameters are

TH - Temperature of the hot surface, K.
 TC - Temperature of the cold surface, K.
 DO - Pre-exponential factor of diffusion coefficient, cm^2/sec .
 QD - Absolute magnitude of the heat of isothermal diffusion, kcal/mole.

QT - Heat of thermal diffusion, kcal/mole.

TI - Time, h.

GRAD - Absolute magnitude of linear temperature gradient, K/cm.

CI - Initial constant concentration of the interstitial element.

APPENDIX E

FORTRAN PROGRAM FOR THE EVALUATION OF THE ANALYTICAL SOLUTION

Listing

The COMP program is written in FORTRAN IV for the CDC-6600. The setup of the deck is as follows.

	PROGRAM WORK (INPUT,OUTPUT)	A	1
	CALL SORS	A	2
	CALL AFUNC	A	3
	CALL FINC	A	4
	CALL COMPR	A	5
	RETURN	A	6
	END	A	7
C			
C			
	SUBROUTINE SORS	B	1
	DIMENSION ALAB(12)	B	2
	COMMON /A1/ ALAB	B	3
	COMMON /A2/ TH,TA,DJ,QD,QT,TI,GRAD,CI	B	4
	READ 10, (ALAB(I),I=1,12)	B	5
	READ 20, TH,TA,DJ,QD,QT,TI,GRAD,CI	B	6
	RETURN	B	7
10	FORMAT (12A6)	B	8
20	FORMAT (6E12.7)	B	9
	END	B	10
C			
C			
	SUBROUTINE AFUNC	C	1
	DIMENSION Y(105), T(105), XR(500), CONC(105), SUM(105), CN1(105),	C	2
	1ALAB(12)	C	3
	COMMON /A1/ ALAB	C	4
	COMMON /A2/ TH,TA,DJ,QD,QT,TI,GRAD,CI	C	5
	COMMON /A3/ D,CP,CN,PI	C	6
	COMMON /A4/ CN1,CN1,T	C	7
	DATA D,CP,CN,PI,2/9.,0.0,0.0,3.14159265358979,1.9872/	C	8
	DO 10 J=1,105	C	9
	SUM(J)=0.0	C	10
10	CONTINUE	C	11
	T1=TH	C	12
	T2=TA	C	13
	T11=T1/T2	C	14
	A=2./(QD/(R*T1)-4.)	C	15
	ORD=((QD-QT)/(R*T1)-2.)/(2D/(R*T1)-4.)	C	16
	B=ORD-2.*(1.+A)	C	17
	TC=GRAD**2*DD*EXP(-QD/(R*T1))*T1/(T1*A)**2*3600.	C	18
	CALL ACO (QT,T1,T2,R,AJ)	C	19
	DTI=(T1-T2)*.01	C	20
	Y(1)=EXP(1./A)	C	21
	Y(102)=EXP(T1/(A*T2))	C	22
	DO 20 I=2,101	C	23
	T(I)=T1-DTI*.5-(I-2)*DTI	C	24
	Y(I)=EXP(T1/(A*T(I)))	C	25
20	CONTINUE	C	26
	RO=Y(102)/Y(1)	C	27
	OR=ORD-1.	C	28
	CALL RQDT (OR,RJ,TC,XR,NR)	C	29
	DO 60 I=1,NR	C	30
	X=XR(I)	C	31
	CALL COEFF (ORD,RJ,RJ,B,X,Y(1),TC,X1J,X1Y,CFF)	C	32
	DO 50 J=2,101	C	33
	X=XR(I)*Y(J)/Y(1)	C	34
	IF (X-20.) 30,40,40	C	35
30	CALL BESSM (ORD,X,AJ,AY)	C	36
	SUM(J)=SUM(J)+CFF*(X1Y*AJ-X1J*AY)/AO	C	37
	GO TO 50	C	38
40	CALL BESLG (ORD,X,AJ,AY)	C	39
	SUM(J)=SUM(J)+CFF*(X1Y*AJ-X1J*AY)/AO	C	40
50	CONTINUE	C	41
60	CONTINUE	C	42
	DO 70 J=2,101	C	43
	CONC(J)=CI*EXP(QT/(R*T(J)))*(1.+SUM(J)*EXP(ORD*ALOG(Y(J))))*AO	C	44
70	CONTINUE	C	45
	PRINT 90	C	46
	PRINT 80, (ALAB(I),I=1,12)	C	47
	PRINT 100, T1,T2,GRAD	C	48
	PRINT 170, T11	C	49
	PRINT 110, DD,2D,2T	C	50
	PRINT 120, CI,TI	C	51

	PRINT 130	C	52
	PRINT 140, ORD, A	C	53
	PRINT 150, B, TC	C	54
	PRINT 160, AD, RD	C	55
	PRINT 180, XR(1), XR(2), XR(3), XR(4), XR(5)	C	56
	RETURN	C	57
90	FORMAT (12A6)	C	58
90	FORMAT (1H1)	C	59
100	FORMAT (5X, *HOT SURFACE = *, F5.0, * K, COLD SURFACE = *, F5.0, * K, G	C	60
	IRAC = *, F5.0, * DEG/CM**//)	C	61
110	FORMAT (5X, *DIFFUSION COEFF = *, 1PE12.5, *EXP(-*, 1PE12.5, */RT) HEA	C	62
	IT OF THERMAL DIFFUSION = *, 1PE12.5**//)	C	63
120	FORMAT (5X, *INITIAL CONC = *, 1PE12.5, * TIME AT TEMP = *, 1PF5.0, *H	C	64
	1R**//)	C	65
130	FORMAT (20X, *CHARACTERISTIC QUANTITIES IN THE CALCULATIONS**//)	C	66
140	FORMAT (5X, *ORDER OF THE BESSEL FUNCTIONS = *, 1PE12.5, * POWER OF	C	67
	1 ARGUMENT IN R SPACE = *, 1PE12.5**//)	C	68
150	FORMAT (5X, *EXPONENT OF THE INITIAL DISTR IN R SPACE = *, 1PE12.5, *	C	69
	1 TIME CONSTANT = *, 1PE12.5**//)	C	70
160	FORMAT (5X, *AD = *, 1PE12.5, * RHO = *, 1PE12.5**//)	C	71
170	FORMAT (5X, *TH/TC = *, 1PE12.5**//)	C	72
180	FORMAT (20X, *FIRST 5 ROOTS OF THE CHARACTERISTIC EQUATION**//5X, *X(	C	73
	11) = *, 1PE12.5, * X(2) = *, 1PE12.5, * X(3) = *, 1PE12.5, * X(4) = *, 1P	C	74
	2E12.5, * X(5) = *, 1PE12.5**//)	C	75
	END	C	76
C			
C			
	SUBROUTINE AC3 (JT, T1, T2, R, AD)	D	1
	IF (QT) 10, 20, 30	D	2
10	W1=-QT/(R*T1)	D	3
	W2=-QT/(R*T2)	D	4
	XX=W1	D	5
	CALL E1 (XX, ANS)	D	6
	G1=ANS	D	7
	XX=W2	D	8
	CALL E1 (XX, ANS)	D	9
	G2=ANS	D	10
	AD=(T1-T2)/((T2*EXP(-W2)*(W2*EXP(W2)*G2-1.)-T1*EXP(-W1)*(W1*EXP(W1)	D	11
	1*G1-1.))	D	12
	GO TO 40	D	13
20	AD=1.	D	14
	GO TO 40	D	15
30	W1=QT/(R*T1)	D	16
	W2=QT/(R*T2)	D	17
	XX=W1	D	18
	CALL E1 (XX, ANS)	U	19
	G1=ANS	D	20
	XX=W2	D	21
	CALL E1 (XX, ANS)	D	22
	G2=ANS	D	23
	AD=(T1-T2)/((T2*EXP(W2)*(W2*EXP(-W2)*G2-1.)-T1*EXP(W1)*(W1*EXP(-W1)	D	24
	1*G1-1.))	D	25
40	RETURN	D	26
	END	D	27
C			
C			
	SUBROUTINE E1 (XX, ANS)	E	1
	C=XX+1.	E	2
	T=1./Q	E	3
	S=T	E	4
	DO 10 J=2, 500	E	5
	A=-(FLOAT(J)-1.)*(FLJAT(J)-1.)	E	6
	B=XX+1.+2.*(FLJAT(J)-1.)	E	7
	T=-T/(1.+Q*(B/A))	E	8
	C=B+A/Q	E	9
	S=S+T	E	10
	IF (ABS(T/S)-1.E-10) 20, 10, 10	E	11
10	CONTINUE	E	12
20	ANS=EXP(-XX)*S	E	13
	RETURN	E	14
	END	E	15
C			

C	SUBROUTINE EI (XX,ANS)	F	1
	T=XX	F	2
	S=T	F	3
	CO 10 J=2,500	F	4
	T=T*XX*(1.-1./FLJAT(J))/FLDAT(J)	F	5
	S=S+T	F	6
	IF (ABS(T/S)-1.E-10) 20,10,10	F	7
10	CONTINUE	F	8
20	ANS=ALOG(XX)+.577215664902+S	F	9
	RETURN	F	10
	END	F	11
C			
C	SUBROUTINE ROOT (OR,RO,TC,XR,NR)	G	1
	DIMENSION XR(500)	G	2
	COMMON /A3/ U,CP,CN,PI	G	3
	OZ=OR	G	4
	OZ=ABS(OZ)	G	5
	OZZ=OZ+.1	G	6
	CO 140 I=1,300	G	7
	IF (I-1) 10,10,20	G	8
10	XX=PI/(RO-1.)-.5	G	9
	GO TO 50	G	10
20	IF (ZT-20.) 40,40,30	G	11
30	XX=PI*(I/(RO-1.))*(1.+(4.*OZ*OZZ-1.)/(8.*RO*(PI*I/(RO-1.))**2))	G	12
	GO TO 130	G	13
40	XX=ZT+.1	G	14
50	CALL FJNC (OZ,RO,XX,FT)	G	15
	IF (FT) 60,70,70	G	16
60	NA=-1	G	17
	GO TO 80	G	18
70	NA=+1	G	19
80	CO 120 KK=1,1000	G	20
	XX=XX+.1	G	21
	CALL FJNC (OZ,RO,XX,FT)	G	22
	IF (FT) 90,100,100	G	23
90	NB=-1	G	24
	GO TO 110	G	25
100	NB=+1	G	26
110	IF (NA+NB) 120,130,120	G	27
120	CONTINUE	G	28
130	CALL INTRA (OZ,OZZ,RO,XX,ZT)	G	29
	XR(I)=ZT	G	30
	IF (EXP(-TC*XR(I)**2)-1.E-08) 150,140,140	G	31
140	CONTINUE	G	32
150	NR=1	G	33
	RETURN	G	34
	END	G	35
C			
C	SUBROUTINE FUNC (OZ,RO,Z1,FT)	H	1
	Z2=RO*Z1	H	2
	IF (Z1-20.) 10,30,30	H	3
10	CALL BESSM (OZ,Z1,AJ,AY)	H	4
	X11J=AJ	H	5
	X11Y=AY	H	6
	IF (Z2-20.) 20,40,40	H	7
20	CALL BESSM (OZ,Z2,AJ,AY)	H	8
	X12J=AJ	H	9
	X12Y=AY	H	10
	GO TO 50	H	11
30	CALL BESLG (OZ,Z1,AJ,AY)	H	12
	X11J=AJ	H	13
	X11Y=AY	H	14
40	CALL BESLG (OZ,Z2,AJ,AY)	H	15
	X12J=AJ	H	16
	X12Y=AY	H	17
50	FT=X11Y*X12J-X11J*X12Y	H	18
	RETURN	H	19
	END	H	20
C			

C	SUBROUTINE INTRA (OZ,OZZ,RO,Z1,ZT)	I	1
	A=1.	I	2
	ZZ=RO*Z1	I	3
	DO 70 K=1,20	I	4
	IF (Z1-20.) 10,30,30	I	5
10	CALL BESSM (OZ,Z1,AJ,AY)	I	6
	X11J=AJ	I	7
	X11Y=AY	I	8
	CALL BESSM (OZZ,Z1,AJ,AY)	I	9
	X21J=AJ	I	10
	X21Y=AY	I	11
	IF (ZZ-20.) 20,40,40	I	12
20	CALL BESSM (OZ,Z2,AJ,AY)	I	13
	X12J=AJ	I	14
	X12Y=AY	I	15
	CALL BESSM (OZZ,Z2,AJ,AY)	I	16
	X22J=AJ	I	17
	X22Y=AY	I	18
	GO TO 50	I	19
30	CALL BESLG (OZ,Z1,AJ,AY)	I	20
	X11J=AJ	I	21
	X11Y=AY	I	22
	CALL BESLG (OZZ,Z1,AJ,AY)	I	23
	X21J=AJ	I	24
	X21Y=AY	I	25
40	CALL BESLG (OZ,Z2,AJ,AY)	I	26
	X12J=AJ	I	27
	X12Y=AY	I	28
	CALL BESLG (OZZ,Z2,AJ,AY)	I	29
	X22J=AJ	I	30
	X22Y=AY	I	31
50	FL=X11Y*X12J-X11J*X12Y	I	32
	IF (ABS(FL)-1.E-11) 80,80,60	I	33
60	GL=X12Y*X21J-X12J*X21Y	I	34
	HL=X22Y*X11J-X22J*X11Y	I	35
	ZT=Z1-FL/(2.*JZ*FL/Z1+GL+RO*HL)	I	36
	Z1=ZT	I	37
	ZZ=RO*Z1	I	38
70	CONTINUE	I	39
80	RETURN	I	40
	END	I	41
C			
C	SUBROUTINE COEFF (JRD,JR,RO,S,X,YYYY,TC,X1J,X1Y,CFF)	J	1
	COMMON /A3/ O,CP,CN,PI	J	2
	OYY=ORD	J	3
	OY=OR	J	4
	TEST=25.	J	5
	X=RO*X	J	6
	IF (X-20.) 10,10,30	J	7
10	CALL BESSM (OY,X,AJ,AY)	J	8
	X2J=AJ	J	9
	X2Y=AY	J	10
	X=X/RO	J	11
20	CALL BESSM (OY,X,AJ,AY)	J	12
	X1J=AJ	J	13
	X1Y=AY	J	14
	GO TO 50	J	15
30	CALL BESLG (OY,X,AJ,AY)	J	16
	X2J=AJ	J	17
	X2Y=AY	J	18
	X=X/RO	J	19
	IF (X-20.) 20,20,40	J	20
40	CALL BESLG (OY,X,AJ,AY)	J	21
	X1J=AJ	J	22
	X1Y=AY	J	23
50	X=X*RU	J	24
	Y=X/RO	J	25
	IF (X-TEST) 60,60,70	J	26

60	CALL SUMS (OYY,B,RO,X,Y,YYYY,D1,D2)	J	27
	Z1=EXP(B*ALOG(YYYY*RC))	J	28
	Z2=EXP(B*ALOG(YYYY))	J	29
	C11=(OYY-B)*(X1Y-X1J*CJT(JYY*PI))	J	30
	C12=(OYY-B)*X1J/SIN(JYY*PI)	J	31
	TAB=Z1*2.*X1J/(PI*X*X2J)-Z2*2./(PI*Y)+C11*D1+C12*D2	J	32
	CFF=(OYY+B)*TAB*(X2J**2/(X1J**2-X2J**2))*PI**2*EXP(-Y**2*TC)*.5	J	33
	GO TO 80	J	34
70	CALL SUML (OYY,B,X,SP)	J	35
	TB=EXP(B*ALOG(YYYY*RC))*SP*2.*X1J/(PI*X*X2J)	J	36
	X=X/RO	J	37
	CALL SUML (OYY,B,X,SP)	J	38
	TA=EXP(B*ALOG(YYYY))*SP*2./(PI*X)	J	39
	CFF=(OYY+B)*(TB-TA)*(X2J**2/(X1J**2-X2J**2))*PI**2*EXP(-X**2*TC)*.	J	40
	15	J	41
80	RETURN	J	42
	END	J	43
C			
C			
	SUBROUTINE SUMS (JSS,B,RO,P,Q,YYYY,DIF1,DIF2)	K	1
	DIMENSION X(2), DSP(2), DSN(2), SP(2), SN(2)	K	2
	DOUBLE PRECISION Z,T,C,DB,S,DSP,DSN,SP,SN,Z1,Z2	K	3
	COMMON /A3/ O,CP,CN,PI	K	4
10	FORMAT (* INTEGER VALUE FOR THE ORDER, TERMINATE *)	K	5
	X(1)=P	K	6
	X(2)=Q	K	7
	OYY=OSS	K	8
	ORCI=OYY	K	9
	IF (OYY) 20,30,30	K	10
20	OYY=-OYY	K	11
30	IF (O-OYY) 40,50,40	K	12
40	O=OYY	K	13
	CALL RGAM	K	14
50	DO 140 I=1,2	K	15
	Z=(X(I)/2.)*2	K	16
	T=-Z/(-O+1.)	K	17
	C=1./(-O+B+2.)	K	18
	DB=T*C	K	19
	S=1./(-O+B)+DB	K	20
	DO 60 J=2,500	K	21
	T=-T*Z/((-O+FLJAT(J))*FLOAT(J))	K	22
	C=C*(-O+B+2.*(FLJAT(J)-1.))/(-O+B+2.*FLOAT(J))	K	23
	DB=T*C	K	24
	S=S+DB	K	25
	IF (ABS(DB/S)-1.D-25) 70,60,60	K	26
60	CONTINUE	K	27
70	DSP(I)=S*EXP(J*ALOG(X(I)/2.))*CP	K	28
	IF (CN) 90,80,90	K	29
80	PRINT 10	K	30
	GO TO 150	K	31
90	T=-Z/(-O+1.)	K	32
	C=1./(-O+B+2.)	K	33
	DB=T*C	K	34
	S=1./(-O+B)+DB	K	35
	DO 100 J=2,500	K	36
	T=-T*Z/((-O+FLJAT(J))*FLOAT(J))	K	37
	C=C*(-O+B+2.*(FLJAT(J)-1.))/(-O+B+2.*FLOAT(J))	K	38
	DB=T*C	K	39
	S=S+DB	K	40
	IF (ABS(DB/S)-1.D-25) 110,100,100	K	41
100	CONTINUE	K	42
110	DSN(I)=S*EXP(-J*ALOG(X(I)/2.))*CN	K	43
	IF (ORDI) 120,130,130	K	44
120	SP(I)=DSN(I)	K	45
	SN(I)=DSP(I)	K	46
	GO TO 140	K	47
130	SP(I)=DSP(I)	K	48
	SN(I)=DSN(I)	K	49

140	CONTINUE	K	50
	Z1=EXP(B*ALOG(YYYY*RC))	K	51
	Z2=EXP(B*ALOG(YYYY))	K	52
	CIF1=Z1*SP(1)-Z2*SP(2)	K	53
	DIF2=Z1*SN(1)-Z2*SN(2)	K	54
150	RETURN	K	55
	ENC	K	56
C			
C			
	SUBROUTINE SUML (JYY,B,X,SP)	L	1
	OR=OYY	L	2
	Z=1./X**2	L	3
	T=(OR-B+?.)*(JR+B-4.)*Z	L	4
	S=1.+T	L	5
	DO 20 J=2,100	L	6
	V=T*Z*(OR-(B-2.*FLOAT(J)))*(OR+3-2.*(FLOAT(J)+1.))	L	7
	IF (ABS(V/T)-1.) 10,3C,3C	L	8
10	T=V	L	9
	S=S+T	L	10
	IF (ABS(T/S)-1.E-10) 30,20,20	L	11
20	CONTINUE	L	12
30	SP=1.+(OR-B)*(JR+B-2.)*S*Z	L	13
	RETURN	L	14
	ENC	L	15
C			
C			
	SUBROUTINE SRGAM (Z,ANS)	M	1
	DIMENSION C(26)	M	2
	DATA C/1.,.5772156649015329,-.6558780715202538,-.0420026350343952,M		3
1	.1665386113822915,-.0421977345555443,-.0096219715278770,M		4
2	.0072189432466630,-.0011651675918591,-.0002152416741149,M		5
3	.0001280502823882,-.0000201348547507,-.0000012504934821,M		6
4	.0000011330272320,-.0000002056338417,.0000000061160950,M		7
5	5.0020075 E-09,-1.1812746 E-09,1.043427 E-10,M		8
6	7.7823 E-12,-3.6968 E-12,5.100 E-13,M		9
7	-2.06 E-14,-5.4 E-15,1.4 E-15,M		10
8	1.0 E-16/	M	11
	T=Z	M	12
	S=T	M	13
	DO 10 I=2,26	M	14
	T=T*Z*C(I)/C(I-1)	M	15
10	S=S+T	M	16
	ANS=S	M	17
	RETURN	M	18
	ENC	M	19
C			
C			
	SUBROUTINE RGAM	N	1
	COMMON /A3/ O,CP,CN,PI	N	2
	ZP=O+1.	N	3
	IF (ZP-1.) 60,60,10	N	4
10	T=O	N	5
	DO 40 J=1,20	N	6
	ZP=O-FLOAT(J)	N	7
	IF (ZP) 20,70,30	N	8
20	ZP=ZP+1.	N	9
	GO TO 50	N	10
30	T=T*ZP	N	11
40	CONTINUE	N	12
50	Z=ZP	N	13
	CALL SRGAM (Z,ANS)	N	14
	CP=ANS/T	N	15
	GO TO 80	N	16
60	CP=1.	N	17
	GO TO 80	N	18
70	CP=1./T	N	19
80	ZN=O+1.	N	20
	IF (ZN) 110,160,90	N	21
90	IF (ZN-1.) 100,160,160	N	22
100	T=1.	N	23
	GO TO 150	N	24

110	T=1./ZN	N	25
	DO 140 J=2, 20	N	26
	ZN=-O+FLOAT(J)	N	27
	IF (ZN) 130,160,120	N	28
120	ZN=ZN-1.	N	29
	T=T*ZN	N	30
	GO TO 150	N	31
130	T=T/ZN	N	32
140	CONTINUE	N	33
150	Z=ZN	N	34
	CALL SRGAM (Z,ANS)	N	35
	CN=ANS/T	N	36
	GO TO 170	N	37
160	CN=0.0	N	38
170	RETURN	N	39
	END	N	40
C			
C			
	SUBROUTINE BESLG (JW,X,AJ,AY)	O	1
	COMMON /A3/ O,CP,CN,PI	O	2
	P=4.*O+O*O	O	3
	Z=1./(8.*X)**2	O	4
	T=-(P-1.)*(P-9.)*Z/2.	O	5
	S=1.+T	O	6
	IF (T) 10,40,10	O	7
10	DO 30 J=2,500	O	8
	V=-T*(P-(4.*FLOAT(J)-3.))**2)*(P-(4.*FLOAT(J)-1.))**2)*Z/(2.*FLOAT(J	O	9
	1)*(2.*FLOAT(J)-1.))	O	10
	IF (ABS(V/T)-1.) 20,40,40	O	11
20	T=V	O	12
	S=S+T	O	13
	IF (ABS(T/S)-1.E-14) 40,30,30	O	14
30	CONTINUE	O	15
40	A=S	O	16
	IF (P-1.) 60,50,60	O	17
50	S=0.0	O	18
	GO TO 100	O	19
60	T=-(P-1.)*(P-9.)*(P-25.)*Z/(48.*X)	O	20
	S=(P-1.)/(8.*X)+T	O	21
	IF (T) 70,100,70	O	22
70	DO 90 J=2,500	O	23
	V=-T*(P-(4.*FLOAT(J)-1.))**2)*(P-(4.*FLOAT(J)+1.))**2)*Z/(2.*FLOAT(J	O	24
	1)*(2.*FLOAT(J)+1.))	O	25
	IF (ABS(V/T)-1.) 80,100,100	O	26
80	T=V	O	27
	S=S+T	O	28
	IF (ABS(T/S)-1.E-14) 100,90,90	O	29
90	CONTINUE	O	30
100	Q=S	O	31
	CHI=X-(2.*O+1.)*PI/4.	O	32
	AJ=(2./(PI*X))**.5*(A*COS(CHI)-2*SIN(CHI))	O	33
	AY=(2./(PI*X))**.5*(A*SIN(CHI)+2*COS(CHI))	O	34
	RETURN	O	35
	END	O	36
C			
C			
	SUBROUTINE BESSM (OS,X,AJ,AY)	P	1
	COMMON /A3/ O,CP,CN,PI	P	2
	DOUBLE PRECISION S,T,Z,DAJ,DAJN	P	3
	OU=OS	P	4
	ORI=OU	P	5
	IF (OU) 10,20,20	P	6
10	OU=-OU	P	7
20	IF (O-OU) 30,40,30	P	8
30	O=OU	P	9
	CALL RGAM	P	10

40	Z=(X/2.):**2	P	11
	T=-Z/(OU+1.)	P	12
	S=1.+T	P	13
	DO 50 K=2,500	P	14
	T=-T*2/(FLJAT(<)*(JU+FLJAT(K)))	P	15
	S=S+T	P	16
	IF (ABS(T/S)-1.D-25) 60,50,50	P	17
50	CONTINUE	P	18
60	CAJ=CP*S*EXP(JU*ALOG(X/2.))	P	19
	IF (CN) 70,90,70	P	20
70	T=-Z/(-OU+1.)	P	21
	S=1.+T	P	22
	DO 80 K=2,500	P	23
	T=-T*2/(FLJAT(<)*(-JU+FLJAT(K)))	P	24
	S=S+T	P	25
	IF (ABS(T/S)-1.D-25) 100,80,80	P	26
80	CONTINUE	P	27
90	PRINT 140	P	28
	GO TO 130	P	29
100	CAJN=CN*S*EXP(-JU*ALOG(X/2.))	P	30
	IF (ORI) 110,120,120	P	31
110	AJ=CAJN	P	32
	AY=(DAJ-COS(OU*PI)*DAJN)/SIN(OU*PI)	P	33
	GO TO 130	P	34
120	AJ=CAJ	P	35
	AY=(DAJ-COS(OU*PI)-DAJN)/SIN(OU*PI)	P	36
130	RETURN	P	37
140	FORMAT (* INTEGER VALUE FOR THE ORDER, TERMINATE*)	P	38
	END	P	39
C			
C			
	SUBROUTINE FINC	Q	1
	DIMENSION T(105), T1(105), T2(105), T3(105), CN(105), C1(105), C2(	Q	2
	1105), CN1(105), D(105), CINC(105)	Q	3
	COMMON /A2/ TH,TA,DS,QD,QT,T1,GRAD,C1	Q	4
	COMMON /A4/ CINC,CV1,T	Q	5
	TC=TA	Q	6
	CX=.01*(TH-TC)/GRAD	Q	7
	AM=10./DX**2	Q	8
	DT=.01*(TH-TC)	Q	9
	DO 10 I=2,101	Q	10
	T1(I)=DT/T1(I)	Q	11
	T2(I)=DT/(1.9872*T1(I)**2)	Q	12
	T3(I)=QT*T2(I)	Q	13
	CN(I)=C1	Q	14
	C(I)=DO*EXP(-QD/(1.9872*T1(I)))	Q	15
10	CONTINUE	Q	16
	CN(1)=CN(3)-2.*T3(2)*CV(2)	Q	17
	CN(102)=CN(100)+2.*T3(101)*CN(101)	Q	18
	DO 20 I=2,101	Q	19
	J=I-1	Q	20
	K=I+1	Q	21
	C1(I)=.5*(CN(K)-CN(J))	Q	22
	C2(I)=CN(K)-2.*CN(I)+CN(J)	Q	23
20	CONTINUE	Q	24
	ITF=IFIX(T1*360.)	Q	25
	DO 60 KK=1,ITF	Q	26
	GO 30 I=2,101	Q	27
	CN1(I)=CN(I)+AM*D(I)*(C2(I)-T3(I)*(C1(I)+2.*T1(I)*CN(I))-CD*T2(I)*	Q	28
	1*(C1(I)-T2(I)*CN(I)))	Q	29
30	CONTINUE	Q	30
	DO 40 I=2,101	Q	31
	CN(I)=CN1(I)	Q	32
40	CONTINUE	Q	33
	CN(1)=CN(3)-2.*T3(2)*CV(2)	Q	34
	CN(102)=CN(100)+2.*T3(101)*CN(101)	Q	35
	GO 50 I=2,101	Q	36
	J=I-1	Q	37
	K=I+1	Q	38
	C1(I)=.5*(CN(K)-CN(J))	Q	39
	C2(I)=CN(K)-2.*CN(I)+CN(J)	Q	40

50	CONTINUE	Q	41
60	CONTINUE	Q	42
	RETURN	Q	43
	ENC	Q	44
C			
	SUBROUTINE COMPR	R	1
	DIMENSION ALAB(12), CONC(105), CN1(105), T(105), PER(105)	R	2
	COMMON /A1/ ALAB	R	3
	COMMON /A4/ CONC,CN1,T	R	4
	DO 10 I=2,101	R	5
	PER(I)=(CONC(I)/CN1(I)-1.)*100.	R	6
10	CONTINUE	R	7
	PRINT 30	R	9
	PRINT 40, (ALAB(I),I=1,12)	R	9
	PRINT 50	R	10
	DO 20 J=2,51	R	11
	PRINT 60, T(J),CONC(J),CN1(J),PER(J),T(J+50),CONC(J+50),CN1(J+50),	R	12
	1PER(J+50)	R	13
20	CONTINUE	R	14
	PRINT 30	R	15
	RETURN	K	16
30	FORMAT (1H1)	R	17
40	FORMAT (12A6)	R	18
50	FORMAT (//2(4X,*T,K*,6X,*CONC*,6X,*CN1*,4X,*PERCENT *)/2(1: X,*1A	R	19
	1A1)*,3X,*1VUMR)*,5X,*DIFF */)	R	20
60	FORMAT (8(1PE10.2))	R	21
	ENC	R	22

Subroutine SORS

Used for data input. The data input format is

- Identification card,
Columns 1 through 72 contain statements pertaining to the problem.
- Data input cards. TH-(Temperature at hot surface, K), TA-(Temperature at cold surface, K), DO-(Pre-exponential factor, cm^2/sec), QD-(Absolute magnitude of the heat of thermal diffusion, kcal/mole), QT-(Heat of transport, kcal/mole), [TI- Time of diffusion process, (h)], GRAD-(Absolute magnitude of linear temperature gradient; K/cm), and CI-(Initial constant concentration distribution, g/cm^3 , etc.).

Subroutine AFUNC

Used for the computation of the analytical solution. During this step, the following parameters are output.

- Identification of problem.
- Temperature at the hot surface and cold surface and the temperature gradient. These values correspond to Eq. (16).
- RATIO of the hot surface temperature to the cold surface temperature, TH/TC. This parameter is correlated with the expected error due to the expansion given by Eq. (25).

• Diffusion parameters DO, QD, and QT as defined by Eqs. (13) and (14).

• Initial constant concentration and time of diffusion run in hours.

• Characteristic parameters of the analytic solution.

- a. Order of Bessel Function [ν in Eq. (36)].
- b. Power of argument in R Space [α in Eq. (36)].
- c. Exponent of the initial distribution in R Space [equivalent to $\nu - 2(1 + x)$ in Eq. (53)].
- d. Time constant [equivalent to $\frac{Z_m^2}{mt}$ in Eq. (58)].
- e. A_0 [A_0 given by Eq. (47)].
- f. RHO [ρ in Eqs. (39) and (40)].
- g. First five roots of characteristic equations [roots of Eq. (39)].

Subroutine FINC

Used for computing the numerical solution of the problem. See Appendix D.

Subroutine COMPR

Compares the concentration at equivalent intervals for the analytical and numerical solution and gives the percentage differences in the solutions.

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