UCRL-17607
cy. 2

University of California

Ernest O. Lawrence Radiation Laboratory

TRANSIENT DIFFUSION IN A COMPOSITE SLAB

Paul Concus and D. R. Olander

June 2, 1967

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 5545

RECEIVED
LAWRENCE
RADIATION LABORATORY
AUG 18 1967
LIBRARY AND
DOCUMENTS SECTION

Berkeley, California

UCRL-17607
Cy. 2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Submitted to International Journal of
Heat and Mass Transfer

UCRL-17607
Preprint

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

TRANSIENT DIFFUSION IN A COMPOSITE SLAB

Paul Concus and D. R. Olander

June 2, 1967

TRANSIENT DIFFUSION IN A COMPOSITE SLAB*

Paul Concus

Lawrence Radiation Laboratory
University of California
Berkeley, California

and

D. R. Olander

Inorganic Materials Research Division,
Lawrence Radiation Laboratory,
and
Department of Nuclear Engineering,
University of California
Berkeley, California

Abstract

The transient response of two slabs of finite thickness in contact at a plane interface and initially containing nonequilibrium amounts of a transferrable solute (or, the response of the analogous heat conduction problem) is found in terms of an eigenfunction series. The approach to equilibrium is depicted graphically for a few values of the parameters, and, with the aid of tables that have been prepared, the solution may be calculated for a larger range of values covering the region of practical interest.

Formulation

The transient response of two slabs of finite thickness in contact at a plane interface and initially containing nonequilibrium amounts of a transferrable solute is of some practical importance. Such a situation may occur in the analysis of porous media in oil fields and in the approach to equilibrium of a solute distributing between two immiscible liquid layers.

For the problem considered here, movement of the solute occurs by molecular diffusion in the two regions, which, in general, have different diffusion coefficients. The slabs are of finite thickness in the direction perpendicular to the interface but are of infinite extent laterally. No transfer occurs across the outer boundaries of the slabs. The concentrations on the two sides of the interface are related by a constant of proportionality m. The fluxes at the interface are the same in both slabs. The quantity of interest is the ratio of the average concentrations in the two media as a function of time. This ratio approaches m as time approaches infinity.

The diffusion equations for the two media are

$$\frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2}, \quad \text{for } -a < x < 0, \quad t > 0,$$

and

$$\frac{\partial c_2}{\partial t} = D_2 \frac{\partial^2 c_2}{\partial x^2}, \quad \text{for } 0 < x < b. \quad t > 0.$$

The outer boundary conditions are

$$\frac{\partial c_1}{\partial x}(t, -a) = \frac{\partial c_2}{\partial x}(t, b) = 0,$$

and the interface conditions are

$$mc_1(t,0^-) = c_2(t,0^+)$$

and

$$D_1 \frac{\partial c_1}{\partial x}(t,0^-) = D_2 \frac{\partial c_2}{\partial x}(t,0^+) .$$

The solution is given here for the general initial condition specifying $c_1(0,x)$ and $c_2(0,x)$, but attention is focused explicitly on the case of special interest,

$$c_1(0,x) = c_{10}, \quad \text{for} \quad -a \leq x < 0,$$
$$c_2(0,x) = 0 \quad , \quad \text{for} \quad 0 \leq x \leq b . \tag{1}$$

A material balance on the solute in the two regions yields

$$\bar{c}_1(t) = c_{10} - \frac{b}{a}\bar{c}_2(t) ,$$

where $\bar{c}_1(t)$ and $\bar{c}_2(t)$ are the average concentrations in regions 1 and 2, respectively, and c_{10} is defined by

$$c_{10} = \frac{1}{a}\left[\int_{-a}^{0} c_1(0,x)\,dx + \int_0^b c_2(0,x)\,dx\right] .$$

The approach to equilibrium is measured by the ratio

$$f(t) = \frac{\bar{c}_2/\bar{c}_1}{m} = \frac{\bar{c}_2/m}{c_{10} - \frac{b}{a}\bar{c}_2}$$

The differential equations and the associated boundary conditions can be written in dimensionless form by letting

$$\tau = \frac{D_1 t}{a^2} ,$$

$$\eta = \begin{cases} x/a , & -1 \leq \eta < 0 \\ \frac{x}{b}\alpha , & 0 \leq \eta \leq \alpha , \end{cases}$$

$$C = \begin{cases} c_1/c_{10}, & -1 \leq \eta < 0 \\ c_2/mc_{10}, & 0 \leq \eta \leq \alpha , \end{cases}$$

(continued)

$$\alpha = \frac{b}{a} \sqrt{\frac{D_1}{D_2}} \tag{2}$$

and

$$M = \frac{b}{a} m . \tag{3}$$

The resulting equations are

$$\frac{\partial C}{\partial \tau} = \frac{\partial^2 C}{\partial \eta^2} , \quad \text{for} \quad \begin{matrix} -1 < \eta < 0 \\ 0 < \eta < \alpha \end{matrix} , \quad \tau > 0 ,$$

$$\frac{\partial C}{\partial \eta} (\tau, -1) = \frac{\partial C}{\partial \eta} (\tau, \alpha) = 0 ,$$

$$C(\tau, 0^-) = C(\tau, 0^+) ,$$

and

$$\frac{\partial C}{\partial \eta} (\tau, 0^-) = \frac{M}{\alpha} \frac{\partial C}{\partial \eta} (\tau, 0^+) .$$

The initial condition, Eq. 1, becomes

$$C(0, \eta) = \begin{cases} 1, & -1 \leq \eta < 0 \\ 0, & 0 \leq \eta \leq \alpha \end{cases} , \tag{4}$$

and the quantity f is

$$f(\tau) = \frac{\overline{C}_2}{1 - M\overline{C}_2} , \tag{5}$$

where

$$\overline{C}_2(\tau) = \frac{1}{\alpha} \int_0^\alpha C(\tau, \eta) d\eta . \tag{6}$$

The manner in which $f(\tau)$ approaches unity as τ approaches ∞ depends upon the parameters α and M. A useful series solution can be obtained directly either by the associated eigenfunction technique or by the Laplace transform method. With the former, general initial conditions can be accommodated more easily, and this scheme is outlined below.

The solution can be applied to the analogous heat conduction situation by replacing D_1/D_2 in Eq. 2 by the ratio of the thermal diffusivities and m in Eq. 3 by the inverse ratio of the volumetric heat capacities. In this case, f is the ratio of the average temperatures in the two regions.

Associated Eigenfunction Technique

Following Lanczos [1], one considers the associated eigenvalue problem for $C_k(\eta)$,

$$\frac{d^2 C_k}{d\eta^2} + \lambda_k^2 C_k = 0 \qquad \text{for } -1 < \eta < 0,\ 0 < \eta < \alpha,$$

with

$$C_k(0^-) = C_k(0^+)\ , \qquad \frac{dC_k}{d\eta}(0^-) = \frac{M}{\alpha}\frac{dC_k}{d\eta}(0^+)\ ,$$

and

$$\frac{dC_k}{d\eta}(-1) = \frac{dC_k}{d\eta}(\alpha) = 0\ .$$

Its solution is

$$C_k(\eta) = A_k \begin{cases} -\sin\lambda_k \sin\lambda_k\eta + \cos\lambda_k \cos\lambda_k\eta, & -1 \leq \eta < 0 \\ -\frac{\alpha}{M}\sin\lambda_k \sin\lambda_k\eta + \cos\lambda_k \cos\lambda_k\eta, & 0 \leq \eta \leq \alpha \end{cases}$$

with the eigenvalues given by

$$\tan\lambda_k = -\frac{M}{\alpha}\tan\alpha\lambda_k\ , \quad \text{for} \quad k = 0, 1, 2, \cdots\ . \tag{7}$$

Only the nonnegative eigenvalues need be considered; let them be ordered so that $\lambda_0 = 0 < \lambda_1 < \lambda_2 < \cdots$.

The eigenfunctions $\left\{C_k(\eta)\right\}$ do not form an orthogonal set over $(-1, \alpha)$ for this problem, but they are biorthogonal with the (discontinuous) functions

$$G_k(x) = \begin{cases} C_k(\eta) & \text{for } -1 \leq \eta < 0 , \\ \frac{M}{\alpha} C_k(\eta) & \text{for } 0 \leq \eta \leq \alpha ; \end{cases}$$

that is,

$$\int_{-1}^{\alpha} C_k(\eta)\, G_j(\eta)\, d\eta \begin{cases} = 0 & \text{if } k \neq j \\ \neq 0 & \text{if } k = j . \end{cases}$$

$$\text{If } A_k = \begin{cases} 1/(1+M)^{1/2} , & \text{for } k = 0 \\ \left[2/\left(1 + \frac{\alpha^2}{M} \sin^2 \lambda_k + M \cos^2 \lambda_k\right)\right]^{1/2} , & \text{for } k = 1, 2, 3, \cdots , \end{cases}$$

then the eigenfunctions are normalized so that

$$\int_{-1}^{\alpha} C_k(\eta)\, G_k(\eta)\, d\eta = 1 .$$

For the general initial condition $C(0, \eta) = g(\eta)$, the solution to the problem in terms of the normalized eigenfunctions is

$$C(\tau, \eta) = \sum_{k=0}^{\infty} B_k\, C_k(\eta) \exp(-\lambda_k^2 \tau) ,$$

where the B_k are the Fourier coefficients of $g(\eta) = \sum_{k=0}^{\infty} B_k C_k(\eta)$,

$$B_k = \int_{-1}^{\alpha} g(\eta)\, G_k(\eta) d\eta .$$

For the specific initial condition, Eq. 4, these are

$$B_k = \begin{cases} A_0 , & \text{for } k = 0 , \\ \frac{A_k}{\lambda_k} \sin \lambda_k , & \text{for } k = 1, 2, 3, \cdots . \end{cases}$$

The quantity $\overline{C}_2(\tau)$ in Eq. 6 is given by

$$\overline{C}_2(\tau) = \sum_{k=0}^{\infty} B_k \exp(-\lambda_k^2 \tau) \int_0^{\alpha} \frac{C_k(\eta)}{\alpha} d\eta$$

$$= \frac{1}{1+M} - \sum_{k=1}^{\infty} \frac{A_k B_k}{M \lambda_k} \sin \lambda_k \exp(-\lambda_k^2 \tau) ;$$

for the initial condition, Eq. 4, this becomes

$$\overline{C}_2(\tau) = \frac{1}{1+M} - \sum_{k=1}^{\infty} \frac{2 \quad \exp(-\lambda_k^2 \tau)}{M \lambda_k^2 \left(\csc^2 \lambda_k + \frac{\alpha^2}{M} \csc^2 \alpha \lambda_k\right)} . \tag{8}$$

The limiting form of the series solution as $\alpha \to \infty$ agrees with the solution given by Lovering for $\eta = 0$ [2] .

Discussion

Even for moderate values of $\lambda_1^2 \tau$ the series Eq. 8 converges extremely rapidly, and only the first term or two need be calculated. The required eigenvalues can be found numerically by solving Eq. 7 by an iterative technique, such as Newton's method, taking care to use the appropriate branches of $\tan \lambda$. Tables have been prepared giving the first ten positive solutions of Eq. 7 to four places for several values of α and M in the range $0.001 \leq \alpha \leq 1.0$ and $0.001 \leq M \leq 1000$ [3]. These tables can also be used to directly obtain the roots for $1.0 \leq \alpha \leq 1000$.

Figures 1 and 2 depict $f(\tau)$, Eq. 5, using $\overline{C}_2(\tau)$ as calculated from Eq. 8, with the series truncated at $k = 40$. This number of terms is required to give plotting accuracy for extremely small values of $f(\tau)$ and $\lambda_1^2 \tau$. Away from the neighborhood of the origin, however, far fewer terms are required. Figure 1 shows the variation of $f(\tau)$ with

M when $\alpha = 1$. If $\alpha = 1$, Eq. 8 becomes simply

$$\overline{C}_2(\tau) = \frac{1}{1+M}\left(1 - \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{8}{k^2\pi^2} \exp\left(-\frac{k^2\pi^2}{4}\tau\right)\right) , \quad (9)$$

so that

$$f(\tau) = \frac{2f_1(\tau)}{1+f_1(\tau) + M[1-f_1(\tau)]} ,$$

where $f_1(\tau)$ denotes $f(\tau)$ when $\alpha = M = 1$. Thus, if $\alpha = 1$, one can obtain $f(\tau)$ directly from $f_1(\tau)$ for values of M not explicitly shown in Fig. 1. Equation 9 agrees with the solution given by Carslaw and Jaeger for $\alpha = M = 1$ [4].

Figure 2 shows the variation of $f(\tau)$ with α when $M = 1$. If $M = 1$ then $\overline{C}_2(\tau)$ for $\alpha = \alpha_0$ and $\overline{C}_2(\tau)$ for $\alpha = 1/\alpha_0$ are related by

$$\overline{C}_2(\tau; \frac{1}{\alpha_0}) = \overline{C}_2(\alpha_0^2\tau; \alpha_0)$$

so that

$$f(\tau; \frac{1}{\alpha_0}) = f(\alpha_0^2\tau; \alpha_0) .$$

Here $\overline{C}_2(\tau; \alpha)$ and $f(\tau;\alpha)$ denote $\overline{C}_2(\tau)$ and $f(\tau)$ for a given α. Thus, if $M = 1$, one can obtain $f(\tau)$ for $\alpha = 1/\alpha_0$ by simply changing the τ scale on the $\alpha = \alpha_0$ curve. In particular, since the curves for $\alpha \leq 0.1$ are essentially indistinguishable from the curve for $\alpha = 0$, $f(\tau)$ for values of α larger than 10 (α_0 less than 0.1) is approximately given by

$$f(\tau; \frac{1}{\alpha_0}) \approx f(\alpha_0^2\tau; 0) .$$

Footnotes and References

*Work done under auspices of the U. S. Atomic Energy Commission.

[1] C. Lanczos, Linear Differential Operators, Van Nostrand, London, 1961, Sec. 8.9, p. 469.

[2] T. S. Lovering, Bull. Geol. Soc. Am. 47, 87 (1936).

[3] P. Concus, "Table of the Solutions of a $\tan(\pi x) = - b \tan(a\pi x)$," Lawrence Radiation Laboratory Report UCRL-17608, June 1967. Also available from Math. Comp., Unpublished Mathematical Tables repository.

[4] H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, 2nd Ed., Oxford Press, 1959, p. 101.

FIGURE LEGENDS

Fig. 1. $f(\tau)$ vs. τ for $\alpha = 1$ and several values of M.

Fig. 2. $f(\tau)$ vs. τ for $M = 1$ and several values of α.

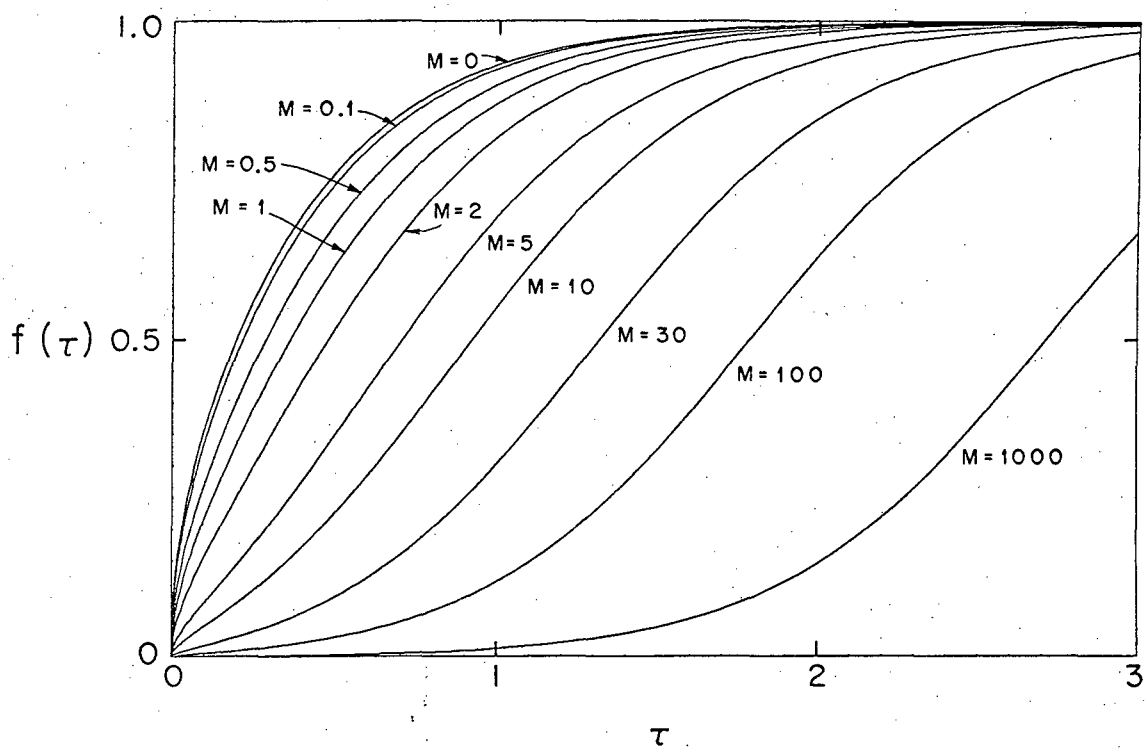

Fig. 1

XBL676-3329

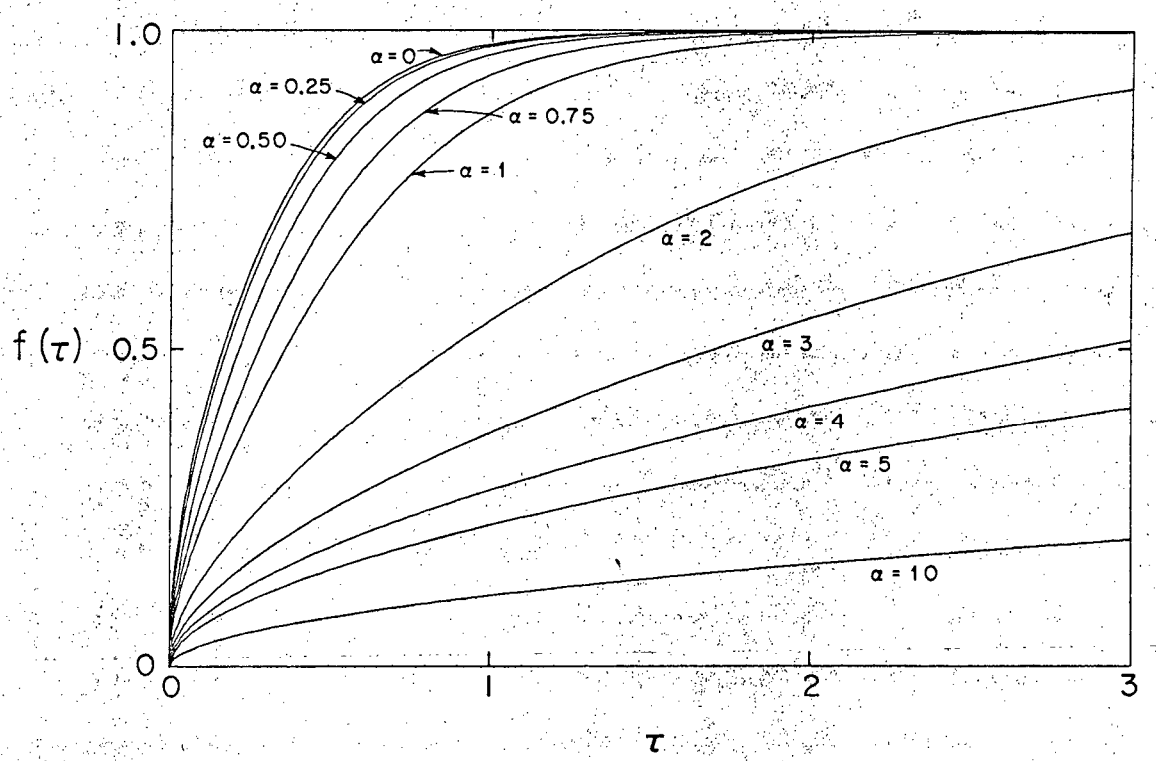

Fig. 2

XBL676-3328

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.