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### Authors

Concus, Paul  
Olander, D.R.

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## Ernest O. Lawrence Radiation Laboratory

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Paul Concus and D. R. Olander

June 2, 1967

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Paul Concus and D. R. Olander

June 2, 1967

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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,

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

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

$$\begin{aligned} \tau &= \frac{D_1 t}{a}, \\ \eta &= \begin{cases} x/a, & -1 \leq \eta < 0 \\ \frac{x}{b} \alpha, & 0 \leq \eta \leq \alpha, \end{cases} \\ C &= \begin{cases} c_1/c_{10}, & -1 \leq \eta < 0 \\ c_2/mc_{10}, & 0 \leq \eta \leq \alpha, \end{cases} \end{aligned}$$

(continued)

$$\alpha = \frac{b}{a} \sqrt{\frac{D_1}{D_2}} \quad (2)$$

and

$$M = \frac{b}{a} m. \quad (3)$$

The resulting equations are

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

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

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

and

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

The initial condition, Eq. 1, becomes

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

and the quantity  $f$  is

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

where

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

The manner in which  $f(\tau)$  approaches unity as  $\tau$  approaches  $\infty$  depends upon the parameters  $\alpha$  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  $C_k(\eta)$ ,

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

with

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

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

$$\tan \lambda_k = -\frac{M}{\alpha} \tan \alpha \lambda_k, \quad \text{for } k = 0, 1, 2, \dots \quad (7)$$

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

The eigenfunctions  $\{C_k(\eta)\}$  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,

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

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

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

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

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

$$\begin{aligned}\bar{C}_2(\tau) &= \sum_{k=0}^{\infty} B_k \exp(-\lambda_k^2 \tau) \int_0^{\alpha} \frac{C_k(\eta)}{\alpha} d\eta \\ &= \frac{1}{1+M} - \sum_{k=1}^{\infty} \frac{A_k B_k}{M \lambda_k} \sin \lambda_k \exp(-\lambda_k^2 \tau); \end{aligned}$$

for the initial condition, Eq. 4, this becomes

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

The limiting form of the series solution as  $\alpha \rightarrow \infty$  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  $\alpha$  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  $\bar{C}_2(\tau)$  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

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

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  $\alpha$  when  $M = 1$ . If  $M = 1$  then  $\bar{C}_2(\tau)$  for  $\alpha = \alpha_0$  and  $\bar{C}_2(\tau)$  for  $\alpha = 1/\alpha_0$  are related by

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

so that

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

Here  $\bar{C}_2(\tau; \alpha)$  and  $f(\tau; \alpha)$  denote  $\bar{C}_2(\tau)$  and  $f(\tau)$  for a given  $\alpha$ . Thus, if  $M = 1$ , one can obtain  $f(\tau)$  for  $\alpha = 1/\alpha_0$  by simply changing the  $\tau$  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  $\alpha$  larger than 10 ( $\alpha_0$  less than 0.1) is approximately given by

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

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.  $\tau$  for  $\alpha = 1$  and several values of  $M$ .

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

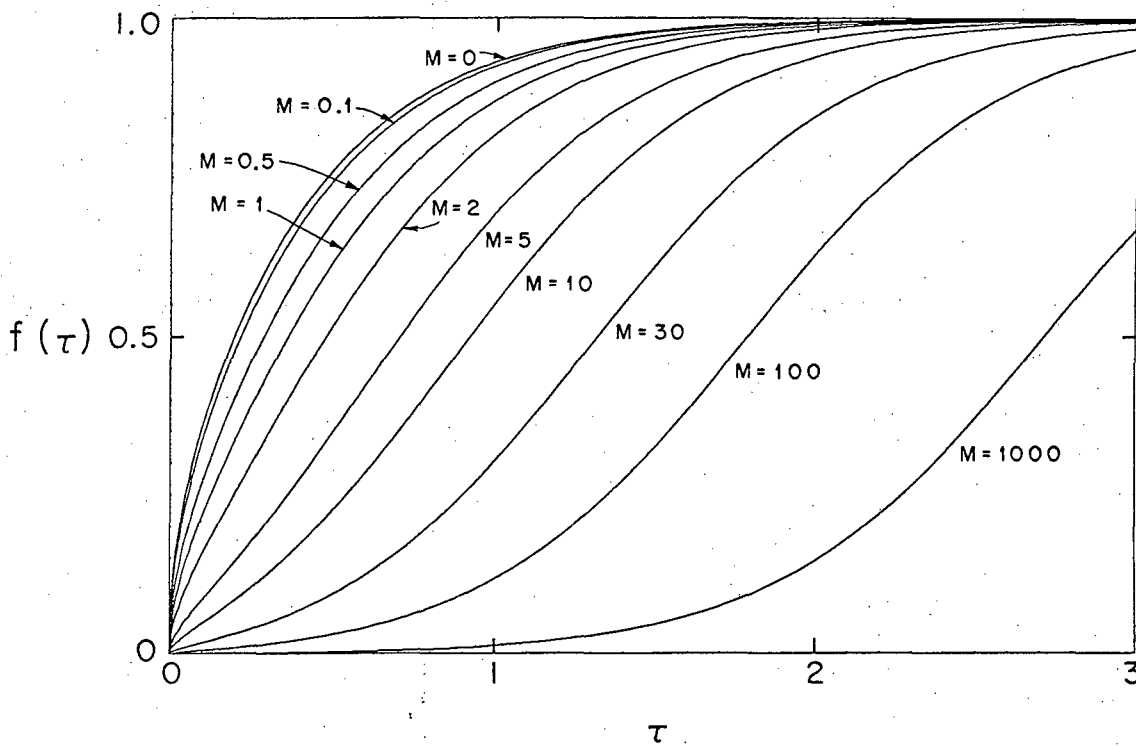


Fig. 1

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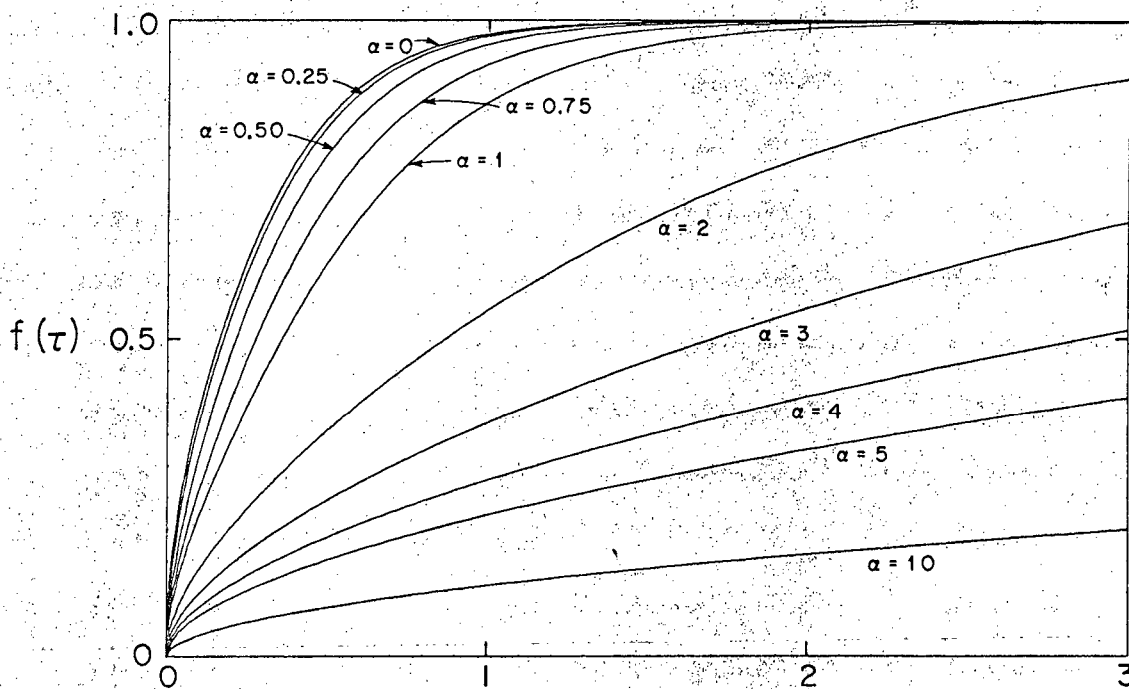


Fig. 2

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