Exact and numerical solutions for effective diffusivity and time lag through multiple layers

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Abstract

We consider diffusion through multiple layers, with application to heat transport. An exact solution is derived and the time lag for heat conduction across the layers is studied. We show the limitations of traditional methods of averaging the diffusivity, which are only applicable in the steady state or for numerous layers.

Contents

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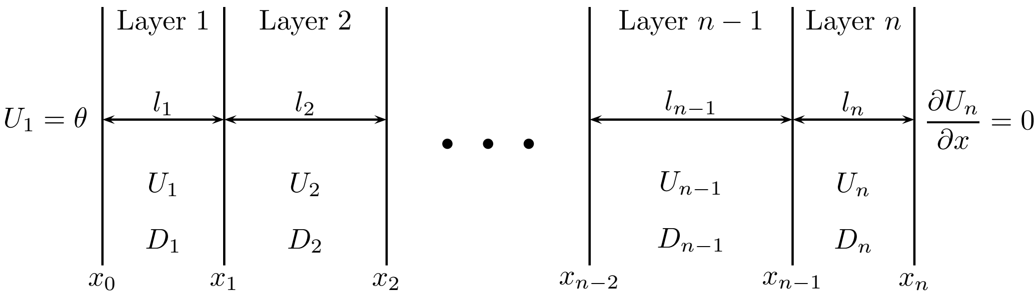

FIGURE 1: n layer problem, with nomenclature explained in the text.

1 Introduction

Diffusion through multiple layers has several applications, including determining when the cold point of a steel coil reaches the annealing temperature [6, 13]. Figure 1 depicts the problem of n layers, with the standard diffusion equation

$$\frac{\partial U_i}{\partial t} = D_i \frac{\partial^2 U_i}{\partial x^2}\,, \quad \text{for } i = 1, 2, 3, \ldots, n\,, \tag{1}$$

applicable in each layer. In Figure 1, U_i is the temperature in layer i at time t, D_i is the diffusivity of a given layer and l_i is the width of the layer. Continuity in temperature and flux is assumed at all the internal boundaries. Various solutions can be found in the literature, for different physical applications, boundary and initial conditions, and with subtly different equations. These include solutions in Cartesian coordinates for two layers [8, 15, 16] and

n layers [9, 11, 14, 18], cylindrical n layer solutions [10], and background on the eigenfunctions [19]. Gilbert and Mathias [12] found semi-analytic solutions by calculating the transfer function for a multiple layered material, although their method involves numerical inversion of the Laplace transform. Azeez and Vakakis [4] found solutions for conduction in composite cylinders using a combined Hankel and Laplace transform method. However, their solution is complicated to implement due to the double numerical inversion of the transformed solution.

A common approach for the n layer problem is to consider an effective diffusivity, and solve the analogous one layer problem. Many authors use the simple approximation for the average diffusivity, D_{av}, of

$$\frac{L}{D_{\text{av}}} = \frac{l_1}{D_1} + \frac{l_2}{D_2} + \cdots\,, \tag{2}$$

where l_i is the width of material with diffusivity D_i, and $L = \sum l_i$. This is true with steady state heat transport or in the case of numerous layers, but is not true in general. Absi et al. [1] describe a brief numerical and experimental comparison of this relationship versus the full coupled numerical system for two layers, illustrating its limitations. Aguirre et al. [2] determined a solution for sinusoidally imposed temperature, calculating an effective diffusivity for a uniform composite material. The effective diffusivity was found in terms of the imposed frequency where Equation (2) is reflected in the low frequency limit when the material is effectively in quasi-steady state. A similar result was obtained by Shigesada et al. [17] for reaction diffusion waves in periodic materials when the layers are thin.

The time lag is a measure of the heat transport time across the layers. It is calculated by determining when the temperature at the end of the region, $x = x_n$, has reached a critical threshold U_c. Several publications in the 1960's dealt with the diffusive time lag through composites, in Cartesian, cylindrical and spherical geometries with Ash et al. [3] giving detailed solutions. These are summarised by Barrer [5] for some of the usual layer configurations. For a single layer, Ash et al. [3] calculate the time lag to be

$$t_L = \frac{L^2}{6D}\,. \tag{3}$$

The general expression given for the time lag in a slab with n layers by Ash et al. [3] is

$$\begin{aligned} t_{Lslab} &= \left[\sum_{i=1}^{n} \frac{l_i}{D_i}\right]^{-1} \left[\sum_{i=1}^{n} \left\{\frac{l_i^2}{2D_i} \sum_{j=i}^{n} \left(\frac{l_j}{D_j}\right) - \frac{l_i^3}{3D_i^2}\right\}\right. \\ &\quad \left. + \sum_{i=1}^{n-1} \left\{\frac{l_i}{D_i} \sum_{k=i+1}^{n} \left(l_k \sum_{j=k}^{n} \left[\frac{l_j}{D_j}\right] - \frac{l_k^2}{2D_k}\right)\right\}\right]. \end{aligned} \tag{4}$$

The exact solution to this n layer diffusion problem is determined in Section 2. We discuss how we calculate the time lag, and the accuracy of the average diffusivity and Ash et al. [3] time lag methods in Section 3.

2 Exact solution

The n layer case has diffusion given by Equation (1) and

$$\begin{aligned} u_1(x_0,t) &= \theta\,, \quad \left.\frac{\partial u_n}{\partial x}\right|_{x_n} = 0\,, && (5)\\ u_i(x_i,t) &= u_{i+1}(x_i,t)\,, \quad \text{for } i = 1,2,3,\ldots,(n-1)\,, && (6)\\ D_i \left.\frac{\partial u_i}{\partial x}\right|_{x_i} &= D_{i+1} \left.\frac{\partial u_{i+1}}{\partial x}\right|_{x_i}\,, \quad \text{for } i = 1,2,3,\ldots,(n-1)\,, && (7)\\ u_i(x,0) &= f_i(x)\,, \quad \text{for } i = 1,2,3,\ldots,n\,. && (8) \end{aligned}$$

Equation (5) represents the external boundary conditions, for constant θ on the left hand side, Equations (6) and (7) represent continuity between layers, and Equation (8) is the initial condition for some $f_i(x)$. Due to the constant boundary condition at $x = x_0$ a transformation described by Carslaw and Jaeger [7] is used, where $U_i = w_i(x) + v_i(x,t)$. That is, U_i is split into the steady state solution, $w_i(x)$, and the transient solution, $v_i(x,t)$, such that $v_i(x,t) \to 0$ as $t \to \infty$.

The steady state solution then satisfies

$$\begin{aligned} D_i \frac{\partial^2 w_i}{\partial x^2} &= 0\,, \quad \text{for } i = 1,2,3,\ldots,n\,, \\ w_1(x_0) &= \theta\,, \quad \left.\frac{\partial w_n}{\partial x}\right|_{x_n} = 0\,, \\ w_i(x_i) &= w_{i+1}(x_i)\,, \quad \text{for } i = 1,2,3,\ldots,(n-1)\,, \\ D_i \left.\frac{\partial w_i}{\partial x}\right|_{x_i} &= D_{i+1} \left.\frac{\partial w_{i+1}}{\partial x}\right|_{x_i}\,, \quad \text{for } i = 1,2,3,\ldots,(n-1)\,. \end{aligned} \tag{9}$$

While this trivially gives $w_i(x) = \theta$, a general solution approach applicable to more general boundary conditions is given. Equation (9) is integrated, giving the steady state solution

$$w_i(x) = q_i(x - x_{i-1}) + h_i\,, \tag{10}$$

where q_i and h_i are constants. The external boundary conditions give $h_1 = \theta$ and $q_n = 0$, and the internal boundary conditions result in recursively defined constants

$$q_{i+1} = \frac{D_i}{D_{i+1}} q_i \quad \text{and} \quad h_{i+1} = h_i + q_i l_i\,. \tag{11}$$

Applying the external boundary conditions gives $q_i = 0$ and $h_i = \theta$. Therefore, the steady state solution is

$$w_i(x) = \theta\,. \tag{12}$$

The transient solution, $v_i(x,t)$, satisfies

$$\frac{\partial v_i}{\partial t} = D_i \frac{\partial^2 v_i}{\partial x^2}\,, \quad \text{for } i = 1,2,3,\ldots,n\,, \tag{13}$$

$$\begin{aligned} v_1(x_0,t) &= 0\,, \quad \left.\frac{\partial v_n}{\partial x}\right|_{x_n} = 0\,, \\ v_i(x_i,t) &= v_{i+1}(x_i,t)\,, \quad \text{for } i=1,2,3,\ldots,(n-1)\,, \\ D_i\left.\frac{\partial v_i}{\partial x}\right|_{x_i} &= D_{i+1}\left.\frac{\partial v_{i+1}}{\partial x}\right|_{x_i}\,, \quad \text{for } i=1,2,3,\ldots,(n-1)\,, \\ v_i(x,0) &= f_i(x)-w_i(x) = g_i(x)\,, \quad \text{for } i=1,2,3,\ldots,n\,, \end{aligned}$$

which is separable. That is, let $v_i(x,t) = X_i(x)T(t)$, resulting in the two ordinary differential equations $T' = \mu\,T$ and $X_i'' = (\mu/d_i^2)X_i$ and the boundary conditions

$$X_1(x_0) = 0 \tag{14}$$

$$X_n'(x_n) = 0 \tag{15}$$

$$X_i(x_i) = X_{i+1}(x_i)\,, \quad \text{for } i=1,2,3,\ldots,(n-1) \tag{16}$$

$$D_i\left.\frac{\partial X_i}{\partial x}\right|_{x_i} = D_{i+1}\left.\frac{\partial X_{i+1}}{\partial x}\right|_{x_i}\,, \quad \text{for } i=1,2,3,\ldots,(n-1)\,, \tag{17}$$

where $d_i = \sqrt{D_i}$ for simplicity later. The cases where $\mu = 0$ and $\mu = +\lambda^2$ yield trivial solutions, but when $\mu = -\lambda^2$,

$$X_i = A_i\sin\left(\frac{\lambda_m}{d_i}(x-x_{i-1})\right) + B_i\cos\left(\frac{\lambda_m}{d_i}(x-x_{i-1})\right)\,. \tag{18}$$

Applying the boundary conditions gives a series of expressions, which can be rewritten in terms of one of the arbitrary constants. For simplicity, A_1 is the chosen constant. Thus Equation (18) becomes

$$X_i = A_1\left[K_{1,i}\sin\left(\frac{\lambda_m}{d_i}(x-x_{i-1})\right) + K_{2,i}\cos\left(\frac{\lambda_m}{d_i}(x-x_{i-1})\right)\right]\,. \tag{19}$$

By definition of the arbitrary constant, $K_{1,1} = 1$ and from Equation (14), $K_{2,1} = 0$. The remaining constants are determined by the internal boundary conditions, Equations (16) and (17), and are recursively defined as

$$K_{1,i+1} = K_{1,i}\frac{d_i}{d_{i+1}}\cos\left(\lambda_m\frac{l_i}{d_i}\right) - K_{2,i}\frac{d_i}{d_{i+1}}\sin\left(\lambda_m\frac{l_i}{d_i}\right)\,, \tag{20}$$

$$K_{2,i+1} = K_{1,i}\sin\left(\lambda_m \frac{l_i}{d_i}\right) + K_{2,i}\cos\left(\lambda_m \frac{l_i}{d_i}\right).$$

The eigenvalue, λ_m, is defined using Equation (15) as

$$K_{1,n}\cos\left(\lambda_m \frac{l_n}{d_n}\right) - K_{2,n}\sin\left(\lambda_m \frac{l_n}{d_n}\right) = 0. \tag{21}$$

Therefore the transient solution is

$$v_i(x,t) = \sum_{m=1}^{\infty} C_m e^{-\lambda_m^2 t} X_i(x), \tag{22}$$

where C_m includes the constant A_1 from X_i. Using the initial condition,

$$v_i(x,0) = g_i(x) = \sum_{m=1}^{\infty} C_m X_i(x). \tag{23}$$

Sturm–Liouville theory yields an orthogonality condition

$$\sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} X_i(x,\lambda_m)\, X_i(x,\lambda_p)\, dx = \begin{cases} 0, & m \neq p, \\ a, & m = p, \end{cases} \tag{24}$$

where a is some constant. The constants $K_{1,i}$ and $K_{2,i}$ in Equation (19) effectively act as weighting terms in the summation, matching the internal boundary conditions. Hence

$$C_m = \frac{\sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} g_i(x) X_i(x)\, dx}{\sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} X_i^2(x)\, dx}. \tag{25}$$

The complete solution is therefore

$$U_i(x,t) = \theta + \sum_{m=1}^{\infty} C_m e^{-\lambda_m^2 t} X_i(x). \tag{26}$$

This exact solution was verified against a numerical solution, using second order central finite differences and an Euler time step. Excellent agreement was found. Equation (26) is also valid for the simpler single uniform region.

3 Results

To measure the accuracy of the average diffusivity approximation, Equation (2), we calculate the time lag. That is, we determine when the temperature has reached the critical threshold U_c at the right hand end of the region, $x = x_n$. A key issue is determining a suitable threshold value, which is discussed shortly.

Two basic methods were employed to calculate the time lag. First, the Ash et al. [3] time lag expressions were used from Equations (3) and (4). Second, the exact solution, Equation (26), is written as

$$U_c - \sum_{m=1}^{\infty} e^{-\lambda_m^2 t_L} X_n(x = x_n) = 0\,, \tag{27}$$

and solved numerically using MATLAB for the unknown time lag t_L.

Our results here use a region $x_0 = 0$ to $x_n = 1$ and equal repeating layers with diffusivities D_a and D_b. Hence, with n layers, $l_i = 1/n$. The initial condition used is $f_i(x) = 0$. We consider two cases (labelled 'Exact 1' and 'Exact 2' in the figures): $D_a = 1/9$ and $D_b = 1$; and $D_a = 1$ and $D_b = 1/9$. Both give $D_{av} = 0.2$ from Equation (2).

Figure 2 depicts the time lag as a function of the number of repeated layers, where $U_c = 0.1665$. The solution labelled 'Exact D_{av}' is the exact solution, Equation (27), with uniform diffusivity D_{av}. The 'D_{av}' solution is where Equation (3) was used. The threshold value, U_c, was chosen such that the 'Exact D_{av}' and 'D_{av}' match, fulfilling an assumption of Ash et al. [3]. The 'Exact 1' and the 'Exact 2' solutions approach the average diffusivity solutions from opposite sides with the 'Exact 2' matching the 'D_{Ash}' solution closer than the 'Exact 1' solution. This suggests the Ash et al. [3] time lag calculation favours one particular combination of layered diffusivities.

Due to the significance of the threshold value on the result, we investigate $U_c = 0.01$ with results presented in Figure 3. However, this threshold value

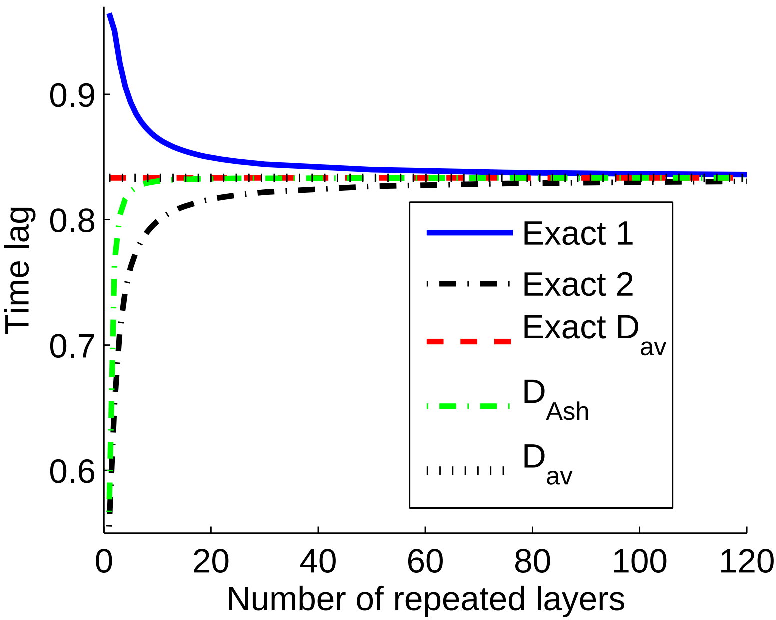

FIGURE 2: Time lag for $U_c = 0.1665$.

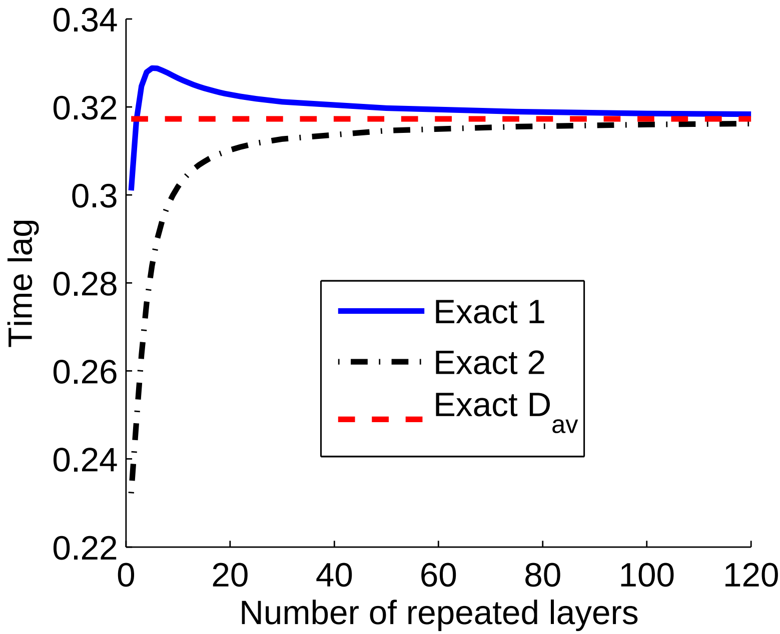

Figure 3: Time lag for $U_c = 0.01$.

transgresses an assumption of Ash et al. [3], thus it is not reasonable to compare their result in this scenario. As expected, the 'Exact 2' solution behaves much the same as in Figure 2. However, the behaviour of the 'Exact 1' solution is intriguing as it crosses the 'Exact D_{av}' solution and warrants further investigation.

In both Figure 2 and Figure 3 it is evident that a substantial number of repeated layers are required to get good agreement with the commonly used approximation given by Equation (2).

4 Conclusions

We expected the average diffusivity solution to hold at steady state and with a sufficient number of layers. However, a remarkably large number of layers were required before the exact solution converged. Therefore, care must be taken when using the average diffusivity approximation as the time lag can be significantly mis-estimated for relatively few layers.

We expected the Ash et al. [3] method, resulting in Equation (4), to give a good approximation of the time lag. However this was only true when the diffusivities were ordered $D_a = 1$ and $D_b = 1/9$, and was quite inaccurate for the other case. In fact, our solution shows a much more complex behaviour. Further work is required in exploring how results vary with other layer configurations.

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