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Semi-analytical solution of multilayer diffusion problems with time-varying boundary conditions and general interface conditions

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ABSTRACT

We develop a new semi-analytical method for solving multilayer diffusion problems with time-varying external boundary conditions and general internal boundary conditions at the interfaces between adjacent layers. The convergence rate of the semi-analytical method, relative to the number of eigenvalues, is investigated and the effect of varying the interface conditions on the solution behaviour is explored. Numerical experiments demonstrate that solutions can be computed using the new semi-analytical method that are more accurate and more efficient than the unified transform method of Sheils [*Appl. Math. Model.*, 46:450–464, 2017]. Furthermore, unlike classical analytical solutions and the unified transform method, only the new semi-analytical method is able to correctly treat problems with both time-varying external boundary conditions and a large number of layers. The paper is concluded by replicating solutions to several important industrial, environmental and biological applications previously reported in the literature, demonstrating the wide applicability of the work.

1. Introduction

Mathematical models of diffusion in layered materials arise in many industrial, environmental, biological and medical applications, such as heat conduction in composite materials [13–15], transport of contaminants, chemicals and gases in layered porous media [10,25], brain tumour growth [1,12], heat conduction through skin [19], transdermal drug delivery [16,21] and greenhouse gas emissions [11]. Another important application is in the field of multiscale modelling: for a large number of layers, layered diffusion is one of the simplest examples of a multiscale problem and is ideal for prototyping macroscopic and multiscale modelling approaches [2,3]. Analytical solutions to such problems are highly valuable as they provide a greater level of insight into the solution behaviour and can be used to benchmark numerical solutions.

The most popular analytical solution approach for multilayer diffusion is classical separation of variables (see, e.g., [6,13,23]). By assuming a separated solution in each layer, one immediately finds that the eigenfunctions are coupled via the internal boundary conditions (BCs) at the interfaces between adjacent layers. Together with the external BCs, a system of algebraic equations is obtained, linear in the (unknown) eigenfunction coefficients. With the requirement that this linear system possess non-trivial solutions, one obtains a transcendental equation satisfied by the unknown eigenvalues formulated

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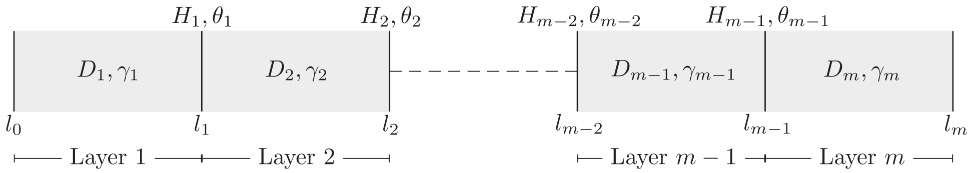

Fig. 1. One-dimensional layered medium. The coefficients D_i and γ_i are constant in each layer ($i = 1, \ldots, m$) while the contact transfer coefficient H_i and partition coefficient θ_i are constants defined at the interfaces ($i = 1, \ldots, m-1$).

by setting the determinant of the coefficient matrix of the linear system equal to zero. Since computing the matrix determinant is numerically unstable for large matrices, using this method to compute the analytical solution performs poorly for a large number of layers as either erroneous eigenvalues/roots are returned during the solution procedure or eigenvalues/roots are skipped altogether (as reported by Carr and Turner [2]).

To overcome these issues, Carr and Turner [2] recently developed a semi-analytical solution approach for multilayer diffusion based on the Laplace transform and an appropriately-defined orthogonal eigenfunction expansion. The attractiveness of this approach is that the solution formulas involve a local set of eigenvalues in each layer satisfying simple transcendental equations, resembling those of the single layer problem, which in most cases can be solved explicitly. As a result, the solution performs well for a large number of layers [2] with the approach classified as *semi-analytical* since computing the inverse Laplace transforms appearing in the solution formulas are carried out numerically.

Recently, Sheils [18] applied the unified transform method, initially proposed by Fokas [4], to the layered diffusion problem and compared the approach to the semi-analytical method of Carr and Turner [2]. Sheils reported that her approach is more accurate, but less efficient and also faulty near the boundaries whenever nonhomogeneous external BCs were applied. We note that her assessment of the accuracy was based on using the default value of 50 terms/eigenvalues in the solution expansions in Carr and Turner [2]'s code. Sheils [18] also remarked that a notable difference between the two methods is that only the unified transform method is applicable to time-dependent external BCs.

In this paper, several key contributions to the literature on multilayer diffusion are presented. Specifically, we:

(i) develop a new semi-analytical solution approach for time-dependent external BCs and a general set of internal BCs (Section 3);
(ii) study the convergence rate of the new semi-analytical method in (i) and compare it to the classical analytical method (Section 4.2);
(iii) carry out a more comprehensive comparison between our semi-analytical method and Sheils' [18] unified transform method, in terms of accuracy and efficiency, by performing an investigation into the effect of the number of terms/eigenvalues on the solution accuracy (Section 4.3);
(iii) explore the effect that changing the interface conditions has on the solution behaviour (Section 4.1);
(iv) extend the classical analytical solution approach to a general set of internal BCs by proposing the correct form of the weight function in the orthogonality condition (Appendix C).

The treatment of time-dependent external BCs addresses a deficiency of Carr and Turner [2]'s semi-analytical method, as reported by Sheils [18], and allows for application of the method to a wider range of problems, for example, contaminant transport modelling in layered porous media involving a time-varying inlet concentration [10]. Our method is also not faulty at the end points as is the case for Sheil's [18] unified transform method whenever nonhomogeneous external BCs are applied. Moreover, general interface conditions permit additional features to be incorporated in the layered diffusion model, such as the volumetric heat capacity in heat conduction problems [7] or the sorption coefficient and partitioning phenomena in chemical transport problems [23].

The remaining sections of this paper are organised in the following manner. Section 2 formulates the multilayer diffusion problem considered in this work while the derivation and implementation of the semi-analytical solution method is outlined in Section 3. Numerical experiments are reported in Section 4. The paper then concludes with a summary and overview of key findings.

2. Multilayer diffusion problem

The one-dimensional multilayer diffusion problem is formulated as follows. Consider a diffusion process on the interval $[l_0, l_m]$, which is partitioned into m subintervals (see Fig. 1):

$$l_0 < l_1 < \cdots < l_{m-1} < l_m. \tag{1}$$

The resulting domain is represented using the notation $[l_0, l_1, \ldots, l_{m-1}, l_m]$. On each subinterval (layer) (l_{i-1}, l_i), that is for all $i = 1, \ldots, m$, we define the diffusion equation:

$$\frac{\partial u_i}{\partial t} = D_i \frac{\partial^2 u_i}{\partial x^2}, \tag{2}$$