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Analytical models of axisymmetric reaction–diffusion phenomena in composite media

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ABSTRACT

Reaction–diffusion equations describe a number of physical, chemical, and biological phenomena, many of which occur in composite environments with piece-wise constant diffusion coefficients. We develop semi-analytical solutions of axisymmetric reaction–diffusion equations with first-order reaction kinetics and continuous transient boundary conditions. These solutions are directly applicable to heat conduction in composite media with transient boundary conditions and heat generation. The solutions lose their robustness in the long time regime, when the Laplace variable tends to zero. This limitation is overcome by the use of corresponding steady-state solutions.

1. Introduction

Transient one-dimensional solutions for heat conduction in composite media have been developed by several authors. Ozisik [10] provides an extensive review of various solutions obtained via Laplace transformations and Green's functions to handle transient problems, and the generalized orthogonal expansion technique to solve homogeneous or steady state problems. Carslaw and Jaeger [3] present solutions derived by means of the Laplace transformation. Sun [11] and de Monte [9] derive solutions utilizing the eigenfunction expansion method. Huang [6] uses Green's functions to derive solutions for periodic boundary conditions. Dias [5] presents a recursive method based on Green's functions to develop a solution. Beck et al. [2] develop a Galerkin-based Green's function method to analyze multidimensional problems. Aviles-Ramos et al. [1] develop a two-layer composite heat conduction solution with periodic boundary conditions using a spectral method with an orthotropic layer to estimate thermophysical properties.

This work employs Laplace transforms to improve previous solutions by solving problems with first-order reaction and source terms in composite media with any number of layers, subject to transient boundary conditions. The first-order reaction term in mass transfer problems is equivalent to the heat generation term in heat conduction problems. Transient boundary conditions of the periodic form are of particular relevance to many problems such as seasonal or diurnal temperature changes outside of a structure. Another application is diffusion through fractured rock [8]. The model developed here can be incorporated as a multi-layered rock medium in the fracture matrix.

More recent work by Sun et al. [11] and de Monte [9] uses eigenfunction expansions to derive nominally analytical solutions, even though the eigenvalues must be calculated numerically and the accuracy of the solution is improved by including more terms in the eigenvalue calculation. The number of required terms in the eigenfunction expansion method increases for small times [11]. The eigenfunction method is advantageous for large-time solutions, as Laplace transform solutions suffer numerical round off for large time values. We overcome this disadvantage by implementing the final value theorem, which produces an exact steady-state solution in real space with no numerical calculation and no need for eigenvalue calculation or increased term inclusion for accuracy. Thus the solution presented here is both valid and accurate for all times. The only exception to this is some intermediate-time regimes characterized by large Damköhler numbers.

A unique advantage of the Laplace transform methods, as it is applied to the current problem, is that the boundary conditions can be isolated as a multiple of the rest of the solution rather than as a component tied inside of an integral. This unique feature allows for various types of boundary conditions to be easily incorporated into the problem. Isolation of the boundary conditions is also useful for linking multiple solutions together in order to create a composite solution. The difficulty often presented by the Laplace

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transform method is the transformation back to real space. Though this inverse transformation can be done for each and every potential boundary condition, this can be a tedious task in systems with a large number of layers. Li et al. [7] presented an analytical solution for a first-order reaction–diffusion problem in a two layer slab, which does not consider arbitrary time-dependent boundary conditions. Extension of this solution to an m-layered solution (where m is any number of layers) is cumbersome. Our method relies on the numerical inverse Laplace transform algorithm developed by De Hoog [4] to handle the m-layered solution. Though this presents a numerical finale to the solution, it yields a very quick and accurate solution for a wide range of problems.

2. Methodology

2.1. The Model

The physical system models used in this paper are layered pieces of material. For cylindrical and spherical coordinate problems the layers are concentric hollow circles or spheres. Fig. 1 depicts the problem in cylindrical coordinates. Each layer is numbered and has its own geometric and physical properties. The solution is robust enough to handle different layer thicknesses, as well as varying diffusion and reaction coefficients and source terms.

A first-order reaction–diffusion equation is based on Fick's law with a first-order reaction term,

$$\frac{\partial \mathcal{C}}{\partial t} = \mathcal{D}\nabla^2\mathcal{C} + (\mathcal{R} + \Phi)\mathcal{C} \tag{1}$$

where $\mathcal{D}$ is the diffusion coefficient, $\mathcal{R}$ is the first-order reaction rate coefficient, and Φ is an unknown source term that is constant with respect to time and space.

2.2. Non-dimensional form

The governing equation is transformed into its non-dimensional form by defining the non-dimensional terms as

$$C = \frac{\mathcal{C}}{\mathcal{C}_c}, \quad D = \frac{\mathcal{D}}{\mathcal{D}_c}, \quad R = \frac{\mathcal{R}}{\mathcal{R}_c}, \quad \psi = \frac{\Phi}{\mathcal{R}_c}$$
$$\xi = \frac{x}{L_c}, \quad \rho = \frac{r}{L_c}, \quad \tau = \frac{t\mathcal{D}_c}{L_c^2} \tag{2}$$

where the subscript c denotes the characteristic value of the relevant quantity. This transforms (1) into

$$\frac{\partial C}{\partial \tau} = D\nabla^2 C + Da(R + \psi)C \tag{3}$$

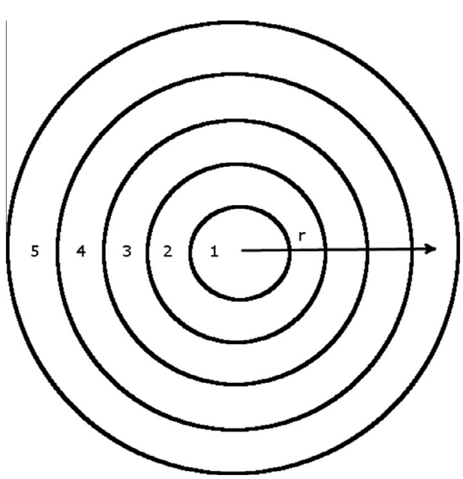

Fig. 1. A radial layered model.

where Da is the Damköhler number defined as

$$Da = \frac{\mathcal{R}_c L_c^2}{\mathcal{D}_c} \tag{4}$$

and $\mathcal{R}_c$ and $\mathcal{D}_c$ are the largest coefficients in the composite medium, such that

$$0 \leqslant D \leqslant 1, \quad 0 \leqslant R \leqslant 1, \quad 0 \leqslant \psi \leqslant 1. \tag{5}$$

2.3. Laplace transform

The Laplace transform is defined as

$$\hat{f}(s) = \mathcal{L}(f(\tau)) = \int_0^\infty f(\tau)e^{-s\tau}\mathrm{d}\tau. \tag{6}$$

It is used in this work for two primary reasons. First, it allows the boundary condition to be a multiplying factor of the equation describing the problem in Laplace space rather than being a component of an integral in the governing equation. Second, it significantly simplifies the derivation of the solution by reducing the dimensionality of a PDE. Since

$$\hat{f}(s) = \mathcal{L}\left(\frac{\partial f(\tau)}{\partial \tau}\right) = s\hat{f}(s) - f(0), \tag{7}$$

taking the Laplace transform of (3) yields

$$s\hat{C} - C_0 = \mathcal{L}\left(D\nabla^2 C + Da(R + \psi)C\right) \tag{8}$$

where $C_0 = \mathcal{C}_0/\mathcal{C}_c$ is the initial condition.

The general Laplace space solutions in each coordinate system (Cartesian, cylindrical, and spherical, respectively) are

$$\hat{C} = Ae^{\beta\xi} + Be^{-\beta\xi} + C_0/\mathcal{S} \tag{9}$$
$$\hat{C} = AI_0(\beta\rho) + BK_0(\beta\rho) + C_0/\mathcal{S} \tag{10}$$
$$\hat{C} = A\frac{e^{-\beta\rho}}{\rho} + B\frac{e^{\beta\rho}}{\beta\rho} + \frac{C_0}{\mathcal{S}} \tag{11}$$

where $\mathcal{S} = s - Da(R + \psi)$, $\beta = \sqrt{\mathcal{S}/D}$ and A and B are constants of integration.

2.4. Special cases

There are three particular cases that are considered in this model. The first is referred to as the finite Neumann case; it has a flux (Neumann) boundary condition at one boundary and a Dirichlet boundary condition at the other. The second is the finite Dirichlet case, with a Dirichlet boundary condition at each boundary. The third is the semi-infinite Dirichlet case, which produces the same results regardless of whether a Neumann or Dirichlet boundary condition is used at infinity. The cases are described in more detail below. Let a and b be the boundaries of each layer and $\hat{\phi}$ denote the time-dependent boundary condition in the Laplace space. Then,

1. Finite Neumann, the solution in the range $a \leqslant \xi \leqslant b$ with boundary conditions

$$\frac{\partial \hat{C}(a,s)}{\partial \xi} = \hat{\phi}_a(s), \quad \hat{C}(b,s) = \hat{\phi}_b(s). \tag{12}$$

2. Finite Dirichlet, the solution in the range $a \leqslant \xi \leqslant b$ with boundary conditions

$$\hat{C}(a,s) = \hat{\phi}_a(s), \quad \hat{C}(b,s) = \hat{\phi}_b(s). \tag{13}$$

3. Semi-infinite Dirichlet, the solution in the range $a \leqslant \xi \leqslant \infty$ with the boundary conditions