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Analytical solution for the advection–dispersion transport equation in layered media

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ABSTRACT

The advection–dispersion transport equation with first-order decay was solved analytically for multi-layered media using the classic integral transform technique (CITT). The solution procedure used an associated non-self-adjoint advection–diffusion eigenvalue problem that had the same form and coefficients as the original problem. The generalized solution of the eigenvalue problem for any numbers of layers was developed using mathematical induction, establishing recurrence formulas and a transcendental equation for determining the eigenvalues. The orthogonality property of the eigenfunctions was found using an integrating factor that transformed the non-self-adjoint advection–diffusion eigenvalue problem into a purely diffusive, self-adjoint problem. The performance of the closed-form analytical solution was evaluated by solving the advection–dispersion transport equation for two- and five-layer media test cases which have been previously reported in the literature. Additionally, a solution featuring first-order decay was developed. The analytical solution reproduced results from the literature, and it was found that the rate of convergence for the current solution was superior to that of previously published solutions.

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1. Introduction

The study of heat and mass transfer in layered media is an important subject in several branches of science and engineering. In heat conduction, for example, multilayer components are important due to the advantages of combining different thermophysical properties as insulation materials, with energy efficiency being improved by optimizing temperature distributions. Layered materials also feature prominently in nuclear reactors, where heat conduction in fuel rods occurs through several layers. In environmental sciences, mass transport often occurs in layered systems, especially in soils, which typically have a layered morphology (where the layers are termed "soil horizons").

The literature contains many analytical solutions for diffusion in a composite medium, with applications to unsteady heat or mass diffusion problems. Methods of solution and citations of classic references can be found in [1–3]. On the other hand, the literature contains relatively few analytical solutions for advection–dispersion transport problems in layered media. The available solutions include [4–8]. These solutions, which we will briefly review here, were all presented in the context of solute transport in composite porous media.

Al-Niami and Rushton [4] used the Laplace transform to obtain analytical solutions for solute transport in finite layered media with constant concentration in the inlet boundary condition. As observed by Leij et al. [5], Al-Niami and Rushton [4] imposed the physically unrealistic assumption that the concentration gradient is zero at the interfaces of the layers.

Leij et al. [5] also used the Laplace transform to develop analytical solutions of the one-dimensional advection–dispersion equation (without decay term) for transport in a semi-infinite, two-layered soil profile with either first- or third-type boundary conditions at the inlet and layer interfaces. Later, Leij and van Genuchten [6] used Laplace transforms to derive an approximate analytical solution for solute transport in a two-layer porous medium and compared the solution with results obtained by numerical inversion of the Laplace transform. These authors noted that the use of Laplace transforms becomes more complicated if the concentration of an upstream layer depends on properties of its downstream layers. This situation arises when both concentration and solute flux are required to be continuous at the interfaces.

Liu et al. [7] used the generalized integral transform technique (GITT) to solve the advection–dispersion multilayer transport equation, using an eigenvalue problem without advection information. The solution of the eigenvalue problem was found using the

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sign-count method to avoid the risk of missing eigenvalues. The resulting transformed problem was truncated and solved analytically using similarity transformation. The authors reported that simulating a two-layer porous medium required 60 terms in the series solution, although in some cases 120 terms were required for convergence. Liu et al. [7] also noted that integral transform methods such as Laplace and Fourier transforms are frequently used to derive analytical solutions for transport in porous media. However, as Liu et al. [7] state, because of the continuity requirement for both concentration and mass flux at layer interfaces, it is difficult to apply integral transforms to space variables in multi-layer problems.

Recently, Li and Cleall [8] presented analytical solutions for conservative solute advection–dispersion in one-dimensional double layered media. Solutions were derived for five scenarios with various combinations of fixed concentration, fixed flux and zero concentration gradient conditions at the inlet and the outlet boundaries considered. The analytical solutions were shown to be in excellent agreement with numerical solutions obtained with a finite element approach and with the Leij and van Genuchten [6] solution.

Analytical solutions for multi-layered media, particularly finite media, tend to be relatively complicated, and the required lengthy solution procedures have likely contributed the relatively small number of available solutions. However, modern software tools such as Mathematica [9], with capabilities for both symbolic and numerical calculations, have made solution procedures such as the classic integral transform technique (CITT) much more tractable [10]. As noted by Ozisik [3], the CITT provides a systematic approach for solving transient and steady problems having homogeneous or non-homogeneous boundary conditions. Heat and mass diffusion problems have been categorized and treated systematically using this technique, creating a unified approach for solving those problems [2]. Transport equations not immediately analytically solvable with the CITT can often be transformed into an amenable form using techniques such as algebraic substitution or integrating factor methods (e.g. [10–13]).

The objective of the present work is to develop a closed-form analytical solution for advection–dispersion transport problems in multilayer, finite media using the CITT. The novel contributions include the use of an associated advection–diffusion eigenvalue problem having the same mathematical form and coefficients as the governing transport equation. It will be shown that when the integral transform procedure uses that associated eigenvalue problem, the procedure converges faster than it does with other possible eigenvalue problems. Also, we overcome a common difficulty associated with the orthogonal expansion technique that is typically used in unsteady heat or mass diffusion problems in composite media, namely the risk of missing some eigenvalues when they are calculated by solving an equation of null determinant [2]. In the present paper, we overcome this problem by developing a transcendental equation for each layer. Lastly, because of our chosen eigenvalue problem and its orthogonality property, we obtain an uncoupled transformed problem and a closed-form analytical solution, which is in contrast to previous solutions which were not closed-from and required the determination of integral coefficients [7].

2. General problem formulation

The one-dimensional unsteady advection–dispersion transport equation for the quantity $c_m \equiv c_m(x,t)$ in a finite composite media of M layers with constant properties in each layer is given by:

$$R_m \frac{\partial c_m}{\partial t} = D_m \frac{\partial^2 c_m}{\partial x^2} - u_m \frac{\partial c_m}{\partial x} - \mu_m c_m = L_m c_m \qquad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{1}$$

where for each layer m the parameter u_m *is* the constant velocity coefficient, μ_m and R_m are constant parameters, and is D_m is the constant dispersion (or diffusion) coefficient.

The operator L_m is defined $L_m \equiv D_m \frac{\partial^2}{\partial x^2} - u_m \frac{\partial}{\partial x} - \mu_m$.

The boundary and initial conditions are, respectively:

$$u_1 c_1 - D_1 \frac{\partial c_1}{\partial x} = u_1 \overline{C}_0; \quad x = x_0 = 0 \tag{2a}$$

$$\left.\begin{array}{l} c_m = c_{m+1} \\ k_m \frac{\partial c_m}{\partial x} = k_{m+1} \frac{\partial c_{m+1}}{\partial x} \end{array}\right\} \quad x = x_m; \quad m = 1,2,3,\ldots,M-1 \tag{2b, c}$$

$$\frac{\partial c_M}{\partial x} = 0; \quad x = x_M \tag{2d}$$

$$c_m = G_m(x); \quad t = 0 \quad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{3}$$

where $\overline{C}_0$ is a reference value and $G_m(x)$ is a known arbitrary function. The generic coefficient k_m preserves continuity in the flux at the layer interfaces and its specification depends on the physical problem being considered; k_m would be, for example, equal to the product of the water content and dispersion coefficient in the case of solute transport in porous media, or equal to thermal conductivity in a general heat conduction problem.

The advection–dispersion transport equation for composite media, Eqs. (1)–(3), is an extension of what is termed Class II problems in the system established by Mikhailov and Ozisik [2] for purely diffusive problems. The problem (Eqs. (1)–(3)) is formulated for perfect contact at layer interfaces. Contact resistances at the interfaces are not considered in the present work, but they could be incorporated into the solution using the procedure given by Mikhailov and Ozisik [2], or by following the procedure given below in Section 3, but with Eq. (2b) replaced by an equation that includes contact resistance. The presented solution procedure could also accommodate entrance and exit boundary conditions different from those given by Eqs. (2a) and (2d), with the alternative formulation resulting in expressions for the coefficients $A_{m,i}$ and $B_{m,i}$ different from those given below. Lastly, although the present problem formulation considers layers with constant coefficients, spatially variable coefficients within layers, including abrupt variations such as considered by Naveira-Cotta et al. [17], could be treated by approximating the spatial variability with stepwise functions. With this technique, the same solution procedure is used, but with the "layers" corresponding to both the material boundaries and the stepwise variations in parameter values.

3. Analytical solution

Our objective is to develop a closed-form analytical solution for the advection–dispersion problem. We will use the Classic Integral Transform Technique (CITT) combined with a mathematical induction procedure to develop the analytical solution.

3.1. Homogenization of the boundary conditions

The boundary conditions of the problem are homogenized by introducing a "filter" function $F_m(x)$ and an unknown function $H_m(x,t)$ such that:

$$c_m(x,t) = F_m(x) + H_m(x,t) \tag{4}$$

When $F_m(x)$ is appropriately chosen, substituting Eq. (4) into Eqs. (1)– (3) leads to a problem with homogeneous boundary conditions in terms of dependent variable $H_m(x,t)$. Appendix A describes in detail the procedure for determining the filter function $F_m(x)$. Once $F_m(x)$ is determined, substituting Eq. (4) into Eqs. (1)–(3) gives:

$$R_m \frac{\partial H_m}{\partial t} = L_m H_m \qquad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{5}$$

$$u_1 H_1 - D_1 \frac{\partial H_1}{\partial x} = 0; \quad x = x_0 = 0 \tag{6a}$$

$$\left.\begin{array}{l} H_m = H_{m+1} \\ k_m \frac{\partial H_m}{\partial x} = k_{m+1} \frac{\partial H_{m+1}}{\partial x} \end{array}\right\} \quad x = x_m; \quad m = 1,2,3,\ldots,M-1 \tag{6b, c}$$

$$\frac{\partial H_M}{\partial x} = 0; \quad x = x_M \tag{6d}$$

$$H_m(x,0) = G_m(x) - F_m(x) \qquad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{7}$$

3.2. The associated advection–dispersion eigenvalue problem

Following the systematized procedure of the CITT [2,3,14], we need to define an auxiliary homogeneous problem for the space variable function $\psi_m(x)$ in the same layers of the original problem. An auxiliary problem can be obtained by applying separation of variables to Eqs. (5)–(7). The resulting advection–dispersion auxiliary problem is,

$$L_m \psi_m + R_m \lambda^2 \psi_m = 0 \qquad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{8}$$

$$u_1 \psi_1 - D_1 \frac{d\psi_1}{dx} = 0; \quad x = x_0 = 0 \tag{9a}$$

$$\left.\begin{array}{l} \psi_m = \psi_{m+1} \\ k_m \frac{d\psi_m}{dx} = k_{m+1} \frac{d\psi_{m+1}}{dx} \end{array}\right\} \quad \begin{array}{l} x = x_m \\ m = 1,2,3,\ldots,M-1 \end{array} \tag{9b-c}$$

$$\frac{d\psi_M}{dx} = 0; \quad x = x_M \tag{9d}$$

The system Eqs. (8) and (9) is an eigenvalue problem and has nontrivial solutions for a discrete spectrum of the parameter $\lambda \equiv \lambda_i$ ($i = 1,2,3,\ldots,\infty$), the eigenvalues, and the corresponding nontrivial solutions $\psi_m(x) \equiv \psi_{m,i}(x)$, the eigenfunctions.

This eigenvalue problem is attractive because it can completely transform Eqs. (5)–(7) such that the resulting system of equations is not coupled [10]. However, this eigenvalue problem is non-self-adjoint, and the orthogonality property is not defined.

Eigenvalue problems with self-adjoint operators have several important and desirable properties: (i) the eigenvalues are real; (ii) the eigenfunctions are orthogonal; and (iii) the eigenfunctions form a complete set. The completeness means that any well-behaved (at least piecewise continuous) function F*(x) can be approximated by a series [15].

To utilize Eqs. (8) and (9), we must transform the non-self-adjoint eigenvalue problem to a self-adjoint one by using an integrating factor, as will be shown below (Section 3.2.2).

3.2.1. Solution of the eigenvalue problem

The general symbolic solution of Eq. (8) can be written in terms of two linearly independent solutions $\phi_{m,i}(x) \equiv \phi_{m,i}(x;\lambda_i)$ and $\theta_{m,i}(x) \equiv \theta_{m,i}(x;\lambda_i)$ and two coefficients $A_{m,i}$ and $B_{m,i}$:

$$\psi_{m,i}(x) = A_{m,i}\phi_{m,i}(x) + B_{m,i}\theta_{m,i}(x) \qquad \begin{array}{l} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{array} \tag{10}$$

Substituting Eq. (10) into Eqs. (9a, b, c) and solving the resulting system for $A_{m,i}$ and $B_{m,i}$ with $m = 1,2,3,\ldots$ reveals a pattern that can be generalized by mathematical induction. The result is the following expressions for the coefficients $A_{m,i}$ and $B_{m,i}$:

$$B_{1,i} = -\frac{u_1\phi_{1,i}(0) - D_1\phi'_{1,i}(0)}{u_1\theta_{1,i}(0) - D_1\theta'_{1,i}(0)} A_{1,i} \tag{11}$$

$$A_{m,i} = \left(\frac{A_{m-1,i}}{k_m}\right) \frac{k_m\phi_{m-1,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - k_{m-1}\theta_{m,i}(x_{m-1})\phi'_{m-1,i}(x_{m-1})}{\phi_{m,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - \theta_{m,i}(x_{m-1})\phi'_{m,i}(x_{m-1})} + \left(\frac{B_{m-1,i}}{k_m}\right) \frac{k_m\theta_{m-1,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - k_{m-1}\theta_{m,i}(x_{m-1})\theta'_{m-1,i}(x_{m-1})}{\phi_{m,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - \theta_{m,i}(x_{m-1})\phi'_{m,i}(x_{m-1})} \tag{12}$$

$$B_{m,i} = \left(\frac{A_{m-1,i}}{k_m}\right) \frac{k_{m-1}\phi_{m,i}(x_{m-1})\phi'_{m-1,i}(x_{m-1}) - k_m\phi_{m-1,i}(x_{m-1})\phi'_{m,i}(x_{m-1})}{\phi_{m,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - \theta_{m,i}(x_{m-1})\phi'_{m,i}(x_{m-1})} + \left(\frac{B_{m-1,i}}{k_m}\right) \frac{k_{m-1,i}\phi_{m,i}(x_{m-1})\theta'_{m-1,i}(x_{m-1}) - k_m\theta_{m-1,i}(x_{m-1})\phi'_{m,i}(x_{m-1})}{\phi_{m,i}(x_{m-1})\theta'_{m,i}(x_{m-1}) - \theta_{m,i}(x_{m-1})\phi'_{m,i}(x_{m-1})} \tag{13}$$

In Eqs. (11)–(13), the prime symbol (′) denotes the first derivative, and $m = 2,3,\ldots,M$. The value of $A_{1,i}$ is arbitrary and is set to $A_{1,i} = 1$.

The solution of the eigenvalue problem can be completed after establishing an equation for the determination of the eigenvalues λ_i. Eqs. (9d) and (10) are used to find a symbolic general transcendental equation. The result suggests a formation rule that can be generalized by mathematical induction for a problem with M layers:

$$A_{M,i}\phi'_{M,i}(x_M) + B_{M,i}\theta'_{M,i}(x_M) = 0 \tag{14}$$

Following Boyce and Di Prima [16] for the case of complex roots in the characteristic equation, the general solution of the advection–dispersion eigenvalue problem (Eq. (8)) can be expressed in terms of exponential and trigonometric functions:

$$\phi_{m,i}(x) = \exp\left(\frac{xu_m}{2D_m}\right)\sin(\beta_{m,i}x) \tag{15a}$$

$$\theta_{m,i}(x) = \exp\left(\frac{xu_m}{2D_m}\right)\cos(\beta_{m,i}x) \tag{15b}$$

where $\beta_{m,i}$ are the layer eigenvalues, $m = 1,2,3,\ldots,M$, which are related to the eigenvalues λ_i by

$$\beta_{m,i} = \frac{\left(4\lambda_i^2 D_m R_m - u_m^2 - 4D_m\mu_m\right)^{1/2}}{2D_m} \tag{15c}$$

From Eqs. (11) and (15), the coefficients for the first layer are:

$$B_{1,i} = \frac{2D_1\beta_{1,i}}{u_1} A_{1,i} \tag{16}$$

For the others layers ($m = 2, 3,\ldots,M$), the following recursive formulas are obtained:

$$A_{m,i} = \exp\left[\frac{x_{m-1}}{2}\left(\frac{u_{m-1}}{D_{m-1}} - \frac{u_m}{D_m}\right)\right]\overline{A}_{m,i} \tag{17}$$

$$\overline{A}_{m,i} = \cos(x_{m-1}\beta_{m,i})[A_{m-1,i}\cos(x_{m-1}\beta_{m-1,i}) - B_{m-1,i} \times \sin(x_{m-1}\beta_{m-1,i})]\frac{k_{m-1}\beta_{m-1,i}}{k_m\beta_{m,i}} + \sin(x_{m-1}\beta_{m,i})[B_{m-1,i} \times \cos(x_{m-1}\beta_{m-1,i}) + A_{m-1,i}\sin(x_{m-1}\beta_{m-1,i})] \tag{18}$$

$$B_{m,i} = \exp\left[\frac{x_{m-1}}{2}\left(\frac{u_{m-1}}{D_{m-1}} - \frac{u_m}{D_m}\right)\right]\overline{B}_{m,i} \tag{19}$$

$$\overline{B}_{m,i} = \cos(x_{m-1}\beta_{m,i})[B_{m-1,i}\cos(x_{m-1}\beta_{m-1,i}) + A_{m-1} \times \sin(x_{m-1}\beta_{m-1,i})] - \sin(x_{m-1}\beta_{m,i})[A_{m-1,i} \times \cos(x_{m-1}\beta_{m-1,i}) - B_{m-1,i}\sin(x_{m-1}\beta_{m-1,i})]\frac{k_{m-1}\beta_{m-1,i}}{k_m\beta_{m,i}} \tag{20}$$

The coefficients $A_{m,i}$ and $B_{m,i}$ are expressed in Eqs. (17)–(20) as the product of exponential and trigonometric functions. Eqs. (10), (15), and (17)–(20) can be combined to yield, after appropriate simplification, an expression for the eigenfunctions $\psi_{m,i}(x)$:

$$\psi_{m,i}(x) = \exp\left(\frac{u_m x}{2D_m} + s_m\right)[\overline{A}_{m,i}\sin(\beta_{m,i}x) + \overline{B}_{mi}\cos(\beta_{m,i}x)] \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \\ i = 1,2,3,\ldots,\infty \end{matrix} \tag{21}$$

where for $m = 1$:

$$\overline{A}_{1,i} = 1; \quad \overline{B}_{1,i} = \frac{2D_1\beta_{1,i}}{u_1}\overline{A}_{1,i} \tag{22a, b}$$

and for $m = 2,3,4,\ldots,M$ the coefficients $\overline{A}_{m,i}$ and $\overline{B}_{m,i}$ were defined previously by Eqs. (18) and (20). The term s_m is given by:

$$s_m = \begin{cases} 0 & (m = 1) \\ \frac{1}{2}\sum_{\bar{m}=2}^{m}\left(\frac{u_{\bar{m}-1}}{D_{\bar{m}-1}} - \frac{u_{\bar{m}}}{D_{\bar{m}}}\right)x_{\bar{m}-1} & (m = 2,3,\ldots,M) \end{cases} \tag{22c}$$

Finally, from Eqs. (14) and (15) the following transcendental equation is obtained:

$$\overline{A}_{M,i}[\sin(x_M\beta_{M,i})u_M + 2\cos(x_M\beta_{M,i})D_M\beta_{M,i}] + \overline{B}_{M,i}[\cos(x_M\beta_{M,i})u_M - 2\sin(x_M\beta_{M,i})D_M\beta_{M,i}] = 0 \tag{23}$$

3.2.2. Orthogonality and norm of the eigenvalue problem

In the classification system given by Mikhailov and Ozisik [2] for self-adjoint problems of heat and mass diffusion, a Class II eigenvalue problem is defined by:

$$\frac{d}{dx}\left[p_m(x)\frac{d\psi_m}{dx}\right] + [\lambda^2 w_m(x) - q_m(x)]\psi_m = 0 \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{24}$$

$$u_1\psi_1 - D_1\frac{d\psi_1}{dx} = 0; \quad x = x_0 = 0 \tag{25a}$$

$$\left.\begin{matrix} \psi_m = \psi_{m+1} \\ p_m\frac{d\psi_m}{dx} = p_{m+1}\frac{d\psi_{m+1}}{dx} \end{matrix}\right\} \quad \begin{matrix} x = x_m \\ m = 1,2,3,\ldots,M-1 \end{matrix} \tag{25a-c}$$

$$\frac{d\psi_M}{dx} = 0; \quad x = x_M \tag{25d}$$

Mikhailov and Ozisik [2] developed the orthogonality relation for this class of (self-adjoint) problems. To determine the orthogonality relation and norm for our study, we will relate Eqs. (8) and (9) with Eqs. (24) and (25) by using the integrating factor concept.

Although Eq. (8) is non self-adjoint, an integrating factor can be used transform Eq. (8) into a form that is equivalent to the self-adjoint Eq. (24). As shown by Pérez Guerrero and Skaggs [10], an integrating factor $p_m(x)$ is obtained by solving the equation:

$$\frac{dp_m(x)}{dx} = -p_m(x)\frac{u_m}{D_m} \quad (m = 1,2,\ldots,M) \tag{26}$$

For a reference position $x = \bar{x}_m$, we define $p_m(\bar{x}_m) = \bar{p}_m$. Thus, an analytical expression for $p_m(x)$ is obtained from Eq. (26):

$$p_m(x) = \bar{p}_m\exp\left[-\int_{\bar{x}_m}^{x}\frac{u_m}{D_m}dx'\right] = \bar{p}_m\exp\left[-\frac{u_m}{D_m}(x - \bar{x}_m)\right] \quad (m = 1,2,\ldots,M) \tag{27}$$

The determination of $\bar{p}_m$ is detailed in Appendix B. Then, the coefficient $p_m(x)$ for each layer is given by:

$$p_m(x) = k_m\exp\left[-\frac{u_m}{D_m}(x - x_m) + g_m\right] \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{28}$$

$$g_m = \begin{cases} 0 & (m = 1) \\ \sum_{\bar{m}=2}^{m}\frac{u_{\bar{m}}}{D_{\bar{m}}}(x_{\bar{m}-1} - x_{\bar{m}}) & (m = 2,3,\ldots,M) \end{cases} \tag{29}$$

Following [10], the others coefficients of Eq. (24) are:

$$q_m(x) = p_m(x)\frac{\mu_m}{D_m}; \quad w_m(x) = p_m(x)\frac{R_m}{D_m} \quad (m = 1,2,\ldots,M) \tag{30,31}$$

Since the non-self-adjoint eigenvalue system was re-written in the form of the Class II self-adjoint diffusion problems, the orthogonality relation is given by [2]:

$$\sum_{m=1}^{M}\int_{x_{m-1}}^{x_m} w_m(x)\psi_{m,i}(x)\psi_{m,j}(x)dx = \delta_{ij}N_i \tag{32}$$

where N_i is the norm. Using Eqs. (21), (18), (20), (22a–c), (28) and (29) in Eq. (30) results in the following closed-form expression for the norm:

$$N_i = \sum_{m=1}^{M}\overline{N}_{m,i} \tag{33a}$$

$$\overline{N}_{m,i} = \frac{k_m R_m\exp\left(\frac{u_1}{D_1}x_1\right)}{4D_m\beta_{m,i}}\left\{\overline{A}_{m,i}^2[\sin(2\beta_{m,i}x_{m-1}) - \sin(2\beta_{m,i}x_m) + 2\beta_{m,i}(x_m - x_{m-1})] + 2\overline{A}_{m,i}\overline{B}_{m,i}[\cos(2\beta_{m,i}x_{m-1}) - \cos(2\beta_{m,i}x_m)] + \overline{B}_{m,i}^2[\sin(2\beta_{m,i}x_m) - \sin(2\beta_{m,i}x_{m-1}) + 2\beta_{m,i}(x_m - x_{m-1})]\right\} \tag{33b}$$

3.3. The integral transform pair

Representing the unknown function $H(x,t)$ as a series expansion in terms of the eigenfunctions $\psi_{m,i}(x)$ and using the orthogonality property (Eq. (30)) results in the following integral transform pair:

$$H_m(x,t) = \sum_{i=1}^{\infty}\frac{\psi_{m,i}(x)}{N_i}\overline{H}_i(t) \quad \text{(Inverse)} \tag{34}$$

$$\overline{H}_i(t) = \sum_{m=1}^{M}\int_{x_{m-1}}^{x_m} w_m(x)\psi_{m,i}(x)H(x,t)dx \quad \text{(Transform)} \tag{35}$$

3.4. Integral transform of the differential equation

Applying the inverse formula (Eq. (32)) to Eq. (5) and recalling the eigenvalue problem (Eq. (8)) results in:

$$R_m\frac{\partial}{\partial t}\sum_{j=1}^{\infty}\frac{\psi_{m,j}(x)}{N_j}\overline{H}_j(t) = -\sum_{j=1}^{\infty}\frac{R_m\lambda_j^2\psi_{m,j}(x)}{N_j}\overline{H}_j(t) \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{36}$$

Now, applying $\sum_{m=1}^{M}\int_{x_{m-1}}^{x_m}\frac{p_m(x)}{D_m}\psi_{m,i}(x)dx$ to both sides of Eq. (36) and grouping resulting terms gives:

$$\frac{\partial}{\partial t}\sum_{j=1}^{\infty}\frac{\overline{H}_j(t)}{N_j}\sum_{m=1}^{M}\int_{x_{m-1}}^{x_m}\frac{p_m(x)}{D_m}R_m\psi_{m,i}(x)\psi_{m,j}(x)dx = -\sum_{j=1}^{\infty}\frac{\overline{H}_j(t)}{N_j}\lambda_j^2\sum_{m=1}^{M}\int_{x_{m-1}}^{x_m}\frac{p_m(x)}{D_m}R_m\psi_{m,i}(x)\psi_{m,j}(x)dx \tag{37}$$

Then, using the orthogonality property (Eq. (32)), the following is obtained:

$$\frac{d\overline{H}_i(t)}{dt} = -\lambda_i^2 \overline{H}_i(t) \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{38}$$

The initial condition (Eq. (7)) is also transformed to yield:

$$\overline{H}_i(0) = \sum_{m=1}^{M} \bar{f}_{m,i} \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{39a}$$

$$\bar{f}_{m,i} = \int_{x_{m-1}}^{x_m} w_m(x)\psi_{m,i}(x)[G_m(x) - F_m(x)]dx \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{39b}$$

Eq. (39) is a generalized expression for any functional form of $G_m(x)$. For situations when $G_m(x) = 0$ and $F_m(x)$ is the general expression given in Appendix A (Eq. (A6)), the following integral coefficient $\bar{f}_{m,i}$ results:

$$\bar{f}_{m,i} = T1_m\left[\frac{a_m T2_{m,i}}{(u_m - 2D_m r1_m)^2 + 4D_m^2\beta_{m,i}^2} + \frac{b_m T3_{m,i}}{(u_m - 2D_m r2_m)^2 + 4D_m^2\beta_{m,i}^2}\right] \tag{40a}$$

$$T1_m = 2k_m R_m \exp\left[g_m + s_m + \frac{u_m}{2D_m}(x_m - x_{m-1})\right] \tag{40b}$$

$$\begin{aligned} T2_{m,i} = {} & \exp\left[\frac{u_m x_m}{2D_m} + r1_m x_{m-1}\right]\sin(x_{m-1}\beta_{m,i})[u_m\overline{A}_{m,i} \\ & - 2D_m(r1_m\overline{A}_{m,i} + \beta_{m,i}\overline{B}_{m,i})] + \cos(x_{m-1}\beta_{m,i}) \\ & \times [2D_m\beta_{m,i}\overline{A}_{m,i} + \overline{B}_{m,i}(u_m - 2D_m r1_m)] \\ & - \exp\left[\frac{u_m x_{m-1}}{2D_m} + r1_m x_m\right]\sin(x_m\beta_{m,i})[u_m\overline{A}_{m,i} \\ & - 2D_m(r1_m\overline{A}_{m,i} + \beta_{m,i}\overline{B}_{m,i})] + \cos(x_m\beta_{m,i})[2D_m\beta_{m,i}\overline{A}_{m,i} \\ & + \overline{B}_{m,i}(u_m - 2D_m r1_m)] \end{aligned} \tag{40c}$$

$$\begin{aligned} T3_{m,i} = {} & \exp\left[\frac{u_m x_m}{2D_m} + r2_m x_{m-1}\right]\sin(x_{m-1}\beta_{m,i})[u_m\overline{A}_{m,i} \\ & - 2D_m(r2_m\overline{A}_{m,i} + \beta_{m,i}\overline{B}_{m,i})] + \cos(x_{m-1}\beta_{m,i}) \\ & \times [2D_m\beta_{m,i}\overline{A}_{m,i} + \overline{B}_{m,i}(u_m - 2D_m r2_m)] \\ & - \exp\left[\frac{u_m x_{m-1}}{2D_m} + r2_m x_m\right]\sin(x_m\beta_{m,i})[u_m\overline{A}_{m,i} \\ & - 2D_m(r2_m\overline{A}_{m,i} + \beta_{m,i}\overline{B}_{m,i})] + \cos(x_m\beta_{m,i})[2D_m\beta_{m,i}\overline{A}_{m,i} \\ & + \overline{B}_{mi}(u_m - 2D_m r2_m)] \end{aligned} \tag{40d}$$

When $G_m(x) = 0$ and $F_m(x) = 1$, the integral coefficient $\bar{f}_{mi}$ is:

$$\begin{aligned} \bar{f}_{m,i} = {} & \frac{2k_m R_m \exp\left[g_m + s_m - \frac{u_m}{2D_m}(x_{m-1} - 2x_m)\right]}{u_m^2 + 4D_m^2\beta_{m,i}^2}\Big\{-\sin(\beta_{m,i}x_{m-1})u_m\overline{A}_{m,i} - 2 \\ & \times\cos(\beta_{m,i}x_{m-1})D_m\beta_{m,i}\overline{A}_{m,i} - \cos(\beta_{m,i}x_{m-1})u_m\overline{B}_{m,i} + 2 \\ & \times\sin(\beta_{m,i}x_{m-1})D_m\beta_{m,i}\overline{B}_{m,i} + \exp\left[\frac{u_m}{2D_m}(x_{m-1} - x_m)\right][(2D_m\beta_{m,i}\overline{A}_{m,i} \\ & + u_m\overline{B}_{m,i})\cos(\beta_{m,i}x_m) + (u_m\overline{A}_{m,i} - 2D_m\beta_{m,i}\overline{B}_{m,i})\sin(\beta_{m,i}x_m)]\Big\} \end{aligned} \tag{41}$$

3.5. Analytical solution for the transformed and original problems

Solving Eq. (38) with initial condition Eq. (39) gives the transformed field:

$$\overline{H}_i(t) = \overline{H}_i(0)\exp\left(-\lambda_i^2 t\right) \tag{42}$$

Finally, invoking the inverse formula Eq. (32) and the relationship in Eq. (4), the closed-form analytical solution is obtained for the advection–dispersion transport equation in multilayered media:

$$c_m(x,t) = F_m(x) + \sum_{i=1}^{\infty}\frac{\psi_{m,i}(x)}{N_i}\overline{H}_i(0)\exp\left(-\lambda_i^2 t\right) \quad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{43}$$

4. Test-case evaluation

The performance of the closed-form analytical solution developed in Section 3 is evaluated by solving the advection–dispersion transport problem in saturated soils for the case of two and five layers, using the same transport parameters given by Liu et al. [7]. The porous medium is assumed to consist of homogeneous layers subject to steady water flow perpendicular to the layer interface. For these cases the coefficient k_m is defined $k_m = \varepsilon_m D_m$, where ε_m and D_m denote the volumetric water content (soil porosity) and the dispersion coefficient in each layer, respectively.

4.1. Two-layer media

Parameter data for the two-layer test-case are given in Table 1 for three different situations. This test-case with $x_1 = 10$ cm and $x_2 = 30$ cm was initially proposed and solved by Leij and van Genuchten [6] with a semi-infinite second layer. Liu et al. [7] solved the same problem with a finite second layer, but they did not report its length.

The series convergence of Eq. (36) is presented in Table 2 for the three cases. For the range of conditions established by Cases 1–3 in Table 1, no more than $N = 15$ terms were necessary to achieve convergence and obtain a solution with the same precision such as reported by Leij and van Genuchten [6] and Liu et al. [7]. Table 3 compares the converged values from the present analytical solution with those obtained previously by Leij and van Genuchten [6] and Liu et al. [7]. Calculations with the present solution were repeated for different values of the exit location, x_2. It was found that any finite domain with $x_2 \geqslant 25$ cm produced a solution which, over the range 0 cm $\leqslant x \leqslant$ 20 cm, matched the semi-infinite solution to the precision reported by Leij and van Genuchten [6] (not shown). The problem was also solved numerically using the method of the lines as implemented in the Mathematica NDSolve library with options set to "ImplicitRungeKutta" [9]. The numerical results matched the analytical solution to the precision reported in Table 3 (not shown).

Liu et al. [7] reported that their analytical solution required $N = 60$ (or in some cases $N = 120$) terms for their series solution to achieve convergence. The faster convergence (no more than $N = 15$ terms) in the current work is because the presented analytical solution utilizes an eigenvalue problem that closely resembles the original problem. The eigenvalue problem used in [7] does not include an advection term. The use of a closely associated eigenvalue problem in the integral transform procedure is convenient because the convergence is faster in relation to other possible eigenvalue problems.

Table 1
Transport parameters for the two-layer test-case.

Case	Layer m	u_m (cm/d)	D_m (cm^2/d)	ε_m	R_m	μ_m (d^{-1})	x_m (cm)
1	1	25	50	0.4	1	0	10
	2	40	20	0.25	1	0	30
2	1	25	20	0.4	1	0	10
	2	40	50	0.25	1	0	30
3	1	40	20	0.25	1	0	10
	2	25	50	0.4	1	0	30
4	1	25	50	0.4	3	3	10
	2	40	20	0.25	2	4	30

Table 2
Convergence of solute concentration in a two-layer porous medium (N is the numbers of terms summed).

Case	x (cm)	t = 0.2 day				t = 0.4 day				t = 0.6 day				t = 0.8 day			
		N = 5	N = 10	N = 15	N = 20	N = 5	N = 10	N = 15	N = 20	N = 5	N = 10	N = 15	N = 20	N = 5	N = 10	N = 15	N = 20
1	0	0.885	0.884	0.884	0.884	0.963	0.963	0.963	0.963	0.987	0.987	0.987	0.987	0.995	0.995	0.995	0.995
	2	0.743	0.742	0.742	0.742	0.915	0.915	0.915	0.915	0.969	0.969	0.969	0.969	0.988	0.988	0.988	0.988
	4	0.560	0.561	0.561	0.561	0.841	0.841	0.841	0.841	0.940	0.940	0.940	0.940	0.977	0.977	0.977	0.977
	6	0.372	0.375	0.375	0.375	0.746	0.746	0.746	0.746	0.901	0.901	0.901	0.901	0.962	0.962	0.962	0.962
	8	0.223	0.222	0.222	0.222	0.645	0.645	0.645	0.645	0.858	0.858	0.858	0.858	0.945	0.945	0.945	0.945
	10	0.149	0.142	0.142	0.142	0.579	0.579	0.579	0.579	0.829	0.829	0.829	0.829	0.933	0.933	0.933	0.933
	10	0.149	0.142	0.142	0.142	0.579	0.579	0.579	0.579	0.829	0.829	0.829	0.829	0.933	0.933	0.933	0.933
	12	0.059	0.063	0.063	0.063	0.480	0.480	0.480	0.480	0.781	0.781	0.781	0.781	0.914	0.914	0.914	0.914
	14	−0.308	0.021	0.021	0.021	0.371	0.372	0.372	0.372	0.722	0.722	0.722	0.722	0.889	0.889	0.889	0.889
	16	−1.950	−0.008	0.005	0.005	0.250	0.264	0.264	0.264	0.651	0.651	0.651	0.651	0.858	0.858	0.858	0.858
	18	0.545	0.089	0.001	0.001	0.153	0.168	0.168	0.168	0.567	0.567	0.567	0.567	0.819	0.819	0.819	0.819
	20	90.700	−0.214	0.000	0.000	0.658	0.094	0.094	0.094	0.476	0.473	0.473	0.473	0.770	0.770	0.770	0.770
2	0	0.980	0.978	0.978	0.978	0.998	0.998	0.998	0.998	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	2	0.873	0.868	0.868	0.868	0.984	0.984	0.984	0.984	0.998	0.998	0.998	0.998	1.000	1.000	1.000	1.000
	4	0.608	0.634	0.634	0.634	0.942	0.942	0.942	0.942	0.991	0.991	0.991	0.991	0.999	0.999	0.999	0.999
	6	0.298	0.345	0.345	0.345	0.848	0.849	0.849	0.849	0.972	0.972	0.972	0.972	0.995	0.995	0.995	0.995
	8	0.382	0.131	0.131	0.131	0.697	0.693	0.693	0.693	0.930	0.930	0.930	0.930	0.986	0.986	0.986	0.986
	10	0.549	0.033	0.033	0.033	0.511	0.496	0.496	0.496	0.853	0.853	0.853	0.853	0.966	0.966	0.966	0.966
	10	0.549	0.033	0.033	0.033	0.511	0.496	0.496	0.496	0.853	0.853	0.853	0.853	0.966	0.966	0.966	0.966
	12	−0.672	0.008	0.011	0.011	0.364	0.370	0.370	0.370	0.783	0.784	0.784	0.784	0.944	0.944	0.944	0.944
	14	−3.950	0.005	0.003	0.003	0.175	0.257	0.257	0.257	0.697	0.699	0.699	0.699	0.913	0.913	0.913	0.913
	16	−6.980	0.012	0.001	0.001	−0.015	0.166	0.166	0.166	0.597	0.601	0.601	0.601	0.871	0.871	0.871	0.871
	18	−0.193	−0.020	0.000	0.000	0.027	0.098	0.098	0.098	0.496	0.498	0.498	0.498	0.817	0.817	0.817	0.817
	20	31.300	−0.036	0.000	0.000	0.724	0.054	0.054	0.054	0.409	0.395	0.395	0.395	0.751	0.751	0.751	0.751
3	0	1.000	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	2	0.994	0.988	0.988	0.988	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	4	0.941	0.928	0.928	0.928	0.999	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	6	0.579	0.765	0.764	0.764	0.994	0.995	0.995	0.995	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	8	−1.090	0.490	0.496	0.496	0.966	0.976	0.976	0.976	0.998	0.998	0.998	0.998	0.999	0.999	0.999	0.999
	10	−3.140	0.181	0.152	0.152	0.742	0.780	0.780	0.780	0.939	0.940	0.940	0.940	0.979	0.979	0.979	0.979
	10	−3.140	0.181	0.152	0.152	0.742	0.780	0.780	0.780	0.939	0.940	0.940	0.940	0.979	0.979	0.979	0.979
	12	1.320	0.045	0.049	0.049	0.600	0.600	0.600	0.600	0.870	0.870	0.870	0.870	0.952	0.952	0.952	0.952
	14	9.610	−0.059	0.013	0.013	0.515	0.418	0.418	0.418	0.774	0.773	0.773	0.773	0.911	0.911	0.911	0.911
	16	6.720	0.100	0.003	0.003	0.355	0.262	0.262	0.262	0.654	0.653	0.653	0.653	0.851	0.851	0.851	0.851
	18	−17.700	0.076	0.000	0.000	−0.015	0.148	0.148	0.148	0.521	0.522	0.522	0.522	0.774	0.774	0.774	0.774
	20	−36.000	−0.346	0.000	0.000	−0.329	0.075	0.075	0.075	0.389	0.393	0.393	0.393	0.681	0.681	0.681	0.681

Table 3
Comparison results among present work (*CITT*), Liu et al. [7] (*GITT*) and Leij and van Genuchten [6] (L^{-1}).

Case	*x* (cm)	*t* = 0.2 day			*t* = 0.4 day			*t* = 0.6 day			*t* = 0.8 day		
		CITT	*GITT*	L^{-1}	*CITT*	*GITT*	L^{-1}	*CITT*	*GITT*	L^{-1}	*CITT*	*GITT*	L^{-1}
1	0	0.884	0.884	0.884	0.963	0.963	0.963	0.987	0.987	0.987	0.995	0.995	0.995
	2	0.742	0.742	0.742	0.915	0.915	0.915	0.969	0.969	0.969	0.988	0.998	0.988
	4	0.561	0.561	0.561	0.841	0.841	0.841	0.940	0.940	0.940	0.977	0.977	0.977
	6	0.375	0.374	0.375	0.746	0.746	0.746	0.901	0.901	0.901	0.962	0.962	0.962
	8	0.222	0.222	0.222	0.645	0.645	0.645	0.858	0.858	0.858	0.945	0.945	0.945
	10	0.142	0.142	0.142	0.579	0.579	0.579	0.829	0.829	0.829	0.933	0.933	0.933
	10	0.142	0.142	0.142	0.579	0.579	0.579	0.829	0.829	0.829	0.933	0.933	0.933
	12	0.063	0.063	0.063	0.480	0.480	0.480	0.781	0.781	0.781	0.914	0.914	0.914
	14	0.021	0.021	0.021	0.372	0.372	0.372	0.722	0.722	0.722	0.889	0.889	0.889
	16	0.005	0.005	0.005	0.264	0.265	0.264	0.651	0.651	0.651	0.858	0.858	0.858
	18	0.001	0.001	0.001	0.168	0.169	0.168	0.567	0.567	0.567	0.819	0.819	0.819
	20	0.000	0.000	0.000	0.094	0.094	0.094	0.473	0.473	0.473	0.770	0.770	0.770
2	0	0.978	0.977	0.978	0.998	0.998	0.998	1.000	1.000	1.000	1.000	1.000	1.000
	2	0.868	0.867	0.868	0.984	0.984	0.984	0.998	0.998	0.998	1.000	1.000	1.000
	4	0.634	0.633	0.634	0.942	0.942	0.942	0.991	0.991	0.991	0.999	0.999	0.999
	6	0.345	0.345	0.345	0.849	0.848	0.849	0.972	0.972	0.972	0.995	0.995	0.995
	8	0.131	0.131	0.131	0.693	0.693	0.693	0.930	0.929	0.930	0.986	0.986	0.986
	10	0.033	0.033	0.033	0.496	0.496	0.496	0.853	0.853	0.853	0.966	0.966	0.966
	10	0.033	0.033	0.033	0.496	0.496	0.496	0.853	0.853	0.853	0.966	0.966	0.966
	12	0.011	0.011	0.011	0.370	0.370	0.370	0.784	0.783	0.784	0.944	0.944	0.944
	14	0.003	0.003	0.003	0.257	0.257	0.257	0.699	0.698	0.699	0.913	0.913	0.913
	16	0.001	0.001	0.001	0.166	0.166	0.166	0.601	0.601	0.601	0.871	0.871	0.871
	18	0.000	0.000	0.000	0.098	0.099	0.098	0.498	0.498	0.498	0.817	0.817	0.817
	20	0.000	0.000	0.000	0.054	0.054	0.054	0.395	0.395	0.395	0.751	0.750	0.751
3	0	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	2	0.988	0.987	0.988	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
	4	0.928	0.928	0.928	0.999	0.999	0.999	1.000	1.000	1.000	1.000	1.000	1.000
	6	0.764	0.763	0.764	0.995	0.995	0.995	1.000	1.000	1.000	1.000	1.000	1.000
	8	0.496	0.495	0.496	0.976	0.976	0.976	0.998	0.998	0.098	0.999	0.999	0.999
	10	0.152	0.152	0.152	0.780	0.779	0.780	0.940	0.939	0.940	0.979	0.978	0.979
	10	0.152	0.152	0.152	0.780	0.779	0.780	0.940	0.939	0.940	0.979	0.978	0.979
	12	0.049	0.050	0.049	0.600	0.600	0.600	0.870	0.870	0.870	0.952	0.952	0.952
	14	0.013	0.013	0.013	0.418	0.418	0.417	0.773	0.773	0.773	0.911	0.910	0.911
	16	0.003	0.003	0.003	0.262	0.262	0.262	0.653	0.653	0.653	0.851	0.851	0.851
	18	0.000	0.000	0.000	0.148	0.148	0.148	0.522	0.522	0.522	0.774	0.774	0.774
	20	0.000	0.000	0.000	0.075	0.075	0.075	0.393	0.393	0.393	0.681	0.681	0.681

Table 4
Transport parameters for the five-layer test-case.

Layer	Velocity ($cm\ d^{-1}$)	Dispersion coefficient ($cm^2\ d^{-1}$)	Porosity	Retardation factor	Constant decay (d^{-1})
Sand	10	7	0.4	4.25	0
Clay	8	18	0.5	14	0

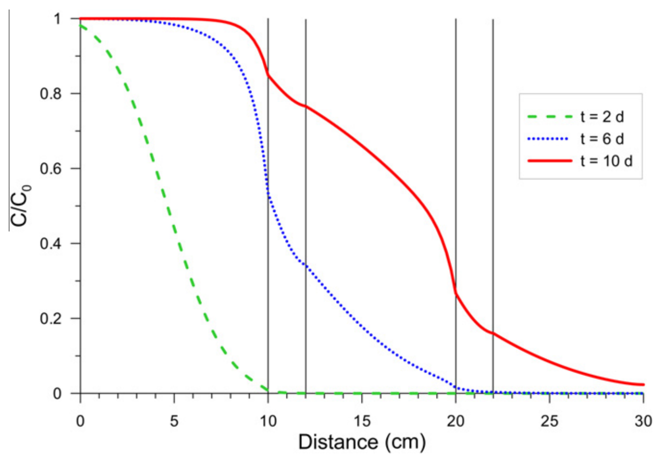

Fig. 1. Relative concentration (C/C_0) as a function of distance at three different times in a composite media with five-layers (sand-clay-sand-clay-sand).

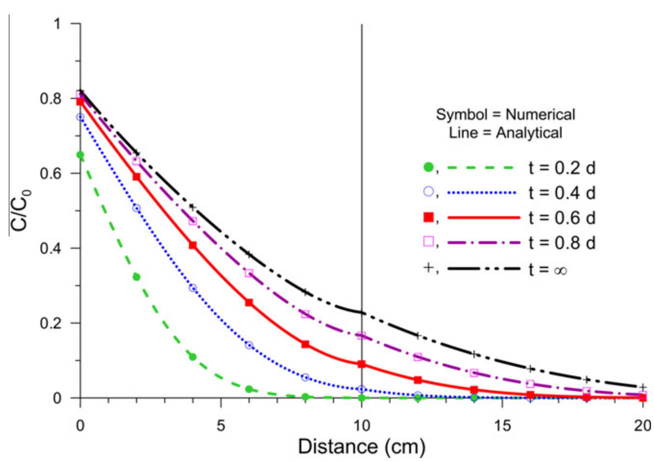

Fig. 2. Relative concentration (C/C_0) as a function of distance at five different times in a composite media with two-layers and solute decay (case 4 of Table 1, x_1 = 10 cm and x_2 = 30 cm).

4.2. Five-layer media

Table 4 gives parameter data for simulating advective–dispersive transport in a composite media consisting of five layers arranged as sand-clay-sand-clay-sand (with x_1 = 10 cm, x_2 = 12 cm, x_3 = 20 cm, x_4 = 22 cm and x_5 = 30 cm), as described in [7]. Fig. 1 illustrates the relative concentration distribution along the layers at the times t = 2, 6 and 10 days. The concentration distributions are in full agreement with those obtained previously in [7].

4.3. Adevection–dispersion transport equation with decay term

Case 4 of Table 1 gives parameter data for a hypothetical test case used to evaluate the present analytical solution when the decay term (μ_m) is nonzero. For this case the filter function developed in Appendix A corresponds to the steady state solution of the transport equation. The numbers of summed terms required in Eq. (43) were N = 30 and N = 40 for layers 1 and 2, respectively. Fig. 2 illustrates the solute concentration in each layer for different times. Also shown are results obtained numerically using the method of the lines as implemented in the Mathematica NDSolve library with options set to "ImplicitRungeKutta" [9]. It is noted that for long times the analytical solution corresponds to the steady state solution.

5. Conclusions

A closed-form analytical solution of the transient, one-dimensional advection–dispersion transport equation with first-order decay was obtained for multi-layered media using the classical integral transform technique (CITT) in conjunction with mathematical induction. The solution procedure used an associated non-self-adjoint advection–diffusion eigenvalue problem that had the same form and coefficients as the original problem. A transcendental equation for determining the eigenvalues was developed, which eliminated the risk of missing eigenvalues, a common potential limitation of these types of solution procedures. The performance of the analytical solution was evaluated by comparing results with those published previously by Liu et al. [7] and Leij and van Genuchten [6] for the case of two layers. The present analytical solution required no more than N = 15 terms to reproduce the previously published results. The number of terms required for convergence was significantly fewer than the N = 60 (or in some cases N = 120) terms reported for the Liu et al. solution [7]. The faster convergence was because the present analytical solution is based on an associated eigenvalue equation having the same form and coefficients as the original problem. A second test case involving a five-layer medium was also simulated and the obtaining concentration distributions were in full agreement with the previously reported results in [7]. A final test case illustrated the concentration distributions that arise in layered media when first-order decay exists.

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Appendix A. Determination of the filter function $F_m(x)$

This appendix explains the procedure for determining the form of the "filter" function $F_m(x)$ needed to transform Eqs. (1)–(3), which has non-homogeneous boundary conditions, into Eqs. (5)–(7), which has homogeneous boundary conditions. In Eq. (4), we introduced the expression:

$$c_m = F_m(x) + H_m(x,t) \qquad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{A1}$$

where $F_m(x)$ is the unknown filter function. Following a procedure similar to that given by Ozisik (1980), we substitute Eq. (A1) into Eqs. (1) and (2), which results in the following:

$$R_m \frac{\partial H_m}{\partial t} = L_m H_m + L_m F_m \qquad \begin{matrix} x_{m-1} < x < x_m \\ m = 1,2,3,\ldots,M \end{matrix} \tag{A2}$$

$$u_1[F_1(x)+H_1(x,t)] - D_1\frac{\partial}{\partial x}[F_1(x)+H_1(x,t)] = u_1\overline{C}_0; \quad x = x_0 = 0 \tag{A3a}$$

$$\left.\begin{matrix} F_m(x)+H_m(x,t) = F_{m+1}(x)+H_{m+1}(x,t) \\ k_m\frac{\partial}{\partial x}[F_m(x)+H_m(x,t)] = \\ k_{m+1}\frac{\partial}{\partial x}[F_{m+1}(x)+H_{m+1}(x,t)] \end{matrix}\right\} \quad \begin{matrix} x = x_m \\ m = 1,2,3,\ldots,M-1 \end{matrix} \tag{A3b,c}$$

$$\frac{\partial}{\partial x}[F_M(x)+H_M(x,t)]=0; \quad x=x_M \tag{A3d}$$

In comparing Eqs. (A2) and (A3) with the desired form of Eqs. (5)–(7), it is evident that Eqs. (5)–(7) will be obtained from Eqs. (A2)–(A3) if F_m satisfies the following:

$$L_mF_m(x)=0 \quad \begin{matrix} x_{m-1}<x<x_m \\ m=1,2,3,\ldots,M \end{matrix} \tag{A4}$$

$$u_1F_1-D_1\frac{\partial F_1}{\partial x}=u_1\overline{C}_0; \quad x=x_0=0 \tag{A5a}$$

$$\left.\begin{matrix} F_m=F_{m+1} \\ k_m\frac{dF_m}{dx}=k_{m+1}\frac{dF_{m+1}}{dx} \end{matrix}\right\} \quad x=x_m; \quad m=1,2,3,\ldots,M-1 \tag{A5b, c}$$

$$\frac{dF_M}{dx}=0; \quad x=x_M \tag{A5d}$$

The filter $F_m(x)$ is the solution of the Eqs. (A4)–(A5). The general solution is given by:

$$F_m(x)=a_m\exp[r1_mx]+b_m\exp[r2_mx] \tag{A6a}$$

$$r1_m=\frac{(u_m-\Delta_m)}{2D_m}; \quad r2_m=\frac{(u_m+\Delta_m)}{2D_m} \tag{A6b}$$

$$\Delta_m=\sqrt{u_m^2-4D_m\mu_m} \tag{A6c}$$

The coefficients a_m and b_m must be determined from the boundary conditions (Eq. (A5)).

Appendix B. Determination of the parameter values $\bar{p}_m$

This appendix gives the procedure for calculating parameter values $\bar{p}_m$ in the expression for the integrating factor $p_m(x)$, Eq. (27). The integrating factor transforms the non-self adjoint equation (8) into a self-adjoint equation with the same dependent quantity, ψ_m. The boundary conditions, Eqs. (9a,b,d) and (25a,b,d), are the same. Eq. (9c) will be re-written in the form of Eq. (25c) by considering an appropriate definition of the coefficient $\bar{p}_m$. For position $x = x_1$, we have:

$$\bar{p}_1\exp\left[-\frac{u_1}{D_1}(x_1-\bar{x}_1)\right]\frac{d\psi_1(x_1)}{dx} = \bar{p}_2\exp\left[-\frac{u_2}{D_2}(x_1-\bar{x}_2)\right]\frac{d\psi_2(x_1)}{dx} \tag{B1}$$

Then considering $\bar{x}_1=x_1$, $\bar{x}_2=x_2$ and $\bar{p}_1=k_1$ leads to

$$\bar{p}_1\frac{d\psi_1(x_1)}{dx}=\bar{p}_2\exp\left[-\frac{u_2}{D_2}(x_1-x_2)\right]\frac{d\psi_2(x_1)}{dx} \tag{B2}$$

By choosing $\bar{p}_2=k_2\exp\left[\frac{u_2}{D_2}(x_1-x_2)\right]$ in Eq. (B2) we obtain Eq. (9c) as required.

Similarly, for position $x = x_2$:

$$\bar{p}_2\exp\left[-\frac{u_2}{D_2}(x_2-\bar{x}_2)\right]\frac{d\psi_2(x_2)}{dx} = \bar{p}_3\exp\left[-\frac{u_3}{D_3}(x_2-\bar{x}_3)\right]\frac{d\psi_3(x_2)}{dx} \tag{B3}$$

Then taking $\bar{x}_2=x_2,\ \bar{x}_3=x_3$ results in,

$$k_2\exp\left[\frac{u_2}{D_2}(x_1-x_2)\right]\frac{d\psi_2(x_2)}{dx}=\bar{p}_3\exp\left[-\frac{u_3}{D_3}(x_2-x_3)\right]\frac{d\psi_3(x_2)}{dx} \tag{B4}$$

Considering again Eq. (9c) leads to:

$$\bar{p}_3=k_3\exp\left[\frac{u_2}{D_2}(x_1-x_2)+\frac{u_3}{D_3}(x_2-x_3)\right] \tag{B5}$$

For position $x = x_3$, we have:

$$\bar{p}_3\exp\left[-\frac{u_3}{D_3}(x_3-\bar{x}_3)\right]\frac{d\psi_3(x_3)}{\partial x} = \bar{p}_4\exp\left[-\frac{u_4}{D_4}(x_3-\bar{x}_4)\right]\frac{d\psi_4(x_3)}{\partial x} \tag{B6}$$

Then for $\bar{x}_3=x_3$ and $\bar{x}_4=x_4$:

$$k_3\exp\left[\frac{u_2}{D_2}(x_1-x_2)+\frac{u_3}{D_3}(x_2-x_3)\right]\frac{d\psi_3(x_3)}{\partial x} = \bar{p}_4\exp\left[-\frac{u_4}{D_4}(x_3-x_4)\right]\frac{d\psi_4(x_3)}{\partial x} \tag{B7}$$

Eq. (9c) requires that:

$$\bar{p}_4=k_4\exp\left[\frac{u_2}{D_2}(x_1-x_2)+\frac{u_3}{D_3}(x_2-x_3)+\frac{u_4}{D_4}(x_3-x_4)\right] \tag{B8}$$

Finally, by using mathematical induction, it is possible to obtain a generalized expression for $\bar{p}_m$ in position x_m:

$$\bar{p}_m=k_m\exp\left[\sum_{\bar{m}=2}^{m}\frac{u_{\bar{m}+1}}{D_{\bar{m}+1}}(x_{\bar{m}-1}-x_{\bar{m}})\right] \tag{B9}$$

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