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Integral transform solution for solute transport in multi-layered porous media with the implicit treatment of the interface conditions and arbitrary boundary conditions

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SUMMARY

Solute transport in multi-layered porous media is of great importance in environmental engineering problems. Its important feature lies in the explicit existence of interface conditions. The previous analytical solutions require explicitly considering the interface conditions in the evaluation of coefficients or in the eigenvalue system. In the present study, an implicit treatment of interface conditions is presented to eliminate the interface conditions from the original system. The generalized integral transform technique is performed with respect to the transformed system to obtain the analytical solution. Compared to the pervious solution strategy, the present eigenfunctions are much simpler. The present analytical solution and eigenvalue system are expressed for the generalized boundary conditions by introducing two boundary factors in the boundary conditions, which applies to arbitrary assembly of boundary conditions without modification and can reduce the effort of programming. The developed analytical solution is validated against two experiments and one analytical solution. Good agreement is shown between the experimental data and analytical as well as numerical solutions.

1. Introduction

Solute transport in single-layered porous media is common in natural environments and artificial environments. Analytical solutions for solute transport in single-layered porous media have been presented in finite and semi-infinite porous media by using Laplace transform technique or the method of variable of separation (Bauer et al., 2001; Chen et al., 2002; Chen and Liu, 2011; Cleary and Dean, 1972; Didierjean et al., 2004; Hassan et al., 2001; Huang et al., 1996; Pérez Guerrero and Skaggs, 2010; Pérez Guerrero et al., 2009, 2010; Van Genuchten, 1982; Xie et al., 2011). In environmental engineering problems, solute transport in multi-layered porous media is often observed, such as leachate transfer in landfills, contaminant diffusion in capping layers over contaminated sediment and stratified soils. Compared to solute transport in single-layered problem, the transport parameters in each layer may be different, resulting in a jump of parameters at the interface of the adjacent layer. In addition to the boundary conditions at the inlet and outlet, there explicitly exist the interface conditions between the adjacent layers, which must be met to guarantee the mass conservation and the continuity of the concentration at the interface of the adjacent layer.

Some authors have presented analytical solutions of solute transport in multi-layered porous media. Leij and van Genuchten (1995) considered the advection and diffusion of solute in semi-infinite two-layered media. The analytical solution in Laplace domain was obtained and an approximate solution in time domain was derived. Liu and Ball (1998) investigated the diffusion of solute in semi-infinite two-layered media with arbitrary boundary and initial conditions. An analytical solution in time domain was derived by using the superposition method, Laplace transform and binomial theorem. Chen et al. (2009) obtained an analytical solution of solute transport in multi-layered media by establishing the analogy between solute transport in multi-layered media and consolidation of layered soil. The coefficients in the analytical solution were obtained by solving a recurrence equation. This analogy virtually means the application of the method of separating variables. Li and Cleall (2010) applied the same analogy as Chen et al. (2009) to derive analytical solutions of solute transport in double-layered media with various boundary conditions. Several forms of solution were required for different boundary conditions. The aforementioned literatures firstly obtained the analytical solutions in Laplace domain or time domain with two undetermined coefficients in each layer and then evaluated these undetermined

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coefficients by using the interface conditions. In other words, the interface conditions must be considered explicitly. Liu et al. (1998) studied the advection–diffusion of solute in multi-layered media. An analytical solution was developed by using the generalized integral transform technique. This study put emphasis on the arbitrary initial condition and inlet boundary condition. The interface conditions appear explicitly in the eigenvalue system.

All the aforementioned solutions require explicitly considering the interface conditions in the evaluation of coefficients or in the eigenvalue system, which bring about a lot of complexity. The aim of the present study is to implicitly treat the interface conditions in the multi-layered solute transport and further simplify the solution of eigenfunctions required in the formal analytical solutions.

2. Problem formulation

For multi-layered porous media, solute transport in each layer can be described by one dimensional transient advection–diffusion equation as follows;

$$R_i \frac{\partial C}{\partial t} + v_i \frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(D_i \frac{\partial C}{\partial x}\right) \quad x_{i-1} \leqslant x \leqslant x_i \tag{1}$$

where C is the concentration, R_i retardation factor, v_i velocity and D_i diffusion coefficient. For simplicity, $x_0 = 0$ is set. The porous media is assumed to contain N homogeneous layer. Due to the existence of layer interface, Eq. (1) should meet the following requirement at the interface of the adjacent layers, which reads

$$C(x_i^-, t) = C(x_i^+, t) \tag{2}$$

$$\varepsilon_i v_i C(x_i^-, t) - \varepsilon_i D_i \frac{\partial C(x_i^-, t)}{\partial x} = \varepsilon_{i+1} v_{i+1} C(x_i^+, t) - \varepsilon_{i+1} D_{i+1} \times \frac{\partial C(x_i^+, t)}{\partial x} \tag{3}$$

where ε_i is the porosity of each layer. Eqs. (2), and (3) guarantee the mass conservation and the continuity of concentration at the layer interface.

At the inlet, the first-type or third-type boundary condition is usually used. At the outlet, the first-type, second-type or third-type boundary condition can be used. All types of boundary conditions can be expressed in a unified form by introducing boundary parameters, which read

$$v_1 (f_i(t) - \Omega_{i,1} C(x_0, t)) = -\Omega_{i,2} D_1 \frac{\partial C(x_0, t)}{\partial x} \tag{4}$$

$$v_N (\Omega_{o,1} C(x_N, t) - f_o(t)) = -\Omega_{o,2} D_N \frac{\partial C(x_N, t)}{\partial x} \tag{5}$$

The values of Ω are unity or zero with constraints of $\Omega_{i,1} + \Omega_{i,2} \neq 0$ and $\Omega_{o,1} + \Omega_{o,2} \neq 0$. The values of Ω determine the kind of boundary condition, as shown in Table 1.

Eq. (1) is subjected to the following initial condition

$$C(x, 0) = g(x) \tag{6}$$

3. The implicit treatment of interface conditions

The solution methodology in the present study is to eliminate the interface conditions firstly and then to perform integral transform. Since the porosity of each layer is a constant, Eq. (1) can be rewritten as follows

$$\varepsilon_i R_i \frac{\partial C}{\partial t} + \varepsilon_i v_i \frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\varepsilon_i D_i \frac{\partial C}{\partial x}\right) \quad x_{i-1} \leqslant x \leqslant x_i \tag{7}$$

Table 1
Types of boundary conditions.

Scenario	Inlet BC	Outlet BC
1	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 0$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 0$
2	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 0$	$\Omega_{o,1} = 0,\ \Omega_{o,2} = 1$
3	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 0$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 1$
4	$\Omega_{i,1} = 0,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 0$
5	$\Omega_{i,1} = 0,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 0,\ \Omega_{o,2} = 1$
6	$\Omega_{i,1} = 0,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 1$
7	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 0$
8	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 0,\ \Omega_{o,2} = 1$
9	$\Omega_{i,1} = 1,\ \Omega_{i,2} = 1$	$\Omega_{o,1} = 1,\ \Omega_{o,2} = 1$

Thus, by defining the following mathematical transform

$$\overline{R}(x) = \begin{cases} \varepsilon_1 R_1 & x_0 \leqslant x \leqslant x_1 \\ \varepsilon_2 R_2 & x_1 \leqslant x \leqslant x_2 \\ \vdots & \vdots \\ \varepsilon_3 R_N & x_{N-1} \leqslant x \leqslant x_N \end{cases} \tag{8}$$

$$\bar{v}(x) = \begin{cases} \varepsilon_1 v_1 & x_0 \leqslant x \leqslant x_1 \\ \varepsilon_2 v_2 & x_1 \leqslant x \leqslant x_2 \\ \vdots & \vdots \\ \varepsilon_N v_N & x_{N-1} \leqslant x \leqslant x_N \end{cases} \tag{9}$$

$$\overline{D}(x) = \begin{cases} \varepsilon_1 D_1 & x_0 \leqslant x \leqslant x_1 \\ \varepsilon_2 D_2 & x_1 \leqslant x \leqslant x_2 \\ \vdots & \vdots \\ \varepsilon_N D_N & x_{N-1} \leqslant x \leqslant x_N \end{cases} \tag{10}$$

Then, Eqs. (1), and 4, 5, 6 can be rewritten as follows;

$$\overline{R}(x) \frac{\partial C}{\partial t} + \bar{v}(x) \frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\overline{D}(x) \frac{\partial C}{\partial x}\right) \tag{11}$$

$$\bar{v}(x_0)(f_i(t) - \Omega_{i,1} C(x_0, t)) = -\Omega_{i,2} \overline{D}(x_0) \frac{\partial C(x_0, t)}{\partial x} \tag{12}$$

$$\bar{v}(x_N)(\Omega_{o,1} C(x_N, t) - f_o(t)) = -\Omega_{o,2} \overline{D}(x_N) \frac{\partial C(x_N, t)}{\partial x} \tag{13}$$

$$C(x, 0) = g(x) \tag{14}$$

Apparently, Eq. (11) reproduces Eq. (1) in each layer with the definition of Eqs. 8–10. Since Eq. (11) describes the same concentration field as Eq. (1), Eq. (2) can be totally guaranteed in Eq. (11). On the other hand, the transport flux at any position can be written as

$$q = \bar{v}(x) C - \overline{D}(x) \frac{\partial C}{\partial x} \tag{15}$$

The mass cannot be accumulated at the interface, which means

$$q|_{x_i^-} = q|_{x_i^+} \tag{16}$$

Taking into account the existence of Eqs. (9), (10), and (15), Eq. (16) is just the same as Eq. (3). Therefore, the interface conditions, i.e., Eqs. (2), and (3), are implied in Eq. (11). It means that the interface conditions, i.e., Eqs. (2), and (3), does not require to be considered explicitly in the system of Eqs. 11–14.

4. Analytical solution

Eq. (11) is virtually a partial differential equation with variable parameters. It can be solved by the use of generalized integral