Semi-analytical solutions to 2D advection-dispersion-reaction equations in a finite domain subject to point-source and boundary-source

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Abstract

Advection-dispersion-reaction equations are widely used to simulate heat and mass transport problems in science and engineering. Analytical and semi-analytical solutions to such problems are highly desirable but are currently limited to a single type of source. This limitation poses significant challenges to the interaction analysis between different types of sources and the accurate inversion of the actual source zone. In this paper, we developed a two-dimensional analytical model for solute transport in a finite domain subject to both internal point sources and boundary sources. The solution approach applies Laplace transform combined with finite Fourier transform and variable substitution to obtain the generalized semi-analytical solution. An instantaneous point source system, together with Dirichlet and Robin inlet boundary, is selected to investigate the solute transport behavior in a multi-source scenario. Results reveal that the solute transport system with point source and Dirichlet boundary source has the largest predicted concentration. The selection of inlet boundaries for the model with low-permeability media (small Péclet number) or highly reactive (large Damköhler number) is of great importance, especially when performing long-term predictions.

Keywords: Solute transport, Advection-dispersion-reaction equation, Analytical solution, Point source, Boundary source

Introduction

Solute fate and transport in porous media are generally modeled using the advection-dispersion-reaction (ADR) equations. Analytical solutions to ADR equations are of great value as they provide more fundamental insight into migration behavior and can serve as a benchmark for complex numerical models. Consequently, a number of analytical or semi-analytical solutions to one- and multi-dimensional ADR equations have been developed to simulate various solute transport problems in porous media [1]. For example, Cleary and Adrian [2] and van Genuchten and Alves [3] presented several analytical solutions to the one-dimensional (1D) ADR equation with various combinations of boundary conditions. Batu [4][5] derived two-dimensional (2D) analytical solutions for solute transport in a unidirectional flow field subject to Dirichlet and Roin influent boundary conditions. Leij et al. [6] and Guerrero et al. [7] formulated analytical solutions for three-dimensional (3D) ADR equations in the semi-infinite and finite spatial domains, respectively. The solute sources in these models mentioned above are imposed by boundary conditions, and such problems are generally referred to as boundary-value problems.

In contrast to the boundary-value problems, another class of transport problems uses the source term of the ADR equation to introduce internal point sources. Bear [8] originally developed an analytical solution for instantaneous injection of a point source. Basha and El-Habel [9] proposed a 1D analytical solution for ADR equations with time-dependent source terms and dispersion coefficients in an infinite domain. Aral and Liao [10] generalized this solution to the two-dimensional infinite system and gave special solutions for instantaneous and constant-rate injection source scenarios. Employing the cosine Fourier series and Laplace transform, Fedi [11] derived an analytical solution for non-reactive solute transport in 2D semi-infinite domain with an instantaneous point injection source. Recently, Ding et al. [12] proposed a 2D analytical solution of ADR equations to investigate the reactive solute transport in a finite domain incorporating multiple arbitrary time-dependent point sources. However, the concentration gradient at the inlet boundary of the multi-point source model is set to zero, which cannot reflect the solute intrusion outside the transport system.

This study extends the method proposed by Ding et al. [12] and develops 2D analytical solutions for reactive solute transport in a finite field involving advection-dispersion-reaction processes subject to internal point sources and boundary sources. The validity of the present solutions is achieved by comparing them against corresponding numerical results. Using these solutions, the influent boundary conditions and transport parameters on the solute migration behavior will be investigated.

Transport model

This study presents a two-dimensional model for solute transport in a finite spatial domain with internal point sources and boundary sources. The groundwater flow is steady and uniform along the horizontal direction. The solute is injected through internal point mass sources and concentration sources at the inlet boundary. The injected solute migrates in the horizontal direction by advection and horizontal dispersion and undergoes vertical dispersion. The transport model also couples linear sorption and first-order reactions of solute, so it is described by the two-dimensional advection-dispersion-reaction equation as follows:

$$\begin{aligned} R\frac{\partial C(x,z,t)}{\partial t} &= D_x\frac{\partial^2 C(x,z,t)}{\partial x^2} + D_z\frac{\partial^2 C(x,z,t)}{\partial z^2} - v\frac{\partial C(x,z,t)}{\partial x} - \mu C(x,z,t) \\ &\quad + \sum_{i=1}^{n} q_i(t)\delta(x-x_i)\delta(z-z_i) \end{aligned} \tag{1}$$

where C is the solute concentration [ML^{-3}] in the finite domain; R is the retardation factor [dimensionless]; D_x and D_z are the hydrodynamic dispersion coefficients [L^2T^{-1}], respectively; v is the pore-water seepage velocity [LT^{-1}]; μ is the first-order reaction constant [T^{-1}]. The time-dependent function $q_i(t)$ [$ML^{-1}T^{-1}$] and Dirac delta function $\delta(x\text{-}x_i)\delta(z\text{-}z_i)$ represents the strength and location of the i-th point sources in the finite domain, respectively.

Initially, the solute concentration in the finite field is assumed to be zero:

$$C(x,z,t=0)=0 \tag{2}$$

The boundary conditions considered herein are:

$$\frac{\partial C(x,z=0,t)}{\partial z}=0 \tag{3}$$

$$\frac{\partial C(x,z=H,t)}{\partial z}=0 \tag{4}$$

$$C(x=0,z,t)=c_s(z) \ \ (\textit{Dirichlet boundary}) \tag{5}$$

$$\text{or } -D_x\frac{\partial C(x=0,z,t)}{\partial x}+vC(x=0,z,t)=vc_s(z) \ \ (\textit{Robin boundary}) \tag{6}$$

$$\frac{\partial C(x=L,z,t)}{\partial x}=0 \tag{7}$$

Two different inlet boundaries are adopted, namely the Dirichlet boundary (or concentration-type) condition of Eq.(5) and the Robin boundary (flux-type) condition of Eq.(6). The concentration of these two types of boundary sources can be an arbitrary depth-dependent function.

Solution method

For mathematical convenience and solution generalization, the following dimensionless parameters are introduced.

$$x_D=\frac{x}{L},z_D=\frac{z}{H},t_D=\frac{tv}{L},\xi=\frac{L}{H},\eta=\frac{D_z}{D_x},\mathrm{Pe}=\frac{vL}{D_x},\mathrm{Da}=\frac{\mu L^2}{D_x},C_D=\frac{C}{C_0},Q_i=\frac{q_i}{C_0D_x} \tag{8}$$

where C_0 is the maximum concentration at the inlet boundary (x = 0), and thus the dimensionless concentration of boundary source $c_{s,D} = c_s/C_0$; Pe is the Péclet number, and Da is the Damköhler number. Then, substituting these above dimensionless parameters into Eqs. (1)-(7), one derives the dimensionless form as follows:

$$\begin{aligned}\mathrm{Pe}R\frac{\partial C_D(x_D,z_D,t_D)}{\partial t_D}&=\frac{\partial^2 C_D(x_D,z_D,t_D)}{\partial x_D^2}+\eta\xi^2\frac{\partial^2 C_D(x_D,z_D,t_D)}{\partial z_D^2}-\mathrm{Pe}\frac{\partial C_D(x_D,z_D,t_D)}{\partial x_D}\\&-\mathrm{Da}C_D(x_D,z_D,t_D)+\sum_{i=1}^{n}\xi Q_i(t_D)\delta(x_D-x_{D,i})\delta(z_D-z_{D,i})\end{aligned} \tag{9}$$

$$C_D(x_D,z_D,t_D=0)=0 \tag{10}$$

$$\frac{\partial C_D(x_D,z_D=0,t_D)}{\partial z_D}=0 \tag{11}$$

$$\frac{\partial C_D(x_D,z_D=1,t_D)}{\partial z_D}=0 \tag{12}$$

$$C_D(x_D=0,z_D,t_D)=c_{s,D}(z_D) \tag{13}$$

$$\text{or } -\frac{\partial C_D(x_D=0,z_D,t_D)}{\partial x_D}+\mathrm{Pe}C_D(x_D=0,z_D,t_D)=\mathrm{Pe}c_{s,D}(z_D) \tag{14}$$

$$\frac{\partial C_D(x_D=1,z_D,t_D)}{\partial x_D}=0 \tag{15}$$

Applying the Laplace transform and finite Fourier transform techniques to the time variable t and spatial variable z of the governing equation (Eq. (9)), combining the initial condition of Eq. (10) and boundary conditions of Eqs. (11)-(12), one can give a second-order ordinary differential equation in the transform domain:

$$\begin{aligned}&\frac{\partial^2 \hat{\bar{C}}_D(x_D,k,s)}{\partial x_D^2} - \mathrm{Pe}\frac{\partial \hat{\bar{C}}_D(x_D,k,s)}{\partial x_D} - (\mathrm{Pe}Rs + \mathrm{Da} + \eta\xi^2 k^2\pi^2)\hat{\bar{C}}_D(x_D,k,s)\\ &= -\sum_{i=1}^{n}\xi\bar{Q}_i(s)\delta(x_D - x_{D,i})\cos(k\pi z_{D,i})\end{aligned} \tag{16}$$

where s and k are the Laplace transform and finite Fourier cosine transform parameters, respectively, and the specific expressions of the two transform techniques are:

$$\bar{f}(s) = L_T\left[f(t_D)\right] = \int_0^{+\infty} f(t_D)e^{-st_D}dt_D \tag{17}$$

$$\hat{g}(k) = F_c\left[g(z_D)\right] = \int_0^1 g(z_D)\cos(k\pi z_D)dz_D \tag{18}$$

where L_T and F_c are the Laplace transform and Fourier cosine transform operators, respectively.

After, the above governing equation (Eq. (16)) can be transformed into:

$$\begin{aligned}&\frac{d}{dx_D}\left(\frac{d\hat{\bar{C}}_D(x_D,k,s)}{dx_D} - \alpha_k\hat{\bar{C}}_D(x_D,k,s)\right) - \beta_k\left(\frac{d\hat{\bar{C}}_D(x_D,k,s)}{dx_D} - \alpha_k\hat{\bar{C}}_D(x_D,k,s)\right)\\ &= -\sum_{i=1}^{n}\xi\bar{Q}_i(s)\delta(x_D - x_{D,i})\cos(k\pi z_{D,i})\end{aligned} \tag{19}$$

where

$$\begin{cases}\alpha_k = (\mathrm{Pe} + \sqrt{\mathrm{Pe}^2 + 4(\mathrm{Pe}Rs + \mathrm{Da} + \eta\xi^2k^2\pi^2)})/2\\ \beta_k = (\mathrm{Pe} - \sqrt{\mathrm{Pe}^2 + 4(\mathrm{Pe}Rs + \mathrm{Da} + \eta\xi^2k^2\pi^2)})/2\end{cases} \tag{20}$$

Using the substitution method [12], the following new variable is introduced:

$$Y(x_D,k,s) = \frac{d\hat{\bar{C}}_D(x_D,k,s)}{dx_D} - \alpha_k\hat{\bar{C}}_D(x_D,k,s) \tag{21}$$

Substituting the variable of Eq. (21) into Eq. (19) yields:

$$\frac{dY(x_D,k,s)}{dx_D} - \beta_k Y(x_D,k,s) + \sum_{i=1}^{n}\xi\bar{Q}_i(s)\delta(x_D - x_{D,i})\cos(k\pi z_{D,i}) = 0 \tag{22}$$

Solving the above two coupled first-order ordinary differential equations (Eqs. (21)-(22)) gives the general solution in the Laplace-Fourier transform domain:

$$\hat{\bar{C}}_D(x_D,k,s) = A_k e^{\alpha_k x_D} + B_k e^{\beta_k x_D} - \sum_{i=1}^{n}\frac{\xi\bar{Q}_i(s)H_v(x_D - x_{D,i})(e^{\alpha_k(x_D - x_{D,i})} - e^{\beta_k(x_D - x_{D,i})})\cos(k\pi z_{D,i})}{(\alpha_k - \beta_k)} \tag{23}$$

where the coefficients A_k and B_k can be determined by inlet and outlet boundary conditions, and they are provided as follows.

Dirichlet inlet boundary scenario:

Applying the Laplace and finite Fourier cosine transforms (Eqs. (17)-(18)) to the inlet and outlet boundary conditions (Eqs. (13) and (15)) yields:

$$\begin{cases} \hat{\bar{C}}_D(x_D=0,k,s)=\hat{c}_{s,D}(k) \\ \dfrac{\partial \hat{\bar{C}}_D(x_D=1,k,s)}{\partial x_D}=0 \end{cases} \tag{24}$$

Substituting the boundary conditions of Eq. (24) in the transform domain into the general solution of Eq. (23), the coefficients A_k and B_k are solved as follows:

$$\begin{cases} A_k=\dfrac{\mathrm{G}(k,s)-\beta_k e^{\beta_k}\hat{c}_{s,D}(k)}{\alpha_k e^{\alpha_k}-\beta_k e^{\beta_k}} \\ B_k=\dfrac{\alpha_k e^{\alpha_k}\hat{c}_{s,D}(k)-\mathrm{G}(k,s)}{\alpha_k e^{\alpha_k}-\beta_k e^{\beta_k}} \end{cases} \tag{25}$$

where

$$\mathrm{G}(k,s)=\sum_{i=1}^{n}\frac{\xi\bar{Q}_i(s)(\alpha_k e^{\alpha_k(1-x_{D,i})}-\beta_k e^{\beta_k(1-x_{D,i})})\cos(k\pi z_{D,i})}{(\alpha_k-\beta_k)} \tag{26}$$

Robin inlet boundary scenario:

Following a similar procedure as above, the Robin inlet and Neumann outlet boundary conditions (Eqs. (14) and (15)) can be rewritten in the Laplace-Finite cosine transform domain as follows:

$$\begin{cases} -\dfrac{\partial \hat{\bar{C}}_D(x_D=0,k,s)}{\partial x_D}+\mathrm{Pe}\hat{\bar{C}}_D(x_D=0,k,s)=\mathrm{Pe}\hat{c}_{s,D}(k) \\ \dfrac{\partial \hat{\bar{C}}_D(x_D=1,k,s)}{\partial x_D}=0 \end{cases} \tag{27}$$

and the corresponding coefficients A_k and B_k are:

$$\begin{cases} A_k=\dfrac{(\mathrm{Pe}-\beta_k)\mathrm{G}(k,s)-\beta_k e^{\beta_k}\mathrm{Pe}\hat{c}_{s,D}(k)}{\alpha_k e^{\alpha_k}(\mathrm{Pe}-\beta_k)-\beta_k e^{\beta_k}(\mathrm{Pe}-\alpha_k)} \\ B_k=\dfrac{e^{\alpha_k}\mathrm{Pe}\hat{c}_{s,D}(k)-(\mathrm{Pe}-\alpha_k)\mathrm{G}(k,s)}{\alpha_k e^{\alpha_k}(\mathrm{Pe}-\beta_k)-\beta_k e^{\beta_k}(\mathrm{Pe}-\alpha_k)} \end{cases} \tag{28}$$

Finally, employing the inverse Fourier cosine transform to Eq. (23) yields a closed-form solution for the solute concentration in the Laplace domain, as follows:

$$\begin{aligned} \bar{C}_D(x_D,z_D,s)&=A_{k=0}e^{\alpha_{k=0}x_D}+B_{k=0}e^{\beta_{k=0}x_D}-\sum_{i=1}^{n}\frac{\xi\bar{Q}_i(s)H_v(x-x_{D,i})(e^{\alpha_{k=0}(x_D-x_{D,i})}-e^{\beta_{k=0}(x_D-x_{D,i})})}{(\alpha_{k=0}-\beta_{k=0})} \\ &+\sum_{k=1}^{\infty}2(A_k e^{\alpha_k x_D}+B_k e^{\beta_k x_D}-\sum_{i=1}^{n}\frac{\xi\bar{Q}_i(s)H_v(x-x_{D,i})(e^{\alpha_k(x_D-x_{D,i})}-e^{\beta_k(x_D-x_{D,i})})\cos(k\pi z_{D,i})}{(\alpha_k-\beta_k)})\cos k\pi z_D \end{aligned} \tag{29}$$

and the Laplace inversion is then implemented using the Stehfest inversion algorithm to give the transient concentration solution.

Result and discussion

In this section, an instantaneous-release source scenario is used as an example to investigate the correctness of the developed solution as well as its practical applications. The mathematical description of the instantaneous source strength is:

$$q_i(t) = M_i \delta(t - t_i) \tag{30}$$

where M_i is the released mass of the i-th point source; and $\delta(t\text{-}t_i)$ is a Dirac delta function where t_i is the release moment.

Two instantaneous point sources are located at the (x = 5m, z = 7.5m) and (x = 5m, z = 12.5m) in a finite domain, and each source has a total release mass of $M_1 = M_2 = 100$ g/m at $t_1 = t_2 = 0$ day. Other material and transport parameters for the finite domain model are given in Table 1.

Table 1. Input Parameters [12].

Parameter description	Symbol	Value
Length of the finite spatial domain	L	30 m
Height of the finite spatial domain	H	20 m
The average seepage velocity	v	0.1 m/day
Horizontal hydrodynamic dispersion coefficients	D_x	0.1 m^2/day
Vertical hydrodynamic dispersion coefficients	D_z	0.03 m^2/day
Sorption retardation factor	R_d	5.3
First-order decay rate coefficient	μ	0.002 day^{-1}

Comparison with analytical solutions and numerical results

As mentioned in the introduction, the Neumann inlet boundary is generally used in previous point source models, which does not reflect the influence of external sources on the transport system. Therefore, this study compared three types of inlet boundary sources on the solute concentration distribution in the transport system (Fig. 1). The predictive model with a constant concentration boundary source (i.e., Dirichlet inlet boundary) presented the maximum solute concentration. The difference in concentration prediction for different inlet boundary cases decreased with an increase in transport distance but gradually increased with time. This implied that solute transport models subject to both the boundary sources and the internal point sources should pay attention to the selection of the inlet boundary conditions, especially when performing long-term predictions. Fig. 1 also shows that the present analytical solutions for Dirichlet-boundary (displayed as solid curves) and Robin-boundary cases (dash-dot curves) agree well with the numerical results (open dots), providing some confidence in the reliability of the developed analytical solution.

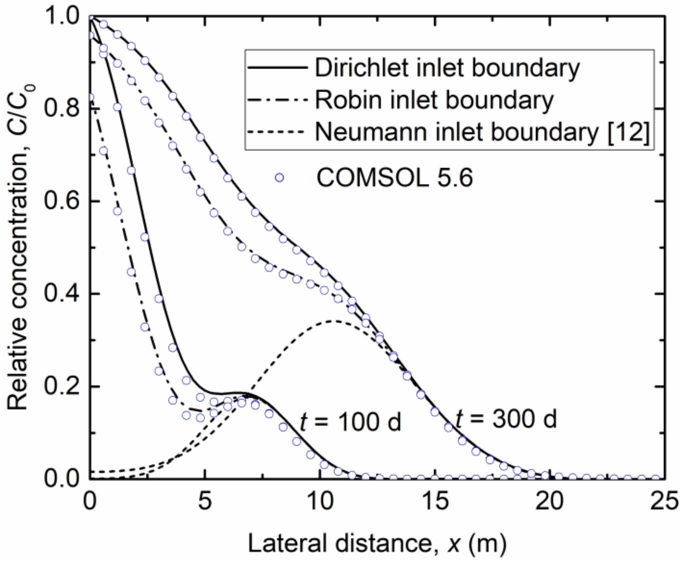

Figure 1. Effect of the inlet boundary condition on the concentration distributions

Effect of Péclet number (Pe) *and Damköhler number* (Da)

The Péclet number (Pe) is a dimensionless number that measures the relative importance of advection and diffusion, where a large number indicates an advection-dominated transport system and a small number indicates a diffuse flow. Fig. 2 investigated the effect of Pe numbers as well as inlet boundary types on the breakthrough curves at different observation locations. One observation is located upstream of the point source (x = 4 m), and the other is located downstream of x = 10 m. The solute concentration at x = 4 m increased significantly with increasing Péclet number Pe, especially in the case of the Robin inlet boundary condition (Fig. 2a). For transport systems with smaller Pe, the difference in predictions between the Dirichlet and Robin boundary source models was greater. For example, at t = 2000 days the relative difference between the predicted concentrations of the two cases for Pe = 20 was 4.4%, while for Pe = 5, this relative difference in prediction could be up to 58.3%. This suggested that the selection of inlet boundary conditions was of particular importance when performing contamination prediction for low permeability sites. For the downstream observation point (x = 10 m), the effect of the inlet boundary condition on the breakthrough curve could be seen after about 300 days (Fig. 2b). Although the observation locations were far from the entrance boundary (x = 10 m), the effect of the Péclet number on the breakthrough curve is still evident. However, the difference in concentrations at x = 10 m predicted by the Dirichlet and Robin boundary source models was relatively smaller compared to the case of a closer observation point (x = 4 m). An important reason is that the concentration at the downstream observation point of x = 10 m is affected by the coupling of point and boundary sources.

A dimensionless number, Damköhler number (Da), is generally used to indicate the rate of the first-order degradation reaction. The increase in Da caused a significant decrease in solute concentration, which is due to the accelerated consumption by biochemical reaction (Fig. 3). Moreover, for a larger Da, the difference in predictions between the Dirichlet and Robin boundary source models was greater. This illustrated that the prediction model for a strongly degradable system also requires careful selection of entrance boundary conditions.

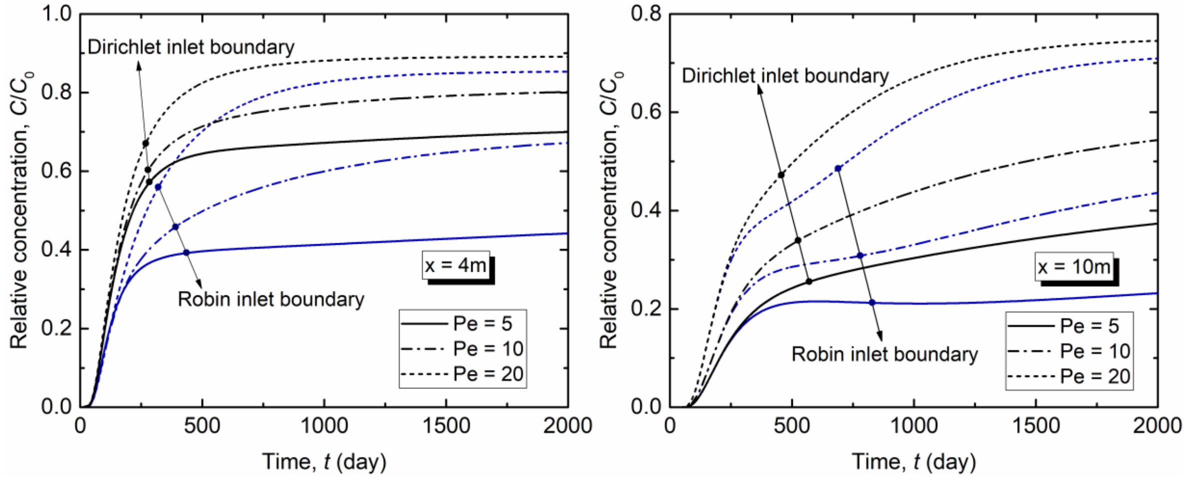

Figure 2. Effect of the Péclet number on the breakthrough curve: (a) the upstream observation point, x = 4 m; (b) the downstream observation point, x = 10 m.

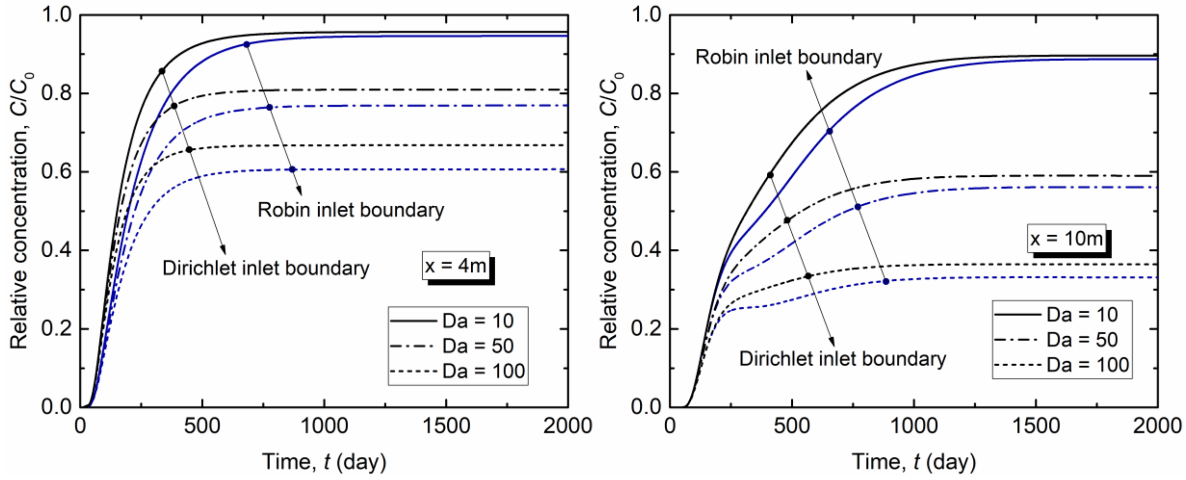

Figure 3. Effect of the Damköhler number on the breakthrough curve: (a) the upstream observation point, x = 4 m; (b) the downstream observation point, x = 10 m.

Conclusion

This study developed a generalized semi-analytical solution for advection-dispersion-reaction equations subject to point-source and boundary-source. Our solution strategy combined Laplace transform, finite Fourier transform, and variable substitution to solve multi-source coupled problems. The derived solutions were tested against numerical results for instantaneous point source scenarios with Dirichlet and Robin inlet boundary and were shown to be accurate and robust. The role of two essential dimensionless parameters was investigated using the proposed solutions. The following main conclusions are obtained:

(1) Point source systems with the Dirichlet boundary condition have a maximum predicted concentration. Predictive models of solute transport subject to both internal point sources and boundary sources should pay attention to the choice of inlet boundary conditions, especially when performing long-term predictions.

(2) For a low permeability system (small Péclet number) or strongly degraded system (large Damköhler number), the boundary source has a significant influence on the solute concentration distribution.

(3) The solutions developed in this paper were programmed into a MATLAB program to facilitate fast calculations. These solutions are mainly used to investigate the forward prediction problem, and they can also be used as a basis for the inverse problem of source zone identification, an essential topic in subsurface transport.

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