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Analytical solution for one-dimensional advection–dispersion transport equation with distance-dependent coefficients

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SUMMARY

Mathematical models describing contaminant transport in heterogeneous porous media are often formulated as an advection–dispersion transport equation with distance-dependent transport coefficients. In this work, a general analytical solution is presented for the linear, one-dimensional advection–dispersion equation with distance-dependent coefficients. An integrating factor is employed to obtain a transport equation that has a self-adjoint differential operator, and a solution is found using the generalized integral transform technique (GITT). It is demonstrated that an analytical expression for the integrating factor exists for several transport equation formulations of practical importance in groundwater transport modeling. Unlike nearly all solutions available in the literature, the current solution is developed for a finite spatial domain. As an illustration, solutions for the particular case of a linearly increasing dispersivity are developed in detail and results are compared with solutions from the literature. Among other applications, the current analytical solution will be particularly useful for testing or benchmarking numerical transport codes because of the incorporation of a finite spatial domain.

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1. Introduction

The literature contains many analytical solutions for solute transport in homogeneous porous media. These solutions, which have been collected in various compendiums (Codell et al., 1982; van Genuchten, 1982; Javandel et al., 1984; Wexler, 1992), were found by solving the linear advection–dispersion transport equation with constant coefficients, subject to appropriate boundary and initial conditions. Solutions are available for one-, two-, and three-dimensional spatial domains, with the vast majority being applicable to semi-infinite or infinite media. However, the advection–dispersion equation with constant coefficients may not be appropriate for transport in heterogeneous media, where transport coefficients can be variable in space and/or time. Relatively few analytical results are available for the case of non-constant coefficients, especially for the case of finite media.

Analytical solutions for heterogeneous porous media include solutions obtained for transport equations with time-dependent coefficients (Barry and Sposito, 1989; Basha and El-Habel, 1993; Aral and Liao, 1996; Marinocchi et al., 1999; Kumar et al., 2010)

or distance-dependent coefficients (Yates, 1990; Chrysikopoulos et al., 1990; Yates, 1992; Huang et al., 1996; Logan, 1996; Zopou and Knight, 1997; Hunt, 1998, 1999, 2002; Pang and Hunt, 2001; Al-Humoud and Chamkha, 2007; Liu and Si, 2008; Chen, 2007; Chen et al., 2003, 2007, 2008a,b; Kumar et al., 2010). While most of these solutions are applicable to a range of problems involving (effectively) semi-infinite or infinite media, other applications require consideration of finite media, such as analysis of transport in lysimeters or columns, or benchmarking numerical transport codes. In these types of problems, the effect of the exit boundary may not be negligible.

One reason for the lack of progress in developing solutions for finite domains is that the solution procedures tend to be relatively complicated, requiring difficult or tedious mathematical derivations and manipulations. However, the advent of software such as Mathematica (Wolfram Research, Inc., 2007) with capabilities for symbolic manipulation has made these solution procedures more tractable.

Also facilitating the development of new solutions are systematized integral transform techniques (ITTs) (Mikhailov and Ozisik, 1984). As noted by Ozisik (1993), the classic ITT (CITT) provides a systematic, efficient, and straightforward approach for the analytical solution of both transient and steady problems, with both homogeneous and non-homogeneous boundary conditions. A large variety of heat and mass diffusion problems have been categorized

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Eq. (2) can then be written more compactly as:

$$A_{01}(\xi) \frac{\partial \omega}{\partial \tau} = L\omega + Q(\xi); \quad \xi_0 < \xi < \xi_1 \tag{4}$$

The transport problem is completed by specifying initial and boundary conditions, respectively, as:

$$\omega(\xi, 0) = \omega_I(\xi); \quad \xi_0 < \xi < \xi_1 \tag{5}$$

$$B_k \omega(\xi_k, \tau) = g(\xi_k); \quad k = 0, 1 \tag{6}$$

The operator B_k can represent a first, second, or third-type boundary condition depending on the specification of the coefficients η_k and H_k :

$$B_k \equiv \eta_k \frac{\partial}{\partial X} + H_k \tag{7}$$

3. General analytical solution

An analytical solution of Eqs. (4)–(6) is obtained in several steps. First the boundary conditions are homogenized using a “filter function” which is found by solving the transport problem in the steady state regime. Next, the general non-self-adjoint transport equation is transformed into an equivalent self-adjoint equation through the use of an appropriate integrating factor. Finally, the resulting self-adjoint equation is solved using the GITT.

3.1. Steady state problem and homogenization of the boundary conditions

For the asymptotic condition $\tau \rightarrow \infty$, the quantity ω in Eqs. (4)–(6) will tend to the steady state regime, $\omega(\xi, \tau) \rightarrow \omega_\infty(\xi)$. The asymptotic system is given by:

$$L\omega_\infty + Q(\xi) = 0; \quad \xi_0 < \xi < \xi_1 \tag{8}$$

$$B_k \omega_\infty(\xi_k) = g(\xi_k); \quad k = 0, 1 \tag{9}$$

Solving Eqs. (8) and (9) gives $\omega_\infty(\xi)$, which may be used as a filter function to obtain a problem with homogeneous boundary conditions. To this end, we express the unknown $\omega(\xi, \tau)$ as the sum of the filter $\omega_\infty(\xi)$ and an unknown function $\theta(\xi, \tau)$:

$$\omega(\xi, \tau) = \omega_\infty(\xi) + \theta(\xi, \tau) \tag{10}$$

The unknown quantity $\omega(\xi, \tau)$ is thus found by determining $\theta(\xi, \tau)$. A system of equations for $\theta(\xi, \tau)$ is obtained by substituting Eq. (10) into Eqs. (4)–(6). The resulting equations for $\theta(\xi, \tau)$ are:

$$A_{01}(\xi) \frac{\partial \theta}{\partial \tau} = L\theta; \quad \xi_0 < \xi < \xi_1 \tag{11}$$

$$\theta(\xi, 0) = \omega_I(\xi) - \omega_\infty(\xi); \quad \xi_0 < \xi < \xi_1 \tag{12}$$

$$B_k \theta(\xi_k, \tau) = 0; \quad k = 0, 1 \tag{13}$$

where the boundary conditions Eq. (13) are homogeneous.

For situations where $\frac{A_{00}(\xi)}{A_{01}(\xi)} = \mu$ is a constant, a simplification is possible. In this case, the last term in the operator L (as defined in Eq. (3)) can be eliminated if the following expression is used instead of Eq. (10):

$$\omega(\xi, \tau) = \omega_\infty(\xi) + \exp(-\mu\tau)\theta(\xi, \tau) \tag{10'}$$

Substituting Eq. (10') into Eq. (4) yields the following equation instead of Eq. (11):

$$A_{01}(\xi) \frac{\partial \theta}{\partial \tau} = L\theta \quad \text{with } A_{00}(\xi) = 0; \quad \xi_0 < \xi < \xi_1 \tag{11'}$$

3.2. Obtaining an equation with a self-adjoint operator

Depending on the functional form of the coefficients $A_{00}(\xi)$, $A_{10}(\xi)$, and $A_{20}(\xi)$, the operator L may or may not be self-adjoint. A second-order differential operator, S , is self-adjoint if and only if it has the form (Sagan, 1961)

$$S \equiv \frac{\partial}{\partial \xi} \left(p(\xi) \frac{\partial}{\partial \xi} \right) + q(\xi) \tag{14}$$

where $p(\xi)$ is differentiable.

The form of S in Eq. (14) indicates that a self-adjoint second-order transport equation is equivalent to a purely diffusive problem such as commonly encountered in heat conduction. Such diffusion equations have been categorized by Mikhailov and Ozisik (1984) into seven classes, and the GITT can be used to obtain formal analytic solutions for each of them (Mikhailov and Ozisik, 1984).

When the operator L is non-self-adjoint, it may be possible to transform the equation to obtain an equivalent problem with a self-adjoint operator. For this purpose, we use an integrating factor to transform Eq. (11). Eq. (11) can be written as:

$$A_{01}(\xi) \frac{\partial \theta}{\partial \tau} = L\theta = A_{20}(\xi) \frac{\partial^2 \theta}{\partial \xi^2} + A_{10}(\xi) \frac{\partial \theta}{\partial \xi} - A_{00}(\xi) \theta \tag{15}$$

We multiply each term by $\frac{p(\xi)}{A_{20}(\xi)}$, where $p(\xi)$ is the unknown integrating factor:

$$\frac{p(\xi)}{A_{20}(\xi)} A_{01}(\xi) \frac{\partial \theta}{\partial \tau} = p(\xi) \frac{\partial^2 \theta}{\partial \xi^2} + \frac{p(\xi)}{A_{20}(\xi)} A_{10}(\xi) \frac{\partial \theta}{\partial \xi} - \frac{p(\xi)}{A_{20}(\xi)} A_{00}(\xi) \theta \tag{16}$$

The idea of the integrating factor is that Eq. (16) should reduce to:

$$\frac{p(\xi)}{A_{20}(\xi)} A_{01}(\xi) \frac{\partial \theta}{\partial \tau} = \frac{\partial}{\partial \xi} \left(p(\xi) \frac{\partial \theta}{\partial \xi} \right) - \frac{p(\xi)}{A_{20}(\xi)} A_{00}(\xi) \theta \tag{17}$$

This requires that:

$$\frac{\partial p(\xi)}{\partial \xi} = \frac{p(\xi)}{A_{20}(\xi)} A_{10}(\xi) \tag{18}$$

Thus the integrating factor is given by:

$$p(\xi) = \exp \left(\int \frac{A_{10}(\xi)}{A_{20}(\xi)} d\xi \right) \tag{19}$$

Note that the integrating factor depends only of the dispersion and advection coefficients.

With the integrating factor defined, Eq. (11) can be written in terms of the self-adjoint operator S Eq. (14):

$$w(\xi) \frac{\partial \theta}{\partial \tau} = S\theta = \frac{\partial}{\partial \xi} \left(p(\xi) \frac{\partial \theta}{\partial \xi} \right) + q(\xi) \theta \tag{20}$$

where the coefficients are given by:

$$w(\xi) = \frac{p(\xi)}{A_{20}(\xi)} A_{01}(\xi); \quad q(\xi) = -\frac{p(\xi)}{A_{20}(\xi)} A_{00}(\xi) \tag{21a, b}$$

It is important to note that the use of the integrating factor does not alter the boundary and initial conditions, Eqs. (12) and (13). Therefore, the unknown $\theta(\xi, \tau)$ is found by solving Eq. (20) subject to Eqs. (12) and (13). For the conditions leading to Eqs. (10') and (11'), the last term in Eq. (20) vanishes ($q(\xi) = 0$).

3.3. Application of the GITT

Having obtained a transport equation (Eq. (20)) with a self-adjoint differential operator and homogeneous boundary conditions Eq. (13), the unknown $\theta(\xi, \tau)$ is found by applying the systematized GITT procedure.

3.3.1. The auxiliary eigenvalue problem

Eigenvalue problems with self-adjoint operators have several interesting properties, including (Zwillinger, 1992): the eigenvalues are real; the eigenvalues are enumerable (with no cluster point); the eigenfunctions corresponding to distinct eigenvalues are orthogonal; and the set of eigenfunctions are complete.

Many eigenvalue problems can be associated with Eq. (20) (subject to Eqs. (12) and (13)). We choose the following one which permits an exact integral transform:

$$\frac{d}{d\xi} \left(p(\xi) \frac{d\psi}{d\xi} \right) + q(\xi)\psi + w(\xi)\beta^2\psi = 0 \tag{22a}$$

$$B_k\psi(\xi_k) = 0; \quad k = 0, 1 \tag{22b}$$

Eq. (22) is the Sturm–Liouville eigenvalue problem, where $\psi \equiv \psi(\xi)$ is the eigenfunction and β is the eigenvalue. The orthogonality property for the set of linearly independent eigenfunctions, $\psi_i(\xi)$, associated with Eq. (22) is given by:

$$\int_{\xi_0}^{\xi_1} w(\xi)\psi_i(\xi)\psi_j(\xi)d\xi = \delta_{ij}N_i \tag{23}$$

where N_i is the norm and δ_{ij} is the Kronecker delta. The normalized eigenfunction is defined:

$$\tilde{\psi}_i(\xi) = \frac{\psi_i(\xi)}{\sqrt{N_i}}; \quad i = 1, 2, 3, \dots \tag{24}$$

3.3.2. Development of the integral transform pair

The unknown function $\theta(\xi, \tau)$ is represented as a series expansion in terms of the eigenfunctions $\psi_i(x)$,

$$\theta(\xi, \tau) = \sum_{i=1}^{\infty} \tilde{\psi}_i(\xi)\bar{\theta}_i(\tau) \quad (\text{Inverse}) \tag{25}$$

where $\bar{\theta}_i(\tau)$ is the transformed “potential”. Eq. (25) is the inverse transform rule. The corresponding transform rule is obtained by following the procedure of Ozisik(1993) and Cotta(1993), i.e. applying the operator $\int_{\xi_0}^{\xi_1} w(\xi)\tilde{\psi}_j(\xi)(\cdot)d\xi$ to both sides of Eq. (20) and using Eq. (23) (the orthogonality property) and (25) to obtain:

$$\bar{\theta}_i(\tau) = \int_{\xi_0}^{\xi_1} w(\xi)\tilde{\psi}_i(\xi)\theta(\xi, \tau)d\xi \quad (\text{Transform}) \tag{26}$$

3.3.3. Integral transform of the differential equation

Substituting the inverse formula into Eq. (20) results in:

$$w(\xi) \frac{\partial}{\partial \tau} \sum_{i=1}^{\infty} \tilde{\psi}_i(\xi)\bar{\theta}_i(\tau) = S \sum_{i=1}^{\infty} \tilde{\psi}_i(\xi)\bar{\theta}_i(\tau) \tag{27}$$

Applying the operator $\int_{\xi_0}^{\xi_1} \tilde{\psi}_j(\xi)(\cdot)d\xi$ to both sides of Eq. (27) and regrouping terms gives:

$$\sum_{i=1}^{\infty} \frac{\partial \bar{\theta}_i(\tau)}{\partial \tau} \int_{\xi_0}^{\xi_1} w(\xi)\tilde{\psi}_i(\xi)\tilde{\psi}_j(\xi)d\xi = \sum_{i=1}^{\infty} \bar{\theta}_i(\tau) \int_{\xi_0}^{\xi_1} \tilde{\psi}_j(\xi)S\tilde{\psi}_i(\xi)d\xi \tag{28}$$

This equation can be simplified using Eqs. (22a), (23), and (26):

$$\frac{d\bar{\theta}_i}{d\tau} = -\beta_i^2 \bar{\theta}_i \tag{29}$$

Analogously the initial condition is also transformed:

$$\bar{\theta}_i(0) = \bar{f}_i = \int_{\xi_0}^{\xi_1} w(\xi)\tilde{\psi}_i(\xi)(\omega_l(\xi) - \omega_{\infty}(\xi))d\xi \tag{30}$$

3.3.4. Analytical solution for the transformed and original problems

Eqs. (29) and (30) are a set of decoupled ordinary differential equations, whose analytical solution is:

$$\bar{\theta}_i(\tau) = \bar{f}_i \exp(-\beta_i^2 \tau) \tag{31}$$

Finally, the original unknown $\omega(\xi, \tau)$ can be calculated analytically from the inverse transform rule and Eq. (10):

$$\omega(\xi, \tau) = \omega_{\infty}(\xi) + \sum_{i=1}^{\infty} \tilde{\psi}_i(\xi)\bar{f}_i \exp(-\beta_i^2 \tau) \tag{32}$$

For situations in which Eqs. (10') and (11') are applicable, the solution is given by:

$$\omega(\xi, \tau) = \omega_{\infty}(\xi) + \exp(-\mu\tau) \sum_{i=1}^{\infty} \tilde{\psi}_i(\xi)\bar{f}_i \exp(-\beta_i^2 \tau) \tag{33}$$

4. Application of the general analytical solution to heterogeneous groundwater systems

The general analytical solution developed above for the advection–dispersion equation with distance-dependent coefficients depends on the existence of an analytical expression for the integrating factor defined in Eq. (19). Such an expression cannot be guaranteed for arbitrary functional forms of the dispersion and advection coefficients. However, in this section we show that for many cases of practical interest in groundwater hydrology, the integrating factor exists.

Contaminant transport in heterogeneous aquifer systems is often modeled in terms of a constant average transport velocity, linear equilibrium sorption, and first-order decay. For a finite medium of length L_0 , this problem can be formulated as:

$$R \frac{\partial C}{\partial T} = \frac{\partial}{\partial X} \left(\bar{D}(X) \frac{\partial C}{\partial X} \right) - V \frac{\partial C}{\partial X} - \lambda RC; \quad 0 < X < L_0 \tag{34}$$

$$C(0, T) = C_0 \quad \text{or} \quad -\bar{D}(0) \frac{\partial C(0, T)}{\partial T} + VC(0, T) = VC_0 \tag{35, 36}$$

$$\frac{\partial C(L_0, T)}{\partial X} = 0 \tag{37}$$

$$C(X, 0) = 0 \tag{38}$$

where $C(X, T)$ is the dimensional concentration (ML^{-3}), C_0 is the boundary Eq. (35) or influent Eq. (36) concentration (ML^{-3}), R is the constant retardation coefficient (-), V is the average constant flow velocity (LT^{-1}), λ is the first-order decay constant (T^{-1}), and $\bar{D}(X)$ is the longitudinal hydrodynamic dispersion coefficient ($L^2 T^{-1}$). The hydrodynamic dispersion coefficient is defined as the sum of the mechanical dispersion and the molecular diffusion, \bar{D}_M ($L^2 T^{-1}$):

$$\bar{D}(X) = V\bar{\alpha}(X) + \bar{D}_M \tag{39}$$

where $\bar{\alpha}(X)$ is the dispersivity (L).

We define the following dimensionless variables:

$$x = \frac{X}{L_0}; \quad t = \frac{T}{\left(\frac{RL_0}{V}\right)}; \quad c = \frac{C}{C_0}; \quad \gamma = \frac{\lambda RL_0}{V} \tag{40a–d}$$

Eqs. (34)–(38) can then be written in dimensionless form:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D(x) \frac{\partial c}{\partial x} \right) - \frac{\partial c}{\partial x} - \gamma c; \quad 0 < x < 1 \tag{41}$$

$$c(0, t) = 1 \quad \text{or} \quad -D(0) \frac{\partial c(0, t)}{\partial x} + c(0, t) = 1 \tag{42, 43}$$

$$\frac{\partial c(1, t)}{\partial x} = 0 \tag{44}$$

$$c(x, 0) = 0 \tag{45}$$

where the dimensionless distance-dependent dispersion parameter $D(x)$ is given by:

$$D(x) = \frac{\bar{D}(xL_0)}{VL_0} = \frac{\bar{\alpha}(xL_0)}{L_0} + \frac{D_M}{L_0V} = \alpha(x) + d_M \tag{46a}$$

$$\alpha(x) \equiv \frac{\bar{\alpha}(xL_0)}{L_0}; \quad d_M \equiv \frac{D_M}{L_0V} \tag{46b, c}$$

where $\alpha(x)$ is the dimensionless dispersivity and d_M the dimensionless diffusion coefficient.

For heterogeneous aquifers, Pickens and Grisak (1981) proposed that the spatial dependence of the dispersivity, $\bar{\alpha}(X)$, may be linear, parabolic, exponential, or asymptotic. Table 1 presents these model dispersivity functions along with the corresponding dimensionless representations, $\alpha(x)$. Note that in each case $\bar{\alpha}(X)$ and $\alpha(x)$ have the same functional form.

To see if the integrating factor exists for the four model functions, Eq. (19) was evaluated analytically for each of the dimensionless models (with the evident variable equivalencies being $\xi = x$, $A_{20}(\xi) = D(x)$, and $A_{10}(\xi) = 1$). Table 2 shows that indeed the integrating factor exists for all four cases, with analytical results being given for both non-negligible ($d_M \neq 0$) and negligible ($d_M = 0$) molecular diffusion (the latter situation yielding less complex mathematical expressions). Hence for each of the forms proposed by Pickens and Grisak (1981) for practical groundwater transport problems, the integrating factor exists and the general analytical solution may be applied. In the remainder of this paper, we apply the general analytical solution to the particular case of groundwater contaminant transport with a linearly increasing dispersivity.

In the event that an analytical expression for the integrating factor is not available, the solution presented in Section 2 may be regarded as a formal solution. In this case, it is possible to evaluate the integrating factor numerically. This formal analytical approach is the subject of ongoing research and will be documented in a future publication.

5. Example: linearly increasing dispersivity

Using the Laplace transform technique, Yates (1990) obtained an analytical solution for advective–dispersive transport in heterogeneous, semi-infinite media in which dispersion increases linearly with transport distance. The equation solved by Yates (1990) is equivalent to our Eq. (41) with $D(x) = ax + d_M$. As a demonstration of the current methodology, we apply our general analytical solution to the specific problem solved by Yates (1990), except that the solution is obtained in the present work for a finite medium of length L_0 .

Two different problems can be formulated depending on the boundary conditions imposed. The first case has the entrance boundary specified by a first-type condition Eq. (42) and the exit boundary by a second-type condition Eq. (44). Signifying the boundary types, we call this formulation “Case 1–2”. The second

case, with entrance boundary given by a third-type condition Eq. (43) and exit boundary by a second-type condition Eq. (44), is called “Case 3–2”.

5.1. Steady transport

Applying the general discussion of Section 3.1 to the current problem, the dimensionless steady state concentration is found by solving:

$$\frac{d}{dx} \left(D(x) \frac{dc_\infty}{dx} \right) - \frac{dc_\infty}{dx} - \gamma c_\infty = 0 \tag{47}$$

$$c_\infty(0) = 1 \quad \text{or} \quad -D(0) \frac{dc_\infty(0)}{dx} + c_\infty(0) = 1 \tag{48, 49}$$

$$\frac{dc_\infty(1)}{dx} = 0 \tag{50}$$

where $D(x) = ax + d_M$. A solution to this problem was obtained using the “DSolve” function of the Mathematica software package, version 6.0 (Wolfram Research, Inc., 2007). The closed-form analytical solutions for Cases 1–2 and 3–2 are, respectively:

$$c_\infty(x) = \left(\frac{D(x)}{D(0)} \right)^{\sigma/2} \frac{I_\sigma[\varphi(x)]K_{\sigma-1}[\varphi(1)] + I_{\sigma-1}[\varphi(1)]K_\sigma[\varphi(x)]}{I_\sigma[\varphi(0)]K_{\sigma-1}[\varphi(1)] + I_{\sigma-1}[\varphi(1)]K_\sigma[\varphi(0)]} \tag{51}$$

$$c_\infty(x) = \left(\frac{1}{\gamma D(0)} \right)^{1/2} \left(\frac{D(x)}{D(0)} \right)^{\sigma/2} \times \frac{I_\sigma[\varphi(x)]K_{\sigma-1}[\varphi(1)] + I_{\sigma-1}[\varphi(1)]K_\sigma[\varphi(x)]}{I_{\sigma-1}[\varphi(1)]K_{\sigma+1}[\varphi(0)] - I_{\sigma+1}[\varphi(0)]K_{\sigma-1}[\varphi(1)]} \tag{52}$$

where

$$\varphi(x) = 2\sigma\sqrt{\gamma D(x)}; \quad \sigma = \frac{1}{a} \tag{53a, b}$$

and where I_σ and K_σ are modified Bessel functions of the first and second kinds, respectively.

5.2. Transient transport

To apply the general solution developed in Section 2, we make the following variable equivalencies (with $\xi \rightarrow x$ and $\tau \rightarrow t$):

$$A_{01}(x) = 1; \quad A_{20}(x) = D(x); \\ A_{10}(x) = \frac{dD(x)}{dx} - 1; \quad A_{00}(x) = \gamma \tag{54a–d}$$

Because the ratio $\frac{A_{00}(x)}{A_{01}(x)} = \gamma$ is a constant, $c(x, t)$ will be represented according to Eq. (10'). For Cases 1–2 and 3–2, the resulting system of equations for the unknown θ is:

$$\frac{\partial \theta}{\partial t} = D(x) \frac{\partial^2 \theta}{\partial x^2} - A_{10}(x) \frac{\partial \theta}{\partial x} \tag{55}$$

$$\theta(0, t) = 0 \quad \text{or} \quad -D(0) \frac{\partial \theta(0, t)}{\partial x} + \theta(0, t) = 0 \tag{56, 57}$$

$$\frac{\partial \theta(1, t)}{\partial x} = 0 \tag{58}$$

$$\theta(x, 0) = -c_\infty(x) \tag{59}$$

The integrating factor $p(x)$ and the coefficient $w(x)$ are (Table 2):

$$p(x) = (ax + d_M)^{1-1/a} = D(x)^{1-\sigma}; \quad w(x) = D(x)^{-\sigma} \tag{60, 61}$$

The Sturm–Liouville problem for Cases 1–2 and 3–2 takes the form:

Table 1
Functional forms for the dimensional ($\bar{\alpha}$) and dimensionless (α) dispersivities.^a

Type	$\bar{\alpha}(X)$	$\alpha(x)$	Coefficients
Linear	aX	ax	
Parabolic	$\bar{b}X^n$	bx^n	$b = \bar{b}L_0^{n-1}$
Exponential	$\bar{A} \left(1 - \frac{\bar{B}}{x+\bar{B}} \right)$	$A \left(1 - \frac{B}{x+B} \right)$	$A = \frac{\bar{A}}{L_0}; B = \frac{\bar{B}}{L_0}$
Asymptotic	$\bar{E} [1 - \exp(-\bar{F}X)]$	$E [1 - \exp(-FX)]$	$E = \frac{\bar{E}}{L_0}; F = \bar{F}L_0$

^a $a, b, A, B, E,$ and F are dimensionless constants, whereas the same symbols with overbars are dimensional constants; n is a dimensionless constant; L_0 is the domain length.

Table 2
Integrating factor $p(x)$ for various model dispersivity functions $\alpha(x)$.^a

$\alpha(x)$	$p(x)$ (non-negligible diffusion, $d_M \neq 0$)	$p(x)$ (negligible diffusion, $d_M = 0$)
ax	$(ax + d_M)^{1-1/a}$	$x^{1-1/a}$
bx^n	$\frac{(bx^n + d_M)}{d_M} \exp \left\{ \frac{x}{(n+1)d_M} [bx^n F_1 \left(1, 1 + \frac{1}{n}; 2 + \frac{1}{n}; -\frac{bx^n}{d_M} \right) - d_M(n+1)] \right\}$	$x^n \exp \left[\frac{x^{1-n}}{b(n-1)} \right]$
$A \left(1 - \frac{B}{x+B} \right)$	$\frac{[Ax + (B+x)d_M]^{1-\frac{AB}{A+d_M}}}{B+x} \exp \left(-\frac{x}{A+d_M} \right)$	$\exp \left[-\frac{x+(B-A) \ln(x) + A \ln(B+x)}{A} \right]$
$E[1 - \exp(-Fx)]$	$\exp(-Fx) [(E + d_M) \exp(Fx) - E]^{1-\frac{1}{F(E+d_M)}}$	$[\exp(Fx) - 1]^{1-\frac{1}{EF}} \exp(-Fx)$

^a d_M is the coefficient of molecular diffusion; $a, b, A, B, E,$ and F are numerical constants; ${}_2F_1(\cdot)$ is the hypergeometric function.

$$\frac{d}{dx} \left(D(x)^{1-\sigma} \frac{d\psi}{dx} \right) + D(x)^{-\sigma} \beta^2 \psi = 0 \tag{62}$$

$$\psi(0) = 0 \quad \text{or} \quad -D(0) \frac{\partial \psi(0)}{\partial x} + \psi(0) = 0 \tag{63, 64}$$

$$\frac{\partial \psi(1)}{\partial x} = 0 \tag{65}$$

This eigenvalue problem was solved in Mathematica using the “DSolve” function in combination with other commands for algebraic simplifications. The set of eigenfunctions are given in terms of Bessel functions of the first (J_σ) and second (Y_σ) kind. The result for Case 1–2 is:

$$\psi_i(x) = D(x)^{\sigma/2} \left(\frac{J_\sigma[2\sigma\beta_i\sqrt{D(x)}]}{J_\sigma[2\sigma\beta_i\sqrt{D(0)}} - \frac{Y_\sigma[2\sigma\beta_i\sqrt{D(x)}]}{Y_\sigma[2\sigma\beta_i\sqrt{D(0)}} \right); \tag{66}$$

$i = 1, 2, 3, \dots$

whereas for Case 3–2 it is:

$$\psi_i(x) = D(x)^{\sigma/2} \left(\frac{J_\sigma[2\sigma\beta_i\sqrt{D(x)}]}{J_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}} + \frac{Y_\sigma[2\sigma\beta_i\sqrt{D(x)}]}{Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}} \right) \tag{67}$$

$i = 1, 2, 3, \dots$

The eigenvalues, β_i , for Cases 1–2 and 3–2 must be calculated, respectively, from the following transcendental equations:

$$\frac{J_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}]}{J_\sigma[2\sigma\beta_i\sqrt{D(0)}} - \frac{Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}]}{Y_\sigma[2\sigma\beta_i\sqrt{D(0)}} = 0 \tag{68}$$

$$\frac{J_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}]}{J_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}} - \frac{Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}]}{Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}} = 0 \tag{69}$$

The analytical expression for the norm (see Eq. (23)) is given by Eq. (70) for Case 1–2 and by Eq. (71) for Case 3–2:

$$N_i = \sum_{m=1}^4 N_{12i}(m) \tag{70a}$$

$$N_{12i}(1) = \sigma D(0) \left(\frac{J_{\sigma-1}[2\sigma\beta_i\sqrt{D(0)}] J_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}]}{J_\sigma[2\sigma\beta_i\sqrt{D(0)}} - 1 \right) \tag{70b}$$

$$N_{12i}(2) = \frac{[1 + \sigma D(0)] \left(J_\sigma^2[2\sigma\beta_i\sqrt{D(1)}] - J_{\sigma-1}^2[2\sigma\beta_i\sqrt{D(1)}] J_{\sigma+1}[2\sigma\beta_i\sqrt{D(1)}] \right)}{J_{\sigma+1}^2[2\sigma\beta_i\sqrt{D(0)}} \tag{70c}$$

$$N_{12i}(3) = \sigma D(0) \left(\frac{Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(0)}] Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}]}{Y_\sigma[2\sigma\beta_i\sqrt{D(0)}} - 1 \right) \tag{70d}$$

$$N_{12i}(4) = \frac{[1 + \sigma D(0)] \left(Y_\sigma^2[2\sigma\beta_i\sqrt{D(1)}] - Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}] Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(1)}] \right)}{Y_\sigma^2[2\sigma\beta_i\sqrt{D(0)}} \tag{70e}$$

$$N_i = \sum_{m=1}^4 N_{32i}(m) \tag{71a}$$

$$N_{32i}(1) = \frac{\sigma D(0) \left(J_{\sigma-1}[2\sigma\beta_i\sqrt{D(0)}] J_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}] - J_\sigma^2[2\sigma\beta_i\sqrt{D(0)}] \right)}{J_{\sigma+1}^2[2\sigma\beta_i\sqrt{D(0)}} \tag{71b}$$

$$N_{32i}(2) = \frac{[1 + \sigma D(0)] \left(J_\sigma^2[2\sigma\beta_i\sqrt{D(1)}] - J_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}] J_{\sigma+1}[2\sigma\beta_i\sqrt{D(1)}] \right)}{J_{\sigma+1}^2[2\sigma\beta_i\sqrt{D(0)}} \tag{71c}$$

$$N_{32i}(3) = \frac{\sigma D(0) \left(Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(0)}] Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(0)}] - Y_\sigma^2[2\sigma\beta_i\sqrt{D(0)}] \right)}{Y_{\sigma+1}^2[2\sigma\beta_i\sqrt{D(0)}} \tag{71d}$$

$$N_{32i}(4) = \frac{[1 + \sigma D(0)] \left(Y_\sigma^2[2\sigma\beta_i\sqrt{D(1)}] - Y_{\sigma-1}[2\sigma\beta_i\sqrt{D(1)}] Y_{\sigma+1}[2\sigma\beta_i\sqrt{D(1)}] \right)}{Y_{\sigma+1}^2[2\sigma\beta_i\sqrt{D(0)}} \tag{71e}$$

The normalized eigenfunction is computed according to Eq. (24).

The transformed initial condition Eq. (30) was determined analytically using the “Integrate” function in Mathematica. Eqs. (72) and (73) give expressions of the transformed initial conditions for Cases 1–2 and 3–2, respectively:

$$\bar{f}_i = \frac{a\varphi(1)T_1 + \pi\sqrt{D(1)}T_2\beta_i}{\pi(T_1 + T_2)J_\sigma \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] Y_\sigma \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] \varphi(1)D(0)^{\sigma/2} (\beta_i^2 + \gamma)\sqrt{N_i}} \tag{72a}$$

$$T_1 = I_\sigma[\varphi(0)]K_{\sigma-1}[\varphi(1)] + I_{\sigma-1}[\varphi(1)]K_\sigma[\varphi(0)] \tag{72b}$$

$$T_2 = J_{\sigma-1} \left[\frac{\varphi(1)}{\sqrt{\gamma}} \beta_i \right] Y_\sigma \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] - J_\sigma \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] Y_{\sigma-1} \left[\frac{\varphi(1)}{\sqrt{\gamma}} \beta_i \right] \tag{72c}$$

$$\bar{f}_i = \frac{2\sqrt{\gamma}}{\pi J_{\sigma+1} \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] Y_{\sigma+1} \left[\frac{\varphi(0)}{\sqrt{\gamma}} \beta_i \right] \varphi(0)D(0)^{\sigma/2} \beta_i (\beta_i^2 + \gamma)\sqrt{N_i}} \tag{73}$$

$$\varphi(x) = 2\sigma\sqrt{\gamma D(x)}. \tag{74}$$

Finally, the solute concentration is found according to Eq. (33).

6. Results for test-case

The GITT analytical solution developed in the previous section was evaluated for a hypothetical test-case whose parameter values

Table 3
Data values for test-case.

Parameter	Value
Domain length, L_0	100 m
Retardation factor, R	1
Molecular diffusion, d_M	$10^{-4} \text{ m}^2 \text{ d}^{-1}$
Average velocity, u	0.25 m d^{-1}
Decay coefficient, λ	0.05 d^{-1}

are given in Table 3. The solution was implemented in Mathematica. The eigenvalues were calculated from the transcendental Eqs. (65) and (66) using the Mathematica function "FindRoot". Solutions were computed using default settings for Mathematica system parameters. The GITT solution was programmed such that dimensionless concentration values less than 10^{-10} were taken to be zero.

For comparison purposes, the formal solution of Yates (1990) for a semi-infinite domain was also implemented in the Mathematica platform. The integrals in the Yates (1990) solution were evaluated numerically using the Mathematica function "NIntegrate".

Table 4 presents the dimensionless steady state concentration c_∞ with the linear dependence of the dispersion coefficient specified by $a = 0.1$. For both Cases 1–2 and 3–2, the results for the finite domain (the current GITT solution) and the semi-infinite domain (the Yates (1990) formal analytical solution) are identical at the entrance boundary and for over more than half of the spatial domain. As expected, however, the solutions diverge further along the domain where the effect of the finite boundary condition becomes apparent. Fig. 1 shows steady state results for different values of a . Field observations of contaminant dispersion, as well as theoretical considerations, indicate that the value of a should be in the range $0 \leq a \leq 1$ (Huang et al., 1996). Fig. 1 demonstrates that the effect of the finite domain, and hence the disagreement with the semi-infinite solution, increases when the value of a increases.

Tables 5–7 show results for the transient concentration at the dimensionless time $t = 0.1$ and various values of the parameter a . The parameter values in Table 4 were again used. Results for finite and semi-infinite domains are presented. The numbers of terms, N , required for convergence of the GITT solution depended on the value of a : $N = 50$ for $a = 0.1$ (Table 5); $N = 30$ for $a = 0.5$ (Table 6); and $N = 10$ for $a = 1$ (Table 7). Increasing a has the effect of increasing dispersion relative to advection, and consequently the number of terms required for convergence is lower. As was the case with the steady state results, the concentration profiles in Tables 5–7 for the finite and semi-infinite domains differ only in the vicinity of the exit boundary.

Table 4
Steady state concentration profiles for $a = 0.1$.

X (m)	Dimensionless concentration			
	Eq. (51) Case 1–2	Yates (1990) Case 1–2	Eq. (52) Case 3–2	Yates (1990) Case 3–2
0	1.	1.	9.99911E-1	9.99911E-1
10	1.35955E-1	1.35955E-1	1.35943E-1	1.35943E-1
20	2.46503E-2	2.46503E-2	2.46481E-2	2.46481E-2
30	5.32019E-3	5.32019E-3	5.31971E-3	5.31971E-3
40	1.29868E-3	1.29868E-3	1.29856E-3	1.29856E-3
50	3.48248E-4	3.48248E-4	3.48217E-4	3.48217E-4
60	1.00682E-4	1.00682E-4	1.00673E-4	1.00673E-4
70	3.09787E-5	3.09779E-5	3.09759E-5	3.09751E-5
80	1.00565E-5	1.00476E-5	1.00556E-5	1.00467E-5
90	3.49118E-6	3.4108E-6	3.49086E-6	3.4105E-6
100	1.82775E-6	1.20497E-6	1.82759E-6	1.20487E-6

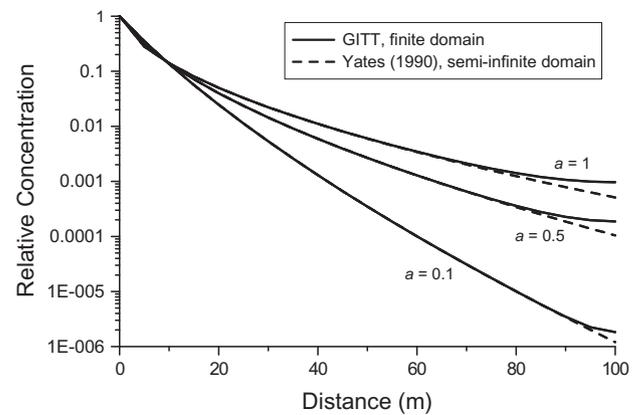


Fig. 1. Steady state concentration profiles for finite (GITT) and semi-infinite (Yates, 1990) domains and for various values of dispersion spatial dependence parameter a . Inlet boundary is a first-type condition.

Table 5
Concentration profiles for $t = 0.1$ and $a = 0.1$.

X (m)	Dimensionless concentration			
	GITT Case 1–2	Yates (1990) Case 1–2	GITT Case 3–2	Yates (1990) Case 3–2
0	1.	1.	9.99911E-11	9.99911E-11
10	9.41422E-2	9.41422E-2	9.41263E-2	9.41263E-2
20	7.8846E-4	7.8846E-4	7.8804E-4	7.8804E-4
30	1.05935E-6	1.05936E-6	1.05834E-6	1.05835E-6
40	5.71943E-10	5.71614E-10	5.71138E-10	5.70811E-10
50	0	3.28618E-13	0	3.23334E-13
60	0	2.14595E-13	0	1.32517E-13
70	0	-3.86535E-13	0	-3.6215E-13
80	0	6.37506E-14	0	7.92379E-14
90	0	3.91891E-13	0	7.30922E-13
100	0	9.99429E-14	0	1.95371E-15

Table 6
Concentration profiles for $t = 0.1$ and $a = 0.5$.

X (m)	Dimensionless concentration			
	GITT Case 1–2	Yates (1990) Case 1–2	GITT Case 3–2	Yates (1990) Case 3–2
0	1.	1.	9.9984E-1	9.9984E-1
10	1.15427E-1	1.15427E-1	1.15402E-1	1.15402E-1
20	1.93139E-2	1.93139E-2	1.93076E-2	1.93076E-2
30	3.21145E-3	3.21145E-3	3.20998E-3	3.20998E-3
40	5.19991E-4	5.19991E-4	5.19677E-4	5.19677E-4
50	8.22096E-5	8.22096E-5	8.21477E-5	8.21477E-5
60	1.2749E-5	1.2749E-5	1.27375E-5	1.27375E-5
70	1.94688E-6	1.94685E-6	1.9448E-6	1.9448E-6
80	2.93698E-7	2.93614E-7	2.9332E-7	2.93258E-7
90	4.45395E-8	4.38308E-8	4.44581E-8	4.3771E-8
100	1.25334E-8	6.48763E-9	1.24949E-8	6.47779E-9

Fig. 2 shows the solute concentration profiles for Case 1–2, calculated with different values of the parameter a and at various dimensionless times t . Results for Case 3–2 are also included in Fig. 2, but at the scale of the figure, they superimpose on the results for the first case and cannot be distinguished. For realistic levels of dispersion ($0 \leq a \leq 1$), the different inlet conditions led to only minor differences in the computed solution. Also shown in Fig. 2 are results computed for constant dispersion, $D = a + d_M$. In comparing the plots of Fig. 2, it can be seen that increasing the value of a increases dispersion and creates a more diffuse concentration front that penetrates more quickly into the finite domain. Also, the divergence from the constant dispersivity case is greater for larger values of a .

Table 7
Concentration profiles for $t = 0.1$ and $a = 1$.

X (m)	Dimensionless concentration			
	GITT Case 1–2	Yates (1990) Case 1–2	GITT Case 3–2	Yates (1990) Caes 3–2
0	1.	1.	9.99336E–1	9.99336E–1
10	1.22758E–1	1.22757E–1	1.2266E–1	1.2266E–1
20	3.41618E–2	3.41612E–2	3.41274E–2	3.41274E–2
30	1.08658E–2	1.08656E–2	1.08525E–2	1.08525E–2
40	3.6527E–3	3.65272E–3	3.64748E–3	3.64748E–3
50	1.26362E–3	1.26374E–3	1.26164E–3	1.26164E–3
60	4.4454E–4	4.44671E–4	4.43865E–4	4.4383E–4
70	1.58159E–4	1.58164E–4	1.57997E–4	1.57829E–4
80	5.71682E–5	5.66704E–5	5.7204E–5	5.65375E–5
90	2.25485E–5	2.04106E–5	2.26559E–5	2.03582E–5
100	1.42596E–5	7.3792E–6	1.43845E–5	7.35863E–6

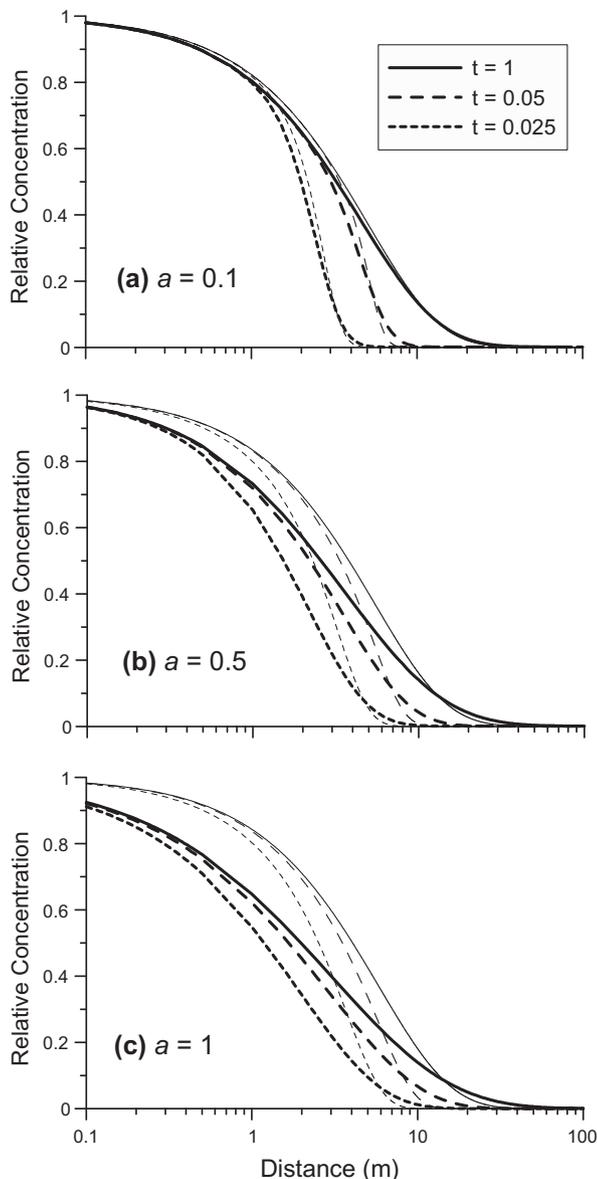


Fig. 2. Concentration distributions in a finite domain at various values of the dimensionless time, t . Inlet boundary is a first-type condition. The thick lines are for a linearly increasing dispersivity, $D(x) = ax + d_M$, whereas the thin lines are for constant dispersivity, $D(x) = a + d_M$.

7. Summary and conclusions

A general analytical solution for solute transport in finite, heterogeneous porous media was developed. The linear advection–dispersion equation with distance-dependent coefficients was solved using an integrating factor in combination with the generalized integral transform technique (GITT). For a number of parameterizations of practical importance to groundwater contaminant transport, we demonstrated that an analytical expression for the integrating factor exists. For the particular case of a linearly increasing dispersivity, solutions were developed in detail and compared with solutions from the literature obtained for semi-infinite media. As expected, the results differed only in the vicinity of the exit boundary. Among other applications, the new solution will be particularly useful analyzing problems where the exit boundary is significant, such as transport in soil columns or lysimeters, or testing and validating numerical transport codes.

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