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Analytical solution of the advection–diffusion transport equation using a change-of-variable and integral transform technique

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ABSTRACT

This paper presents a formal exact solution of the linear advection–diffusion transport equation with constant coefficients for both transient and steady-state regimes. A classical mathematical substitution transforms the original advection–diffusion equation into an exclusively diffusive equation. The new diffusive problem is solved analytically using the classic version of Generalized Integral Transform Technique (GITT), resulting in an explicit formal solution. The new solution is shown to converge faster than a hybrid analytical–numerical solution previously obtained by applying the GITT directly to the advection–diffusion transport equation.

1. Introduction

Analytical solutions of advective–diffusive transport problems continue to be of interest in many areas of science and engineering, such as heat and mass transfer and pollutant dispersion in air, soils, and water. They are useful for a variety of applications [1–5], such as providing initial or approximate analyses of alternative pollution scenarios, conducting sensitivity analyses to investigate the effects of various parameters or processes on contaminant transport, extrapolation over large times and distances where numerical solutions may be impractical, serving as screening models or benchmark solutions for more complex transport processes that cannot be solved exactly, and for validating more comprehensive numerical solutions of the governing transport equations.

The literature presents several methods to analytically solve the partial differential equations governing transport phenomena [6–10]. For example, the method of separation-of-variables is one of the oldest and most widely used techniques. Similarly, the classical Green's function method can be applied to problems with source terms and inhomogeneous boundary conditions on finite, semi-infinite, and infinite regions [10,11].

Integral transform techniques, such as the Laplace and Fourier transform methods, employ a mathematical operator that produces a new function by integrating the product of an existing function and a kernel function between suitable limits. The kernel of an integral transform, along with the integration limits, distinguishes one integral transform from another. Exact solutions of linear diffusion problems by classical integral transform techniques were reviewed and classified by Mikhailov and Ozisik [12]. They identified and unified seven classes of problems and demonstrated many applications in heat and mass diffusion. Cotta [13] generalized and extended the classical integral transform method presented by Mikhailov and Ozisik [12], thereby creating a new systematic procedure referred to as the Generalized Integral Transform Technique (GITT).

The literature also features the use of mathematical substitutions in obtaining analytical solutions to partial differential equations. Mathematical substitutions can simplify the structure of an equation, thereby facilitating more flexible applications of certain solution methods. Compilations of transformations and substitutions are presented by Zwillinger [14] and Polyanin [15]. Most existing analytical solutions for advection–diffusion transport problems [3,16–18], including problems with growth and decay terms, are for semi-infinite or infinite regions, with solutions for finite domains being mostly limited to one-dimensional problems.

The aim of this paper is to present an analytical methodology to solve advection–diffusion transport problems in a finite domain for both transient and steady-state regimes. The proposed methodology uses change-of-variables in combination with the classic version of the Generalized Integral Transform Technique (GITT).

2. Problem formulation

We study transport in a finite domain and consider a three-dimensional linear problem with decay and source terms. The

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Nomenclature

a	generic position on the boundary
C	dimensionless solute concentration
D_x, D_y, D_z	dispersion–diffusion constants
F	filter function
$\bar{f}_i$	integral transform of ρ
G	source term
$\bar{G}$	integral transform of G
H_1, H_2	coefficients
i,j	indices
L	mathematical operator
L_0	domain length
M	function with homogeneous boundary conditions
N_i	norm
Pe	Peclet number
p_1, p_2, p_3	constants for the algebraic substitution
q_1, q_2, q_3	constants for the algebraic substitution
R	coefficient
S	source term
T	scalar quantity
t	time
u, v, w	advection (convection) components
$\bar{v}$	symbolic coordinates for integration
V	generic finite volume
x, y, z	spatial coordinates

Greek symbols

β_i	eigenvalue
γ	dimensionless coefficient
δ_{ij}	Kronecker delta
θ	function in purely diffusive equation
$\bar{\theta}_i$	integral transform of the function θ
λ	generic decay constant (Eq. (2))
λ^*	decay constant for the second test case
μ_i	eigenvalue
π	number Pi
ρ	generic initial condition
τ	auxiliary variable
∇^2	Laplacian operator
ψ_i	eigenfunction
$\tilde{\psi}_i$	normalized eigenfucntion

boundary conditions can be any combination of the first, second, or third kinds. We begin with formal mathematical definitions for both transient and steady-state problems.

2.1. Transient problem

The transient transport equation for a scalar quantity $T(x,y,z,t)$ undergoing constant advection (or convection) and dispersion (or diffusion) is given by:

$$R\frac{\partial T(x,y,z,t)}{\partial t} + LT(x,y,z,t) + S(x,y,z,t) = \nabla^2 T(x,y,z,t) \tag{1}$$

where the operators L and ∇^2 are defined by:

$$L \equiv u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z} + \lambda R \tag{2}$$

$$\nabla^2 \equiv D_x\frac{\partial^2}{\partial x^2} + D_y\frac{\partial^2}{\partial y^2} + D_z\frac{\partial^2}{\partial z^2} \tag{3}$$

in which the parameters u, v, and w are constant velocity coefficients, λ is a constant decay term, D_x, D_y, and D_z are constant dispersion (or diffusion) coefficients, and $S(x,y,z,t)$ is a source term. The coefficient R in Eq. (1) is also a constant parameter (e.g., the retardation factor in many subsurface contaminant transport problems).

A general initial condition can be established as:

$$T(x,y,z,0) = \rho(x,y,z) \tag{4}$$

2.2. Steady-state problem

The transport equation for a steady-state transport regime independent of time, t, follows from Eq. (1) as:

$$\nabla^2 T(x,y,z) = LT(x,y,z) + S(x,y,z) \tag{5}$$

3. Mathematical analysis

3.1. Generalized Integral Transform Technique (GITT)

The transient and steady-state problems given by Eqs. (1) and (5), respectively, can be solved using integral transform methods as systematized by Cotta [13]. In this technique, termed the Generalized Integral Transform Technique (GITT), the unknown function is represented in terms of an eigenfunction series expansion. Basically, the GITT has the following steps:

(a) Choose an appropriate auxiliary eigenvalue problem and find the associated eigenvalues, eigenfunctions, norm, and orthogonalization property.
(b) Develop the integral and inverse transforms.
(c) Transform the partial differential equation into a system of ordinary differential or algebraic equations.
(d) Solve the ordinary differential or algebraic system.
(e) Use the inverse transform to obtain the unknown function.

3.2. Transient regime

Considering a more general case we assume that the boundary conditions associated with Eq. (1) are non-homogeneous. To homogenize the boundary conditions, we rewrite Eq. (1) using the following filter strategy:

$$T(x,y,z,t) = M(x,y,z,t) + F(x,y,z;t) \tag{6}$$

where $F(x,y,z;t)$ is any function satisfying exactly the original boundary conditions of $T(x,y,z,t)$. Eq. (1) now becomes:

$$R\frac{\partial M(x,y,z,t)}{\partial t} + LM(x,y,z,t) = \nabla^2 M(x,y,z,t) + G(x,y,z,t) \tag{7}$$

where $G(x,y,z,t)$ is the new source term which includes the original source term as well as terms containing the filtering function. The filtered initial condition is given by:

$$M(x,y,z,0) = \rho(x,y,z) - F(x,y,z;0) \tag{8}$$

Using a change-of-variable, similar to that used by [19,20,10] we define $M(x,y,z,t)$ in terms of a new function, $\theta(x,y,z,t)$:

$$M(x,y,z,t) = \theta(x,y,z,t)\exp[p_1x + p_2y + p_3z + t(q_1 + q_2 + q_3)] \tag{9}$$

where p_1, p_2, p_3, q_1, q_2, and q_3 are constants that need to be determined.

A comparable substitution was used by Brenner [19] to obtain a transient, one-dimensional solution for miscible fluid displacement in finite length beds. Selim and Mansell [20] similarly presented an analytical solution for reactive solutes with linear adsorption, a sink/source term, a finite domain, and continuous and flux-plug type inlet conditions at the inlet boundary. Recently, Goltz [21] used an equivalent substitution studying convective–dispersive solute transport with constant production, first-order decay, and equilibrium sorption in a porous medium. All of these studies used integral transforms and changes-of-variables, but were limited to unsteady, one-dimensional problems.

The idea of the substitution in Eq. (9) is to transform the transient advection–dispersion (or diffusion) problem into an equivalent heat conduction problem involving a purely diffusive type equation. Applying the substitution to Eq. (7) leads to:

$$\begin{aligned} R\frac{\partial\theta(x,y,z,t)}{\partial t} &+ \theta(x,y,z,t)[R(q_1+q_2+q_3+\lambda) \\ &+p_1(-D_xp_1+u)+p_2(-D_yp_2+v)+p_3(-D_zp_3+w)] \\ &+(-2D_zp_3+w)\frac{\partial\theta(x,y,z,t)}{\partial z}-D_z\frac{\partial^2\theta(x,y,z,t)}{\partial z^2} \\ &+(-2D_yp_2+v)\frac{\partial\theta(x,y,z,t)}{\partial y}-D_y\frac{\partial^2\theta(x,y,z,t)}{\partial y^2} \\ &+(-2D_xp_1+u)\frac{\partial\theta(x,y,z,t)}{\partial x}-D_x\frac{\partial^2\theta(x,y,z,t)}{\partial x^2} \\ =&\frac{G(x,y,z,t)}{\exp[(q_1+q_2+q_3)t+p_1x+p_2y+p_3z]} \end{aligned} \tag{10}$$

Inspection of Eq. (10) shows that the advection terms can be eliminated by choosing the constants p_1, p_2, p_3, q_1, q_2 and q_3 as follows:

$$p_1=\frac{u}{2D_x};\quad p_2=\frac{v}{2D_y};\quad p_3=\frac{w}{2D_z} \tag{11a–c}$$

$$q_1=-\left(\frac{u^2}{4D_xR}+\lambda\right);\quad q_2=-\frac{v^2}{4D_yR};\quad q_3=-\frac{w^2}{4D_zR} \tag{11d–f}$$

Note that the coefficient multiplying the term $\theta(x,y,z,t)$ in Eq. (10) then reduces to zero, which allows us to write the transient transport equation for $\theta(x,y,z,t)$ as:

$$R\frac{\partial\theta(x,y,z,t)}{\partial t}=\nabla^2\theta(x,y,z,t)+\frac{G(x,y,z,t)}{\exp[(q_1+q_2+q_3)t+p_1x+p_2y+p_3z]} \tag{12a}$$

The new transport Eq. (12) is a diffusion equation that has a modified source term which contains all of the advection and decay information from the original problem. Using Eqs. (8) and (9), the modified initial condition in terms of $\theta(x,y,z,t)$ is now:

$$\theta(x,y,z,0)=\frac{\rho(x,y,z)-F(x,y,z;0)}{\exp(p_1x+p_2y+p_3z)} \tag{12b}$$

The boundary conditions must be similarly redefined in terms of $\theta(x,y,z,t)$. As a general situation, we consider three kinds of homogeneous boundary conditions in only the x-direction at the generic boundary position at $x=a$. These conditions are summarized in Table 1, in which η and H are coefficients. Boundary conditions for the other directions can be obtained by inspection.

Table 1
Boundary conditions at the generic position $x=a$ on the boundary for transient, $M\equiv M(a,y,z,t)$, and steady state, $M\equiv M(a,y,z)$, problems.

Boundary conditions for M	Boundary conditions for θ
$M=0$	$\theta=0$
$\frac{\partial M}{\partial x}=0$	$\frac{\partial\theta}{\partial x}+p_1\theta=0$
$\eta\frac{\partial M}{\partial x}+HM=0$	$\eta\frac{\partial\theta}{\partial x}+(H+\eta p_1)\theta=0$

To implement the GITT, we selected an eigenvalue problem with the same kind of boundary conditions as specified for $\theta(x,y,z,t)$.

In that case the problem is given by:

$$\nabla^2\psi(x,y,z)+\mu^2\psi(x,y,z)=0 \tag{13}$$

The eigenvalue problem given by Eq. (13) has nontrivial solutions only for certain values of the parameter $\mu\equiv\mu_i$ ($i=1,2,\ldots,\infty$), called eigenvalues. The corresponding nontrivial solutions $\psi(x,y,z)\equiv\psi_i(x,y,z)$ are eigenfunctions obeying the following orthogonality property:

$$\int_V\psi_i(x,y,z)\psi_j(x,y,z)d\bar{v}=N_i\delta_{ij} \tag{14}$$

where N_i is the normalization integral (or the norm) and δ_{ij} the Kronecker delta. Using this orthogonality property, the integral transform pair is readily derived as:

$$\bar{\theta}_i(t)=\int_V\tilde{\psi}_i(x,y,z)\theta(x,y,z,t)d\bar{v}\quad\text{(Transform)} \tag{15a}$$

$$\theta(x,y,z,t)=\sum_{i=1}^{\infty}\tilde{\psi}_i(x,y,z)\bar{\theta}_i(t)\quad\text{(Inverse)} \tag{15b}$$

where $\tilde{\psi}_i(x,y,z)$ are the normalized eigenfunctions defined by

$$\tilde{\psi}_i(x,y,z)=\frac{\psi_i(x,y,z)}{\sqrt{N_i}} \tag{16}$$

The integral transformation of Eq. (12a) can now be carried out by applying the operator $\int_V\tilde{\psi}_i(x,y,z)d\bar{v}$ and using Eq. (15a,b), leading to an infinite system of decoupled ordinary differential equations of the form

$$R\frac{d\bar{\theta}_i(t)}{dt}+\mu_i^2\bar{\theta}_i(t)=\bar{G}_i(t);\quad i=1,2,\ldots \tag{17a}$$

where

$$\bar{G}_i(t)=\int_V\tilde{\psi}_i(x,y,z)\frac{G(x,y,z,t)}{\exp[(q_1+q_2+q_3)t+p_1x+p_2y+p_3z]}d\bar{v} \tag{17b}$$

The initial conditions in Eq. (12b) must also be transformed to give:

$$\bar{\theta}_i(t=0)=\bar{f}_i=\int_V\tilde{\psi}_i(x,y,z)\frac{\rho(x,y,z)-F(x,y,z;0)}{\exp(p_1x+p_2y+p_3z)}d\bar{v} \tag{17c}$$

The ordinary differential system Eq. (17a,b) with initial condition Eq. (17c) has as formal solution:

$$\bar{\theta}_i(t)=\exp\left(-\frac{\mu_i^2}{R}t\right)\left[\bar{f}_i+\frac{1}{R}\int_0^t\bar{G}_i(\tau)\exp\left(\frac{\mu_i^2}{R}\tau\right)d\tau\right] \tag{18}$$

The unknowns $\theta(x,y,z,t)$ and $T(x,y,z,t)$ can now be obtained by using the inverse formula given by Eq. (15b), and Eqs. (6), (9), respectively, to give:

$$\theta(x,y,z,t)=\sum_{i=1}^{\infty}\tilde{\psi}_i(x,y,z)\exp\left(-\frac{\mu_i^2}{R}t\right)\left[\bar{f}_i+\frac{1}{R}\int_0^t\bar{G}_i(\tau)\exp\left(\frac{\mu_i^2}{R}\tau\right)d\tau\right] \tag{19}$$

$$T(x,y,z,t)=\theta(x,y,z,t)\exp\left\{\frac{ux}{2D_x}+\frac{vy}{2D_y}+\frac{wz}{2D_z}-t\left[\left(\frac{u^2}{4D_xR}+\lambda\right)+\frac{v^2}{4D_yR}+\frac{w^2}{4D_zR}\right]\right\}+F(x,y,z;t) \tag{20}$$

3.3. Steady-state regime

Eq. (5) defined a steady-state transport problem with non-homogeneous boundary conditions. The boundary conditions can again be made homogeneous using the filter strategy:

$$T(x,y,z) = M(x,y,z) + F(x,y,z) \tag{21}$$

where $F(x,y,z)$ satisfies exactly the original boundary conditions of $T(x,y,z)$. Therefore, the steady-state problem can be re-written as

$$LM(x,y,z) = \nabla^2 M(x,y,z) + G(x,y,z) \tag{22}$$

where $G(x,y,z)$ is the new source term containing information about the original source and the filter function.

For the steady-state problem we use a change-of-variable similar to Eq. (9) but without the time domain:

$$M(x,y,z) = \theta(x,y,z)\exp(p_1 x + p_2 y + p_3 z) \tag{23}$$

This substitution eliminates the advection terms when p_1, p_2, and p_3 are chosen judiciously. In this case the choices are the same as for the transient case, Eq. (11a–c). Therefore, the new formulation for the steady transport equation in terms of $\theta(x,y,z)$ is

$$\left(\frac{u^2}{4D_x} + \frac{v^2}{4D_y} + \frac{w^2}{4D_z} + \lambda R\right)\theta(x,y,z) = \nabla^2\theta(x,y,z) + \frac{G(x,y,z)}{\exp\left(\frac{u}{2D_x}x + \frac{v}{2D_y}y + \frac{w}{2D_z}z\right)} \tag{24}$$

Eq. (24) is also a diffusion equation, but with a modified source term that contains the advection information of the original problem. The boundary conditions in terms of $\theta(x,y,z)$ are summarized in Table 1.

The eigenvalue problem in this case is the same as for the transient problem, and is given by Eq. (13). The integral transform pair is given by:

$$\bar{\theta}_i = \int_V \tilde{\psi}_i(x,y,z)\theta(x,y,z)d\bar{v} \quad \text{(Transform)} \tag{25a}$$

$$\theta(x,y,z) = \sum_{i=1}^{\infty}\tilde{\psi}_i(x,y,z)\bar{\theta}_i \quad \text{(Inverse)} \tag{25b}$$

Note that the transformed potentials $\bar{\theta}_i$ are constants for each value of i.

Applying the operator $\int_V \tilde{\psi}_i(x,y,z)d\bar{v}$ to Eq. (24) and using Eq. (25a,b), results in the following transformed equation:

$$\left(\frac{u^2}{4D_x} + \frac{v^2}{4D_y} + \frac{w^2}{4D_z} + \lambda R\right)\bar{\theta}_i + \mu_i^2\bar{\theta}_i = \bar{G}_i; \quad i = 1,2,\ldots \tag{26a}$$

$$\bar{G}_i = \int_V \tilde{\psi}_i(x,y,z)\frac{G(x,y,z)}{\exp\left(\frac{u}{2D_x}x + \frac{v}{2D_y}y + \frac{w}{2D_z}z\right)}d\bar{v} \tag{26b}$$

The solution of this equation is:

$$\bar{\theta}_i = \frac{\bar{G}_i}{\mu_i^2 + \left(\frac{u^2}{4D_x} + \frac{v^2}{4D_y} + \frac{w^2}{4D_z} + \lambda R\right)} \tag{27}$$

Finally, invoking the inverse formula, Eq. (25b), and recalling Eqs. (21), (23), we obtain:

$$\theta(x,y,z) = \sum_{i=1}^{\infty}\tilde{\psi}_i(x,y,z)\frac{\bar{G}_i}{\mu_i^2 + \left(\frac{u^2}{4D_x} + \frac{v^2}{4D_y} + \frac{w^2}{4D_z} + \lambda R\right)} \tag{28}$$

$$T(x,y,z) = \theta(x,y,z)\exp\left(\frac{u}{2D_x}x + \frac{v}{2D_y}y + \frac{w}{2D_z}z\right) + F(x,y,z) \tag{29}$$

4. Test cases

4.1. First test case

As a test case for the general analytical solution, we consider the particular problem of solving the linearized Burgers equation [13]. The partial differential equation for this test case is

$$R\frac{\partial T(x,t)}{\partial t} + u\frac{\partial T(x,t)}{\partial x} = D_x\frac{\partial^2 T(x,t)}{\partial x^2} \tag{30a}$$

with initial and boundary conditions:

$$T(x,0) = 1; \quad 0 \le x \le 1 \tag{30b}$$

$$T(0,t) = 1; \quad T(1,t) = 0; \quad t > 0 \tag{30c,d}$$

Because Eq. (30c) is not homogeneous, it is necessary to define a filter function to homogenize the boundary condition. A suitable filter may be found by solving the steady-state version of Eq. (30a):

$$u\frac{dF(x)}{dx} = D_x\frac{d^2F(x)}{dx^2} \tag{31a}$$

with boundary conditions

$$F(0) = 1; \quad F(1) = 0 \tag{31b,c}$$

This differential equation has the following analytic solution:

$$F(x) = \frac{1 - \exp\left(-\frac{u}{D_x}(1-x)\right)}{1 - \exp\left(-\frac{u}{D_x}\right)} \tag{32}$$

Eq. (30) can be written in terms of $M(x,t)$ by using Eq. (6):

$$R\frac{\partial M(x,t)}{\partial t} + u\frac{\partial M(x,t)}{\partial x} = D_x\frac{\partial^2 M(x,t)}{\partial x^2} \tag{33a}$$

$$M(x,0) = 1 - F(x); \quad 0 \le x \le 1 \tag{33b}$$

$$M(0,t) = 0; \quad M(1,t) = 0; \quad t > 0 \tag{33c,d}$$

The values of p_1 and q_1 that transform Eq. (33a) into an exclusively diffusive equation are given by:

$$p_1 = \frac{u}{2D_x}; \quad q_1 = -\left(\frac{u^2}{4D_x R}\right) \tag{34a,b}$$

According to the general solution presented above, we need to specify the eigenfunction and eigenvalues problem in a form such as defined by Eq. (13). In this case the eigenvalue problem is a Sturm–Liouville problem with the set of eigenvalues given by:

$$\beta_i = i\pi; \quad \mu_i = \beta_i\sqrt{D_x}; \quad i = 1,2,\ldots \tag{35a,b}$$

and with the norms and the normalized eigenfunctions as:

$$N_i = \frac{1}{2}; \quad \tilde{\psi}_i = \sqrt{2}sin(\beta_i x) \tag{36,37}$$

We note that these eigenfunctions and eigenvalues satisfy the following orthogonality property:

$$\int_0^1 \tilde{\psi}_i(x)\tilde{\psi}_j(x)dx = \delta_{ij} \tag{38}$$

The next step according to the general analytical solution procedure is to calculate the initial coefficient $\bar{f}_i$ established in Eq. (17c), whose analytic expression is given by

$$\bar{f}_i = -\frac{(-1)^i 4\sqrt{2}D_x^2\mu_i\exp(-\frac{u}{2D_x})}{u^2 + 4D_x^2\mu_i^2} \tag{39}$$

The structure of Eq. (37) implies that for specified values of u and D_x, the absolute value of $\bar{f}_i$ decreases monotonically as the eigenvalue order increases. Such behavior is expected in the GITT approach.

We can now compose the analytical solution for the linearized Burgers equation:

$$T(x,t) = \exp\left(\frac{u}{2D_x}x - \frac{u^2}{4D_xR}t\right)\sum_{i=1}^{\infty}\tilde{\psi}_i(x)\exp\left(-\frac{\mu_i^2}{R}t\right)\bar{f}_i + F(x) \quad (40)$$

Numerical results were obtained for the following two sets of parameter values: $t = 0.1$, $R = 1$, $D_x = 1$, $u = 1$, $\lambda = 0$ and $t = 0.1$, $R = 1$, $D_x = 1$, $u = 10$, $\lambda = 0$. These cases were chosen to permit a comparison with previous results presented by Cotta [13]. Cotta obtained a solution for the linearized Burgers equation using a hybrid analytical–numerical GITT approach in which the transformed infinite system of ordinary differential equations was truncated and solved numerically using the DIVAPG subroutine from the IMSL Library [22].

Tables 2 and 3 compare the convergence of the present solution with the hybrid solution of Cotta [13], the latter results shown in parentheses. The parameter N in the tables is the number of terms summed in the truncated infinite series for both the present analytic solution and the hybrid solution of [13]. Also shown are results for a fully numerical solution obtained by Cotta [13] using the DMOLCH subroutine from the IMSL Library [22]. In both cases (with $u = 1$ and $u = 10$) the new analytical solution required only $N = 5$ terms to achieve convergence to six decimal places. In fact, the solution for only $N = 1$ term already provides an excellent approximation to the true solution. The converged analytical solution agreed excellently with the hybrid GITT and the full numerical results reported by Cotta [13].

The faster convergence demonstrated in Tables 2 and 3 is due to the change-of-variable used in the present analytic solution that transformed the original advection–diffusion partial differential equation into a pure diffusive equation. The hybrid solution of [13] applied the GITT directly to the advection–diffusion equation.

4.2. Second test case

As a second example, we solve a transport problem that, among other applications, has been employed to model nutrient and contaminant transport in soils (e.g., van Genuchten [23]). In his paper, van Genuchten [23] used Laplace transforms to derive the analytic solution for solute transport of up to four species involved in sequential decay chain reactions. Here, we compare results from the present formulation with earlier results obtained in [23] for the first species, ammonium (NH_4^+). The transport of ammonium is of interest both as a plant nutrient and a possible groundwater contaminant.

The dimensionless transport equation, in terms of the solute concentration, is given by:

$$R\frac{\partial C(x,t)}{\partial t} + \frac{\partial C(x,t)}{\partial x} + \gamma C(x,t) = \frac{1}{Pe}\frac{\partial^2 C(x,t)}{\partial x^2} \quad (41a)$$

with initial condition:

$$C(x,0) = 0; \quad t = 0 \quad (41b)$$

and boundary conditions:

$$-\frac{\partial C(0,t)}{\partial x} + PeC(0,t) = Pe; \quad \frac{\partial C(1,t)}{\partial x} = 0 \quad (41c, d)$$

The dimensionless parameters Pe and γ in Eq. (39) are defined by:

$$Pe = \frac{L_0 u^*}{D_x^*}; \quad \gamma = \frac{\lambda^* R L_0}{u^*} \quad (42a, b)$$

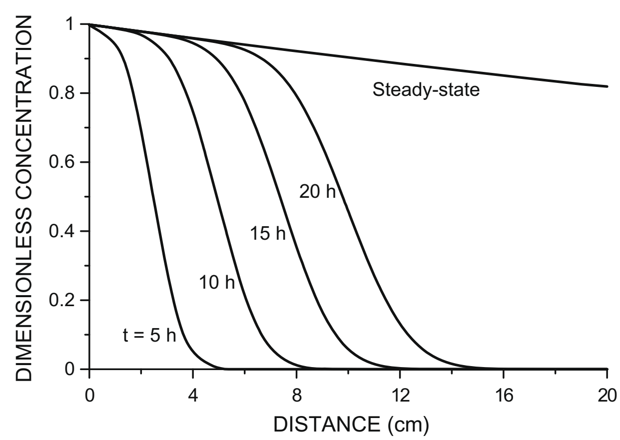

Fig. 1. Distribution of the dimensionless concentration at various times ($L_0 = 20$ cm).

Table 2
Convergence comparison of the analytical and hybrid solutions for $u = 1$, $t = 0.1$, $R = 1$, $D_x = 1$, and $\lambda = 0$.

x	Analytical solution (hybrid solution, Ref. [13])					Ref. [13]
	$N = 1$	$N = 5$	$N = 10$	$N = 15$	$N = 30$	
0.1	0.983264	0.981048 (0.98145)	0.981048 (0.98101)	0.981048 (0.98104)	0.981048 (0.98105)	0.9810
0.3	0.925062	0.921078 (0.92105)	0.921078 (0.92107)	0.921078 (0.92109)	0.921078 (0.92108)	0.9210
0.5	0.798233	0.798211(0.79842)	0.798211(0.79823)	0.798211(0.79821)	0.798211(0.79821)	0.7981
0.7	0.567179	0.57206 (0.57225)	0.57206 (0.57211)	0.57206 (0.57207)	0.57206 (0.57206)	0.5720
0.9	0.216888	0.220238 (0.21993)	0.220238 (0.22033)	0.220238 (0.22026)	0.220238 (0.22024)	0.2202

Table 3
Convergence comparison of the analytical and hybrid solutions for $u = 10$, $t = 0.1$, $R = 1$, $D_x = 1$, and $\lambda = 0$.

x	Analytical solution (hybrid solution, Ref. [13])					Ref. [13]
	$N = 1$	$N = 5$	$N = 10$	$N = 15$	$N = 30$	
0.1	0.999941	0. 999939 (1.00020)	0.999939 (0.99993)	0. 999939 (0.99994)	0.999939 (0.99994)	0.9999
0.3	0.999268	0.999259 (0.99953)	0.999259 (0.99923)	0.999259 (0.99927)	0.999259 (0.99926)	0.9993
0.5	0.99376	0.99376 (0.99476)	0.99376 (0.99370)	0.99376 (0.99377)	0.99376 (0.99376)	0.9938
0.7	0.951251	0.951317 (0.95264)	0.951317 (0.95122)	0.951317 (0.95135)	0.951317 (0.95132)	0.9513
0.9	0.633182	0.633293 (0.63477)	0.633293 (0.63322)	0.633293 (0.63322)	0.633293 (0.63329)	0.6333

where L_0 is the length of the domain, u^* is he advective velocity, D_x^* is the dispersion coefficient, λ^* is the first-order decay coefficient, and R is the retardation factor. Parameter values for the transport of ammonium were taken as [23]: u^*=1 cm h^{-1}, $D_x^* = 0.18$ cm^2 h^{-1}, R = 2, $\lambda^* = 0.005$ h^{-1}.

The parameters of the general analytical solution and the variables in the present test problem correspond as:

$$D_x = \frac{1}{Pe}; \quad u = 1; \quad \lambda = \frac{\gamma}{R} \tag{43a-c}$$

Therefore, parameter p_1 and q_1 are given by:

$$p_1 = \frac{Pe}{2}; \quad q_1 = -\frac{1}{R}\left(\frac{Pe}{4} + \gamma\right) \tag{44a, b}$$

The eigenfunction for this case is obtained from the following Sturm–Liouville problem:

$$\frac{d^2\psi(x)}{dx^2} + \mu^2\psi(x) = 0 \tag{45a}$$

with boundary conditions:

$$-\frac{d\psi(0)}{dx} + Pe\psi(0) = 0; \quad \frac{d\psi(1)}{dx} + Pe\psi(1) = 0 \tag{45b, c}$$

It is interesting that, due to the change-of-variables, the boundary condition at x = 1 is now a third-type boundary condition, similarly as the condition at x = 0.

The analytic solution of the eigenvalue problem is [10]:

$$\psi_i = \beta_i cos(\beta_i x) + H_1 sin(\beta_i x) \tag{46}$$

The norms and eigenvalues are obtained from the following equations:

$$N_i = \frac{(\beta_i^2 + H_1^2) + H_1 + H_2}{2} \tag{47}$$

$$tan(\beta_i) = \frac{\beta_i(H_1 + H_2)}{\beta_i^2 - H_1H_2} \tag{48}$$

respectively, where $H_1 = \frac{Pe}{2} and H_2 = \frac{Pe}{2}$.

The filter function is obtained by solving the equation:

$$\frac{dF(x)}{dx} + \gamma F(x) = \frac{1}{Pe}\frac{d^2F(x)}{dx^2} \tag{49a}$$

with the boundary conditions:

$$-\frac{dF(0)}{dx} + PeF(0) = Pe; \quad \frac{dF(1)}{dx} = 0 \tag{49b, c}$$

This ordinary differential equation can be solved analytically, leading to the following expression for the filter function:

Table 4
Solution convergence for L_0 = 200 cm and t = 200 h (N = number of terms summed).

X (cm)	Dimensionless concentration			Ref.[23]
	N = 250	N = 350	N = 400	
0	0.9982064510	0.9982064510	0.9982064510	0.99821
5	0.9496085026	0.9496085026	0.9496085026	0.94961
10	0.9033765583	0.9033765583	0.9033765583	0.90338
15	0.8593954286	0.8593954286	0.8593954286	0.85940
20	0.8175555319	0.8175555319	0.8175555319	0.81756
25	0.7777526219	0.7777526219	0.7777526219	0.77775
30	0.7398875272	0.7398875272	0.7398875272	0.73989
35	0.7038659047	0.7038659047	0.7038659047	0.70387
40	0.6695980046	0.6695980046	0.6695980046	0.66960
45	0.6369984464	0.6369984464	0.6369984464	0.63700
50	0.6059860065	0.6059860065	0.6059860065	0.60599
55	0.5764834154	0.5764834154	0.5764834154	0.57648
60	0.5484171659	0.5484171659	0.5484171659	0.54842
65	0.5217173284	0.5217173284	0.5217173284	0.52172
70	0.4963172806	0.4963172806	0.4963172806	0.49632
75	0.4721485541	0.4721485541	0.4721485541	0.47215
80	0.4490140056	0.4490140056	0.4490140056	0.44901
85	0.4250786668	0.4250786668	0.4250786668	0.42508
90	0.3894312160	0.3894312160	0.3894312160	0.38943
95	0.3149047564	0.3149047564	0.3149047564	0.31490
100	0.1927162768	0.1927162768	0.1927162768	0.19272
105	0.07678511830	0.07678511830	0.07678511830	0.07679
110	0.01794434192	0.01794434192	0.01794434192	0.01794
115	0.002312432594	0.002312432594	0.002312432594	0.00231
120	0.0001586398313	0.0001586398313	0.0001586398313	0.00016
125	$5.675789878 \times 10^{-6}$	$5.675789878 \times 10^{-6}$	$5.675789878 \times 10^{-6}$	0.00001
130	$1.045824992 \times 10^{-7}$	$1.045824992 \times 10^{-7}$	$1.045824992 \times 10^{-7}$	0.00000
135	$9.845112917 \times 10^{-10}$	$9.845112917 \times 10^{-10}$	$9.845112917 \times 10^{-10}$	0.00000
140	0.000000000	0.000000000	0.000000000	0.00000
145	$-1.325484431 \times 10^{-10}$	0.000000000	0.000000000	0.00000
150	0.0001250537544	0.000000000	0.000000000	0.00000
155	336.4850318	0.000000000	0.000000000	0.00000
160	$3.536666357 \times 10^{8}$	0.000000000	0.000000000	0.00000
165	$1.365890562 \times 10^{14}$	0.000000000	0.000000000	0.00000
170	$-2.043458682 \times 10^{20}$	0.000000000	0.000000000	0.00000
175	$-4.597385308 \times 10^{26}$	0.000000000	0.000000000	0.00000
180	$-4.459462906 \times 10^{32}$	0.000000000	0.000000000	0.00000
185	$-1.312702502 \times 10^{38}$	0.000000000	0.000000000	0.00000
190	$3.199088984 \times 10^{44}$	0.000000000	0.000000000	0.00000
195	$6.267155179 \times 10^{50}$	0.000000000	0.000000000	0.00000
200	$5.611318166 \times 10^{56}$	0.000000000	0.000000000	0.00000

$$F(x) = \frac{4\gamma\sqrt{Pe}\exp\left[-w\sqrt{Pe}+\frac{1}{2}\left(Pe+w\sqrt{Pe}\right)x\right]+2\exp\left[\frac{1}{2}\left(Pe-w\sqrt{Pe}\right)x\right]\sqrt{Pe}\left(Pe+w\sqrt{Pe}+2\gamma\right)}{-\exp\left(-w\sqrt{Pe}\right)\left(\sqrt{Pe}+w\right)\left(Pe-w\sqrt{Pe}+2\gamma\right)+\left(\sqrt{Pe}+w\right)\left(Pe+w\sqrt{Pe}+2\gamma\right)} \tag{50}$$

where $w=\sqrt{Pe+4\gamma}$.

Finally, we find the transformed initial condition coefficient:

$$\bar{f}_i = \frac{num}{den} \tag{51a}$$

$$num = 8\exp(-w\sqrt{Pe})Pe(w-\sqrt{Pe})\gamma\beta_i - 4Pe(w+\sqrt{Pe})(Pe+w\sqrt{Pe}+2\gamma)\beta_i + 2\exp\left(-\frac{w}{2}\sqrt{Pe}\right)\sin(\beta_i)\left[-Pe^{5/2}\left(Pe+w\sqrt{Pe}+4\gamma\right) + 4w(Pe+w\sqrt{Pe})\beta_i^2\right] \tag{51b}$$

$$den = (w+\sqrt{Pe})(Pe+w\sqrt{Pe}+2\gamma-\exp\left[-w\sqrt{Pe}\right] \times (Pe-w\sqrt{Pe}+2\gamma))(Pew^2+4\beta_i^2)\sqrt{N_i} \tag{51c}$$

The symbolic and numerical computations were made in the Mathematica platform [24]. When we used for this purpose the Mathematica function *FindRoot* to solve the transcendental Eq. (48) and compute the eigenvalues, it was necessary to set the Mathematica parameter *WorkingPrecision* to 200.

Fig. 1 shows dimensionless concentration profiles computed for different times with a relatively short domain length of L_0 = 20 cm. The figure shows the concentration distribution progressing toward a linear, steady-state profile.

Table 4 illustrates the convergence of the solution computed for t = 200 h, where N is again the number of terms summed in the truncated series expansion. For comparison purposes, all values less than 10^{-10} were discarded. The results show that convergence is obtained for the entire spatial domain of L_0 = 200 cm with N = 350 terms; the concentration values did not change when additional (N = 400 or more) terms were used. The converged values are in complete agreement with the previous results of van Genuchten [23]. Table 4 also demonstrates that solution convergence slowly progressed towards the end of the spatial domain as the number of terms in the series increased. For example, convergence for $X \leqslant 135$ cm was obtained

Table 6
Solution convergence for L_0 = 20 cm and t = 20 h (N = number of terms summed).

X (cm)	Dimensionless concentration			Ref. [25]
	N = 20	N = 50	N = 100	
0	0.998206	0.998206	0.998206	0.99821
1	0.988291	0.988291	0.988291	0.98829
2	0.978469	0.978469	0.978469	0.97847
3	0.968683	0.968683	0.968683	0.96868
4	0.958554	0.958554	0.958554	0.95855
5	0.946242	0.946242	0.946242	0.94624
6	0.925461	0.925461	0.925461	0.92546
7	0.881528	0.881528	0.881528	0.88153
8	0.792957	0.792956	0.792956	0.79296
9	0.646514	0.646526	0.646526	0.64653
10	0.458117	0.457931	0.457931	0.45793
11	0.268772	0.271654	0.271654	0.27165
12	0.175886	0.131256	0.131256	0.13126
13	−0.639369	0.0506341	0.0506341	0.05063
14	10.673	0.0153803	0.0153803	0.01538
15	−164.519	0.00364344	0.00364344	0.00364
16	2538.9	0.000668586	0.000668586	0.00067
17	−39170.	0.0000945846	0.0000945846	0.00009
18	604111.	0.0000102798	0.0000102798	0.00001
19	-9.31184×10^6	8.55118×10^{-7}	8.55118×10^{-7}	0.00000
20	1.43399×10^8	6.81699×10^{-8}	6.81699×10^{-8}	0.00000

Table 5
Solution convergence for L_0 = 140 cm and t = 200 h (N = number of terms summed).

X (cm)	Dimensionless concentration			
	N = 100	N = 150	N = 200	N = 250
0	0.9982064510	0.9982064510	0.9982064510	0.9982064510
5	0.9496085026	0.9496085026	0.9496085026	0.9496085026
10	0.9033765583	0.9033765583	0.9033765583	0.9033765583
15	0.8593954286	0.8593954286	0.8593954286	0.8593954286
20	0.8175555319	0.8175555319	0.8175555319	0.8175555319
25	0.7777526219	0.7777526219	0.7777526219	0.7777526219
30	0.7398875272	0.7398875272	0.7398875272	0.7398875272
35	0.7038659047	0.7038659047	0.7038659047	0.7038659047
40	0.6695980046	0.6695980046	0.6695980046	0.6695980046
45	0.6369984464	0.6369984464	0.6369984464	0.6369984464
50	0.6059860065	0.6059860065	0.6059860065	0.6059860065
55	0.5764834154	0.5764834154	0.5764834154	0.5764834154
60	0.5484171659	0.5484171659	0.5484171659	0.5484171659
65	0.5217173284	0.5217173284	0.5217173284	0.5217173284
70	0.4963172806	0.4963172806	0.4963172806	0.4963172806
75	0.4721485541	0.4721485541	0.4721485541	0.4721485541
80	0.4490137609	0.4490140056	0.4490140056	0.4490140056
85	0.1320360358	0.4250786668	0.4250786668	0.4250786668
90	103148.4364	0.3894312160	0.3894312160	0.3894312160
95	$3.904198455 \times 10^{11}$	0.3149047564	0.3149047564	0.3149047564
100	$1.109849736 \times 10^{17}$	0.1927162768	0.1927162768	0.1927162768
105	$-3.774497734 \times 10^{23}$	0.07678511830	0.07678511830	0.07678511830
110	$-3.448237131 \times 10^{29}$	0.01794434192	0.01794434192	0.01794434192
115	$2.298888763 \times 10^{35}$	0.002312432594	0.002312432594	0.002312432594
120	$5.264401526 \times 10^{41}$	0.0001586227102	0.0001586398313	0.0001586398313
125	$4.119631336 \times 10^{46}$	0.02564681436	$5.675789878 \times 10^{-6}$	$5.675789878 \times 10^{-6}$
130	$-5.803900012 \times 10^{53}$	−2020.240884	$1.045824992 \times 10^{-7}$	$1.045824992 \times 10^{-7}$
135	$-3.829622487 \times 10^{59}$	$-2.788998787 \times 10^{10}$	$9.845112917 \times 10^{-10}$	$9.845112917 \times 10^{-10}$
140	4.484729306 × 1065	2.605574947 × 1016	0	0

with $N = 250$ terms, while $N = 350$ terms were required to achieve convergence over the entire 200 cm domain.

Because in this example the concentration was zero for $X > 140$ cm, the simulation could have been performed with a shorter domain (e.g., $L_0 = 140$ cm). Table 5 shows that convergence for $L_0 = 140$ cm is faster, occurring now with $N = 200$. The faster convergence is due to the fact that a smaller value of L_0 corresponds to a smaller Peclet number, which causes the transport problem to become more diffusive. This faster convergence for smaller L_0 can be exploited when making early time calculations for large domains (i.e., when the solute has moved in only a small fraction of the transport domain). This idea is demonstrated in Table 6, which shows results for the same transport parameters as before at the early time $t = 20$ h and $L_0 = 20$ cm. Convergence was achieved now with only $N = 50$ terms and verified with $N = 100$. We note that the converged results duplicated exactly the earlier analytic solution [23] as implemented within the STANMOD computer software [25]. We note also that it was possible to obtain these same results with default values for the *WorkingPrecision* parameter.

5. Conclusions

Using the Generalized Integral Transform Technique (GITT), in its classic formulation, in combination with a simple algebraic substitution, it was possible to obtain a formal exact solution of the linear advection–dispersion (or diffusion) transport equation for both transient and steady-state regimes. The mathematical substitution, which transformed the original advection–diffusion problem, into an exclusively diffusive problem, proved to be very advantageous by improving convergence of the GITT series solution.

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