



Dimensionless analysis of two analytical solutions for 3-D solute transport in groundwater

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Abstract

Analytical solutions are widely used as screening tools for estimating the potential for contaminant transport in groundwater, or for interpreting tracer tests or groundwater quality data. A solution for three-dimensional solute migration from a plane-source source that is frequently used in practice is the approximate solution of Domenico [J. Hydrol. 91 (1987) 49–58]. A more rigorous solution to the same problem was provided by Sagar [ASCE, J. Hydraul. Div. 108, no. HY1 (1982) 47–62]. A comprehensive and unambiguous comparison between these two solutions is provided using dimensionless analysis. The solutions are first cast in terms of dimensionless parameters and then used to provide type curves covering a wide range of dimensionless parameter values. Results show that while discrepancies between the two solutions are relatively negligible along the plume centreline (for flow regimes dominated by advection and mechanical dispersion), large concentration differences can be observed as lateral distance from the centreline increases, especially in the presence of solute decay. © 2004 Elsevier B.V. All rights reserved.

Keywords: Analytical solutions; Solute transport; Dimensionless variables; Decay

1. Introduction

Analytical solutions are popular tools for estimating the potential for contaminant transport in groundwater. While numerical models are able to account for the complexity of the subsurface and may accommodate complicated boundary conditions, information

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concerning this complexity may often be lacking, particularly at an early stage of a project. Analytical solutions then provide a useful alternative approach for making screening-level calculations. Analytical solutions are also ideal for addressing uncertainty under conditions of limited information. In general, they can be evaluated much more quickly than numerical solutions, making it feasible to compute a large number of results for Monte Carlo analysis, for example.

For a given transport equation, analytical solutions will differ according to the assumed domain geometry, the source geometry and boundary conditions. Huyakorn et al. (1987) compared several analytical solutions for three-dimensional transport in groundwater that have different source geometries and boundary conditions. This paper focuses on two solutions that have the same geometries and boundary conditions, and can therefore be expected to provide similar results. The first solution is the approximate solution proposed by Domenico (1987) for three-dimensional transport with first-order decay. This solution is one of the most widely used analytical solutions for three-dimensional solute transport in the field of contaminant hydrogeology and has been implemented in several risk assessment models, for example, RBCA (ASTM, 1995) and BIOSCREEN (Newell et al., 1996). The second solution was proposed by Sagar (1982); it addresses the same problem as the Domenico solution but its derivation is more rigorous.

Although it is well known that the Domenico solution can yield discrepancies, particularly at early times and close to the source (see Domenico and Robbins, 1985; Huyakorn et al., 1987), to date there has been no comprehensive assessment of the solution's range of validity, particularly in the presence of first-order decay. A comprehensive and unambiguous comparison between these two analytical solutions is provided here using dimensionless parameters. First, certain assumptions underlying the original solutions and their derivation are presented. The starting points of the two solutions are presented in some detail for the sake of clarity. Next, the solutions are cast in terms of dimensionless parameters and compared using type curves covering a wide range of dimensionless parameter values. A numerical example using typical site parameter values illustrates the potential magnitude of the discrepancies between the Domenico and Sagar solutions.

2. Analytical solutions

The geometry of the problem addressed by the Domenico and Sagar solutions is illustrated schematically in Fig. 1. The equation describing advective–dispersive transport in a uniform flow field, with linear retardation and first-order decay, can be written as:

$$R \frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - v \frac{\partial c}{\partial x} - R\lambda c \quad (1)$$

with:

$$D_x = \alpha_x v + D_0 \psi, \quad D_y = \alpha_y v + D_0 \psi, \quad D_z = \alpha_z v + D_0 \psi \quad (2)$$

where c is the solute concentration at points x , y , z and at time t ; v is the average linear groundwater velocity; α_x is longitudinal dispersivity (in the direction of flow); α_y is

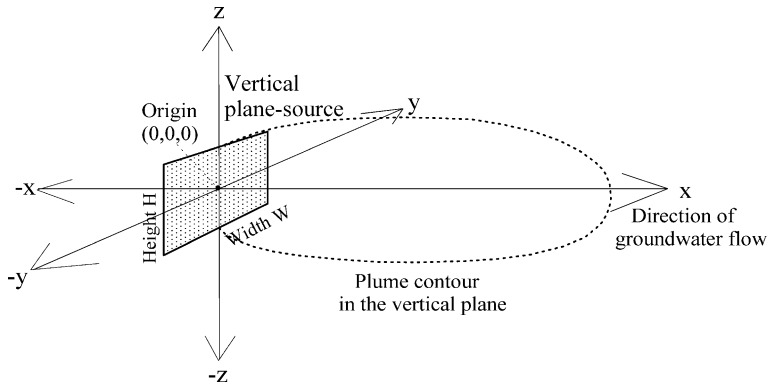


Fig. 1. Geometry and axis coordinate system for a vertical source-plane.

horizontal-transverse dispersivity; α_z is vertical-transverse dispersivity; D_0 is free-solution diffusion coefficient; ψ is tortuosity; R is retardation coefficient in the aquifer; and λ is the first-order constant for decay in the aquifer.

Embedded in Eq. (1) are the following assumptions:

- Groundwater flow is steady and uni-directional along the x -axis;
- Material properties are homogeneous;
- Partitioning between dissolved and sorbed phases is instantaneous and reversible;
- Solute undergoes first-order degradation at the same rate in the dissolved and sorbed phases.

Solutions to Eq. (1) exist for a variety of boundary conditions (see for example Lenda and Zuber, 1970; Wexler, 1992). For the case of a constant source concentration, an analytical solution that is used frequently for three-dimensional solute transport is the “approximate” solution proposed by Domenico (1987). The starting equation (or Green’s function) used by Domenico and Robbins (1985) is the solution for a point source in an infinite aquifer. The governing equation for the Green’s function is:

$$R \frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - v \frac{\partial c}{\partial x} - R\lambda c + \frac{M}{\theta} \delta(x - x') \delta(y - y') \delta(z - z') \delta(t - t') \quad (3)$$

subject to boundary conditions:

$$c(\pm \infty, y, z, t) = 0 \quad (4)$$

$$c(x, \pm \infty, z, t) = c(x, y, \pm \infty, t) = 0 \quad (5)$$

and initial condition:

$$c(x, y, z, 0) = 0 \quad (6)$$

In Eq. (3), M is the mass released instantaneously at point (x', y', z') at time t' , θ is aquifer porosity and δ is the Dirac delta function. The boundary conditions (Eqs. (4) and (5)) incorporate the implicit assumption that the aquifer is infinitely wide and infinitely thick. The analytical solution is (Lenda and Zuber, 1970):

$$c(x, y, z, t) = \frac{M}{\theta} \frac{1}{8\pi^{3/2}} \frac{1}{\sqrt{D_x D_y D_z / R}} \frac{1}{(t - t')^{3/2}} \exp[-\lambda(t - t')] \cdot \exp\left[-\frac{\{(x - x') - v(t - t')/R\}^2}{4D_x(t - t')/R}\right] \cdot \exp\left[-\frac{(y - y')^2}{4D_y(t - t')/R}\right] \cdot \exp\left[-\frac{(z - z')^2}{4D_z(t - t')/R}\right] \quad (7)$$

There are two ways to extend the solution for a point source to the case of a continuous plane-source of width W and height H . The first approach is by analytic integration and yields an expression that includes an integral that must be evaluated numerically. Domenico and Robbins (1985) and Domenico (1987) describe a second approach, presented as “more heuristic than rigorous” (Domenico, 1987), that involves the combination of two simpler solutions; one to account for dispersion in the x direction and another for dispersion in the y and z directions. The transient solution proposed by Domenico (1987) is:

$$c(x, y, z, t) = \frac{c_0}{8} \exp\left[\frac{vx}{2D_x} \left(1 - \sqrt{1 + \frac{4\lambda RD_x}{v^2}}\right)\right] \cdot \operatorname{erfc}\left[\frac{x - \frac{vt}{R} \sqrt{1 + \frac{4\lambda RD_x}{v^2}}}{2\sqrt{D_x t / R}}\right] \cdot \left(\operatorname{erf}\left[\frac{y + W/2}{2\sqrt{D_y x / v}}\right] - \operatorname{erf}\left[\frac{y - W/2}{2\sqrt{D_y x / v}}\right]\right) \cdot \left(\operatorname{erf}\left[\frac{z + H/2}{2\sqrt{D_z x / v}}\right] - \operatorname{erf}\left[\frac{z - H/2}{2\sqrt{D_z x / v}}\right]\right) \quad (8)$$

where erf is the error function and $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$.

The steady-state solution along the plume centreline is (Domenico, 1987):

$$c(x, 0, 0, \infty) = c_0 \exp\left[\frac{vx}{2D_x} \left(1 - \sqrt{1 + \frac{4\lambda RD_x}{v^2}}\right)\right] \cdot \operatorname{erf}\left[\frac{W}{4\sqrt{D_y x / v}}\right] \cdot \operatorname{erf}\left[\frac{H}{4\sqrt{D_z x / v}}\right] \quad (9)$$

As the solution is symmetrical with respect to the surface $z=0$ (Fig. 1), this surface can be interpreted either as the middle of the source located within an infinitely thick aquifer, or as the top of a semi-infinite aquifer (see Fig. 6c of Huyakorn et al., 1987). In this case, H is selected as twice the “true” height of the source.

As stated previously, an “exact” solution to the problem of a plane-source in an infinite domain can be obtained by integrating Eq. (5) over the duration of the release and over the dimensions of the source in the y and z directions. To represent a continuous release from a source with concentration (c_o), an expression must be provided for the mass flux M . If the plane-source is a surface of constant concentration, the mass flux has two components; an advective component, and a dispersive component. However, because the value of the dispersive flux is unknown a priori, it is neglected and the mass flux is approximated by only the advective mass flux:

$$\bar{M} = v\theta c_o \tag{10}$$

The solution is:

$$c(x,y,z,t) = \frac{vc_o \exp\left[\frac{vx}{2D_x}\right]}{8\sqrt{\pi D_x/R}} \int_0^t \frac{1}{\tau^{1/2}} \exp\left[-\left(\lambda + \frac{v^2}{4RD_x}\right)\tau - \frac{Rx^2}{4D_x\tau}\right] \cdot \left(\operatorname{erfc}\left[\frac{y-W/2}{2\sqrt{D_y\tau/R}}\right] - \operatorname{erfc}\left[\frac{y+W/2}{2\sqrt{D_y\tau/R}}\right]\right) \cdot \left(\operatorname{erfc}\left[\frac{z-H/2}{2\sqrt{D_z\tau/R}}\right] - \operatorname{erfc}\left[\frac{z+H/2}{2\sqrt{D_z\tau/R}}\right]\right) d\tau \tag{11}$$

where τ is a dummy variable of integration.

A shortcoming of this solution is that because the dispersive component of the source mass flux is neglected, the concentration near the source may be underestimated. In order to actually constrain the concentration at the source to a specified value c_o , the solution must be derived for a domain that is semi-infinite in the x direction. The following source boundary condition is applied to Eq. (1) subject to Eqs. (5) and (6):

$$c(0,y,z,t) = c_o \quad \text{for } -W/2 \leq y \leq W/2 \text{ and } -H/2 \leq z \leq H/2$$

$$c(0,y,z,t) = 0 \quad \text{for } |y| > W/2 \text{ and } |z| > H/2 \tag{12}$$

The solution, which is nearly identical to the previous one, is presented in Sagar (1982) and Wexler (1992):

$$c(x,y,z,t) = \frac{c_o x \exp\left[\frac{vx}{2D_x}\right]}{8\sqrt{\pi D_x/R}} \int_0^t \frac{1}{\tau^{3/2}} \exp\left[-\left(\lambda + \frac{v^2}{4RD_x}\right)\tau - \frac{Rx^2}{4D_x\tau}\right] \cdot \left(\operatorname{erfc}\left[\frac{y-W/2}{2\sqrt{D_y\tau/R}}\right] - \operatorname{erfc}\left[\frac{y+W/2}{2\sqrt{D_y\tau/R}}\right]\right) \cdot \left(\operatorname{erfc}\left[\frac{z-H/2}{2\sqrt{D_z\tau/R}}\right] - \operatorname{erfc}\left[\frac{z+H/2}{2\sqrt{D_z\tau/R}}\right]\right) d\tau \tag{13}$$

The corresponding steady-state solution is slightly awkward to compute as it involves two successive numerical integrations (one in y and another in z). It is more convenient to obtain the steady-state solution by computing Eq. (13) for large values of time. In the comparison provided below, we compare results obtained from Eqs. (8) and (13).

3. Dimensionless analysis

Dimensionless parameters (see for example Sauty, 1977) are particularly useful for comparing analytical solutions because a much wider range of parameter values can be covered in a compact fashion than when dimensional parameters are used. For comparison purposes, type curves can be derived that provide a specific solution's "fingerprint".

First, the following dimensionless parameters are defined (see also Guyonnet et al., 1995, 1996, Perrochet, 1996):

$$C_D = \frac{c}{c_0} \quad X_D = \frac{x}{x_0} \quad Y_D = \frac{vy}{\sqrt{D_x D_y}} \quad Z_D = \frac{vz}{\sqrt{D_x D_z}} \quad (14)$$

$$W_D = \frac{vW}{\sqrt{D_x D_y}} \quad H_D = \frac{vH}{\sqrt{D_x D_z}} \quad t_D = \frac{vt}{Rx_0} \quad Pe = \frac{vx_0}{D_x} \quad \lambda_D = \frac{R\lambda D_x}{v^2} \quad (15)$$

where C_D is relative concentration, X_D , Y_D and Z_D are dimensionless distances in directions x , y and z , respectively, x_0 is an arbitrary distance from the source in the x direction, W_D and H_D are dimensionless source width and height, respectively, t_D is dimensionless time, Pe is the Peclet number and λ_D is the dimensionless decay constant.

The Peclet number is a measure of the relative importance of advection and dispersion in the transport process. The dimensionless distance X_D is defined relative to an arbitrary distance from the source x_0 . Taking $X_D=1$ implies therefore that results are applicable to any point $x=x_0$. The dimensionless decay constant λ_D combines decay and retardation. As indicated previously, it is assumed that solute undergoes first-order degradation at the same rate in the dissolved and sorbed phases. As seen in the expression of λ_D , retardation enhances the effect of decay.

With dimensionless parameters as defined above, the Domenico solution Eq. (8) becomes:

$$C_D = \frac{1}{8} \exp \left[\frac{Pe}{2} \left(1 - \sqrt{1 + 4\lambda_D} \right) \right] \cdot \operatorname{erfc} \left[\frac{X_D - t_D \sqrt{1 + 4\lambda_D}}{2\sqrt{t_D/Pe}} \right] \\ \cdot \left(\operatorname{erfc} \left[\frac{Y_D - W_D/2}{2\sqrt{Pet_D}} \right] - \operatorname{erfc} \left[\frac{Y_D + W_D/2}{2\sqrt{Pet_D}} \right] \right) \\ \cdot \left(\operatorname{erfc} \left[\frac{Z_D - H_D/2}{2\sqrt{Pet_D}} \right] - \operatorname{erfc} \left[\frac{Z_D + H_D/2}{2\sqrt{Pet_D}} \right] \right) \quad (16)$$

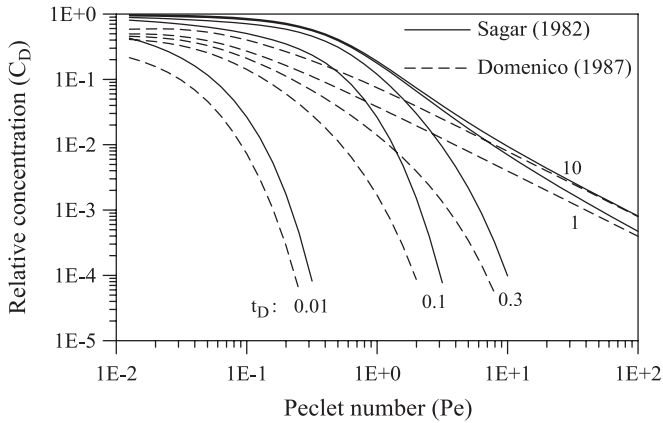


Fig. 2. Comparison between the Domenico (1987) and Sagar (1982) solutions along the plume centreline for different values of dimensionless time (t_D).

While the Sagar solution Eq. (13) becomes:

$$\begin{aligned}
 C_D = & \frac{X_D \sqrt{Pe} \exp\left[\frac{PeX_D}{2}\right]}{8\sqrt{\pi}} \int_0^{t_D} \frac{1}{\tau^{3/2}} \exp\left[Pe\tau(-\lambda_D - 1/4) - \frac{X_D^2 Pe}{4\tau}\right] \\
 & \cdot \left(\operatorname{erfc}\left[\frac{Y_D - W_D/2}{2\sqrt{Pe\tau}}\right] - \operatorname{erfc}\left[\frac{Y_D + W_D/2}{2\sqrt{Pe\tau}}\right] \right) \\
 & \cdot \left(\operatorname{erfc}\left[\frac{Z_D - H_D/2}{2\sqrt{Pe\tau}}\right] - \operatorname{erfc}\left[\frac{Z_D + H_D/2}{2\sqrt{Pe\tau}}\right] \right) d\tau \tag{17}
 \end{aligned}$$

where τ is the dimensionless integration variable (t_D). Replacing the dimensionless parameters by their expressions in Eqs. (14) and (15), it is easily verified that the original solutions expressed in terms of dimensional parameters Eqs. (8) and (13) are recovered.

Fig. 2 presents a graph of relative concentrations versus Peclet number, calculated using the two solutions, without decay and for different values of dimensionless time. Calculations are performed along the plume centreline ($Y_D=Z_D=0$) for a source of dimensions $W_D=H_D=1$ and at a dimensionless distance from the source $X_D=1$ (Table 1).

Table 1
Values of dimensionless parameters used to produce the type curves

	X_D	Y_D	Z_D	Pe	W_D	H_D	t_D	λ_D
Fig. 2	1	0	0	var	1	1	var	0
Fig. 3	1	var	0	var	1	1	100	0
Fig. 4	1	0	0	var	1	1	100	var
Fig. 5	1	1	0	var	1	1	100	var
Fig. 7	1	var	0	1	1	1	100	var
Fig. 8	1	var	0	var	1	1	100	0

var: variable.

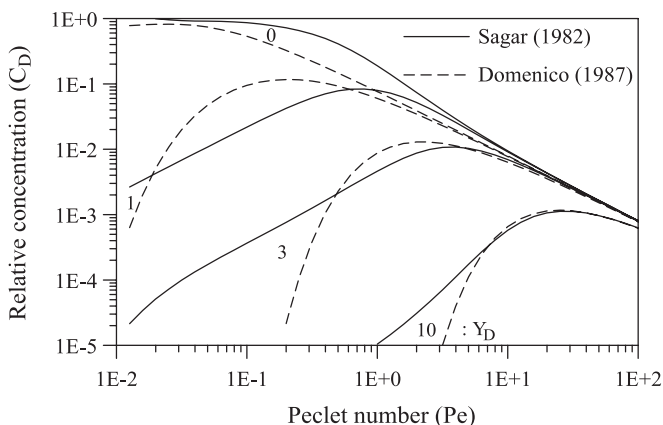


Fig. 3. Steady-state concentrations: effect of lateral distance to the plume axis (Y_D).

Results are presented for a range of dimensionless time from 0.01 to 10. Quasi steady-state conditions are reached beyond dimensionless time values of 10.

Discrepancies between the Domenico and Sagar solutions are observed in particular for intermediate values of Peclet number between 0.1 and 6. According to Pfannkuch (1963), such values correspond to the range where mechanical dispersion and molecular diffusion both influence the transport process. At steady-state the difference may reach a factor of up to 3, while at earlier times, differences may attain an order of magnitude. Although the Domenico solution is seen in Fig. 2 to slightly underestimate relative concentrations compared to the Sagar solution, the figure suggests that in the case of relatively permeable aquifers ($Pe > 6$), the difference between the two solutions for concentrations located along the plume centreline is relatively small and therefore the Domenico solution appears to be a suitable approximation. Calculations also show that for a given value of the Peclet number, differences between the two solutions decrease as the dimensions of the source increase (increasing W_D, H_D).

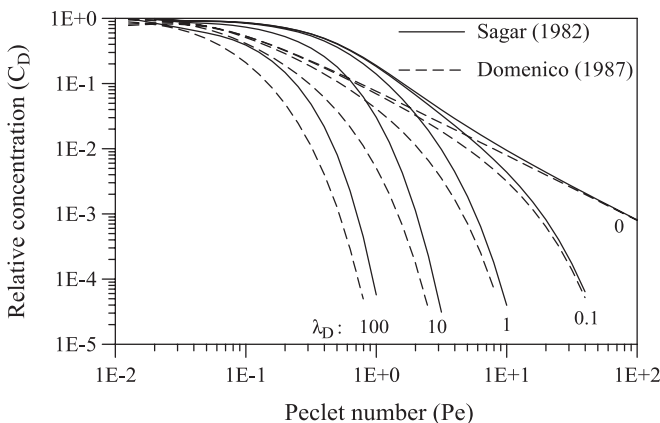


Fig. 4. Steady-state concentrations along the plume centreline: effect of dimensionless decay.

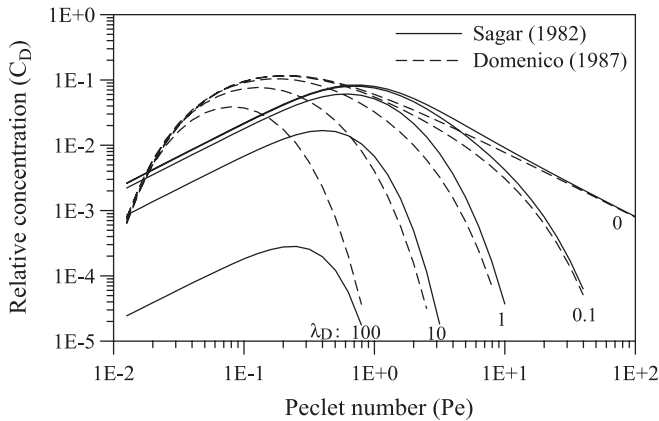


Fig. 5. Steady-state concentrations: effect of decay for a lateral distance to the plume axis $Y_D=1$.

In Fig. 3, calculations are performed at steady-state ($t_D=100$) for different values of dimensionless lateral distance Y_D , with Z_D kept equal to zero. Results suggest that the error in the Domenico solution is significantly influenced by lateral distance to the plume centreline, especially at low values of Peclet number. Discrepancies are increased by non-zero values of Z_D .

The effect of decay on concentrations calculated along the plume centreline and at steady-state is illustrated in Fig. 4. It is seen that an increase of the dimensionless decay constant does not have a significant influence on the discrepancy between the two solutions along the plume centreline. Concentrations off the plume centreline are shown in Fig. 5. In contrast to the results in Fig. 4, Fig. 5 shows that the value of dimensionless decay does have a strong influence on the discrepancy observed at low to intermediate values of Peclet number.

4. Example calculations

This discrepancy between the two solutions outside the plume centreline is illustrated below with a numerical example using typical site parameters. The source width is taken as 10 m while the zone of contamination extends 5 m below the water table ($H=10$ m in Fig. 1). The pollutant decays with a half-life $T_{0.5}=100$ days ($\lambda=\ln(2)/T_{0.5}=0.27$ year $^{-1}$) and undergoes retardation with a factor $R=5$. Aquifer permeability, hydraulic gradient and porosity are 10^{-4} m/s, 0.7% and 0.25, respectively, yielding an average groundwater velocity of 88.3 m/year. Longitudinal, horizontal-transverse and vertical-transverse dispersivities are taken as 8, 2 and 0.5 m, respectively. Calculations are performed at steady-state and at the water table ($z=0$). Fig. 6 shows relative concentrations as a function of longitudinal distance from the source along the plume centreline ($y=0$ m) and at a lateral distance $y=50$ m. While the differences between the two solutions are relatively small along the centreline, there is up to a factor 30 difference at a lateral distance of 50 m. The Domenico solution is seen to overestimate concentrations compared to the Wexler

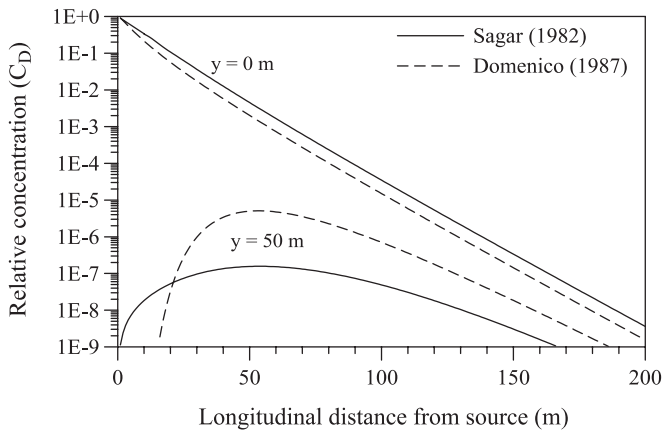


Fig. 6. Numerical example. Comparison between the Domenico (1987) and Sagar (1982) solutions along the plume centreline and at a lateral distance of 50 m.

solution. Whether it over or underestimates concentrations depends primarily on the distance from the source and on the value of dimensionless decay. Although the discrepancy in Fig. 6 affects low concentration values located along the plume fringes, it could be significant in the case of soluble contaminants that are potentially toxic at low concentrations, such as, for example, chlorinated organic solvents. Trichloroethylene (TCE), for example, has a solubility on the order of 1 g/l. Taking this concentration as a constant source concentration, the peak concentration obtained in Fig. 6 at a lateral distance of 50 m would be 5 $\mu\text{g/l}$ with the Domenico (1987) solution and 0.16 $\mu\text{g/l}$ with the Sagar (1982) solution. Considering that certain health authorities (for example, the California Department of Health Services) mandate a maximum allowable concentration for TCE in drinking water of 5 $\mu\text{g/l}$, differences between the solutions of this magnitude could have an influence on decisions relative to potential risks.

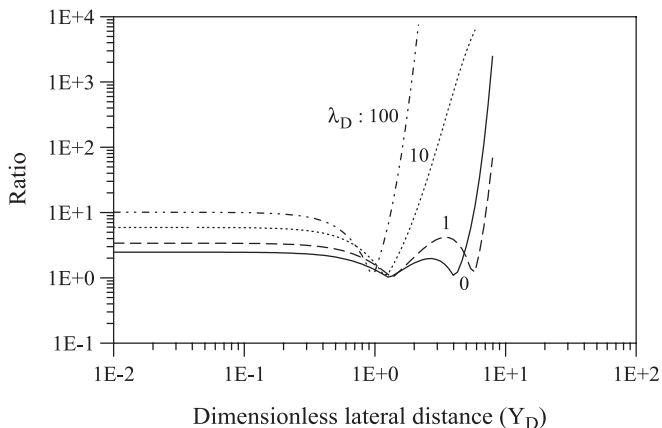


Fig. 7. Discrepancies between the two solutions as a function of dimensionless lateral distance (Y_D) for $Pe=1$ and several values of dimensionless decay (λ_D).

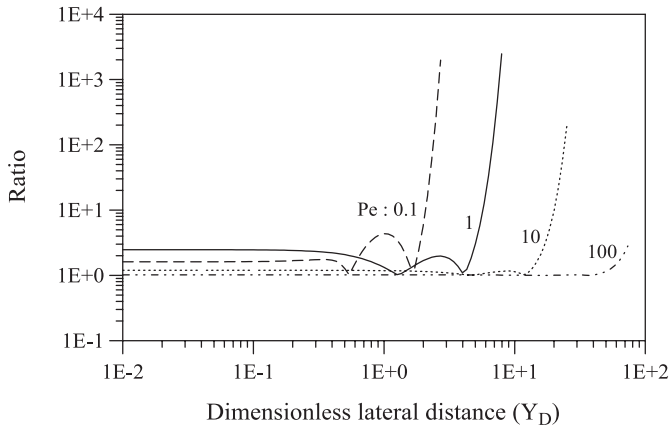


Fig. 8. Discrepancies between the two solutions as a function of dimensionless lateral distance for several values of Pe (no decay).

To assess the magnitude of the discrepancies between the two solutions for increasing lateral distance from the source, ratios are plotted in Figs. 7 and 8. As concentration profiles obtained with the two solutions tend to crossover, the ratios plotted in Figs. 7 and 8 were taken as the higher value of either $C_{\text{Domenico}}/C_{\text{Sagar}}$ or $C_{\text{Sagar}}/C_{\text{Domenico}}$. Therefore the plotted ratios cannot be lower than unity. Fig. 7 presents the ratios for a Peclet number of 1 and for different values of dimensionless decay. Dimensionless depth (Z_D) was taken as zero. The figure shows that as lateral distance from the source (Y_D) increases, the ratios are at first stable (concentrations from the Sagar solution are slightly higher than those from the Domenico solution) and then decrease to unity (equal concentrations) for a lateral distance of 1. Beyond this lateral distance discrepancies increase significantly. For values of λ_D of 0 and 1, concentration profiles cross each other twice which explains the “bumps” in the ratio curves (Fig. 7). Fig. 8 shows the ratio curves for different values of Peclet number ($\lambda_D=0$). It is seen that for large lateral distances, if the Peclet number is large there is little to no discrepancy between the two solutions.

5. Conclusions

The approximate analytical solution proposed by Domenico (1987), for calculating three-dimensional solute transport with decay for a vertical plane-source at a constant concentration, has been evaluated against the more rigorous solution of Sagar (1982). The evaluation has been conducted in dimensionless space and time, thereby allowing a more general consideration of the differences between the two solutions.

The results of the evaluation confirm that along the plume centreline, and for groundwater flow regimes dominated by advection and mechanical dispersion rather than by molecular diffusion, discrepancies between the two solutions can be considered negligible for practical purposes. However, the errors in the Domenico (1987) solution may increase significantly outside the plume centreline. These errors are amplified when

the solute undergoes first-order decay and magnified further if the solute is retarded. If calculations are to be performed outside the plume centreline, the Sagar (1982) solution should be preferred to the Domenico (1987) solution.

List of symbols used

c	solute concentration at points x , y , z and at time t
c_o	constant source concentration
C_D	relative concentration
D_o	free-solution diffusion coefficient
D_x	longitudinal diffusion–dispersion coefficient
D_y	horizontal-transverse diffusion–dispersion coefficient
D_z	vertical-transverse diffusion–dispersion coefficient
erf	error function
erfc	complementary error function
H	height of source zone (along the z -axis)
H_D	dimensionless height of source zone (along the z -axis)
M	mass of slug release
\bar{M}	mass flux from source
Pe	Peclet number
R	retardation coefficient
t	time
t_D	dimensionless time
v	groundwater velocity
W	width of source zone (along the y -axis)
W_D	dimensionless width of source zone (along the y -axis)
x	distance along the x -axis
X_D	dimensionless distance along the x -axis
y	distance along the y -axis
Y_D	dimensionless distance along the y -axis
z	distance along the z -axis (depth)
Z_D	dimensionless distance along the z -axis
α_x	longitudinal dispersivity (in the direction of flow)
α_y	horizontal-transverse dispersivity
α_z	vertical-transverse dispersivity
λ	first-order decay constant
λ_D	dimensionless first-order decay constant
θ	aquifer porosity or soil volumetric water content
τ	integration variable
ψ	tortuosity

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