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Domenico Solution—Is It Valid?

by V. Srinivasan[1], T.P. Clement[2], and K.K. Lee[3]

Abstract

The Domenico solution is widely used in several analytical models for simulating ground water contaminant transport scenarios. Unfortunately, many textbook as well as journal article treatments of this approximate solution are full of empirical statements that are developed without mathematical rigor. For this reason, a rigorous analysis of this solution is warranted. In this article, we present a mathematical method to derive the Domenico solution and explore its limits. Our analysis shows that the Domenico solution is a true analytical solution when the value of longitudinal dispersivity is zero. For nonzero longitudinal dispersivity values, the Domenico solution will introduce a finite amount of error. We use an example problem to quantify the nature of this error and suggest some general guidelines for the appropriate use of this solution.

Introduction

Analytical solutions provide computationally efficient tools for modeling the fate and transport of ground water contaminant plumes (Aziz et al. 2000; Clement et al. 2002). In addition, they are also useful for testing complex numerical models (Clement et al. 1998; Clement 2001; Quezada et al. 2004). One of the most popular analytical solutions used for modeling ground water contaminant plumes is the Domenico (1987) solution. The Domenico solution is an approximate three-dimensional (3D) solution that describes the fate and transport of a decaying contaminant plume evolving from a finite patch source. This solution was based on an approach previously published by Domenico and Robbins (1985) for modeling a nondecaying contaminant plume. Prior to this work, Cleary and Ungs (1978) presented an analytical solution to a similar 3D transport problem for a domain finite in y and z directions. Later, Sagar (1982) published an exact analytical solution to the transport problem considered by Domenico and Robbins (1985). Wexler (1992) extended the Sagar (1982) solution to include the effects of reaction and presented an exact analytical solution to the transport problem considered by Domenico (1987). However, these solutions are not closed form expressions since they involve numerical evaluation of a definite integral. This numerical integration step can be computationally demanding and can also introduce numerical errors. The key advantage of the Domenico and Robbins (1985) approach is that it provides a closed form solution without involving numerical integration procedures. Due to this computational advantage, the Domenico solution has been widely used in several public domain design tools, including the U.S. EPA tools BIOCHLOR and BIOSCREEN (Newell et al. 1996; Aziz et al. 2000).

Although the Domenico solution is extensively employed in several ground water transport models, its approximate nature has received mixed reviews over the years. For example, West and Kueper (2004) compared the BIOCHLOR model against a more rigorous analytical solution and observed considerable discrepancies. By comparing the near field concentration profiles, they concluded that the Domenico solution can produce errors up to 50%. Guyonnet and Neville (2004) compared the Domenico solution against the Sagar (1982) solution and presented the results in a nondimensional form. They concluded that for ground water flow regimes dominated by advection

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and mechanical dispersion, the discrepancies between the two solutions can be considered negligible along the plume centerline. They further added that the errors may increase significantly outside the plume centerline.

The previous review indicates that there are conflicting opinions regarding the performance of the Domenico solution. Furthermore, since the development of the Domenico solution was based on a heuristic approach, researchers have expressed skepticism regarding its validity (West and Kueper 2004). Currently, there are several unanswered issues related to the performance of this solution that include: Is there a mathematical basis for deriving the Domenico solution? If so, what are the approximations involved in deriving the solution? What are the errors associated with these approximations? Finally, under what conditions are these approximations valid? To answer these questions, we need a fundamental understanding of the nature of the approximations involved in the Domenico solution. The focus of this article is to perform a rigorous mathematical analysis on the origin and development of the Domenico solution. The outcomes of this analysis are used to develop some general guidelines for the appropriate use of the solution.

Governing Equations

The transport problem considered by Domenico (1987) assumes a patch source of constant concentration c_o located at $x = 0$ in a clean, semi-infinite aquifer. The contaminant is subjected to advection in the x direction and dispersive mixing in all three directions. Furthermore, it is assumed that the contaminant decays through a first-order process. The governing transport equation considered by Domenico (1987) is:

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

The initial and boundary conditions are:

$$\begin{aligned}
&c(x,y,z,0) = 0,\ \forall\ 0<x<\infty,\ -\infty<y<\infty,\ -\infty<z<\infty\\
&c(0,y,z,t) = c_o,\ -\frac{Z}{2}<z<\frac{Z}{2},\ -\frac{Y}{2}<y<\frac{Y}{2},\ \forall\ t>0\\
&\qquad = 0,\ \text{otherwise}\ \forall\ t>0\\
&\lim_{x\to\infty}\frac{\partial c(x,y,z,t)}{\partial x} = 0\\
&\lim_{y\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial y} = 0\\
&\lim_{z\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial z} = 0
\end{aligned} \quad (2)$$

where c is the concentration of the contaminant [ML^{-3}]; c_o is the concentration at the source [ML^{-3}]; Y and Z are the source dimensions in y and z directions, respectively [L]; D_x, D_y, and D_z are the dispersion coefficients in x, y, and z directions, respectively [L^2T^{-1}]; v is the advection velocity in the x direction [LT^{-1}]; and k is the first-order decay coefficient [T^{-1}].

Review of the Domenico Solution

The Domenico (1987) solution was based on an approximate approach given by Domenico and Robbins (1985). Therefore, we first present a detailed review of the development of the Domenico and Robbins (1985) solution. Domenico and Robbins (1985) began their analysis by presenting the following exact analytical solution that describes the transport of an instantaneous pulse source in a 3D domain (Hunt 1978):

$$\begin{aligned}
&c(x,y,z,t) = \frac{c_o}{8}\tilde{f_x}(x,t)\tilde{f_y}(y,t)\tilde{f_z}(z,t),\\
&\text{where } \tilde{f_x}(x,t) = \left[\operatorname{erf}\left\{\frac{x-vt+\frac{X}{2}}{2(D_xt)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{x-vt-\frac{X}{2}}{2(D_xt)^{1/2}}\right\}\right]\\
&\tilde{f_y}(y,t) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(D_yt)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(D_yt)^{1/2}}\right\}\right]\\
&\tilde{f_z}(z,t) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(D_zt)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(D_zt)^{1/2}}\right\}\right]
\end{aligned} \quad (3)$$

They then present the following one-dimensional (1D) analytical solution (Crank 1975):

$$\begin{aligned}
c(x,t) &= \frac{c_o}{2}f_x(x,t),\\
\text{where}\quad f_x(x,t) &= \operatorname{erfc}\left\{\frac{x-vt}{2(D_xt)^{1/2}}\right\}
\end{aligned} \quad (4)$$

Note that the previous expression is the solution to the standard 1D advection-dispersion equation for an instantaneous source extending from zero to negative infinity (Bear 1979).

To account for the transverse dispersion due to a finite-sized two-dimensional (2D) source, they employed the following two analytical solutions (Crank 1975):

$$\begin{aligned}
&c(y,t) = \frac{c_o}{2}f_y(y,t)\ \text{ and }\ c(z,t) = \frac{c_o}{2}f_z(z,t),\\
&\text{where } f_y(y,t) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(D_yt)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(D_yt)^{1/2}}\right\}\right]\\
&\text{and } f_z(z,t) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(D_zt)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(D_zt)^{1/2}}\right\}\right]
\end{aligned} \quad (5)$$

Note that $c(y,t)$ and $c(z,t)$ are solutions to two independent 1D transient diffusion equations subjected to an instantaneous line source of widths Y and Z, respectively. Further, it can be observed that the terms $f_y(y,t)$ and $f_z(z,t)$

in Equation 5 are identical to the terms $\tilde{f_y}(y,t)$ and $\tilde{f_z}(z,t)$ in the Hunt (1978) solution.

Domenico and Robbins (1985) multiplied the 1D solution $f_x(x,t)$ with these "transverse spreading terms" $f_y(y,t)$ and $f_z(z,t)$ and presented the following expression:

$$c(x,y,z,t) = \frac{c_o}{8} f_x(x,t) f_y(y,t) f_z(z,t) \tag{6}$$

However, the authors did not justify this superposition step. Note that the Hunt solution was never used in this analysis. At this stage, Domenico and Robbins presented the following arguments: "The product of these three integral solutions [Equation 6] describes a semi-infinite contaminated parcel which moves in the positive x direction with a 1D velocity but which continuously expands in size in directions transverse to x throughout the whole domain of x, i.e., in the positive and negative regions. This is because the time t in the transverse spreading terms is interpreted as running time. Reinterpreting this time as x/v for a moving coordinate system, as is common in all transverse spreading models (Bruch and Street, 1967; Ogata, 1970; Domenico and Palciauskas, 1982) has the effect of maintaining the original source dimensions at $x = 0$ so that the condition $C = Co$ is maintained at $x = 0$ for $t > 0$." Using these arguments, they reinterpret the time term t in the transverse spreading terms $f_y(y,t)$ and $f_z(z,t)$ as x/v. However, the authors did not provide a mathematical reasoning for this time reinterpretation step. Further, all the references cited in the previous text solve fundamentally different problems and we will address this issue in a later section. Using this time reinterpretation step, Equation 6 was modified as:

$$\begin{aligned} c(x,y,z,t) &= \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x), \\ \text{where } f_x(x,t) &= \operatorname{erfc}\left\{\frac{x - vt}{2(D_x t)^{1/2}}\right\} \\ f_y(y,x) &= \left[\operatorname{erf}\left\{\frac{y + \frac{Y}{2}}{2(D_y x/v)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y - \frac{Y}{2}}{2(D_y x/v)^{1/2}}\right\}\right] \\ f_z(z,x) &= \left[\operatorname{erf}\left\{\frac{z + \frac{Z}{2}}{2(D_z x/v)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z - \frac{Z}{2}}{2(D_z x/v)^{1/2}}\right\}\right] \end{aligned} \tag{7}$$

Equation 7 was presented as the final solution to the continuous finite patch source problem considered by Domenico and Robbins (1985).

Domenico (1987) incorporated the effects of first-order decay by replacing the $f_x(x,t)$ term with an analytical solution for the semi-infinite pulse source problem with a decay term presented by Bear (1979). The final solution was given as (Domenico 1987):

$$\begin{aligned} c(x,y,z,t) &= \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x), \\ \text{where } f_x(x,t) &= \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 - \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x - vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) \\ f_y(y,x) &= \left[\operatorname{erf}\left\{\frac{y + \frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y - \frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\}\right] \\ f_z(z,x) &= \left[\operatorname{erf}\left\{\frac{z + \frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z - \frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\}\right] \end{aligned} \tag{8}$$

where $\alpha_x = D_x/v$, $\alpha_y = D_y/v$, and $\alpha_z = D_z/v$ are the dispersivities in the x, y, and z directions, respectively [L].

Martyn-Hayden and Robbins (1997) later modified the Domenico (1987) solution, referred in this work as the modified-Domenico solution, by incorporating the following 1D solution (which describes a constant source-boundary) in the $f_x(x,t)$ term (Bear 1979):

$$\begin{aligned} f_x(x,t) = &\left(\exp\left\{\frac{x}{2\alpha_x}\left[1 - \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x - vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) \\ &+ \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 + \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x + vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) \end{aligned} \tag{9}$$

As pointed out by Bear (1979), if the value of x/α_x is sufficiently large, a condition usually satisfied in practice, the additional term in the previous equation can be safely ignored.

The previous review shows that the development of various forms of the Domenico solution does not have a rigorous mathematical basis. The empirical arguments provided by the authors are vague because the mathematical procedures implied by these arguments are inexplicit and nebulous. In the following section, we provide a more rigorous approach to derive the Domenico solution, clearly stating the approximations involved.

A Rigorous Approach to Derive the Domenico Solution

The exact semi-analytical solution for the 3D transport problem described by Equations 1 and 2,

considered by Domenico (1987), was provided by Wexler (1992) as:

$$c(x,y,z,t) = \frac{c_o}{8}\int_{\tau=0}^{\tau=t} f_x'(x,\tau) f_y'(y,\tau) f_z'(z,\tau)\mathrm{d}\tau,$$

$$\text{where } f_x'(x,\tau) = \frac{x}{\sqrt{\pi D_x}}\exp\left(\frac{vx}{2D_x}\right) \times \frac{\exp\left(\frac{-v^2}{4D_x}\tau - k\tau + \frac{-x^2}{4D_x\tau}\right)}{\tau^{3/2}}$$

$$f_y'(y,\tau) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(D_y\tau)^{1/2}}\right\}\right]$$

$$f_z'(z,\tau) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(D_z\tau)^{1/2}}\right\}\right] \quad (10)$$

To obtain the Domenico solution from the previous exact solution, we replace the value of τ in the transverse spreading terms $f_y'(y,\tau)$ and $f_z'(z,\tau)$ with x/v (the validity of this substitution will be discussed later). This yields the following expression:

$$c(x,y,z,t) = \frac{c_o}{8} f_y(y,x) f_z(z,x)\int_{\tau=0}^{\tau=t} f_x'(x,\tau)\mathrm{d}\tau,$$

$$\text{where } f_y(y,x) = \left[\operatorname{erf}\left\{\frac{y+\frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y-\frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\}\right]$$

$$f_z(z,x) = \left[\operatorname{erf}\left\{\frac{z+\frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z-\frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\}\right] \quad (11)$$

where $\alpha_y = D_y/v$ and $\alpha_z = D_z/v$. Note that by substituting $\tau = x/v$, we have made the transverse spreading terms $f_y(y,x)$ and $f_z(z,x)$ independent of time; hence, they will not participate in the integration process. Without the transverse terms, the definite integral can be evaluated analytically as shown in Appendix 1. Therefore, the previous equation can be simplified as:

$$c(x,y,z,t) = \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x),$$

$$\text{where } f_x(x,t) = \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 - \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x - vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) + \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 + \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x + vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) \quad (12)$$

Equation 12 is identical to the modified-Domenico solution shown in Equation 9. If we set the first-order decay coefficient k to zero, Equation 12 reduces to:

$$c(x,y,z,t) = \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x),$$

$$\text{where } f_x(x,t) = \operatorname{erfc}\left\{\frac{x - vt}{2(\alpha_x vt)^{1/2}}\right\} + \exp\left\{\frac{x}{\alpha_x}\right\}\operatorname{erfc}\left\{\frac{x + vt}{2(\alpha_x vt)^{1/2}}\right\} \quad (13)$$

Equation 13 is similar to the Domenico and Robbins (1985) solution given by Equation 7. The additional expression in the $f_x(x,t)$ term in Equations 12 and 13 is due to the use of the expanded form of the 1D solution that describes a constant concentration boundary condition instead of a semi-infinite pulse source boundary condition.

The previous analysis shows that the only approximation required for rigorously deriving the Domenico solution is the time reinterpretation step, where τ is replaced by x/v in the transverse dispersion terms. In the following section, we perform a detailed mathematical analysis to investigate the validity of this approximation.

Mathematical Analysis of the Validity of the Approximation Involved in the Domenico Solution

Review of transport modeling literature indicates that it is common to replace τ with x/v in the transverse dispersion terms when solving convection-dominated problems that have low longitudinal mixing. For example, Bruch and Street (1967) used a similar assumption to solve the advection-dispersion problem when the longitudinal mixing was smaller than the transverse mixing. Another example of a convection-dominated problem that employs this approximation is the air pollution model used for predicting the fate and transport of smoke plumes evolving from chimneys (Wark and Warner 1981). Here, the transport is dominated by convection along the wind direction, and dispersive mixing is restricted to the transverse directions only. Neglecting the effects of longitudinal dispersion in such problems simplifies the governing transport equation as:

$$\frac{\partial c}{\partial t} = -v\frac{\partial c}{\partial x} + D_y\frac{\partial^2 c}{\partial y^2} + D_z\frac{\partial^2 c}{\partial z^2} - kc \quad (14)$$

We consider solution to the previous transport problem subject to the following Domenico type initial and boundary conditions:

$$c(x,y,z,0) = 0 \;\forall\; 0<x<\infty,\; -\infty<y<\infty,\; -\infty<z<\infty$$
$$c(0,y,z,t) = c_o,\; -\frac{Z}{2}<z<\frac{Z}{2},\; -\frac{Y}{2}<y<\frac{Y}{2},\; \forall\; t>0$$
$$= 0 \text{ otherwise},\; \forall\; t>0$$
$$\lim_{y\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial y} = 0$$
$$\lim_{z\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial z} = 0 \quad (15)$$

In Appendix 2, we use Laplace transform techniques to solve the previous problem and the resulting exact analytical solution is:

$$c(x,y,z,t) = \frac{c_o}{8} f_x^o(x,t) f_y(x,y) f_z(x,z),$$

where $f_x^o(x,t) = 2\exp\left(-\frac{kx}{v}\right) u\left\{t - \frac{x}{v}\right\}$

where $u\left\{t - \frac{x}{v}\right\}$ is the step function given by,

$$u\left\{t - \frac{x}{v}\right\} = \begin{cases} 0 \text{ if } t \le \frac{x}{v} \\ 1 \text{ if } t > \frac{x}{v} \end{cases} \tag{16}$$

where $f_y(x,y)$ and $f_z(x,z)$ are identical to the expressions given in Equation 11.

Since the Domenico approach approximates τ as x/v in the transverse dispersion terms, we hypothesize that the Domenico approximation must be valid when α_x is zero. To test this hypothesis, we perform a limiting analysis of the modified-Domenico solution by forcing α_x to zero; this is expressed as:

$$c(x,y,z,t) = \lim_{\alpha_x \to 0} \frac{c_o}{8} f_x(x,t) f_y(y,x) f_z(z,x) \tag{17}$$

The mathematical details of this limiting analysis are given in the supplementary material. The analysis shows that when α_x approaches zero, the modified-Domenico solution relaxes to the exact analytical solution given by Equation 16. This proves that the Domenico approximation indeed yields an exact analytical solution when α_x is equal to zero.

Analysis of the Error Associated with the Domenico Solution

The mathematical analysis presented in the previous section demonstrates that the time reinterpretation step, where τ is replaced with x/v, is exactly valid when $\alpha_x = 0$. From these results, one could also infer that this time reinterpretation process provides a reasonable approximation when longitudinal dispersion plays an insignificant role in the overall transport. Hence, the Domenico solution can be expected to produce reasonable estimates for advection-dominated problems; however, it can introduce significant errors for longitudinal dispersion-dominated problems.

Another important feature of the time reinterpretation step is that it forces a quasi-steady-state condition along the transverse directions at all times. In other words, the "conceptual" residence time (x/v value) associated with a point located at the centerline to disperse contaminant mass in the transverse directions is independent of the simulation time. Further, this residence time is also assumed to increase linearly with respect to x. These unrealistic assumptions regarding residence times will lead to erroneous predictions, especially beyond the advective front. For example, consider a problem where $v = 50$ m/year, and we are interested in predicting the concentration distribution of a 2-year-old plume ($t = 2$ years) at a location $x = 200$ m. The Domenico solution will estimate the residence time τ for our location of interest $x = 200$ m as $\tau = x/v = 4$ years; this in fact is greater than the total simulation time itself. This is an unrealistic assumption since a 2-year-old plume simply cannot have the time to disperse for 4 years. For a particle located at the advective front, the residence time assumed by the Domenico solution is 2 years (the simulation time), and for all the particles located behind the advective front, the residence time assumed by the Domenico solution will be equal to x/v (which will be < 2 years); these seem to be reasonable estimates. However, for all points beyond the advective front, i.e., $x > 100$ m, the Domenico solution will assign unrealistic conceptual residence times, which will be greater than the simulation time $t = 2$ years. It must be noted that this incorrect behavior will vanish when α_x is zero because, for this case, the plume will abruptly end at the advective front, and the residence time for each particle located at or behind the advective front will in fact be equal to x/v.

When solving steady-state problems, the assumption related to residence time should be a reasonable approximation. This is because, at steady state, the theoretical advective front will be at infinity. Therefore, the time reinterpretation should be reasonable for any finite domain. Hence, the performance of the Domenico solution under steady-state conditions can be expected to be better. However, it is important to note that even under steady-state conditions, the solution will not be exact because it will still ignore the transport due to longitudinal mixing. In general, it can be concluded that the Domenico solution can be expected to perform better behind the advective front. In the following section, we use an example problem to illustrate the implication of these theoretical results.

Example Problem

The example problem presented by Domenico and Robbins (1985) is considered in this analysis. The transport parameters used in the problem are summarized in Table 1. The performance of the modified-Domenico solution was tested by comparing its results against those generated using the exact solution given by Wexler (1992).

It has been established in the previous sections that the Domenico approximation makes unreasonable assumptions regarding the residence time beyond the advective front and reasonable assumptions behind the

Table 1
Parameters Used in the Example Problem

Parameter	Value
Longitudinal dispersivity (α_x)	42.58 m
Transverse dispersivity (α_y)	8.43 m
Transverse dispersivity (α_z)	0.00642 m
Velocity (v)	0.2151 m/d
Source width in Y direction (Y)	240.0 m
Source width in Z direction (Z)	5.0 m
Source concentration (C)	850 mg/L
Simulation Time (t)	5110 d

front. Therefore, we analyze the results of this comparison in two parts— one behind the advective front and the other beyond the advective front (note that for our base case the front is at $x = 1100$ m).

Plume Comparison Analysis behind the Advective Front

Figures 1a and 1b compare the 2D concentration contours of both solutions on the X-Y and X-Z planes. (Note: an aspect ratio of "2.2:1" was maintained for the X-Y plots, and an aspect ratio of "55:1" was maintained for the X-Z plots.) Since the problem is symmetric about the X-axis, only half of the plume is presented. It can be observed from Figure 1 that the modified-Domenico solution is reasonably close to the true solution, though there are some noticeable discrepancies. To explore the limits of these discrepancies, we performed a series of sensitivity simulations.

In the first set of sensitivity simulations, we varied the value of the longitudinal dispersivity (α_x) by an order of magnitude above and below the assumed baseline value. Figures 2a and 2b compare the 2D concentration contours of the solutions for both cases. Comparison of the data shown in Figures 1a and 2 indicates that the discrepancies between the two solutions were large when the value of longitudinal dispersivity was high. Also, as expected, when the longitudinal dispersivity was low, there was an excellent match between the solutions. Similar trends were also observed in the concentration contours predicted on the X-Z plane. Since the spreading terms in the y and z directions are identical in structure, the contours in the X-Y and X-Z planes will exhibit identical trends. Therefore, from this point onward, our analysis will be restricted to X-Y contours.

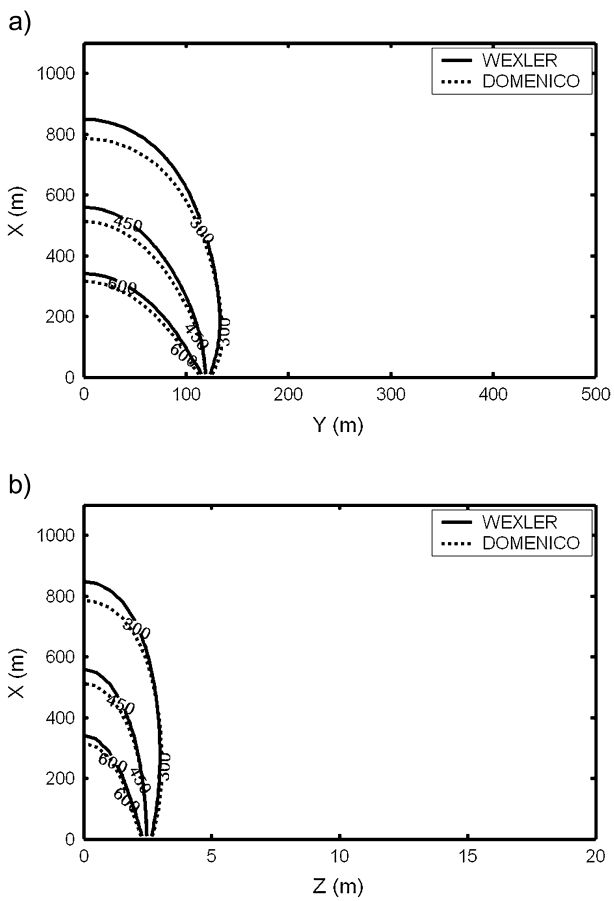

Figure 1. Concentration contours predicted by the Domenico and Wexler solutions for the base case: solutions behind the advective front for (a) X-Y plane and (b) X-Z plane.

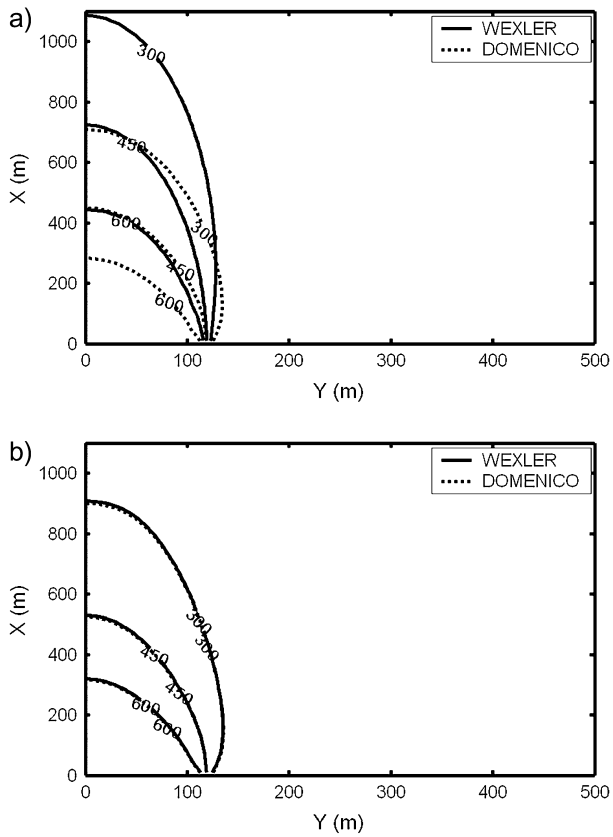

Figure 2. Sensitivity results for variations in the longitudinal dispersivity value: solutions behind the advective front for (a) α_x □ 10 and (b) α_x/10.

In the second set of sensitivity simulations, we varied the value of the transverse dispersivity (α_y) by an order of magnitude above and below the baseline value. These results (Figures S1 and S2) indicated that the transverse dispersivity in the y direction does not play a significant role in influencing the error associated with the modified-Domenico solution. Similar sensitivity analysis performed on other transport parameters, including the transverse dispersivity α_z and the source dimensions Y and Z, also showed minimal sensitivity.

Although the original problem considered by Domenico and Robbins (1985) does not involve reactions, in order to test the performance of the modified-Domenico solution in the presence of first-order decay, a third set of sensitivity simulations were completed for a decaying contaminant plume by assuming various first-order rate coefficients (k). Comparison of the concentration contours for k values of 0.0001 and 0.001/d (Figures S1 and S2) indicated that the presence of a decay term does not introduce any significant additional error.

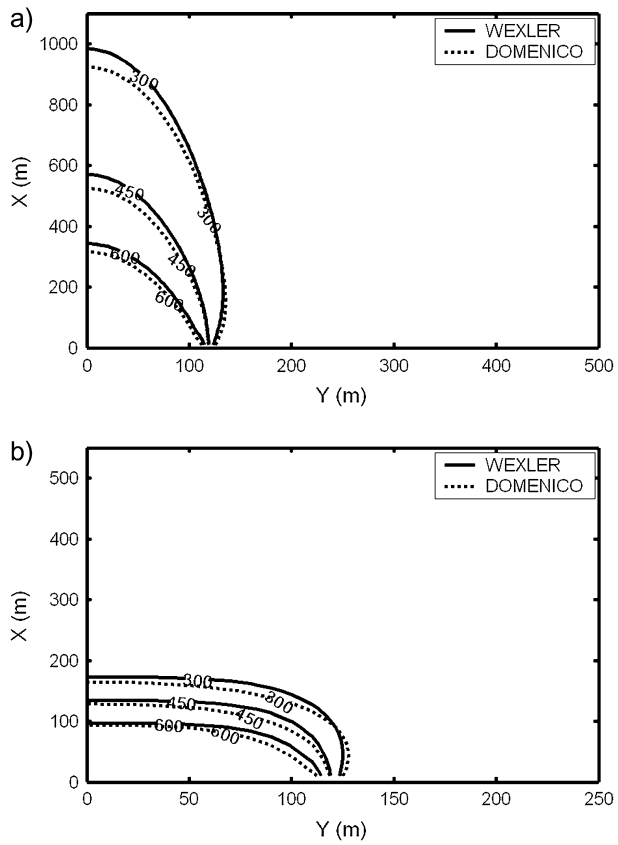

Figure 3. Sensitivity results for variations in the transport velocity: solutions behind the advective front for (a) v □ 10 and (b) v/10.

The fourth set of sensitivity simulations involved varying the advection velocity (v) by an order of magnitude above and below the baseline value. Figures 3a and 3b compare the concentration contours of the solutions for the two cases. From these figures, it can be concluded that the advection velocity has very little effect in determining the accuracy of the solution. Note that in the absence of first-order decay, varying the advection velocity will have the same effect as varying the total simulation time (t). Since decay does not play any significant role in determining the accuracy of the modified-Domenico solution, it can be safely concluded that variations in the total simulation time will have little sensitivity on its accuracy.

The previous results indicate that within the advective front, the longitudinal dispersivity plays a very important role in determining the accuracy of the modified-Domenico solution. All the other transport parameters have negligible effect on the accuracy of the solution.

Plume Comparison Analysis beyond the Advective Front

Figure 4 compares the concentration contours of the two solutions in the X-Y plane for the base case parameters. (Note: here an aspect ratio of "4:1" is maintained for the X:Y plane to capture the plume beyond the advective front; also, the location of the advective front is indicated by an arrow on the x-axis.) It can be observed from Figure 4 that, as we move beyond the advective front, the accuracy of the modified-Domenico solution reduces rapidly. As pointed out in the earlier sections, this is due

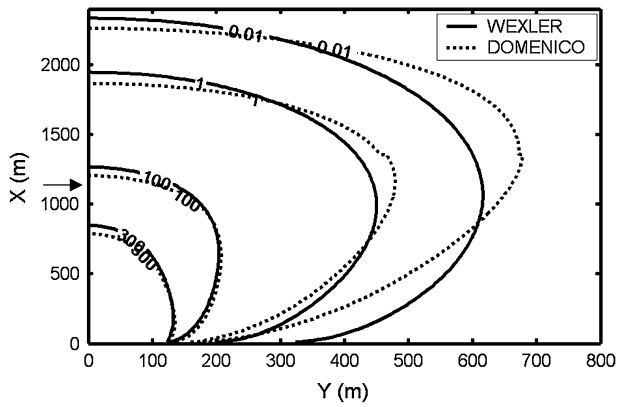

Figure 4. Concentration contours predicted by the Domenico and Wexler solutions for the base case: solutions include concentration contours beyond the advective front.

to the unrealistic assumptions made by the Domenico solution when computing the conceptual residence times beyond the advective front.

The results of a sensitivity analysis performed on the parameter α_x are summarized in Figures 5a and 5b. These figures indicate a trend similar to those present for regions within the advective front. The higher the value of the longitudinal dispersivity, the greater the error associated with the modified-Domenico solution. Further, it can be observed that the error systematically increases when the contaminant is transported beyond the advective front.

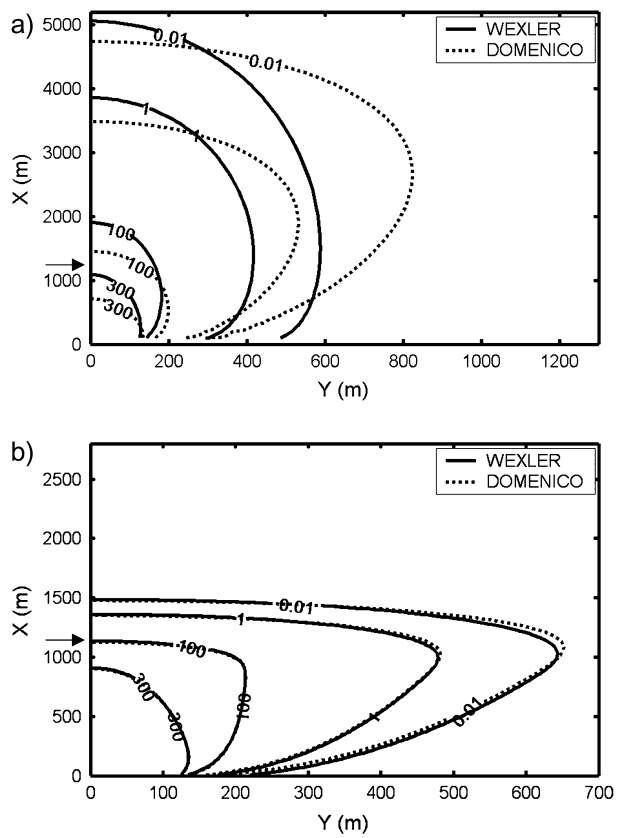

Figure 5. Sensitivity results for variations in the longitudinal dispersivity value: solutions include concentration contours beyond the advective front for (a) α_x □ 10 and (b) α_x/10.

A similar set of sensitivity simulations were performed on different transport parameters, including α_y, α_z, Y, Z, and K for regions beyond the advective front as well. As expected, the results indicated that these parameters had negligible contribution in determining the accuracy of the solution.

A final set of sensitivity simulations were performed by varying the value of the advection velocity (v) by an order of magnitude above and below the baseline value. The results of this sensitivity analysis are summarized in Figures 6a and 6b. Initial observations of these figures may indicate that at higher velocities the modified-Domenico solution appears to perform better. However, a closer analysis of these figures with respect to their respective advective front locations indicates that at higher velocities a greater portion of the plume is behind the advective front, whereas at lower velocities a relatively lesser portion of the plume is behind the advective front. Comparison of these figures made in the light of their respective advective fronts reveals that the advection velocity has little effect in determining the accuracy of the solution. However, it must be noted that the advection velocity itself plays an important role in determining the location of the advective front, which is one of the key parameters that affects the performance of the solution. Variations in the total simulation time (t) will have a similar effect as that of the advection velocity.

From the results of these sensitivity simulations, it can be safely concluded that the two most important factors that affect the accuracy of the modified-Domenico solution are the value of the longitudinal dispersivity (α_x) and the position of the advective front (vt). The solution will have minimal errors when the value of α_x is low and when the advective front is farther away from the source. It must be noted that the conclusions obtained for the modified-Domenico solution apply to the Domenico solution as well, provided the value of x/α_x is sufficiently large (Bear 1979).

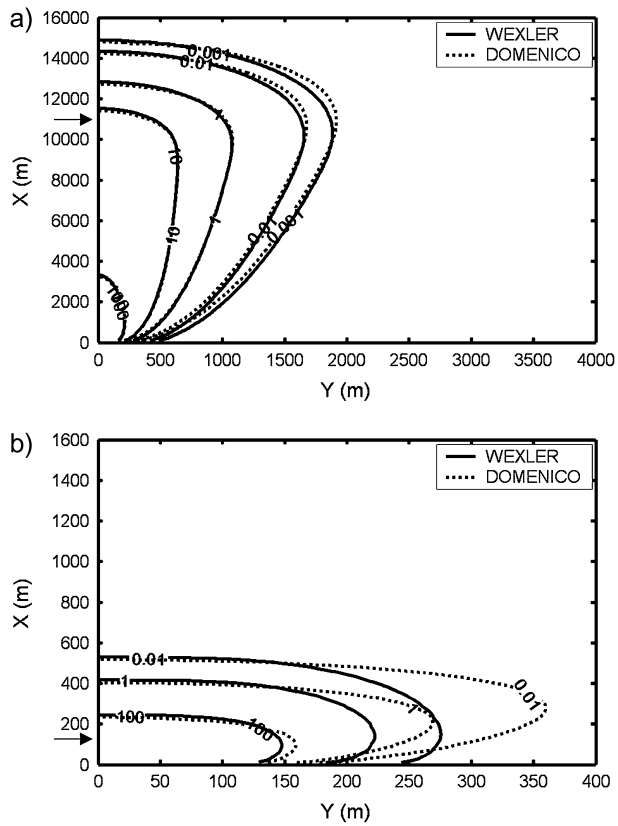

Figure 6. Sensitivity results for variations in the transport velocity: solutions include concentration contours beyond the advective front for (a) v □ 10 and (b) v/10.

General Discussions Regarding the Accuracy of the Domenico Solution

Since the original Domenico solution lacked a theoretical basis, several misconceptions regarding its performance have evolved over the years. One of the common misconceptions is that the error will be a minimum along the plume centerline. For example, Guyonnet and Neville (2004) compared the Domenico solution against the Sagar solution and concluded that "the results of the evaluation confirm that along the plume centerline, and for ground water flow regimes dominated by advection and mechanical dispersion rather than by molecular diffusion, discrepancies between the two solutions (namely the Domenico solution and the Sagar solution) can be considered negligible for all practical purposes. However the errors in the Domenico (1987) solution may increase significantly outside the plume centerline." However, our simulation results indicate that this conclusion might not be true for all cases. To illustrate this, we compare the y and z concentration transects predicted by the two solutions for our base case scenario. Figure 7a compares the concentration profiles along the y direction at $x = 1000$ and 1500 m, and similar results for the z direction are shown in Figure 7b. It is evident from these figures that the error is not minimal along the centerline, but rather at a point, which will always be away from the centerline. This error pattern can also be observed in all the 2D contours. Further, it can be observed from Figures 7a and 7b that the absolute error is, in fact, maximum along the plume centerline.

Another important issue that we would like to address here is the nature in which the error associated with the Domenico approximation is propagated spatially. Our results show that the plumes predicted by the modified-Domenico solution are always wider than the actual plumes. This phenomenon can easily be observed in all the figures presented in this study. This can be attributed to the fact that the Domenico approximation overpredicts the conceptual residence times of all particles along the centerline (hence allows more time to disperse in the transverse directions). This overprediction would lead to a decrease in the centerline concentrations; therefore, solutions that employ the Domenico approximation will always underpredict the overall extent of the plume in the longitudinal direction.

An important transport parameter not addressed so far is the retardation factor (R). Retardation affects the advection velocity and possibly the decay constant (depending on the phase where the decay occurs). Since the presence of a decay term does not introduce any significant additional error to the Domenico solution, its effect can be ignored. However, retardation changes the location of the advective front by changing the advection velocity

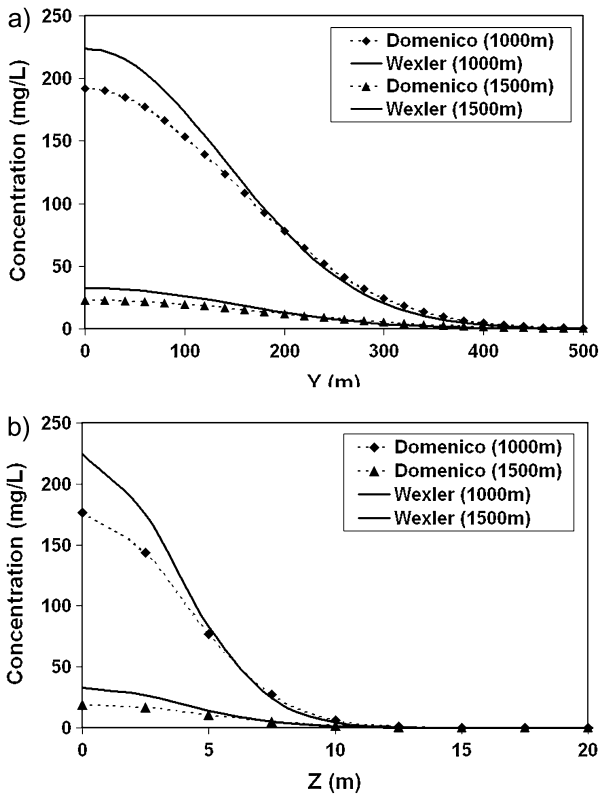

Figure 7. Concentration profiles predicted by the Domenico solution compared with the Wexler solution at $x = 1000$ m and 1500 m (a) along Y-axis and (b) along Z-axis.

and hence would influence the overall accuracy of the Domenico solution.

Conclusions

Based on the theoretical results presented in this study, we conclude that the key assumption used to derive the Domenico solution is the time reinterpretation step, where the time τ in the transverse dispersion terms is replaced with x/v. Our derivations prove that this substitution process is valid only when the longitudinal dispersivity is zero. For all nonzero longitudinal dispersivity values, the solution will have a finite error. The spatial distribution of this error is highly sensitive to the value of α_x and the position of the advective front (vt), and is relatively less sensitive to other transport parameters. Based on the results of this study, we conclude that the error in the Domenico solution will be low when solving transport problems that have low longitudinal dispersivity values, high advection velocities, and large simulation times.

Despite its limitations, the Domenico approximation offers a simple alternative for extending 1D analytical solutions to 3D analytical solutions. This approach is useful for developing approximate solutions for unsolved, 3D, multispecies reactive transport problems that have explicit 1D solutions. However, such solutions should be used carefully after understanding the limitations identified in this study.

Finally, it is of the authors' opinion that the performance of the Domenico solution can be improved by using a better approximation for the time reinterpretation step. This improved approximation should include the effects of transport due to longitudinal dispersion (currently ignored by the Domenico solution). Furthermore, it will be useful to develop some quantitative guidelines for the use of the Domenico solution. This could be accomplished by using a set of nondimensional parameters.

Acknowledgments

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Supplementary Material

The following supplementary material available for this article:

Appendix S1. Limiting Analysis of the Domenico solution ($\alpha_x = 0$).

Figure S1. Sensitivity results for variations in the transverse dispersivity value; solutions behind the advective front for (a) α_y*10 and (b) α_y/10.

Figure S2. Sensitivity results for variations in the decay rate; solutions behind the advective front for (a) $K = 0.0001$ day^{-1} and (b) $K = 0.001$ day^{-1}.

This material is available as part of the online article from: http://www.blackwell-synergy.com/doi/abs/10.1111/j.1745-6584.2006.00281.x

(This link will take you to the article abstract).

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Appendix 1

The integral in Equation 11 can be evaluated as:

$$I = \int_{\tau=0}^{\tau=t} f_x' \mathrm{d}\tau = \frac{x}{\sqrt{\pi D_x}} \exp\left\{\frac{vx}{2D_x}\right\} \times \int_{\tau=0}^{\tau=t} \frac{\exp\left\{\frac{-v^2}{4D_x}\tau - k\tau + \frac{-x^2}{4D_x\tau}\right\}}{\tau^{3/2}} \mathrm{d}\tau \quad \text{(A1)}$$

Applying Laplace transform to Equation A1, we get:

$$1[I] = \frac{x}{\sqrt{\pi D_x}} \exp\left\{\frac{vx}{2D_x}\right\}\frac{1}{s} \times \square 1\left[\frac{\exp\left\{\frac{-v^2}{4D_x}\tau - k\tau + \frac{-x^2}{4D_x\tau}\right\}}{\tau^{3/2}}\right] \quad \text{(A2)}$$

where 1 is the Laplace transform operator and s is the Laplace variable. Equation A2 can be expressed as:

$$1[I] = \frac{x}{\sqrt{\pi D_x}}\frac{1}{s}\exp\left\{\frac{vx}{2D_x}\right\} \times \square 1\left[\exp\left\{-\frac{v^2}{4D_x} + k\tau\right\}\frac{\exp\left\{\frac{-x^2}{4D_x\tau}\right\}}{\tau^{3/2}}\right] \quad \text{(A3)}$$

The second term within the Laplace operator can be evaluated by using Selby (1971, Equation 82, 497) as:

$$1\left[\frac{\exp\left\{\frac{-x^2}{4D_x\tau}\right\}}{\tau^{3/2}}\right] = \left[\frac{2\sqrt{\pi D_x}}{x}\exp\left\{-\frac{x}{\sqrt{D_x}}\sqrt{s}\right\}\right] \quad \text{(A4)}$$

The entire expression within the Laplace operator can be evaluated by using Selby (1971, Equation 11, 491) and Equation A4 as:

$$1[I] = \frac{2}{s}\exp\left\{\frac{vx}{2D_x}\right\}\left[\exp\left\{-\frac{x}{\sqrt{D_x}}\sqrt{s + \left(\frac{v^2}{4D_x} + k\right)}\right\}\right] \quad \text{(A5)}$$

Inverse Laplace transform of the previous equation yields (Bear 1979):

$$I = \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 - \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x - vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right) + \left(\exp\left\{\frac{x}{2\alpha_x}\left[1 + \left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}\right]\right\} \times \operatorname{erfc}\left\{\frac{x + vt\left(1 + \frac{4k\alpha_x}{v}\right)^{1/2}}{2(\alpha_x vt)^{1/2}}\right\}\right), \quad \text{(A6)}$$

where $\alpha_x = \frac{D_x}{v}$

Appendix 2

The governing transport equation is:

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} - D_y\frac{\partial^2 c}{\partial y^2} - D_z\frac{\partial^2 c}{\partial z^2} = -kc \quad \text{(B1)}$$

The initial and boundary conditions are:

$$c(x,y,z,0) = 0,\ \forall\ 0 < x < \infty,\ -\infty < y < \infty,\ -\infty < z < \infty$$
$$c(0,y,z,t) = c_o,\ -\frac{Z}{2} < z < \frac{Z}{2},\ -\frac{Y}{2} < y < \frac{Y}{2},\ \forall\ t > 0$$
$$= 0,\ \text{otherwise}\ \forall\ t > 0$$
$$\lim_{y\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial y} = 0$$
$$\lim_{z\to\pm\infty}\frac{\partial c(x,y,z,t)}{\partial z} = 0 \quad \text{(B2)}$$

Applying Laplace transform to *c(x,y,z,t)* in Equation B1 gives:

$$\frac{\partial p}{\partial x} - \alpha_y\frac{\partial^2 p}{\partial y^2} - \alpha_z\frac{\partial^2 p}{\partial z^2} = -\frac{(s+k)}{v}p,$$
$$\text{where}\quad \alpha_y = \frac{D_y}{v}\quad\text{and}\quad \alpha_z = \frac{D_z}{v} \quad \text{(B3)}$$

where s is the Laplace variable and p is the concentration in the Laplace domain.

The boundary conditions get modified as:

$$p(0,y,z) = \frac{c_o}{s},\quad -\frac{Z}{2} < z < \frac{Z}{2},\quad -\frac{Y}{2} < y < \frac{Y}{2}$$
$$= 0,\quad \text{otherwise}$$
$$\lim_{y\to\pm\infty}\frac{\partial p(x,y,z)}{\partial y} = 0$$
$$\lim_{z\to\pm\infty}\frac{\partial p(x,y,z)}{\partial z} = 0 \quad \text{(B4)}$$

Equation B3 can be interpreted as a transient 2D diffusive reactive transport problem. Its boundary conditions given by Equation B4 represent an instantaneous pulse of a plane source. The solution to this problem without the decay term can be readily deduced from Hunt (1978) by ignoring the advection term and reducing the problem to two dimensions. Thus, the solution to the previous problem without the reaction term is given by:

$$p'(x,y,z) = \frac{c_o}{4s}f_y(x,y)f_z(x,z),$$
$$\text{where}\ f_y(x,y) = \left[\operatorname{erf}\left\{\frac{y + \frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{y - \frac{Y}{2}}{2(\alpha_y x)^{1/2}}\right\}\right]$$
$$f_z(x,z) = \left[\operatorname{erf}\left\{\frac{z + \frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\} - \operatorname{erf}\left\{\frac{z - \frac{Z}{2}}{2(\alpha_z x)^{1/2}}\right\}\right] \quad \text{(B5)}$$

Now, we make use of a method similar to the Danckwert's method described by Crank (1975) to include the reaction term. If p' is the solution for the diffusion problem without reaction; the solution for the same problem with a first-order reaction, with a rate constant $\left(\frac{s+k}{v}\right)$, for the same initial and boundary condition is given as:

$$p = p'\exp\left\{-\left(\frac{s+k}{v}\right)x\right\} \quad \text{(B6)}$$

This can be easily verified by checking if the solution p satisfies the governing equation and the initial and boundary conditions. Since p' is the solution to Equation B3 without the reaction term, it must satisfy:

$$\frac{\partial p'}{\partial x} - \alpha_y \frac{\partial^2 p'}{\partial y^2} - \alpha_z \frac{\partial^2 p'}{\partial z^2} = 0 \qquad \text{(B7)}$$

Also, differentiating p with respect to x, y, and z to the respective orders yields:

$$\begin{aligned}
\frac{\mathrm{d}p}{\mathrm{d}x} &= -\left(\frac{s+k}{v}\right)\exp\left\{-\left(\frac{s+k}{v}\right)x\right\}p' \\
&\quad + \exp\left\{-\left(\frac{s+k}{v}\right)x\right\}\frac{\mathrm{d}p'}{\mathrm{d}x} \\
\frac{\partial^2 p}{\partial y^2} &= \exp\left\{-\left(\frac{s+k}{v}\right)x\right\}\frac{\partial^2 p'}{\partial y^2} \\
\frac{\partial^2 p}{\partial z^2} &= \exp\left\{-\left(\frac{s+k}{v}\right)x\right\}\frac{\partial^2 p'}{\partial z^2}
\end{aligned} \qquad \text{(B8)}$$

From Equations B6 through B8, we get Equation B3. This proves that solution p satisfies the governing differential equation. To check for the initial condition, we substitute $x = 0$ in Equation B6. When $x = 0$, the exponential term becomes unity and hence Equation B6 reduces to $p = p'$; thus, the initial condition is satisfied. In order to check for the boundary condition in the y direction, we need to take the derivative of the solution p with respect to y. This is given as:

$$\frac{\mathrm{d}p}{\mathrm{d}y} = \exp\left\{-\left(\frac{s+k}{v}\right)x\right\}\frac{\mathrm{d}p'}{\mathrm{d}y} \qquad \text{(B9)}$$

In the limiting case, when y approaches $\pm\infty$, the derivative of p' with respect to y becomes 0. From Equation B9, we can conclude that the derivative of p with respect to y also becomes 0. This proves that the boundary condition in the y direction is satisfied. On similar lines, we see that the boundary condition is also satisfied in the z direction. Hence, it is proved that Equation B6 is the solution for the system of equations described by Equations B3 and B4.

Equation B6 can be written as:

$$p(x,y,z) = \frac{c_o}{4s}\exp\left\{-\left(\frac{s+k}{v}\right)x\right\}f_y(x,y)f_z(x,z) \qquad \text{(B10)}$$

Inverse Laplace transform of Equation B10 gives the final solution as (Selby 1971, Equation 61, 495):

$$c(x,y,z,t) = \frac{c_o}{8}f_x^{\mathrm{o}}(x,t)f_y(x,y)f_z(x,z)$$

$$f_x^{\mathrm{o}}(x,t) = 2\exp\left(-\frac{kx}{v}\right)u\left\{t-\frac{x}{v}\right\},$$

where $u\left\{t-\frac{x}{v}\right\}$ is the step function given by,

$$u\left\{t-\frac{x}{v}\right\} = \left\{\begin{array}{ll} 0 & \text{if } t \le \frac{x}{v} \\ 1 & \text{if } t > \frac{x}{v} \end{array}\right\} \qquad \text{(B11)}$$

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