

Reactive Contaminant Transport with Space-Dependent Dispersion and Time-Dependent Concentration Source

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ABSTRACT

This work is focused on the modeling of a one-dimensional contaminant transport in a uniform porous medium with a spatially dependent dispersion coefficient and time-dependent source concentration in the presence of a first-order reaction. Two types of source concentration boundary conditions are employed. These are the type I and type III boundary conditions with an increasing time-dependent power law function multiplied by a decaying time-dependent exponential function. The variable dispersion coefficient is represented by an exponentially increasing function with the downstream distance. Various analytical solutions for special cases of the problem are presented, and the general nonlinear problem is solved numerically by an implicit finite difference method. The numerical method is validated by various comparisons with the analytical solutions and is found to be in excellent agreement. A parametric study of all physical parameters is conducted, and the results are presented graphically to illustrate interesting features of the solutions.

NOMENCLATURE

a, b	constants used in exponential dispersion coefficient	n	power law source concentration exponent
b^*	exponential source concentration exponent (T^{-1})	Pe	Peclet number
c	concentration of contaminant ($M L^{-3}$)	t	time (T)
c_0	boundary concentration source ($M L^{-3}$)	u	flow velocity ($L T^{-1}$)
C	dimensionless concentration of contaminant	x	longitudinal distance (L)
D	hydrodynamic dispersion coefficient ($L^2 T^{-1}$)	x_0	characteristic longitudinal distance (L)
D_c	molecular diffusion coefficient ($L^2 T^{-1}$)	Greek Symbols	
D_0	characteristic dispersion constant ($L^2 T^{-1}$)	α	dispersivity (L)
D^*	dimensionless hydrodynamic dispersion coefficient	β	dimensionless exponential source concentration exponent
erf	error function	η	dimensionless longitudinal distance coefficient
erfc	complementary error function	λ	dimensionless chemical reaction rate
H	unit step function	τ	dimensionless time
k	chemical reaction rate coefficient of contaminant (T^{-1})		

I. INTRODUCTION

Modeling of contaminant transport in soil, groundwater, and surface water has been a popular research topic for many years. This is due to increased public awareness of significant contamination of groundwater and surface water by industrial, municipal, and agricultural chemicals, accidental spills, and the effect of soil contamination resulting from landfill dumps and burial of hazardous materials. Most transport studies assume that the source contaminant concentration is constant. However, in many applications, the source contaminant loading is time-dependent. For example, the study of one-dimensional reactive transport of a contaminant in a porous medium with time-dependent source loading is needed as part of the preliminary performance assessment for nuclear waste disposal in crystalline rocks. Van Genuchten (1981) reported

various analytical solutions for chemical transport with simultaneous adsorption, zero-order production, and first-order decay with an exponentially decaying source concentration. Shih et al. (2002) studied contaminant transport in fractured media with pulse, Dirac delta, and single-sinusoid input sources and reported analytical solutions obtained using the Laplace transform method. Also, a number of analytical solutions for steady flow and different boundary and initial conditions were given by van Genuchten and Alves (1982) for problems with linear adsorption and zero- and first-order production and decay.

Most previously published analytical solutions to advective-dispersive transport model (Bear, 1970) problems are obtained based on the assumption of a homogeneous porous medium (van Genuchten, 1981; van Genuchten and Alves, 1982). In reality, subsurface porous media through which the contaminant

moves are seldom homogeneous, and significant spatial variability of transport properties should be expected (Gelhar, 1986; Dagan, 1988; Liu et al., 1998). As a result of the heterogeneity of the porous media, the dispersion coefficients in all directions vary with the space coordinate, and the resulting contaminant transport equation contains spatially dependent coefficients.

Limited analytical solutions for scale-dependent dispersion coefficients have been reported in the literature. Yates (1990, 1992) obtained one-dimensional solutions for uniform flow with constant concentration or constant concentration flux boundary conditions when the medium has a linearly or exponentially increasing dispersion coefficient with the spatial coordinate. Huang et al. (1996) also presented analytical solutions for a scale-dependent dispersion coefficient that increased linearly with the distance until some distance, after which it reached an asymptotic value. Logan (1996) derived an analytical solution for the one-dimensional equations incorporating rate-limited sorption and first-order decay under time-varying boundary conditions, assuming an exponentially increasing dispersion coefficient. Zi-ting (2001) reported an analytical solution for an exponential-type dispersion process. However, the solutions given by Yates (1990, 1992), Huang et al. (1996), Logan (1996), and Zi-ting (2001) are complex and difficult to evaluate numerically.

The objective of this work is to report accurate numerical solutions based on the finite difference methodology for one-dimensional contaminant transport through a semi-infinite porous medium domain in the presence of a first-order reaction and to study the relative influence of variable dispersion effects on predictions using type I and type III source concentration boundary conditions. The transport of the contaminant is assumed to start from a time-dependent concentration source, and the dispersion coefficient is assumed to be spatially dependent. The exponential-type dispersion coefficient used by Zi-ting (2001) is employed in the present work, and the temporal source concen-

tration is assumed to be a multiplication of an increasing power law function and a decaying exponential function. The study of one-dimensional reactive solute transport with this source loading should be needed as part of the preliminary performance assessment for nuclear waste disposal and safety analysis.

2. FORMULATION

Consider transient one-dimensional advective-dispersive contaminant transport in a porous medium from a time-dependent source with a first-order reaction. The flow of the contaminant takes place in the semi-infinite region $0 \leq x < \infty$ with a uniform velocity, and the dispersion coefficient is assumed to be spatially dependent. The governing equation for this situation can be written as

$$\frac{\partial c(x,t)}{\partial t} + u \frac{\partial c(x,t)}{\partial x} = \frac{\partial}{\partial x} \times \left[D(x) \frac{\partial c(x,t)}{\partial x} \right] - kc(x,t) \quad (1)$$

where t is time, x is the one-dimensional spatial coordinate ($0 \leq x < \infty$) (or longitudinal distance), $c(x,t)$ is the concentration, u is the uniform velocity, k is the chemical reaction rate coefficient, and $D(x)$ is the spatially variable hydrodynamic dispersion coefficient representing the sum of both the effects of molecular diffusion (D_e) and mechanical dispersion (αu , where α is usually called the dispersivity). In most solute transport studies, the molecular diffusion is usually neglected compared to the mechanical dispersion. For simplicity, this assumption is made in this work. It should be noted that the first term on the left-hand side of Eq. (1) represents the transient or accumulation effect. The second term on the left-hand side of the equation represents the advection or convection effect, which is defined as the transport of contaminant by the mean velocity in the flow stream. The first term on the right-side of the equation accounts for the dispersion or diffusion effect, which is responsible for the spreading of the contaminant in the medium. The last term of Eq. (1) represents the linear first-order

reaction effect that may take place between the contaminant and the medium, such as the transport of a landfill leachate in soils.

Equation (1) can be expanded and written as

$$\frac{\partial c(x,t)}{\partial t} + u \frac{\partial c(x,t)}{\partial x} = D(x) \frac{\partial^2 c(x,t)}{\partial x^2} + \frac{\partial D(x)}{\partial x} \frac{\partial c(x,t)}{\partial x} - kc(x,t) \quad (2)$$

The initial and boundary conditions for this problem are given by

$$c(x,0) = 0 \quad (3a)$$

Type I Boundary Condition:

$$c(0,t) = c_0 \left(\frac{ut}{x_0} \right)^n \exp(-b^*t) \quad (3b)$$

Type III Boundary Condition:

$$-D(0) \frac{\partial c(0,t)}{\partial x} + uc(0,t) = uc_0 \left(\frac{ut}{x_0} \right)^n \exp(-b^*t) \quad (3c)$$

$$\frac{\partial c(\infty,t)}{\partial x} = 0 \quad (3d)$$

where b^* , c_0 , and n are positive constants and D_0 is a characteristic dispersion constant. It should be noted that when $n = 0$ and $b^* = 0$ and $b^* \rightarrow \infty$ in Eqs. (3b) and (3c), the continuous and pulse source boundary conditions are recovered, respectively. Equation (3d) indicates that the end boundary has a zero-dispersive condition.

It is convenient to work with dimensionless equations. This can be accomplished by using

$$\eta = \frac{x}{x_0} \quad \tau = \frac{ut}{x_0} \quad C(\eta, \tau) = \frac{c(x,t)}{c_0} \quad D^*(\eta) = \frac{D(x)}{D_0} \quad (4)$$

where x_0 is a characteristic longitudinal distance.

Substituting Eq. (4) into Eqs. (2) and (3) gives, respectively,

$$\frac{\partial C(\eta, \tau)}{\partial \tau} + \frac{\partial C(\eta, \tau)}{\partial \eta} = \frac{D^*(\eta)}{Pe} \frac{\partial^2 C(\eta, \tau)}{\partial \eta^2} + \frac{1}{Pe} \frac{\partial D^*(\eta)}{\partial \eta} \frac{\partial C(\eta, \tau)}{\partial \eta} - \lambda C(\eta, \tau) \quad (5)$$

$$C(\eta, 0) = 0 \quad (6a)$$

Type I Boundary Condition:

$$C(0, \tau) = \tau^n \exp(-\beta\tau) \quad (6b)$$

Type III Boundary Condition:

$$-\frac{D^*(0)}{Pe} \frac{\partial C(0, \tau)}{\partial \eta} + C(0, \tau) = \tau^n \exp(-\beta\tau) \quad (6c)$$

$$\frac{\partial C(\infty, \tau)}{\partial \eta} = 0 \quad (6d)$$

where

$$Pe = \frac{ux_0}{D_0} \quad \lambda = \frac{kx_0}{u} \quad \beta = \frac{b^*x_0}{u} \quad (7)$$

are the Peclet number, dimensionless reaction rate constant, and dimensionless exponential source concentration exponent, respectively.

The spatially dependent dispersion coefficient is assumed to take the following form:

$$D^*(\eta) = 1 - a \exp(-b\eta) \quad (8)$$

where a and b are dimensionless constants. When a is equated to zero in the above equation, the constant dispersion case is recovered. As mentioned by Zi-ting (2001), the exponential form of the dispersion coefficient was deduced from measured data on reservoirs with heterogeneous media. It should be noted that Zi-ting (2001) derived a complicated analytical solution for a transport problem with the exponential-type dispersion coefficient given by Eq. (8).

3. ANALYTICAL SOLUTIONS

Analytical solutions play an important role in modeling because they offer fundamental insight into governing physical processes, provide useful tools for validating numerical approaches, and are sometimes more computationally efficient (Liu et al. 1998). Therefore it is helpful to have some analytical solutions for special cases of the general problem to use as standards of comparison for the numerical procedure to be discussed in the next section.

Consider the special case where $D^*(\eta) = 1$ (constant dispersion coefficient) and $n = 0$ (exponentially decaying source concentration), for which Eqs. (5) and (6) are simplified to read

$$\frac{\partial C(\eta, \tau)}{\partial \tau} + \frac{\partial C(\eta, \tau)}{\partial \eta} = \frac{1}{Pe} \frac{\partial^2 C(\eta, \tau)}{\partial \eta^2} - \lambda C(\eta, \tau) \tag{9}$$

$$C(\eta, 0) = 0 \tag{10a}$$

Type I Boundary Condition:

$$C(0, \tau) = \exp(-\beta\tau) \tag{10b}$$

Type III Boundary Condition:

$$-\frac{D^*(0)}{Pe} \frac{\partial C(0, \tau)}{\partial \eta} + C(0, \tau) = \exp(-\beta\tau) \tag{10c}$$

$$\frac{\partial C(\infty, \tau)}{\partial \eta} = 0 \tag{10d}$$

These equations are linear and can be solved analytically by the Laplace transformation methods. Without going into detail, the solution of the above initial-value problem can be shown to be

Type I Boundary Condition:

$$C(\eta, \tau) = \frac{1}{2} \exp(-\beta\tau) \left\{ \begin{aligned} & \exp \left[\frac{[Pe - \sqrt{Pe^2 + 4Pe(\lambda - \beta)}]}{2} \eta \right] \\ & \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta - \sqrt{Pe + 4(\lambda - \beta)}\tau}{2\sqrt{\tau}} \right] \\ & + \exp \left[\frac{[Pe + \sqrt{Pe^2 + 4Pe(\lambda - \beta)}]}{2} \eta \right] \\ & \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta + \sqrt{Pe + 4(\lambda - \beta)}\tau}{2\sqrt{\tau}} \right] \end{aligned} \right\} \tag{11}$$

$$\operatorname{erfc}(\zeta) = 1 - \operatorname{erf}(\zeta) = \frac{2}{\sqrt{\pi}} \int_{\zeta}^{\infty} \exp(-\theta^2) d\theta \tag{12}$$

where erf and erfc are the error function and complementary error function, respectively, and θ is a dummy variable. It should be noted that Eq. (11) is consistent with and represents the dimensionless form of that reported earlier by van Genuchten (1981). The constant source concentration case is easily obtained from Eq. (11) by simply setting $\beta = 0$ to yield

$$C(\eta, \tau) = \frac{1}{2} \left\{ \begin{aligned} & \exp \left[\frac{(Pe - \sqrt{Pe^2 + 4\lambda Pe})}{2} \eta \right] \\ & \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta - \sqrt{Pe + 4\lambda}\tau}{2\sqrt{\tau}} \right] \\ & + \exp \left[\frac{(Pe + \sqrt{Pe^2 + 4\lambda Pe})}{2} \eta \right] \\ & \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta + \sqrt{Pe + 4\lambda}\tau}{2\sqrt{\tau}} \right] \end{aligned} \right\} \tag{13}$$

The above result is consistent with the result reported by van Genuchten and Alves (1982).

As $Pe \rightarrow \infty$ (no diffusivity), Eq. (11) reduces to

$$C(\eta, \tau) = \exp[-(\lambda\eta + \beta\tau)]H(\tau - \eta) \tag{14}$$

where H is the unit step function. For small amounts of diffusivity ($1/Pe \ll 0$), the discontinuity exhibited by Eq. (14) at $\eta = \tau$ is replaced by a narrow continuous transition layer.

For the special case in which $\lambda = 0$ (no chemical reaction), Eq. (5) becomes a simple convection-diffusion equation. Equations (11) and (14) are valid with $\lambda = 0$. This leads to the respective results

$$C(\eta, \tau) = \frac{1}{2} \exp(-\beta\tau) \tag{15}$$

$$\times \left\{ \begin{aligned} &\exp \left[\frac{[Pe - \sqrt{Pe^2 - 4Pe\beta}]}{2} \eta \right] \\ &\operatorname{erfc} \left[\frac{\sqrt{Pe}\eta - \sqrt{Pe - 4\beta\tau}}{2\sqrt{\tau}} \right] \\ &+ \exp \left[\frac{[Pe + \sqrt{Pe^2 - 4Pe\beta}]}{2} \eta \right] \\ &\operatorname{erfc} \left[\frac{\sqrt{Pe}\eta + \sqrt{Pe - 4\beta\tau}}{2\sqrt{\tau}} \right] \end{aligned} \right\}$$

$$C(\eta, \tau) = \exp(-\beta\tau)H(\tau - \eta) \tag{16}$$

Type III Boundary Condition:

$$C(\eta, \tau) = \exp(-\beta\tau) \tag{17}$$

$$\times \left\{ \begin{aligned} &\frac{1}{1 + \sqrt{\frac{1+4(\lambda-\beta)}{Pe}}} \\ &\times \exp \left[\frac{[Pe - \sqrt{Pe^2 + 4Pe(\lambda - \beta)}]}{2} \eta \right] \\ &\operatorname{erfc} \left[\frac{\sqrt{Pe}\eta - \sqrt{Pe + 4(\lambda - \beta)\tau}}{2\sqrt{\tau}} \right] \end{aligned} \right\}$$

+ $\exp(-\beta\tau)$

$$\times \left\{ \begin{aligned} &\frac{1}{1 - \sqrt{\frac{1+4(\lambda-\beta)}{Pe}}} \\ &\times \exp \left[\frac{[Pe + \sqrt{Pe^2 + 4Pe(\lambda - \beta)}]}{2} \eta \right] \\ &\operatorname{erfc} \left[\frac{\sqrt{Pe}\eta + \sqrt{Pe + 4(\lambda - \beta)\tau}}{2\sqrt{\tau}} \right] \end{aligned} \right\}$$

$$+ \frac{Pe}{2(\lambda - \beta)} \exp(Pe\eta - \lambda\tau) \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta + \tau)}{2\sqrt{\tau}} \right]$$

for $\beta \neq \lambda$

$$C(\eta, \tau) = \exp(-\lambda\tau) \left\{ \frac{\sqrt{Pe\tau}}{\sqrt{\pi}} \exp \left[-\frac{Pe(\eta - \tau)^2}{4\tau} \right] + \frac{1}{2} \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta - \tau)}{2\sqrt{\tau}} \right] \right\} - \exp(-\lambda\tau) \times \left\{ + \frac{1}{2} [1 + Pe(\eta + \tau)] \exp(Pe\eta) \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta + \tau)}{2\sqrt{\tau}} \right] \right\} \quad \text{for } \beta = \lambda \tag{18}$$

The above solutions are consistent with those reported by van Genuchten (1981) and later by Kaluarachchi and Morshed (1995).

For the special case of $\beta = 0$, Eq. (17) reduces directly to

$$C(\eta, \tau) = \frac{1}{1 + \sqrt{\frac{1+4\lambda}{Pe}}} \times \exp \left[\frac{[Pe - \sqrt{Pe^2 + 4Pe\lambda}]}{2} \eta \right] \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta - \sqrt{Pe + 4\lambda\tau}}{2\sqrt{\tau}} \right] + \frac{1}{1 - \sqrt{\frac{1+4\lambda}{Pe}}} \times \exp \left[\frac{[Pe + \sqrt{Pe^2 + 4Pe\lambda}]}{2} \eta \right] \operatorname{erfc} \left[\frac{\sqrt{Pe}\eta + \sqrt{Pe + 4\lambda\tau}}{2\sqrt{\tau}} \right] + \frac{Pe}{2\lambda} \exp(Pe\eta - \lambda\tau) \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta + \tau)}{2\sqrt{\tau}} \right] \tag{19}$$

This solution is the dimensionless form of the solution given by van Genuchten and Alves (1982) with the retardation coefficient set to unity. Also, for $\lambda = 0$, Eq. (17) reduces to

$$C(\eta, \tau) = \frac{\sqrt{Pe\tau}}{\sqrt{\pi}} \exp \left[-\frac{Pe(\eta - \tau)^2}{4\tau} \right] + \frac{1}{2} \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta - \tau)}{2\sqrt{\tau}} \right] - \frac{1}{2} [1 + Pe(\eta + \tau)] \exp(Pe\eta) \operatorname{erfc} \left[\frac{\sqrt{Pe}(\eta + \tau)}{2\sqrt{\tau}} \right] \tag{20}$$

which is consistent with the result of Lindstrom et al. (1967).

4. NUMERICAL METHOD

The initial value problem represented by Eqs. (5) and (6) is nonlinear. Therefore an analytical solution to this problem is unlikely, and a numerical solution is required. Accurate numerical solutions of these equations are important to ensure physically realistic predictions of contaminant transport in a variety of applications. Many existing computer codes employ a finite difference approach for the solution of transport equations. In the present work an accurate implicit iterative tridiagonal finite difference method similar to that discussed by Blottner (1970) is employed. A two-point backward difference quotient is used to represent the dimensionless time τ derivative, and three-point central difference quotients are used to represent the dimensionless space η derivatives. The computation starts at $\tau = 0$ and marches forward in time. At each time a system of nonlinear algebraic equations must be solved to determine the η distributions of C . An iterative procedure is employed for this purpose. At each iteration an equivalent linear system of algebraic equations (the linearization being effected by representing some quantities by their values from the previous iteration) must be solved. These equations have a tridiagonal form and can be solved by the Potter's method variables, which can be determined by a forward sweep in the η direction. Then the physical variables can be found from a corresponding backward sweep. This process avoids the need for matrix inversion. Iteration is continued until convergence is obtained at a given time. The procedure moves forward for the next time. The computational domain for this problem was divided up into 501 points in the η direction and 1001 points in the τ direction, with variable step sizes in both directions. The initial step sizes and growth factors employed in the η and τ directions were 0.001, 0.001, 1.055, and 1.03, respectively. These values were arrived at after performing various numerical experiments to access grid-independent

results. The convergence criterion required that the difference between the current and previous iterations be 10^{-7} .

The accuracy of the numerical method discussed above is validated by direct comparisons with the analytical results given in Eqs. (11), (17), and (18). These comparisons are presented in Figs. 1a, 1b, and 2 for $Pe = 1$ and $Pe = 100$ and the type I boundary condition and $Pe = 1$ and the type III boundary condition, respectively. It is clear from these figures that excellent agreement between the numerical and analytical results exists. These favorable comparisons lend confidence to the numerical results reported in the next section.

5. RESULTS AND DISCUSSION

In this section a representative set of selected numerical results is presented in Figs. 3–12. These results are chosen to illustrate the influence of the power law source concentration exponent n , the Peclet number Pe , the reaction rate constant λ , the scale-dependent dispersion constant α , and the exponential source concentration exponent β . In Figs. 3 and 4, the dispersion coefficient is constant, while in Figs. 5–10, the dispersion coefficient is spatially variable.

Figure 3 presents the temporal development of the contaminant concentration for various values of the power law source concentration exponent n for the case of constant dispersion effects at a specific location ($\eta = 0.232$) for two different Peclet numbers corresponding to moderate dispersion ($Pe = 1$) and small dispersion ($Pe = 1000$) effects. In this and all subsequent figures, the horizontal coordinate (time or space) is represented by a logarithmic scale so as to capture the complete transition from unsteady conditions at small dimensionless time τ to steady state conditions at $\tau = \infty$ or to capture spatial gradients in the flow direction. It is observed that as the exponent n increases, a distinctive peak in the concentration temporal development occurs, and this peak moves forward in time, increases in value, and becomes more distinctive as n is increased further and further. How-

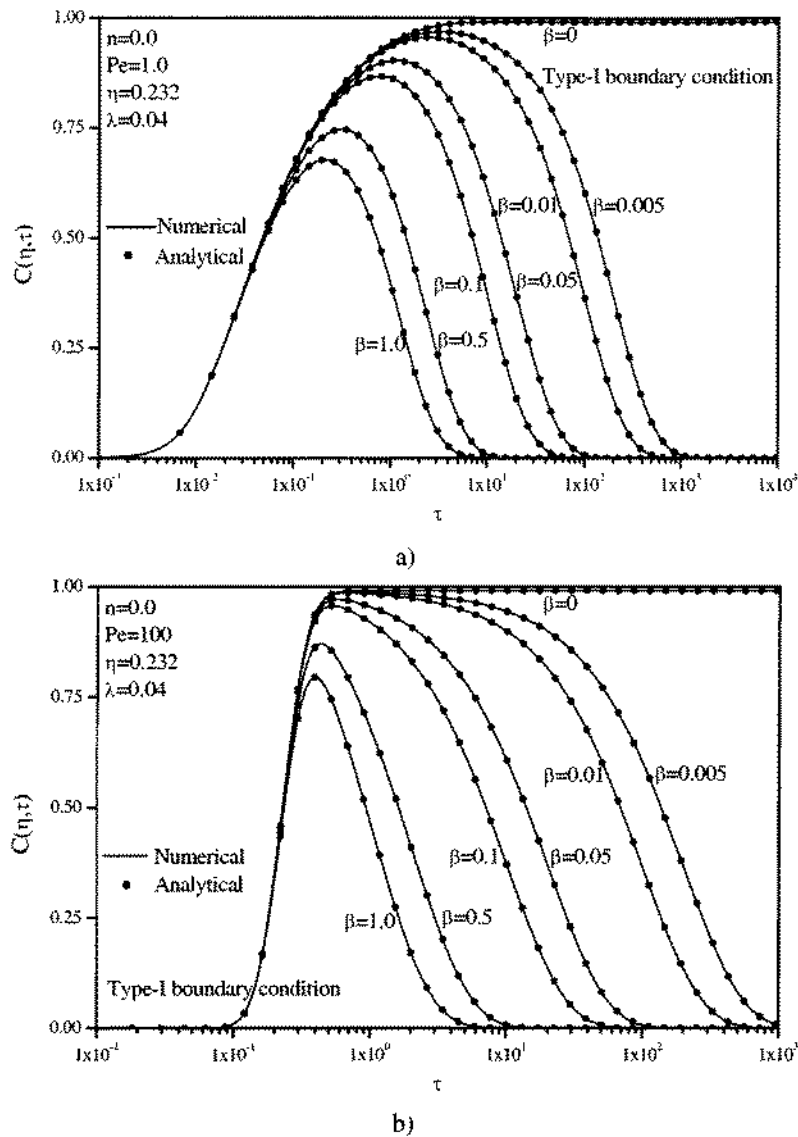


Figure 1. a) Comparison of temporal development of concentration for different values of β for $Pe = 1.0$ and b) comparison of temporal development of concentration for different values of β for $Pe = 100$

ever, the initial temporal slope tends to decrease as n is increased. Therefore, at the spatial location $\eta = 0.232$, it is predicted that increases in the exponent n increase the concentration for values of $\tau > 1$ and decrease it for values of $\tau < 1$. The dimensionless time $\tau = 1$ appears to be a transition time. In addition, the approach toward steady state conditions becomes slower as n increases. Furthermore, as Pe increases

from 1 to 1000, the same general features are observed, except that for $Pe = 1000$, the concentration level remains zero for quite some time and increases more sharply as time progresses than observed for $Pe = 1$. Also, the effect of increasing Pe at this location ($\eta = 0.232$) appears to be limited only to early times ($\tau < 1$) for which the concentration level for $Pe = 1000$ is higher than that for $Pe = 1$ for values of $n \leq 0.3$

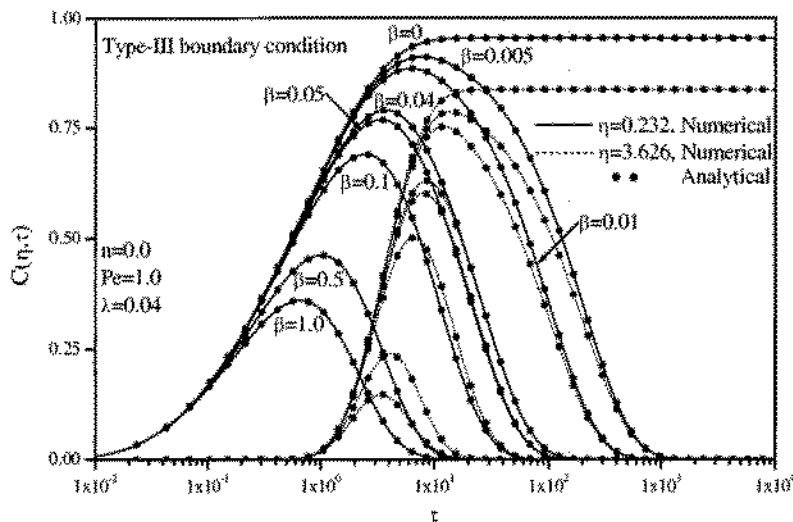


Figure 2. Comparison of temporal development of concentration for different values of β at $\eta = 0.232$ and $\eta = 3.626$

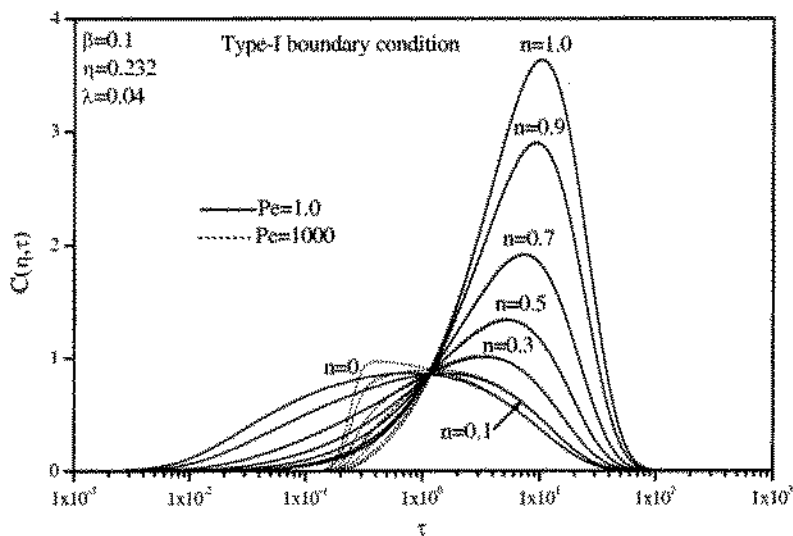


Figure 3. Effects of n and Pe on the temporal development of concentration

and lower for $n > 0.3$. This is only true in the small time range $0.3 \leq \tau \leq 1$.

Figure 4 illustrates the relative influence of the reaction rate constant λ on the temporal development of concentration at two different spatial locations ($\eta = 0.232$ and $\eta = 3.626$). Physically speaking, a chemical reaction term represents a concentration sink or decay term. This means that as λ increases, the decaying effect increases, causing the contaminant con-

centration to decrease everywhere in the flow region away from the boundaries and for all times. Thus, as expected, the concentration level decreases as λ increases. However, it is predicted that the decreases in the concentration levels are more pronounced for the downstream location $\eta = 3.626$ than for the upstream location $\eta = 0.232$. Also, it is observed that the concentration level decreases as the flow moves downstream and that the formation of the distinctive

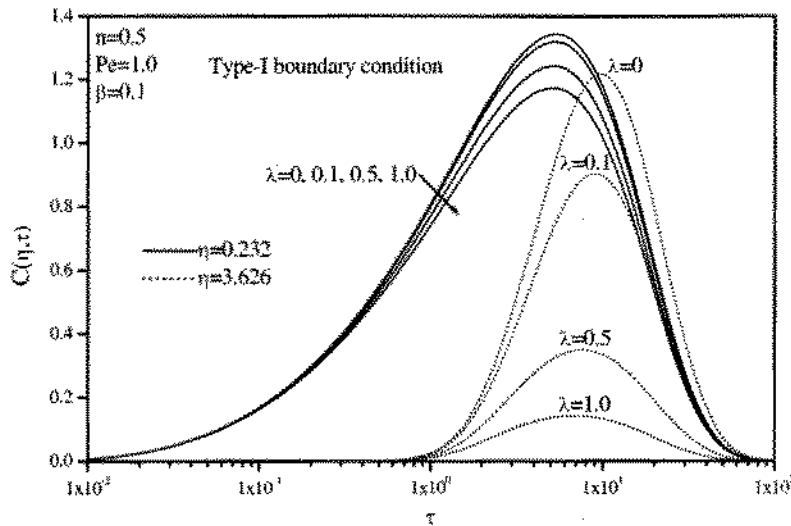


Figure 4. Effects of λ on the temporal development of concentration of two different locations

peaks moves forward in time as η increases. These behaviors are clearly shown in Fig. 4.

Figure 5 depicts the influence of the exponential-type dispersion coefficient constant a and n on the temporal development of concentration at the specific location $\eta = 0.232$. In general, it is observed that increasing the value of the constant a causes appreciable decreases in the contaminant concentration level at small time stages for values of $n > 0.3$ and insignif-

icant changes at high time stages for all values of n . However, for a limited time range ($0.3 \leq \tau \leq 1$), the concentration level increases as a increases for $n \leq 0.3$.

Figure 6 shows the changes in the concentration profiles that are brought about as a result of increasing the constant a for various values of n at $\tau = 0.6$. This figure clearly supports the statements made above in the discussion of the effect of a on the contaminant

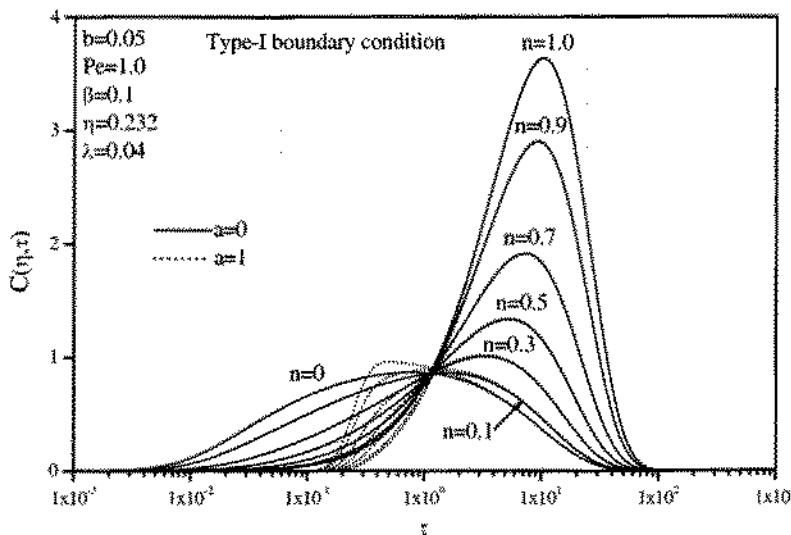


Figure 5. Effects of n and a on the temporal development of concentration at $\eta = 0.232$ for $Pe = 1.0$ and Type-I boundary condition

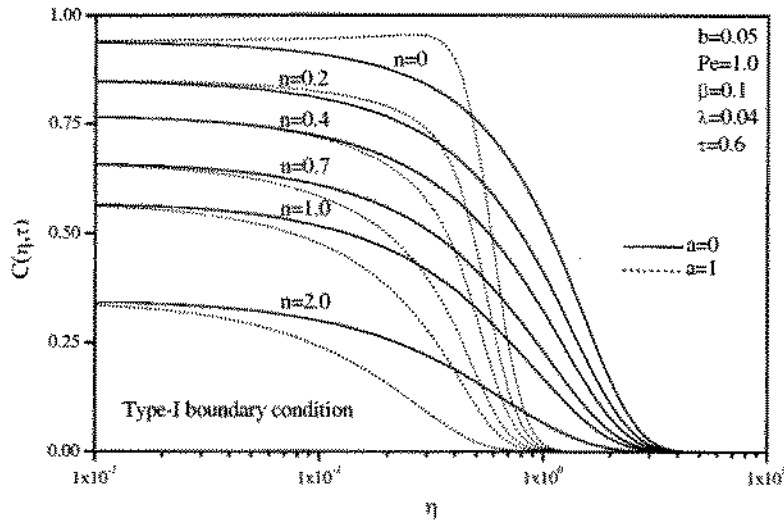


Figure 6. Effects of n and a on the concentration profiles at $\tau = 0.6$

concentration level. Again, it is clear that for values of $n \leq 0.3$, the concentration profile increases as a increases before it reaches the downstream boundary, while it decreases as a increases for $n > 0.3$. It is also important to note that the concentration boundary layer thickness decreases as either a or n , or both, increases.

Figures 7 and 8 present the effects of a and n on the temporal development of concentration for the type III boundary condition for $Pe = 1$ (moder-

ate dispersion effects) and $Pe = 100$ (small dispersion effects) at $\eta = 0.232$, respectively. Unlike the case corresponding to the type I boundary condition, it is predicted that increases in the value of the exponential-type dispersion constant a cause increases in the concentration level at all times away from the initial and steady state conditions. In addition, and as expected, the influence of a on the temporal development of concentration is more pronounced for $Pe = 1$ than for $Pe = 100$. The effect of increasing the expo-

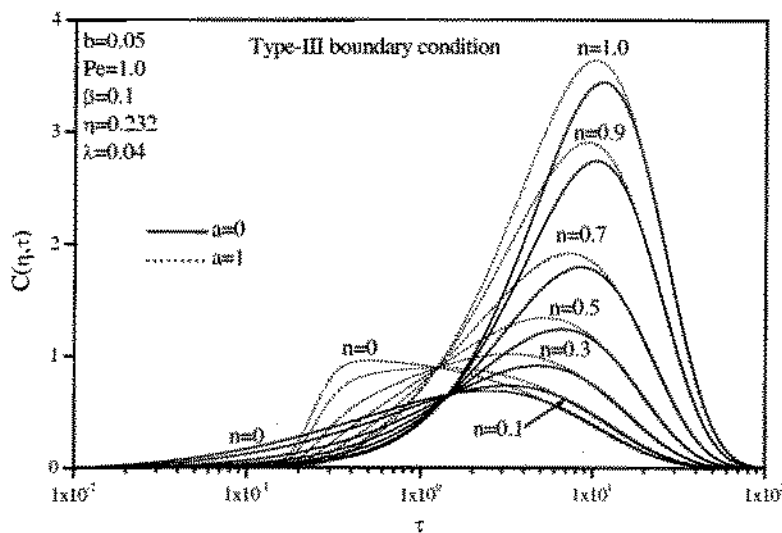


Figure 7. Effects of n and a on the temporal development of concentration at $\eta = 0.232$ for $Pe = 1.0$ and Type-III boundary condition

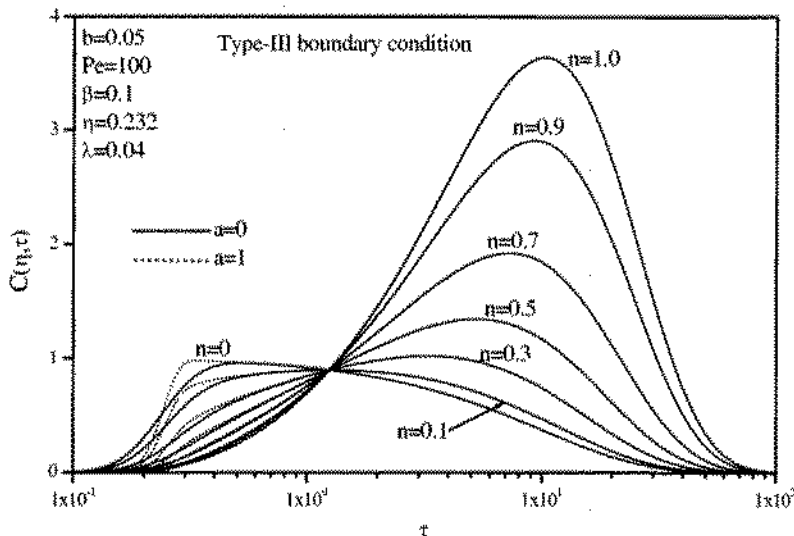


Figure 8. Effects of n and a on the temporal development of concentration at $\eta = 0.232$ for $Pe = 100$ and Type-III boundary condition.

ment n for this case of the type III boundary condition is the same as for the case of the type I boundary condition; that is, as n increases, a distinctive peak in the temporal development of concentration is formed. These behaviors are obvious from Figs. 7 and 8.

Figure 9 shows the effect of increasing either the Peclet number Pe or the reaction rate constant λ on the temporal development of the contaminant concentration at $\eta = 0.232$ for the type III boundary

condition and variable dispersion. As in the case of the type I boundary condition, increasing the value of λ produces reductions in the concentration level at all times. However, the temporal development of the concentration varies considerably and nonmonotonically with changes in the value of Pe in the significant dispersion range $0.0001 \leq Pe \leq 1$. As Pe increases from $Pe = 0.0001$ to $Pe = 0.001$, the temporal concentration level decreases, and then it increases as Pe

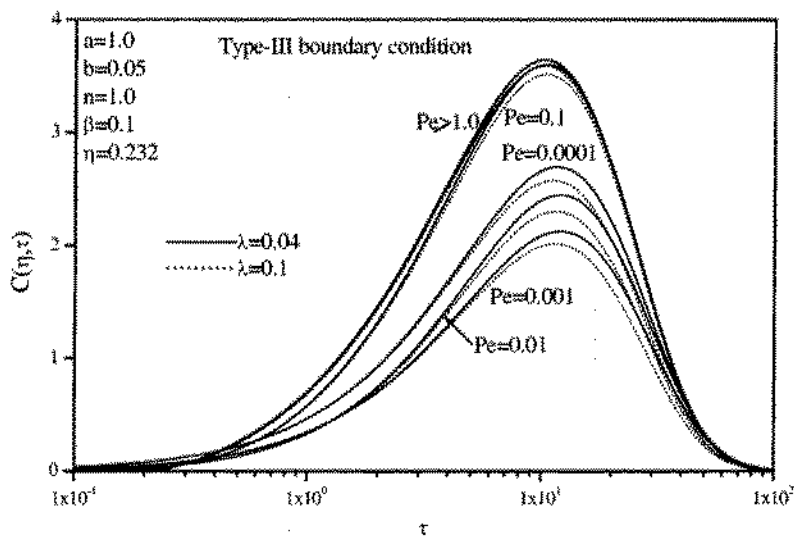


Figure 9. Effects of Pe and λ on the temporal development of concentration at $\eta = 0.232$

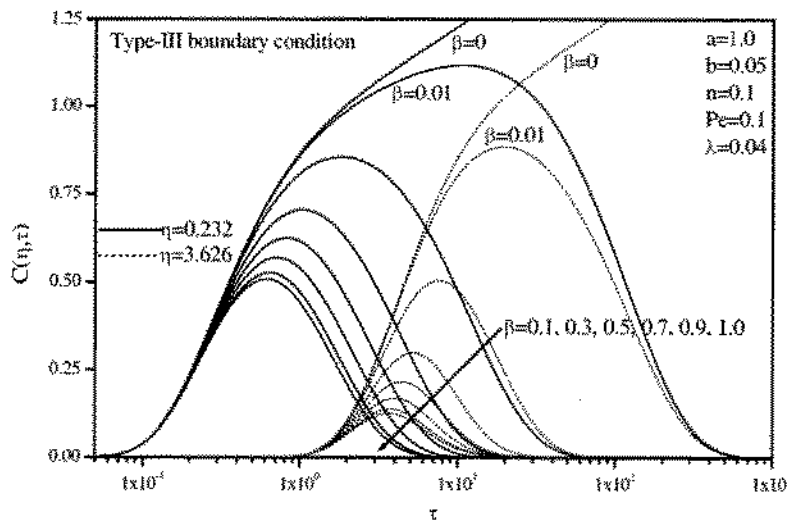


Figure 10. Effects of β and λ on the temporal development of concentration at two different locations

is increased beyond the value of 0.001. It should be noted that when Pe was increased beyond the values of unity, no significant changes were observed.

Figure 10 reports the effects of the dimensionless exponential source concentration exponent β on the temporal development of concentration at two different space locations ($\eta = 0.232$ and $\eta = 3.626$) for the type III boundary condition and variable dispersion. It is clearly observed that as β increases, the concentration level decreases at all times. This is true for both space locations considered. It should be mentioned that for the case of $\beta = 0$, the front concentration becomes a power law function of time. As time progresses, the concentration level increases without bound. The rate of increase in the concentration level is controlled by the value of exponent n .

6. CONCLUSION

This work was focused on the modeling of a one-dimensional contaminant transport in a uniform porous medium with a spatially dependent dispersion coefficient and time-dependent source concentration in the presence of a first-order reaction. Two types of source concentration boundary conditions were employed. These were the type I and type III boundary

conditions with an increasing time-dependent power law function multiplied by a decaying time-dependent exponential function. The variable dispersion coefficient was represented by an exponentially increasing function with the downstream distance. Various analytical solutions for special cases of the problem were presented, and the general nonlinear problem was solved numerically by an efficient implicit iterative tridiagonal finite difference method. The accuracy of the numerical method was validated by various favorable comparisons with known analytical solutions for special cases of the general transport problem. Several numerical solutions based on the general model were reported, assuming a uniform flow field. A parametric study was conducted, and the results were presented graphically to illustrate interesting features of the solutions. It was found that the spatially dependent dispersion coefficient has a significant effect on the contaminant concentration level within the porous medium. This is especially true when a type III boundary condition is employed for the source concentration. In general, as the dispersion coefficient increased with the downstream distance, the concentration level increased. In addition, while the temporal concentration level for a specific location in the porous medium increased as the power

law source concentration exponent increased, it was decreased as the exponential source concentration exponent increased. This was true for both type I and type III source concentration boundary conditions. Furthermore, reductions in the concentration levels were predicted as either the reaction rate constant or the space location was increased. It is hoped that this work will be used as a vehicle for understanding the relative influence of variable dispersion effects on predictions using type I and type III source concentration boundary conditions.

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