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# First- and Third-Type Boundary Conditions in Two-Dimensional Solute Transport Modeling

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This paper presents a general analytical solution for convective-dispersive solute transport in a two-dimensional, semiinfinite porous medium. The solute is assumed to be subject to linear equilibrium sorption and first-order decay. Solutions are derived for several third-type (Cauchy) or flux-type boundary conditions at the input surface. After presenting a generally applicable solution a special solution is given for a strip-type solute source. It is shown that the third-type boundary condition correctly conserves mass in the two-dimensional system and that the first-type (Dirichlet) or concentration-type boundary condition corresponds to a situation that the solute flux at the source decreases with time and at large time approaches to the solute flux of the third-type boundary condition. This can lead to significant discrepancies in the calculated concentrations, especially near the source boundaries.

## INTRODUCTION

During the past several decades a large number of analytical solutions have been developed for estimating the fate and transport of various constituents in the subsurface environment. Application of these solutions is generally limited to steady groundwater flow fields and to relatively simple initial and boundary conditions. Nevertheless, these analytical solutions play an important role in contaminant transport studies, giving initial or approximate estimates of solute concentration distributions in soil and aquifer systems, and allowing for verification of the accuracy of more elaborate numerical models.

The convection-dispersion equation has remained the basis of most analytical and numerical studies of solute transport. With few exceptions, almost all currently used two-dimensional solutions and documented computer codes are based on first-type (Dirichlet) boundary conditions which specify given concentrations at the input surface (e.g., *Bruch and Street* [1967], *Carnahan and Remer* [1984], *Cleary and Ungs* [1978], *Batu* [1983], and *Javandel et al.* [1984], among others). Following earlier work by *Brigham* [1974], *Kreft and Zuber* [1978], and others, *Parker and van Genuchten* [1984*a*] showed that these solutions do not conserve mass in one-dimensional systems if concentrations are interpreted to represent the usual volume-average (or resident) quantities (i.e., amount of solute per unit volume of fluid in the system). However, the one-dimensional solutions did conserve mass when concentrations were considered to be flux-averaged values (amount of solute per unit volume of fluid passing through a unit cross section during a unit time interval). Improper distinction between volume-averaged (resident) concentrations $C_r$ and flux-averaged concentrations $C_f$, and the associated boundary conditions, can easily lead to significant concentration discrepancies, especially for relatively short one-dimensional finite or semiinfinite systems with large dispersivities [*van Genuchten and Parker*, 1984].



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Recently, a number of studies also stressed the importance of distinguishing between volume-averaged and flux-averaged quantities in two-dimensional approaches. For example, *Tang and Peaceman* [1987] and *Chen* [1987] used a third-type condition at the injection well boundary to derive analytical solutions for radial dispersion and convection in an aquifer, while *Sposito and Barry* [1987] discussed the problem of $C_r$ versus $C_f$ in a stochastic framework. The purpose of this paper is to develop a general analytical solution for two-dimensional solute transport subject to a third-type input boundary condition. Specific solutions are also derived for a single strip source. We shall show that the third-type solution for $C_r$ correctly conserves mass in the system, and the first-type solution corresponds to a situation that the solute flux at the source decreases with time, which results in significant discrepancies between the corresponding concentrations in certain situations.

## GOVERNING EQUATIONS

The partial differential equation describing convective-dispersive solute transport in a multidimensional porous medium is

$$\frac{\partial(nR_dC_r)}{\partial t} = \nabla \cdot \mathbf{F} - \nu n R_d C_r \qquad (1)$$

where $\nabla$ is the vector differential operator, $\mathbf{F}$ is the solute flux density vector, $n$ is the porosity, $C_r$ is the volume-averaged (resident) concentration, $R_d$ is a solute retardation factor arising from linear equilibrium sorption onto the solid phase, and $\nu$ is a first-order decay coefficient which assumes equal rates of decay in the solid and liquid phases of the soil (e.g., as for radioactive decay). Equation (1) in a Cartesian coordinate system takes the form

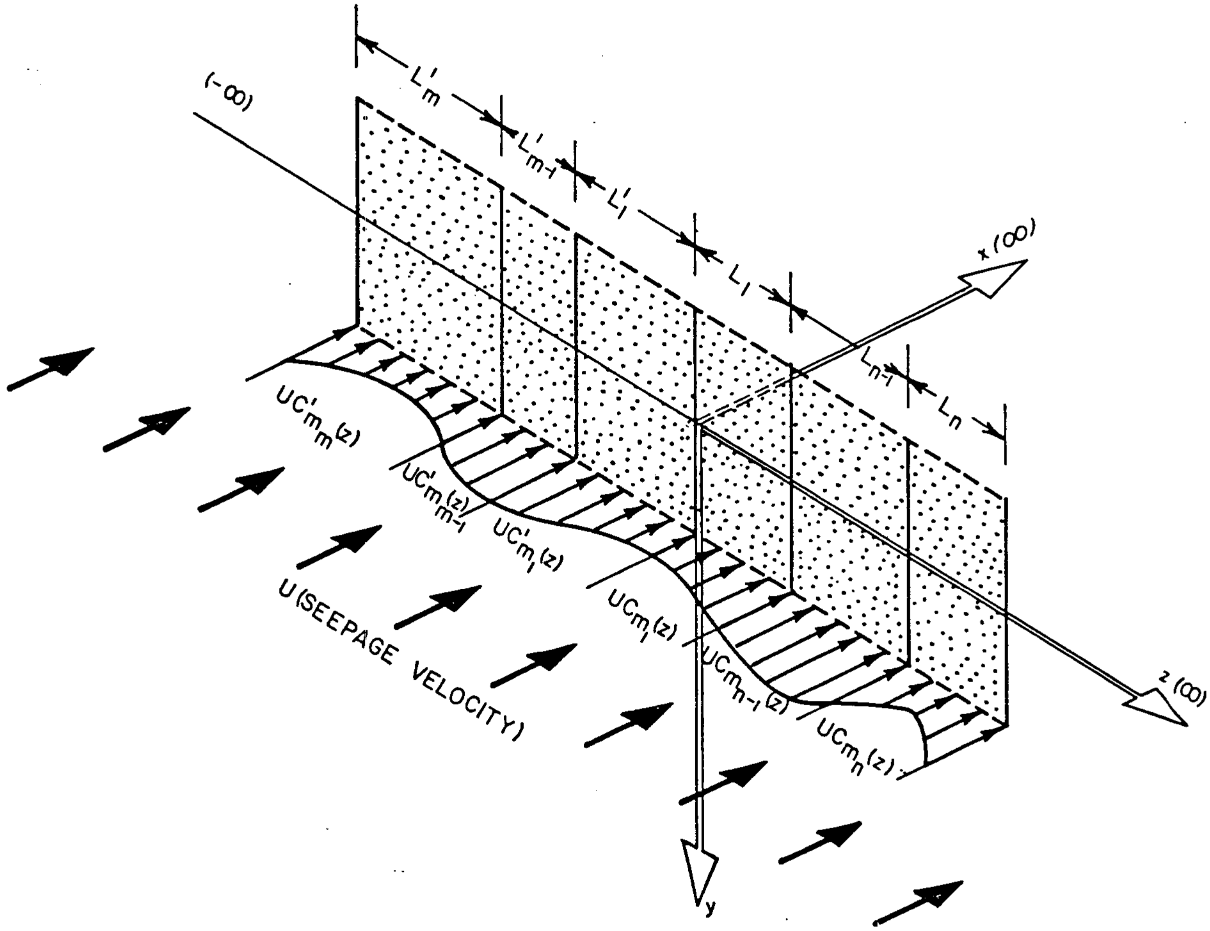


Fig. 1. Schematic representation of semi-infinite porous medium in unidirectional flow field with flux-type inputs at the boundary sources.

$$\frac{\partial(nR_dC_r)}{\partial t} = -\frac{\partial F_x}{\partial x} - \frac{\partial F_y}{\partial y} - \frac{\partial F_z}{\partial z} - \nu nR_dC_r \tag{2}$$

where $F_x$, $F_y$, and $F_z$ are the convective-dispersive flux components in the $x$, $y$, and $z$ directions, respectively. We limit our analysis to a groundwater flow system with a uniform seepage (or average pore water velocity) field $U$. Assuming that the $x$ coordinate is aligned with the direction of flow, the convective-dispersive flux components can be written as

$$F_x = nUC_r - nD_x\,\partial C_r/\partial x \tag{3}$$

$$F_y = -nD_y\,\partial C_r/\partial y \tag{4}$$

$$F_z = -nD_z\,\partial C_r/\partial z \tag{5}$$

where $D_x$, $D_y$, and $D_z$ are the dispersion coefficients in the $x$, $y$, and $z$ directions, respectively. Substituting equations (3), (4), and (5) into (2) and assuming a homogeneous and isotropic medium at constant water porosity leads to the solute transport equation

$$R_d\frac{\partial C_r}{\partial t} = D_x\frac{\partial^2 C_r}{\partial x^2} + D_y\frac{\partial^2 C_r}{\partial y^2} + D_z\frac{\partial^2 C_r}{\partial z^2} - U\frac{\partial C_r}{\partial x} - \nu R_dC_r \tag{6}$$

which will be solved below for a two-dimensional $x$–$z$ coordinate system.

## INITIAL AND BOUNDARY CONDITIONS

Consider a unidirectional flow field containing strip solute sources whose concentrations are functions of the $z$ coordinate, as shown schematically in Figure 1. The medium is semiinfinite in the $x$ direction ($0 < x < \infty$) and infinite in the $z$ direction ($-\infty < z < \infty$). Because the source concentration is a function of the $z$ coordinate, the flux component at $x = 0$ will be a function of $z$ as well. Note that all concentrations are independent of $y$.

The initial condition of the two-dimensional ($x$, $z$) system is taken as

$$C_r(x, z, 0) = 0 \tag{7}$$

From (3), the boundary conditions at the sources ($x = 0$) can be written as

$$F_x(0, z) = nUC_{m_i}(z) \qquad H_{i-1} < z < H_i \tag{8}$$

$$(i = 1, 2, \ldots, n)$$

$$F_x(0, z) = nUC'_{m_i} \qquad -H'_i < z < -H_{i-1} \tag{9}$$

$$(i = 1, 2, \ldots, m)$$

where $H_0 = H_0' = 0$, and (see Figure 1)

$$H_i = \sum_{j=1}^{i} L_j \tag{10a}$$

$$H_i' = \sum_{j=1}^{i} L_j' \tag{10b}$$

At infinity the following boundary condition can be assumed:

$$\lim_{r \to \infty} C_r(x, z, t) = 0 \tag{11}$$

$$r = (x^2 + z^2)^{1/2} \tag{12}$$

## GENERAL SOLUTION

The two-dimensional form of (6) in $x$-$z$ coordinates with the preceding initial and boundary conditions is solved using Laplace transform and Fourier analysis techniques. After taking the Laplace transforms of (6), using the initial condition described by (7) and involving the boundary condition at infinity (11), the following solution in the Laplace domain results [*Batu*, 1983, equation (25)]:

$$\bar{C}_r(x, z, s) = \int_0^{\infty} \exp\left\{\left[\frac{U}{2D_x} - \frac{k(\lambda)}{D_x}\right]x\right\} \cdot [A(\lambda)\sin(\lambda z) + B(\lambda)\cos(\lambda z)]\, d\lambda \tag{13}$$

in which

$$\bar{C}_r = \bar{C}_r(x, z, s) = \int_0^{\infty} e^{-st} C_r(x, z, t)\, dt \tag{14}$$

$$k(\lambda) = \left[D_x D_z \lambda^2 + R_d D_x (s + \nu) + \frac{U^2}{4}\right]^{1/2} \tag{15}$$

where $A(\lambda)$ and $B(\lambda)$ are constants. After implementing the boundary conditions at $x = 0$ into the Fourier integral formula one obtains the following closed form solution for $\bar{C}_r(x, z, s)$ (see Appendix A for details):

$$\bar{C}_r(x, z, s) = \frac{1}{\pi}\int_0^{\infty} \frac{\exp\{[(U/2D_x) - (k(\lambda)/D_x)]x\}}{s[(U/2) + k(\lambda)]} J(\lambda)\, d\lambda \tag{16}$$

where

$$J(\lambda) = \int_{-\infty}^{\infty} \frac{F_x(0, p)}{n} \cos[\lambda(z - p)]\, dp \tag{17}$$

The inverse Laplace transform solution of (16) is derived in Appendix B. We obtained the following result:

$$C_r(x, z, t) = \frac{1}{\pi}\int_0^{\infty} \frac{\exp(Ux/2D_x)}{D_x} \cdot \left\{\int_0^t \exp[-K_1(u, \lambda)][G_1(u) - G_2(u)]\, du\right\} J(\lambda)\, d\lambda \tag{18}$$

where

$$K_1(u, \lambda) = \nu u + \frac{U^2 u}{4R_d D_x} + \frac{D_z u}{R_d}\lambda^2 \tag{19}$$

$$G_1(u) = \left(\frac{D_x}{\pi R_d u}\right)^{1/2} \exp[-K_2(u)] \tag{20}$$

$$G_2(u) = \frac{U}{2R_d} \exp[K_3(u)]\,\mathrm{erfc}[K_4(u)] \tag{21}$$

$$K_2(u) = \frac{R_d x^2}{4D_x u} \tag{22}$$

$$K_3(u) = \frac{Ux}{2D_x} + \frac{U^2 u}{4R_d D_x} \tag{23}$$

$$K_4(u) = \frac{R_d x}{2(R_d D_x u)^{1/2}} + \frac{U}{2D_x}\left(\frac{D_x u}{R_d}\right)^{1/2} \tag{24}$$

## SPECIAL SOLUTIONS

### *Single Strip Source Solution*

Using the general solution given by (18), special solutions can be obtained for any combinations of solute strip sources as shown in Figure 1. For example, Figure 2 shows the geometry of a single strip source in which case $L_1 = L_1' = B$. The boundary conditions at $x = 0$ take the form

$$\frac{F_x(0, z)}{n} = UC_m \qquad -B < z < B \tag{25a}$$

$$\frac{F_x(0, z)}{n} = 0 \qquad \text{otherwise} \tag{25b}$$

Introducing (25) in (17) gives

$$J(\lambda) = \frac{2UC_m}{\lambda} \sin(\lambda B)\cos(\lambda z) \tag{26}$$

Substituting (26) in (18) gives

$$C_r(x, z, t) = \frac{2UC_m}{\pi D_x} \exp\left(\frac{Ux}{2D_x}\right) \int_0^t J_s(\lambda) \cdot \exp\left(-\nu u - \frac{U^2 u}{4R_d D_x}\right)[G_1(u) - G_2(u)]\, du \tag{27}$$

where

$$J_s(\lambda) = \int_0^{\infty} \exp\left(-\frac{D_z u \lambda^2}{R_d}\right) \frac{1}{\lambda} \sin(\lambda B)\cos(\lambda z)\, d\lambda \tag{28}$$

This integral can be evaluated in a manner similar to *Batu* [1982, equations (61)–(72)]. The final result is

$$J_s(\lambda) = \frac{\pi}{4}\left\{\mathrm{erf}\left[\frac{R_d(z + B)}{2(D_z R_d u)^{1/2}}\right] - \mathrm{erf}\left[\frac{R_d(z - B)}{2(D_z R_d u)^{1/2}}\right]\right\} \tag{29}$$

Finally, introducing (29) in (27) gives the following equation for the volume-averaged concentration distribution:

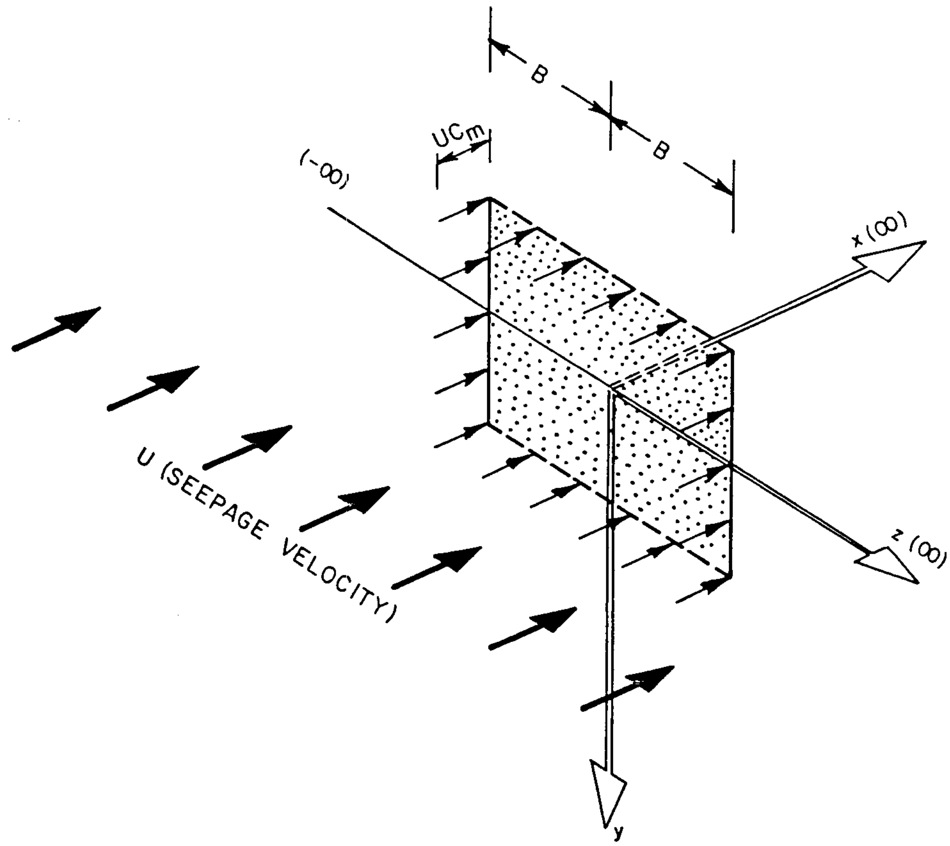


Fig. 2. The geometry of a single strip source.

$$C_r(x, z, t) = \frac{UC_m}{2(\pi R_d D_x)^{1/2}} \int_0^t \frac{1}{u^{1/2}} F_1(u)[F_4(u) - F_5(u)]\, du$$
$$- \frac{U^2}{4R_d D_x} C_m \int_0^t \exp(-\nu u) F_2(u)[F_4(u) - F_5(u)]\, du \quad (30)$$

where

$$F_1(u) = \exp\left[\frac{Ux}{2D_x} - \nu u - \frac{U^2 u}{4R_d D_x} - K_2(u)\right] \quad (31)$$

$$F_2(u) = \exp\left(\frac{Ux}{D_x}\right) F_3(u) \quad (32)$$

$$F_3(u) = \text{erfc}\,[K_4(u)] \quad (33)$$

$$F_4(u) = \text{erf}\left[\frac{R_d(z + B)}{2(D_z R_d u)^{1/2}}\right] \quad (34)$$

$$F_5(u) = \text{erf}\left[\frac{R_d(z - B)}{2(D_z R_d u)^{1/2}}\right] \quad (35)$$

*Solutions for Two or More Strip Sources*

Equation (17) represents the geometrical distribution of the sources and their source concentrations. For any number of sources, only the integral $J(\lambda)$ needs to be evaluated. The other part of the general solution (18) remains the same for any arbitrary combination of the individual sources. The general solution is also valid for any type of $z$-dependent source concentration. For $C_m = C_m(z)$, (17) can be evaluated either analytically or numerically depending on the functional distribution of $C_m(z)$.

## MODEL EVALUATION AND VERIFICATION

Equation (30) gives residence concentration distribution for a single strip source. The integrals in (30) were evaluated numerically by means of Gaussian integration using 256 quadrature points. Normalized concentration distributions calculated with (30) for the third-type boundary conditions were first checked by comparison with the analytical solution for the one-dimensional case [*Lindstrom et al.*, 1967]. Comparisons were made for the parameters (and results) given in Table 6 of *van Genuchten and Alves* [1982, p. 118] that is, $U$ = 1 m/d, $D_x$ = 4 m$^2$/d and $R_d$ = 1. In order to reproduce correctly the one-dimensional results we used a very small transverse dispersion coefficient $D_z$ of $10^{-10}$ m$^2$/d and a very large strip source width $B$ of $10^4$ m. Essentially identical results were obtained for the one- and two-dimensional solutions (results not shown).

Analytical results based on (30) were also compared with numerical results generated with a finite-element groundwater flow and solute transport code called GEOFLOW [*International Technology Corporation*, 1986], International Technology Corporation's in-house semi-three-dimensional groundwater flow and solute transport code. A domain of 75 × 50 m$^2$ was used in the numerical model which contained 432 four-node quadrilateral elements. No-flux concen-

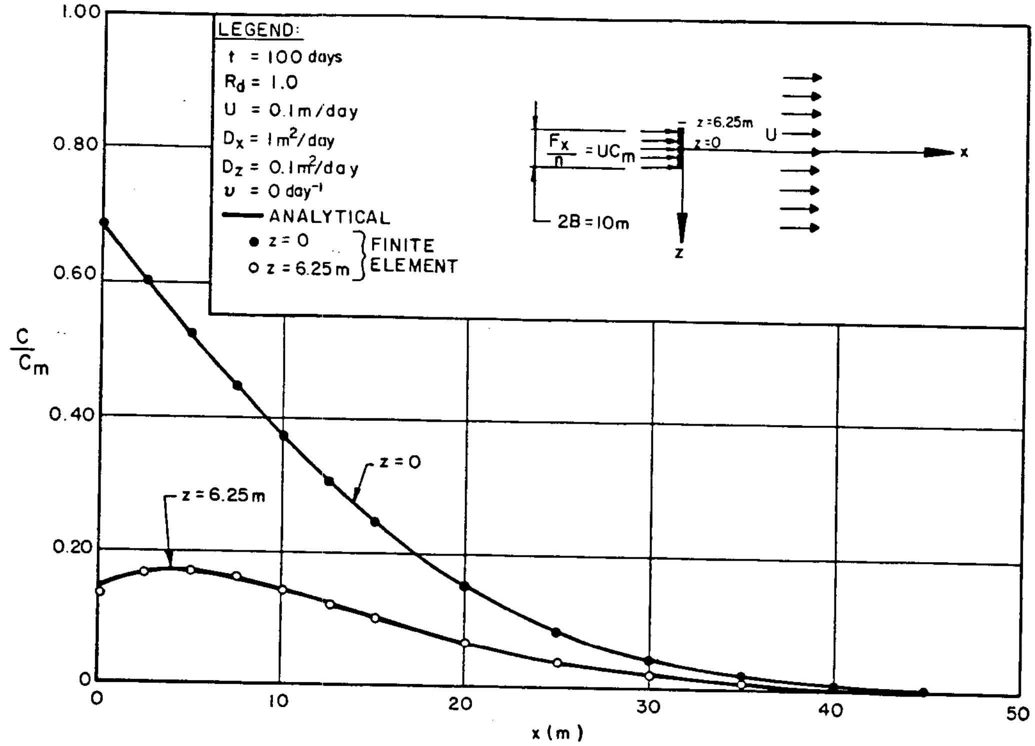


Fig. 3. Comparison of the analytical and finite-element results for the normalized concentrations obtained in the longitudinal direction with third-type boundary condition ($R_d$ = 1, $t$ = 100 days).

tration boundaries were imposed at $z = \pm 25$ m, while a zero-concentration gradient was assumed along the downstream boundary at $x = 75$ m. The finite element dimensions were between 1.25 and 5 m, with a fine grid near the source boundary. The width of the source strip was taken to be 10 m. Calculated normalized concentration distributions versus $x$ and $z$ after 100 days for a retardation factor $R_d$ of 1 are shown in Figures 3 and 4, respectively. Note that the

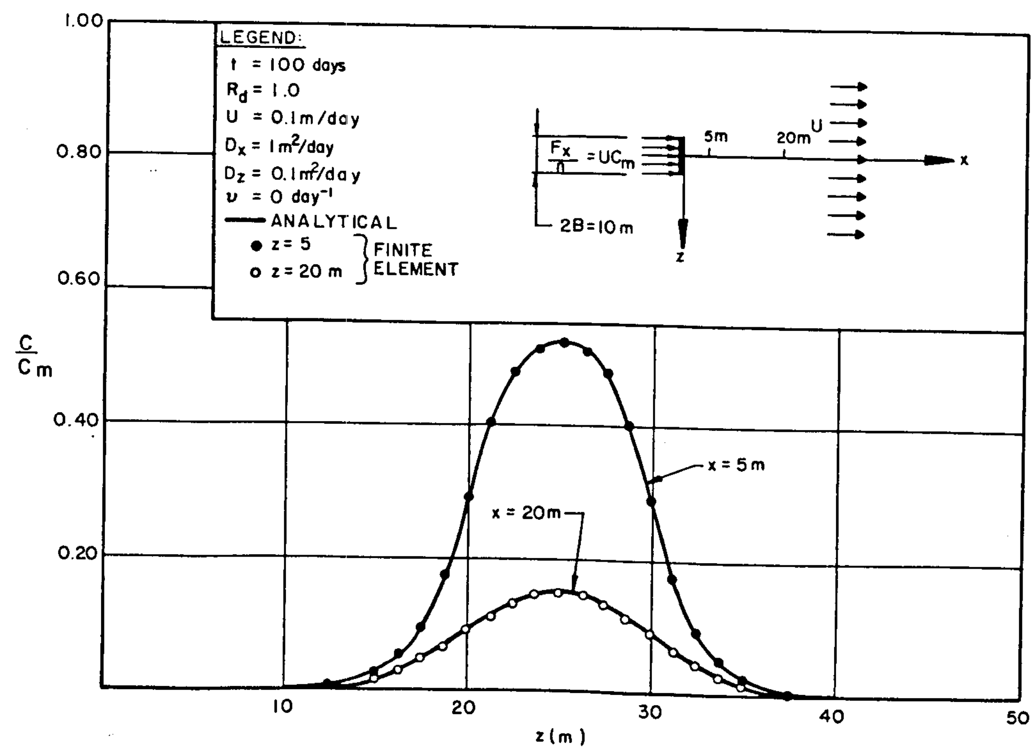


Fig. 4. Comparison of the analytical and finite-element results for the normalized concentrations obtained in the transverse direction with the third-type boundary condition ($R_d$ = 1, $t$ = 100 days).

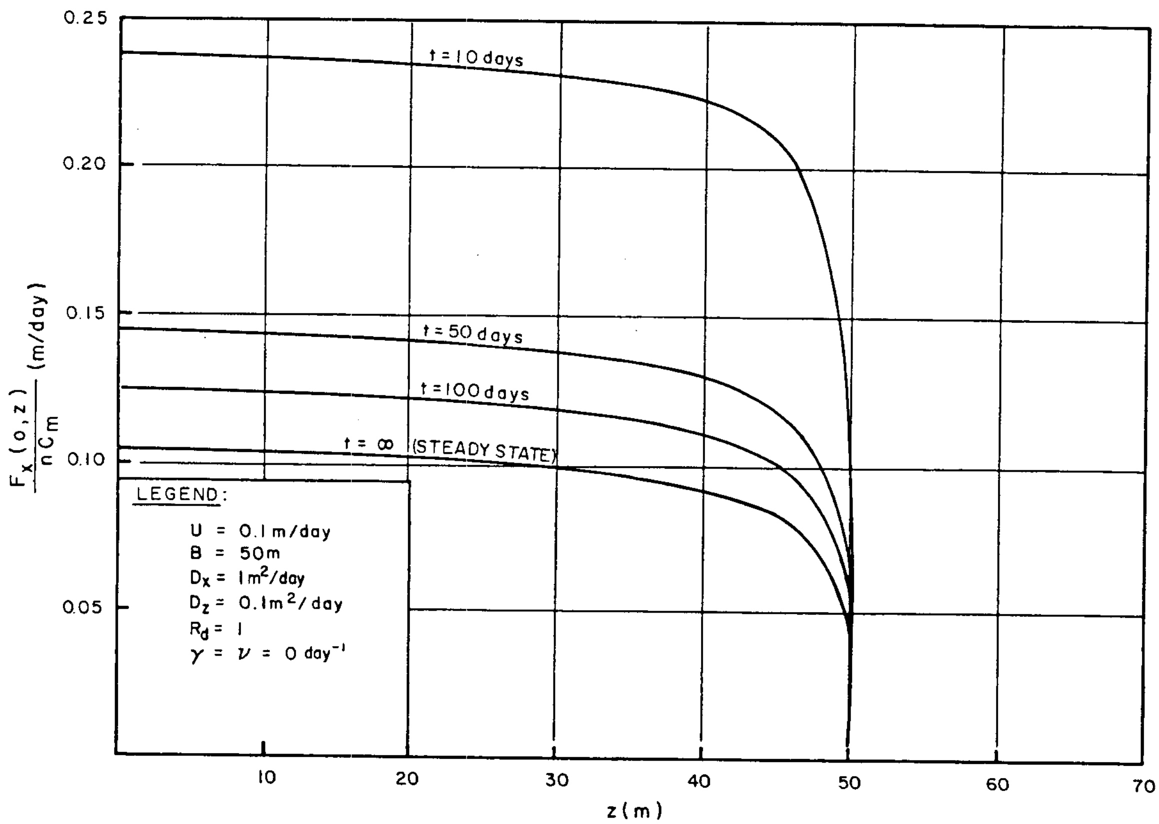


Fig. 5. Temporal and spatial variations of $F_x(0, z)/nC_m$ at $x = 0$ for the first-type boundary condition.

analytical model holds for a semi-infinite domain in the $x$ direction, while the numerical solution assumes a finite domain with a downstream boundary at $x = 75$ m. However, the calculated numerical normalized concentrations should be unaffected by the location of downstream boundary as long as the concentration front does not reach that boundary. As can be seen from Figures 3 and 4, the comparison of the two-dimensional analytical and finite-element results for the third-type boundary condition is excellent.

We also verified the accuracy of the first-type analytical solution as given by *Batu* [1983] by comparison with data listed in the work by *Javandel et al.* [1984, pp. 134, 137], based on the solution of *Cleary and Ungs* [1978]. The answers were essentially the same and are not presented here.

In Figure 5 the convective-dispersive flux component for the first-type (Dirichlet) boundary condition along the $z$ axis, $F_x/(nC_m)$, is presented at $x = 0$. Because of symmetry, only half of the curves are given. Figure 5 clearly shows that the flux decreases with the increase of time and becomes constant when the system reaches steady state. This is in contrast to similar results for the third-type boundary condition whose flux component at $x = 0$ remains constant at $F_x/(nC_m) = U$ (=0.1 m/d).

Figures 6–8 compare the concentration distributions for the first-type and third-type boundary conditions for $t$ at =10, 100, and ∞ (steady state) days. The concentration profiles correspond to $z = 25$ m. These graphs clearly show that the first-type boundary condition predicts normalized concentrations with significant discrepancies with the third-type boundary condition during transient conditions, especially near the input boundary. The principal reason for this situation is that the first-type boundary condition corresponds to the situation that the solute flux at the source decreases with time (Figure 5), whereas the solute flux for the third-type boundary condition case is constant. For large times and steady state transport conditions the results become approximately the same. For example, the first-type boundary condition in this example predicts more than 3 times higher concentrations at $t = 100$ days than the third-type boundary condition does.

## MASS BALANCE CONSTRAINTS

Assuming no decay ($\nu = 0$), mass balance considerations lead to the following equality for the solute transport situation depicted in Figure 2:

$$2BnUC_mt = nR_d \int_{x=0}^{\infty} \int_{z=\infty}^{\infty} C_r(x, z, t)\,dx\,dz \qquad (36)$$

Equation (36) is the two-dimensional equivalent of (6) of *van Genuchten and Parker* [1984]. With (25), the left-hand side of (36) is equivalent to $2BF_x(0, z)t$. This quantity gives the mass of the solute entering into the medium through the strip source between times 0 and $t$. The thickness of the source perpendicular to the $x$-$z$ plane is considered to be of unit length. The right-hand side of (36) gives the total mass of the solute recovered in the system during the same time period. In other words, whatever is added at the source (term on the left) must be found inside the solute transport medium (term on the right).

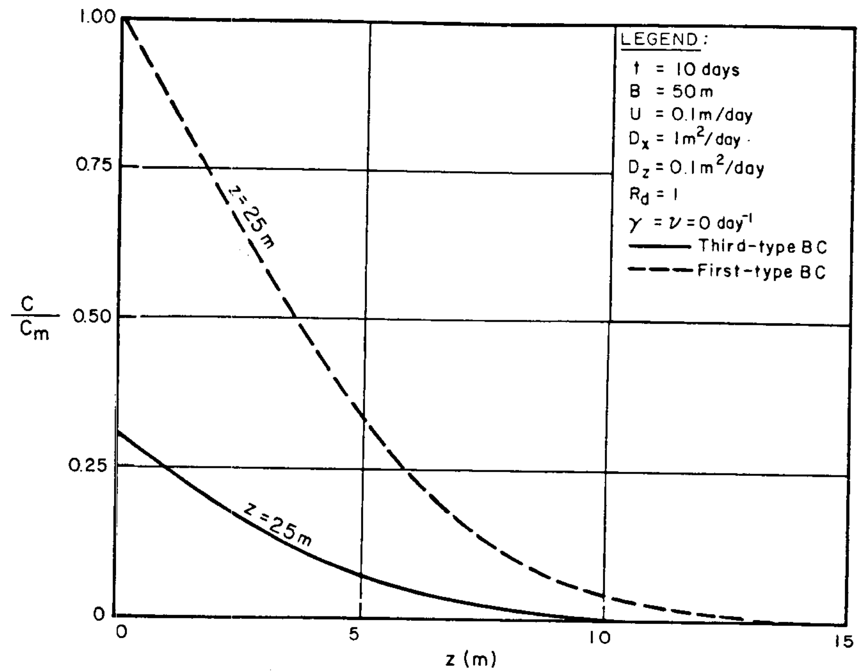


Fig. 6. Comparison of the normalized concentrations for the first-type and third-type boundary conditions for $t = 10$ days.

We will now show that the mass balance constraint imposed on (36) is indeed met if $C_r$ is given by (30). To do this, let us take the Laplace transform of (36) to give

$$2BUC_m \frac{1}{s^2} = R_d \int_{x=0}^{\infty} \int_{z=-\infty}^{\infty} \bar{C}_r(x, z, s)\, dx\, dz \quad (37)$$

Mathematically, it is easier to work with (37) than with (36). Appendix C shows that, with the introduction of (16) and (26), the right-hand side of (37) results in exactly the same form as its left-hand side. This means that the mass balance requirement is satisfied exactly for the third-type (Cauchy) boundary condition.

However, large discrepancies in (36) may occur when the first-type solution is substituted into the mass balance constraint, especially for large longitudinal dispersivities. The potential magnitude of these discrepancies are illustrated indirectly by the differences between the first- and third-type

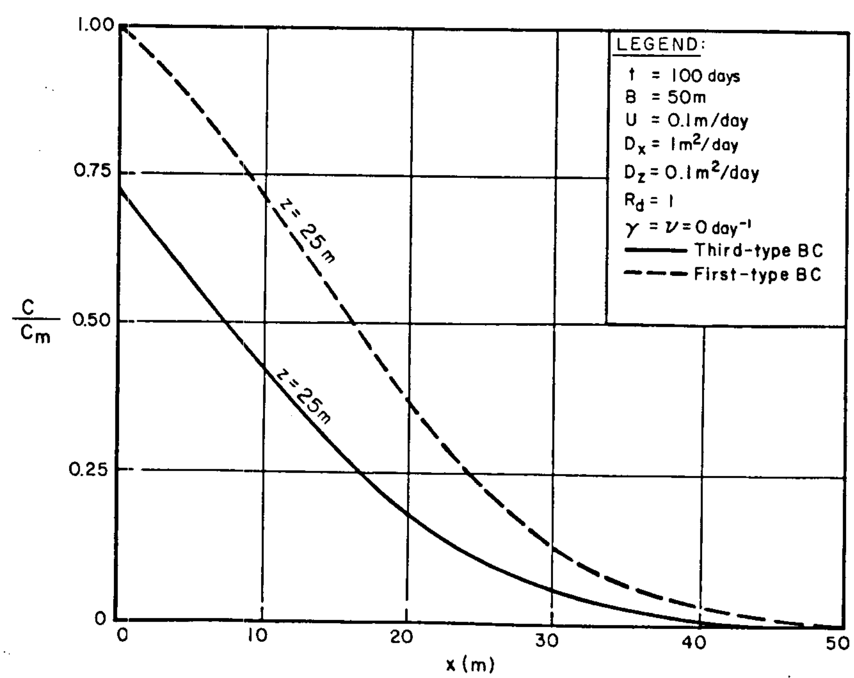


Fig. 7. Comparison of the normalized concentrations for the first-type and third-type boundary conditions for $t = 100$ days.

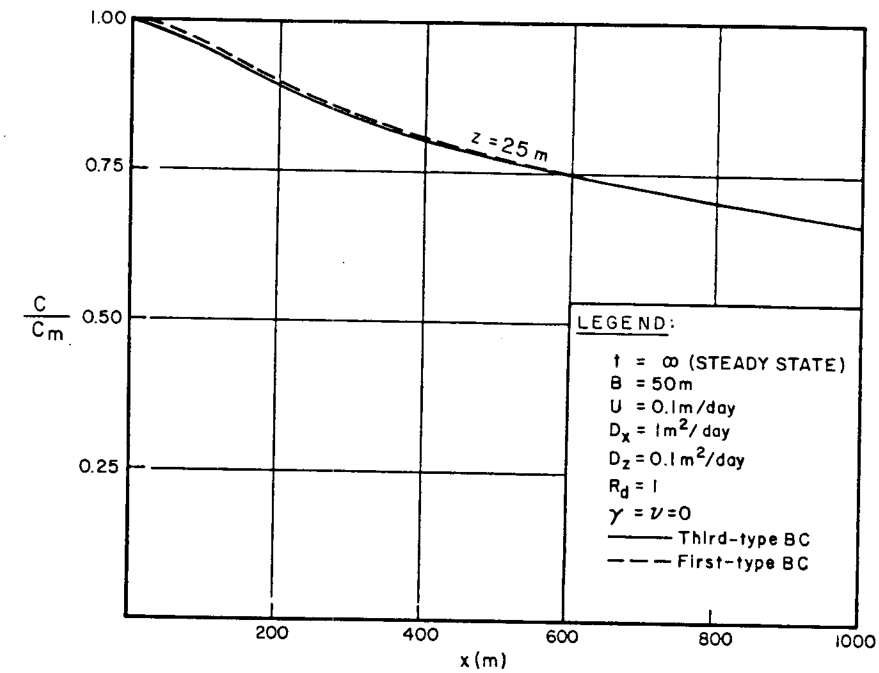


Fig. 8. Comparison of the normalized concentrations for the first-type and third-type boundary conditions for $t = \infty$ (steady state).

solutions shown in Figures 6–8. The discrepancies for the limiting case of one-dimensional transport were previously given by equation (8) of *van Genuchten and Parker* [1984] and plotted in their Figure 1 as a function of the dimensionless variable $\zeta = U^2t/D_xR$.

## VOLUME-AVERAGED VERSUS FLUX-AVERAGED CONCENTRATIONS

Several papers previously discussed the importance of distinguishing between volume-averaged (resident) concentrations $C_r$ and flux-averaged (flowing) concentrations $C_f$ during one-dimensional solute transport [*Brigham*, 1974; *Kreft and Zuber*, 1978; *Parker and van Genuchten*, 1984*a*]. These studies established the following relationship between $C_f$ and $C_r$:

$$C_f = C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x} \tag{38}$$

This transformation was shown to leave the one-dimensional transport equation invariant, indicating that the transport equation can be formulated in terms of both $C_r$ and $C_f$ [*Kreft and Zuber*, 1979; *Parker and van Genuchten*, 1984*b*]. Equation (38) also applies to the two-dimensional case described by our (6) and the invoked initial and boundary conditions. The invariance of (6) to the transformation given by (38) is most easily shown by rewriting (6) in the form

$$R_d\frac{\partial C_r}{\partial t} = D_x\frac{\partial^2 C_r}{\partial z^2} + D_z\frac{\partial^2 C_r}{\partial z^2} - U\frac{\partial C_r}{\partial x} - \nu R_d C_r$$
$$+ \frac{D_x}{U}\frac{\partial}{\partial x}\left[R_d\frac{\partial C_r}{\partial t} - D_x\frac{\partial^2 C_r}{\partial x^2}\right.$$
$$\left. - D_z\frac{\partial^2 C_r}{\partial z^2} + U\frac{\partial C_r}{\partial x} + \nu R_d C_r\right] \tag{39}$$

Note that the last term (in square brackets) is identical to zero as predicted by (6). Combining terms in (39) gives

$$R_d\frac{\partial}{\partial t}\left(C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x}\right) = \left(D_x\frac{\partial^2 C_r}{\partial x^2} - \frac{D_x^2}{U}\frac{\partial^3 C_r}{\partial x^3}\right)$$
$$+ \left(D_z\frac{\partial^2 C_r}{\partial z^2} - \frac{D_xD_z}{U}\frac{\partial^3 C_r}{\partial x\,\partial z^2}\right)$$
$$- U\frac{\partial C_r}{\partial x} + D_x\frac{\partial^2 C_r}{\partial x^2} - \nu R_d C_r + \frac{\nu D_x R_d}{U}\frac{\partial C_r}{\partial x} \tag{40}$$

or with some rearranging

$$R_d\frac{\partial}{\partial t}\left(C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x}\right) = D_x\frac{\partial^2}{\partial x^2}\left(C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x}\right)$$
$$+ D_z\frac{\partial^2}{\partial z^2}\left(C_r - \frac{D_x}{U}\frac{\partial C}{\partial x}\right) - U\frac{\partial}{\partial x}$$
$$\cdot\left(C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x}\right) - \nu R_d\left(C_r - \frac{D_x}{U}\frac{\partial C_r}{\partial x}\right) \tag{41}$$

and hence with (40)

$$R_d\frac{\partial C_f}{\partial t} = D_x\frac{\partial^2 C_f}{\partial x^2} + D_z\frac{\partial^2 C_f}{\partial z^2} - \nu R_d C_f \tag{42}$$

which is of the same form as (6). Application of (37) to (8) and its associated equations transforms the third-type boundary condition in terms of $C_r$ into a first-type condition for $C_f$, that is,

$$C_f(0, z, t) = C_{m_i}(z) \qquad H_{i-1} < z < H_i \qquad (i = 1, 2, \cdots, n) \tag{43a}$$

$$C_f(0, z, t) = C'_{m_i}(z) \qquad -H'_i < z < -H'_{i-1} \tag{43b}$$

$$(i = 1, 2, \cdots, m)$$

Because the remaining initial and boundary conditions remain invariant under transformation (38), it follows that the first-type solution given previously by *Batu* [1983] represents the flux-averaged concentration.

Equation (38) gives the flux-averaged concentration $C_f$ in terms of the volume-averaged concentration $C_r$. The equation can be used immediately to derive the first-type solution from the third-type solution. Alternatively, the third-type solution may be derived from the first-type solution by using the inverse of (38) (see also *van Genuchten et al.* [1984, equations (74*a*) and (74*b*)]):

$$C_r(x, z, t) = \frac{U}{D_x} \exp\left(\frac{Ux}{D_x}\right) \int_x^\infty \exp\left(-\frac{U\xi}{D_x}\right) C_f(\xi, z, t)\, d\xi \tag{44}$$

One may verify that (44) indeed transforms the Laplace domain solution for the first-type case (see equation (33) of *Batu* [1983], with $\gamma = 0$) into the Laplace solution for the third-type boundary condition (equation (16) of this paper).

The above considerations show that the analytical solutions of (6) for the first- and third-type boundary conditions are related to each other through (38) and (43) and that these solutions represent flux-averaged and volume-averaged concentrations, respectively. This interpretation is analogous to the one-dimensional situation described by *Parker and van Genuchten* [1984*a*]. However, we emphasize that the above relationships (38 and 43) between the first- and third-type analytical solutions of (6) only hold for the simplified transport problem considered in this study, that is, for undirectional steady flow perpendicular to the input boundary at $x = 0$. In more general situations (including radial flow), additional terms in (42) will be generated when (38) is used to derive the flux-averaged concentration from the volume-averaged concentration [see *Sposito and Barry*, 1987]. Thus first-type analytical solutions do not always represent flux-averaged concentrations in two-dimensional transport models.

## Summary and Conclusions

A general analytical solution given by equation (18) has been developed for solute transport in a two-dimensional, semi-infinite system subject to a third-type, Cauchy, or flux-type boundary condition at the source boundary. The governing equation includes terms accounting for convective (advective) transport, dispersion, linear equilibrium adsorption, and first-order decay. Special solutions for a single-strip source are also derived. Mass balance principles were applied to the third-type solution as well as to a previously derived first-type solution for the same problem [*Batu*, 1983]. Assuming no decay, it is shown that only the third-type solution satisfied the global mass balance of the transport system and that the first-type solution corresponds to a situation that the solute flux at the source decreases with time, which results in significant discrepancies between the corresponding concentrations, especially near the source boundary. We have also shown that for the simplified transport problem of this study the first-type solution represents flux-averaged concentration.

## Appendix A: Derivation of Equation (18)

The Laplace transform of (3) is

$$\frac{\bar F_x}{n} = \left(U\bar C_r - D_x \frac{\partial \bar C_r}{\partial x}\right) s \tag{A1}$$

From (15)

$$\frac{\partial \bar C_r}{\partial x} = \left[\frac{U}{2D_x} - \frac{k(\lambda)}{D_x}\right] \int_0^\infty \exp\left\{\left[\frac{U}{2D_x} - \frac{k(\lambda)}{D_x}\right] x\right\} \cdot [A(\lambda)\sin(\lambda z) + B(\lambda)\cos(\lambda z)]\, d\lambda \tag{A2}$$

and introducing $x = 0$ in (15) and (A2), respectively, gives

$$\bar C_r|_{x=0} = \int_0^\infty [A(\lambda)\sin(\lambda z) + B(\lambda)\cos(\lambda z)]\, d\lambda \tag{A3}$$

$$\left.\frac{\partial \bar C_r}{\partial x}\right|_{x=0} = \left[\frac{U}{2D_x} - \frac{k(\lambda)}{D_x}\right] \cdot \int_0^\infty [A(\lambda)\sin(\lambda z) + B(\lambda)\cos(\lambda z)]\, d\lambda \tag{A4}$$

Introducing (A3) and (A4) in (A1) gives

$$\frac{\bar F_x(0, z)}{n} = \int_0^\infty [\bar A(\lambda)\sin(\lambda z) + \bar B(\lambda)\cos(\lambda z)]\, d\lambda \tag{A5}$$

where

$$\bar A(\lambda) = A(\lambda)\left\{U - D_x\left[\frac{U}{2D_x} - k(\lambda)\right]\right\} s \tag{A6}$$

$$\bar B(\lambda) = B(\lambda)\left\{U - D_x\left[\frac{U}{2D_x} - k(\lambda)\right]\right\} s \tag{A7}$$

The general form of the Fourier integral formula [*Churchill*, 1941, p. 114] is

$$f(z) = \frac{1}{\pi}\int_0^\infty \sin(\lambda z) \int_{-\infty}^\infty f(p)\sin(\lambda p)\, dp\, d\lambda + \frac{1}{\pi}\int_0^\infty \cos(\lambda z)\int_{-\infty}^\infty f(p)\cos(\lambda p)\, dp\, d\lambda \tag{A8}$$

Here $f(z)$ and $f(p)$ correspond to $\bar F_x(0, z)/n$ and $\bar F_x(0, p)/n$, respectively. Introducing these values in (A8) gives

$$\frac{\bar F_x(0, z)}{n} = \frac{1}{\pi}\int_0^\infty \sin(\lambda z)\int_{-\infty}^\infty \frac{\bar F_x(0, p)}{n}\sin(\lambda p)\, dp\, d\lambda + \frac{1}{\pi}\int_0^\infty \cos(\lambda z)\int_{-\infty}^\infty \frac{\bar F_x(0, p)}{n}\sin(\lambda p)\, dp\, d\lambda \tag{A9}$$

or

$$\frac{F_x(0, z)}{n} = \int_0^\infty \left[\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{F_x(0, p)}{n} \cdot \sin(\lambda p)\, dp\right] \sin(\lambda z)\, d\lambda + \int_0^\infty \left[\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{F_x(0, p)}{n} \cdot \cos(\lambda p)\, dp\right] \cos(\lambda z)\, d\lambda \qquad \text{(A10)}$$

From (A5) and (A10)

$$\bar{A}(\lambda) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{F_x(0, p)}{n} \sin(\lambda p)\, dp \qquad \text{(A11)}$$

$$\bar{B}(\lambda) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{F_x(0, p)}{n} \cos(\lambda p)\, dp \qquad \text{(A12)}$$

Substituting (A11) and (A12) into (A6) and (A7), respectively, the values of $A(\lambda)$ and $B(\lambda)$ can be determined. Then introducing $A(\lambda)$ and $B(\lambda)$ in (15) leads to the final solution as given by (18).

## APPENDIX B: THE INVERSE LAPLACE TRANSFORM OF EQUATION (18)

To evaluate the inverse Laplace transform of (18), the first translation or shifting property [*Spiegel*, 1965] will be used. Equation (17) may be written as

$$k(\lambda) = [R_d D_x(s - b)]^{1/2} \qquad \text{(B1)}$$

where

$$b = -\nu - \frac{U^2}{4R_d D_x} - \frac{D_z}{R_d}\lambda^2 \qquad \text{(B2)}$$

Introducing (B1) and (B2) in (18), $\bar{C}_r$ takes the form

$$\bar{C}_r(x, z, s) = \frac{1}{\pi} \cdot \int_0^\infty \frac{\exp\{[(U/2D_x) - (1/D_x)(R_d D_x(s - b))^{1/2}]x\}}{sD_x\{(U/2D_x) + (1/D_x)[R_d D_x(s - b)]^{1/2}\}} J(\lambda)\, d\lambda \qquad \text{(B3)}$$

or

$$\bar{C}_r(x, z, s) = \frac{1}{\pi}\int_0^\infty \frac{f(s - b)}{s} J(\lambda)\, d\lambda \qquad \text{(B4)}$$

where

$$f(s - b) = \frac{\exp\{[(U/2D_x) - (1/D_x)[R_d D_x(s - b)]^{1/2}]x\}}{D_x\{(U/2D_x) + (1/D_x)[R_d D_x(s - b)]^{1/2}\}} \qquad \text{(B5)}$$

If

$$L^{-1}\{g(s)\} = G(t) \qquad \text{(B6)}$$

then

$$F(t) = L^{-1}\{f(s - b)\} = e^{bt}G(t) \qquad \text{(B7)}$$

$$C_r(x, z, t) = L^{-1}\{\bar{C}_r(x, z, s - b)\} = L^{-1}\left\{\frac{1}{\pi}\int_0^\infty \frac{f(s - b)}{s} J d\lambda\right\} = \frac{1}{\pi}\int_0^\infty \int_0^t F(u)\, J du d\lambda \qquad \text{(B8)}$$

where

$$g(s) = \left[\frac{U}{2D_x} + D_x^{-1}(R_d D_x s)^{1/2}\right]^{-1} \exp[-D_x^{-1}(R_d D_x s)^{1/2} x] \qquad \text{(B9)}$$

The inverse of (B9) is [*Carslaw and Jaeger*, 1959, p. 494, equation 12]

$$G(t) = E_1(t) - E_2(t) \qquad \text{(B10)}$$

where

$$E_1(t) = \left(\frac{D_x}{\pi R_d t}\right)^{1/2} \exp\left(-\frac{R_d x^2}{4D_x t}\right) \qquad \text{(B11)}$$

$$E_2(t) = \frac{U}{2R_d} \exp\left(\frac{Ux}{2D_x} + \frac{U^2 t}{4R_d D_x}\right) \cdot \operatorname{erfc}\left[\frac{R_d x}{2(R_d D_x t)^{1/2}} + \frac{U}{2D_x}\left(\frac{D_x t}{R_d}\right)^{1/2}\right] \qquad \text{(B12)}$$

and from (B2), (B7), and (B10)

$$F(t) = \exp\left[-\nu t - \frac{U^2}{4R_d D_x} t - \frac{D_z \lambda^2}{R_d} t\right] G(t) \qquad \text{(B13)}$$

By writing $u$ instead of $t$ and introducing $F(u)$ in (B8) leads to the final solution as given by (18).

## APPENDIX C: PROOF OF THE MASS BALANCE FOR THE THIRD-TYPE (CAUCHY) BOUNDARY CONDITION

In this appendix we show that the right-hand side of (37) is exactly equivalent to its left-hand side. Introducing (26) into (16) with $\nu = 0$ gives

$$\bar{C}_r(x, z, s) = \frac{1}{\pi}\int_0^\infty \frac{\exp\{[(U/2D_x) - k(\lambda)]x\}}{D_x\{(U/2D_x) + (1/D_x)[R_d D_x(s - b)]^{1/2}\}} \cdot \frac{2UC_m}{\lambda} \sin(\lambda B) \cos(\lambda z)\, d\lambda \qquad \text{(C1)}$$

With (B1), (C1) takes the form

$$\bar{C}_r(x, z, s) = \frac{1}{\pi}\int_0^\infty \frac{\exp\{(Ux/2D_x) - (1/D_x)[R_d D_x(s - b)]^{1/2}x\}}{\{(U/2) + [R_d D_x(s - b)]^{1/2}\}s} \cdot \frac{2UC_m}{\lambda} \sin(\lambda B) \cos(\lambda z)\, d\lambda \qquad \text{(C2)}$$

Introducing (C2) in the right-hand side of (37) (denoted by $I_R$) gives

$$I_R = R_d \int_{\lambda=0}^{\infty} \left[ \frac{1}{\pi} \int_{x=0}^{\infty} \int_{z=-\infty}^{\infty} \left\{ \exp\left( \frac{Ux}{2D_x} - \frac{1}{D_x} \cdot [R_d D_x(s-b)]^{1/2} x \right) \left[ \left( \frac{U}{2} + [R_d D_x (s-b)]^{1/2} \right) s \right]^{-1} \right\} \cdot \cos(\lambda z)\, dx\, dz \right] \frac{2UC_m}{\lambda} \sin(\lambda B)\, d\lambda \quad \text{(C3)}$$

Integrating (C3) with respect to $x$ gives

$$I_R = R_d \int_{\lambda=0}^{\infty} \left[ \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{(R_d s + D_z \lambda^2) s} \cos(\lambda z)\, dz \right] \cdot \frac{2UC_m}{\lambda} \sin(\lambda B)\, d\lambda \quad \text{(C4)}$$

Because of the symmetrical property of the integrand in (C4) with respect to $z$, $I_R$ can also be written as

$$I_R = \frac{4UC_m R_d}{\pi s} \int_0^{\infty} \left[ \int_0^{\infty} \frac{\sin(\lambda B)\cos(\lambda z)}{(R_d s + D_z \lambda^2)\lambda} d\lambda \right] dz \quad \text{(C5)}$$

By considering Figure 2, (C5) can be written as

$$I_R = \frac{4UC_m R_d}{\pi s} \int_0^{B} \left( \int_0^{\infty} \frac{1}{D_z} \frac{\sin(\lambda B)\cos(\lambda z)}{\lambda[\lambda^2 + (R_d s/D_z)]} d\lambda \right) dz + \frac{4UC_m R_d}{\pi s} \int_B^{\infty} \left( \int_0^{\infty} \frac{1}{D_z} \frac{\sin(\lambda B)\cos(\lambda z)}{\lambda[\lambda^2 + (R_d s/D_z)]} d\lambda \right) dz \quad \text{(C6)}$$

This equation can also be written as

$$I_R = \frac{4UC_m a}{\pi s} \left[ \int_0^{B} I_1\, dz + \int_B^{\infty} I_2\, dz \right] \quad \text{(C7)}$$

where

$$I_1 = \frac{1}{D_z} \int_0^{\infty} \frac{\sin(\lambda B)\cos(\lambda z)}{\lambda[\lambda^2 + (R_d s/D_z)]} d\lambda \qquad 0 < z < B \quad \text{(C8)}$$

$$I_2 = \frac{1}{D_z} \int_0^{\infty} \frac{\sin(\lambda B)\cos(\lambda z)}{\lambda[\lambda^2 + (R_d s/D_z)]} d\lambda \qquad B < z < \infty \quad \text{(C9)}$$

The integrals given by (C8) and (C9) can be evaluated analytically with the equation given by *Gradshteyn and Ryzhik* [1965, p. 408,equation 3.725-3]:

$$I_1 = \frac{\pi}{2R_d s} \exp\left[ -B \left( \frac{R_d s}{D_z} \right)^{1/2} \right] \cdot \cosh\left[ z \left( \frac{R_d s}{D_z} \right)^{1/2} \right] + \frac{\pi}{2R_d s} \quad \text{(C10)}$$

$$I_2 = \frac{\pi}{2R_d s} \exp\left[ -\left( \frac{R_d s}{D_z} \right)^{1/2} z \right] \sinh\left[ B \left( \frac{R_d s}{D_z} \right) \right] \quad \text{(C11)}$$

With (C10), the first integral of (C7) can be developed as

$$\int_0^{\infty} I_1\, dz = -\frac{\pi}{4R_d s} \left( \frac{D_z}{R_d s} \right)^{1/2} \cdot \left\{ \exp\left[ -2B \left( \frac{R_d s}{D_z} \right)^{1/2} \right] \right\} + \frac{\pi B}{2R_d s} \quad \text{(C12)}$$

Similarly, the second integral of (C7) can be written as

$$\int_B^{\infty} I_2\, dz = \frac{\pi}{4R_d s} \left( \frac{D_z}{R_d s} \right)^{1/2} \left\{ 1 - \exp\left[ 2B \left( \frac{R_d s}{D_z} \right)^{1/2} \right] \right\} \quad \text{(C13)}$$

Introducing (C12) and (C13) in (C7) and after some manipulations, the following expression can be obtained

$$I_R = 2BUC_m \frac{1}{s^2} \quad \text{(C14)}$$

which is exactly the same as the left-hand side of (37).

## REFERENCES

Batu, V., Time-dependent, linearized two-dimensional infiltration and evaporation from nonuniform and nonperiodic strip sources, *Water Resour. Res.*, *18*(6), 1725–1733, 1982.

Batu, V., Two-dimensional dispersion from strip sources, *J. Hydraul. Eng.*, *109*(6), 827–841, 1983.

Brigham, W. E., Mixing equations in short laboratory columns, *Soc. Pet. Eng. J.*, *14*, 91–99, 1974.

Bruch, J. C., and R. L. Street, Two-dimensional dispersion, *J. Sanit. Eng. Div. Am. Soc. Civ. Eng.*, *93*, 17–39, 1967.

Carnahan, C. L., and J. S. Remer, Nonequilibrium and equilibrium sorption with a linear sorption isotherm during mass transport through an infinite porous medium: Some analytical solutions, *J. Hydrol.*, *73*, 227–258, 1984.

Carslaw, H. S., and J. C. Jaeger, *Conduction of Heat in Solids*, 2nd ed., Clarendon, Oxford, 1959.

Chen, C. S., Analytical solutions for radial dispersion with Cauchy boundary at injection well, *Water Resour. Res.*, *23*(7), 1217–1224, 1987.

Churchill, R. V., *Fourier Series and Boundary Value Problems*, McGraw-Hill, New York, 1941.

Cleary, R. W., and M. J. Ungs, Analytical methods for ground water pollution and hydrology, *Rep. 78-WR-15*, Water Resour. Program, Princeton Univ., Princeton, N. J., 1978.

Gradshteyn, I. S., and I. W. Ryzhik, *Table of Integrals, Series, and Products*, edited by A. Jeffrey, translated from Russian by Scripta Technica, Academic, San Diego, Calif., 1965.

International Technology Corporation (IT), *GEOFLOW, Ground Water Flow and Solute Transport Computer Program, User's Manual*, Monroeville, Pa., 1986.

Javandel, I., C. Doughty, and C. F. Tsang (Eds.), *Groundwater Transport: Handbook of Mathematical Models, Water Resour. Monogr. Ser.*, vol. 10, AGU, Washington, D. C., 1984.

Kreft, A., and A. Zuber, On the physical meaning of the dispersion equation and its solution for different initial and boundary conditions, *Chem. Eng. Sci.*, *33*, 1471–1480, 1978.

Kreft, A., and A. Zuber, On the use of the dispersion model of fluid flow, *Int. J. Appl. Radiat. Isot.*, *30*, 705–708, 1979.

Lindstrom, F. T., R. Haque, V. H. Freed, and L. Boersma, Theory on the movement of some herbicides in soils: Linear diffusion and convection of chemicals in soils, *Environ. Sci. Technol.*, *1*, 561–565, 1967.

Parker, J. C., and M. T. van Genuchten, Flux-averaged and volume-averaged concentrations in continuum approaches to solute transport, *Water Resour. Res.*, *20*, 866–872, 1984*a*.

Parker, J. C., and M. T. van Genuchten, Determining transport parameters from laboratory and field tracer experiments, *Bull. 84-3*, Va. Agric. Exp. Sta., Blacksburg, 1984*b*.

Speigel, M. R., *Theory and Problems of Laplace Transforms*, Shaum's Outline Ser., McGraw-Hill, New York, 1965.

Sposito, G., and D. A. Barry, On the dagan model of solute transport in groundwater: Foundational aspects, *Water Resour. Res.*, *23*, 1867–1875, 1987.

Tang, D. E., and D. W. Peaceman, New analytical and numerical solutions for the radial convection-dispersion problem, paper presented at the Ninth Symposium on Reservoir Simulation, Soc. of Pet. Eng., San Antonio, Tex., 75–92, 1987.

van Genuchten, M. T., and W. J. Alves, Analytical solutions of the one-dimensional convective-dispersive solute transport equation, *Tech. Bull. 1661*, U. S. Dep. of Agric., Washington, D. C., 1982.

van Genuchten, M. T., and J. C. Parker, Boundary conditions for displacement experiments through short laboratory soil columns, *Soil Sci. Soc. Am. J.*, *48*, 703–708, 1984.

van Genuchten, M. T., D. H. Tan, and R. Guennelon, Some exact solutions for solute transport through soils containing large cylindrical macropores, *Water Resour. Res.*, *20*(3), 335–346, 1984.

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