

Analysis of Point-Source and Boundary-Source Solutions of One-Dimensional Groundwater Transport Equation

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Abstract: The solute transport equation is commonly used to describe the migration and fate of solutes in a groundwater flow system. Depending on the problem nature, the source of the solute may be represented as a point source term in the equation or specified as the first-type or third-type boundary condition. The solutions derived under the condition that the solute introduced into the flow system is from the boundary is herein considered as the boundary-source solutions. The solution obtained when solving the transport equation with a point-source term is considered as the point-source solution. The Laplace transform technique is employed to derive the formulas for those solutions expressed in terms of the normalized mass release rate. The underlying nature of different source release modes and the differences among those boundary-source solutions and the constant point-source solution can be easily and clearly differentiated based on the derived formulas for one-dimensional transport. The methodology could, however, be easily extended to two- and three-dimensional problems.

DOI: 10.1061/(ASCE)0733-9372(2007)133:11(1032)

CE Database subject headings: Analytical solutions; Groundwater management; Mathematical models; Solutes.

Introduction

The mathematical statement of the solute transport equation, also called the advective-dispersion equation, is generally an accepted model for describing the migration and fate of solutes in groundwater (Bedient et al. 1999). For a simplified case, the transport equation includes the processes of advective and dispersive transports. The solution of the transport equation may serve as a tool for the prediction of the spatial and temporal distribution of the solute in an aquifer, a reference to verify a numerical code, or a means to compare laboratory or field experimental results. In addition, the analytical solution coupled with an optimization algorithm is often employed to analyze tracer-test data for determining the best-fit aquifer parameters.

van Genuchten and Alves (1982) published a technical report that contains many mathematical models and associated solutions for one-dimensional solute transport in semi-infinite media or finite-length columns. The governing equations of the transport models include terms accounting for advection, diffusion and dispersion, and linear equilibrium adsorption. The effects of zero-order production and first-order decay of both the source term and the contaminant are also included in some cases. In the report, two different conditions considered to specify the boundary at

the origin (i.e., $x=0$) are the first-type (or concentration-type) and the third-type (or flux-type) boundary conditions. Derivations of the analytical solutions using the Laplace transform technique for the transport equation with the terms of zero-order production subject to first- and third-type boundary conditions were given in van Genuchten (1981). In addition, van Genuchten and Parker (1984) presented a discussion of the physical and mathematical significance of various boundary conditions applicable to one-dimensional solute transport through short soil columns. They pointed out that the use of volume-average or resident concentrations and flux-averaged or flowing concentrations is pertinent to the choice of a suitable boundary condition and corresponding analytical solution. Kreft and Zuber (1978) gave a solution for continuous injection of solutes in an infinite bed with a fixed concentration at upstream remote boundary and a hybrid pulse type initial condition at the origin. Their solution obtained by solving the transport equations with the boundary and initial conditions will be given later. These solutions were derived under the condition that the solutes introduced into the flow system are from the boundary. Therefore, they are considered as the boundary-source solutions in this study.

Instead of solving the boundary-value problem, one can obtain the solution for the transport equation using the Green's function with a constant point source in an infinite domain. Assuming that an injection rate of water per unit area is equal to Darcy's velocity, Sauty (1980) presented a solution in a dimensionless form for the transport equation with a point source of constant input located at the origin of the coordinate in an infinite medium. The same solution was also presented in Kreft and Zuber (1978) and Hunt (1978) and later given in Sun (1996) with a detailed derivation. This solution herein is referred to as the constant-point source solution.

Many analytical solutions for the solute transport equation in a one-dimensional medium can be found in the groundwater literature (e.g., Kreft and Zuber 1978; Sauty 1980; van Genuchten and Alves 1982), yet care must be taken for choosing a proper one to estimate the concentration distribution of solutes or to determine

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Note. Discussion open until April 1, 2008. Separate discussions must be submitted for individual papers. To extend the closing date by one month, a written request must be filed with the ASCE Managing Editor. The manuscript for this paper was submitted for review and possible publication on August 10, 2005; approved on June 1, 2007. This paper is part of the *Journal of Environmental Engineering*, Vol. 133, No. 11, November 1, 2007. ©ASCE, ISSN 0733-9372/2007/11-1032-1041/\$25.00.

the aquifer parameters for a specific site in engineering practice. The objective of this article is to present a methodology based on the concept of source release mode for obtaining the formulas in relation to the analytical solutions. The formulas for those solutions are derived by the Laplace transform technique and expressed in terms of the normalized mass release rate. Those formulas can be used to differentiate the differences among those analytical solutions due to different source release modes and to examine the physical character of the normalized mass release rate for the selection of those solutions. In addition, the underlying nature of different source release modes and the differences among those boundary-source solutions and the constant-point source solution can be easily and clearly differentiated based on the derived formulas.

Analytical and Approximate Solutions

One-Dimensional Solute Transport Equation

Considering a one-dimensional flow in a homogeneous and isotropic porous medium with a constant velocity along the x -direction, the advection-dispersion equation for nonreactive solute derived based on the conservation of mass is (Freeze and Cherry 1979)

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} \quad (1)$$

where $c=c(x,t)$ =solute concentration [M/L^3]; D =dispersion coefficient [L^2/T]; u =average linear velocity [L/T]; t =time; and x =spatial coordinate. For the sake of simplicity, the initial concentration is assumed zero. That is

$$c(x,0) = 0 \quad (2)$$

For a groundwater system of infinite extent in the $+x$ direction, an appropriate downstream boundary condition at $x=\infty$ is

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

Solution for First-Type Boundary Condition

If the input solute is well mixed and its concentration is continuous across the inlet boundary for a semi-infinite aquifer, the first-type boundary condition may then be applied at $x=0$ as

$$c(0,t) = c_0 \quad (4)$$

where c_0 represents a fixed concentration.

The solution of Eqs. (1)–(4) is (Lapidus and Amundson 1952; Ogata and Banks 1961)

$$c(x,t) = \frac{c_0}{2} \left[\operatorname{erfc} \left(\frac{x-ut}{\sqrt{4Dt}} \right) + \exp \left(\frac{ux}{D} \right) \operatorname{erfc} \left(\frac{x+ut}{\sqrt{4Dt}} \right) \right] \quad (5)$$

where $\operatorname{erfc}()$ =complementary error function. Introducing two dimensionless parameters, $\xi=ut/x$ and $\eta=D/ux$, Ogata and Banks (1961) plotted c/c_0 versus ξ curves under various values of η on a logarithmic probability graph using Eq. (5).

We can define a dimensionless time $t_R=ut/x$ and a dimensionless parameter $P=ux/D$, which is known as Péclet number if x is chosen as a characteristic length (Bear 1979). The Péclet number represents the ratio of the rate of transport by advection to that by dispersion (Bear 1979). Commonly, the groundwater system is

considered as under the dispersion-dominant condition when P is small and advection-dominant condition when P is large. A dimensionless concentration for Eq. (5) was written in terms of P and t_R by Sauty (1980) as

$$c_R(P,t_R) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1-t_R) \right] + \exp(P) \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1+t_R) \right] \right\} \quad (6)$$

where $c_R(=c/c_0)$ is a dimensionless concentration. Sauty (1980) also pointed out that P practically ranges between 1 and 100 for flow in aquifers.

Solution for Third-Type Boundary Condition

Specified at $x=0$, the flux-type boundary condition, which leads to conservation of mass inside the medium while the outside medium has a well-mixed concentration C_0 with a constant flow rate entering the medium, may be expressed as (Bear 1979)

$$\left(-D \frac{\partial c}{\partial x} + uc \right)_{x=0} = uc_0 \quad (7)$$

The solution of Eqs. (1)–(3) and (7) given by Lindstrom et al. (1967) is

$$c(x,t) = \frac{c_0}{2} \left\{ \operatorname{erfc} \left(\frac{x-ut}{\sqrt{4Dt}} \right) - \left(1 + \frac{ux}{D} + \frac{u^2t}{D} \right) \exp \left(\frac{ux}{D} \right) \operatorname{erfc} \left(\frac{x+ut}{\sqrt{4Dt}} \right) + \frac{4ut}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x-ut)^2}{4Dt} \right] \right\} \quad (8)$$

Note that they also gave plots of the concentration ratio c/c_0 as a function of time at a fixed x for different values of the velocity. The dimensionless concentration for Eq. (8) in terms of P and t_R can be derived as

$$c_R(P,t_R) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1-t_R) \right] - (1+P+Pt_R) \exp(P) \times \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1+t_R) \right] + 2 \left(\frac{Pt_R}{\pi} \right)^{\frac{1}{2}} \times \exp \left[-\left(\frac{P}{4t_R} \right) (1-t_R)^2 \right] \right\} \quad (9)$$

Solution for Initial and Boundary Conditions Given by Kreft and Zuber (1978)

Kreft and Zuber (1978) considered a case for solute distribution in an infinite medium when the detection is the fluid flux rather than resident fluid. They gave an initial condition for this case as

$$c(x,0) = \begin{cases} c_0 & x < 0 \\ \frac{c_0}{2} \left[1 + \frac{2D}{u} \delta(x) \right] & x = 0 \\ 0 & x > 0 \end{cases} \quad (10)$$

where $\delta(x)$ is the Dirac delta function. The upstream and downstream boundary conditions, respectively, are

$$c(-\infty, t) = c_0 \quad (11)$$

and

$$c(\infty, t) = 0 \quad (12)$$

The solution for the one-dimensional solute transport equation (Eq. (1)), subject to the initial and boundary conditions of Eqs. (10)–(12), is

$$c(x, t) = \frac{c_0}{2} \left\{ \operatorname{erfc} \left(\frac{x-ut}{\sqrt{4Dt}} \right) + \frac{2D}{u} \frac{1}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x-ut)^2}{4Dt} \right] \right\} \quad (13)$$

The dimensionless concentration of Eq. (13) in terms of P and t_R can be expressed as

$$c_R(P, t_R) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1-t_R) \right] + \left(\frac{1}{\pi P t_R} \right)^{\frac{1}{2}} \exp \left[-\left(\frac{P}{4t_R} \right) (1-t_R)^2 \right] \right\} \quad (14)$$

We define the influence function, or Green's function as

$$G(x, t; x_0, 0) = \frac{1}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x-x_0)^2}{4Dt} \right] \quad (15)$$

where x_0 denotes the location of the point source. It can be shown that (Haberman 1987)

$$\lim_{t \rightarrow 0} G(x, t; x_0, 0) = \delta(x-x_0) \quad (16)$$

Note that Kreft and Zuber (1978) published solution contains an error. When $t=0$ and with the relationships of $\operatorname{erfc}(x \rightarrow \infty)=0$, $\operatorname{erfc}(x \rightarrow -\infty)=2$, Eqs. (15), (16), it is easy to prove that Eq. (13) satisfies the conditions of Eqs. (10)–(12), while the values of u and t are finite. The equation of Kreft and Zuber (1978) is identical to Eq. (13) except that c_0 is not divided by 2. Their solution leads to a result of $2c_0$ when $x \rightarrow -\infty$ and the value of t is finite.

Solution for a Constant Point Source Condition

For a constant point source at $x=0$, the solution of Eq. (1) with a source term $m/n_e \delta(x)$ in an infinite medium can be obtained by use of Green's function (Yeh 1981; and Beck et al. 1992) as

$$c(x, t) = \int_0^t \frac{m/n_e}{\sqrt{4\pi D(t-\tau)}} \exp \left\{ -\frac{[x-u(t-\tau)]^2}{4D(t-\tau)} \right\} d\tau \quad (17)$$

where m =constant mass release rate of the point source [M/L^2]; n_e =effective porosity; and τ =dummy variable. Here, m/n_e =rate of material source entering into the groundwater system and the Green's function is the fundamental solution of the one-dimensional transport equation. Obviously, a different source release rate at the origin will have a different concentration distribution in the flow system.

Assuming that continuous mass release rate of the constant point source (m/n_e) at $x=0$ entering the flow system is equal to uc_0 , Sun (1996) derived a solution by integrating Eq. (17) as

$$c(x, t) = \frac{c_0}{2} \left[\operatorname{erfc} \left(\frac{x-ut}{\sqrt{4Dt}} \right) - \exp \left(\frac{ux}{D} \right) \operatorname{erfc} \left(\frac{x+ut}{\sqrt{4Dt}} \right) \right] \quad (18)$$

Actually, this solution was mentioned in Kreft and Zuber (1978) and Hunt (1978) and was presented in a dimensionless form in Sauty (1980) as

$$c_R(P, t_R) = 0.5 \left\{ \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1-t_R) \right] - \exp(P) \operatorname{erfc} \left[\left(\frac{P}{4t_R} \right)^{\frac{1}{2}} (1+t_R) \right] \right\} \quad (19)$$

Numerical Results

We assume that the dispersion coefficient $D=1.0$ m²/day and the average linear velocity $u=1.0$ m/day. The dimensionless concentrations (c/c_0) for analytical solutions of Eqs. (5), (8), (13), and (18) plotted against the distance x are shown in Fig. 1 at times of 2, 20, and 50 days. These results illustrate that the first-type boundary solution (Eq. (5)), gives the highest concentration, the solution of Kreft and Zuber (1978) (Eq. (13)), gives the second highest, the third-type boundary solution (Eq. (8)), the third, and the constant point source solution (Eq. (18)), yields the lowest among these four solutions. It is noteworthy from computed results that at $x=0$ and short source release period such as $t=2$ days, the first-type boundary solution maintains the fixed concentration (c/c_0) and the others give results below 1.0. The estimated c/c_0 for Kreft and Zuber's solution, the third-type boundary, and the constant point source solution are, respectively, 0.96, 0.85, and 0.68.

Fig. 2 shows the dimensionless concentrations for analytical solutions of Eqs. (5), (8), (13), and (18) plotted against the time at the origin, i.e., $x=0$. This figure reveals that the first-type boundary solution has the fixed value of $c/c_0=1$ and the highest dimensionless concentration after the time of 0.75 days among these four solutions. The solution of Kreft and Zuber (1978) has an extremely high dimensionless concentration at a very short time, rapidly drops to lowest value of $c/c_0=0.9623$ at $t=2.0$ days, and then gradually increases and approaches $c/c_0=1$ at $t=28$ days. Obviously, their solution yields extremely high dimensionless concentrations when both time and distance are very small. The dimensionless concentrations of both third-type boundary solution and constant point source solution start from zero, gradually increase, and finally reach one for the third-type boundary solution at $t=25$ days and the constant point source solution at $t=33$ days; moreover, the third-type boundary solution always has a higher concentration than the point source solution even at large dimensionless time.

Approximate Solution

It is interesting to note that only the signs of the second term on the right-hand side (RHS) of Eqs. (5) and (18) are different and the first terms on the RHS of Eqs. (5), (8), (13), and (18) are all the same. Mathematically, Eqs. (5) and (8) can be considered as the boundary source solutions, Eq. (13) as the initially distributed source solution (or hybrid pulse type solution), and Eq. (18) as a constant point source solution. Freeze and Cherry (1979) pointed out that the second term on the RHS of Eq. (5) is negligible when the dispersivity of the porous medium is large or when x and t are large. The approximate solution for Eq. (5) is expressed as (Freeze and Cherry 1979)

$$c(x, t) = \frac{c_0}{2} \left[\operatorname{erfc} \left(\frac{x-ut}{\sqrt{4Dt}} \right) \right] \quad (20)$$

that may also be considered as an approximate solution for the other three solutions mentioned above. Sauty (1980) gave a plot

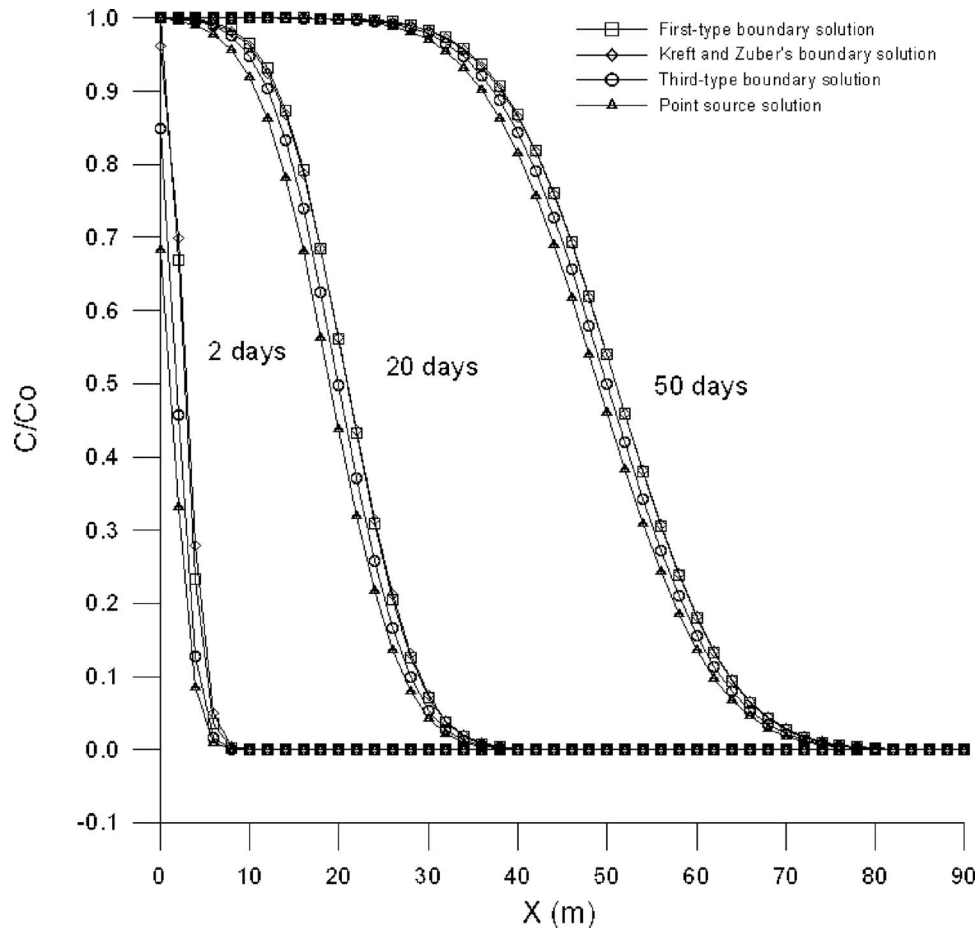


Fig. 1. Plot of dimensionless concentration versus distance for analytical solutions of the first type, third type, and Krefit and Zuber (1978) and the constant-point source solution at times of 2, 20, and 50 days. Dispersion coefficient $D=1.0 \text{ m}^2/\text{day}$ and average linear velocity $u=1.0 \text{ m/day}$.

of the dimensionless concentration curves for $P=1, 10,$ and 100 and t_R ranging from 0 to 2.5 for Eq. (6), Eq. (19), and the dimensionless form of Eq. (20). For $P=1$, Eq. (6) (dimensionless form of Eq. (5)) and Eq. (19) give quite different results, whereas for $P=100$, they are very close and the curve of Eq. (20) lies midway between them. For P greater than 10, Saaty suggested that Eq. (20) is probably acceptable, especially as P approaches 100. Besides, Ogata and Banks (1961) showed that Eq. (20) gives an error of less than 3% if compared to Eq. (5) when $ux/D > 500$. Obviously, Eq. (20) gives a good approximate result for advection-dominated transport.

Normalized Mass Release Rates for Solutions under Different Source Conditions

Formulas for Laplace Transforms

Based on two formulas in Erdelyi [1954, (5) on p. 129 and (27) on p. 146], the following relationship can be derived

$$L\left\{\frac{e^{-at}e^{-b/4t}}{\sqrt{t}}\right\} = \sqrt{\frac{\pi}{s+a}} \exp(-\sqrt{b(s+a)}) \quad (21)$$

where a and b are constants, $L\{\}$ denotes the Laplace transform, and s is a Laplace variable. Accordingly, the Laplace transform of the influence function of Eq. (17) when setting $\tau=0$ is

$$L\left\{\frac{\exp\left[\frac{-(x-ut)^2}{4Dt}\right]}{\sqrt{4\pi Dt}}\right\} = \frac{\exp\left(\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{\sqrt{4D(s+u^2/4D)}} \quad (22)$$

The formula in Spiegel [1965, (88) on p. 250] may be written in a different form as

$$L\left\{e^{b^2t} \operatorname{erfc}\left(b\sqrt{t} + \frac{a}{2\sqrt{t}}\right)\right\} = \frac{e^{-a(\sqrt{s+b})}}{\sqrt{s(\sqrt{s+b})}} \quad (23)$$

Furthermore, using the formula in Spiegel [1965, (3) on p. 243], Eq. (25) can be transformed to

$$L\left\{\operatorname{erfc}\left(b\sqrt{t} + \frac{a}{2\sqrt{t}}\right)\right\} = \frac{e^{-a(\sqrt{s+b^2+b})}}{\sqrt{s+b^2(\sqrt{s+b^2+b})}} \quad (24)$$

Normalized Mass Release Rates of Constant Point Source Solution

Taking the Laplace transform of Eq. (17), the Green's function solution (Beck et al. 1992), by aid of convolution theorem (Haberman 1987) and using the relationship of Eq. (24) yields

$$L\{c(x,t)\} = \frac{m/n_e}{\sqrt{4D}} \frac{\exp\left(\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{\sqrt{s+u^2/4D}} \quad (25)$$

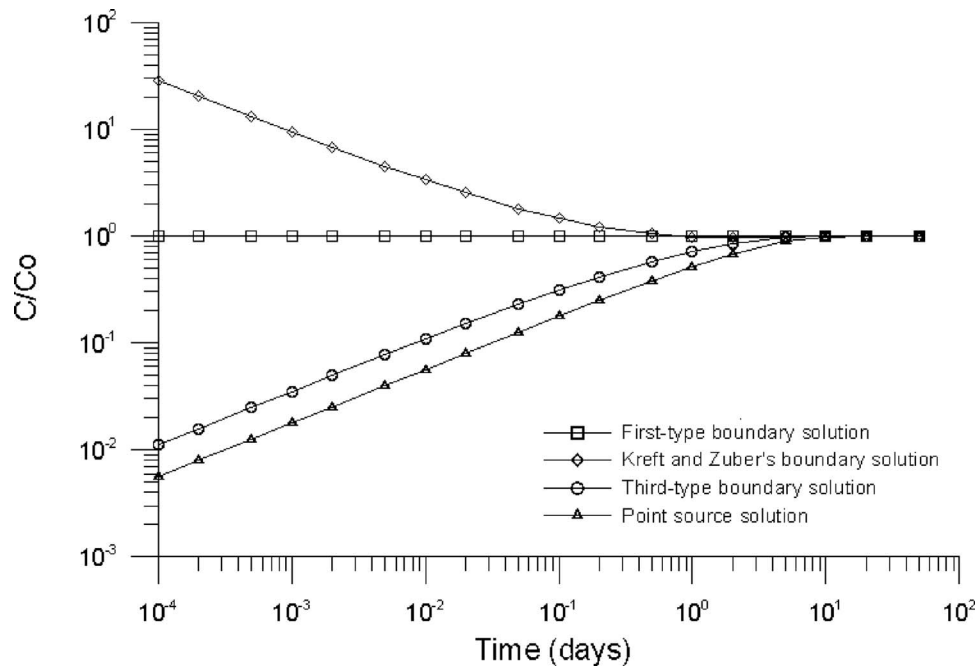


Fig. 2. Plot of dimensionless concentration versus time for analytical solutions of the first-type, third-type, and Krefit and Zuber (1978) and the constant point source solution at origin. Dispersion coefficient $D=1.0$ m²/day and average linear velocity $u=1.0$ m/day.

Application of the Laplace transform to the first term on the RHS of Eq. (18) yields

$$L\left\{\frac{c_0}{2} \operatorname{erfc}\left(\frac{x-ut}{\sqrt{4Dt}}\right)\right\} = \frac{c_0}{2} \left[\frac{\sqrt{s+u^2/4D} + \sqrt{u^2/4D} \exp\left(\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{s} \right] \quad (26)$$

Likewise, applying the Laplace transform to the second term on the RHS of Eq. (18) gives

$$L\left\{\frac{c_0}{2} \exp\left(\frac{ux}{D}\right) \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right)\right\} = \frac{c_0}{2} \left[\frac{\sqrt{s+u^2/4D} - \sqrt{u^2/4D} \exp\left(\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{s} \right] \quad (27)$$

Based on the property of linearity of the transform (Spiegel 1965) and subtracting Eq. (27) from Eq. (26), the Laplace transform of Eq. (18) becomes

$$L\{c(x,t)\} = \frac{uc_0}{\sqrt{4D}s} \frac{1}{\sqrt{s+u^2/4D}} \exp\left(\frac{xu}{D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right) \quad (28)$$

The inverse transform after setting Eq. (28) equal to Eq. (25) and using the formula in Spiegel [1965, (1) on p. 243] produces

$$\frac{m/n_e}{uc_0} = 1 \quad (29)$$

that confirms that the constant mass release rate of the point source while entering the flow system is equal to uc_0 , the advective flux of the source concentration in the flow system. This result is consistent with the one derived by Sun (1996) in the case of constant release of a point source.

Normalized Mass Release Rates of the Other Three Solutions

As discussed before, there are three different types of boundary source solutions that can be seen in the groundwater literature. Those solutions are derived under different conditions that the solutes are mainly introduced at the inlet (i.e., $x=0$) and enter the groundwater system. One might have interest to know what the mass release rates are that form those source boundaries in those three solutions. Thus, similar procedures are taken in the following to derive the normalized mass release rates expressed as the ratio of m/n_e to uc_0 for those three boundary source solutions. Physically, the derived normalized mass release rate represents the relative magnitude of the release mass rate from each inlet boundary. We define a dimensionless variable:

$$z = \sqrt{u^2 t / 4D} \quad (30)$$

where z can also be related to the Péclet number P and dimensionless time t_R as $z = \sqrt{Pt_R}/4$.

The normalized mass release rate for the first-type boundary solution [Eq. (5)], obtained by combining Eqs. (26) and (27) and using the definition of Eq. (30) gives

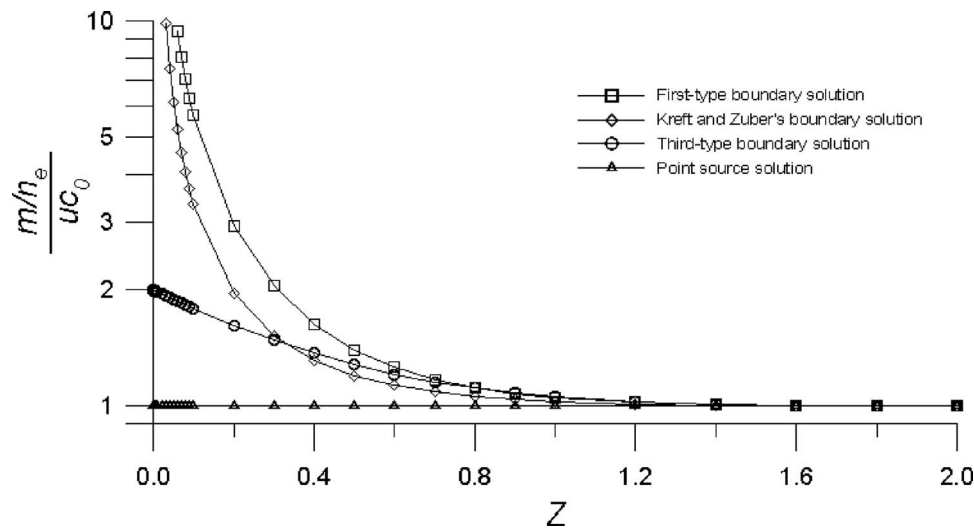


Fig. 3. Plot of normalized mass release rate versus z for the constant-point source solution and the boundary solutions of the first type, third type, and Kreft and Zuber (1978)

$$\frac{m/n_e}{uc_0} = \frac{1}{\sqrt{\pi}} \frac{e^{-z^2}}{z} + \text{erf}(z) \quad (31)$$

where $\text{erf}()$ =error function.

The detailed derivation of the normalized mass release rate for the third-type solution Eq. (9) is listed in the Appendix and the result is

$$\frac{m/n_e}{uc_0} = 1 + (2z^2 + 1)\text{erfc}(z) - \frac{2z}{\sqrt{\pi}}e^{-z^2} \quad (32)$$

The normalized mass release rate for Eq. (13), the solution of Kreft and Zuber (1978), can be derived and expressed in a similar fashion as

$$\frac{m/n_e}{uc_0} = \frac{1}{2} \left[\frac{1}{\sqrt{\pi}} \frac{e^{-z^2}}{z} + \text{erf}(z) + 1 + \frac{2D}{u^2} \delta(t) \right] \quad (33)$$

The derived formulas for those boundary solutions shown in Eqs. (31)–(33) give the values of normalized mass release rates. Those formulas provide a means to explore the physical significance after the release of the solute mass and may be used as a guide to choose appropriate boundary type for modeling the real world physical situations.

Results and Discussion

Normalized Mass Release Rates in Terms of Dimensionless Variable z

The normalized mass release rate for the constant point source solution and the boundary solutions of the first type, third type, and Kreft and Zuber (1978) are shown in Fig. 3. The vertical axis represents the mass release rate m/n_e normalized with uc_0 and the horizontal axis is the dimensionless variable z , defined in Eq. (30), which represents the dimensionless distance or time. It can be seen that mathematically, the first-type boundary solution produces the largest amount of solute mass, the solution of Kreft and Zuber (1978) the second largest, the third-type boundary solution the third, and the constant-point source solution the least. This figure gives a clear picture to depict that the first-type bound-

ary solution yields the highest concentration distribution, the solution of Kreft and Zuber (1978) the second highest, the third-type boundary solution the third, and the constant-point source solution the lowest. It also shows that the normalized values for these four solutions are very close to one at $z=1.0$; that is 1.0568 for the third-type boundary solution, 1.050 for the first-type boundary solution, and 1.038 for the solution of Kreft and Zuber (1978).

The normalized mass release rate is equal to 1.0 in the medium for the constant-point source case shown in Fig. 3. Physically, this situation may occur in aquifers at the cases of a system of waste-disposal injection wells or a surface canal having percolation with a constant solute concentration into an aquifer (Sauty 1980). Figures were also given in Sauty (1980) to illustrate these two cases for constant injection of the solute into an aquifer. The normalized values for the first-type solution and the solution of Kreft and Zuber (1978) approach infinity when z approaches zero. This implies that there are tremendous amounts of solute particles released at the origin in both cases. Therefore, the concentration at $x=0$ for the first-type boundary solution is capable of maintaining the constant value of c_0 , as indicated in Fig. 1 even within a very short period of source release time. Roughly speaking, these two solutions may be chosen when modeling the migration of leachate from old or poorly designed landfills to the groundwater system. The normalized value for the third-type boundary solution is equal to 2.0 at $z=0$ in Fig. 3. This means that the magnitude of the mass release rate into the aquifer happens to be twice that for the case of the constant mass release. Accordingly, the third-type boundary solution may be used to describe a finite amount of solutes from surface impoundment, which serves as the disposal site for hazardous and nonhazardous wastes (Bedient et al. 1999), discharged into the nearby aquifer. Physically, the impoundment provides driving forces to produce the dispersive and advective fluxes for the solute entering the adjacent aquifer.

Furthermore, examining the normalized mass release rate of Eq. (33), which is derived based on the solution of Kreft and Zuber (1978), it can be proved that the first three terms on the RHS of Eq. (33) equal the normalized mass release rate of the approximate solution of Eq. (20). The last term on the RHS of

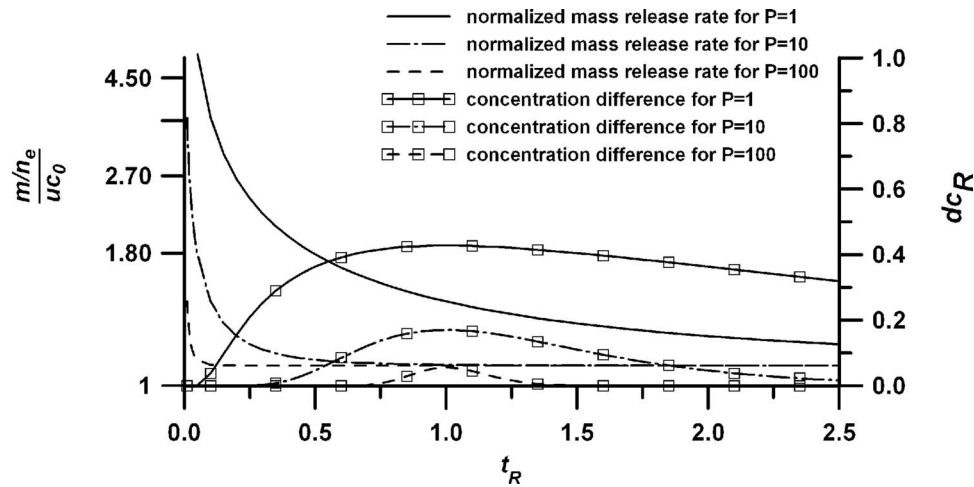


Fig. 4. Plot of normalized mass release rate versus dimensionless time t_R for the first-type boundary solution and the dimensionless concentration differences dc_R between that solution and the constant point source solution

Eq. (33), accounting for the initial condition of Eq. (10), basically is generated from a fundamental solution for a hybrid pulse type point source.

Normalized Mass Release Rates in Terms of Péclet Number and Dimensionless Time

Fig. 4 shows the normalized mass release rates for the first-type boundary solution and the dimensionless concentration differences (dc_R) between the first-type boundary solution and the constant-point source solution. Both the normalized rates and the dimensionless concentration differences are expressed in terms of the Péclet number P at values of 1, 10, and 100 and the dimensionless time t_R ranging from 0 to 2.5. For the case of $P=1$, considered as in a dispersion-dominant flow regime, the normalized values for the first-type boundary solution are very large as $t_R \rightarrow 0$ and rapidly drop as time elapses. However, the normalized rates are always greater than 1.1, even as t_R approaches 2.5. Also, the dimensionless concentration differences for t_R ranging from 0.4 to 2.5 are even higher than 0.3, while the values of the constant point source solution range from 0.091 to 0.33. Those results reveal that large errors will be made if one chooses the constant-point source solution to model the solute released from a constant concentration boundary in a mainly dispersive transport system. For $P=10$, the normalized rates are moderately large as t_R close to 0, then decrease dramatically and tend to be less than 1.04 when $t_R > 0.45$. The differences of the dimensionless concentration between the first-type boundary solution and the constant point source solution as indicated in Fig. 4 are in the range of 0.1 and 0.18 for t_R ranging from 0.65 to 1.55. Yet, these values of differences are moderate if comparing to that of $P=1$. For the situation of $P=100$, that is under the advection-dominant condition, the normalized values for the first-type boundary solution are equal to 1 for most of t_R except within the period of $t_R < 0.2$. The differences of the dimensionless concentration range between 0.03 and 0.057, which is minor, for t_R ranging from 0.9 to 1.15, while the relative difference, defined as the ratio of the difference to the dimensionless concentration of the constant-point source solution, is less than 20% at all times. It is of interest to note that the maximum concentration differences between the first-type boundary solution and the constant-point source solution occur right at $t_R=1$, no matter what the value of P is.

The normalized mass release rate for the solution of Kreft and Zuber (1978) and the dimensionless concentration difference between their solution and the constant point source solution are plotted against t_R for $P=1$, 10, and 100 in Fig. 5. The shapes of those curves are similar to those of Fig. 4. Yet, the values of maximum dc_R do not necessarily occur at $t_R=1$, though it may be very close to $t_R=1$ when P is moderately large. We need to point out when P is equal to or less than 0.1, Eq. (14) yields values of c_R over 1. For example, c_R equals 2.5661 when $t_R=0.1$ and $P=0.1$. That c_R is greater than 1.0 is due to the pulse of $c_0 D/u$ applied at $x=0$ initially. Obviously the solution of Kreft and Zuber (1978) is suitable to apply for a catastrophic event that the pollutant was massively and instantaneously released into the aquifer.

The normalized mass release rates for the third-type boundary solution and the point-source solution are drawn against t_R , ranging from 0 to 2.5, in Fig. 6 for $P=1$, 10, and 100. For $t_R \rightarrow 0$, the normalized mass release rates for $P=1$ and 10 will approach 2. These results coincide with the one being observed in Fig. 3 for the case of the third-type boundary solution. The dispersive flux is equal to the advective flux, if the normalized mass release rate, carried by the advective and dispersive processes in the flow field, is double the advective flux, i.e., uc_0 . The dispersive process of the flow system is, on the other hand, minor when $P=100$ as indicated in Fig. 6 since the normalized values are equal to 1 for most of t_R except within the period of $t_R < 0.2$. Table 1 gives the maximum differences and relative maximum differences of the dimensionless concentration between the third-type solution and the constant point source solution. It shows that the maximum relative difference is 5.98% at $t_R=1$ for $P=100$, implying the differences of the predictions between the third-type solution and constant point source solution are small. Note that for $P=1$, the normalized mass fluxes are always greater than 1, indicating that there are some contributions from the dispersive flux. The maximum relative differences of the dimensionless concentration is noticeable (33.11%) and the difference of the dimensionless concentration is fairly high (>0.15) for $t_R > 1.35$ when $P=1$, as illustrated in Fig. 6. Figs. 4–6 indicate that the influence due to the dispersive transport can be apparent in a fairly advection-dominant system.

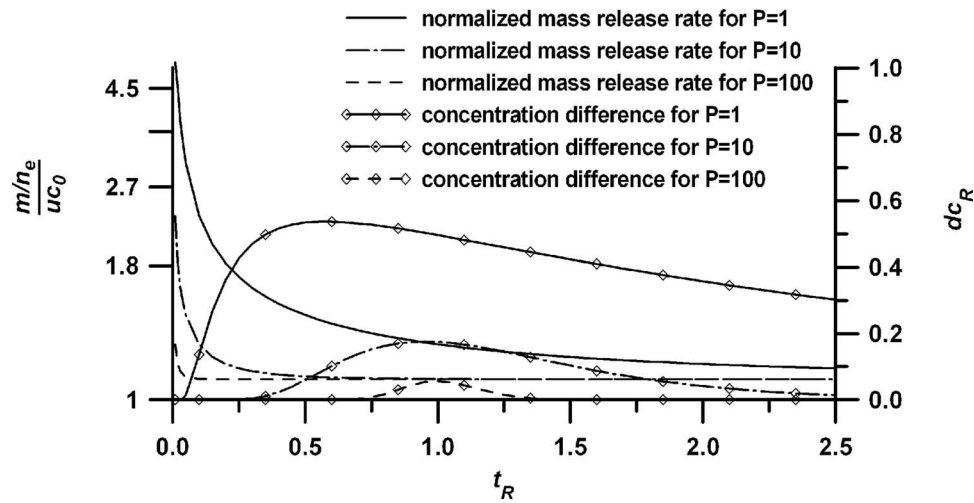


Fig. 5. Plot of normalized mass release rate versus dimensionless time t_R for the solution of Kreft and Zuber (1978) and the dimensionless concentration differences dc_R between their solution and the constant-point source solution

Summary and Conclusions

A methodology was developed based on the concept of source release mode to compare the formulas of some analytical solutions of the solute transport equation. The formulas for those solutions are expressed in terms of the normalized mass release rate and derived by the Laplace transform technique. The derived formulas can be used to differentiate between various analytical solutions due to different source release modes and to examine physical character of the normalized mass release rate for the selection of the solutions. In addition, based on the derived formulas, the underlying nature of different source release modes and the different solutions can be easily and clearly differentiated.

Four analytical solutions for the solute transport equation, subject to various boundary and initial conditions, in a one-dimensional semi-infinite or infinite medium were investigated. The boundary conditions considered herein are the first-type, third-type conditions. The initial conditions include zero concentration and the one suggested by Kreft and Zuber (1978) with a hybrid pulse type source at the origin. In addition, a solution was derived for a point source representing a constant mass rate released into the medium.

The analyzed results indicate that the first-type boundary solution yields the largest amount of solute mass, the solution of Kreft and Zuber (1978) the second, the third-type boundary solution the third, and the constant point source solution the least when z is not large. The more the amount of release solute mass, the higher the solute concentration will be. Those results are consistent with the plots of the concentration curves from the analytical solutions where the first-type boundary solution gives the highest concentration distribution, the solution of Kreft and Zuber (1978) the second, the third-type boundary solution the third, and the constant-point source the lowest.

The dimensionless concentrations of those three boundary source solutions and the constant-point source solution were also expressed as function of Péclet number and the dimensionless time. The difference of the dimensionless concentration between each boundary source solution and the constant point source solution was also computed for those three boundary solutions. Under the dispersion-dominant flow condition, the results show that the difference of the dimensionless concentration is very large when comparing the first-type boundary solution to the constant point source solution. On the other hand, the first-type solution produces a relative difference less than 20% to the constant

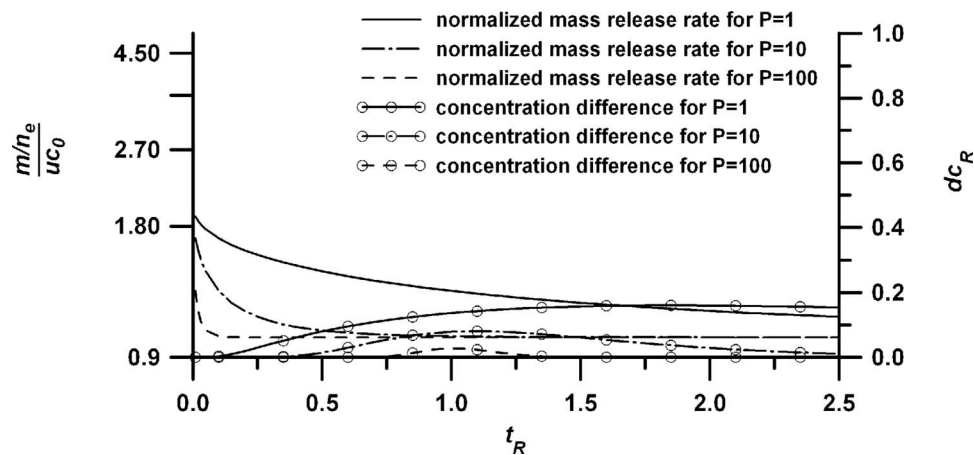


Fig. 6. Plot of normalized mass release rate versus dimensionless time t_R for the third-type boundary solution and the dimensionless concentration differences dc_R between that solution and the constant point source solution

Table 1. Maximum Difference and Relative Maximum Difference of the Dimensionless Concentration between the Third-Type Boundary Solution and Constant Point Source Solution

P	t_R	c_{R-3}	c_{R-P}	dc_R	dc_R/c_R
1	1.85	0.642	0.483	0.160	33.11%
10	1.10	0.581	0.501	0.080	16.00%
100	1.00	0.500	0.472	0.028	5.98%

Note: c_{R-3} denotes the dimensionless concentration for the third-type boundary solution, c_{R-P} denotes the dimensionless concentration for the constant point source solution, and dc_R/c_R denotes the relative difference of the dimensionless concentration.

point source solution when the flow is advection dominant. The difference of the dimensionless concentration between the third-type boundary solution and the constant-point source solution is small when the flow is advection dominant, while the difference is significant when the flow is dispersion dominant. The differences of the dimensionless concentration between the first-type boundary solution and the constant-point source solution happen to be a maximum when the dimensionless time is equal to one no matter what the value of P is.

Acknowledgments

This study was partly supported by the Taiwan National Science Council under Grant No. NSC95-2221-E-009-019. M. H. Li is acknowledged for his help in the preparation of this manuscript and figures. The writers sincerely thank three anonymous reviewers for constructive comments and suggested revisions.

Appendix. Derivations of Normalized Mass Release Rate for Third-Type Boundary Solution

The analytical solution, which contains five terms on the RHS of Eq. (8), for the solute transport equation with the third-type boundary condition expressed as the normalized mass release rate is derived here.

The normalized mass release rate for the first and second terms on the RHS of Eq. (8) has been derived as Eq. (29). That is expressed as

$$\left. \frac{m/n_e}{uc_0} \right|_{1+2} = 1 \quad (34)$$

where the index 1+2 after the vertical line represents the normalized mass release rate due to the first term plus second term (with negative sign) of the RHS of Eq. (8).

Similar to the derivation of Eq. (27), the Laplace transform of the third term on the RHS of Eq. (8) is

$$\begin{aligned} & L \left\{ -\frac{c_0 ux}{2D} \exp\left(\frac{ux}{D}\right) \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right) \right\} \\ &= -\frac{c_0 ux}{2D} \frac{\sqrt{s+u^2/4D} - \sqrt{u^2/4D}}{s} \frac{\exp\left(\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{\sqrt{s+u^2/4D}} \end{aligned} \quad (35)$$

Setting Eq. (35) equal to Eq. (25), the inverse transform based on the formula in Erdelyi [1954, (22) on p. 235] with $\beta=0$ and $\alpha=u^2/4D$ is

$$\left. \frac{m/n_e}{uc_0} \right|_3 = \frac{ux}{2D} \left[-\frac{1}{\sqrt{\pi}} \frac{e^{-z^2}}{z} + \operatorname{erfc}(z) \right] \quad (36)$$

where the index 3 after the vertical line denotes the normalized mass release rate due to the third term of the RHS of Eq. (8).

The Laplace transform for the fourth term on the RHS of Eq. (8) is

$$\begin{aligned} & L \left\{ -\frac{c_0 u^2 t}{2D} \exp\left(\frac{ux}{D}\right) \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right) \right\} \\ &= \frac{c_0 u^2}{2D} \exp\left(\frac{ux}{D}\right) L \left\{ -t \times \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right) \right\} \end{aligned} \quad (37)$$

Using the formula in Spiegel [1965, (8) on p. 243] and deriving the derivative term, one can obtain

$$\begin{aligned} & L \left\{ -t \times \operatorname{erfc}\left(\frac{x+ut}{\sqrt{4Dt}}\right) \right\} \\ &= \frac{-\exp\left(-\frac{xu}{2D} - \frac{x}{\sqrt{D}}\sqrt{s+u^2/4D}\right)}{\sqrt{s+u^2/4D}} \\ &\quad \times \left\{ \frac{x/\sqrt{4D}}{\sqrt{s+u^2/4D} \left(\sqrt{s+u^2/4D} + \frac{u}{\sqrt{4D}}\right)} \right. \\ &\quad \left. + \frac{1}{\sqrt{s+u^2/4D} \left(\sqrt{s+u^2/4D} + \frac{u}{\sqrt{4D}}\right)^2} \right. \\ &\quad \left. + \frac{u/\sqrt{4D}}{\left(s+u^2/4D\right) \left(\sqrt{s+u^2/4D} + \frac{u}{\sqrt{4D}}\right)^2} \right\} \end{aligned} \quad (38)$$

Let Eq. (37) equal (25) after substituting Eq. (38) into Eq. (37). The normalized mass release rate accounting for the first term inside the bracket of Eq. (38), which is in the fourth term of Eq. (8), can be found by using two formulas in Spiegel [1965, (1) on p. 245 and (63) on p. 248] with $a=u^2/4D$ as

$$\left. \frac{m/n_e}{uc_0} \right|_{4-1} = \frac{x}{\sqrt{4D}} [1 - \operatorname{erf}(z)] \quad (39)$$

Likewise, the normalized mass release rate accounting for the second term inside the bracket of Eq. (38) obtained based on the formula in Erdelyi [1954, (12) p. 234] with $\alpha=u/\sqrt{4D}$ is

$$\left. \frac{m/n_e}{uc_0} \right|_{4-2} = 2\sqrt{tz} \left[\frac{e^{-z^2}}{\sqrt{\pi z}} - \operatorname{erfc}(z) \right] \quad (40)$$

The normalized mass release rate accounting for the third term inside the bracket of Eq. (38) can be derived in a similar way and based on the formula in Erdelyi [1954, (11) p. 234] with $\alpha=u/\sqrt{4D}$ as

$$\left. \frac{m/n_e}{uc_0} \right|_{4-3} = \frac{\sqrt{tz}}{2} \left[\left(\frac{1}{z} - \frac{2}{\sqrt{\pi}} \right) \frac{e^{-z^2}}{z} + \left(2 - \frac{1}{z^2} \right) \operatorname{erfc}(z) \right] \quad (41)$$

Therefore, the fourth term on the RHS of Eq. (8) in terms of the normalized value can be gotten by adding Eqs. (39)–(41) as

$$\frac{m/n_e}{uc_0} \Big|_4 = \left(2z^2 + 1 - \frac{ux}{2D} \right) \operatorname{erfc}(z) - \left(1 + \frac{2z}{\sqrt{\pi}} \right) e^{-z^2} \quad (42)$$

Finally, the Laplace transform of the last term on the RHS of Eq. (8) based on the formula in Erdelyi [1954, (26) on p. 146] is expressed as

$$L \left\{ \frac{2utc_0}{\sqrt{4\pi Dt}} \exp \left[-\frac{(x-ut)^2}{4Dt} \right] \right\} \\ = \frac{uc_0}{\sqrt{4D}} \frac{\exp \left(\frac{xu}{2D} - \frac{x}{\sqrt{D}} \sqrt{s+u^2/4D} \right)}{\sqrt{s+u^2/4D}} \left(\frac{1}{s+u^2/4D} + \frac{x/\sqrt{D}}{\sqrt{s+u^2/4D}} \right) \quad (43)$$

Let Eq. (43) equal (25) and take the inverse transform. The normalized value for the last term on the RHS of Eq. (8) can be derived based on the formulas in Spiegel [1965, (3) on p. 243 and (1) on p. 245] and the formula in Spiegel [1965, (65) on p. 248] with $a=-u^2/4D$ and $b=0$ as

$$\frac{m/n_e}{uc_0} \Big|_5 = \left(1 + \frac{x}{\sqrt{\pi Dt}} \right) e^{-z^2} \quad (44)$$

Thus, the complete form of the normalized mass release rate, composed of those five terms shown in Eqs. (34), (36), (42), and (44), for the analytical solution of the transport equation with the third-type boundary condition is obtained as

$$\frac{m/n_e}{uc_0} = 1 + (2z^2 + 1) \operatorname{erfc}(z) - \frac{2z}{\sqrt{\pi}} e^{-z^2} \quad (45)$$

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