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ANALYTICAL SOLUTIONS FOR CHEMICAL TRANSPORT WITH SIMULTANEOUS ADSORPTION, ZERO-ORDER PRODUCTION AND FIRST-ORDER DECAY*[1]

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ABSTRACT

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Analytical solutions are presented for the movement of a chemical in a porous medium as influenced by linear equilibrium adsorption, zero-order production, and first-order decay. Solutions, obtained by means of Laplace transforms, are given for different initial and boundary conditions. Some typical examples, furthermore, demonstrate the effects of the two rate terms on resulting chemical concentration distributions.

INTRODUCTION

A look at recent literature shows that much has been learned about the effects of dispersion, adsorption, and decay on chemical transport in soils. Numerous analytical solutions have been developed to quantitatively describe one-dimensional convective—dispersive solute transport (Lapidus and Amundson, 1952; Ogata and Banks, 1961; Brenner, 1962; Ogata, 1964; Lindstrom et al., 1967; Gershon and Nir, 1969; Cleary and Adrian, 1973; Lindstrom and Stone, 1974a, b; Marino, 1974a, b; Selim and Mansell, 1976). Many other solutions, undoubtedly, will follow. Such solutions are needed, not only by those of us interested in actually predicting the movement of such chemicals as pesticides, fertilizers, heavy metals, or radioactive waste materials in field soils, but also by those more interested in an analysis of the different mechanisms affecting chemical transport (for example, in conjunction with column displacement studies).

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Generally, several processes will act simultaneously on a chemical constituent while being transported through the soil. This necessitates that quantitative descriptions of chemical transport include as many processes as realistically feasible. This paper presents several analytical solutions of the one-dimensional, single-ion convective—dispersive transport equation; which includes terms accounting for linear equilibrium adsorption, zero-order production and first-order decay. Solutions are derived for a semi-infinite medium and several sets of initial and soil surface boundary conditions. Some examples are given to show the effects of various terms in the transport equation on computed chemical concentration distributions.

THE GOVERNING TRANSPORT EQUATION

The partial differential equation describing one-dimensional chemical transport during transient fluid flow is taken as (see also the Notation for symbols used in this paper):

$$\frac{\partial}{\partial x}\left(\theta D\frac{\partial c}{\partial x} - qc\right) - \frac{\partial}{\partial t}(\theta c + \rho S) = \alpha\theta c + \beta\rho S - \gamma\theta \tag{1}$$

where c is the solution concentration ($\mathrm{M\,L^{-3}}$); S is the adsorbed concentration ($\mathrm{M^0}$); θ is the volumetric moisture content ($\mathrm{L^0}$); D is the dispersion coefficient ($\mathrm{L^2\,T^{-1}}$); q is the fluid flux density ($\mathrm{L\,T^{-1}}$); and ρ is the porous medium bulk density ($\mathrm{M\,L^{-3}}$). The coefficients α and β are first-order rate constants for decay, and are associated with the liquid and solid phases of the soil, respectively ($\mathrm{T^{-1}}$). The coefficient γ represents a zero-order liquid-phase source term ($\mathrm{M\,L^{-3}\,T^{-1}}$).

NOTATION

List of symbols used

A	term defined by eq. 11
B	term defined by eq. 12
c	solution concentration
$\bar{c}$	Laplace transform of c
$c_i(x)$	general initial concentration
C_i	constant initial concentration
$c_0(t)$	general surface boundary concentration
C_0	constant surface boundary concentration
C_b	background concentration
D	dispersion coefficient
E	term defined by eq. 17
F	term defined by eq. 21
G	term defined by eq. 23
H	term defined by eq. 27
I_i	terms defined in Appendix A ($i = 1,5$)

NOTATION (*continued*)

J_i	terms defined in Appendix B ($i = 1,3$)
k	distribution coefficient defined in eq. 2
M	term defined by eq. 28
N	term defined by eq. 30
P	term defined by eq. 34
q	fluid flux density
Q	term defined by eq. 38
R	retardation factor defined by eq. 4
s	Laplace transform variable
S	adsorbed concentration
t	time
u	$= v[1 + 4\mu D/v^2]^{1/2}$
U	term defined by eq. C-4
v	pore water velocity
V	term defined by eq. C-5
w	$= v[1 + 4(\mu - \lambda R)D/v^2]^{1/2}$
W	term defined by eq. C-10
x	distance
X	term defined by eq. C-14
Y	term defined by eq. C-15
Z	term defined by eq. C-20
α	first-order liquid phase decay constant
β	first-order solid phase decay constant
γ	zero-order liquid phase source term
θ	volumetric moisture content
λ	decay constant for surface boundary condition
μ	general first-order decay constant (eq. 5)
ξ	$= v[1 - 4\lambda DR/v^2]^{1/2}$
ρ	porous medium bulk density

The solution of eq. 1 requires an expression relating the adsorbed concentration (S) with the solution concentration (c). Several types of models for adsorption or ion exchange can be used, such as equilibrium and non-equilibrium models. In this study, only single-ion equilibrium transport is considered and the general adsorption isotherm is described by a linear (or linearized) isotherm of the form:

$$S = kc \tag{2}$$

where k is an empirical constant ($M^{-1} L^3$). Substitution of eq. 2 into eq. 1 gives:

$$\frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x} - qc\right) - \frac{\partial(\theta R c)}{\partial t} = \theta \mu c - \gamma\theta \tag{3}$$

where the retardation factor R is defined by:

$$R = 1 + \rho k/\theta \tag{4}$$

and where the general decay constant μ is given by

$$\mu = \alpha + \beta\rho k/\theta \tag{5}$$

Note that μ reduces to αR when α equals β.

When the volumetric moisture content and the volumetric fluid velocity remain constant in time and space (steady-state flow), the transport equation reduces to:

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - R\frac{\partial c}{\partial t} = \mu c - \gamma \tag{6}$$

where v ($= q/\theta$) is the interstitial or pore-water velocity. Eq. 6, or appropriate simplifications thereof, has been used widely in soil science, chemical and environmental engineering, and water resources. Some of the known applications are the movement of ammonium or nitrate in soils (Gardner, 1965; Reddy et al., 1976; Misra and Mishra, 1977), pesticide movement (Kay and Elrick, 1967; Van Genuchten and Wierenga, 1974), transport of radioactive waste materials (Arnett et al., 1976; Duguid and Reeves, 1977), fixation of certain iron and zinc chelates (Lahav and Hochberg, 1975), and precipitation and dissolution of gypsum (Kemper et al., 1975; Keisling et al., 1978; Glas et al., 1979) or other salts (Melamed et al., 1977). Transport equations similar to eq. 6 have also been applied to salt-water intrusion problems in coastal aquifers (Shamir and Harleman, 1966), to thermal and contaminant pollution in rivers and lakes (Cleary, 1971; Thomann, 1973; DiToro, 1974; Baron and Wajc, 1976), and to convective heat transfer problems in general (Carslaw and Jaeger, 1959; Lykov and Mikhailov, 1961).

Eq. 6 will be solved for a semi-infinite porous medium and for different initial and surface boundary conditions. In its most general form the initial condition is given by:

$$c(x,0) = c_i(x) \tag{7}$$

Two different sets of boundary conditions associated with the surface ($x = 0$) are considered: a general third-type (or flux-type) boundary:

$$\left(-D\frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = vc_0(t) \tag{8a}$$

and a general first-type (or concentration-type) boundary condition of the form:

$$c(0,t) = c_0(t) \tag{8b}$$

Several analytical solutions of eq. 6, subject to some specific initial (eq. 7) and soil surface boundary conditions (eq. 8a or eq. 8b), will now be derived.

THEORETICAL

Solutions for a third-type boundary condition

Case A1. Eq. 6 is solved subject to the following initial and boundary conditions:

$$c(x,0) = C_i \tag{9a}$$

$$\left(-D\frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = \begin{cases} vC_0 & 0 < t \leqslant t_0 \\ 0 & t > t_0 \end{cases} \tag{9b}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0 \tag{9c}$$

where C_i and C_0 are constants. Appendix A gives a complete derivation of the solution, using Laplace transforms. The solution is:

$$c(x,t) = \begin{cases} (C_0 - \gamma/\mu)\,A(x,t) + B(x,t) & 0 < t \leqslant t_0 \\ (C_0 - \gamma/\mu)A(x,t) + B(x,t) - C_0 A(x,\,t - t_0) & t > t_0 \end{cases} \tag{10}$$

where

$$A(x,t) = \frac{v}{(v+u)}\exp\left[\frac{(v-u)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] + \frac{v}{(v-u)}\exp\left[\frac{(v+u)x}{2D}\right]$$
$$\times\ \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] + \frac{v^2}{2\mu D}\exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right)\operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \tag{11}$$

$$B(x,t) = \left(\frac{\gamma}{\mu} - C_i\right)\exp\left(-\frac{\mu t}{R}\right)\left\{\frac{1}{2}\operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi RD}\right)^{1/2}\right.$$
$$\times\ \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] - \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp\left(\frac{vx}{D}\right)\left.\operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\}$$
$$+\ \frac{\gamma}{\mu} + \left(C_i - \frac{\gamma}{\mu}\right)\exp\left(-\frac{\mu t}{R}\right) \tag{12}$$

and

$$u = v(1 + 4\mu D/v^2)^{1/2} \tag{13}$$

Case A2. The steady-state solution of the same problem (case *A1*) follows immediately from eq. 10 by letting t and t_0 go to infinity:

$$c(x) = \frac{\gamma}{\mu} + \left(C_0 - \frac{\gamma}{\mu}\right)\left(\frac{2v}{v+u}\right)\exp\left[\frac{(v-u)x}{2D}\right] \tag{14}$$

Eq. 14 is hence the solution of:

$$D\frac{\mathrm{d}^2c}{\mathrm{d}x^2} - v\frac{\mathrm{d}c}{\mathrm{d}x} - \mu c + \gamma = 0 \tag{15}$$

subject to:

$$\left.\left(-D\frac{\mathrm{d}c}{\mathrm{d}x} + vc\right)\right|_{x=0} = vC_0 \tag{16a}$$

$$\frac{\mathrm{d}c}{\mathrm{d}x}(\infty) = 0 \tag{16b}$$

Note that the retardation factor R does not appear in eq. 14. This shows that the steady-state solution is not affected by adsorption.

Case A3. Eq. 10 gives the solution of eq. 6 subject to a constant initial concentration C_i. Such a constant initial concentration may not be realistic in all situations. Suppose, for example, that the porous medium was leached earlier with a feed solution having a concentration equal to some characteristic "background" value, C_b (not necessarily zero). It seems more realistic to replace the constant initial concentration in this situation with the steady-state solution, i.e. by eq. 14 with C_0 replaced by C_b. The problem now is to solve eq. 6 subject to the initial condition:

$$c(x,0) \equiv E(x) = \frac{\gamma}{\mu} + \left(C_b - \frac{\gamma}{\mu}\right)\left(\frac{2v}{v+u}\right)\exp\left[\frac{(v-u)x}{2D}\right] \tag{17}$$

and boundary conditions (9b) and (9c). Using Laplace transform techniques similar to those for case *A1* in Appendix A, the following solution is obtained:

$$c(x,t) = \begin{cases} (C_0 - C_b)A(x,t) + E(x) & 0 < t \leqslant t_0 \\ (C_0 - C_b)A(x,t) + E(x) - C_0A(x,t-t_0) & t > t_0 \end{cases} \tag{18}$$

where $A(x,t)$ is given by eq. 11 and $E(x)$ exactly by the initial condition (17).

Case A4. Eq. 6 is solved for the following initial and boundary conditions:

$$c(x,0) = C_i \tag{19a}$$

$$\left.\left(-D\frac{\partial c}{\partial x} + vc\right)\right|_{x=0} = vC_0\exp(-\lambda t) \quad \text{and} \quad \frac{\partial c}{\partial x}(\infty,t) = 0 \tag{19b, c}$$

These conditions are the same as for case *A1*, except that the pulse-type surface boundary condition (eq. 9b) is replaced by an exponentially decaying one (eq. 19b). The parameter λ in eq. 19b represents a first-order rate constant for decay (T^{-1}). The derivation for this case again follows closely the derivation given in Appendix A for case *A1*. The solution is:

$$c(x,t) = \begin{cases} C_0 F(x,t) + B(x,t) - \dfrac{\gamma}{\mu} A(x,t) & (\mu \neq \lambda R) \\ \\ C_0 G(x,t) + B(x,t) - \dfrac{\gamma}{\mu} A(x,t) & (\mu = \lambda R) \end{cases} \tag{20}$$

where $A(x,t)$ and $B(x,t)$ are given by eqs. 11 and 12, respectively, and:

$$F(x,t) = \exp(-\lambda t)\left\{\frac{v}{(v+w)} \exp\left[\frac{(v-w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] + \right.$$

$$\left. \frac{v}{(v-w)x} \exp\left[\frac{(v+w)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right]\right\} +$$

$$\frac{v^2}{2D(\mu - \lambda R)} \exp\left(\frac{vx}{D} - \frac{\mu t}{R}\right) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \tag{21}$$

$$w = v[1 + 4D(\mu - \lambda R)/v^2]^{1/2} \tag{22}$$

$$G(x,t) = \exp(-\mu t/R)\left\{\frac{1}{2} \operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \times \right.$$

$$\exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] - \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right) \exp(vx/D) \times$$

$$\left. \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\} \tag{23}$$

Case A5. This case is the same as the previous one, except that the constant initial concentration (eq. 19a) is replaced by the steady-state solution as used in case *A3*. The problem, hence, is to solve eq. 6, subject to the initial condition (17) and boundary conditions (19b) and (19c). The solution is:

$$c(x,t) = \begin{cases} C_0 F(x,t) - C_b A(x,t) + E(x) & (\lambda \neq \mu R) \\ C_0 G(x,t) - C_b A(x,t) + E(x) & (\lambda = \mu R) \end{cases} \tag{24}$$

where $F(x,t)$ and $G(x,t)$ are defined by eqs. 21 and 23, respectively, $A(x,t)$ by eq. 11 and $E(x)$ by the initial condition (17).

Solutions for a first-type boundary condition

Case B1. Eq. 6 is solved subject to the following initial and boundary conditions:

$$c(x,0) = C_i \tag{25a}$$

$$c(0,t) = \begin{cases} C_0 & 0 < t \leqslant t_0 \\ 0 & t > t_0 \end{cases} \tag{25b}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0 \tag{25c}$$

Appendix B gives a complete derivation of the analytical solution for this case, again using Laplace transforms. The solution is as follows:

$$c(x,t) = \begin{cases} (C_0 - \gamma/\mu)H(x,t) + M(x,t) & 0 < t \leqslant t_0 \\ (C_0 - \gamma/\mu)H(x,t) + M(x,t) - C_0 H(x, t - t_0) & t > t_0 \end{cases} \tag{26}$$

where

$$H(x,t) = \frac{1}{2}\exp\left[\frac{(v-u)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx - ut}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp\left[\frac{(v+u)x}{2D}\right] \times \operatorname{erfc}\left[\frac{Rx + ut}{2(DRt)^{1/2}}\right] \tag{27}$$

$$M(x,t) = \left(\frac{\gamma}{\mu} - C_i\right)\exp\left(-\frac{\mu t}{R}\right)\left\{\frac{1}{2}\operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp\left(\frac{vx}{D}\right)\operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\} + \frac{\gamma}{\mu} + \left(C_i - \frac{\gamma}{\mu}\right)\exp\left(-\frac{\mu t}{R}\right) \tag{28}$$

and where u is the same as before (eq. 13).

Case B2. The steady-state solution of case *B1* follows from eq. 26 by letting t and t_0 go to infinity:

$$c(x) = \frac{\gamma}{\mu} + \left(C_0 - \frac{\gamma}{\mu}\right)\exp\left[\frac{(v-u)x}{2D}\right] \tag{29}$$

Eq. 29 is hence the solution of eq. 15 subject to condition (16b) and the surface boundary condition $c(0) = C_0$.

Case B3. Similar to case *A3*, eq. 6 is again solved with the initial constant concentration replaced by the steady-state solution:

$$c(x,0) \equiv N(x) = \frac{\gamma}{\mu} + \left(C_b - \frac{\gamma}{\mu}\right)\exp\left[\frac{(v-u)x}{2D}\right] \tag{30}$$

where C_b, as before, represents the background concentration of the applied water before the pulse of concentration C_0 was added to the profile. The analytical solution for this case [i.e. of eq. 6 subject to conditions (30), (25b) and (25c)] is given by:

$$c(x,t) = \begin{cases} (C_0 - C_b)H(x,t) + N(x) & 0 < t \leqslant t_0 \\ (C_0 - C_b)H(x,t) + N(x) - C_0 H(x,t-t_0) & t > t_0 \end{cases} \tag{31}$$

where $H(x,t)$ is given by eq. 27 and $N(x)$ by eq. 30.

Case B4. This case is the same as case *A4*, except that the exponentially decaying boundary condition at the surface is now given by:

$$c(0,t) = C_0 \exp(-\lambda t) \tag{32}$$

The derivation of the analytical solution of eq. 6, subject to conditions (25a), (25c) and (32) is nearly identical to the derivation of the analytical solution of case *B1* given in Appendix B. The solution is:

$$c(x,t) = C_0 P(x,t) + M(x,t) - \frac{\gamma}{\mu} H(x,t) \tag{33}$$

where $H(x,t)$ and $M(x,t)$ are given by eqs. 27 and 28, respectively, and where:

$$P(x,t) = \exp(-\lambda t)\left\{\frac{1}{2}\exp\left[\frac{(v-w)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx - wt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp\left[\frac{(v+w)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx + wt}{2(DRt)^{1/2}}\right]\right\} \tag{34}$$

with w given by eq. 22.

Case B5. The last problem considered is again analogous to case *A5*. Eq. 6 is solved, subject to the steady-state-type initial concentration of case *B3* (eq. 30), an exponentially decaying surface boundary condition (eq. 32), and for a semi-infinite medium (eq. 25c). The analytical solution for this case is:

$$c(x,t) = C_0 P(x,t) - C_b H(x,t) + N(x) \tag{35}$$

where $P(x,t)$, $H(x,t)$ and $N(x)$ are given by eqs. 34, 27 and 30, respectively.

Limiting cases and some results

The analytical solutions given thus far were derived for non-zero values of the parameters γ and μ. In many situations, one or both of these parameters will be zero. Mathematically, the simplest case arises when the zero-order source term (γ) vanishes. The transport equation reduces then to:

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - R\frac{\partial c}{\partial t} = \mu c \tag{36}$$

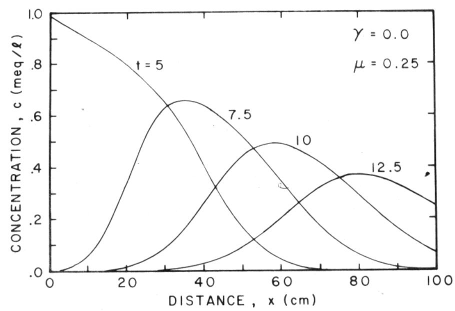
All previous solutions of eq. 6 now reduce to solutions of eq. 36 by simply setting the parameter γ equal to zero in the different expressions. For example, the solution of eq. 36 subject to initial condition (9a) and boundary conditions (9b) and (9c) follows immediately from case *A1* by setting $\gamma = 0$ in eqs. 10 and 12. Hence the solution is:

$$c(x,t) = \begin{cases} C_0A(x,t) + C_iQ(t) - C_iG(x,t) & 0 < t \leqslant t_0 \\ C_0A(x,t) + C_iQ(t) - C_iG(x,t) - C_0A(x,t-t_0) & t > t_0 \end{cases} \tag{37}$$

where $A(x,t)$ and $G(x,t)$ are given by eqs. 11 and 23, respectively, and where:

$$Q(t) = \exp(-\mu t/R) \tag{38}$$

The analytical solution (37) was given earlier by Lindstrom and Oberhettinger (1975), and for $C_i = 0$ and $t \leqslant t_0$ by Parlange and Starr (1978). To provide for a better presentation of subsequent results, some curves based on solution (37) are shown in Fig. 1. Results were obtained for the following parameter values: $v = 25\,\text{cm day}^{-1}$; $D = 37.5\,\text{cm}^2\,\text{day}^{-1}$; $\mu = 0.25\,(\text{day}^{-1})$, $R = 3$; $t_0 = 5$ (days); $C_i = 0$ and $C_0 = 1$ (meq l^{-1}). Note that the peak solute concentration decreases when the 5-day-long pulse travels through the profile. Because of decay also the total amount of salt in the profile (i.e. the area under the curves) decreases with time.



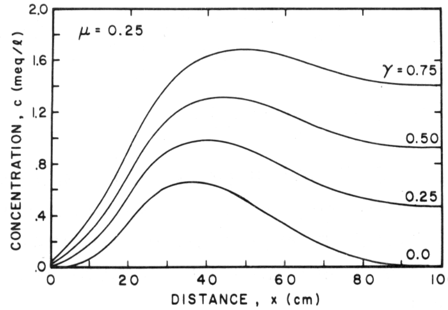


Fig. 1. Calculated concentration distributions at different times after applying a 5-day long solute pulse to a semi-infinite medium. Calculated curves are based on eq. 37.

Fig. 2. Effect of the zero-order source term on calculated solute distributions after 7.5 days ($t_0 = 5$). Calculated curves are based on eq. 10.

Fig. 2 shows the effect of the zero-order source term (γ) on the calculated solute distributions after 7.5 days, again for a pulse length (t_0) of 5 days. The remaining parameters have the same values as before. The curve labelled $\gamma = 0$ in Fig. 2 is hence the same as the curve labelled $t = 7.5$ in Fig. 1. The curves in Fig. 2 are based on eq. 10. It is evident that the source term leads to an increase in concentration over the entire depth of the medium, but especially away from the surface. After reaching a maximum, the concentration levels off to a constant value when x increases. This constant value is determined by the magnitudes of the rate parameters γ and μ, and is given by the expression:

$$c(t) = \gamma/\mu + (C_i - \gamma/\mu)\exp(-\mu t/R) \tag{39}$$

Eq. 39 is simply the solution of eq. 6 for $D = 0$, $v = 0$, and initial condition (9a).

The effect of the parameter μ on the calculated distributions after 7.5 days and with t_0 again set at 5 days is shown in Fig. 3. The different parameters are again the same as before, except that the zero-order source term is now fixed at 0.5 (meq l^{-1} day^{-1}). The curve labelled $\mu = 0.5$ is therefore the same as the curve labelled $\gamma = 0.25$ in Fig. 2. When μ increases, i.e. when degradation increases, the concentrations in the profile clearly decrease in value. The concentration is maximum when μ becomes zero. Inspection of the analytical solution (eq. 10) shows that the solution does not hold when μ becomes zero because of a division by zero. This same problem occurs with all other solutions presented in the theoretical section. The governing transport equation for $\mu = 0$ reduces to:

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - R\frac{\partial c}{\partial t} = -\gamma \tag{40}$$

Analytical solutions of eq. 40 may be obtained from the solutions of eq. 6 by rearranging certain terms in the solutions and subsequent application of l'Hopital's rule. Alternatively, one may apply Laplace transform techniques directly to eq. 40 itself and its associated initial and boundary conditions.

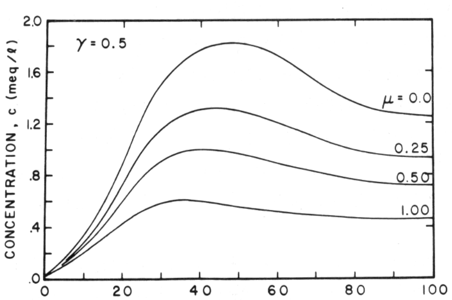


Fig. 3. Effect of the first-order decay constant on calculated solute distributions after 7.5 days ($t_0 = 5$). Calculated curves for $\mu > 0$ are based on eq. 10; the curve labelled $\mu = 0$ is based on eq. C-3.

Appendix C lists the different analytical solutions of eq. 40, using initial and boundary conditions which are similar to those used for cases *A1*—*A5* and *B1*—*B5* before. The curve labelled $\mu = 0$ in Fig. 3 was obtained with the analytical solution of case *C1* in Appendix C (eq. C-3).

Fig. 4, finally, shows some curves based on eq. 18, i.e. for the steady-state initial condition (eq. 17 with $C_b = 0$), and for a continuous feed solution at $x = 0$ ($t < t_0$ in eq. 18). The values of the remaining parameters are again the same as before, except that $\gamma = 0.25$ (meq l^{-1} day^{-1}) and $\mu = 0.50$ (day^{-1}). The curves in Fig. 4 are bounded by the initial condition and the steady-state solution for $t \to \infty$ (eq. 14 with $C_0 = 1$). These two boundary curves converge to γ/μ when x increases.

All curves in Figs. 1—4 were obtained for a third or flux-type boundary condition at the soil surface (eq. 8a). Slightly different results may be expected when this boundary condition is replaced by a first-type (or constant concentration) boundary condition (eq. 8b), especially near the soil surface boundary and close to the calculated concentration fronts. The effect of the type of boundary condition used is most significant for large values of D/v.

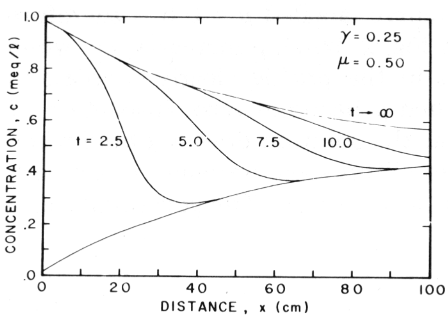


Fig. 4. Calculated concentration profiles based on eq. 18 with $t < t_0$. The curve labelled $t \to \infty$ represents the steady-state solution given by eq. 14.

CONCLUDING REMARKS

Several analytical solutions have been developed for the movement of a chemical in a one-dimensional semi-infinite system. The governing transport equation includes terms accounting for linear equilibrium adsorption, zero-order production, and first-order decay. All solutions also hold for the limiting case when the zero-order production term becomes zero. When, on the other hand, the first-order decay coefficient becomes zero, the solutions have to be modified accordingly. Appendix C gives a list of these modified analytical solutions.

The analytical solutions given in this paper may be used to predict the movement of various chemicals in field soils. In addition, the solutions should be useful for those more interested in a study of the actual chemical transport mechanisms; for example, when analyzing data obtained from miscible displacement experiments.

APPENDIX A — ANALYTICAL SOLUTION FOR CASE $A1$

This Appendix gives a derivation of the analytical solution of the following set of equations:

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - R\frac{\partial c}{\partial t} = \mu c - \gamma \tag{A-1}$$

$$c(x,0) = C_{\mathrm{i}} \tag{A-2}$$

$$\left(-D\frac{\partial c}{\partial x} + vc\right)\Bigg|_{x=0} = \begin{cases} vC_0 & 0 < t \leqslant t_0 \\ 0 & t > t_0 \end{cases} \tag{A-3}$$

$$\frac{\partial c}{\partial x}(\infty,t) = 0 \tag{A-4}$$

The solution can be obtained by means of Laplace transforms. The Laplace transform of c with respect to t is defined by:

$$\bar{c} = \bar{c}(x,s) = \int_0^\infty \exp(-st)c(x,t)\mathrm{d}t \tag{A-5}$$

The Laplace transform of (A-1) which satisfies the initial condition (A-2) is:

$$\frac{D}{R}\frac{\partial^2 \bar{c}}{\partial x^2} - \frac{v}{R}\frac{\partial \bar{c}}{\partial x} - \left(s + \frac{\mu}{R}\right)\bar{c} = -\frac{\gamma}{Rs} - C_{\mathrm{i}} \tag{A-6}$$

The transforms of eqs. A-3 and A-4 take the form:

$$\left(-D\frac{\partial \bar{c}}{\partial x} + v\bar{c}\right)\Bigg|_{x=0} = vC_0[1 - \exp(-t_0 s)] \tag{A-7}$$

$$\frac{\partial \bar{c}}{\partial x}(\infty,s) = 0 \tag{A-8}$$

The direct solution of eqs. A-6—A-8 is:

$$\bar{c}(x,s) = \frac{\dfrac{v}{D}\left(C_0 - \dfrac{\gamma}{\mu}\right)\exp\left[\dfrac{vx}{2D} - x\left(\dfrac{v^2}{4D^2} + \dfrac{s+\mu/R}{D/R}\right)^{1/2}\right]}{s\left[\dfrac{v}{2D} + \left(\dfrac{v^2}{4D^2} + \dfrac{s+\mu/R}{D/R}\right)^{1/2}\right]} -$$

$$\frac{\dfrac{vC_0}{D}\exp(-t_0 s)\exp\left[\dfrac{vx}{2D} - x\left(\dfrac{v^2}{4D^2} + \dfrac{s+\mu/R}{D/R}\right)^{1/2}\right]}{s\left[\dfrac{v}{2D} + \left(\dfrac{v^2}{4D^2} + \dfrac{s+\mu/R}{D/R}\right)^{1/2}\right]} +$$

$$\frac{\frac{v}{D}\left(\frac{\gamma}{\mu}-C_{\mathrm{i}}\right)\exp\left[\frac{vx}{2D}-x\left(\frac{v^2}{4D^2}+\frac{s+\mu/R}{D/R}\right)^{1/2}\right]}{(s+\mu/R)\left[\frac{v}{2D}+\left(\frac{v^2}{4D^2}+\frac{s+\mu/R}{D/R}\right)^{1/2}\right]}+$$

$$\frac{\gamma/R}{s(s+\mu/R)}+\frac{C_{\mathrm{i}}}{s+\mu/R} \tag{A-9}$$

The inverse Laplace transform of the first term in eq. A-9 can be obtained by first letting $p = s$, $h = v/(2D)$, $\kappa = D/R$, and $\alpha = \mu/R + v^2/(4DR)$ in eq. 31 of Appendix A of Carslaw and Jaeger (1959), and subsequently using $a = -\mu/R - v^2/(4DR)$ in equation (29.2.12) of Abramowitz and Stegun (1970). The following expression was obtained for this term:

$$I_1(x,t) = (C_0 - \gamma/\mu)\,A(x,t) \tag{A-10}$$

where $A(x,t)$ is given by eqs. 11 and 13 in the text.

The inverse of the second term in eq. A-9 follows immediately from the first term and eq. A-10 by making use of equation (29.2.15) of Abramowitz and Stegun (1970):

$$I_2(x,t) = \begin{cases} 0 & 0 < t \leqslant t_0 \\ -C_0 A(x,t-t_0) & t > t_0 \end{cases} \tag{A-11}$$

The inverse transform of the third term in eq. A-9 may be obtained by first considering eq. A-1 without the two rate terms, i.e.:

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - R\frac{\partial c}{\partial t} = 0 \tag{A-12}$$

The Laplace transform solution of this equation subject to the same initial and boundary conditions as before, but with $C_{\mathrm{i}} = 0$ in eq. A-2, and with $C_0 = 1$ and $t_0 \to \infty$ in eq. A-3 (i.e. a continuous feed solution), is given by:

$$\bar{c}(x,s) = \frac{\frac{v}{D}\exp\left[\frac{vx}{2D}-x\left(\frac{v^2}{4D^2}+\frac{s+\mu/R}{D/R}\right)^{1/2}\right]}{s\left[\frac{v}{2D}+\left(\frac{v^2}{4D^2}+\frac{s}{D/R}\right)^{1/2}\right]} \tag{A-13}$$

The direct solution of eq. A-12 subject to these same initial and boundary conditions, however, is known (Lindstrom et al., 1967):

$$c(x,t) = \frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi R D}\right)^{1/2} \exp\left[-\frac{(Rx-vt)^2}{4DRt}\right] -$$

$$\frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp(vx/D)\,\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \qquad \text{(A-14)}$$

Eq. A-14 is hence the inverse transform of eq. A-13. Application of equation (29.2.12) of Abramowitz and Stegun (1970) to eqs. A-13 and A-14 leads now directly to the Laplace inverse of the third term in eq. A-9:

$$I_3(x,t) = \left(\frac{\gamma}{\mu} - C_i\right)\exp\left(-\frac{\mu t}{R}\right)\left\{\frac{1}{2}\,\mathrm{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \right.$$

$$\left(\frac{v^2 t}{\pi R D}\right)^{1/2} \exp\left[-\frac{(Rx-vt)^2}{4DRt}\right] -$$

$$\left.\frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp(vx/D)\mathrm{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right]\right\} \qquad \text{(A-15)}$$

The inverse transforms of the fourth and fifth terms in eq. A-9 follow from equations (29.3.12) and (29.3.8) of Abramowitz and Stegun (1970):

$$I_4(x,t) = \frac{\gamma}{\mu}\,[1 - \exp(-\mu t/R)] \qquad \text{(A-16)}$$

$$I_5(x,t) = C_i \exp(-\mu t/R) \qquad \text{(A-17)}$$

The inverse transform of eq. A-9, which is the solution of eqs. A-1—A-4, is hence given by (see also eqs. 10—13):

$$c(x,t) = I_1(x,t) + I_2(x,t) + I_3(x,t) + I_4(x,t) + I_5(x,t) \qquad \text{(A-18)}$$

APPENDIX B — ANALYTICAL SOLUTION FOR CASE *B1*

The governing equations for this case are the same as those for case *A1* in Appendix A, except that eq. A-3 has to be replaced by:

$$c(0,t) = \begin{cases} C_0 & 0 < t \leqslant t_0 \\ 0 & t > t_0 \end{cases} \qquad \text{(B-1)}$$

The Laplace transform of eq. B-1 is:

$$\bar{c}(0,s) = \frac{C_0}{s}\exp(-t_0 s) \qquad \text{(B-2)}$$

The Laplace transform solution for the present case hence follows by solving eqs. A-6, A-8 and B-2. The solution is:

$$\bar{c}(x,s) = \frac{1}{s}\left(C_0 - \frac{\gamma}{\mu}\right)\exp\left[\frac{vx}{2D} - x\left(\frac{v^2}{4D^2} + \frac{s+\mu/R}{D/R}\right)^{1/2}\right] -$$

$$\frac{C_0}{s}\exp(-t_0 s)\exp\left[\frac{vx}{2D} - x\left(\frac{v^2}{4D^2} + \frac{s+\mu/R}{D/R}\right)^{1/2}\right] + \frac{(\gamma/\mu - C_i)}{(s+\mu/R)} \times$$

$$\exp\left[\frac{vx}{2D} - x\left(\frac{v^2}{4D^2} + \frac{s+\mu/R}{D/R}\right)^{1/2}\right] + \frac{\gamma/R}{s(s+\mu/R)} + \frac{C_i}{s+\mu/R} \qquad \text{(B-3)}$$

The inverse Laplace transform of the first term in eq. B-3 can be obtained by first letting $p = s$, $h = v/(2D)$, $\kappa = D/R$, and $\alpha = \mu/R + v^2/(4DR)$ in equation (19) of Appendix A of Carslaw and Jaeger (1959), and subsequently using $a = -\mu/R - v^2/(4DR)$ in equation (29.2.12) of Abramowitz and Stegun (1970). This results in the following inverse transform of the first term in eq. B-3:

$$J_1(x,t) = (C_0 - \gamma/\mu)\, H(x,t) \qquad \text{(B-4)}$$

where $H(x,t)$ is given by eq. 26. The inverse of the second term in eq. B-3 follows again directly from the first term and eq. B-4 by using equation (29.2.15) of Abramowitz and Stegun (1970):

$$J_2(x,t) = \begin{cases} 0 & 0 < t \leqslant t_0 \\ -C_0\, H(x,t-t_0) & t > t_0 \end{cases} \qquad \text{(B-5)}$$

The inverse transform of the third term in eq. B-3 follows again by making use of equation (19) of Carslaw and Jaeger (1959) and equation (29.2.12) of Abramowitz and Stegun (1970). By first letting $p = s$, $\kappa = D/R$, and $\alpha = v^2/(4DR)$ in the equation of Carslaw and Jaeger, and subsequently using $-\mu/R - v^2/(4DR)$ for a in the equation of Abramowitz and Stegun, the following expression for the inverse of the third term in eq. B-3 results:

$$J_3(x,t) = \left(\frac{\gamma}{\mu} - C_i\right)\exp(-\mu t/R)\left\{\frac{1}{2}\operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \right.$$

$$\left.\exp(vx/D)\operatorname{erfc}\left[\frac{Rx+vt}{2(DRt)^{1/2}}\right]\right\} \qquad \text{(B-6)}$$

The inverse transforms of the fourth and fifth terms in eq. B-3 are already given by eqs. A-16 and A-17 of Appendix A. The inverse transform of eq. B-3, which is hence the solution of the present problem, is therefore (see also eqs. 26—28):

$$c(x,t) = J_1(x,t) + J_2(x,t) + J_3(x,t) + I_4(x,t) + I_5(x,t) \qquad \text{(B-7)}$$

APPENDIX C — ANALYTICAL SOLUTIONS FOR ZERO-ORDER PRODUCTION ONLY

This Appendix presents solutions of:

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} + \gamma \tag{C-1}$$

for various initial and boundary conditions. The initial and boundary conditions are the same as for cases $A1$—$A5$ and $B1$—$B5$, except that $\mu \to 0$ in the initial conditions of cases $A3$, $A5$, $B3$ and $B5$, and that the semi-infinite system is more correctly described by:

$$\left.\frac{\partial c}{\partial x}\right|_{x\to\infty} = \text{(finite)} \qquad (t \geqslant 0) \tag{C-2}$$

Eq. C-2 requires that the concentration gradient remains finite when x goes to infinity. All solutions were obtained by Laplace transform techniques. Details of the derivation are omitted.

Case C1. The solution of eq. C-1 subject to conditions (9a), (9b) and (C-2) is:

$$c(x,t) = \begin{cases} C_i + (C_0 - C_i)\,U(x,t) + V(x,t) & 0 < t \leqslant t_0 \\ C_i + (C_0 - C_i)\,U(x,t) + V(x,t) - C_0\,U(x,t-t_0) & t > t_0 \end{cases} \tag{C-3}$$

where

$$U(x,t) = \frac{1}{2}\,\text{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \left(\frac{v^2 t}{\pi DR}\right)^{1/2} \exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] - \frac{1}{2}\left(1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right)\exp(vx/D)\,\text{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \tag{C-4}$$

$$V(x,t) = \frac{\gamma}{R}\left\{t - \left(\frac{t}{2} - \frac{Rx}{2v} - \frac{DR}{2v^2}\right)\text{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \left(\frac{t}{4\pi DR}\right)^{1/2} \times \left(Rx + vt + \frac{2DR}{v}\right)\exp\left[-\frac{(Rx - vt)^2}{4DRt}\right] + \left[\frac{t}{2} - \frac{DR}{2v^2} + \frac{(Rx + vt)^2}{4DR}\right] \times \exp(vx/D)\,\text{erfc}\left[\frac{(Rx + vt)}{2(DRt)^{1/2}}\right]\right\} \tag{C-5}$$

Case C2. The steady-state solution of case *C1* ($\partial c/\partial t = 0$ in eq. C-1) follows from eq. C-3 by letting t and t_0 go to infinity:

$$c(x) = C_0 + \gamma(vx + D)/v^2 \tag{C-6}$$

Case C3. The solution of eq. C-1 subject to the initial concentration:

$$c(x,0) = C_b + \gamma(vx + D)/v^2 \tag{C-7}$$

and boundary conditions (9b) and (C-2), is:

$$c(x,t) = \begin{cases} C_b + (C_0 - C_b)U(x,t) + \dfrac{\gamma(vx + D)}{v^2} & 0 < t \leqslant t_0 \\ C_b + (C_0 - C_b)U(x,t) + \dfrac{\gamma(vx + D)}{v^2} - C_0\, U(x, t - t_0) & t > t_0 \end{cases} \tag{C-8}$$

where $U(x,t)$ is given by eq. C-4.

Case C4. The solution of eq. C-1 subject to conditions (19a), (19b) and (C-2) is:

$$c(x,t) = C_i - C_i U(x,t) + C_0 W(x,t) + V(x,t) \tag{C-9}$$

where $U(x,t)$ and $V(x,t)$ are given by eqs. C-4 and C-5, respectively, and where:

$$\begin{aligned} W(x,t) = \exp(-\lambda t)\Bigg\{ & \frac{v}{(v+\xi)} \exp\left[\frac{(v-\xi)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx - \xi t}{2(DRt)^{1/2}}\right] + \\ & \frac{v}{(v-\xi)} \exp\left[\frac{(v+\xi)x}{2D}\right] \operatorname{erfc}\left[\frac{Rx + \xi t}{2(DRt)^{1/2}}\right]\Bigg\} - \\ & \frac{v^2}{2\lambda DR} \exp(vx/D) \operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \end{aligned} \tag{C-10}$$

with

$$\xi = v[1 - 4\lambda DR/v^2]^{1/2} \tag{C-11}$$

Case C5. The solution of eq. C-1 subject to conditions (C-7), (19b) and (C-2) is:

$$c(x,t) = C_b - C_b U(x,t) + C_0 W(x,t) + \gamma(vx + D)/v^2 \tag{C-12}$$

where $U(x,t)$ and $W(x,t)$ are given by eqs. C-4 and C-10, respectively.

Case D1. The solution of eq. C-1 subject to conditions (25a), (25b) and (C-2) is:

$$c(x,t) = \begin{cases} C_i + (C_0 - C_i)\, X(x,t) + Y(x,t) & 0 < t \leqslant t_0 \\ C_i + (C_0 - C_i)\, X(x,t) + Y(x,t) - C_0\, X(x,t-t_0) & t > t_0 \end{cases} \tag{C-13}$$

where

$$X(x,t) = \frac{1}{2}\operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp(vx/D)\operatorname{erfc}\left[\frac{Rx + vt}{2(DRt)^{1/2}}\right] \tag{C-14}$$

$$Y(x,t) = \frac{\gamma}{R}\left\{t + \frac{(Rx - vt)}{2v}\operatorname{erfc}\left[\frac{Rx - vt}{2(DRt)^{1/2}}\right] - \frac{(Rx + vt)}{2v}\exp(vx/D)\operatorname{erfc}\left[\frac{(Rx + vt)}{2(DRt)^{1/2}}\right]\right\} \tag{C-15}$$

Case D2. The steady-state solution of case *D1* ($\partial c/\partial t = 0$ in eq. C-1) follows from eq. C-13 by letting t and t_0 go to infinity:

$$c(x) = C_0 + \gamma x/v \tag{C-16}$$

Case D3. The solution of eq. C-1 subject to the initial condition:

$$c(x,0) = C_b + \gamma x/v \tag{C-17}$$

and boundary conditions (25b) and (C-2) is:

$$c(x,t) = \begin{cases} C_b + (C_0 - C_b)X(x,t) + \gamma x/v & 0 < t \leqslant t_0 \\ C_b + (C_0 - C_b)X(x,t) + \gamma x/v - C_0 X(x,t-t_0) & t > t_0 \end{cases} \tag{C-18}$$

where $X(x,t)$ is given by eq. C-14.

Case D4. The solution of eq. C-1 subject to conditions (25a), (32) and (C-2) is:

$$c(x,t) = C_i - C_i X(x,t) + C_0 Z(x,t) + Y(x,t) \tag{C-19}$$

where $X(x,t)$ and $Y(x,t)$ are given by eqs. C-14 and C-15, respectively, and where:

$$Z(x,t) = \exp(-\lambda t)\left\{\frac{1}{2}\exp\left[\frac{(v-\xi)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx - \xi t}{2(DRt)^{1/2}}\right] + \frac{1}{2}\exp\left[\frac{(v+\xi)x}{2D}\right]\operatorname{erfc}\left[\frac{Rx + \xi t}{2(DRt)^{1/2}}\right]\right\} \tag{C-20}$$

with ξ given by eq. C-11.

Case D5. The solution of eq. C-1 subject to conditions (C-17), (32) and (C-2) is:

$$c(x,t) = C_b - C_b X(x,t) + C_0 Z(x,t) + \gamma x/v \tag{C-21}$$

where $X(x,t)$ and $Z(x,t)$ are given by eqs. C-14 and C-20, respectively.

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