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AN ANALYTICAL SOLUTION FOR PREDICTING SOLUTE TRANSPORT DURING PONDED INFILTRATION

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An analytical solution is presented for one-dimensional solute transport in soil during ponded infiltration. The pore-water velocity $v = q/\theta$ in the convection-dispersion transport equation was obtained by assuming that the water flux density q in the soil can be calculated with the Green-Ampt infiltration model, $q = a + b/I$, in which a and b are constants and I is the cumulative infiltration rate evaluated using Philip's two-term infiltration equation. The water content θ was approximated by the saturated water content, θ_s. Through an appropriate transformation, the solute transport equation for transient unsaturated flow conditions was linearized and solved analytically for a general initial concentration profile given by an arbitrary number of straight line segments. The solution compared well with more complete numerical solutions of the transport problem, as well as with several experimental data sets.

Many numerical techniques have been developed in recent years for the purpose of providing comprehensive quantitative descriptions of agrochemical transport in soils. While numerical methods can be applied to a wide variety of soil and water flow conditions, they generally require extensive input information that is not always readily available. Moreover, numerical solutions sometimes exhibit undesired numerical oscillations and nonphysical dispersion, especially when steep concentration fronts exist such as is the case during ponded infiltration in initially very dry, coarse-textured soils. Hence, analytical solutions remain useful tools in a number of applications, including the simulation of simplified transport scenarios in the field, carrying out sensitivity analyses, estimation of important soil-hydraulic or solute transport parameters, and verification of the accuracy of numerical solutions. Compared with numerical models, analytical solutions often provide more insight into the conceptual behavior of the system being studied.

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In this paper we develop an approximate analytical solution for simulating solute transport in unsaturated soil during ponded infiltration of water and a dissolved tracer. The solution was derived through an appropriate variable transformation of a transport model that uses for the water flux density, q, a combination of the infiltration models of Green and Ampt (1911) and Philip (1969). The proposed model improves upon previous approximate solutions (Warrick et al. 1971; De Smedt and Wierenga 1978), which either assumed q to be a constant (equal to the saturated hydraulic conductivity) or calculated q independently, using numerical techniques. The proposed solution will be tested by means of comparisons with numerical solutions, previously published approximate analytical solutions, and experimental data.

MATHEMATICAL PROBLEM

The partial differential equation describing one-dimensional convective-dispersive chemical transport in soils is given by

$$\frac{\partial(\rho s)}{\partial t} + \frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z}\right) - \frac{\partial qc}{\partial z} \qquad (1)$$

where c is the solution concentration (ML^{-3}), s is the adsorbed concentration (MM^{-1}), θ is the volumetric water content (L^3L^{-3}), D is the dispersion coefficient (L^2T^{-1}), q is the volumetric flux density (LT^{-1}), ρ is the bulk density (ML^{-3}), z is the distance from the soil surface (L), and t is time (T). For simplicity, no production and decay reactions are considered here. The adsorption isotherm is described by a linear (or linearized) equation of the form

$$s = kc \qquad (2)$$

where k is an empirical distribution coefficient ($M^{-1}L^3$). Neglecting molecular diffusion, the dispersion coefficient is given by (*Bear* 1972)

$$D = \frac{\alpha q}{\theta} \qquad (3)$$

where α is the dispersivity (L). Substitution of Eqs. (2) and (3) into (1), and using the continuity equation for water flow

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \tag{4}$$

yields

$$\frac{\theta R}{q}\frac{\partial c}{\partial t} = \alpha\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} \tag{5}$$

where the retardation factor R is given by

$$R = 1 + \rho k/\theta \tag{6}$$

Adopting the Green-Ampt infiltration model (Green and Ampt 1911), the infiltration rate during ponding with a negligible depth of water on the soil surface is given by

$$q = K_s\left[1 + \left(\theta_s - \theta_i\right)\frac{h_f}{I}\right] \tag{7}$$

where K_s is the saturated hydraulic conductivity (L/T), θ_i and θ_s are the initial and final (saturated) water contents, respectively, h_f is the suction head (negative pressure head) at the wetting front (L), and I is the cumulative infiltration rate (L). The above model assumes that the wetting front can be represented by a sharp interface separating a saturated zone above the wetting front from a semi-infinite unsaturated zone having a constant water content below the wetting front. Although the wetting front itself can be readily monitored, the suction head, h_f, at the wetting front is more difficult to determine. Whisler and Bouwer (1970) suggested that h_f be approximated by the more easily measured air entry value. More precisely, Bouwer (1964) suggested that h_f be linked to measurable soil characteristics using the relationship

$$h_f = \int_0^{h_i} k_r(h)\,dh \tag{8}$$

where h_i is the initial pressure head (L), and $k_r(h)$ the relative hydraulic conductivity ($0 \le k_r \le 1$) as a function of the pressure head, h. An alternative physically based expression was later derived by Neuman (1976) for the early stages of infiltration as follows

$$h_f = \frac{1}{2}\int_0^{h_i}\left(1 + \frac{\theta - \theta_i}{\theta_s - \theta_i}\right)k_r(h)\,dh \tag{9}$$

The cumulative infiltration, I, in Eq. (7) will be approximated here with Philip's expression for infiltration (Philip 1969):

$$I = S\sqrt{t} + K_s t \tag{10}$$

in which S is the sorptivity that can be measured experimentally (Lin and Gray 1971) or estimated from the diffusivity function, $D(\theta)$ (L^2T^{-1}) using (Parlange 1975)

$$S^2 \approx \int_{\theta_i}^{\theta_s}\left(\theta_s + \theta - 2\theta_i\right)D(\theta)\,d\theta \tag{11}$$

Neuman (1976) showed previously that Eq. (9) is consistent with the form of Eq. (11). The set of equations (7) and (9) through (11) gives a physics-based description of infiltration consistent with the approximate mechanistic approach of Green and Ampt (1911), but incorporating features of Philip's infiltration equation (10) and Parlange's sorptivity function (11) such that the infiltration rate can be linked directly to measurable soil hydraulic parameters.

Application of the transformation

$$T = \int_0^t \frac{q}{\theta}\,dt \tag{12}$$

reduces Eq. (5) to the linearized form

$$R\frac{\partial c}{\partial T} = \alpha\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} \tag{13}$$

Substituting Eqs. (7) and (10) into (12) and using for θ the saturated water content, θ_s, we obtain

$$T = \frac{K_s t + 2\left(\theta_s - \theta_i\right)h_f \ln\left(1 + \frac{K_s\sqrt{t}}{S}\right)}{\theta_s} \tag{14}$$

Note that since the Green-Ampt model implies a uniform velocity profile within the saturated zone, and a zero flux below the wetting front, the transformed transport equation is only valid between the soil surface and the wetting front. The depth of the wetting front, z_f, at time t can be estimated from the implicit Green-Ampt equation as follows

$$t = \frac{\theta_s - \theta_i}{K_s}\left[z_f - h_f \ln\left(1 + \frac{z_f}{h_f}\right)\right] \tag{15}$$

This equation follows from Eq. (7), the definition of infiltration rate as $q = dI/dt$, as well as the basic assumption of the Green-Ampt model that $I = (\theta_s - \theta_i)\, z_f$.

ANALYTICAL SOLUTION

Equation (13) will be solved analytically for a general initial concentration distribution given by an arbitrary number of connecting straight lines as shown in Fig. 1, i.e.,

$$c(z,0)=\begin{cases} a_1+b_1z & z\epsilon[0,z_1] \\ a_2+b_2z & z\epsilon[z_1,z_2] \\ \dots & \dots \\ a_n+b_nz & z\epsilon[z_{n-1},z_n] \\ c_n & z>z_n \end{cases} \tag{16}$$

where a_i and b_i for each line segment are given by, respectively,

$$a_i=c_{i-1}-b_iz_{i-1} \qquad b_i=\frac{c_i-c_{i-1}}{z_i-z_{i-1}} \tag{17}$$

in which c_i is the value of initial concentration at depth $z_i(z_0=0)$. Note that for a step-wise initial concentration distribution profile, all b_i equal zero.

The transport problem will be solved for a semi-infinite soil profile, i.e.,

$$\frac{\partial c}{\partial z}(\infty,t)=0 \tag{18}$$

and for both a first- or concentration-type and a third- or flux-type boundary condition at the soil surface.

First-type boundary condition

The following equation defines a first-type inlet condition describing the step-wise application of a solute tracer

$$c(0,t)=\begin{cases} C_{01} & 0<t\le t_0 \\ C_{02} & t>t_0 \end{cases} \tag{19}$$

in which t_0 is the applied injection time period, and C_{01} and C_{02} are concentrations of the injected fluid before and after t_0. After implementing the transformation from t to T in Eq. (19) and applying Laplace transform techniques as discussed in detail by van Genuchten (1981), using transforms listed in van Genuchten and Alves (1982) and Spiegel (1991), we obtained the following solution of Eq. (13) subject to the invoked initial and boundary conditions

$$\begin{aligned} c=C_{02}+(C_{01}-C_{02}) & \\ &\left[A(z,T)-A(z,T-T_0)U(T-T_0)\right] \\ &+\sum_{i=1}^{n+1}\left[(a_i-C_{02})G_i(z,T)+b_iE_i(z,T)\right] \end{aligned} \tag{20}$$

where $U(T-T_0)$ is Heaviside's unit function, $T_0=T(t_0)$, and

$$A(z,T)=\frac{1}{2}\left\{\operatorname{erfc}\left[\frac{Rz-T}{2\sqrt{R\alpha T}}\right]+e^{\frac{z}{\alpha}}\operatorname{erfc}\left[\frac{Rz+T}{2\sqrt{R\alpha T}}\right]\right\} \tag{20a}$$

$$\begin{aligned} G_i(z,T)=&\frac{1}{2}\left\{\operatorname{erfc}\left[\frac{R(z-z_i)-T}{2\sqrt{R\alpha T}}\right]-\operatorname{erfc}\left[\frac{R(z-z_{i-1})-T}{2\sqrt{R\alpha T}}\right]\right\} \\ &+\frac{1}{2}e^{\frac{z}{\alpha}}\left\{\operatorname{erfc}\left[\frac{R(z_i+z)+T}{2\sqrt{R\alpha T}}\right]-\operatorname{erfc}\left[\frac{R(z_{i-1}+z)+T}{2\sqrt{R\alpha T}}\right]\right\} \end{aligned} \tag{20b}$$

$$\begin{aligned} E_i(z,T)=&\sqrt{\frac{\alpha T}{\pi R}}\left\{\exp\left[-\frac{R}{4\alpha T}\left(z-z_{i-1}-\frac{T}{R}\right)^2\right]\right. \\ &-\exp\left[-\frac{R}{4\alpha T}\left(z-z_i-\frac{T}{R}\right)^2\right] \\ &-e^{\frac{z}{\alpha}}\left(\exp\left[-\frac{R}{4\alpha T}\left(z+z_{i-1}+\frac{T}{R}\right)^2\right]\right. \\ &\left.\left.-\exp\left[-\frac{R}{4\alpha T}\left(z+z_i+\frac{T}{R}\right)^2\right]\right)\right\} \\ &+\frac{z-T/R}{2}\left\{\operatorname{erfc}\left[\frac{R(z-z_i)-T}{2\sqrt{R\alpha T}}\right]-\operatorname{erfc}\left[\frac{R(z-z_{i-1})-T}{2\sqrt{R\alpha T}}\right]\right\} \\ &-\frac{z+T/R}{2}e^{\frac{z}{\alpha}}\left\{\operatorname{erfc}\left[\frac{R(z_i+z)+T}{2\sqrt{R\alpha T}}\right]-\operatorname{erfc}\left[\frac{R(z_{i-1}+z)+T}{2\sqrt{R\alpha T}}\right]\right\} \end{aligned} \tag{20c}$$

Third-type boundary condition

The inlet boundary condition is now given by

$$\left.\left(-\theta D\frac{\partial c}{\partial z}+qc\right)\right|_{z=0}=\begin{cases} qC_{01} & t\le t_0 \\ qC_{02} & t>t_0 \end{cases} \tag{21}$$

As pointed out by van Genuchten and Parker (1984), among others, a third-type condition is generally more realistic inasmuch as this condition conserves solute mass in the simulated system. The analytical solution of Eq. (13) subject to Eqs. (16), (18), and (21) is again given by Eq. (20) in which now

$$
\begin{aligned}
A(z,T) = {} & \frac{1}{2}\operatorname{erfc}\left[\frac{Rz - T}{2\sqrt{R\alpha T}}\right] \\
& - \frac{1}{2}\left(1 + \frac{z}{\alpha} + \frac{T}{\alpha R}\right) e^{\frac{z}{\alpha}} \operatorname{erfc}\left[\frac{Rz + T}{2\sqrt{R\alpha T}}\right] \\
& + \sqrt{\frac{T}{\pi\alpha R}}\ \exp\left[\frac{(Rz - T)^2}{2\sqrt{R\alpha T}}\right]
\end{aligned}
\tag{22a}
$$

$$
\begin{aligned}
G_i(z,T) = {} & \frac{1}{2}\left\{\operatorname{erf}\left[\frac{R(z_i - z) + T}{2\sqrt{R\alpha T}}\right] - \operatorname{erf}\left[\frac{R(z_{i-1} - z) + T}{2\sqrt{R\alpha T}}\right]\right\} \\
& + \sqrt{\frac{T}{R\alpha\pi}}\, e^{\frac{z}{\alpha}} \left\{\exp\left[-\frac{R}{4\alpha T}\left(z + z_i + \frac{T}{R}\right)^2\right] - \exp\left[-\frac{R}{4\alpha T}\left(z + z_{i-1} + \frac{T}{R}\right)^2\right]\right\} \\
& + \frac{1}{2} e^{\frac{z}{\alpha}} \left\{\left(1 + \frac{z_{i-1} + z}{\alpha} + \frac{T}{\alpha R}\right) \cdot \operatorname{erfc}\left[\frac{R(z_{i-1} + z) + T}{2\sqrt{R\alpha T}}\right] \right. \\
& \left. - \left(1 + \frac{z_i + z}{\alpha} + \frac{T}{R\alpha}\right) \operatorname{erfc}\left[\frac{R(z_i + z) + T}{2\sqrt{R\alpha T}}\right]\right\}
\end{aligned}
\tag{22b}
$$

$$
\begin{aligned}
E_i(z,T) = {} & e^{z/\alpha}\sqrt{\frac{\alpha T}{\pi R}}\left\{\left(1 + \frac{z - z_{i-1} + T/R}{2\alpha}\right) \cdot \exp\left[-\frac{R}{4\alpha T}\left(z + z_{i-1} + \frac{T}{R}\right)^2\right] \right. \\
& \left. - \left(1 + \frac{z - z_i + T/R}{2\alpha}\right) \cdot \exp\left[-\frac{R}{4\alpha T}\left(z + z_i + \frac{T}{R}\right)^2\right]\right\} \\
& + \sqrt{\frac{\alpha T}{\pi R}}\left\{\exp\left[-\frac{R}{4\alpha T}\left(z - z_{i-1} - \frac{T}{R}\right)^2\right] - \exp\left[-\frac{R}{4\alpha T}\left(z - z_i - \frac{T}{R}\right)^2\right]\right\} \\
& + \frac{z - T/R}{2}\left\{\operatorname{erfc}\left[\frac{R(z - z_i) - T}{2\sqrt{R\alpha T}}\right] - \operatorname{erfc}\left[\frac{R(z - z_{i-1}) - T}{2\sqrt{R\alpha T}}\right]\right\} \\
& + \frac{1}{2} e^{z/\alpha}\left\{\left(z + \frac{2T}{R} + \frac{(z + T/R)^2 - z_i^2}{2\alpha}\right) \cdot \operatorname{erfc}\left[\frac{R(z_i + z) + T}{2\sqrt{R\alpha T}}\right] \right. \\
& \left. - \left(z + \frac{2T}{R} + \frac{(z + T/R)^2 - z_{i-1}^2}{2\alpha}\right) \cdot \operatorname{erfc}\left[\frac{R(z_{i-1} + z) + T}{2\sqrt{R\alpha T}}\right]\right\}
\end{aligned}
\tag{22c}
$$

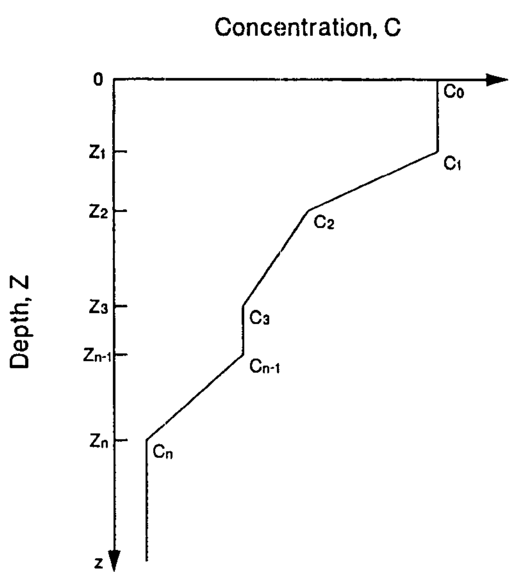

FIG. 1. General initial concentration distribution used for the analytical solution.

APPLICATIONS

We now present three examples illustrating the applicability of the analytical solution to several infiltration scenarios. The examples also serve as tests of the accuracy of the proposed solution by showing comparisons against numerical results, previous approximate analytical solutions, and experimental data.

Example 1: Infiltration into a coarse-textured soil

The first example considers solute transport in a relatively coarse-textured soil. The soil hydraulic properties were described with the parametric functions (van Genuchten 1980)

$$S_e(h) = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left(1 + |\alpha_h h|^n\right)^m}$$
$$K(h) = K_s \sqrt{S_e}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{23}$$

in which K_s = 50 cm/h, θ_s = 0.4, θ_r = 0.05 (θ_r is the residual water content), α_h = 0.05 cm^{-1} and n = 3.0 are empirical shape parameters, and m = 1 − 1/n. The transport experiment assumed that the soil was initially solute free, i.e., $c(x, 0) = 0$, and had a uniform initial volumetric water content, θ_i, of 0.051. The dispersivity, α, was assumed to be 2.727 cm, and no adsorption was considered (R = 1). The suction head, h_f, of the wetting front as calculated with Eq. (9) was 10.85 cm, whereas the sorptivity, S, according to Eq. (11), was found to be 19.45 cm/h$^{1/2}$. Assuming ponding, the irrigation water contained a tracer at a concentration of 1 g/cm^3 (C_{01} = 1) for a period of 0.25 h (t_0 = 0.25), after which the irrigation water was again free of solute (C_{02} = 0). Figure 2 compares the analytical solution using a third-type boundary condition, with numerical results generated with the HYDRUS code of Kool and van Genuchten (1991) based on the Richards equations for transient, variably saturated water flow and the convection-dispersion equation for solute transport. The figure shows close agreement between the analytical and numerical solutions, with the analytical solution being slightly ahead of the numerical simulation. The calculations for this case, as well as for the examples below, were obtained using Eq. (9) for the suction head h_f of the wetting front. Using Eq. (8) rather than (9) did not lead to a visibly different curve in Fig. 2. For the current example 1, Eq. (9) produced a value of 10.85 for h_f, which is close to the value of 11.3 cm generated with Eq. (8).

Example 2: Column infiltration

A laboratory solute transport experiment during ponded infiltration was carried out by Bresler and Laufer (1974) using a 45-cm-long soil column filled with Gilat loam. The soil had an initial water content of 0.03 and an initial chloride concentration of 165 meq/L. The column was flood-irrigated for about 0.35 hours, such that 3 cm of water containing 10 meq/L $CaCl_2$ infiltrated. Other parameters included K_s = 0.72 cm/h, θ_s = 0.44, and α = 0.08 cm. The suction head of the wetting front was h_f = 30 cm (Eq. 9), and S equaled 4.645 cm/hr$^{1/2}$. These values for h_f and S were estimated from the hydraulic properties of Gilat loam as shown in Fig. 1 of Bresler et al. (1971). Figure 3 shows good agreement between the analytical solution and the experimental data. The analytical solution also closely approximated the nu-

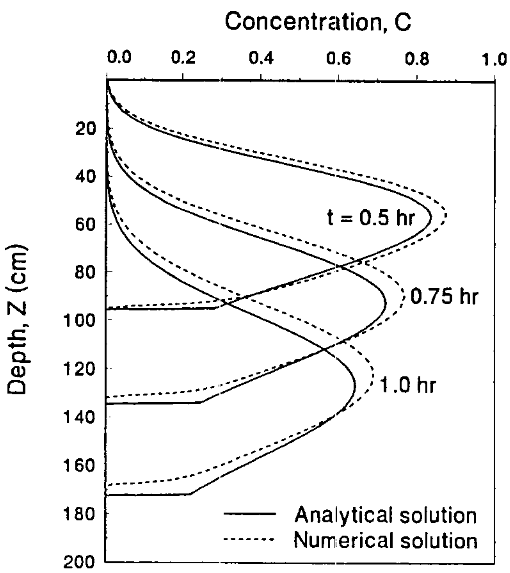

FIG. 2. Comparison of the proposed analytical solution with numerical results for solute transport in a coarse-textured soil.

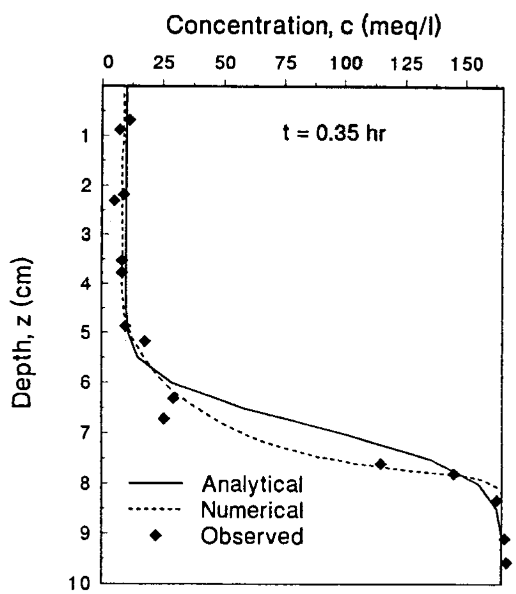

FIG. 3. Observed (diamonds) and calculated chloride concentration distributions during ponded infiltration. The solid line denotes the proposed analytical solution, whereas the dashed line represents the numerical solution of Bresler and Laufer (1974).

merical results obtained by Bresler and Laufer (1974).

Example 3: Field infiltration

The model was also tested against results from a field infiltration experiment reported previously by Warrick et al. (1971). The experiment involved the application of a 7.62-cm pulse of water having a concentration of 0.2 N $CaCl_2$ (t_0 = 2.8 h), followed by 22.9 cm of solute-free water. The soil profile was assumed to have a constant initial water content of 0.2 and a saturated water content at the soil surface of 0.38. No adsorption or ion exclusion was considered in the calculations. Using the measured hydraulic functions $\theta(h)$ and $K(\theta)$ (Figs. 2 and 3 of Warrick et al. 1971), the values of h_f and S were estimated to be 10.2 cm and 2.375 cm/h$^{1/2}$, respectively. The dispersivity was assumed to be 1.02 cm (De Smedt and Wierenga 1978), although Bresler (1973) used somewhat lower values. Figure 4 shows that our analytical solution agrees closely with the complete numerical solution of van Genuchten (1982) for essentially the same transport problem (the initial water content profiles differed slightly). The analytical solution also agreed closely with an approximate solution previously obtained by De Smedt and Wierenga (1978) and applied to the same infiltration problem. Notice that the analytically and numerically calculated chloride profiles all lagged behind the measured data. Deviations between the observed and calculated curves may be explained in terms of anion exclusion (Bresler 1973; De Smedt and Wierenga 1978), having imprecise estimates of the unsaturated hydraulic properties and/or the general problems of soil heterogeneity and preferential flow.

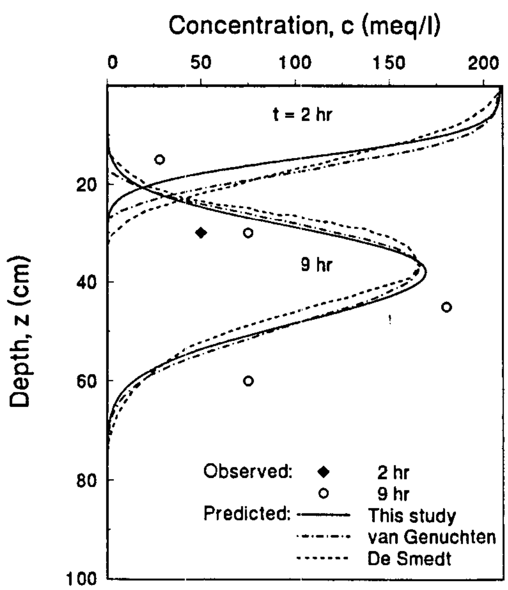

FIG. 4. Observed and calculated chloride concentration profiles during ponded infiltration in a Panoche clay loam (Warrick et al. 1971).

SUMMARY AND CONCLUSIONS

The analytical solution developed in this paper assumes that the Darcian fluid flux density in the transport equation can be approximated using the Green-Ampt infiltration model combined with Philip's infiltration equation, whereas the water content behind the wetting front can be taken as the saturated (or maximum) water content during infiltration. Using these approximations, the unsaturated convection-dispersion transport equation may be linearlized and solved analytically using an appropriate variation transformation. Analytical solutions were derived for both first- and third-type boundary conditions at the soil surface and assumed a very general initial concentration distribution approximated by an arbitrary number of connecting straight lines. The analytical solution agreed well with solutions generated with more comprehensive numerical variably saturated flow/transport models for three solute transport problems involving ponded infiltration, as well as with several experimental data sets. The results demonstrate that the approximate analytical solution provides a good approximation of solute transport during ponded infiltration.

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