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Average concentration of soluble salts in leached soils inferred from the convective–dispersive equation

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Abstract The convective–dispersive, or advective–dispersive, equation (CDE) has long been the model of choice for solute transport in soils. Using the average concentration of soluble salts in soil profile to evaluate changes in salinity due to irrigation can be beneficial when spatial variability of soil salinity at selected depths is larger than spatial variability of soil salinity in the layer encompassing these depths, and when soil salinity is evaluated with electric conductivity measurements that give layer-average rather than depth-specific salinity values. The objective of this work was to present analytical solutions of the CDE that express the average soluble salt content in soil profile as the function of time, water flux, and solute dispersion parameter. The solutions were developed for both semiinfinite and finite domain and implemented in a computer code. Examples are presented of using these solutions to develop a nomogram for the dispersion coefficient estimation and to evaluate the applicability of the semiinfinite domain solution to soil monolith leaching experiments. In cases when the CDE application is justified, the analysis of the salt leaching based on the average salt concentrations in soil profile provides estimates of the effective salt dispersion parameter useful in land evaluation and soil reclamation.

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Introduction

The convective–dispersive, or advective–dispersive, equation (CDE) has long been the model of choice for solute transport in soils (Rolston 2007). It has been widely used to simulate changes in soil salinity under irrigation (e.g., Misra and Mahapatra 1989). Analytical solutions of the CDE have been summarized in the exhaustive compendium by van Genuchten and Alves (1982), and the search for the methods of solving it continues (Pérez Guerrero et al. 2009).

Published analytical solutions usually present the dependencies of solute concentrations on time and depth. In case of soil salinity studies, however, it can be beneficial to use the analytical solutions of CDE that present the dependencies of total mass of soluble salts, or average concentration of salts, in soil profile on time. There are at least three reasons for that. First, the spatial variability of soil salinity at selected depth intervals is often larger than the spatial variability of soil salinity in the layer encompassing these depth intervals (e.g., Utset et al. 1998). Therefore, more reliable values of the dispersivity parameter can be found from data on the salinity change in soil profile to represent salt leaching across the field under irrigation. Second, electrical conductivity measurements become the method of choice to obtain and characterize the variability of soil salinity with great spatial detail (Herrero et al. 2003). These methods allow one to obtain average soil salinity values for large soil profiles, often 0–100 cm, or even deeper. Third, historic data on the effect of irrigation and leaching on soil salinity are often presented for soil profiles rather than for separate soil layers. Analysis of these data has to be based on total mass in soil profile.

The objective of this work is to present analytical solutions of the CDE that express the average soluble salt content in soil profile as a function of time and water flux.

Analytical solutions of the CDE

The CDE is used in this work in the form

$$\frac{\partial}{\partial t}(\theta C + \rho b) = \theta D \frac{\partial^2 C}{\partial x^2} - \theta v \frac{\partial C}{\partial x}, \quad b = kC \tag{1}$$

where $C(x, t)$—the solute concentration [ML^{-3}]; $b(x, t)$—the concentration of the adsorbed solute [MM^{-1}]; θ—the volumetric soil water content [$L^{-3}L^{-3}$]; ρ—soil bulk density [ML^{-3}]; D—the dispersion coefficient [L^2T^{-1}]; $v = q/\theta$—average pore water velocity [LT^{-1}]; q—the water flux per unit of soil cross-sectional area [LT^{-1}]; k—the distribution coefficient [L^3M^{-1}]; t—time [T]; x—distance from the soil surface [L].

The initial condition is

$$C(0, t) = C_0. \tag{2}$$

At soil surface, we consider boundary conditions of the third type:

$$vC(x, t) - D\frac{\partial C}{\partial x} = v\hat{C}_i, \\ t_i < t \leq t_{i+1} \left(i = \overline{0, n}; t_0 = 0; t_{n+1} = \infty\right). \tag{3}$$

Here, $\hat{C}_i$ is the concentration of soluble salts in the irrigation water. This boundary condition is recommended to simulate the resident concentrations, measured as mass of solute per unit volume of water (e.g., van Genuchten and Parker 1984).

Solute transfer is considered both in the finite layer of thickness L with boundary condition

$$\frac{\partial C(L, t)}{\partial x} = 0, \quad 0 < t < \infty \tag{4}$$

and in the semiinfinite domain with the boundary condition

$$\frac{\partial C(x, t)}{\partial x}\bigg|_{x \to \infty} = 0, \quad 0 < t < \infty \tag{5}$$

Equation 1 has analytical solutions that allow one to compute concentrations at an arbitrary depth x on arbitrary time. These solutions have been summarized by van Genuchten and Alves (1982). The general form of these analytical solutions is

$$C(\zeta, \xi, \xi_i) = C_0\Phi(\zeta, \xi) + \sum_{i=0}^{n} \left(\hat{C}_i - \hat{C}_{i-1}\right) \\ \times [1 - \Phi(\zeta, \xi - \xi_i)], \quad (\hat{C}_{-1} = 0) \tag{6}$$

where $\zeta = \frac{x}{L}$, $\xi = \frac{vt}{RL}$, $R = 1 + \frac{\rho}{\theta}k$.

Function $\Phi(\zeta, \xi)$ has different forms dependent on boundary conditions on the surface and type of domain considered. For the third type, or flux boundary condition (3) at the surface and semininfinite transport domain, the function $\Phi(\zeta, \xi)$ is

$$\Phi(\zeta, \xi) = \frac{1}{2}erfc[z_-(\zeta, \xi)] + \frac{1}{2}\{erfc[z_+(\zeta, \xi)] \\ -4\sqrt{\eta\xi} \cdot ierfc[z_+(\zeta, \xi)]\}e^{4\eta\zeta} \tag{7}$$

where $ierfc(u) = \exp(-u^2)/\sqrt{\pi} - u[1 - erf(u)]$, $erfc(u) = 1 - erf(u)$, $\eta = \frac{vL}{4D}$, $erf(u) = \frac{2}{\pi}\int_0^u \exp(-t^2)dt$, $z_\pm(\zeta, \xi) = (\xi \pm \zeta)\sqrt{\frac{\eta}{\xi}}$.

For the finite domain with the boundary condition (3), the function $\Phi(\zeta, \xi)$ is

$$\Phi(\zeta, \xi) = \sum_{n=1}^{\infty} \left\{ \frac{2\eta h_n \cdot [h_n \cos(2h_n\zeta) + \eta \sin(2h_n\zeta)]}{(h_n^2 + \eta^2)(h_n^2 + \eta^2 + \eta)} \right\} \\ \times \exp\left[2\eta\zeta - (h_n^2 + \eta^2)\frac{\xi}{\eta}\right] \tag{8}$$

for the finite layer. In Eq. 8, h_n are roots of the equation $tg(2h) = \frac{2h\eta}{h^2-\eta^2}$.

The average concentration of readily soluble salts

The average concentration in the layer with the thickness ℓ ($0 \leq \ell \leq L$) is found as

$$\overline{C}(t, \ell) = \frac{1}{\ell}\int_0^\ell C(x, t)dx = \frac{1}{a}\int_0^a C(y, \xi)dy = \overline{C}(a, \xi) \tag{9}$$

where $a = \ell/L$. Using Eq. 6, one obtains

$$\overline{C}(a, \xi) = C_0 E(a, \xi) + \sum_{i=0}^{n} \left(\hat{C}_i - \hat{C}_{i-1}\right) \\ \times [1 - E(a, \xi - \xi_i)], \quad (\hat{C}_{-1} = 0). \tag{10}$$

Function $E(a, \xi)$ has different forms dependent on surface boundary and type of domain considered. For the semiinifinite domain and the third type, or flux, boundary condition (3) at the surface, the integration (9) applied to $C(x, t)$ from Eq. 7 with $\Phi(\zeta, \xi)$ from Eq. 7 results in

$$E(a, \xi) = \frac{1}{2a}\{(\xi + a)e^{4a\eta}erfc[z_+(a, \xi)] \\ -(\xi - a)erfc[z_-(a, \xi)]\} \tag{11}$$

where $z_\pm(a, \xi) = (\xi \pm a)\sqrt{\frac{\eta}{\xi}}$.

For the finite thickness layer, the integration (9) applied to $C(x, t)$ from Eq. 5 with $\Phi(\zeta, \xi)$ from Eq. 8 leads to

$$E(a, \xi) = \sum_{n=1}^{\infty} (-1)^{n+1} \left[\frac{\sin(2h_n)\sin(2ah_n)}{2a(h_n^2 + \eta^2 + \eta)} \right] \\ \times \exp\left[2a\eta - (h_n^2 + \eta^2)\frac{\xi}{\eta}\right]. \tag{12}$$

Applications of the solutions

The PC program ASC for computations based on Eq. 10 is available from the corresponding author upon request. The program works in three modes for both seminifinite and finite domains. In the mode 1 (forecast mode), the program computes the average concentration according Eq. 10 when the dispersion coefficient D is known, and parameters $\xi = \frac{vt}{R_L}$ and $\eta = \frac{vL}{4D}$ can be computed from projected leaching conditions. In the mode 2 (inverse mode), the program is used for determining parameter D from experimental data on salt leaching from soil. In this mode, the average concentration and the parameter ξ are known, and the parameter η is found to match the simulated and measured average concentration. The value of D is then found as $D = vL/4\eta$. In the mode 3 (design mode), the program is used to determine the time t or volume of water vt to bring the average solute concentration to the predefined level. In this mode, the average concentration and the parameter η are known, and the parameter ξ is found to bring the average solute concentration to the predefined level. The value of t is then found as $t = \xi RL/v$. Algorithms *zbrac* and *rtbis* from Press et al. (1992) were applied to solve Eq. 10 and 11 or 10 and 12 with respect to η and ξ in modes 2 and 3, respectively, using bracketing and bisection. The program was validated using the CXFIT (Toride et al. 1999) code that computes concentrations according to Eq. 6 at the arbitrary depths and time for both seminifinite and finite domains. We computed the concentration profiles in soil with CXFIT for 10 randomly chosen pairs of η and ξ values, integrated them numerically using the trapezoidal method to obtain the average concentrations, compared the integration results with results from ASC, and observed the agreement of four significant digits.

An example of application of this program is shown in Fig. 1 where dimensionless parameters ξ and η are related to the fraction of salts $\bar{C}(1, \xi)/C_0$ left in the soil profile after one leaching tact. The average concentrations were computed using ASC in the mode 1 with parameters ξ and η incremented within the limits shown at the graph, and the nomograph was drawn as a contour graph using the SigmaPlot software (MathWorks, Cambridge, MA). The solution for the seminifinite domain has been used.

The arrows show an example of using this nomograph. Consider the case when leaching with the flux of irrigation water q of 0.06 m d^{-1} for 9 days resulted in the 1-m average salinity decrease to 19% of the initial amount. The soil porosity was $\theta = 0.4$, and the velocity v was $q/\theta = 0.15$. In this case the value of parameter ξ was $0.15 \times 9 = 1.35$. This gives the point A at the graph where the arrow AB starts. This arrow ends in the point B where the residual concentration is 0.19. Arrow BC shows the
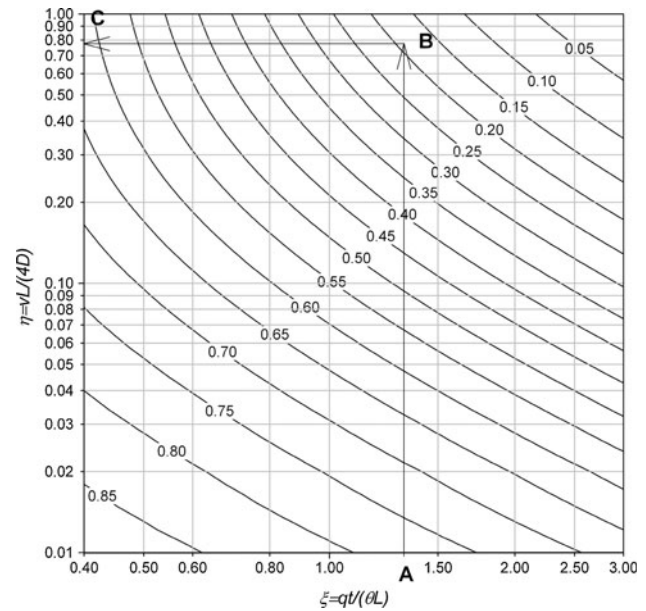

Fig. 1 Nomograph showing the dependence of the residual average salt content in soil profile on dimensionless parameters ξ and η after single application of the irrigation water for leaching. Parameter ξ is the amount of leaching water measured in pore volumes in the leached layer, parameter η quantifies the relative importance of convective and dispersive transport mechanisms, convection dominates when η is large. The solution for the seminifinite domain was used to construct the graph. See text for more details

point C where the corresponding value of η is found. Then, the dispersion coefficient $D = vL/(4\eta)$ is 0.05 m^2 d^{-1}.

Another example of using the ASC program was developed to evaluate the error resulting from the application of the solution for the seminifinite domain to cases when the solution for the finite domain should be applied. Previous research showed the good agreement between the solute breakthrough computed for seminifinite and infinite domains for large values of the parameter Peclet $Pe = 4\eta$ values. Van Genuchten and Parker (1984) indicated such good agreement at $Pe > 5$ whereas Schwartz et al. (1999) recommended values of $Pe > 10$. The substantial volume of historic data on leaching efficiency was obtained from experiments in monoliths, and the dispersion coefficient was found by applying the solution for the seminifinite domain (e.g., Klykov et al. 1975). Values of the dispersion coefficient were large in some cases in these historic data, and therefore values of the parameter η appeared to be relatively small.

Dependencies of average solute concentrations after leaching on parameters ξ and η are compared in Fig. 2 for the seminifinite and finite transport domains. The graph in this figure was obtained using the ASC in the mode 1 in the same way as in Fig. 1. Relatively good agreement between two solutions can be seen for values of $\eta = 3$ corresponding to $Pe = 12$. However, the average concentrations in the profile are substantially different for the two
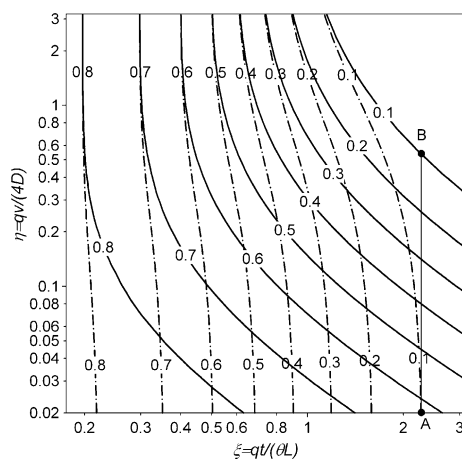
Fig. 2 Comparison of dependences of the residual average salt content in soil profile on dimensionless parameters ξ and η obtained from the semiinfinite (*solid line*) and finite (*dash-dot line*) solutions. A single application of the irrigation water for leaching is simulated. See text for details

solutions at smaller η. The value of η appears to be overestimated if the solution for the semiinfinite domain has been used in place of the solution for the finite domain. The AB segment in the graph demonstrates an extreme case of such underestimation. The point A shows the set of parameters corresponding to the residual concentration of 10% of the initial assuming that the finite domain solution is applicable (e.g., monolith leaching). The value of η is 0.02. If the semiinfinite domain solution is used to estimate η in the same way as in Fig. 1, then the value of $\eta = 0.52$ will be found that corresponds to the point B on the 10% concentration isoline. Since D is inversely proportional to η, the D value found from the semiinfinite domain solution will be $0.52/0.02 \approx 25$ times less than the actual value. These results show that the cautions should be exercised when using historic data on the dispersion coefficient value obtained from the monolith leaching experiments.

Discussion

The applicability of presented solutions is limited to the extent of applicability of the convective–dispersive equation to the leaching process in a specific soil. The CDE is the most useful for homogeneous, uniform soils. It does not perform well in all soils. If soil structure results in zones with different mobility of soil water, CDE may not describe the leaching process correctly (Wallender et al. 2006). Similarly, the use of (1) is limited if the solution chemistry greatly changes during the leaching and greatly affects soil structure and infiltrability (Bauder et al. 2008).

The assumption of the stationary flow in Eq. 1 applies reasonable well to the field leaching of saline soils. Its applicability to the situations when soil water dynamics includes substantial periods of evaporation is limited. Therefore, the values of the dispersion coefficients obtained by averaging temporally variable soil pore velocities will be affected by the specifics of soil water regime and should not be treated as transport parameters of the soil.

In cases when the application of the Eq. 1 is justified, the analysis of the salt leaching process based on the average concentrations of salts in soil profile can provide useful estimates of the effective salt dispersion parameter that can be used in land evaluation and soil reclamation in areas with salt-affected soils.

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