Average Pollutant Concentration in Soil Profile

Simulated with Convective-Dispersive Equation

Model and Manual

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Abstract

Different parts of soil solution move with different velocities, and therefore chemicals are leached gradually from soil with infiltrating water. Solute dispersivity is the soil parameter characterizing this phenomenon. To characterize the dispersivity of soil profile at field scale, it is desirable to use changes in total chemical mass in the whole soil profile rather than chemical content in individual soil layers. The computer program ASC implements the analytical solution of the model of dispersive transport in soils and allows a user to (a) fit this solution to field data to obtain soil dispersivity parameter, (b) estimate the average concentration in soil profile when the dispersivity parameter is known, and (c) determine the amount of leaching water needed to bring the average concentration to the desired level. The program is written in FORTRAN and compiled at PC. Examples of input and output files are given.

Disclaimer

Although the code has been tested by its developers, no warranty, expressed or implied, is made as to the accuracy and functioning of the program modifications and related program material, nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the developers in connection therewith.

1. The analytical solution

The PC program ASC (Average Salt Concentration) implements analytical solution of the CDE used in the form

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

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

The initial condition is

$$C(0,t)=C_0 \qquad (2)$$

Boundary conditions of the third type are set at the soil surface

$$vC(x,t)-D\frac{\partial C}{\partial x}=v\hat{C}_i\ ,\ \text{при}\ \ t_i<t\le t_{i+1}\left(i=\overline{0,n}\ ;\ t_0=0\ ;\ t_{n+1}=\infty\right) \qquad (4)$$

Here $\hat{C}_i$ is the concentration of soluble salts in the irrigation water. Solute transfer is considered both in the finite layer of thickness L with boundary condition

$$\frac{\partial C(L,t)}{\partial x}=0\ ,\ 0<t<\infty \qquad (5)$$

and in the semiinfinite domain with the boundary condition

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x\to\infty}=0\ ,\ 0<t<\infty \qquad (6)$$

Equation (1) has analytical solutions that allow one to compute concentrations at an arbitrary depth *x* on arbitrary time. The general form of these analytical solutions is

$$C(\zeta,\xi,\xi_i) = C_0\Phi(\zeta,\xi) + \sum_{i=0}^{n}\left(\hat{C}_i - \hat{C}_{i-1}\right)[1-\Phi(\zeta,\xi-\xi_i)]\ ,\ \left(\hat{C}_{-1}=0\right) \tag{7}$$

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

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 (4) at the surface and semininfinite transport domain, the function $\Phi(\zeta,\xi)$ is

$$\Phi(\zeta,\xi) = \frac{1}{2}erfc\left[z_-(\zeta,\xi)\right] + \frac{1}{2}\left\{erfc\left[z_+(\zeta,\xi)\right] - 4\sqrt{\eta\xi}\cdot ierfc\left[z_+(\zeta,\xi)\right]\right\}e^{4\eta\zeta} \tag{8}$$

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 (4), the function $\Phi(\zeta,\xi)$ is

$$\Phi(\zeta,\xi) = \sum_{n=1}^{\infty}\left\{\frac{2\eta h_n\cdot\left[h_n\cos(2h_n\zeta)+\eta\sin(2h_n\zeta)\right]}{(h_n^2+\eta^2)(h_n^2+\eta^2+\eta)}\right\}\exp\left[2\eta\zeta - \left(h_n^2+\eta^2\right)\frac{\xi}{\eta}\right] \tag{9}$$

for the finite layer. In Eq. (9), h_n are roots of the equation $tg(2h) = \frac{2h\eta}{h^2-\eta^2}$,.

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

$$\overline{C}(t,\ \ell) = \frac{1}{\ell}\int_0^{\ell} C(x,t)dx = \frac{1}{a}\int_0^{a} C(y,\xi)dy = \overline{C}(a,\xi) \tag{10}$$

where $a = \ell / L$. Using Eq. (7), one obtains

$$\overline{C}(a,\xi) = C_0\, E(a,\xi) + \sum_{i=0}^{n}\left(\hat{C}_i - \hat{C}_{i-1}\right)[1 - E(a,\xi - \xi_i)]\ , \left(\hat{C}_{-1} = 0\right) \tag{11}$$

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 (4) at the surface, the integration (10) applied to *C(x,t)* from Eq. (7) with $\Phi(\zeta,\xi)$ from Eq. (8) results in

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

(12)

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

For the finite thickness layer, the integration (10) applied to *C(x,t)* from Eq. (7) with $\Phi(\zeta,\xi)$ from Eq. (9) leads to

$$E(a,\xi) = \sum_{n=1}^{\infty}(-1)^{n+1}\left[\frac{\sin(2h_n)\sin(2ah_n)}{2a\left(h_n^2 + \eta^2 + \eta\right)}\right]\exp\left[2a\eta - \left(h_n^2 + \eta^2\right)\frac{\xi}{\eta}\right] \tag{13}$$

2. The ASC program

The program ASC works in three modes for both seminifinite and finite domains. In the mode 1 (forecast mode), the program computes the average concentration according Eq. (11) when the dispersion coefficient D is known and parameters $\xi = \frac{vt}{\mathrm{R}L}$ 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 $t = \xi RL/v$.

Measurement units have to be consistent. We recommend to express the pore water velocity v in m day^{-1}, L (the thickness of the soil layer where the average salt concentration is found) in m, time t in days, and the dispersion coefficient D in m^2 day^{-1}.

An example of the input file is shown below.

```
MODE (1 - forward, 2 - inverse, 3 - design)
2
DOMAIN (1 - semiinfinite, 2 - finite)
2
NUMBER OF CASES
3
AVERAGE_CONCENTRATION    KSI    ETA
  0.7                     0.600  0.3
  0.6                     0.5    1.0
  0.3                     1.1    1.0
```

Note that values of AVERAGE_CONCENTRATION (average residual salt concentration), KSI(ξ), and ETA(η) have to be entered for any mode and domain values. In the mode 1, the entered value of the AVERAGE_CONCENTRATION is be arbitrary, in the mode 2, the entered value of ETA is arbitrary, and in the mode 3 the entered value of KSI is arbitrary. The correct values will be found in the found in the output file ASC_OUT.txt.

The example of output file ASC_OUT.txt corresponding to the above ASC_IN.txt is shown below.

```
MODE (1 - forward, 2 - inverse, 3 - design)
        2
DOMAIN (1 - semiinfinite, 2 - finite)
        2
NUMBER OF CASES
        3
Case No      AVERAGE_CONCENTRATION    KSI    ETA
        1   NO SOLUTION
        2   .600                  .500   .033
        3   .300                 1.100   .148
```

For the first case, no solution of the CDE exists. If the numbers for AVERAGE CONCENTRATION and KSI came from an experiment, the “NO SOLUTION” message means that the CDE is not applicable in these experimental conditions (see the paper "Average concentration of soluble salts in leached soils inferred from the convective-dispersive equation" for explanations). For the second and third cases, values of AVERAGE CONCENTRATION and KSI in the output file ASC_OUT.txt are the same as in the input file ASC_IN.txt. The output file contains correct values of ETA whereas the input file contained arbitrary values of ETA.

The input file ASC_IN.txt file has to be placed to the same directory as the executable ASC.exe.