

Soil Trace Element Model (Profile Distribution)

Documentation

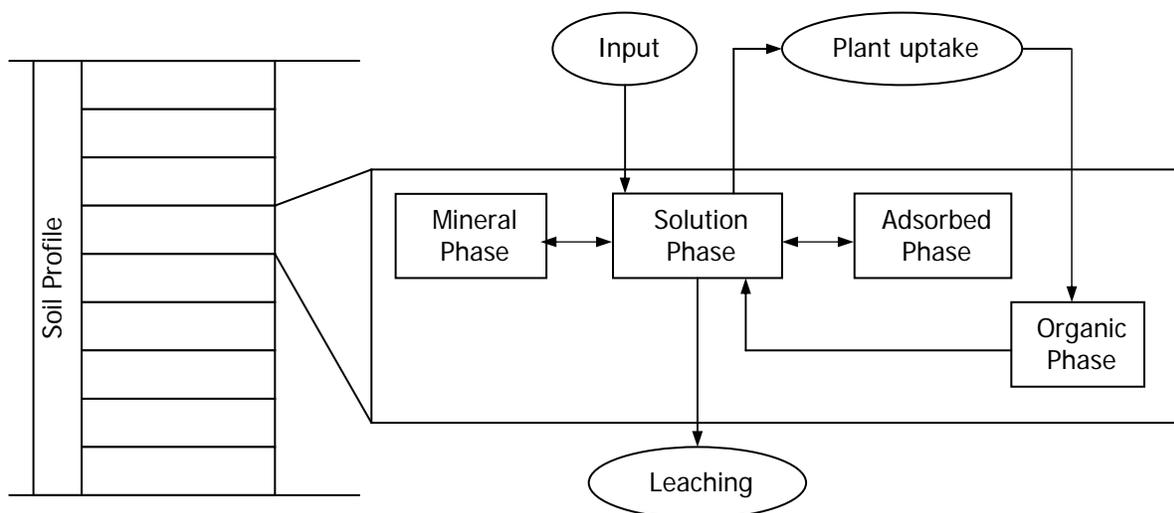
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Introduction

Trace elements such as Arsenic and Cadmium may be added to soils through atmospheric deposition, irrigation, fertilizers, and other amendments. The mass balance approach was used in the model to examine the flow of trace elements as influenced by the interactive processes in soils including adsorption-desorption, precipitation-dissolution, and organic matter mineralization. In the model, leaching was related with soil characteristics and plant uptake with crop characteristics. The model was solved numerically to evaluate the long-term behavior of trace elements in cropland soils and to evaluate the effects of soil characteristics, plant uptake factors, and inputs sources on trace element accumulation in receiving soils.

Model Structure

The simulated soil profile is discretized into a number of uniform adjoining sections. For each section, there are three fluxes: inputs (external inputs or internal inputs from other sections), leaching out the section, and plant uptake. These three fluxes are influenced by interactions among four phases: solution phase, adsorbed phase, mineral phase, and organic phase. The block diagram of the trace element mass balance model is depicted below:



Model Approach

- Call water flow and root water uptake subroutines from HYDRUS 1D (Šimunek et al., 1998); get water content and water flux velocities. Model assumptions are atmospheric boundary condition with surface layer for upper boundary condition, free drainage for lower boundary condition, van Genuchten [1980] hydraulic model without hysteresis, and Feddes [1978] water uptake reduction model without solute stress.

- Apply convective-dispersive transport equation to each section.

$$(K_d + \theta) \frac{\partial C}{\partial t} = - \frac{\partial}{\partial z} [qC - \theta D(\theta, q) \frac{\partial C}{\partial z}] - U + I + k_{im} \cdot O - (k_f(K_d + \theta)C - k_b M)$$

$k_f(K_d + \theta)C - k_b M$ represents the precipitation-dissolution kinetics of mineral phase (M).

$k_{im} \cdot O$ represents the mineralization kinetics of organic phase.

- Get section water flux and water content (θ), which is calculated by averaging the water content of adjoining nodes. Calculate dispersion coefficient (θD) as follows:

$$\theta D = D_L |q| + \theta D_w \tau_w \quad [\text{Bear, 1972}]$$

$$\tau_w = \theta^{7/3} / \theta_s^2 \quad [\text{Millington and Quirk, 1961}]$$

- Calculate Input:

- Input from atmospheric deposition are added to the mineral phase or mobile phase (solution phase plus adsorbed phase) of the top section.
- Input from irrigation is calculated by the flux and TE concentration at the top section and is incorporated into the solution phase of the top section.
- Input from fertilizers, micronutrients, and so on are added to the mineral phase or mobile phase of the plow layer.
- Depending on the direction, the TE transport with water fluxes and diffusion are considered as either input or leaching for a specified section.

- Calculate trace element uptake:

$$U = RD \cdot J \quad \text{where } J = \frac{J_{\max} \cdot C}{K_M + C} \quad \text{and } RD \text{ is the root density for the section.}$$

- Get root density distribution

- The classical Verhulst-Pearl logistic growth function is used to simulate root development.

$$RD(t) = \frac{RD_0 \cdot RD_m}{RD_0 + (RD_m - RD_0) e^{-rt}}$$

where RD_0 and RD_m are the initial and maximum root densities, respectively.

- The growth rate is calculated based on the assumption that 50% of the root density will be reached after 50% of the growing season has elapsed.
 - An exponential function is used to describe the spatial root distribution.
- Apply 4th order Runge-Kutta method on spatial and temporal scale, get the TE pools and change in fluxes.

Model Input

The input window is divided into seven tabs: Basic Information, Soil Properties, Initial Conditions, Input, Boundary Fluxes, Plant Growth and Uptake, and Root Water Uptake. The user can open an existing input file or enter his/her data and save it as a new file. The parameters are described in the following sections. The user can also search it by selecting Parameter Description from the Help menu (Ctrl+F1).

Basic Information

Space and time discretization and trace element specified constant is defined in this interface.

Soil Geometry. The space discretization is defined by four variables. The Profile Depth will specify the depth of the soil profile simulated in the model. The Depth of Plow Layer defines a layer where the biomass return, trace element pool redistribution, and discrete source input will take place. If there is more than one layer in the simulated system (different soil materials or different initial trace element pools), the user needs to specify that in Layers of Soil. Otherwise, set the value to 1. Correspondingly, the depth, initial trace element pools, and soil hydraulic properties for each soil layers needs to be provided in the later sections. The Number of Discretized Sections specifies the space discretization. In the model, the simulated soil profile is discretized into number of uniformly-sized adjoining sections. Thus, the thickness of each section is determined by dividing soil profile depth by the number of sections.

Time Information. The Simulation Duration provides the number of years to be simulated. The Initial Time Step specifies the initial time increment, which should be a function of the type of problem being solved. Problems with high-pressure gradients (e.g., infiltration into an initially very dry soil) require relatively small initial time steps. The Minimum Time Step and Maximum Time Step will specify the minimum and maximum permitted values for the time increment. The actual computation time step will automatically adjusted between these two numbers inside the model based on number of iterations required for the numerical solution of Richards' Equation. Generally, the relative error of the water balance is highly dependent on the minimum and maximum time step. Larger time steps may lead to inaccurate simulation results. Smaller time steps may provide more accurate computation but will take longer to simulate. Appropriate care should be taken to set appropriate time steps. The Output Time Step determines the temporal separation between two entries in the output data table.

Trace Element Constants. In this section, reaction constants that affect the transformation of trace elements among pools (solution phase, adsorbed phase, mineral phase, and organic phase) and constants that define solute transport are entered. Before setting the constants, the user should select the element to be evaluated. The Precip./Dissol. Rate and Dissol./Precip. Rate refers to the forward and backward precipitation-dissolution rates, respectively. In the model, the precipitation-dissolution process is simulated by a modified first order kinetics equation. The Mineralization Rate refers to the first order mineralization rate of the trace element in organic phase. The Adsorption Constant refers to the linear distribution coefficient between the solution

phase and adsorbed phase. The Longitudinal Dispersivity refers to the characteristic length that defines the spatial extent of dispersion of solutes along the flow path. The Molecular Diffusion Coeff. refers to molecular diffusion coefficient in free water.

Soil Properties

In this section, information on the properties of the soil including the soil bulk density and the soil hydraulic properties is provided. The van Genuchten soil hydraulic functions are implemented in the model and are given by:

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \\ \theta_s \end{cases}$$

$$K = K_s \sqrt{S_e} \left[1 - (1 - S_e^{1/m})^m \right]^2$$

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$m = 1 - \frac{1}{n}$$

Consequentially, five independent parameters are necessary. Theta_r is the residual water content; Theta_s is saturated water content; K_s is the saturated hydraulic conductivity; Alpha is the inverse of the air-entry value or bubbling pressure; n is a pore-size distribution index. A database of soil properties for different soils was constructed from Carsel and Parrish (1988) and Rosetta Lite (Schaap, 2001). The user can choose one of the 12 major soil textural groups and set the parameters for a specified layer. The Density refers to the soil bulk density, which is used inside the model for unit conversion. For each soil material, the user needs to enter these values. When entering Depth, the value to be entered refers to the depth of the **bottom** of the soil material layer. It does not refer to the thickness of the layer.

Initial conditions

Initial conditions for water flow and TE pools will be set in this interface. The model uses pressure head as initial conditions for water flow and will linearly interpolate it within the soil profile based on the Top Pressure Head and Bottom Pressure Head. Based on the model concept, the trace element in soils was distributed into several pools: soil solution phase, adsorbed phase, mineral phase, and organic matter phase. The soil solution phase is represented by soil solution concentration. The adsorbed phase is determined by the linear adsorption constant and soil solution concentration.

The user needs to enter the data related to initial TE pools, which include: the initial soil solution concentration (C_0), initial TE content in mineral phase (Min_0), initial TE content in organic

phase (Org_0) and total TE soil content (Total_0). The model assumes that the trace element is distributed uniformly along the soil material layer at the beginning of the simulation. If this is not the case, the user can change the number of soil materials, keep soil parameters the same, and just change the initial conditions. In other words, the user can divide a larger layer into a few smaller layers and set different initial conditions for each of them.

Inputs

In this section, the user enters information regarding input sources for the trace element. In the model, the external trace element inputs are sorted into three categories. The continuous input from Atmospheric Fallout is added to the top element of the soil profile in the mineral phase or in the mobile phase (soil solution phase plus the adsorbed phase) depending on the Fraction to Mineral Phase. The Discrete Sources from fertilizers, micronutrient, and waste disposal and so on are added uniformly as the combination of mobile, mineral and/or organic phases to the plow layer, depending on user specifications. The user can use the self-explanatory command buttons on right side to edit the information for the discrete sources, including the Time when it is applied, the Amount (g/ha), fraction to the mineral phase (Frac to Min), and fraction to the organic phase (Frac to Org). Input from irrigation water will be set in the boundary fluxes tab.

Boundary Fluxes

The atmospheric boundary condition with surface layer is set as the upper boundary condition for the water flow simulation. Thus the user needs to provide the time variable top boundary fluxes including the Precipitation (irrigation), Evaporation and Transpiration. Again the user can use the self-explanatory command buttons on right side to edit the boundary fluxes table. The default beginning time is 0. So the Time in the table is the ending time for each set of boundary fluxes, the beginning time is 0 or the time specified in the previous row. In addition, the trace element Concentration in irrigation/precipitation water needs to be provided to consider the input from irrigation.

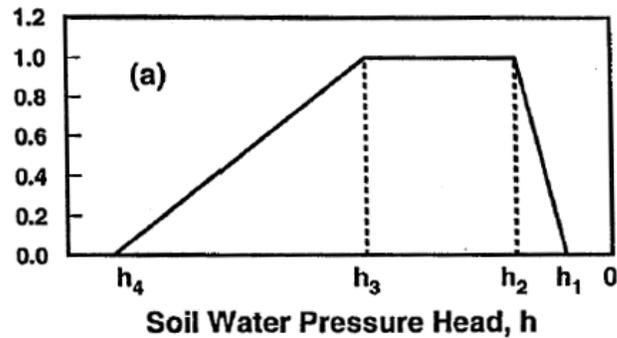
Plant Growth and Uptake

In this section, the parameters that define the plant growth and uptake of trace elements are specified. First, the user needs to specify the Number of Crops Per Annual Cycle (the default setting is 2). Inside the model, it will recycle annually. The length of each crop season is defined by the two variables the Beginning of Season and the Harvest Time. In the model, the root development is simulated by the classical Verhulst-Pearl logistic growth function with the assumption that the rooting depth will reach half of the maximum root depth in the middle of the growing season. Four parameters need to be provided for the simulation of root growth, including the Initial Root Depth, Initial Root Density, Maximum Root Depth, Maximum Root Density. A Root Distribution Coefficient is needed for distributing the root length density exponentially with soil depth. In addition, the Root Permeability Coefficient and Maximum Influx of the Michaelis-Menten kinetics equation are necessary for simulate the kinetic plant uptake of trace element. The fraction of the harvested biomass (Biomass Return Factor) that is

reincorporated should also be specified. It is assumed that comparable amounts of the trace element absorbed by plants in the previous crop season will reenter the soil in the organic form.

Root Water Uptake

The Feddes model was used for simulating the water uptake, in which the root water uptake equals the product of transpiration and a prescribed dimensionless water stress response function. The function is schematically described in the following figure (Šimunek et al., 1998).



Four pressure heads are necessary to define the water stress response function. Pressure head h_1 (P_0) represents the pressure head below which roots start to extract water from the soil. Pressure head h_2 (P_{Opt}) represents the pressure head below which roots start to extract water at the maximum possible rate. Pressure head h_3 represents the pressure head below which the roots cannot extract water at the maximum rate. Pressure head h_4 (P_3) represents the pressure head below which root water uptake ceases. Instead of giving h_3 directly, the model calculates h_3 as a function of the potential transpiration rate (T_p). The interpolation scheme is given by:

$$h_3 = \begin{cases} P_{2H} + \frac{P_{2L} - P_{2H}}{r_{2H} - r_{2L}}(r_{2H} - T_p) & \text{for } r_{2L} < T_p < r_{2H} \\ P_{2L} & \text{for } T_p \leq r_{2L} \\ P_{2H} & \text{for } T_p \geq r_{2H} \end{cases}$$

where r_{2H} and r_{2L} are the high (0.5 cm day^{-1} as default) and low potential transpiration rate (0.1 cm day^{-1} as default); P_{2H} and P_{2L} are the corresponding pressure heads for r_{2H} and r_{2L} . In all, seven parameters are necessary for the simulation of root water uptake. A database of values related to different plant types from HYDRUS 1D are available. The user can choose a set of values and set them for specified crop.

Model Output

When the computation completes, the results window will automatically appear. The outputs are organized in tabs. The model output include four parts: Input Information, Profile Distribution, Temporal Results, and Balance. The user can save the output in one folder, which will save the graphs and the data (as text and comma-separated values, which can be opened in most spreadsheet programs). The user can also use the keyboard shortcuts Ctrl+C or Ctrl+Shift+C copy any data from the data table without or with headings, respectively, onto the clipboard, from where it can be pasted into a spreadsheet program.

Input Information

The folder Input Information summarizes the input data used in the simulation.

Profile Distribution

The time dependent trace element pools distribution along with the soil profile is summarized in this tab. The user can specify the time at which the data is tabulated by the combo box of At time. Under this tab, there are more tabs containing a Data Table and plots of the concentration of each of the trace element pools at different depths in the profile. The soil depth at the middle of each section is used to represent that section. The abbreviations (C, Q, M, O, T) on the data columns represent the soil solution concentration, mobile phase, mineral phase, organic phase, and total trace element concentrations in soil, respectively.

Temporal Results

The temporal changes of trace element pools and fluxes in the entire soil profile layer or plow layer are summarized in this tab. The user can choose the layer from the Data Table tab (Choose layer combo box). The Temporal Results tab contains a Data Table tab and tabs containing plots of individual output parameters.

Balance

There are three Balance tables. The user can examine the balance between any two points in time by selecting from the Beginning time and Ending time combo boxes.

The Water Balance table summarizes the water fluxes and actual volume of water content changes in the specified period. It is used to check whether the numerical solution from HYDRUS 1D is good. If the relative error of water balance is great (for example greater than 1%), it means the time step was not well chosen, and the user should reduce the minimum time step or the maximum time step.

The Trace Element (TE) Balance table summarizes the trace element fluxes in specified period. The total trace element change should equal the sum of the three kinds of input minus the uptake and plus leaching (since leaching is negative).

The Trace Element Pools table summarizes the trace element pools in the specified period. In the model, the change in total trace element content is calculated based on the fluxes at every time step. The relative error was calculated based on the following equation:

$$E_{rel}(\%) = \frac{\int TE_{flux} - \Delta TE_{pools}}{\int TE_{flux}} \cdot 100\%$$

It is the difference between the net total flux calculated from the user interface and the calculated change in TE concentration based on fluxes at each time step, divided by the former, and multiplied by 100%.

References

- Bear J.. 1972. Dynamics of Fluid in Porous Media. Elsevier, New York, NY.
- Carsel, R.F. and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. *Water Resources Research*, 24:755-769.
- Feddes, R. A., P. J. Kowalik, and H. Zaradny. 1978. *Simulation of Field Water Use and Crop Yield*, John Wiley & Sons, New York, NY.
- Millington, R. J. and J. M. Quirk. 1961. Permeability of porous solids, *Trans. Faraday Soc.*, 57:1200-1207.
- Schaap, M.G., F.J. Leij and M. Th. van Genuchten. 2001. Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. *Journal of Hydrology*. 251:163-176.
- Šimunek, J., M. Šejna and M. Th. van Genuchten, The HYDRUS-1D software package for simulating the one-dimensional movement of water, heat, and multiple solutes in variably saturated media. Version 2.0, U.S. Salinity Laboratory, USDA, ARS, Riverside, California, 178 pp., 1998.
- van Genuchten, M. Th.. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, 44, 892-898.

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