

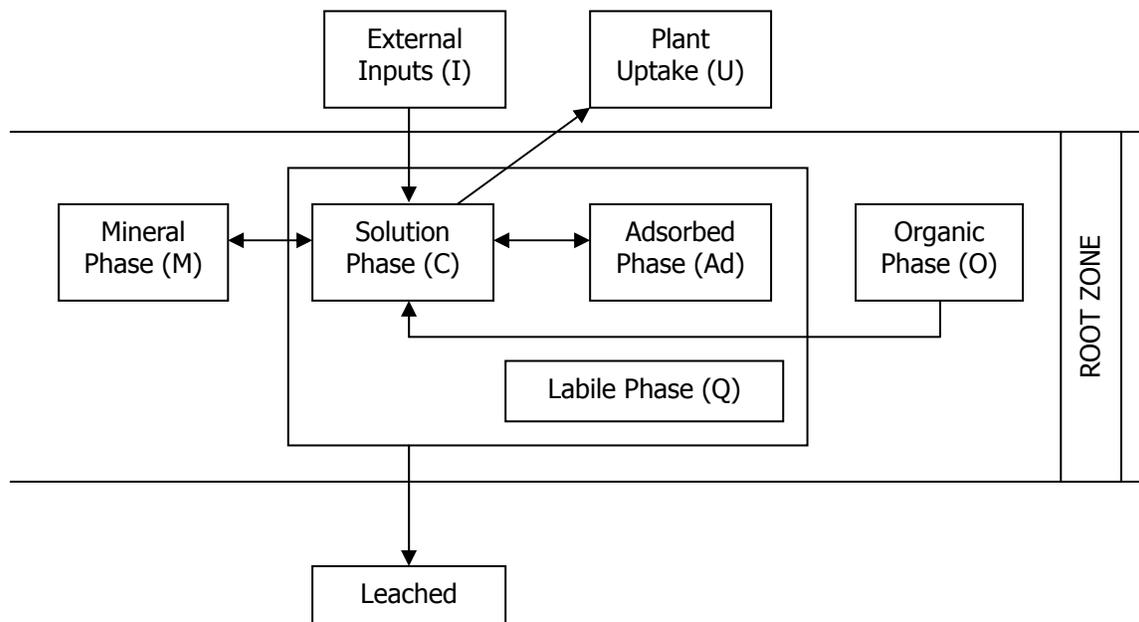
# Soil Trace Element Model (Single Layer)

## Documentation

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### Model Structure

The model was used to evaluate the long-term behavior of trace elements (TE) in cropland soils and to evaluate the effects of soil characteristics, plant uptake factors, and input sources on trace element accumulation in receiving soils. The model frame is based on mass balance. The change in total metal content (T) in the root zone is balanced with the input (I) at the soil surface, the output caused by leaching from the root zone, and by uptake removal in harvested products. In the model, dynamic uptake and leaching related to trace element soil solution concentration were adopted; two important chemical processes, adsorption-desorption and precipitation-dissolution, were considered as well, which affect the soil solution concentration dynamically. In addition, part of the plant uptake will be reintroduced into the soil through biomass return in organic form and the mineralization of the TE in organic phase will in turn contribute to the change in the soil solution. An illustration of the model structure follows.



The change in the mobile trace element concentration in soil ( $Q$ ,  $\mu\text{mol/L}$  soil) with time in a completely mixed soil layer is described by the continuity equation:

$$\frac{\partial Q}{\partial t} = -\frac{\partial F}{\partial z} + \frac{\partial M}{\partial t} + \frac{\partial O}{\partial t} - U + I \quad [\text{Eq. 1}]$$

In the model, the trace elements in mobile phase  $Q$  ( $\mu\text{mol/L}$  soil) are represented by those in solution and those adsorbed by the soil (exchangeable and surface adsorbed part), which is in instantaneous equilibrium with soil solution concentration. Thus,

$$Q = Ad + \theta \cdot C = K_d \cdot C + \theta \cdot C \quad [\text{Eq. 2}]$$

where  $K_d$  is the linear adsorption constant (L soil solution/L soil),  $\theta$  is the volumetric water content of the soil (L/L), and  $C$  is the trace element concentration in the soil solution ( $\mu\text{M}$ ).

$M$  represents another important chemical process: precipitation-dissolution, which also affects the soil solution concentration. The trace element solubility is controlled by the mineral phase and the kinetics is described by:

$$\frac{\partial M}{\partial t} = k_f(K_d + \theta)C - k_b M \quad [\text{Eq. 3}]$$

where  $k_f$  and  $k_b$  ( $\text{hr}^{-1}$ ) are the forward and backward precipitation/dissolution rate constants, respectively.

In the model, the first order mineralization process of organic matter was used:

$$\frac{\partial O}{\partial t} = -k_{im} * O \quad [\text{Eq. 4}]$$

where  $k_{im}$  is the mineralization rate constant ( $\text{hr}^{-1}$ ) and  $O$  is the organic matter content ( $\mu\text{mol/L}$  soil).

The term  $L$  represents the downward transport flux (leaching), which is described by:

$$L = K_{bf} \cdot \theta_f \cdot C \quad [\text{Eq. 5}]$$

where  $K_{bf}$  is the percolation rate ( $\text{cm hr}^{-1}$ ) at the field water content  $\theta_f$ .

The term  $U$  represents the plant uptake process that is described by:

$$U = \frac{R \cdot J}{d} \quad [\text{Eq. 6}]$$

where  $R$  is root density (cm root  $\text{cm}^{-2}$  soil) in the soil layer of depth  $d$  (cm), and  $J$  ( $\mu\text{mol cm}^{-1}$  root  $\text{hr}^{-1}$ ) is the flux of trace element uptake by the roots described by the Michaelis-Menten kinetics equation:

$$J = \frac{J_{\max} \cdot C}{K_m + C} \quad [\text{Eq. 7}]$$

where  $J_{\max}$  is the maximum  $J$  and  $K_m$  is the root permeability coefficient ( $\mu\text{M}$ ).

The term  $I$  represents the input flux of the addition of trace elements to the soil. It comprises the trace element that is found in P fertilizers, irrigation water, atmospheric deposition, and other sources.

The model integrates all of these processes and equations to evaluate the long-term behavior of TE in cropland soils.

## **Model Application**

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For running the model, the user needs to enter the data for simulation or open an existing input file. There are 7 separate sections for entering different types of information, which will be described below.

**General Information.** Here, the user specifies the simulation type to be conducted—standard, sensitivity, or uncertainty analysis. The standard analysis will perform one simulation according to the data entered, the sensitivity analysis allows the user to conduct multiple simulations by varying the value of one model parameter, and the uncertainty analysis allows the user to conduct Monte Carlo simulations according to the probability distributions of the uncertain parameters. Then, the user enters the trace element to be evaluated. This entry globally sets the element name to be displayed in all of the data summary and output files. Finally, the user selects the number of simulations to be run when uncertainty analysis is selected. This option is only available when running the uncertainty analysis. The computation time is directly dependent on the number of simulations to be conducted.

The user may go to the File menu on top left corner of the screen and selects Open Input File... (Ctrl+O). When this menu option is selected, an Open File dialog box appears to let the user choose from previously saved input files. This model ships with some default files. The data entry boxes will be loaded with data from the file. When all the boxes are filled, the user may proceed by clicking on the  button at the bottom right corner of the window. The user may manually change a value in a data entry box should it need modification. To reset the data entry boxes to a clean state, the user may selected New Input (Ctrl+N) from the File menu. The data entry boxes will be cleared and ready for entering the new data. The user may also save his/her own inputs by selected Save (Ctrl+S) or Save File As... (F12) from the File menu. Selecting Save after modifying an opened file will overwrite that file.

**Simulation Period.** The time parameters for the simulation are provided in this section. The beginning time usually is 0 and the ending time is dependent on the number of years to be simulated. Specifying 0 for beginning time and 10 for ending time should give the same result as specifying 1990 for beginning time and 2000 for ending time. The Computation Time Step specifies the time resolution of the simulation; the user enters the number of hours that each simulation time step spans. It may be set at 10 or larger. Smaller time steps may provide more accurate computation but will take longer for the simulation to finish and will require more memory. The Output Summary Time Step determines the temporal separation of each entry in the output data table.

**Initial TE Pools.** In this section, the user needs to enter the initial values for the trace element pools of the soils. TE denotes the trace element under consideration. Each entry box is self-explanatory (see Model Structure for more details). They include: concentrations in soil solution, mineral phase, organic phase, and total TE content in the soil.

**Input Information.** In this section, the user enters information on trace element inputs. The Continuous Input mode will uniformly distribute the specified input rate over each computation time step. The Point Source Input mode allows the user to enter specific days on which to add trace element to the soil. To edit the Point Source Input, click the data entry box and a table will appear for entering the inputs in tabulated form.

The model can accept continuous inputs (i.e. atmospheric fallout) and point source inputs (i.e. fertilizer applications and irrigation) simultaneously.

**Soil Properties.** In this section, information on the properties of the soil is provided. Profile Depth refers to the depth of soil being considered in the simulation. Usually, it is the depth of the root zone. Other parameters to be entered (Bulk Density, Percolation Rate, and Volumetric Water Content) are self-explanatory and correspond to the same parameters defined in the mathematical forms of the model (see Model Structure). For standard simulation and sensitivity analysis only the mean values are needed. For uncertainty analysis, the variance and probability distribution of the parameters also need to be specified.

**Plant Uptake Information.** In this section, the parameters that define the plant uptake of trace elements are specified. They include the Root Permeability Coefficient ( $K_m$ ), Maximum Influx ( $V_{max}$ ), and Root Density ( $R$ ). They correspond to the parameters in the mass balance model described in Model Structure. Among them, the Maximum Influx and Root Density are uncertain parameters and their variance and probability distribution should be specified for uncertainty analysis. In addition, the fraction of the harvested biomass that is reincorporated should also be specified. It is assumed that comparable amounts of the trace elements absorbed by plants in the previous half year will reenter the soil in the organic form.

**Constants.** In this section, reaction constants that define the transformation of trace elements among different pools are entered. They are the TE Adsorption Constant ( $K_d$ ), Mineralization Rate ( $K_{im}$ ), and the forward and backward Precipitation/Dissolution Rate ( $k_f$  and  $k_b$ ). (See equations 2, 3, and 4.)

## Results

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When data entry is completed, Click the **Run** button at the lower right corner of the screen. The simulation begins and a small screen will appear to track the progress of the computation. It generally takes only a few seconds for a standard simulation to complete. The time required for the sensitivity and uncertainty analysis is dependent on the number of simulations to be run.

When the simulation completes, a window will appear with the results. The outputs are organized into tabs.

The Simulation Parameters tab summarizes the input data used in the simulation. The user can go to the file menu on top left corner of the output screen and select Save Output (Ctrl+S) to save all the results, including simulation parameters, data tables, and graphs.

The Mass Balance tab shows the mass balance of trace element over the simulation period, including the fluxes balance (input, leaching, and uptake removal) and the pools balance (mobile phase, mineral phase, and organic phase). Theoretically, the change in total soil trace element content based on these two types of mass balance should be equal. The user can check it. If the changes are not equal, it means the model computation was not good. The user will have to adjust the time step. If the user wants to check the mass balance at any other period, it can be obtained by setting the Beginning Time and Ending Time in the output interface and clicking the Recompute button.

The Simulation Results tab show the temporal change of all the components of the trace element mass balance over the simulation period. It is further divided into tabs, one for output data table, and the rest for plots of individual output parameters. The Data Table tab tabulates the entire set of output data. A legend explaining the abbreviations in each data column is located at the bottom of the screen. Click on **Copy Selection** at the bottom right corner of the window to copy the data onto the clipboard, from where the user can paste the data into a word processing or spreadsheet program. The tabulated data in the Simulation Parameters and Mass Balance may be exported in the same manner.

## Contact

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If you encounter any bugs, please contact Weiping or Xuan as soon as possible.