

Model MIM_column

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Contents

1 Objectives	1
2 Modules	1
3 Test cases	2

1 Objectives

The model simulates solutes transport in a porous media or a soil column with a steady water flow. It uses the concept of Mobile and Immobile water to model the displacement of solute species. The model can transport several solute species at a time. Sorption of solute species is modeled with the Local Equilibrium Assumption (LEA) and linear isotherms. The steady water flow module is used to force the mobile and immobile water content and the water flux. The soil structure module is used to indicate the volume distribution and the size of soil aggregates containing the immobile water.

2 Modules

- **MIM_LEA** To solve the set of equations related to the MIM approach. Will provide the concentrations, the amount of solute species, the flux at the boundary and the cumulated flux at several time scales. The module, its inputs, outputs and parameters are described in a file attached to the module.
- **steady_water_flow** To provide the mobile and immobile water content and the steady flux of water inside the column. Please check that the flux inside the column is equal to the flux of water provided by the **sprink_solutes_file**.
- **sprink_solutes_file** To provide as function of time the concentrations of the solute species and the flux at which they are applied. Uses a file containing this information. An example is provided.
- **soil_structure_forced** To provide the bulk density and the porosity of the soil. These variables are used in the solution of the equation and in calculating the dispersivity. The module provides also the volume distribution and the size of the aggregates composing the porous media. The size of the aggregates is used by the **MIM_LEA** module to calculate the exchange rate between the mobile and immobile water.
- **homogeneous_soil_temperature** To impose a soil temperature that is used by the **MIM_column** model to calculate the diffusion coefficients.
- **bottom_solutes_conc_forced** To provide a concentration imposed at the bottom of the column. The value is used if the boundary condition of the **MIM_LEA** module is of the Dirichlet type. This is not the case in tracer transport experiments.
- **no_climate** To indicate that there is no rain.
- **no_water_runoff** To indicate that there is no runoff in this model.

3 Test cases

- **MIM_tracer_1site** Simulation with one class of aggregates (the immobile water regions are all the same). One tracer. A step input is used. A file with name **tracer_step.dat** is used containing the characteristics of the step input. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case.
- **MIM_tracer_1site_leach** Simulation with one class of aggregates (the immobile water regions are all the same). One tracer. Leaching of tracer initially in the immobile phase is simulated. A file with name **leach.dat** is used containing the characteristics of the imposed flux and concentration of the leachingsolution. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case.
- **MIM_tracer_2sites** Simulation with two classes of aggregates (the immobile water regions have two size nd occupied each a fraction of the soil volume). Size of the aggregates are provided in the module **soil_structure_forced**. One tracer. A step input is used. A file with name **tracer_step.dat** is used containing the characteristics of the step input. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case.
- **MIM_tracer_2sites_leach** Simulation with two classes of aggregates (the immobile water regions have two size nd occupied each a fraction of the soil volume). One tracer. Leaching of tracer initially in the immobile phase is simulated. A file with name **leach.dat** is used containing the characteristics of the imposed flux and concentration of the leachingsolution. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case.
- **MIM_tracer_2sites_leach_init_in_file** Simulation with two classes of aggregates (the immobile water regions have two size nd occupied each a fraction of the soil volume). One tracer. Leaching of tracer initially distributed heterogeneously in the immobile water regions is simulated. A file with name **Init_ag_MIM.dat** contains the initial situations for the immobile regions and the solutes used. This file can be duplicated and adapted to your situation. A file with name **leach.dat** is used containing the characteristics of the imposed flux and concentration of the leachingsolution. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case.
- **MIM_tracer_1site_LM** Example of parameter estimation with the Levenberg-Marquardt method. The estimated parameter is the size of the immobile water regions. A file containing the observed breakthrough curve is given as an example of file needed by the LM method. Simulation with one class of aggregates (the immobile water regions are all the same). One tracer. A step input is used. A file with name **tracer_step.dat** is used containing the characteristics of the step input. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case. ■
- **MIM_LEA_1site** Simulation with one class of aggregates (the immobile water regions are all the same). One tracer and one sorbed species. A step input is used. A file with name **tracer_step.dat** is used containing the characteristics of the step input. This file can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. It is attached to the module **sprink_solutes_file**. This file can be copied and adapted to your case.
- **MIM_LEA_2sites** Simulation with two classes of aggregates (the immobile water regions have two size nd occupied each a fraction of the soil volume). One tracer and one sorbed species. A step input is used. A file with name **tracer_step.dat** is used containing the characteristics of the step input. This file is attached to the module **sprink_solutes_file** and can be find in the directory: *.vsoil/modules/sprink_solutes_file/user_datafiles*. This file can be copied and adapted to your case. ■