Model
pest_fate_in_column

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Contents

1 Objectives

This model is an example of models that can be easily developped to simulate the fate of pesticides molecules in column experiments. The model is based on transport module **CDE_PEST** simulating concentrations in the liquid phase and concentrations on two types of sorption sites. The degradation and the sorption and desorption of a pesticide on the solid phase are simulated by a module **pest_soil_two_sites**. In this model this module also simulates the production of a metabolite. In a copy of the model, this module for pesticides degradation and sorption can be changed and replaced by another module simulating the same phenomena. The only condition is that the new module produces the inputs required by the transport module. A module is used to provide a biomass associated to organic matter decomposition. This biomass can be used in the module for pesticides degradation if required. Temperature and soil water potential are provided by two modules that return constant values (in modules homogeneous_soil_temperature and steady_water_flow). The model uses several neutral modules because the module **CDE_PEST** is the module used for building the model that simumlate the fate of pesticides in the field. In the case of laboratory experiments, some of the mechanisms existing in field conditions are ignored.

2 Modules

- **CDE_PEST** Simulates the balance of the species involved in: sorption, degradation and transport. Sorption is supposed to occur on “fast” and “slow” sites. Only one water phase is considered. The module carries out the integration of the mass balance equation for the species in solution and for the “fast” and “slow” sorption sites. A Cranck-Nicholson schema is used for integrating the differential equations. This module was specifically adapted for the simulation of pesticides fate in transport experiments, but can be easily reused or modified for any situation with sorption, degradation and exchange with a sorbent.

- **pest_soil_two_sites** Calculates the sink and source terms for a pesticides in the soil solution. A cometabolism mechanism and/or a specific metabolism are used to simulate degradation and eventually the production of a metabolite. It simulates the growth of the specific biomass.
- **OM_NRM_2001_basic** This is a organic matter decomposition module used to get a biomass carrying out the degradation by cometabolism. This module is proposed as an example and can be changed.
- **steady_water_flow** To provide the steady water content and the steady flux of water inside the column. You must check that the flux provided by the module is equal to the flux of water provided by the rain of the **climate** module added to the flux of water provided by the **sprink_solutes_file**.
- **homogeneous_soil_temperature** To impose a soil temperature that is used by the the degradation modules for PAH and organic matter.
- **soil_structure_forced** To provide the bulk density and te porosity of the soil. These variables are used in the solution of the transport equation and in calculating the dispersivity.
- **sprink_solutes_file** To impose the flux of water applied at the surface and the concentrations of the pesticides species in the applied water. Uses a file to prescribe the flux of water and the concentrations. You must check that the flux provided by the module added to the flux provided by the climate module are equal to the flux of water provided by the **steady_water_flow** module.
- The model uses also the following "neutral_" or "no_" modules:
  - **no_climate**
  - **no_crop**
  - **no_evapotranspiration**
  - **no_mulch_dynamic**
  - **no_root_water_uptake**
  - **no_water_runoff**
  - **canopy_water_transfer_neutral**
  - **split_climate**
  - **mulch_water_neutral**
  - **mulch_leaching_neutral**
  - **hydraulic_properties**

3 Test case

- **column_prodmeta_degcomet** Example of configuration file. This is transport of a pesticide **parathion**, with sorption and two types of sites, with degradation by cometabolism and production of a metabolite **paraoxon**. The metabolite is also involved in the degradation and sorption processes. This file can be copied and adapted to your case. In particular you can change the options about degradation and metabolite production in the module **pest_soil_two_sites**