

Module CDE_PEST

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1 Introduction

The platform VSOIL provides several modules for solutes transport modeling based on the convection dispersion equation (CDE). These modules differ mainly by (1) the sink and/or source terms they are able to handle, (2) the way they deal with adsorption and (3) the possible interactions with colloids and/or particle transport. This module was developed to simulate the fate of pesticides. It handles sink and source terms due sorption and desorption from two types of sites, and degradation. The module calculates the concentration of pesticides in the soil solution and the concentrations of the pesticides on the sorbing sites. This module can be associated in a model with any module simulating pesticides fate (sorption, desorption, degradation, etc) and providing the inputs described below.

2 Assumptions

- Transport in the porous medium obeys the convection dispersion equation.
- The model can deal with a water layer at the soil surface (runoff) exchanging solutes with the soil water.
- The module can handle several species at the same time.
- The module accepts sink and source terms due to sorption, desorption, degradation.

3 Balance equation for sorbed species

In addition to the part of the module solving the transport equation, the solution for the equations modeling the balance of the sorbed species is added to the compute part of the module. A Crank-Nicolson schema is used to solve the two following ordinary differential equations.

For each pesticide species the module solves a balance equation for the fast sorbing sites and the slow sorbing sites. The equation is the same for the two sites. If $S(kg.kg^{-1})$ is the sorbed concentration on a site, the equation is:

$$\frac{dS}{dt} = R - D \quad (1)$$

where $R(kg.kg^{-1}.s^{-1})$ is the sorption rate from the solution to the site, $D(kg.kg^{-1}.s^{-1})$ is the desorption rate from the site to the soil solution. R, D are provided by a module simulating the sorption and desorption processes. An example of module is for example: `pest_soil_two_sites`. When using this transport module in a model, you can use your own module to provide the R, D terms.

4 Numerical solution

Please refer to the documentation of the module `CDE_LEA` for details on the numerical solution. The two modules use the same routines and differ only by the sink/source terms and the possibility to account for mineral fertilisation.

5 Inputs

All the informations (localisation, type, description, unit) concerning a variable are available inside the VSOIL-MODULES application. Some of the inputs below are *tagged* in the sense of the VSOIL platform. The *taggs* are used to identify which transported species are concerned by the input terms. Tagged variables are indicated below by the following keyword: *[tagged]*.

- **mulch with soil contact leachate concentration** This is the concentration of the water flowing throught the mulch that is in contact with the soil. $[kg.m^{-3}]$ *[tagged]*
- **mulch without soil contact leachate concentration** This is the concentration of the water flowing throught the mulch that is not in contact with the soil. $[kg.m^{-3}]$ *[tagged]*
- **rain intensity** Rain intensity applied to the vegetation-mulch-soil continuum. $[m.s^{-1}]$.
- **rain solute mass concentration** Concentrations of the solute species in the rain. $[kg.m_w^{-3}]$ *[tagged]*
- **soil bottom solution solutes concentration** Concentrations of the solute species applied at the bottom boundary when the boundary condition is of the Dirichlet type. $[kg.m_w^{-3}]$ *[tagged]*.
- **soil bulk density** Bulk density of the soil as function of depth. $[kg.m^{-3}]$
- **soil fast sites sorbed pesticides desorption rate** Rtae of desorption of the pesticides from the fast sites. $[kg.kg^{-1}.s^{-1}]$ *[tagged]*

- **soil fast sites sorbed pesticides sorption rate** Rate of sorption of the pesticides on the fast sites. [$kg.kg^{-1}.s^{-1}$] [*tagged*]
- **soil hydraulic** Allows to access the hydraulic properties. [-]
- **soil pore volume per volume** Porosity of the soil. [$m^3.m^{-3}$].
- **soil slow sites sorbed pesticides desorption rate** Rate of desorption of the pesticides from the slow sites. [$kg.kg^{-1}.s^{-1}$] [*tagged*]
- **soil slow sites sorbed pesticides sorption rate** Rate of sorption of the pesticides on the slow sites. [$kg.kg^{-1}.s^{-1}$] [*tagged*]
- **soil solution pesticides sink** Contains the pesticides sink terms for the soil solution. Usually the sink term accounts for sorption, degradation and uptake by other mechanisms. [$kg.m_w^{-3}.s^{-1}$] [*tagged*].
- **soil solution pesticides source** Contains the pesticides source terms for the soil solution. Usually the source term accounts for desorption. [$kg.m_w^{-3}.s^{-1}$] [*tagged*].
- **soil surface runoff height** Thickness of the water layer at the soil surface [m].
- **soil surface runoff volumetric flux density** Runoff flux. [$m.s^{-1}$].
- **soil surface sprinkling irrigation rate** Instantaneous water flux applied to the vegetation-mulch-soil continuum. [$m.s^{-1}$].
- **soil surface sprinkling irrigation solute concentration** Concentrations of the solute species in the water applied. [$kg.m_w^{-3}$] [*tagged*].
- **soil surface water volumetric flux density** This is the water flux applied to the soil after influences of crop canopy and mulch have been accounted for. When there is no mulch and vegetation, this variable is equal to the soil surface sprinkling irrigation rate. [$m.s^{-1}$].
- **soil temperature** Temperature of the soil as function of depth. [K]
- **soil water volumetric content** Water volumetric content. [$m_w^3.m^{-3}$].
- **soil water volumetric flux density** This is the water flux in the soil as function of depth. [$m.s^{-1}$].

6 Outputs

The module provides the following variables. All the informations (localisation, type, description, unit) concerning a variable are available inside the VSOIL-MODULES application. Tagged variables are indicated by the following keyword: [*tagged*].

- **soil bottom solutes mass flux** Instantaneous flux of the solute species at the bottom. [$kg.m^{-2}.s^{-1}$] [*tagged*]
- **soil bottom solutes mass flux daily cumulated** Flux of the solute species at the bottom cumulated on a daily basis. [$kg.m^{-2}$] [*tagged*]

- **soil bottom solutes mass flux time cumulated** Flux of the solute species at the bottom cumulated since the start of the simulation. [$kg.m^{-2}$] [*tagged*]
- **soil fast sites sorbed pesticides mass concentration** Mass concentration of the pesticides on the fast sites. [$kg.kg^{-1}$] [*tagged*]
- **soil fast sites sorbed pesticides mass concentration profile cumulated** Amount of pesticides sorbed on the fast sites for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil slow sites sorbed pesticides mass concentration** Mass concentration of the pesticides on the slow sites. [$kg.kg^{-1}$] [*tagged*]
- **soil slow sites sorbed pesticides mass concentration profile cumulated** Amount of pesticides sorbed on the slow sites for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil solution solutes mass concentration** Concentrations of the solute species as function of depth and time. [$kg.m^{-3}$] [*tagged*] **Initial values are required for all the species. At least two points are required: surface and bottom boundaries.**
- **soil solution solutes mass concentration profile cumulated** Amount of solute species contained in the mobile water for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil surface water layer solutes exchange rate** Rate of exchange of the species between the water layer at the soil surface and the soil solution. [$kg.m^{-2}.s^{-1}$] [*tagged*]
- **soil surface water layer solutes exchange rate time cumulated** Rate of exchange of the species between the water layer at the soil surface and the soil solution cumulated in time. [$kg.m^{-2}$] [*tagged*]
- **soil surface water layer solutes molar concentration** Molar concentrations of the species in the water layer at the soil surface. [$mol.m^{-3}$] [*tagged*]
- **soil surface water layer solutes runoff rate** Amount of solute species lost by run off per unit of time and surface. [$kg.m^{-2}.s^{-1}$] [*tagged*]
- **soil surface water layer solutes runoff rate daily cumulated** Amount of solute species lost by run off during the day for a unit area. [$kg.m^{-2}$] [*tagged*]
- **soil surface water layer solutes runoff rate time cumulated** Amount of solute species lost by run off during the whole simulation period for a unit area. [$kg.m^{-2}$] [*tagged*]

7 Parameters

The description of the parameters and their characteristics are available inside the VSOIL-MODULES application when editing the module and in the Graphic User Interface. The parameters are however described hereafter. Default values are available within the platform when this is possible. **These values are given to ease the use of the module but they are not warranted and probably not correct for all the situations. The user must verify the default values.**

- **consurf**, [*logical*]. If set to **.true.** the concentration is imposed at the surface, otherwise the third-type boundary condition is used.
- **conbot**, [*logical*]. If set to **.true.** the concentration is imposed at the bottom, otherwise the free flow boundary condition is used.

- **upwind**, [*logical*]. Logical to use a upwind uncentered finite difference schema for spatial derivatives of convective terms.
- **upwind_cor**, [*logical*]. Logical to allow correction of numerical dispersion induced when UPWIND is set to **true**.
- **ech_lame**, [*listofchoices*]. To choose the mode of solute exchange between runoff water and soil water. 0: no exchange; 1: diffusion like (first-order)
- **lambda** [*m*] Dispersivity coefficient. Can be layer dependent.
- **adscoef** [$m^3.kg^{-1}$] Equilibrium constant in the linear Freundlich isotherm. As many values as species considered. Can be layer dependent. This parameter is useful if pesticide sorption is considered as instantaneous and is calculated in this module. If pesticides sorption is calculated by another module, this parameter should be left to its default value: 0.
- **codif** [$m^2.s^{-1}$] Diffusion coefficients in pure water for the simulated species. Corrections for porosity, water content and temperature are made in the module.