Modules

balance_batch_PAH

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Summary

1 Introduction

This module calculates the balance of the solutes species involved in: sorption and desorption with the soil solid phase, degradation in solution and exchange between soil solution and a sorbent (release from a compost for example) and exchange between the sorbent and the sorption sites. The module carries out the integration of the mass balance equation for the species in solution and for the "weak" and "strong" sorption sites. This module was specifically developped for the simulation of PAH fate in batch experiments, but it can be easily re-used/modified/simplified for any situation with sorption, degradation and pollutant release by added organic matter.

2 Assumptions

- Only one water phase is considered.
- Molecules are released in solution directly from the compost (hydrolysis).
- Sorption occurs on two types of sites : strong sorption sites and weak sorption sites.
- Weak sorption sites are in contact with the soil solution. For these sites, sorption and desorption are modeled as first-order kinetic processes.

- Molecules sorbed on the weak sorption sites can be reversibly exchanged with the strong sorption sites. This exchange is also modeled as a first-order kinetic process.
- Molecules in solution can be degraded.

3 Equations

With the above assumptions, the balance equation for the species in solution writes :

$$\theta \frac{dC}{dt} = So - Si - D + SSC \tag{1}$$

where

- C is the concenration of the PAH in the mobile water.
- θ is the soil mobile water volumetric content
- So is the source term due to desorption from the weak sorption sites
- Si is the sink term due to sorption on the weak sorption sites
- D is the sink term due to degradation in the soil solution
- SSC is the exchange term between the compost and the mobile water

The balance equation for the weak sorption sites writes :

$$\rho \frac{dS_w}{dt} = -So + Si - E \tag{2}$$

where :

- S_w is the mass concenration of the PAH sorbed on the weak sorption sites. Its unit is kg of PAH per kg of soil.
- ρ is the bulk density.
- So is the source term due to desorption from the weak sorption sites
- Si is the sink term due to sorption on the weak sorption sites
- E is the rate of exchange between the weak and the strong sorption sites.

The balance equation for the strong sorption sites writes :

$$\rho \frac{dS_s}{dt} = E + CSS \tag{3}$$

where :

- S_s is the mass concenration of the PAH sorbed on the weak sorption sites. Its unit is kg of PAH per kg of soil.
- ρ is the bulk density.
- E is the rate of exchange between the weak and the strong sorption sites.
- CSS is the rate of exchange between the compost and the strong sorption sites.

4 Solution

The three differential equations are solved using a Crank-Nicholson schema.

5 Inputs

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*].

- **soil bulk density** Bulk density of the soil. $[kg.m^{-3}]$
- **soil mobile water volumetric content** Soil mobile water volumetric content. $[m^3.m^{-3}]$
- **soil mobile solution organic pollutant sink** Sink term for the mobile solution corresponding to the sorption on the weak sites. This is variable Si in equations 1,2. $[kg.m^{-3}.s^{-1}]$
- **soil mobile solution organic pollutant source** Source term for the mobile solution corresponding to the desorption from the weak sites. This is variable So in equations 1,2. $[kg.m^{-3}.s^{-1}]$
- **soil mobile solution solutes degradation rate** Rate of degradation of the molecules in the soil solution. This is variable D in equation 1. $[kg.m^{-3}.s^{-1}]$
- **soil pah compost to mobile solution exchange rate** The rate of release of pah from the compost into the soil solution. This is variable SSC in equation 1. $[kg.m^{-3}.s^{-1}]$
- **soil pah compost to strong sorption sites exchange rate** The exchange rate of pah from the compost to the strong sorption sites. This is variable CSS in equation 3. $[kg.kg^{-1}.s^{-1}]$
- **soil pah weak sites to strong sites exchange rate** The exchange rate of pah from weak sorption sites to the strong sorption sites. This is variable E in equations 2,3. $[kg.kg^{-1}.s^{-1}]$

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 mobile solution concentration** Concentrations of PAH in the mobile water. $[kg.m^{-3}]$.
- **soil mobile solution concentration profile cumulated** Concentrations of PAH in the mobile water cumulated for the profile. $[kg.m^{-2}]$.

- **soil PAH weakly sorbed** Mass concentration of the PAH sorbed on the weak sites. $[kg.kg^{-1}]$. [*tagged*].
- **soil PAH weakly sorbed profile cumlated** Mass concentration of the PAH sorbed on the weak sites cumulated for the profile. $[kg.m^{-2}]$. [*tagged*].
- **soil PAH strongly sorbed** Mass concentration of the PAH sorbed on the strong sites. $[kg.kg^{-1}]$. [*tagged*].
- **soil PAH strongly sorbed profile cumulated** Mass concentration on the PAH sorbed of the strong sites cumulated for the profile. $[kg.m^{-2}]$. [*tagged*]. .
- **soil PAH solutes sorbed concentration profile cumulated** Total amount of solutes sorbed on the solid phases. Corresponds to weak and strong sites. $[kg.m^{-2}]$ [*tagged*].
- **soil solutes amount** Total amount of solutes sorbed on the solid phases and in the soil solution. $[kg.m^{-2}]$ [*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 decribed hereafter. Default values are available within the platform when this is possible. **These values are gven to ease the use of the module but they are not waranted and probably not correct for all the situations. The user must verify the default values.**

This module does not have parameter.