Modules

PAH_compost

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1 Introduction

This document is based on the publication K., Ouvrard, S., Houot, S., Lafolie, F., Garnier, P. (2018). Modelling the fate of PAH added with composts in amended soil according to the origin of the exogenous organic matter. Science of the Total Environment, 616-617, 658-668. , DOI : 10.1016/j.scitotenv.2017.10.269

The module simulates the release of PAH molecules contained in organic matter.

2 Assumptions

The module assumes that the hydrolysis of the organic matter releases PAH molecules. We assume that the PAH molecules are initially evenly retained by all the pools describing the organic matter. Given that some pools will hydrolyse faster, the amount of PAHs on the various pools will change with time. The released molecules are dissolved in the soil solution. The module also assumes that the molecules can be directly exchanged with the strong sorption sites of the soil solid phase. The module provides the PAH concentration sorbed on strong sorption sites, the flux of PAH towards the soil solution and the amount of PAH remaining within the organic matter. Organic matter containing PAH can be added at any time.

3 Equations

The mass concentration of the PAH retained in the organic matter obeys the following differential equation :

$$\frac{dS}{dt} = \frac{1}{MO}\frac{dMO}{dt}S - k_{cs}S \tag{1}$$

where

- S is the mass concenration of the PAH retained on the organic matter. Its unit is kg of PAH per kg of carbon of the organic matter.
- MO is the organic matter mass ratio with unit : kilogram of carbon per kilogram of soil
- $\frac{dMO}{dt}$ is the hydrolysis rate of the organic matter. It is the sum of the mass ratio changes of the various pools. Pools with a mass ratio increasing are not considered.
- k_{cs} is the time constant for the sorption process from the organic matter towards the strong sorption sites.

Following this equation, the flux of PAH towards the mobile water phase is simply given by : $-\rho\frac{dMO}{dt}S$. The multiplication by the bulk density ρ allows to have a rate expressed in mass per volume of soil per time unit.

The flux of PAH towards the strong sorption sites is simply given by :$k_{cs}S$. Its unit is mass of PAH per mass of soil per time unit.

4 Solution

The first order differential equations (eq. 1) is solved with a fully implicit method. This gives :

$$S(t+dt) = \frac{1}{1 + k_{cs}dt - \frac{dtdMO/dt}{MO}} \tag{2}$$

where dt is the time increment used. The time constant k_{cs} for kinetic sorption on the strong sorption sites is usually small. In consequence, there is no constraint on the time increment being assumed that it is usually less than 1 hour in simulations involving transport.

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*].

- **organic fertilizer pah surfacic mass** Mass of PAH contained in the organic fertilizer applied. Unit is kg of PAH per m2 of soil. $[kg.m^{-2}]$.
- **soil organic fertilizer incorporation depth** Depth of soil considered for incorporation of the organic fertilizer applied. $[m]$.

- **soil bulk density** Bulk density of the soil. $[kg.m^{-3}]$
- **soil organic matter pools carbon mass ratio** Amount of carbon in the pools used to describe the organic matter. Unit is : kgC/kg soil. $[kg.kg^{-1}]$. [*tagged*].
- **soil organic matter pools decomposition rate** Organic matter pools decomposition rates. Unit is : kgC/kg soil/s. $[kg.kg^{-1}.s^{-1}]$. [*tagged*].

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*].

- **c_co2 pah production rate by cometabolism** Production rate of CO2 due to PAH decomposition by the cometabolism pathway. Expressed as C_CO2. $[kgC.kg^{-1}.s^{-1}]$
- **c_co2 pah production rate by specific biomass** Production rate of CO2 due to PAH decomposition by the specific biomass. Expressed as C_CO2. $[kg.kg^{-1}.s^{-1}]$
- **c_co2 pah metabolites production rate** Production rate of CO2 due to metabolites decomposition. Expressed as C_CO2. $[kg.kg^{-1}.s^{-1}]$
- **c_co2 pah production rate** Global production rate of CO2 due to PAH decomposition. It is the sum of the three previous variables. $[kg.kg^{-1}.s^{-1}]$
- **c_co2 pah production rate profile cumulated** Global production rate of CO2 due to PAH decomposition cumulated for the whole profile. $[kg.m^{-2}.s^{-1}]$
- **c_co2 pah production rate profile time cumulated** Global production rate of CO2 due to PAH decomposition cumulated in time and for the whole profile . $[kg.m^{-2}]$
- **soil mobile solution solutes degradation rate** Degradation rate of molecules in liquid mobile phase. Unit is : kg.m-3.s-1 or mol.m-3.s-1 depending on the unit used for the concentrations.. $[kg.m^{-3}.s^{-1}]$ [*tagged*]
- **soil mobile solution solutes degradation rate profile cumulated** Degradation rate of molecules in liquid mobile phase for the whole profile .$[kg.m^{-2}.s^{-1}]$ [*tagged*]
- **soil mobile solution solutes degradation rate profile time cumulated** Degradation rate of molecules in liquid mobile phase for the whole profile cumulated in time $[kg.m^{-2}]$ [*tagged*]
- **soil pah metabolites mass concentration** Mass concentration of the metabolites produced by the degrdation of the PAH $[kg.kg^{-1}]$ **Initial values are required for all the species. At least two points are required : surface and bottom boundaries.**

- **soil pah metabolites mass concentration profile cumulated** Mass concentration of the metabolites produced by the degrdation of the PAH for the whole profile $[kg.m^{-2}]$
- **soil pah non extractible mass concentration** Total amount of non extractible PAH. It corresponds to the sum of the biologically bounded residues and of the strongly sorbed residues.$[kg.kg^{-1}]$ $[tagged]$
- **soil pah non extractible mass concentration profile cumulated** Total amount of non extractible PAH for the whole profile. $[kg.m^{-2}]$ $[tagged]$
- **soil pah residues biological bounded** Non extractable residues (NER) formed by microbiological processes and bounded to the biomass. $[kg.kg^{-1}]$ $[tagged]$ **Initial values are required for all the species. At least two points are required : surface and bottom boundaries.**
- **soil pah residues biological bounded profile cumulated** Non extractable residues for the whole profile $[kg.m^{-2}]$ $[tagged]$
- **soil specific microbial biomass mass ratio** Quantity of specific microbial and/or micorhizal biomass that contributes to the degradation. $[kg.kg^{-1}]$ **Initial values are required. At least two points are required : surface and bottom boundaries.**
- **soil specific microbial biomass mass ratio profile cumulated** Quantity of specific microbial and/or micorhizal biomass for the whole profile. $[kg.m^{-2}]$

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.**

- **deg_hap**, $[kg.kg^{-1}.s^{-1}]$, Degradation time constant for the cometabolism way (kg C of PAH/kg soil/s). This is parameter δ in equation 3.
- **beta** $[NA]$. Ratio of metabolites to CO_2 productions for the cometabolism degradation pathway (0 to 1) This is parameter β in equation 3.
- **k_MB** $[s^{-1}]$, Time constant for transformation of metabolites into residues bounded to the biomass compartment. This is parameter k_{mb} in equation 2.
- **k_BC** $[s^{-1}]$, Time constant for mineralization of metabolites bounded to the biomass compartment. This is parameter k_{bc} in equation 4.

- **Ks_spe** $[kg.kg^{-1}]$,Half saturation constant for PAH degradation by a specific biomass with a Monod equation. This is parameter K_s in equation 1.
- **k_M** $[s^{-1}]$ Mortality time constant for the specific biomass degrading PAH. This is parameter k_m in equation 1.
- **mu_spe_max** $[kg.kg^{-1}.s^{-1}]$ Maximum growth rate for the specific biomass degrading PAH. It is the maximum amount of carbon from PAH per unit mass of specific biomass per unit time that can be transformed into microbial specific biomass. Used to calculate the parameter μ (eq.1) using the vantHoff and Andren models for accounting for temperature and soil water potential effects on microbial activity.
- **y_spe** $[NA]$ Specific biomass yield for the decomposition of the PAH by a specific biomass (kg biomass/kg metabolite). This parameter Y_s used in equations 3 and 7.
- **alpha** $[NA]$ Ratio: (metabolites production rate) / (PAH degradation rate) by the specific degradation way. This is parameter α in equations 3 and 7.
- **tempref** $[K]$ Reference temperature for vantHoff model.
- **qvanthoff** $[NA]$ Parameters of the vantHoff model.
- **pot_opt** $[m]$ Optimum potential for Andren model
- **pot_min** $[m]$ Minimum potential for Andren model
- **init_biomass_soil** $[kg.kg^{-1}]$ The initial cometabolism microbial biomass concentration in soil before compost application. This is parameter B_{ini} in equation 3.