

# Modules

## PAH\_sorption

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### Summary

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Assumptions</b>	<b>1</b>
<b>3</b>	<b>Equations</b>	<b>2</b>
<b>4</b>	<b>Solution</b>	<b>2</b>
<b>5</b>	<b>Inputs</b>	<b>3</b>
<b>6</b>	<b>Outputs</b>	<b>3</b>
<b>7</b>	<b>Parameters</b>	<b>4</b>

## 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 calculates the rates of sorption and desorption of PAH molecules on the soil solid phase.

## 2 Assumptions

Sorption is assumed to occur on two types of sites : strong sorption sites and weak sorption sites. On weak sorption sites, sorption and desorption can occur and are modeled as first-order kinetic processes. In addition, it is assumed that molecules sorbed on the weak sorption sites can be reversibly exchanged with the strong sorption sites. This exchange is modeled as a first-order kinetic process.

### 3 Equations

With the above assumptions, the rate of exchange from the weak sorption sites to the mobile solution writes :

$$desorp = k_{wa}W_S\rho \quad (1)$$

and *sorp* the rate of sorption writes :

$$sorp = k_{aw}C\theta \quad (2)$$

where

- $W_S$  is the mass concentration of the PAH sorbed on the weak sorption sites. Its unit is kg of PAH per kg of soil.
- $C$  is the concentration of the PAH in the mobile water.
- $\rho$  is the bulk density.
- $\theta$  is the soil mobile water volumetric content
- $k_{wa}$  is the time constant for the sorption process from the mobile water to the weak sorption sites.
- $k_{aw}$  is the time constant for the desorption process from the weak sorption sites to the mobile water.

The exchange of PAH between the weak sorption sites and the strong sorption sites is simply given by :

$$exchws = k_{ws}W_S - k_{sw}S_S \quad (3)$$

where :

- $W_S$  is the mass concentration of the PAH sorbed on the weak sorption sites. Its unit is kg of PAH per kg of soil.
- $S_S$  is the mass concentration of the PAH sorbed on the strong sorption sites. Its unit is kg of PAH per kg of soil.
- $k_{ws}$  is the time constant for the sorption process from the weak to the strong sorption sites.
- $k_{sw}$  is the time constant for the desorption process from the strong to the weak sorption sites.

### 4 Solution

The evaluation of the terms at each node grid is straightforward. An upper bound for the time increment is calculated by :

$$dt_{max} = \frac{1}{\max(k_{aw}, k_{wa}, k_{ws}, k_{sw})} \quad (4)$$

## 5 Inputs

Some of the inputs below are *tagged* in the sense of the VSOIL platform. The *tags* are used to identify which transported species are concerned by the input terms. Tagged variables are indicated below by the following keyword : [*tagged*].

- **soil mobile solution concentration** Concentrations of PAH in the mobile water. [ $kg.m^{-3}$ ].
- **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 PAH weakly sorbed** Mass concentration of the PAH sorbed of the weak sites. [ $kg.kg^{-1}$ ]. [*tagged*].
- **soil PAH strongly sorbed** Mass concentration of the PAH sorbed of the strong sites. [ $kg.kg^{-1}$ ]. [*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*].

- **soil mobile solution organic pollutant sink** This is the sorption rate for organic pollutants contained in mobile water. The term will be used as a sink term in a transport or balance module for species in solution. Beware of the unit. 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 organic pollutant sink profile cumulated** This is the sorption rate for organic pollutants contained in mobile water cumulated for the profile. Beware of the unit. Unit is :  $kg.m^{-2}.s^{-1}$  or  $mol.m^{-2}.s^{-1}$  depending on the unit used for the concentrations. [ $kg.m^{-2}.s^{-1}$ ] [*tagged*]
- **soil mobile solution organic pollutant sink profile time cumulated** This is the sorption rate for organic pollutants contained in mobile water cumulated for the profile and cumulated in time. Beware of the unit. Unit is :  $kg.m^{-2}$  or  $mol.m^{-2}$  depending on the unit used for the concentrations. [ $kg.m^{-2}$ ] [*tagged*]
- **soil mobile solution organic pollutant source** This is the desorption rate for organic pollutants sorbed on the weak sites. The term will be used as a source term in a transport or balance module for species in solution. Beware of the unit. 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 organic pollutant source profile cumulated** This is the desorption rate for organic pollutants sorbed on the weak

sites cumulated for the profile. Beware of the unit. Unit is :  $\text{kg.m-2.s-1}$  or  $\text{mol.m-2.s-1}$  depending on the unit used for the concentrations.  $[\text{kg.m}^{-2}.\text{s}^{-1}]$  *[tagged]*

- **soil mobile solution organic pollutant source profile time cumulated** This is the desorption rate for organic pollutants sorbed on the weak sites cumulated for the profile and cumulated in time. Beware of the unit. Unit is :  $\text{kg.m-2}$  or  $\text{mol.m-2}$  depending on the unit used for the concentrations.  $[\text{kg.m}^{-2}]$  *[tagged]*
- **soil pah weak sites to strong sites exchange rate** Exchange rate of oranic pollutants between the weakly sorbed compartment and the strongly sorbed one. Beware of the unit. Unit is :  $\text{kg.kg-1.s-1}$  or  $\text{mol.kg-1.s-1}$  depending on the unit used for the concentrations.  $[\text{kg.kg}^{-1}.\text{s}^{-1}]$  *[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 given 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.**

- **k\_wa** [ $\text{s}^{-1}$ ], Time constant for desorption from the weak sorption sites to the mobile water. This is parameter  $k_{wa}$  in equation 1.
- **k\_aw** [ $\text{s}^{-1}$ ], Time constant for sorption from the mobile water to the weak sorption sites. This is parameter  $k_{aw}$  in equation 2.
- **k\_ws** [ $\text{s}^{-1}$ ], Time constant for sorption from the weak sorption sites to the strong sorption sites. This is parameter  $k_{ws}$  in equation 3.
- **k\_sw** [ $\text{s}^{-1}$ ], Time constant for desorption from the strong sorption sites to the weak sorption sites. This is parameter  $k_{sw}$  in equation 3.