

Modules

pest_two_sites

François Lafolie

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1 Introduction

This document is based on the publication:

K. Saffih-Hdadi, L. Bruckler, F. Lafolie, E. Barriuso, 2006. A Model for Linking the Effects of Parathion in Soil to its Degradation and Bioavailability Kinetics. *J. of Environmental Quality*. <https://doi.org/10.2134/jeq2005.0059>

The module simulates the degradation and the sorption of a pesticides and its metabolite produced by degradation. Characteristics of this module derived for the Parathion and its metabolite Paraoxon are described below and in the publication. This module can be used for other situations similar to this one.

2 Assumptions

The module calculates the rates of degradation of a mother molecule and the production of the metabolite molecule. Degradation of the two molecules can be due: (1) a specific biomass growing with the degradation of the molecules, (2) a cometabolism degradation using a biomass involved in the organic matter cycle, (3) degradation by the two ways. Degradation rates depend on the temperature and the soil water potential. Options are available to choose the degradation mechanism for the two molecules. The module simulates also the rates of sorption and desorption of the two molecules on the soil solid phase. Sorption is assumed to occur on two types of sites: fast sorption sites and slow sorption sites. Sorption and desorption mechanisms are modeled as first-order kinetic processes.

Equations are available in the publication.

3 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 fast sites sorbed pesticides mass concentration** Concentration of the pesticides molecules on the fast sorption sites of the soil matrix. [$kg.kg^{-1}$]
- **soil hydraulic** Indicates that the module has access to the hydraulic properties.
- **soil organic matter pools carbon mass ratio** Ratio between the mass of carbon and the mass of solid phase in the pools used to described the organic matter. [$kg.kg^{-1}$]
- **soil slow sites sorbed pesticides mass concentration** Concentration of the pesticides molecules on the slow sorption sites of the soil matrix. [$kg.kg^{-1}$]
- **soil solution solutes mass concentration** Concentrations of the solute species (among which pesticides) in the soil water. [$kg.m^{-3}$].
- **soil temperature** Temperature of the soil. [K].
- **soil water matrix potential** Water matrix potential at grid nodes. [m].
- **soil water volumetric content** Soil water volumetric content. [$m^3.m^{-3}$]

4 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 fast sites sorbed pesticides desorption rate** This is the rate the pesticides molecules are desorbed from the fast sorption sites. The term will be used as a source term in a transport or balance module for species in solution. [$kg.kg^{-1}.s^{-1}$] *[tagged]*
- **soil fast sites sorbed pesticides sorption rate** This is the rate the pesticides molecules are sorbed on the fast sorption sites. The term will be used as a sink term in a transport or balance module for species in solution. [$kg.kg^{-1}.s^{-1}$] *[tagged]*
- **soil slow sites sorbed pesticides desorption rate** This is the rate the pesticides molecules are desorbed from the slow sorption sites. The term will be used as a source term in a transport or balance module for species in solution. [$kg.kg^{-1}.s^{-1}$] *[tagged]*
- **soil slow sites sorbed pesticides sorption rate** This is the rate the pesticides molecules are sorbed on the slow sorption sites. The term will be used as a sink term in a transport or balance module for species in solution. [$kg.kg^{-1}.s^{-1}$] *[tagged]*
- **soil solution pesticides degradation rate** Degradation rate of the pesticides molecules in the soil solution. [$kg.m^{-3}.s^{-1}$] *[tagged]*

- **soil solution pesticides sink** This term is the soil solution pesticides sink resulting from the sorption rates. To be used in a module carrying the mass balance or transport. [$kg.m^{-3}.s^{-1}$] [*tagged*]
- **soil solution pesticides source** This term is the soil solution pesticides source resulting from the desorption rates. To be used in a module carrying the mass balance or transport. [$kg.m^{-3}.s^{-1}$] [*tagged*]

5 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.**

- **ioprod_met** [*choices*] To produce or not a metabolite during degradation of the mother molecule.
- **iopbiodeg** [*choices*] To choose among the following choices for the mother molecule: No degradation, Degradation by cometabolism, Degradation by specific metabolism, Degradation by the two metabolisms together.
- **iopbiodeg_met** [*choices*] To choose among the following choices for the metabolite molecule: No degradation, Degradation by cometabolism, Degradation by specific metabolism, Degradation by the two metabolisms together. ■
- **convspe** [], Convergence criteria for the algorithm used with the specific metabolism.
- **itermaxspe** [], Maximum number of iterations for the algorithm used with the specific metabolism.
- **tref_pest** [K] Reference temperature at which the parameters below for the pesticide were obtained.
- **tref_met** [K] Reference temperature at which the parameters below for the metabolite were obtained.
- **psiref_pest** [m] Soil water potential at which the parameters below for the pesticide were obtained.
- **psiref_met** [m] Soil water potential at which the parameters below for the metabolite were obtained.
- **pfopt** [] pF of the optimum soil water potential for microbial activity.
- **pfmin** [] pF of the minimum soil water potential for microbial activity.
- **qpest** [] Parameters of the Van'Hoff model for effects of soil temperature on microbial activity. 9 values are required for the 5 degrees temperature interval.
- **k1_pest** [s^{-1}] Time constant for sorption of pesticide on fast sites.
- **k2_pest** [s^{-1}] Time constant for desorption of pesticide from the fast sites.

- **k3_pest** [s^{-1}] Time constant for sorption of pesticide on slow sites.
- **k4_pest** [s^{-1}] Time constant for desorption of pesticide from the slow sites.
- **vcom_pest** [s^{-1}] Time constant for biodegradation by cometabolism.
- **bmspe_pest_init** [$kg.kg^{-1}$] Initial value of Specific biomass for degradation of pesticide. Unit is kg par kg of soil.
- **yspe_pest** [$kg.kg^{-1}$] Yield of pesticide degradation by the specific biomass growth. Unit is kg of biomass per kg of pesticide.
- **vmax_spe_pest** [s^{-1}] Maximum growth time constant for the specific biomass on the pesticide.
- **km_spe_pest** [kg] Michaelis constant for the growth rate of the specific biomass on the pesticide.
- **dead_spe_pest** [s^{-1}] Time constant for the mortality of the specific biomass.
- **k1_meta** [s^{-1}] Time constant for sorption of metabolite on fast sites.
- **k2_meta** [s^{-1}] Time constant for desorption of metabolite from the fast sites.
- **k3_meta** [s^{-1}] Time constant for sorption of metabolite on slow sites.
- **k4_meta** [s^{-1}] Time constant for desorption of metabolite from the slow sites.
- **vcom_met** [s^{-1}] Time constant for biodegradation of metabolite by cometabolism.
- **fcom_met** [] Ratio of metabolite produced by biodegradation of the pesticide by the cometabolism biomass.
- **bmspe_met_init** [$kg.kg^{-1}$] Initial value of Specific biomass for degradation of the metabolite. Unit is kg par kg of soil.
- **yspe_met** [$kg.kg^{-1}$] Yield of metabolite degradation by the specific biomass growth. Unit is kg of biomass per kg of metabolite.
- **vmax_spe_met** [s^{-1}] Maximum growth time constant for the specific biomass on the metabolite.
- **km_spe_met** [kg] Michaelis constant for the growth rate of the specific biomass on the metabolite.
- **fspe_met** [] Ratio of metabolite produced by biodegradation of the pesticide by the specific biomass.
- **dead_spe_met** [s^{-1}] Time constant for the mortality of the specific biomass for the metabolite.
- **biomass_tag** [s^{-1}] Tag of the required biomass pool for cometabolism. The tag is needed to find the biomass pool among the organic matter pools passed to the module. A default value is the tag: **AUB**