Module
MIM_LEA

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Contents

1 Introduction

The platform VSOIL provides several modules for solutes transport modeling based on the mobile-immobile water concept. 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 particles transport. The hypotheses and the main characteristics of the resolution of the equations appearing in the MIM module are decribed hereafter for the case of species acting as tracers or species for which interactions with the solid phase can be modeled by mean of the LEA (Local Equilibrium Assumption) model, i.e. instantaneous equilibrium.

2 Assumptions

- Two regions are considered for water: mobile water where the flux takes place and immobile water acting as a reservoir interacting with the mobile water [1] [4].

- Transport in the mobile water region obeys the convection dispersion equation.
- Exchange of solute species between the two water regions obeys a first-order equation based on concentrations gradients
- The exchange coefficient between the mobile and immobile water depends on the characteristic size of the immobile regions and on the saturation index of the mobile region.
- We assume that the immobile region can be made of soil volumes having different characteristic sizes and thus exchanging solutes with the mobile water at different rates [2].
- Interactions with the solid phase uses the LEA assumption for the mobile and immobile regions. We restrict to linear isotherms.
- There is no interaction with particles transport.
- The model can deal with a water layer at the soil surface (runoff) exchanging solutes with the soil water.

3 Equations

For the mobile water, the equation combines the convection dispersion, the exchange term with the immobile regions, and sink and source terms. It writes:

$$\underbrace{\frac{\partial R_m C_m}{\partial t}}_{Storage} = \underbrace{\frac{\partial}{\partial z}(\theta D \frac{\partial C_m}{\partial z})}_{Dispersion} - \underbrace{\frac{\partial q C_m}{\partial z}}_{Convection} \underbrace{- (1-n_s)\sum_{j=1}^{N_C} f_j \gamma_j (C_m - Cag_j)}_{Exchange} + \underbrace{\Gamma_m}_{Sinks-Sources} \quad (1)$$

The terms appearing in the equation are described hereafter. They all depend on depth z, either directly or indirectly because they depend on variables that are depth dependent.

One have the following definitions:

1. R_m $[-]$ Retardation factor. R_m is calculated by: $R_m = 1 + \frac{\rho k}{\theta_m}$
2. θ_m $[m_w^3.m^{-3}]$ Mobile water volumetric content. The index $_w$ indicates a volume of soil solution.
3. ρ $[kg.m^{-3}]$ Bulk density of the soil.
4. k $[m_w^3.kg^{-1}]$ Slope of the linear isotherm for sorption on the solid phase.
5. t $[s]$ Time
6. z $[m]$ Depth
7. C_m $[kg.m_w^{-3}]$ Concentration (s) of the mobile water.
8. D $[m^2.s^{-1}]$ Hydrodynamic dispersion.
9. q $[m.s^{-1}]$ Darcy's flux.
10. n_s Maximum ratio of the volume occupied by the mobile water.
11. N_C is the number of classes of immobile water regions having a different characteristic size

12. f_j is the fraction of soil volume occupied by the immobile water region j. $\sum f_j = 1$

13. γ_j $[s^{-1}]$ is the exchange rate coefficient for the class j.

14. Ca_j $[kg.m_w^{-3}]$ is the solutes concentration in the immobile water regions of class j.

15. Γ_m $[kg.m^{-3}.s^{-1}]$ is a term accounting for the sink and sources acting on the solutes species transported.

For each immobile water region j, the mass balance equation writes:

$$\underbrace{\frac{\partial Ra_j Ca_j}{\partial t}}_{Storage} = \underbrace{\gamma_j(C_m - Ca_j)}_{Exchange} + \underbrace{\Gamma_j}_{Sink-Sources} \tag{2}$$

One have the following definitions:

1. Ra_j $[-]$ Retardation factor. Ra_j is calculated by: $Ra_j = 1 + \frac{\rho_a k}{\theta_a}$

2. θ_a $[m_w^3.m_a^{-3}]$ water volumetric content in the region j. The index $_w$ indicates a volume of soil solution. The index $_a$ indicates a volume of soil in the immobile region j.

3. ρ_a $[kg.m^{-3}]$ Bulk density of the soil of region j.

4. k $[m_w^3.kg^{-1}]$ Slope of the linear isotherm for sorption on the solid phase.

5. t $[s]$ Time

6. C_m $[kg.m_w^{-3}]$ Concentration (s) of the mobile water.

7. Γ_j $[kg.m^{-3}.s^{-1}]$ is a term accounting for the sink and sources acting on the solutes species in the class j

In the following we assume that the water volumetric content θ_a and the bulk density ρ_a are the same for all the immobile water regions. The storage term in this equation is expressed with respect to the volume of the immobile region and so has the unit: $[kg.m_a^{-3}.s^{-1}]$. Multiplying each member by the term $n'_s = (1 - n_s)$ we obtain the unit: $[kg.m_s^{-3}.s^{-1}]$ for all the terms (storage, exchange and sinks). Using n'_s, and the homogeneous values of θ and k for the classes, we have:

$$n'_s Ra_j = n'_s(\theta_a + \rho_a k) =$$
$$n'_s(\theta_a) + n'_s \rho_a k = \theta_{im} + \rho_d k = R_{im}$$

The storage coefficient Ra_j is indepedent of the class considered. The equation becomes:

$$\frac{\partial R_{im} Ca_j}{\partial t} = n'_s \gamma_j (C_m - Ca_j) + n'_s \Gamma_j$$

wher R_{im} is the retardation factor for the immobile regions.

3.1 Surface boundary condition

At the soil surface a Cauchy condition is used (flux imposed). During evaporation periods, the flux is zero. During infiltration periods, this flux is the product of the water flux entering the soil q by the concentration of the water C_s (concentration of the rain, irrigation water, runoff water). When there is no water accumulation at the soil surface, the boundary condition writes:

$$\left[-\theta D \frac{\partial C_m}{\partial z} + qC_m\right]_{z=0} = qC_s \tag{3}$$

When water accumulates at the soil surface, one must account for possible exchanges between the water layer and the water in the porous medium. This requires also to have an equation to simulate the concentrations in the water layer at the soil surface in response to exchanges with the soil and to inputs from either water application or runoff.

3.1.1 Balance equation for the water layer and corresponding boundary condition

Let $\epsilon(t)$ be the thickness of the water layer. In case of runoff, $\epsilon(t)$ is calculated by a module managing runoff. Let C_l be the concentrations of the species in the water layer. The mass balance equation for the species in the water layer writes:

$$\underbrace{\frac{d\epsilon C_l}{dt}}_{Storage} = \underbrace{PC_p}_{Inputs} - \underbrace{qC_l + \gamma_l(C_1 - C_l)}_{ExchangesWaterLayer-Soil} \tag{4}$$

The term *Inputs* corresponds to amounts brought in by the rain or the irrigation, where P is the flux applied and C_p is the corresponding concentrations. The exchange term has a convective part qC_l where q is the water flux entering the soil and a first-order term $\gamma_l(C_1 - C_l)$ to account for the diffusive exchanges between the water layer and the soil. Estimation of γ_l is analogous to what is done to calculate characteristic times for exchange between aggregates and mobile water in chemical engineering models. γ_l is given by:

$$\gamma_l = \frac{2D_0}{\epsilon(t)} \tag{5}$$

where D_0 is the diffusion coefficient in the soil.

With this assumption, the boundary condition writes:

$$\left[-\theta D \frac{\partial C_m}{\partial z} + qC_m\right]_{z=0} = qC_l - \gamma_l(C_{m_{z=0}} - C_l) \tag{6}$$

The only difference with the previous (eq. 3) is the presence of the first-order exchange term. This term vanishes when there is no water layer at the soil surface. This condition is used in the module.

3.2 Boundary condition at the bottom of the profile

The module offers two possibilities: Imposed concentrations or a free drainage condition. This last condition corresponds to a flux of solutes downwards due only to convection (no concentration gradients at the boundary). This condition is most often used. It writes:

$$\left[\frac{\partial C_m}{\partial z}\right]_{z=L} = 0 \tag{7}$$

3.3 Initial Conditions

The module requires that initial concentrations be provided for the mobile water concentration and for the immobile water. For the immobile water, one have the possibility to impose the same concentrations in all the classes of immobile water or to impose the initial situation for each class of immobile water. Parameters are available for select among these two possibilities. Values must be given at least for the soil surface and the bottom boundary. A linear interpolation is used to calculate the initial situation at grid nodes from the values provided.

3.4 Estimation of Hydrodynamic Dispersion

The hydrodynamic dispersion is linked to the diffusion coefficient and to the water flux by the following relationship:

$$D(z) = D_0 + \lambda \frac{q}{\theta_m} \tag{8}$$

where θ_m is the water volumetric content D_0 is the diffusion coefficient in the soil $[m^2.s^{-1}]$ and λ is the dispersivity of the porous medium. λ has the dimension of a length $[m]$.

The parameter λ acconts for the dispersion coefficient dependence on the geometry of the water fill pore space. The dispersion coefficients depends also on D_0 but essentially for low velocity flows. The diffusion coefficients depends on the water content and on temperature. The following relationship is used is the module:

$$D_0 = D_{mol} \frac{T}{293} \frac{\theta_m^{10/3}}{n^2} \tag{9}$$

where D_{mol} is the molecular diffusion coefficient, n the porosity and T the temperature (K) The subroutine `vsoil_dispers`, available in the platform, uses this formulation to provide the dispersion coefficient.

3.5 Estimation of Exchange Coefficients

We assume that immobile water regions with different characteristic size are present simultaneously. The characteristic diffusion time inside the aggregates (or immobile water regions) is given by:

$$t_D = \frac{1}{\gamma} = r^2/15D \tag{10}$$

where r is a characteristc size (radius) and D the diffusion coefficient within the immobile water. Given that the macroporosity can be unsaturated and given that the aggregates have contact surfaces corresponding to no-flux conditions, an effective radius can be calculated as follows (see the option `corrected_radii`). First for an aggregate with surface S, the surface in contact with other aggreates is estimated by [3]:

$$S_c = \frac{0.44 - n_s}{0.44} S \tag{11}$$

The surface in contact with the mobile water is estimated as:

$$S_m = \sqrt{i_{ns}}(S - S_c) \tag{12}$$

where i_{ns} is the saturation index of the macroporosity. Combining these equations gives the external surface in contact with mobile water:

$$Sm = \frac{\sqrt{\theta_m n_s}}{0.44} S \tag{13}$$

The ratio volume versus surface gives the effective radius or characteristic size:

$$r_{eff} = \frac{0.44}{\sqrt{\theta_m n_s}} r \tag{14}$$

The exchange coefficient γ is then calculated by:

$$\gamma = \frac{15D}{r_{eff}^2} \tag{15}$$

The subroutine `vsoil_MIM_CN_cal_echcoef`, available in the platform, does this calculus and provides outputs used to build the linear system.

4 Numerical solution

The module uses first the routine `vsoil_dispers` to calculate the hydrodynamic dispersion. Next, the routine `vsoil_MIM_CN_cal_echcoef` is used to calculate the exchange coefficients and variables used by the routine `vsoil_MIM_CN_contri_twph` to caclulate the contributions of the exchange process to the second member of the linear system. The module uses the routines `vsoil_calfluxhyd_int` to calculate the internodal water flux and the routine `vsoil_cal_part_const_cde_c` to calculate the contribution of convection to the matrix of the linear system. This is done only one time if several solute species are considered. Next,the routine `vsoil_MIM_CN` which implements a Crank-Nicholson time schema with a second-order finite difference approximation for the space derivatives is used to build the linear system. The solution is obtained with the routine `vsoil_thomas`. The solution in the immobile regions is next calculated with the routine `vsoil_MIM_CN_resimo`. The module has an option to use centered or upwind schema for the spatial discretisation of the convective term. If needed, the equation for the exchange with a soil surface water layer is solved simultaneously with the transport equation and this leads to a modified term in the second member of the linear system. For this, the module uses the routine `vsoil_res_lam_dif`. The module uses the finite difference grid provided by the platform. This grid can be irregular. The parameters can be depth dependent. Please refer to the documentation of the routine `vsoil_MIM_CN` to have more details.

This module can be used for steady and unsteady water flow. For unsteady water flow, the mobile water content can reach zero at some locations. To deal with this, the numerical solution checks if the mobile water content is greater than zero at all the nodes. If the mobile water content is zero at some nodes, the matrix and the second member are modified to account for this.

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*]. If the module requires also the value of an input variable at the previous time step, this is indicated by the keyword: [*valid_input*]

- **rain intensity** Rain intensity. $[m.s^{-1}]$
- **rain solutes mass concentration**. Concentration of solute species in the rain. $[kg.m_w^{-3}]$ [*tagged*].

- **soil aggregates size class proportion**. The volumetric fraction of each class of aggregates or immobile water regions. At any depth the sum must equal 1.[*ratio*] [*tagged*].
- **soil aggregates size**. The mean radii of the various aggregate or immobile water regions classes considered. [m] [*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. [$mol.m_w^{-3}$] [*tagged*].
- **soil bulk density** Bulk density of the soil as function of depth. [$kg.m^{-3}$]
- **soil immobile water volumetric content**. Immobile water volumetric content. [$m^3.m^{-3}$] [*valid_input*]
- **soil mobile water volumetric content**. Mobile water volumetric content. [$m^3.m^{-3}$] [*valid_input*]
- **soil pore volume per volume** Porosity of the soil. [$m^3.m^{-3}$].
- **soil structural pore volume per volume** Structural porosity of the soil. This porosity correspond to large pores by which most of the water flux passes. Mobile water content is at most equal to this porosity. [$m^3.m^{-3}$].
- **soil surface evaporation volumetric flux density**. Evaporation volumetric flux density substracted from the rain or the irrigation flux density. [$m.s^{-1}$]
- **soil surface runoff height**. Height of the water layer at the soil surface during run-off. [m] [*valid_input*]
- **soil surface sprinkling irrigation rate** Instantaneous water flux applied to the vegetation-mulch-soil continuum. [$m.s^{-1}$].
- **soil surface sprinkling irrigation solute mass concentration** Concentrations of the solute species in the water applied. [$kg.m_w^{-3}$] [*tagged*].
- **soil temperature** Temperature of the soil as function of depth. [K]
- **soil textural pore volume per volume** Porosity of soil aggregates related to their texture. The immobile water content is less or equal to tis porosity. [$m_w^3.m^{-3}$].
- **soil water volumetric flux density** This is the water flux in the soil as function of depth. [$m.s^{-1}$]. [*valid_input*]

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 time cumulated** Flux of the solute species at the bottom cumulated since the start of the simulation. [$kg.m^{-2}$] [*tagged*]

- **soil immobile solution diffusion length**. Effective diffusion length in immobile water regions. Depends on the aggregates classes considered. The variable account for the ratio between the immobile region volume and the area in contact with the mobile water. [m] [*tagged*]
- **soil immobile solution solutes mass concentration**. Concentrations in the immobile water. This concentration is averaged between the various immobile regions if needed. [$kg.m^{-3}$] [*tagged*]
- **soil immobile solution solutes mass concentration profile cumulated**. For each solute species, total amout dissolved in the immobile water for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil immobile solution solutes sorbed concentration**. Concentrations of the species sorbed on the sites with instantaneous sorption (Local Equilibrium Assumption) in contact with immobile water. [$kg.kg^{-1}$] [*tagged*]
- **soil immobile solution solutes sorbed concentration profile cumulated**. Concentrations of the species sorbed on the sites with instantaneous sorption in contact with the immobile water cumulated for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil mobile solution immobile solution solutes exchange rate**. Rate of exchange of the solutes between the mobile and immobile soil solutions. A positive value indicates a gain for the mobile solution. [$kg.m^{-3}.s^{-1}$] [*tagged*]
- **soil mobile solution immobile solution solutes exchange rate profile time cumulated**. Rate of exchange between the mobile and immobile water regions cumulated in time and depth. [$kg.m^{-2}$] [*tagged*]
- **soil mobile solution immobile solution solutes exchange rate time cumulated**. Rate of exchange between the mobile and immobile water regions cumulated in time. A positive value indicates a gain for the mobile solution. [$kg.m^{-3}$] [*tagged*]
- **soil mobile solution solutes mass concentration**. Concentrations in the mobile water. [$kg.m^{-3}$] [*tagged*]
- **soil mobile solution solutes mass concentration profile cumulated**. Amount of solutes in the mobile water for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil mobile solution solutes sorbed concentration**. Concentrations of the species sorbed on the sites with instantaneous sorption (Local Equilibrium Assumption) in contact with mobile water. [$kg.kg^{-1}$] [*tagged*]
- **soil mobile solution solutes sorbed concentration profile cumulated**. Concentrations of the species sorbed on the sites with instantaneous sorption in contact with the mobile water cumulated for the whole profile. [$kg.m^{-2}$] [*tagged*]
- **soil solution solutes balance terms cumulated**. For each solute species, this is the sum of the time cumulated breakthrough flux cumulated, with the amount of solutes retained in the solution, the amount of solutes eventually sorbed on the solid phase and the amount of solutes degraded. This term minus the initial amount of solute species in the profile must be compared to the time cumulated inputs. Based on the absence of production terms. [kg] [*tagged*]

- **soil solution solutes instantaneous sites sorbed concentration profile cumulated**. For each solute species, total amount (profile cumulated) sorbed on sites with instantaneous sorption (LEA assumption). This variable is the sum of quantities sorbed on sites in contact with mobile and immobile water. $[kg.m^{-2}]$ $[tagged]$

- **soil solution solutes mass concentration profile**. For each solute species, total amount (profile cumulated) in the soil solution. This variable is the sum of quantities in mobile and immobile water. $[kg.m^{-2}]$ $[tagged]$

- **soil surface solutes applied amount time cumulated**. Time cumulated amount of solute species received by the soil surface. This amount is calculated from the concentrations of the rain and the irrigation after influence of the crop canopy and the mulch have been acounted. $[kg.m^{-2}]$ $[tagged]$

- **soil surface water layer solutes molar concentration**. Solutes concentration of the water layer at the soil surface. This water layer may result from runoff or agricultural practices (temporary or permanent submersion). $[kg.m^{-3}]$ $[tagged]$

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.**

- **init_ag**, $[logical]$. If **true**, the module reads the initial situation for the aggregate classes in a file. The mean initial concentration in the immobile phase is calculated from these data. If **false**, the initial concentration in the aggregates is set equal to the immobile concentration read in the interface.

- **init_ag_path**, $[filename]$.Pathname of the file containing the initial situation in the aggregates.

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

- **upwind**, $[logical]$. If set to **true** the module uses a upwind uncentered finite difference schema for spatial derivatives of convective terms. If **false**, a centered shema is used.

- **upwind_cor**, $[logical]$. If set to **true** allows the correction of numerical dispersion induced when UPWIND is set to **true**. If **false**, no correction is applied.

- **ech_lame**, $[logical]$. If set to **true** allows the solute exchange with a water layer at the soil surface. If **false**, the exchange is not allowed.

- **correction_radii**, $[logical]$. To choose if the correction of the aggregates radii must be used or not. The correction allows to account for the saturation of the macropore space and for the contact between aggregates when calculating the exchange areas between the mobile and immobile water.

- **lambdah** $[m]$ Dispersivity coefficient used to calculate the hydrodynamic dispersion coefficient (eq.7). Can be layer dependent.

- **adscoef** $[m^3.kg^{-1}]$ Adsorption coefficient for a linear isotherm.
- **codif** $[m^2.s^{-1}]$ Diffusion coefficients in pure water for the simulated species. Corrections for porosity, water content and temperature are made in equation 8.
- **degcoef** $[s^{-1}]$ Degradation time constant for a first-order degradation term.

References

[1] J-P. Gaudet. 1978. Transferts d'eau et de soluté dans les sols non-saturés. Mesure et simulation. *Thèse de Docteur d'Etat, Université de Grenoble, 230pp.*

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