

# Module

## Ross\_FHAVeT

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## 1 Introduction

The module `Ross_FHAVeT` provides a solution of the water flow in the soil. The Ross method proposes a fast and efficient algorithm to solve the conservation equation for the water volumetric content coupled with the Darcy's law. The module is based on the publications of **Ross, 2003** and **Crevoisier et al., 2009**. This module was developed by **Tinet, 2015** with some ameliorations for a mass and energy balance model.

## 2 Equations

The water flow modeling is based on the mass conservation equation :

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} \quad (1)$$

and Darcy's equation :

$$q = -K(h) \frac{\partial h}{\partial z} \quad (2)$$

The method uses a discretization of the profile in cells, the state variables being calculated at the center of the cells. Discretization of the mass balance equation for the cells writes :

$$(\theta_s - \theta_r)_i e_i \frac{\Delta S_i}{\Delta t} = -(q_i^\sigma - q_{i-1}^\sigma) \quad (3)$$

where  $\theta_s$  and  $\theta_r$  are the saturated and residual water content for the cell  $i$ ,  $e_i$  is the thickness of the cell and  $S_i$  is the saturation index. The flux entering the cell  $q_{i-1}$  and leaving the cell  $q_i$  are evaluated at a fraction  $\sigma$  of the time step  $\Delta t$ .

The flux  $q_i$  leaving a cell  $i$ , depends on the saturation index in the cell  $S_i$  and also in the cell below  $S_{i+1}$ . A Taylor first-order development is used to express the flux  $q_i^\sigma$  with respect to the saturation index  $S_i$  and  $S_{i+1}$ . It comes :

$$q_i^\sigma = q_i^0 + \sigma \left( \frac{dq_i}{dS_i} \Big|_0 \Delta S_i + \frac{dq_i}{dS_{i+1}} \Big|_0 \Delta S_{i+1} \right) \quad (4)$$

where the superscript 0 indicates the values at the beginning of the time step. The parameter  $\sigma$  is a stability coefficient equal to 0.5. If one of the cells becomes saturated,  $\sigma$  is set to 1. Combining this expression with the mass balance leads for each cell  $i = 2, N - 1$  of the profile to :

$$\frac{dq_{i-1}}{dS_{i-1}} \Delta S_{i-1} + \left[ -\frac{\Omega_i}{\sigma \Delta t} + \frac{dq_{i-1}}{dS_i} - \frac{dq_i}{dS_i} \right] \Delta S_i - \frac{dq_i}{dS_{i+1}} \Delta S_{i+1} = \frac{q_i^0 - q_{i-1}^0}{\sigma} \quad (5)$$

where  $\Omega_i = (\theta_s - \theta_r)_i e_i$ . For the first cell the first term disappears and we have :

$$\left[ -\frac{\Omega_1}{\sigma \Delta t} + \frac{dq_0}{dS_1} - \frac{dq_1}{dS_1} \right] \Delta S_1 - \frac{dq_1}{dS_2} \Delta S_2 = \frac{q_1^0 - q_0}{\sigma} \quad (6)$$

where  $q_0$  is the flux applied at the upper boundary of the cell.

For the last cell  $N$  the the term with  $\Delta S_{N+1}$  disappears because cell  $N + 1$  does not exist and we have :

$$\frac{dq_{N-1}}{dS_{N-1}} \Delta S_{N-1} + \left[ -\frac{\Omega_N}{\sigma \Delta t} + \frac{dq_{N-1}}{dS_N} - \frac{dq_N}{dS_N} \right] \Delta S_N = \frac{q_N - q_{N-1}^0}{\sigma} \quad (7)$$

where  $q_N$  denotes the flux at the lower boundary of the last cell.

This leads to a tri-diagonal system whose solution is the variation of the saturation index during the time step used. There is no non-linearity and iterations are not required. The saturation index is updated with :  $S(t + \Delta t) = S(t) + \Delta S$ . The volumetric water content is calculated from the saturation index and the matric potential using the retention curve. Flux  $q_0$  and  $q_N$  must be known to solve the system. The evaluation of the terms of the matrix requires to calculate the terms  $dq/dS$ .

In the Ross method, the Kirchhoff transformation is used. Using the transformation, the matric flux potential  $\Phi$  is given by :

$$\Phi(h) = \int_{-\infty}^h K(x) dx \quad (8)$$

Using the Kirchhoff transformation, the flux given by the Darcy's law is related to the variable  $\Phi$  by :

$$q = -\frac{d\Phi}{dz} + K \quad (9)$$

This linearizes the term related to matric potential gradients in the Darcy's law. So the flux  $q_i^0$  in equation 4 is calculated by :

$$q_i^0 = \frac{\Phi_i^0 - \Phi_{i+1}^0}{\Delta z_i} + K_{i+1/2} \quad (10)$$

where  $K_{i+1/2}$  is a ponderation between  $K_i$  and  $K_{i+1}$ . Calculation of ponderation coefficients between  $K_i$  and  $K_{i+1}$  is explained later.

Using the expression for  $q_i^0$  and equation 4 the terms  $dq_i/dS_i$  and  $dq_i/dS_{i+1}$  appearing in the linear system can be calculated by :

$$\frac{dq_i}{dS_i} = \frac{d\Phi_i/dS_i}{\Delta z_i} + \omega \frac{dK_i}{dS_i} \quad (11)$$

$$\frac{dq_i}{dS_{i+1}} = \frac{d\Phi_{i+1}/dS_{i+1}}{\Delta z_i} + (1 - \omega) \frac{dK_{i+1}}{dS_{i+1}} \quad (12)$$

where  $\Delta z_i$  is the distance between the centers of cells  $i$  and  $i + 1$ .

The evaluation of the terms depends on the evaluation of  $d\Phi/dS$  and  $dK/dS$ . A module as been developped `hydraulic_properties_FHAVeT` providing the hydraulic functions and the derivatives needed to calculate the terms of the matrix. The modules contains several formulations for the hydraulic properties : Linear (Gardner), Brooks - Corey, Van Genuchten - Mualem, modified Van Genuchten - Mualem, Van Genuchten - Corey. Refer to the documentation of this module to have more informations.

Once the system of equations solved, the variable  $\Phi$  in the cells is calculated from the saturation index. When a cell becomes saturated, there is no change of the saturation index. For these cells, the variable  $\Phi$  is substituted to  $S$  when building the linear system. In this case, the resolution of the system provides the changes of  $\Phi$  in the saturated cells. The variable  $\Phi$  is available in all the cells and its gradient can be calculated (evaluation of Darcy's flux). When a cell is saturated, the stability coefficient  $\sigma$  is equal to 1.

Ponderation coefficient  $\omega$  for a cell  $i$  is calculated as follows. Let  $h_b$  be the water matrix potential at the bottom of the cell. We define  $h_0 = h_b - dz_i$  and  $h_{12} = (h_b - dz_i + h_e)/2$  where  $dz_i$  is the width of the cell. If  $h_0$  is greater than the air entry potential  $h_e$ , then  $\omega = 0$ . If  $h_b$  is greater than  $h_e$ , then  $\omega$  is given by :

$$\omega = \frac{(K_b - 1/6(K_0 + K_b) + 2/3K_{12})(dz_i - h_b + h_e) + K_b(h_b - h_e)}{dz_i(K_b - K_0)} \quad (13)$$

If  $h_b$  is less than  $h_e$  we define  $h_{12} = h_b - dz_i/2$  and  $\omega$  is given by :

$$\omega = \frac{(K_b - 1/6(K_0 + K_b) + 2/3K_{12})}{K_b - K_0} \quad (14)$$

## 2.1 Boundary conditions

### Negative flux at surface

As indicated above, the flux at the boundaries must be given to solve the system. For an negative flux (evaporation), the boundary condition is inbedded as long as the flux can be satisfied by the soil. The maximum evaporative flux allowed by the soil at the current time is calculated with :

$$q_{ev} = \frac{\Phi_1 - \Phi_0}{0.5\Delta z_1} + 0.5K_1 \quad (15)$$

where  $\Delta z_1$  is the tickness of the first cell.  $\Phi_0$  is set to 0 to assume that the soil water potential at soil surface is very low to estimate the maximum evaporative flux at the soil surface for the actual water volumetric content profile. If  $q_{ev}$  is less than the flux imposed by the boundary condition,  $q_{ev}$  is used to impose the flux at the soil surface.

## Positive flux at surface

For positive flux applied at the surface (rains or irrigations), if saturation does not occur, the condition is already included in the system. If saturation occurs at the soil surface, the module simulates the creation and the evolution of a water layer at the soil surface until it disappears. The flux entering the soil is calculated from the thickness of the water layer and the saturation index of the first cell. A cell corresponding to the water layer is considered and the equation simulating the thickness dynamic of the water layer is :

$$\frac{\Delta h}{\Delta t} = q_L - q_0^\sigma \quad (16)$$

where  $q_L$  is the water flux applied at soil surface (balance between rain and evaporation) and  $q_0$  is the water flux through the soil surface. This flux depends on the height of water  $h$  and on the saturation index or the matric flux potential  $\Phi$  in the first cell. Application of a Taylor first order development for  $q_0^\sigma$  leads to :

$$\frac{\Delta h}{\Delta t} = q_L - q_0 - \sigma \frac{dq}{dh} \Delta h - \sigma \frac{dq}{dS_1} \Delta S_1 \quad (17)$$

This leads to the following equation with unknown  $\Delta h$  and  $\Delta S_1$ :

$$\left[ -\frac{1}{\Delta t} - \sigma \frac{dq}{dh} \right] \Delta h - \sigma \frac{dq}{dS_1} \Delta S_1 = -(q_L - q_0) \quad (18)$$

The parameter  $\sigma$  is equal to 1 because of saturation. This equation is added to the system of equations modeling the water flow in the cells (see ). When the water layer is not present, the coefficient of  $\Delta h$  is 1, the coefficient of  $\Delta S_1$  and the second member are set to 0. The term  $\frac{dq}{dh}$  is calculated by :

$$\frac{dq}{dh} = \frac{dq}{d\Phi} \frac{d\Phi}{dh} \quad (19)$$

The function  $\Phi(h)$  is given by :

$$\Phi(h) = \int_{-\infty}^h K(x) dx = \int_{-\infty}^0 K(x) dx + \int_0^h K(x) dx = \Phi(0) + hK_s \quad (20)$$

The derivative  $d\Phi/dh$  is then  $K_s$ . The equation added to the system of equations is :

$$\left[ -\frac{1}{\Delta t} - K_s \frac{dq}{d\Phi} \right] \Delta h - \sigma \frac{dq}{dS_1} \Delta S_1 = -(q_L - q_0) \quad (21)$$

## Imposed water potential

When the soil water matrix potential is imposed at the soil surface or at the bottom, the module calculates the flux resulting from the imposed potentials and uses these flux as boundary conditions.

## Initial Conditions

The module requires that an initial situation is provided for at least the soil surface and the bottom boundary. A linear interpolation is used to calculate the initial situation at cells center from the values provided. The initial conditions can be provided in either : soil matric potential, soil total pressure head, soil volumetric water content or soil saturation index.

### 3 Numerical solution

The numerical solution use a Thomas algorithm to solve the linear system.

The cells used in the method are defined using the successive nodes of the VSoil grid as upper and lower bounds of the cells. If there is  $N$  nodes in the VSoil grid, there is  $N - 1$  cells. The outputs at the nodes of the VSoil grid are calculated by interpolation using the outputs calculated at the center of the cells.

The main point is the control of the time step. The module uses the methods proposed in the article **Crevoisier et al., 2009** to calculate the optimum time step. For this, a maximum variation of the saturation index in the cells is used :  $\Delta S_{max}$ . During a time step, a variation of the saturation index in a cell is given by :

$$\Delta S_i = \Delta t \left| \frac{q_{i-1} - q_i}{(\theta_s - \theta_r) \Delta z_i} \right| \quad (22)$$

The maximum time step is then calculated as :

$$\Delta t = \frac{\Delta S_{max}}{\max_{i=1,N} \Delta S_i} \quad (23)$$

At the end of the time step, if  $\max_{i=1,N} \Delta S_i$  is greater than  $(1 + e1 * \Delta S_{max})$  then the time step is reduced proportionnaly and the solution is calculated with the new time step :

$$dt = dt \frac{\Delta S_{max}}{\max_{i=1,N} \Delta S_i} \quad (24)$$

If saturation occurs during the time step, then a new time step is calculated as well as a stock error and the solution is recalculated. Let  $imax$  be the cell with maximum change , then the new time step is given by :

$$\Delta t_{new} = \frac{(1 + S_{max})/2. - S_{imax}}{\Delta S_{imax}} \Delta t_{prec} \quad (25)$$

where  $S_{max}$  is a parameter.

If a water layer appears at the soil surface, the time step is also reduced to a minimal value and the solution is recalculated.

If the water layer vanishes, then the time step is calculated as :

$$\Delta t_{new} = \frac{h_{min}/2. - \max(0., h)}{\Delta h} \Delta t_{prec} \quad (26)$$

where  $h_{min}$  is a parameter .

All these parameters are described in the section of parameters below.

### 4 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]`.

- **root water volumetric uptake rate cell** Water uptake rates by roots calculated for the cells.  $[m^3.m^{-3}.s^{-1}]$
- **soil bottom water pressure head** Total pressure head imposed as a boundary condition at the bottom of the soil profile.  $[m]$

- **soil bottom water volumetric flux density** Imposed water flux as a boundary condition at the lower boundary. [ $m.s^{-1}$ ]
- **soil surface maximum evaporation volumetric flux density** This is the evaporative demand that is applied at the soil surface. [ $m.s^{-1}$ ]
- **soil surface water pressure head** This is a surface pressure head imposed as a boundary condition. [ $m$ ]
- **soil surface water volumetric flux density** This is the water flux applied to the soil after influences of crop canopy and mulch have been accounted for. [ $m.s^{-1}$ ]
- **soil temperature** Temperature of the soil as function of depth. [ $K$ ]

## 5 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 saturation index** Soil saturation index at grid nodes. [*ratio0* : 1]
- **soil saturation index cell** Soil saturation index in a cell. [*ratio0* : 1]
- **soil surface evaporation volumetric flux density** Actual evaporation from the soil surface. [ $m^3.m^{-2}.s^{-1}$ ]
- **soil surface evaporation volumetric flux density daily** Actual evaporation from the soil surface at a daily scale. [ $m^3.m^{-2}$ ]
- **soil surface evaporation volumetric flux density deficit** Instantaneous soil evaporation deficit. Difference between demand and actual evaporation as controled by the soil. [ $m^3.m^{-2}.s^{-1}$ ]
- **soil surface evaporation volumetric flux density deficit time cumulated** Evaporation deficit at a daily scale. [ $m^3.m^{-2}$ ]
- **soil surface evaporation volumetric flux density time cumulated** Time cumulated evaporation at the soil surface. [ $m^3.m^{-2}$ ]
- **soil water height** Total water amount in the soil profile. [ $m$ ]
- **soil water Kirchoff potential** The Kirchoff potential is defined as the integral of the hydraulic conductivity between two values of the soil water potential. Kirchoff transformation is used to get a transport equation with less non linearities. The problem is to have a relation between the Kirchoff potential (solution of the transformed Richards equation) and the soil water potential. This requires tabulation or strong hypotheses on the analytical form of the hydraulic conductivity. [ $m^2.s^{-1}$ ]
- **soil water matrix potential** Soil water matrix potential at grid nodes. [ $m$ ]
- **soil water matrix potential cell** Soil water matrix potential at center of the cells. [ $m$ ]
- **soil water volumetric content** Soil water volumetric content. [ $m^3.m^{-3}$ ]
- **soil water volumetric flux density** Volumetric water flux at grid nodes. [ $m.s^{-1}$ ]

## 6 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.**

- **hmin** [ $m$ ] Minimal value for matric potential when unsaturated. A default value of 0.001 m is given. This parameter is used to avoid numerical errors when saturation changes from saturated to unsaturated and to calculate the optimal dt in these situations.
- **Smax** [ $m^3.m^{-3}$ ] Maximal value of saturation index. A default value of 1.005 is given. The parameter is used to detect saturation index too large and to calculate the optimal time steps.
- **dSmax** [ $m^3.m^{-3}$ ] Maximal value of saturation index variation during a time increment. A default value of 0.1 is given. This parameter is used for calculating the maximum time increment.
- **e1** [ $NA$ ] A parameter for error calculation. A default value of 0.25 is given.
- **typ\_CL\_top** [*Choice*] Type of boundary condition for surface: 1: Flux.Manages : evaporation deficit, surface saturation. 2: Constant head 3: Flux. Manages : surface saturation. Coupled with energy. Choice 1 : if the flux applied is positive the module handles the cases where the flux is larger than the soil infiltrability. If the flux is negative, the module will handle the situations where the evaporative flux allowed by the soil is less than the imposed flux. Choice 2 : To apply a soil water potential at the soil surface. The flux entering or leaving the soil is calculated by the module. Choice 3 : if the flux applied is positive the module handles the cases where the flux is larger than the soil infiltrability. The evaporative flux must be acceptable by the soil. This option is for coupling the module with an energy balance module providing the evaporative flux.
- **typ\_CL\_bot** [*Choice*] Type of boundary condition for bottom: 1: Imposed flux. The imposed flux is an input of the module. 2: Imposed matrix water potential. The resulting water flux is calculated by the module. 3: Free drainage.
- **init\_situation\_variable** [*Choice*] Choice of the variable for the initial situation. Choice in the following list : matrix potential, total pressure head, volumetric water content, saturation index.

## 7 References

- **Ross, P. J. 2003.** Modeling soil water and solute transport. Fast, simplified numerical solutions. *Agronomy Journal*, 95, 1352-1361.
- **Crevoisier, D., Chanzy, A. and M. Voltz. 2009.** Evaluation of the Ross fast solution of Richards' equation in unfavourable conditions for standard finite element method. *Adv. Water Resour.*, 32, 936-947.

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