The hydrol module of ORCHIDEE: scientific documentation

[rev 3977] and on, work in progress, towards CMIP6v1

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1 Introduction

1.1 Roles of this module in ORCHIDEE

The `hydrol.f90` module computes the water budget of the land surface grid-cells at each time step of ORCHIDEE. It distinguishes three main reservoirs with separate water budgets : the canopy interception reservoir, the snow pack, and the soil, described here using a multi-layer scheme to solve the Richards diffusion equation.

The main input variables are precipitation (liquid and solid) and the different terms of evapotranspiration (transpiration, bare soil evaporation, interception loss, sublimation, which are previously computed, for the current time step, by the `diffuco` then `enerbil` subroutines. The module organizes the required initialisation of water prognostic variables, their integration at each time step given the above forcings, and the required output (writing of restart file, updated prognostic variables, diagnostic variables).

We focus here on the soil moisture processes, which relate water redistribution in the soil by diffusion, drainage at the soil bottom, infiltration at the soil surface, bare soil evaporation and transpiration. **The snow processes are not detailed here.**

Unless otherwise mentioned, all the grid-cell values that are imported to or exported from `hydrol.f90` are grid-cell avearges, expressed in m^2 of land area in the grid-cell. This is also true in the code.

1.2 Spatial framework for the water and energy budgets

1.2.1 Overview

The standard version of ORCHIDEE builds on the concept of metaclasses (MC) to describe vegetation distribution: by default it distinguishes 13 MCs (one for bare soil, eight for forests, two for grasslands and two for croplands), and each MC is associated to a predefined plant functional type (PFT) with default parameters. In this document, PFTs and MCs are used as synonyms.

The soil water fluxes are computed in ORCHIDEE within ”soiltiles”, which define separate soil water columns within the grid-cell, in which independent soil water budgets are computed (water input by throughfall and snow melt, water output by total runoff, transpiration and soil evaporation). When using the diffusive multi-layer soil hydrology scheme described here (also known as the CWRR, or Dublin, or ORC11 model), the number of soil columns is reduced to a maximum of three: one gathering every forest MC, one for every MC with grass and crops, and one for the bare soil PFT. Since [rev 3588], the ”nobio” surface types, such as ice, free water, cities, etc., are kept apart, and described as glaciers, with a simple parametrization of snow accumulation and melting (Figure 1).

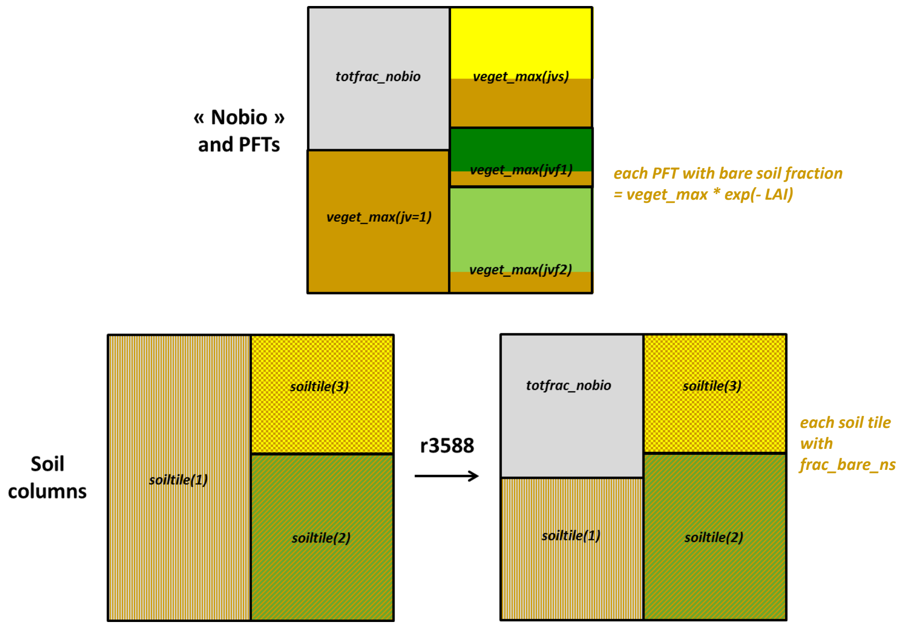

Figure 1: Areal composition of an ORCHIDEE grid-cell using the multi-layer soil hydrology scheme described in this document, and the resulting soiltiles, before and after [rev 3588]. ORCHIDEE's variable names are defined in section 8.

The total land surface of an ORCHIDEE grid-cell, A_L, can then be subdivided between the bare soil area of the grid-cell (called A_g), the vegetated area of the grid-cell (called A_v), and the "nobio" area (called A_n):

$$A_L = A_g + A_v + A_n = A_{vg} + A_n \tag{1}$$

Further notations are introduced in 1.2.2, while the correspondence with ORCHIDEE's variable names is given in section 8.

At any time, the two soil columns, or "soiltiles", with vegetation, release water via both transpiration and soil evaporation. The latter is commensurate to the fraction of soil that is not covered by vegetation, while transpiration originates from the fraction effectively covered with vegetation, which increases with LAI:

$$f_v^j = f^j (1 - \exp(-k_{\text{ext}} \, \text{LAI}_\text{j})). \tag{2}$$

This equation holds in each PFT j, where f^j is the fraction of A_L covered by the PFT j, and f_v^j is the fraction of A_L covered by effective vegetation in this PFT j.

Before [rev 3524], the extinction coefficient k_{ext} was identical here and to define the extinction of light by the canopy for photosynthesis, with a value of 0.5. Two parameters are now differentiated, and the parameter k_{ext} used to control the PFT fractions effectively covered by vegetation and bare soil (called `ext_coeff_vegetfrac_mtc` in the code) has now been increased to 1, to reduce the bare soil fraction and bare soil evaporation.

1.2.2 Further notations

In ORCHIDEE, many areal fractions are fractions of the grid-cell total land area A_L.

Let's introduce f_n the fraction of A_L covered with "nobio", while f_{vg} is the "bio" fraction (called `vegtot` in the code). The latter is comprised of f^j, f_v^j and f_g^j, which are the fractions of A_L covered by the PFT j, by the effective vegetation in PFT j (see Eq. 2, and by the effective bare soil in PFT j (this is different from ORCHIDEE's code for the bare soil PFT):

$$f^j = f_v^j + f_g^j \tag{3}$$

$$\sum f_v^j = A_v/A_L = f_v \tag{4}$$

$$\sum f_g^j = A_g/A_L = f_g \tag{5}$$

$$\sum f^j = (A_v + A_g)/A_L = f_v + f_g = f_{vg} \tag{6}$$

$$f_n + f_{vg} = 1 \tag{7}$$

A different decomposition of A_L is into soiltiles (Figure 1), each of them with a fraction g^c of f_{vg} (since [rev 3594]), so that $\sum g^c = 1$.

1.2.3 Link with the energy budget

The spatial framework is crucial for the calculation of evapotranspiration, E, which makes the link between the water and energy budgets. In ORCHIDEE, it is calculated from the potential evaporation E_{pot} limited by a stress function β:

$$E = \beta E_{\mathrm{pot}}, \tag{8}$$

$$E_{\mathrm{pot}} = \frac{\rho}{r_a}\left(q_{\mathrm{sat}}(T_s) - q_{\mathrm{a}}\right), \tag{9}$$

where ρ is air density, q_a specific humidity of air at the reference height, $q_{\mathrm{sat}}(T_s)$ saturated specific humidity at the surface temperature T_s, and r_a is the aerodynamic resistance, depending on the reference height, wind speed, roughness length, and air stability.

Because of the requirements for the coupling with the boundary layer when ORCHIDEE is coupled to an atmospheric model, all the variables in Eqs. 8 and 9 are defined at the grid-cell scale, and a single energy budget is solved per grid-cell at each time step. In particular, E and E_{pot} are mean water fluxes per m^2 of A_L, in $kg.m^{-2}$ per time step of ORCHIDEE's code.

In absence of snow and flood-plains, evapotranspiration E can be decomposed in (i) bare soil evaporation, E_g, which occurs over the bare fraction of the grid-cell, (ii) interception loss E_i and transpiration E_t, which both come from the effectively vegetated fraction:

$$E = E_i + E_t + E_g \tag{10}$$

In this framework, the stress function β conveys two kinds of information:

i) the different stresses limiting the local values of bare soil evaporation, interception loss and transpiration compared to the potential rate E_{pot}, which stands for the entire grid-cell;

ii) how the mean value of E in the grid-cell results from the local subfluxes, as a function of A_g and A_v.

If we further assume the absence of "nobio" surfaces ($A_n = 0$, $A_L = A_v + A_g$), we have :

$$\beta = (A_v(\beta_2 + \beta_3) + A_g\beta_4)/A_L, \tag{11}$$

where β_2, β_3, and β_4, are the *individual* stress functions on interception loss, transpiration, and bare soil evaporation respectively. By construction, we get $\beta_2 = 1$, since the local evaporation flux from the intercepted water proceeds at potential rate. The local stress functions β_3 and β_4 are ≤ 1, and all the closer to zero as soil moisture gets limiting. The stress function on transpiration, β_3, depends on soil moisture via the U_s variable defined in sections 4.1 and 7.2. **Does it depend on other stresses, depending on `control%ok_co2` and the coupling with `stomate.f90` ?**

The `vbeta` variables found in the code combine the control of individual stress functions and the supporting fractions, and it would be helpful to disentangle these two contributions, cf Ticket #350.

1.2.4 The itching question of the "nobio" fraction

We should now wonder what should be the expression of β in presence of "nobio" surfaces. Before [rev3588], A_n was included in the "bare" soiltile as shown in Figure 1, so that bare soil evaporation was also also proceeding from A_n. It should be pointed out that this led to assign the same evaporation properties to A_n ("nobio") as to A_g (bare soil), which may contribute to the tendency of the multi-layer soil hydrology to produce very high bare soil evaporation. This strategy led to some inconsistencies. For instance, the total evaporating bare soil fraction, `tot_bare_soil`, was not including A_n; and hydrol was applied on the sum of all three soil tiles, i.e. on A_L, but the resulting soil moisture was multiplied by `vegtot` = A_L - A_n for water budget computations.

Since [rev3588], A_n has been excluded from the "bare" soiltile, which has now the same areal support as PFT1. Further details and discussion can be found in Ticket #222.

1.3 Important preliminary remarks

- Unless otherwise mentioned, the following text uses SI units. For instance, water flux variables X in are in kg.m^{-2}.s^{-1}. It is important to keep in mind that ORCHIDEE's code, in contrast, works with integrated fluxes over the calculation time step : $Y = X\Delta t$.

- Since the "MergeHydro" in summer 2012, the trunk version of ORCHIDEE defines the same soil texture for the three soil columns, or soiltiles, in an ORCHIDEE grid-cell. It is a simplification compared to older versions where an alternative was also allowed to define soil columns with different soil textures. Some traces of this option remain in the code, but the user is not advised to use this option without a very careful work on the code.
- This documentation is not official and still in construction. It highlights the questions of the author in bold. It may also contain errors. If you suspect one, or can answer some of the questions, you are kindly invited to contact the author to improve this documentation and the corresponding code.

2 Water diffusion and redistribution in the soil

2.1 Main equations

A physically-based description of unsaturated soil water flow was introduced in ORCHIDEE by De Rosnay et al. (2002). It relies on a one-dimensional Fokker-Planck equation, combining the mass and momentum conservation equations using volumetric water content θ ($m^3.m^{-3}$) as a state variable, instead of pressure head as in the Richards equation.

Due to the large scale at which ORCHIDEE is usually applied, we neglect the lateral fluxes between adjacent grid cells. We also assume all variables to be horizontally homogeneous, so that the mass conservation equation relating the vertical distribution of θ to its flux field q ($m.s^{-1}$) is:

$$\frac{\partial \theta(z,t)}{\partial t} = -\frac{\partial q(z,t)}{\partial z} - s(z,t). \tag{12}$$

In this equation, z is depth below the soil surface, and t is time (in m and s respectively). The sink term s ($m^3.m^{-3}.s^{-1}$) is due to transpiration and depends on the root's density profile.

The flux field q comes from the equation of motion known as Darcy (1856) equation in the saturated zone, and extended to unsaturated conditions by Buckingham (1907):

$$q(z,t) = -D(\theta(z,t))\frac{\partial \theta(z,t)}{\partial z} + K(\theta(z,t)), \tag{13}$$

$K(\theta)$ and $D(\theta)$ are the hydraulic conductivity and diffusivity (in $m.s^{-1}$ and $m^2.s^{-1}$ respectively). The latter defines the link between the volumetric soil moisture θ and the matric potential ψ (in m):

$$D(\theta(z,t)) = K(\theta(z,t))\,\frac{\partial \psi}{\partial \theta}(\theta(z,t)). \tag{14}$$

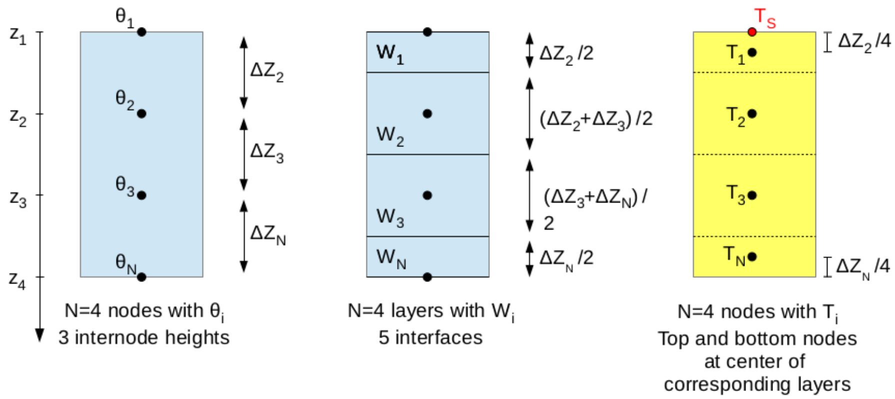

Figure 2: Soil vertical discretization: for hydrol in blue on the left, with links between node positions, their local volumetric water content θ_i, the soil layers, their depth and integrated soil moisture W_i, in the simple case of four equidistant nodes. Link with code's names in Table 3. The correspondence with the nodes for the soil thermics appears on the yellow column on the right.

2.2 Vertical discretization and finite difference integration

The Fokker-Planck equation, as defined by the combination of Eqs. 12-13, is solved using a finite difference method. To this end, the soil column is discretized using N nodes, defined by an index i increasing from top to bottom, and where we calculate the values of θ (Figure 2). The middle of each consecutive couple of nodes represents the limit between two soil layers, except for the upper and the lower layers, for which the top/bottom interfaces are defined by the first/last nodes respectively.

As a consequence, each soil layer holds only one node i, and we define layer i as the layer holding node i. We can thus define the thickness h_i of each layer by:

$$h_i = [\,\Delta Z_i\, + \Delta Z_{i+1}\,]/2,\;\; i \in [2, N-1] \tag{15}$$

$$h_1 = \Delta Z_2/2 \tag{16}$$

$$h_N = \Delta Z_N/2 \tag{17}$$

In this expressions, ΔZ_i is the distance between nodes $(i-1)$ and i (`dz` in the code), which have volumetric water contents θ_{i-1} and θ_i (Figure 2). In ORCHIDEE's code, ΔZ_i, thus h_i, are expressed in mm, and $\sum_i h_i = 1000\,\texttt{zmaxh}$.

The total water content of each layer i, W_i (mm), is obtained by integration of $\theta(z)$, assumed to undergo linear variations between two consecutive nodes. Following De Rosnay (1999, p56, 57), this leads to the following expressions

$$W_i = [\,\Delta Z_i\,(3\,\theta_i + \theta_{i-1}) + \Delta Z_{i+1}\,(3\,\theta_i + \theta_{i+1})\,]/8,\;\; i \in [2, N-1] \tag{18}$$

$$W_1 = [\,\Delta Z_2\,(3\,\theta_1 + \theta_2)\,]/8 \tag{19}$$

$$W_N = [\,\Delta Z_N\,(3\,\theta_N + \theta_{N-1})\,]/8 \tag{20}$$

As the ΔZ_i are expressed in mm in ORCHIDEE's code, this leads to W_i in mm, or kg.m^{-2}.

Equation 12 can then be integrated between the nodes and over the time step dt, over which q is assumed to be constantly equal to its value at $t + dt$ (implicit scheme). This allows defining the water budget of each layer i:

$$\frac{W_i(t+dt) - W_i(t)}{dt} = Q_{i-1}(t+dt) - Q_i(t+dt) - S_i, \tag{21}$$

where S_i is the integrated sink term and Q_i the water flux at the interface between layers i and $(i+1)$.

The above flux is deduced from Equation 13, by approximating $\partial\theta/\partial z$ by the rate of increase between the equidistant neighbouring nodes $(i-1)$ and i, and this leads to:

$$\frac{Q_i}{A} = -\frac{D(\theta_{i-1}) + D(\theta_i)}{2} \frac{\theta_i - \theta_{i-1}}{\Delta Z_i} + \frac{K(\theta_{i-1}) + K(\theta_i)}{2}, \tag{22}$$

where A is the area of the grid mesh. To get this expression, we also approximate the values of K and D at the layers' interfaces by the arithmetic average of their values at the neighbouring nodes. The $K(\theta)$ and $D(\theta)$ are also linearized (section 3), so that it becomes possible to construct a tridiagonal matrix system to solve $\theta_i(t+dt)$, at least for the inner nodes (i in $[2, N-1]$). See section 2.4 for details.

Additional information is required to solve θ_1 and θ_N. It consists of water fluxes Q_0 and Q_N at the top and bottom of the soil column respectively. These fluxes need to be prescribed as boundary conditions at each time step, and thus drive the evolution of the soil moisture profile (section 4).

2.3 How to define the vertical discretization?

Starting at [rev2917], the trunk uses the same vertical discretization for the vertical fluxes of heat and moisture, with the exception of the first and last node position (Fig. 2). It is possible, however, to extend the domain for heat fluxes below the one for moisture, and several options are available, to adjust both vertical discretizations. As a general rule, thin layers must be used close to interfaces where high gradients of θ can develop, such as the soil-atmosphere interface, or the soil bottom interface if one changes the free drainage boundary condition (section 4).

These options are controlled by externalized parameters (see grey box) and all assume that inter-node distance increases geometrically in the top part of the soil, and can become constant (see Figure 3 right), then increase geometrically again at further depth. This is set in `hydrol_var_init.f90`, with values calculated in `src_parameters/vertical_soil.f90`.

In the trunk version of `hydrol.f90`, the default setting includes a 2-m soil column, and 11 nodes with a geometric progression of the internode distance, as illustrated in Figure 3(left). The top layer has a thickness of 1 mm, corresponding to a top internode distance of 2 mm. Further values defining the default discretization are given in Table 1, and Table 2 gives an alternative discretization with a finer regular discretization in the deepest 1.75m of soil, similar to the one tested by Campoy et al. (2013) and recommended in case of impermeable bottom.

Keywords to adjust the vertical discretization in run.def:

Keyword	Default value	Unit	Meaning
DEPTH_MAX_H	2.0	m	Depth of soil for moisture
DEPTH_MAX_T	10.0	m	Depth of soil for thermodynamics
DEPTH_TOPTHICK	9.77517107e-04	m	Thickness of top layer
DEPTH_CSTTHICK	DEPTH_MAX_H	m	Depth at which constant layer thickness starts
DEPTH_GEOM	DEPTH_MAX_H	m	Depth at which geometrical increase resumes (for temperature)
RATIO_GEOM_BELOW	2.0	-	Ratio of geometrical series defining thickness below DEPTH_GEOM (to cover the depth needed for temperature with fewer layers)

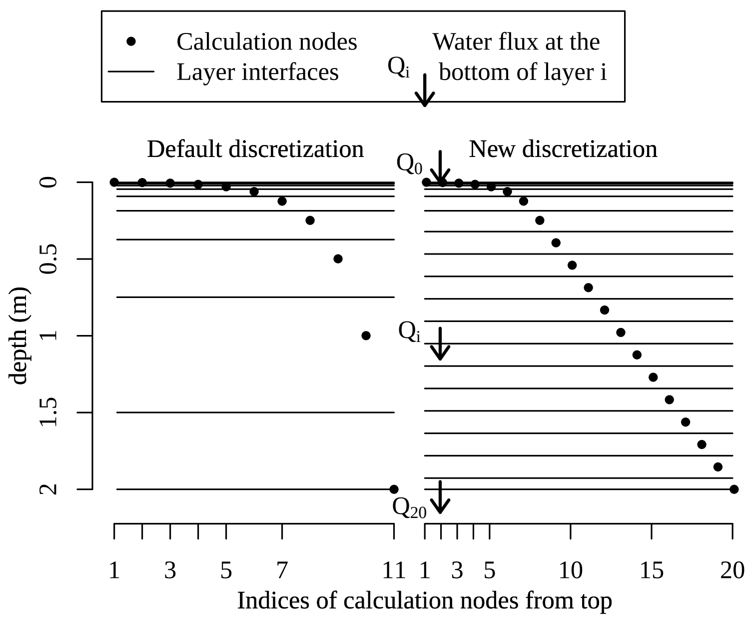

Figure 3: Soil vertical discretization: (left) default 11-layer discretization from De Rosnay et al. (2002), (right) 20-layer discretization from Campoy et al. (2013).

2.4 Numerical solution

The diffusion calculations are done in subroutine `hydrol_soil`. They rely on a tridiagonal matrix, as explained in De Rosnay (1999, p57 + annexe B p155-157). Since we solve one independent water budget per soiltile, the number of times the diffusion scheme is used per grid-cell is defined by the number of soiltiles.

Index of node or layer	z_i (m)	ΔZ_i (m)	h_i (m)	$\Sigma_1^i h_i$ (m)
1	0.000	-	0.001	0.001
2	0.002	0.002	0.003	0.004
3	0.006	0.004	0.006	0.010
4	0.014	0.008	0.012	0.022
5	0.030	0.016	0.023	0.045
6	0.062	0.032	0.047	0.092
7	0.125	0.063	0.094	0.186
8	0.250	0.125	0.188	0.374
9	0.500	0.250	0.375	0.750
10	1.000	0.500	0.750	1.500
11	2.000	1.000	0.500	2.00

Table 1: Default vertical discretization for water fluxes.

Index of node or layer	z_i (m)	ΔZ_i (m)	h_i (m)	$\Sigma_1^i h_i$ (m)
1	0.000	-	0.001	0.001
2	0.002	0.002	0.003	0.004
3	0.006	0.004	0.006	0.010
4	0.014	0.008	0.012	0.022
5	0.030	0.016	0.023	0.045
6	0.062	0.032	0.047	0.092
7	0.125	0.063	0.094	0.186
8	0.250	0.125	0.125	0.311
9	0.375	0.125	0.125	0.436
10	0.500	0.125	0.125	0.561
11	0.625	0.125	0.125	0.686
1	0.750	0.125	0.125	0.811
13	0.875	0.125	0.125	0.936
14	1.000	0.125	0.125	1.062
15	1.125	0.125	0.125	1.187
16	1.250	0.125	0.125	1.312
17	1.375	0.125	0.125	1.437
18	1.500	0.125	0.125	1.562
19	1.625	0.125	0.125	1.687
20	1.750	0.125	0.125	1.812
21	1.875	0.125	0.125	1.937
22	2.000	0.125	0.063	2.000

Table 2: Vertical discretization for water fluxes in a 2-m soil with 22 layers and constant thickness below 20cm. It is obtained with the following keywords in run.def: DEPTH_MAX_H = 2.0; DEPTH_CSTTHICK = 0.2 (values in m). Note the above values are slightly rounded for simplicity compared to the exact values calculated by the code.

3 Hydrodynamic parameters

3.1 Van Genuchten relationships

The hydraulic parameters required by the diffusion equation solved in ORCHIDEE are the hydraulic conductivity and diffusivity, K and D, which depend on volumetric water content θ. These relationships are given in ORCHIDEE by the Mualem (1976) - Van Genuchten (1980) model:

$$K(\theta) = K_s \sqrt{\theta_f} \left(1 - \left(1 - \theta_f^{1/m}\right)^m\right)^2, \tag{23}$$

$$D(\theta) = \frac{(1-m)K(\theta)}{\alpha m} \frac{1}{\theta - \theta_r} \theta_f^{-1/m} . \left(\theta_f^{-1/m} - 1\right)^{-m}, \tag{24}$$

which also writes:

$$D(\theta) = \frac{K(\theta)}{\alpha m n} \frac{1}{\theta - \theta_r} \theta_f^{-1/m} . \left(\theta_f^{-1/m} - 1\right)^{-m}. \tag{25}$$

There, K_s is the saturated hydraulic conductivity (m.s^{-1}), α (m^{-1}) corresponds to the inverse of the air entry suction, and m is a dimensionless parameter, related to the classical Van Genuchten parameter n by:

$$m = 1 - 1/n. \tag{26}$$

The last Van Genuchten relationship defines the link between the matric potential ψ (m), involved in the hdraulic diffusivity (Eq. 14), and the volumetric water content θ:

$$\psi(\theta) = -\frac{1}{\alpha} \left(\theta_f^{-1/m} - 1\right)^{1/n} \tag{27}$$

These equations, illustrated in Figure 4, assume that θ varies between the residual water content θ_r and the saturated water content θ_s, which leads to define relative humidity as $\theta_f = (\theta - \theta_r)/(\theta_s - \theta_r)$.

3.2 Modifications of Ks with depth

3.2.1 Decrease with depth: `kfact`

Following d'Orgeval (2006, p81-82) and d'Orgeval et al. (2008, section 2.1.3), several modifications of K_s, thus $K(\theta)$, with depth are implemented in ORCHIDEE. Firstly, as suggested by Beven and Kirkby (1979), K_s is assumed to decrease exponentially with depth (below the top 30 centimeters with the default parameters):

$$K_s(z) = K_s^{\text{ref}} F_K(z), \tag{28}$$

$$F_K(z) = \min(\max(\exp(-f(z - z_{\text{lim}}), 1/F_K^{\max}), 1). \tag{29}$$

Here, z is the depth below the soil surface, K_s^{ref} is the reference value of K_s based on soil texture (section 6). The other three parameters are constants, which are independent

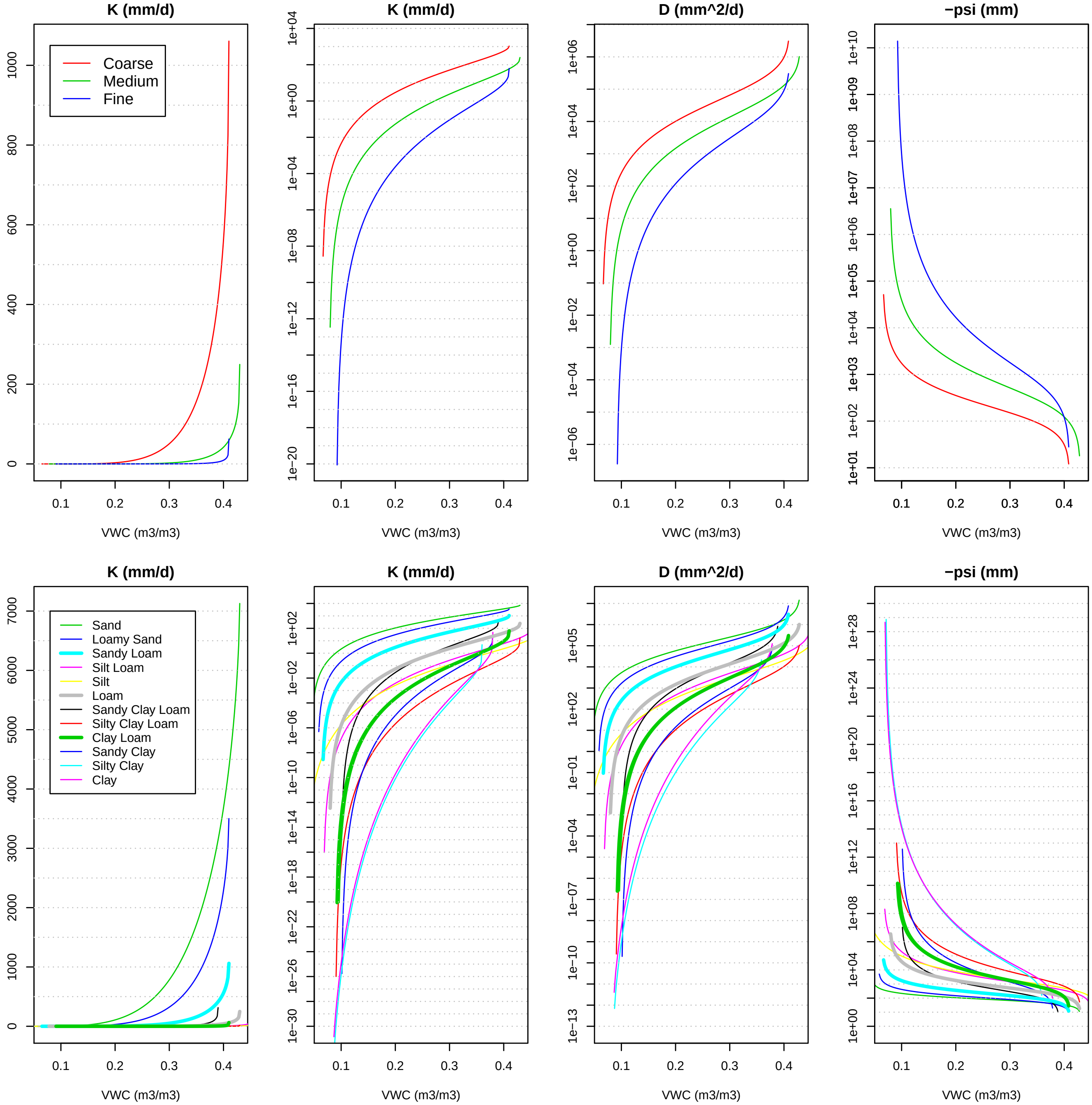

Figure 4: Van Genuchten relationship $K(\theta)$, $D(\theta)$, and $\psi(\theta)$, for θ in $[\theta_r, \theta_s]$, based on Eqs. 23, 25, and 27: (top) for the three Zobler texture classes (Table 5); (bottom) for the 12 USDA texture classes (Table 4). The difference between the first two panels in each row is that the second one uses a logarithmic axis for $K(\theta)$.

from the PFT, the soiltile, and the soil texture: z_{lim} is the depth at which the decrease of K_s starts; f is the decay factor (in m^{-1}); and $F_K(z)$ cannot be smaller than $1/F_K^{\max}$.

In the trunk, the default values are $f = 2$ m, $z_{\text{lim}} = 0.3$ m, and $F_K^{\max} = 10$, so that K_s is identical for all nodes below 1.45 m.

In run.def, you can cancel the decrease of Ks with depth by setting $f = 0$:
KFACT_DECAY_RATE = 0.0

3.2.2 Increase with depth: `kfact_root`

An increase of K_s towards the soil surface is also taken into account, because the presence of vegetation tends to increase the soil porosity in the root zone and therefore to increase infiltration capacity (Beven, 1982, 1984). For each MC j, a multiplicative factor F_{Kj} depending on depth z is defined:

$$F_{Kj}(z) = \max\left(1, \left(\frac{K_s^{\max}}{K_s^{\text{ref}}}\right)^{\frac{1-c_j z}{2}}\right), \tag{30}$$

where $K_s^{\max} = 7128.0$ mm.d^{-1} is a constant taken as the maximum K_s given by (Carsel and Parrish, 1988), for the sandy texture, and c_j is the root profile decay factor (in m^{-1}) for vegetation type $j \geq 2$. This formula allows to increase exponentially the saturated conductivity for $z < 1/c_i$ (which ranges between 0.25 m for grasses and crops, to 1.25 m for forests; when using the defaults values of c_j for the multi-layer hydrology, defined in `constantes_mtc.f90`).

The resulting saturated conductivity for the soiltile c is eventually given by the following expressions:

$$K_s^*(z, c) = K_s(z)\, F_{K\text{root}}(z, c), \tag{31}$$

$$F_{K\text{root}}(z, c) = \prod_{j \in c} F_{Kj}(z)^{f^j/2} = \prod_{j \in c} \max\left(1, \left(\frac{K_s^{\max}}{K_s^{\text{ref}}}\right)^{f^j(1-c_j z)/4}\right), \tag{32}$$

where $K_s(z)$ is given by Eq. 28, and f^j is the fraction of MCs j belonging to the soiltile c (f^j is equivalent to `veget_max(ji,jv)` in the code).

The above expression assumes that $K_s(z, c)$ is not modified by roots in the bare soil PFT ($j = 1$), and has first been introduced by d'Orgeval et al. (2008) to obtain a reasonable evapotranspiration variability in Hapex-Sahel simulations. This work used f_v^j instead of $0.5 f^j$, leading to variable $K_s^*(z, c)$ over time, since $f_v^j = f^j(1 - \exp(-k_{\text{ext}}\,\text{LAI}_\text{j}))$. It was changed in [rev2916], to make $F_{K\text{root}}$ constant if the PFT does not change.

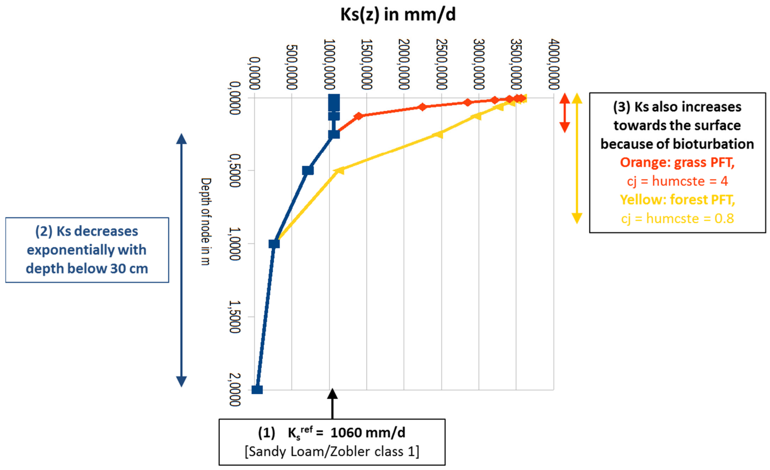

Figure 5: Profiles of saturated hydraulic conductivity for a sandy loam soil. The final profiles are in orange for a grass PFT, and in yellow for a forest PFT.

3.2.3 Combined effect

Eventually, the vertical profile of the effective saturated hydraulic conductivity is given in each soiltile c by:

$$K_s^*(z,c) = K_s^{\mathrm{ref}} F_K(z)\, F_{K\mathrm{root}}(z,c). \tag{33}$$

Since [rev4764], the corresponding variable is output under the name `ksat`, but it is not explicitely calculated and stored: the saturated conductivity profiles are only defined by the factors F_K and $F_{K\mathrm{root}}$, called `kfact` and `kfact_root` in the code, and both available at the end of in subroutine `hydrol_var_init`. The effect of each factor is illustrated in Figure 5.

These two factors are thus used to calculate infiltration and to solve the Richards equation: (i) in `hydrol_soil_infilt` to define both the saturated and non-saturated hydraulic conductivity for the infiltration; (ii) in `hydrol_soil_coef` to define the non saturated hydraulic conductivity and diffusivity (see section 3.5) required for the redistribution. These non saturated parameters also depend on the Van Genuchten parameters n and α, which are modified according to F_K as explained in below (section 3.3).

3.3 Resulting modifications of other soil parameters with depth

To introduce a consistency between K_s and the parameters α and n, the latter can also modified, based on their log-log regression with K_s, using the values given by Carsel and Parrish (1988) for the 12 USDA soil textures. The resulting regressions appear in Fig 4.14 of d'Orgeval (2006, p82), and are defined by:

$$n(K_s) = n_0 + A_n (K_s)^{B_n} \tag{34}$$
$$\alpha(K_s) = \alpha_0 + A_\alpha (K_s)^{B_\alpha} \tag{35}$$

where $n_0 = 0.95$, $B_n = 0.34$, $\alpha_0 = 0.12\ \mathrm{m}^{-1}$, and $B_\alpha = 0.53$. The parameters A_n and A_α equal 42 and 2500 respectively, but they vanish when combining equations.

In ORCHIDEE, these relationships are used to define changes in n and α resulting from the decrease of K_s with depth below 30 cm (section 3.2.1), **but they are not used to change n and α as a result of K_s increase with roots** (section 3.2.2).

Given the texture, we know K_s^{ref}, and $K_s(z) = K_s^{\text{ref}}.F_K$ (Eqs. 28 and 29). From Eqs. 34 and 35, it comes:

$$n(K_s(z)) - n_0 = (n(K_s^{\text{ref}}) - n_0).(F_K)^{B_n} = (n^{\text{ref}} - n_0).(F_K)^{B_n} \quad (36)$$

$$\alpha(K_s(z)) - \alpha_0 = (\alpha(K_s^{\text{ref}}) - \alpha_0).(F_K)^{B_\alpha} = (\alpha^{\text{ref}} - \alpha_0).(F_K)^{B_\alpha} \quad (37)$$

This is done in subroutine `hydrol_var_init`.

In run.def, to keep vertically uniform α and n, add the following:

CWRR_AKS_A0 = 0.
CWRR_AKS_POWER = 0.
CWRR_NKS_N0 = 0.
CWRR_NKS_POWER = 0.

3.4 Linearization

Equation 22 is not linear at first-order with respect to θ, because of the strong non-linearity of $K(\theta)$ and $D(\theta)$ in Equations 23 and 24. To solve this issue, the interval $[\theta_r; \theta_s]$ is discretized in ORCHIDEE into 50 regular smaller sub-domains where K and D are described by piecewise functions, respectively linear in θ and constant (De Rosnay, 1999, p149):

$$K_k = a_k \theta_k + b_k \quad (38)$$

$$D_k = d_k \quad (39)$$

In practice, for each soil depth and texture allowed in ORCHIDEE, we define $K_s(z)$ from Eq. 28, and $n(K_s(z))$ and $\alpha(K_s(z))$ as explained in the above section 3.3. Then, we define k=51 uniformly increasing θ_k^b between θ_r and θ_s (bounds of the 50 intervals), and for each of them:

- We define $K(\theta_k^b)$ from Eq. 23, except for $K(\theta_1^b = \theta_r)$, which would be zero. To prevent from numerical problems, we ensure that the small values of K are always strictly positive and increasing with θ_k^b. To this end, we find the highest k so that $K(\theta_k^b) < 10^{-32}$ mm.d^{-1}, and all the $K(\theta_k^b)$ with a lower k are recursively deduced by successive divisions by 10. This adjustment can be necessary for all clayish textures (Table 4) and the number of adjusted bins depends on the soil texture, and on the changes to α and n described in section 3.3.
- We calculate $D(\theta_k^b)$ from Eq. 25 but the special case of $\theta_1^b = \theta_r$, which leads to D=NaN, is adapted, see below.

The values of a_k, b_k, and d_k can then be defined for the 50 $[\theta_k^b, \theta_{k+1}^b]$ bins:

- We deduce a_k and b_k based on continuity between successive segments described by Eq.38, which applies for all the θ_k between θ_k^b and θ_{k+1}^b,
- The constant d_k is the arithmetic mean two successive values : $d_k = 0.5(D(\theta_k^b) + D(\theta_{k+1}^b)$ for k in [2,49] ; except for $d_{50} = D(\theta_{50}^b)$ and d_1=d_2/1000. Finally, all the bins where $K(\theta_k^b)$ has been modified to ensure an increase are also adjusted for d_k. Note we stopped using $d_1 = 0$ (for the first bin and all θ below the residual value) as it does not have a strong physical sense and can create numerical problems. For near-saturation values, the convergence towards the saturated case is not explicitly treated, since it is not possible when solving Richards equation in θ.

All this is done in subroutine `hydrol_var_init`. The results are `k_lin(i,jsl, jsc)`, `a_lin(i,jsl, jsc)`, `b_lin(i,jsl, jsc)`, and `d_lin(i,jsl, jsc)`, in which the three dimensions correspond respectively to the soil moisture bins k, the soil layers i, and the different possible textures (see Table 7 for details regarding the indices in ORCHIDEE). As already noted, these variables include the effect of `kfact` but not the one of `kfact_root` (section 3.2).

3.5 Final values of K and D for soil diffusion calculations

These values are calculated at each time step in subroutine `hydrol_soil_coef` called in `hydrol_soil`.

The above parameters a_k, b_k,d_k (which include the effect of F_K, and its consequences on α and m), and $F_{K\text{root}}$, all produced by subroutine `hydrol_var_init`, allow to define the appropriate K and D for each calculation node depending on the value of θ_i in a soil layer at the beginning of each time step.

The position of θ_i in $[\theta_r, \theta_s]$ defines the index k to select the good a_k, b_k and d_k, and the increase of the conductivity by the roots is taken into account here :

$$K(\theta_i) = F_{K\text{root}} \, (a_k \theta_i + b_k) \quad (40)$$

$$D(\theta_i) = F_{K\text{root}} \; d_k \quad (41)$$

The output variables from `hydrol_soil_coef` are defined at each time step for each soil layer and each soiltile, and are called: `d` $= D(\theta_i)$, `k` $= K(\theta_i)$, `a` $= F_{K\text{root}} \, a_k$, `b` $= F_{K\text{root}} \, b_k$.

Since it is the only place where $F_{K\text{root}}$ is used in the code, the increase of K_s by roots does not lead to changes of α and m, contrarily to the decrease of K_s by means of compaction with depth.

3.6 Link with ORCHIDEE's variable names

See Table 3.

Symbol	SI unit	ORCHIDEE's name	ORCHIDEE's unit	Subroutine
z_i	m	`zz`	mm	`vertical_soil.f90`
ΔZ_i	m	`dz`	mm	
K_s^{ref}	m.s^{-1}	`ks`	mm.d^{-1}	`constantes_soil_var.f90`
K_s^{max}	m.s^{-1}	`ks_usda`	mm.d^{-1}	
n^{ref}	-	`nvan`	-	
α^{ref}	m^{-1}	`avan`	mm^{-1}	
n_0	-	`n0`	-	
B_n	-	`nk_rel`	-	
α_0	m^{-1}	`a0`	mm^{-1}	
B_α	-	`ak_rel`	-	
z_{lim}	m	`dp_comp`	m	??
f	-	`f_ks`	-	??
c_j	-	`humcste`	-	`constantes_mtc.f90`
f_v^j	-	`veget`	-	`slowproc.f90`
f^j	-	`veget_max`	-	`slowproc.f90`
z	m	`zz`	mm	
F_K	-	`kfact`	-	`hydrol_var_init`
$F_{K\mathrm{root}}$	-	`kfact_root`	-	
$(F_K)^{B_n}$	-	`nfact`	-	
$(F_K)^{B_\alpha}$	-	`afact`	-	
$n(K_s(z))$	-	`nvan_mod`	-	
$\alpha(K_s(z))$	m^{-1}	`avan_mod`	mm^{-1}	
θ_f	-	`frac`	-	
θ_k^b	m^3.m^{-3}	`mc_lin`	m^3.m^{-3}	
a_k	m.s^{-1}	`a_lin`	mm.d^{-1}	
b_k	m.s^{-1}	`b_lin`	mm.d^{-1}	
		`k_lin`	mm.d^{-1}	
d_k	m^2.s^{-1}	`d_lin`	mm^2.d^{-1}	
	-		-	

Table 3: Links between this document's symbols and variable names in subroutine `hydrol_var_init`.

3.7 Link with soil texture and particular soil moisture values

All the parameters involved in the Van Genuchten relationships depend on soil texture, which is deduced from soil maps as explained in the following section. Table 4 gives the main properties of the 12 USDA soil textures, including the values of d_2 (if not modified to follow K) and d_{50} (section 3.4). Table 5 gives the same information for the three classes obtained from the Zobler soil map.

In particular, the field capacity and wilting point are important threshold soil moistures, which control available water capacity, and are related to soil moisture stresses (section 4.1). The corresponding volumetric water contents, further noted θ_c and θ_w, can be related to n and α (Van Genuchten relationships), by means of characteristic soil matric potentials. These parameters are derived using the Van Genuchten relationships, based on a soil matric potential of -3.3 m (-1 m for sandy soils following Richards and Weaver (1944)) for θ_c, and -150 m (permanent wilting point) for θ_w, so they vary with soil texture. The resulting values of θ_c and θ_w used in ORCHIDEE are also given in Tables 4 and 5. As an example, Figure 6 shows the spatial distribution of wilting point and field capacity when using the USDA texture map (section 6.2) and an horizonal resolution of 144 $\times$ 142.

ORCHIDEE introduces another important threshold to constrain transpiration, and noted $W_{\%}$ in this document (`sm_nostress` in the code). It is the soil moisture above which transpiration is maximum, i.e. not limited by water stress (section 4.1). This threshold is defined via the parameter `pcent`=$p_{\%}$ in `constantes_soil_var.f90`:

$$W_{\%} = W_w + p_{\%}(W_c - W_w)$$

$p_{\%}$ is constant for all soil textures : $p_{\%} = 0.8$.

Two other special soil moisture values are defined in ORCHIDEE, thus in `hydrol.f90`, to characterize albedo changes with soil moisture. Albedo remains constant to the value $a_{\rm dry}$ when $\theta < \theta_{\rm dry}$, and it remains constant to $a_{\rm wet}$ when $\theta > \theta_{\rm wet}$. The parameters $\theta_{\rm dry}$ and $\theta_{\rm wet}$ are defined in `constantes_soil_var.f90`, while $a_{\rm dry}$ and $a_{\rm wet}$ are defined in the `condveg` module. **Since [rev3740], these variables are not used anymore**, and the background albedo file must now contain the variables `bg_alb_vis` and `bg_alb_nir` as in file `alb_bg_modisopt_2D.nc`.

4 Boundary conditions and sink terms: simulated fluxes

4.1 The transpiration sink term

The transpiration sink $s(z,t)$ in Eq. 12 describes the interplay between the transpiration flux, E_t, the soil moisture profile, and the root density profile, $R_j(z)$, which is assumed to decrease exponentially with depth in a way that is PFT dependent :

$$R_j(z) = \exp(-c_j z), \tag{42}$$

	Code's unit	1 Sand	2 Loamy Sand	**3 Sandy Loam**	4 Silt Loam	5 Silt	**6 Loam**
K_s^{ref}	mm.d^{-1}	7128.0	3501.6	1060.8	108.0	60.0	249.6
n^{ref}	-	2.68	2.28	1.89	1.41	1.37	1.56
α^{ref}	mm^{-1}	0.0145	0.0124	0.0075	0.0020	0.0016	0.0036
θ_s	m^3.m^{-3}	0.43	0.41	0.41	0.45	0.46	0.43
θ_c	m^3.m^{-3}	0.0493	0.0710	0.1218	0.2402	0.2582	0.1654
θ_w	m^3.m^{-3}	0.0450	0.0570	0.0657	0.1039	0.0901	0.0884
θ_r	m^3.m^{-3}	0.045	0.057	0.065	0.067	0.034	0.078
AWC(2m)	mm	9	28	112	273	336	154
$\log_{10}(d_2)$	m^3.m^{-3}	1.916	1.419	0.552	-2.229	-2.901	-0.926
$\log_{10}(d_{50})$	m^3.m^{-3}	6.724	6.478	6.105	5.375	5.126	5.642

	Code's unit	7 Sandy Clay Loam	8 Silty Clay Loam	**9 Clay Loam**	10 Sandy Clay	11 Silty Clay	12 Clay
K_s^{ref}	mm.d^{-1}	314.4	16.8	62.4	28.8	4.8	48.0
n^{ref}	-	1.48	1.23	1.31	1.23	1.09	1.09
α^{ref}	mm^{-1}	0.0059	0.0010	0.0019	0.0027	0.0005	0.0008
θ_s	m^3.m^{-3}	0.39	0.43	0.41	0.38	0.36	0.38
θ_c	m^3.m^{-3}	0.1695	0.3383	0.2697	0.2672	0.3370	0.3469
θ_w	m^3.m^{-3}	0.1112	0.1967	0.1496	0.1704	0.2665	0.2707
θ_r	m^3.m^{-3}	0.100	0.089	0.095	0.100	0.070	0.068
AWC(2m)	mm	117	283	240	194	141	152
$\log_{10}(d_2)$	m^3.m^{-3}	-1.483	-6.061	-3.754	-6.173	**-Inf**	**-Inf**
$\log_{10}(d_{50})$	m^3.m^{-3}	5.554	4.639	5.117	4.527	3.870	4.634

Table 4: Values of important soil parameters, as found in `constantes_soil_var.f90` for the 12 USDA texture classes (section 6). AWC(2m) gives the available water capacity of a 2m soil, calculated in mm as AWC(2m) = 2000 $(\theta_c - \theta_s)$. The values of d_2 and d_{50} are calculated assuming vertically uniform α and n (the very fine textures, for classes 11 and 12, lead to problematic values at very low soil moistures, at least in R, used here to compute d_2).

Parameter	ORCHIDEE's unit	1= Coarse (sandy loam)	2 = Medium (loam)	3 = Fine (clay loam)
K_s^{ref}	mm.d^{-1}	1060.8	249.6	62.4
n^{ref}	-	1.89	1.56	1.31
α^{ref}	mm^{-1}	0.0075	0.0036	0.0019
θ_s	m^3.m^{-3}	0.41	0.43	0.41
θ_c	m^3.m^{-3}	0.1218	0.1654	0.2697
θ_w	m^3.m^{-3}	0.0657	0.0884	0.1496
θ_r	m^3.m^{-3}	0.065	0.078	0.095
AWC(2m)	mm	112	154	240

Table 5: Values of important soil parameters, as found in `constantes_soil_var.f90` for the three soil texture classes kept when reading the Zobler map. See above for AWC(2m).

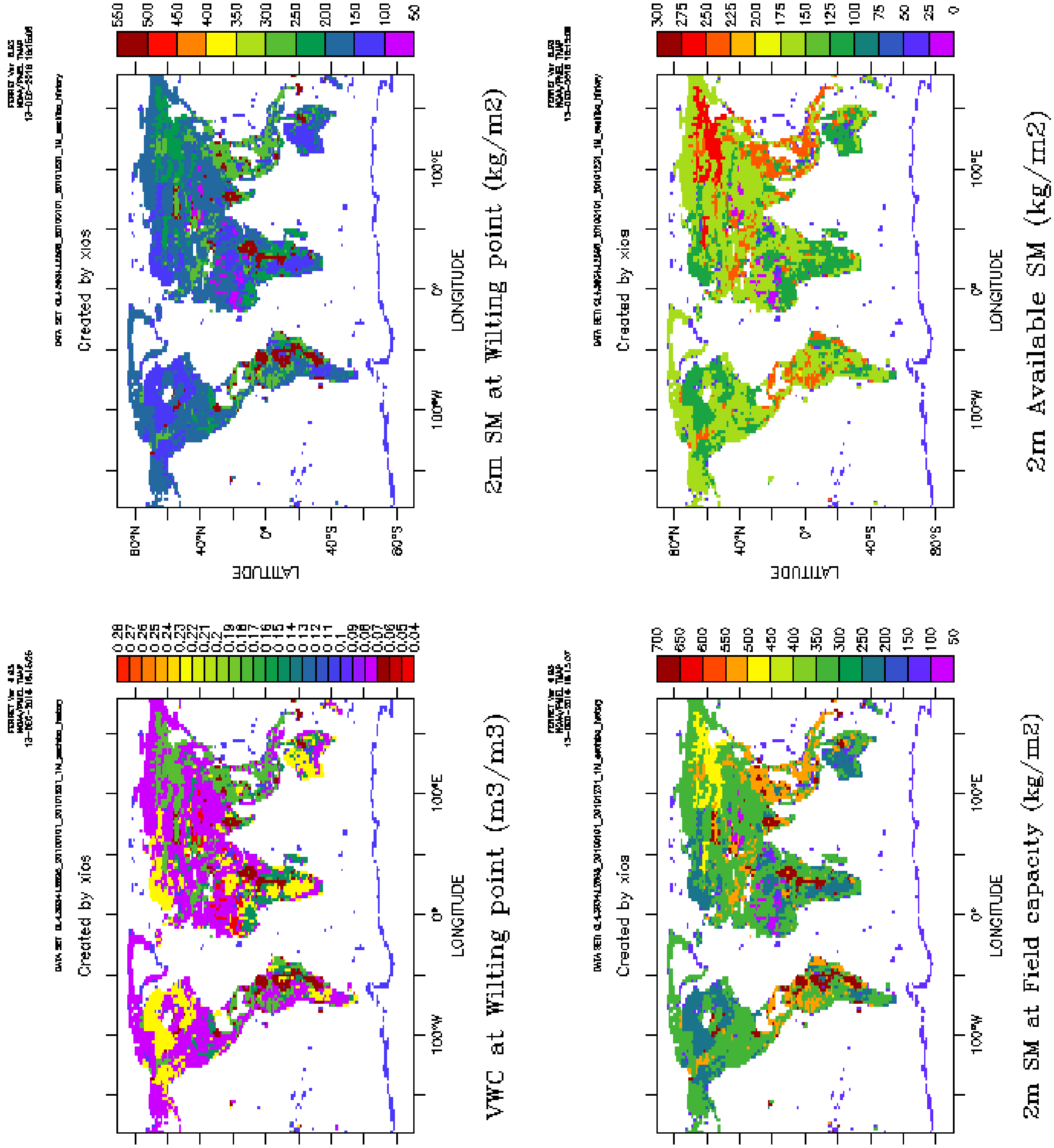

Figure 6: Particular moisture values with the USDA map at the 144 × 142 resolution: volumetric water content at wilting point θ_w in m3/m−3; total soil moisture at wilting point and at field capacity for a 2m soil (kg.m^{-2}); corresponding available water content, defined as the difference betwen the two previous maps.

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since the decay factor c_j is a PFT characteristic (see De Rosnay (1999, p158)).

In all the soil layers (but the top one, which does not contribute to transpiration), the local transpiration sink S_i (Eq. 21) is linked to the water stress factor U_s controlling E_t:

$$S_i = u_i \, E_t / U_s \tag{43}$$

$$E_t = \sum_{i>1} S_i \tag{44}$$

$$U_s = \sum_{i>1} u_i \tag{45}$$

In these equations, i identifies the soil layer, and u_i defines the local water stress factor, called `us` in the code (see section 7.2). It varies linearly from 0 (full stress) at the wilting point W_w to 1 (no stress) at $W_{\%}$, which is smaller or equal to the field capacity W_c. The stress factor u_i in each soil layer also depends on the mean relative root density in the layer i, called $n_{\text{root}}(i)$, with $\sum_i n_{\text{root}}(i) = 1$:

$$u_1 = 0 \tag{46}$$

$$u_i = n_{\text{root}}(i) \max(0, \min(1, (W_i - W_w)/(W_{\%} - W_w))) \tag{47}$$

As detailed in section 3.7, since [r3473], the default behavior in ORCHIDEE assumes that $W_{\%} = W_w + 0.8(W_c - W_w)$, and the corresponding shapes of the transpiration stress factor are illustrated in Figure 7 for the the various soil textures considered in ORCHIDEE.

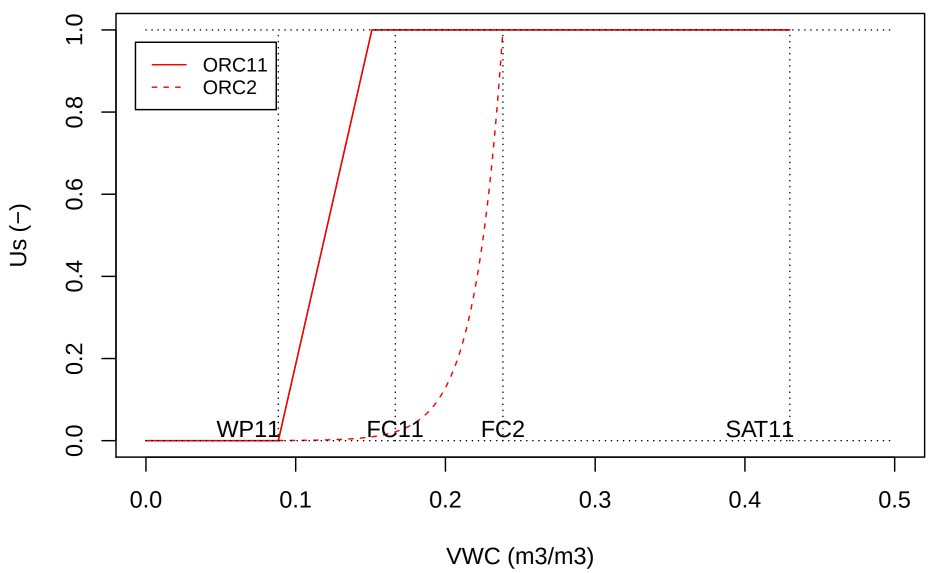
Importantly, all above variables are actually defined at the PFT level, but the index of the PFT was omitted for simplicity. The aggregation at the grid-cell scale is additive, for both the transpiration flux and the total sink term S_t, which correspond to the same quantity by construction:

$$E_t = \sum_j E_t^j = \sum_j \sum_{i>1} S_i^j = S_t \tag{48}$$

Eventually, in each PFT, the water stress factor U_s is involved in two ways:

- its value from the previous time step defines the root sink term thus the water budget of the current time step;
- once updated at the end of the current time step, based on the corresponding soil moisture, it is used at the beginning of the following timestep to calculate the stress function β_3 controlling the transpiration of the PFT thus the surface energy budget of the following time step.

In the code, U_s is called `humrelv` or `humrel`. As detailed in sections 7.2 and 7.3, **these two variables only differ by the absence/presence of a dimension for the soiltiles, and the code could be simplified by removing one of them**.



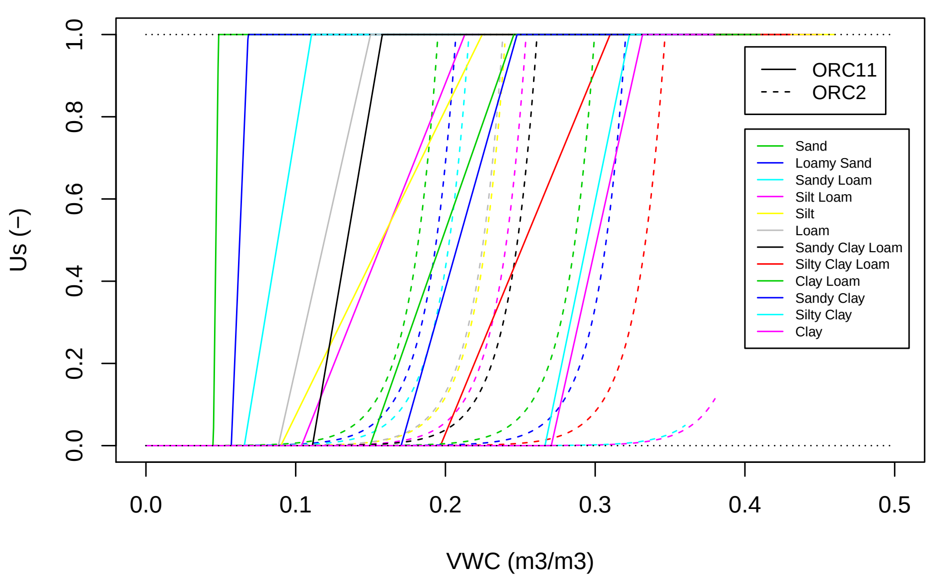


Figure 7: Function U_s computed in the case of uniform θ profiles. The dotted curves show the values of U_s in the 2-layer soil hydrology scheme, assuming a 2-m soil with a water-holding capacity of 150 kg.m^{-2} above wilting point, and no top layer. (top) Case of a loamy soil (texture class n^{o}6, in grey below), (bottom) all 12 texture classes. In all cases, we assume $c_j = 4$, as in the herbaceous PFTs. Note that n_{root} is taken into account for ORC11, but with no visible effect given the assumption of uniform θ profile.

4.2 At the soil surface: soil evaporation

Q_0 (section 2.2) is defined by the difference between infiltration into the soil (section 4.3) and soil evaporation, E_g.

The latter is a parallel flux to transpiration, which originates from the entire bare soil column, and from the bare soil fraction of the other soil columns. It is calculated using a **supply/demand approach, assuming it can proceed at the potential rate** (Eq. 9), **unless water becomes limiting**, i.e. if the upward diffusion to the top soil layer cannot provide enough water to sustain the required potential rate. If this is not the case, the diffusion needs to be recalculated assuming a lower soil evaporation.

This is explained in French in De Rosnay (1999, p60-61), but the strategy has slightly changed since. In particular, the potential rate is now calculated using the correction of Milly (1992), as briefly explained in d'Orgeval (2006, p74). The corrected potential evaporation is further called E^*_{pot}. The limitation of bare soil evaporation by upward diffusion is also estimated differently, now using a dummy integration at the end of `hydrol.f90`, as justified in French in Campoy (2013, p41-42).

In each soiltile c, we define the stress factor β_g^c aiming at controling the calculation of bare soil evaporation E_g^c, by

$$\beta_g^c = E_g^c / E_{\text{pot}}, \tag{49}$$

$$E_g^c = \min(E^*_{\text{pot}}, Q^c_{\text{up}}). \tag{50}$$

The demand is defined by E^*_{pot}, the potential evaporation reduced following Milly (1992), and the supply by Q^c_{up}, the maximum amount of water that can be extracted from the soiltile given the moisture profile (thus at the soil column scale).

To prevent from mass conservation violation, Q^c_{up} is estimated by dummy integrations of the Richards redistribution equation at the end of each time step, in which two boundary conditions are successively tested:

- firstly a flux condition favoring the demand ($E_g^c = E^*_{\text{pot}}$),
- then, if the previous case leads to any node with $\theta_i^c < \theta_r$, a Dirichlet condition ($\theta_1^c = \theta_r$ at the top node), which strongly limits E_g^c.

In both cases, if the total moisture in the top 4 soil layers (assumed to be representative of the litter) is below the wilting point, E_g^c thus β_g^c are arbitrarily reduced by a factor 2. Eventually, E_g^c can proceed at the potential rate of Milly (1992), unless water becomes limiting, i.e. if upward diffusion to the top soil layer cannot provide enough water to sustain the demanded rate. This is usually less frequent than the former case, but, as $E^*_{\text{pot}} < E_{\text{pot}}$ in most conditions, $\beta_g^c < 1$.

Since [rev3975], it is possible to reduce the demand, thus the soil evaporation, owing to a soil resistance following the formulation of Sellers et al. (1992):

$$r_{\text{soil}} = \exp(8.206 - 4.255 L/L_s), \tag{51}$$

$$E_g^c = \min(E_{\text{pot}}^*/(1 + r_{\text{soil}}/r_a), Q_{\text{up}}^c). \tag{52}$$

L is the soil moisture in the top 4 layers of the soil (litter zone, corresponding to 2.5 cm with the default vertical discretization, including soil ice), L_s is the corresponding moisture at saturation, and r_a is the aerodynamic resistance (Eq. 9).

In run.def, to use the soil resistance:
DO_RSOIL = y *(default = n)*

The fluxes E_g^c and Q_{up}^c, thus the factor β_g^c, are estimated after the update of the soil moisture profile as a function of the surface forcing (precipitation and evaporations fluxes required by the current time step's energy budget), thus at the end of `hydrol_soil.f90`. It will serve to control the bare soil evaporation and surface energy budget of the following time step, after spatial averaging towards the grid-cell scale. At this stage, β_g^c and E_g^c are local, in the sense that they do not depend on the fraction of bare soil in the soiltile.

The spatial integration of the stress factor at the grid-cell scale is performed at the very end of `hydrol_soil.f90`, by:

```
evap_bare_lim_ns(ji,jst) = evap_bare_lim_ns(ji,jst)
        * frac_bare_ns(ji,jst)/ evapot(ji)
evap_bare_lim(ji) = SUM(evap_bare_lim_ns(ji,:)*vegtot(ji)*soiltile(ji,:))
```

The right-hand side `evap_bare_lim_ns` in the first line corresponds to the flux E_g^c from a soiltile that would be fully covered with bare soil(in kg per m^2 of soiltile per time step in the code).

Link with diffuco:

`evap_bare_lim` is used at the following time step in diffuco, as $\beta_4^b = \min($`evap_bare_lim`$, 1 - \Sigma\beta_2^b - \Sigma\beta_3^b)$, to eventually constrain the surface energy budget. This expression uses the bulk stress functions β^b (called `vbeta` in the code), which come from the local stress functions of section 1.2 after multiplication by the grid-cell fraction from which the flux originates (A_v/A_L for the interception loss and transpiration, A_g/A_L for the bare soil evaporation). Note that diffuco uses `evapot` (E_{pot}) and `evapot_penm` (E_{pot}^*) that were calculated during the previous time step (by enerbil which is called after diffuco in sechiba.f90), i.e. the same timestep at which β_g^c and `evap_bare_lim(ji)` were calculated.

The limitation by $1 - \Sigma\beta_2^b - \Sigma\beta_3^b$ is due to the fact that bare soil evaporation is possible together with transpiration and interception loss from the same PFT, and we should in no case have a higher than potential ETR rate. Priority is given to transpiration (and IL), which somehow balances the fact that `evap_bare_lim` is defined by a "dummy" integration of the soil water diffusion which neglects the root sink. Thus, we can consider that the dummy integration only deals with the evaporation from the `frac_bare` fraction, independently from the transpiration, supposed to act on the `veget` fraction.

Eventually, we get (after [rev 3594]):

$$\texttt{evap\_bare\_lim} = \frac{A_g}{A_L}\beta_4 = \frac{A_g}{A_L}\min(\text{supply}, \text{demand})/E_{\text{pot}}.$$

4.3 At the soil surface: infiltration vs surface runoff

The main elements of the infiltration parametrization (`hydrol_soil_infilt.f90`) are described in d'Orgeval (2006); d'Orgeval et al. (2008). What relates to the soil conductivity has been detailed in section 3.3. Another element is a "time-splitting" procedure to describe the wetting front depth as a function of its speed. The parameterization also depends on a sub-grid distribution of infiltration (based on an exponential pdf), and on the mean slope of the grid-cell, with ponding that is only possible at low slopes. This is described in details (but in French) in d'Orgeval (2006, p77-80). A summary is provided below.

4.3.1 Local scale

The parametrization of infiltration into the soil is inspired by the model of Green and Ampt (1911), with a sharp wetting front propagating like a piston. A time-splitting procedure is used to describe the wetting front propagation during a time step as a function of its speed. To this end, the saturation of each soil layer is described iteratively from top to bottom. The time to saturate one layer depends on its water content, and on the infiltration rate from the above layer, which is saturated by construction (the top layer, with a 1-mm depth using the 11-mode discretization, is assumed to saturate instantaneously).

The input flux I_0 is composed of throughfall and snowmelt, plus the return flow from the routing scheme if the options allow for it. The procedure accumulates the time to saturate the soil layers from top to bottom, and if all the available water I_0 can infiltrate before the end of the time step, then no surface runoff is produced. Else, the part of I_0 that has not infiltrated during the time step becomes **surface runoff, produced by an infiltration-excess, or Hortonian, mechanism**.

For simplification, the effect of soil suction is neglected, which leads to gravitational infiltration fluxes. The infiltration rate is thus equal to the hydraulic conductivity at the wetting front interface, called K_i^{int}, and defined as the arithmetic average of $K(\theta_i)$ in the unsaturated layer i reached by the wetting front and at the deepest saturated node $(i-1)$:

$$K_i^{\text{int}} = (K(\theta_i) + K_s^*(z_i))/2. \tag{53}$$

d'Orgeval (2006, p78) reminds that geometric means of K should be preferred for diffusion in non saturated soils, based on Haverkamp and Vauclin (1979). Yet, arithmetic averaging of K_s is used for the wetting front propagation (`k_m`).

4.3.2 Subgrid scale

The parameterization also includes a **sub-grid distribution of infiltration**, which reduces the effective infiltration rate into each successive layer of the wetting front. In practice, the mean infiltrability over the grid-cell (K_i^{int} if we assume uniform properties) is spatially distributed using an exponential pdf, then compared locally to the amount of water to infiltrate (I_0, called `flux_tmp` in the code). As a result, infiltration-excess runoff is produced over the fraction of the soil column where I_0 is larger than the local k defined by the exponential distribution of the mean K_i^{int}, with the following cdf:

$$F(k) = 1 - \exp(-k/K_i^{\text{int}}). \tag{54}$$

A spatial integration is conducted for each soil layer i that becomes saturated when the wetting front propagates, giving the mean infiltration excess runoff R_i produced from the saturation of each soil layer i:

$$R_i = I_0 - K_i^{\text{int}}\,(1 - \exp(-I_0/K_i^{\text{int}})). \tag{55}$$

Eventually, this leads to define an effective conductivity $K_i^{\text{int}*}$ in each leayer:

$$K_i^{\text{int}*} = K_i^{\text{int}}\,(1 - \exp(-I_0/K_i^{\text{int}}). \tag{56}$$

Since this effective conductivity is smaller than the one of the uniform case (K_i^{int}), the sub-grid distribution increases surface runoff, given by the sum of R_i from all the layers saturated during the time step. This sub-grid distribution can be seen as the opposite to the parametrization of Warrilow et al. (1986), detailed in Ducharne (1997, Annex D p 187), since the conductivity K rather than the precipitation rate is spatially distributed within the grid-cells.

Finally, **a fraction γ of surface runoff is allowed to pond in flat areas**, to account for the effect of pond systems on infiltration (d'Orgeval et al., 2008). This fraction is constant over time, but varies spatially, based on an input slope map, which gives the slope in % at the 0.25° resolution and called `cartepente2d_15min.nc`. This file has been introduced by Tristan D'Orgeval during his PhD defended in 2006, and its headers refer to ETOPO, which suggests the 0.25° slope has been calculated based on the DEM ETOPO5 (1988) or ETOPO2 (2001).

The fraction γ (called `reinf_frac` in the code) is calculated in `slowproc_slope`. It is defined in each grid-cell based on S, the weighted area mean of the high-resolution slope (calculated by `interpweight_2Dcont`, and shown in Figure 8), and a threshold slope $S_{\max}$ (with a default value of 0.5%), such that local reinfiltration fraction decreases from 1 when $S = 0$, to 0 when $S \geq S_{\max}$:

$$\gamma = 1 - \min(1, S/S_{\max}) \tag{57}$$

The parameter $S_{\max}$ is externalized (using keyword `SLOPE_NOREINF`) and may be changed to modify the effectiveness of ponding. **However, it is probably not possible to use $S_{\max} = 0$ to cancel ponding**, because the code divides by $S_{\max} = 0$ without protection.

Surface runoff is then reduced by the fraction γ, which is temporarily stored in the variable `water2infilt`, kept to be infiltrated at the following time step with the following throughfall, snowmelt, and return flows from the routing scheme if any. The variable `water2infilt` thus conveys memory of water storage, and belongs to the prognostic variables. Note, however, that it is integrated to the total soil moisture variables `tmc` and `humtot` (sections 7.2 and 7.3)

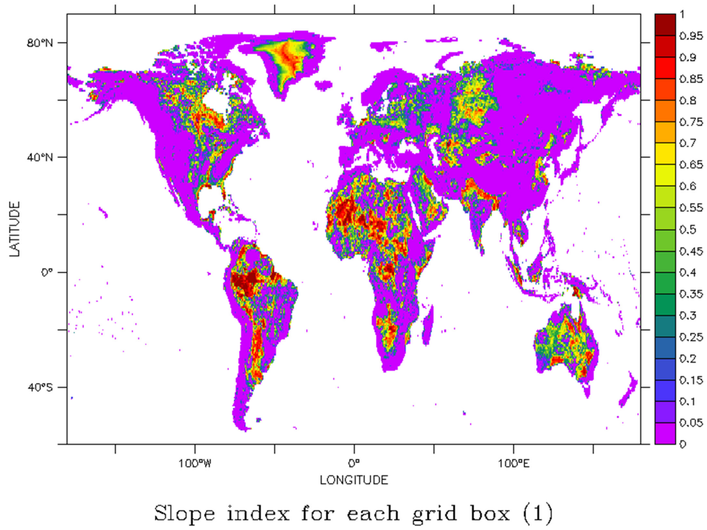


Figure 8: Map of the reinfiltration fraction γ produced by ORCHIDEE at the 0.5° resolution.

4.4 At the soil bottom: drainage, etc.

By default, the bottom boundary condition to water flow in the soil is defined by free gravitational drainage:

$$Q_N = K(\theta_N). \tag{58}$$

But two other options are possible. The first one, originally proposed by De Rosnay (1999), consists in reducing the free drainage calculation by a coefficient F:

$$Q_N = F.K(\theta_N), \tag{59}$$

where $0 \leq F \leq 1$. This condition is equivalent to reducing the hydraulic conductivity K under the bottom of the soil column, which could be achieved alternatively by enhancing the exponential decay of K with depth. Setting $F = 0$ makes the bottom totally impermeable as in the two-layer soil hydrology scheme of ORCHIDEE.

The second new boundary condition, proposed since Campoy (2013), is to impose saturation under the calculation node n_{sat} chosen by the user:

$$\theta_{i \geq n_{\mathrm{sat}}} = \theta_s. \tag{60}$$

This implies the presence of a water table inside the modeled soil column. To do so, we first solve the diffusion equation over the 2-m soil column assuming that $F = 0$, then we adjust the resulting soil moisture to bring it back to saturation at nodes n_{sat} and below, if either upward diffusion or root absorption made it drop to unsaturated values. The required water flux is assumed to enter the soil column through the soil bottom interface, and thus represents negative drainage.

WARNING:
Reduced drainage or having a water table in the soil column can create sharper θ gradients than with the free drainage boundary conditions. In such cases, you need to revise the vertical discretization, with thinner soil layers at depth (Campoy et al., 2013).

4.5 Total runoff

Eventually, the two runoff terms in ORCHIDEE are a surface runoff (Hortonian runoff minus reinfiltration), and drainage, gravitational by default, at the bottom of soil column. The input water flux feeding infiltration (I_{pot}) is the sum of throughfall and snowmelt during the time step, plus reinfiltration from the previous time step, and return flows from the routing scheme (from the flood plains and irrigation, see section 8.3), also from the previous time step.

For numerical convenience, infiltration proceeds before soil water redistribution, and bare soil evaporation (E_g, see next section) is subtracted from the input water flux. If the former exceeds the latter, there is no infiltration, and the top boundary condition to water redistribution is a water demand amounting $E_g - I_{\text{pot}}$.

Note that the runoff terms can be modified during the time step to correct the cases of "oversaturation" ($\theta > \theta_s$), which may arise from numerical errors when θ approaches saturation. If the drainage coefficient $F \leq 0.5$, or if soil freezing is allowed, all moisture above saturation is sent to surface runoff. Else, this "excess" moisture is sent to drainage. This involves `hydrol_soil_smooth_over_mcs2.f90`

5 Link to soil thermodynamics

5.1 Heat diffusion in the soil

The soil thermodynamic model in ORCHIDEE was developed by assuming the heat conduction to be the main process of the heat transfer in the soil vertical direction Hourdin (1992), which can be described by the classical one-dimensional Fouriers law:

$$C_v(\theta, \text{st})\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda\left(\theta, \text{st}\right)\frac{\partial T}{\partial z}\right], \tag{61}$$

where C_v and λ are respectively the soil volumetric heat capacity(J/m^3/K) and soil apparent thermal conductivity (J/m/s/K); T is the soil temperature (K). The heat diffusion is solved using an implicit finite difference method, with zero heat flux condition at the lower boundary of LSM Hourdin (1992); Wang et al. (2016). By default, the latter is set at 10 m, and the same vertical discretization as the one used for moisture is adopted for the top 2 m, so that the soil moisture profile does not need to be interpolated in order to diagnose the moisture-dependent thermal properties when solving the heat transfer equation (see section 2.2 for further details). In this framework, the soil below 2 m and down to 10 m is discretized into 3 additional layers of increasing thickness.

The trunk does not offer the possibility to describe the transport of heat by the water flow, which was shown to have a very weak effect by Wang et al. (2016).

5.2 Influence of soil freezing on water fluxes and STOMATE

Soil freezing is optional in ORCHIDEE, and controlled by the keyword `ok_freeze`. In this case, a part of the soil moisture can freeze depending on the temperature, following Gouttevin et al. (2012), with impacts on infiltration and the water stresses.

5.2.1 Profile of frozen fraction

The frozen fraction x_i^{ice} is defined at each time step and in each soil layer i at the begining of `hydrol_soil`, via `hydrol_soil_froz`, which calculates two complementary terms:

- x_i, which is the liquid saturation degree above θ_r: `(mcl-mcr)/(mcs-mcr)`
- $1-x_i = x_i^{\text{ice}}$, the frozen saturation degree above residual, exported as `profil_froz_hydro`

Of course, x_i varies with the soil layer temperature T_i: $x_i = 1$ if $T_i > 1^o$C and $x_i = 0$ if $T_i < -1^o$C. The transition is either linear or based thermodynamica considerations, following Gouttevin et al. (2012).

This formulation tends to induce an overestimation of total runoff, particularly in areas where soil freezing is moderate and undergoes strong seasonal variations (as the Mississippi and Danube river basins). An alternative formulation has been introduced in [r4202] to decrease the vertical profile $x_i(z)$ based on the vertical averages of:

- the frozen fraction, to reduce the effect of soil freezing on infiltration where a few layers only are frozen;
- the soil wetness (based on liquid and solid water in the top 1 meter), as freezing cannot markedly reduce the soil infiltration in dry soils where infiltration is already weak.

The vertical averages of the frozen fraction over the entire hydrological depth (2m by default) and of the soil wetness over the first meter are weighted by the thickness of each layer and called X^{ice} and $S_{\text{tot}}^{1\text{m}}/S_s^{1\text{m}}$. The frozen fraction of each layer is then modified as follows:

$$x_i^{\text{ice}*} = x_i^{\text{ice}}\,(X^{\text{ice}})^{n_F}\,(S_{\text{tot}}^{1\text{m}}/S_s^{1\text{m}})^{n_W} < x_i^{\text{ice}}. \tag{62}$$

The exponents n_F and n_W serve to modulate the attenuation of the frozen profile: the frozen fractions are maximum (equal to $x_i$ice) when $n_F = n_W = 0$; and they decrease all the more as n_F and n_W increase above 1, since both X^{ice} and S^{tot}/S_s belong to $[0, 1]$.

In the code, n_F and n_W are called `froz_frac_corr` and `smtot_cor`, and correspond the keywords FROZ_FRAC_CORR and SMTOT_CORR which have a default value of 1 and 2 respectively.

5.2.2 Impact on soil moisture and related fluxes

In `hydrol_soil`, we then distinguish the total volumetric water content at each node (`mc`, noted θ) from the liquid volumetric water content (`mcl` noted θ_i^{liq}):

$$\theta_i^{\text{liq}} = \min(\theta,\, x_i(\theta - \theta_r)) \leq \theta \leq \theta_s \tag{63}$$

$$\theta_{\text{ice}} = \theta - \theta_i^{\text{liq}} \tag{64}$$

$$\theta_i^{(new)} = \max(\theta_i^{\text{liq}},\, \theta_i^{\text{liq}} + (1 - x_i)(\theta_i^{(old)} - \theta_r)) \tag{65}$$

The soil moisture redistribution (Richards equation) is performed on θ_i^{liq}, and updates this variable. The required hydrodynamic parameters are defined in `hydrol_soil_coef`, based on θ_i^{liq} in each soil layer. The larger the frozen fraction, the smaller θ_i^{liq}, so the hydrodynamic parameters correspond to a drier soil (lower K and D).

Before the redistribution, the infiltration also depends on the reduced K if the soil is frozen (at least partially). The wetting front propagation, which depends on the soil moisture deficit of each layer compared to θ_s, is calculated based on θ, and this explicitely increases this variable. θ_i^{liq} is not explicitely updated, but it also increases since it is linked to θ by Equation 63.

The critical values of θ (θ_s, θ_c, θ_w, θ_r, see section 3.7) are constants that correspond to total soil moisture (liquid+solid). As a result, the sequences in `hydrol_soil` that involve these critical values for the corrections of over-saturation and under-residual cases values rely on total water content θ.

Finally, **all soil moisture variables which control evaporative or biological processes in ORCHIDEE are based on the liquid water content** θ_i^{liq}, although it was omitted for simplicity in the previous section:

- the calculation of the water stress factor U_s for transpiration (section 4.1) is based on θ_i^{liq} since plants cannot transpire solid water;
- the resistance r_{soil} to bare soil evaporation (section 4.2) is based on the liquid soil moisture in the top soil layers (L^{liq});
- the water stress factors for phenology (`vegstress`), for soil carbon decomposition (`shumdiag`), and for litter decomposition (`litterhumdiag`), all described in section 7.3), are also based on θ_i^{liq}.

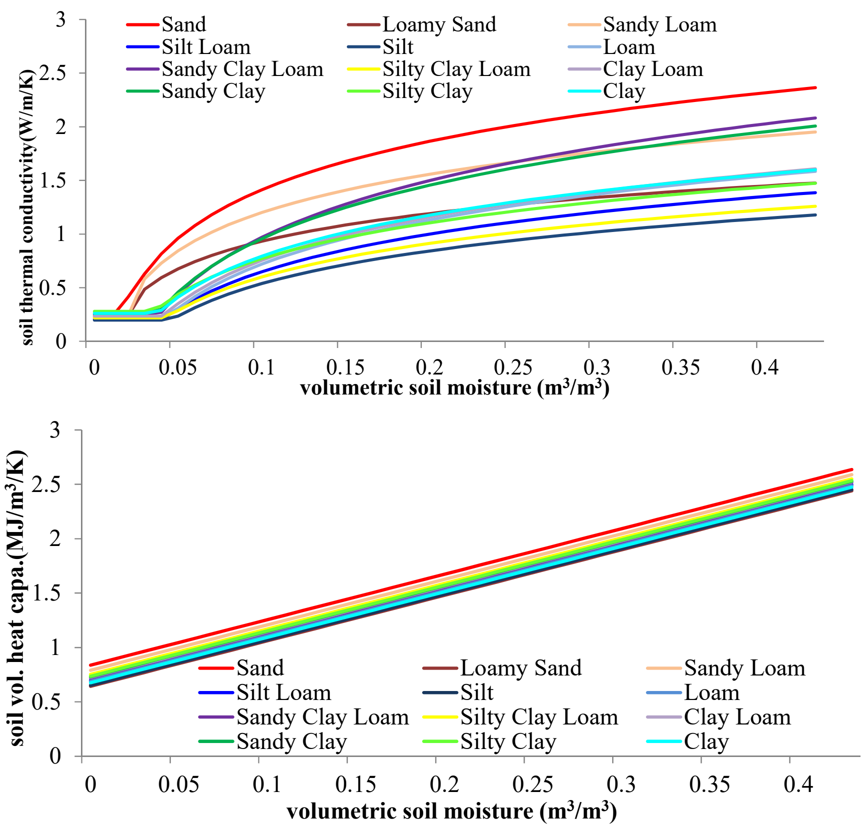


Figure 9: Dependance of heat conductivity κ (top) and heat capacity C_v (bottom) on volumetric water content θ and soil texture, for the 12 USDA classes.

5.3 Thermal properties depend on water content and soil texture

Since [r2922], the volumetric heat capacity C_v and the heat conductivity κ are parameterized as a function of soil texture and soil moisture θ, as illustrated in Figure 9. These dependences are detailed below, and include a different impact of the frozen and liquid water content (if the soil freezing is activated). Bugs were corrected in [r4767] and [r4768].

5.3.1 Heat conductivity

To compute the soil thermal conductivity κ (in $\mathrm{W\,m^{-1}\,K^{-1}}$), we followed the semi-empirical method proposed by Johansen (1975), modified by assuming a density of the soil solids of

2700 kg.m^{-3} as in Peters-Lidard et al. (1998). This leads to the following equations:

$$\kappa_i = \kappa_{\text{dry}} + (\kappa_{\text{sat}} - \kappa_{\text{dry}})\, K_e(\theta_i^*, \text{st}), \tag{66}$$

$$K_e = \log(\theta_i^*/\theta_s) + 1 \;\text{ if fine texture} \tag{67}$$

$$= 0.7\log(\theta_i^*/\theta_s) + 1 \;\text{ if coarse texture,} \tag{68}$$

$$\kappa_{\text{dry}} = \frac{0.135\,(1-\theta_s) + 0.024}{1 - 0.947\,(1-\theta_s)}, \tag{69}$$

$$\kappa_{\text{sat}} = (\kappa_{\text{q}}^q\, \kappa_{\text{o}}^{1-q})^{1-\theta_s}\, \kappa_{\text{liq}}{}^{x_i\theta_s}\, \kappa_{\text{ice}}{}^{(1-x_i)\theta_s}. \tag{70}$$

K_e is called the Kersten number and is described by two different formulations depending on soil texture. In ORCHIDEE, we assigned the first three textures of the USDA classification (Sand, Loamy sand, Sandy loam) to be "coarse" and so is the "Coarse" texture based on the Zobler map, which has the same hydrodynamic parameters as the USDA Sandy loam. κ_{dry} and κ_{sat} are the dry and saturated thermal conductivities (W m^{-1} K^{-1}), which depend on soil texture via the porosity θ_s and the quartz content q, defined in `constantes_var_soil`. The thermal conductivities of liquid water, ice, quartz, and other minerals (κ_{liq}, κ_{ice}, κ_{q}, and κ_{o} in W m^{-1} K^{-1}) are obtained from Peters-Lidard et al. (1998) and hard-coded in `thermosoil_cond`. The effect of ice on the thermal conductivity is controlled by the unfrozen volume x_i which depends on temperature as explained in section 5.2.

Finally, the heat diffusion scheme requires the soil thermal conductivities at the layers' interfaces, which are calculated based on θ^* values that are linearly interpolated at the interfaces according to the thickness of the layers and the depth of the nodes.

Note that the thermal conductivity values in `constantes_var` are not used anymore to calculate κ, so the code could be cleaned here.

5.3.2 Heat capacity

In contrast to heat conductivity, the heat capacities are required inside the layers, and are based on the mean θ of each layer. In each soil layer, $C_{v,i}$ (in J m^{-3} K^{-1}) is computed as the sum of heat capacities of soil and water in both liquid and solid phase:

$$C_{v,i} = (1-\theta_s)\, C_{v,\text{d}} + \frac{W_i^{\text{liq}}}{h_i}\, C_{v,\text{liq}} + \frac{W_i^{\text{ice}}}{h_i}\, C_{v,\text{ice}}. \tag{71}$$

The parameters that depend on soil texture are the porosity θ_s and the volumetric heat capacity of the soil solids, $C_{v,\text{d}}$ (J m^{-3} K^{-1}), which is defined in `constantes_var_soil` following Pielke (2002); Wang et al. (2016). W_i^{liq} and W_i^{ice} are the total water content in the soil layer i under liquid and solid phase (m), h_i is the thickness of the soil layer (m), so the ratios W_i^{liq}/h_i and W_i^{ice}/h_i give the mean values of θ_i^{liq} and θ_i^{ice} in the layer. $C_{v,\text{liq}}$ and $C_{v,\text{ice}}$ are the volumetric heat capacities for liquid water (4.186 10^6 J m^{-3} K^{-1}) and for ice (2.640 10^6 J m^{-3} K^{-1}), defined in `constantes_var_soil` and `constantes_var` respectively. Equation 71 assumes that the heat capacity of air is negligible.

To diagnose the specific heat capacity $C_{m,i}$ in $\mathrm{J\,kg^{-1}\,K^{-1}}$, we need to define the density of the soil layers:

$$\rho_i = (1-\theta_s)\,\rho_{\mathrm{d}} + \frac{W_i^{\mathrm{liq}}}{h_i}\,\rho_{\mathrm{liq}} + \frac{W_i^{\mathrm{ice}}}{h_i}\,\rho_{\mathrm{ice}}, \tag{72}$$

where ρ_{liq} = 1000 kg.m^{-3} and ρ_{ice} = 920 kg.m^{-3}. The density of the solid particles, ρ_{d} = 2700 kg.m^{-3}, is taken from Peters-Lidard et al. (1998), as already mentioned above. Eventually, the specific heat capacity is simply given by:

$$C_{m,i} = C_{v,i}/\rho_i. \tag{73}$$

6 Soil texture

In this framework, ORCHIDEE takes into account the soil's characteristics through parameters K_s, θ_s, θ_r, α and m, which directly depend on soil texture. This involves subroutines `slowproc_soilt` of `slowproc.f90` and `constantes_soil_var.f90`. As explained above, secondary parameters also depend on soil texture, in particular the wilting point and field capacity.

We only describe here the three cases that are presently coded into ORCHIDEE's Trunk: (i) soil texture is read from the Zobler (1986) texture map at the 1 ^{o} resolution; (ii) since [rev2419], soil texture can be read as USDA texture classes, provided at the 1/12 resolution from Reynolds et al. (2000); (iii) soil texture is forced in a 1D application after setting the two flags IMPVEG and IMPSOIL to true.

6.1 Definitions

Soil texture is defined by the soil's granulometric composition (in terms of particle size). It is usually defined as the % in three granulometric classes (`ntext=3`): coarse/sand (diameter $>$ 0.05 mm), medium/silt (diameter in $[0.002, 0.02]$ mm), and fine/clay (diameter $<$ 0.002 mm) particles. This granulometric composition can be visualized in texture triangles. One example is the USDA texture triangle, which defines 12 texture classes (domains within the triangle in Figure 10). In ORCHIDEE, this is defined by the array `textfrac_table`, which holds the correspondence between textural classes and their granulometric composition. The areal fractions of each textural class in each grid-cell is held in `soilclass`, and the dominant textural class is `njsc(kjpindex)`.

6.2 USDA map

Since [rev2419], the trunk correctly deals with the `CASE('usda')`, which effectively allows reading a map defining the USDA by indices ranging from 1 to 12, with the following order:

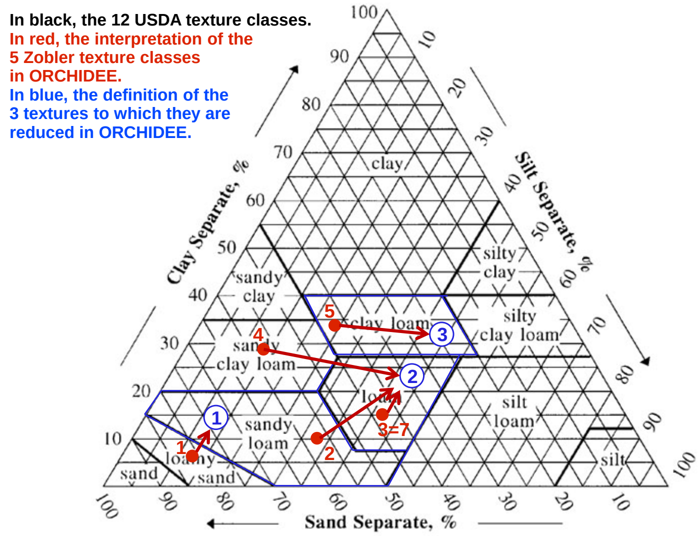


Figure 10: USDA triangle and its 12 texture classes (black), with the interpretation of the five Zobler classes (red), and the resulting three main texture classes kept in ORCHIDEE with this map (blue).

1. Sand
2. Loamy Sand
3. Sandy Loam
4. Silt Loam
5. Silt
6. Loam
7. Sandy Clay Loam
8. Silty Clay Loam
9. Clay Loam
10 Sandy Clay
11. Silty Clay
12. Clay

The related sequence of instructions is the following:

1. We read the USDA texture classes (0 to 12, with 0 in ocean points, and 1:12 for the texture classes). The "standard" file is called `soil_param_usda.nc`, at the 5' resolution, and originates from Reynolds et al. (2000).

2. Each class is defined by a granulometric composition in `get_soilcorr_usda`, assuming three main granulometric classes (`ntext=3`), for silt, sand and clay with indices from 1 to 3 respectively. In particular, this defines the % of clay particles for each texture. The granumometric composition for each USDA class are the mean values from Carsel and Parrish (1988), thus are consistent with the corresponding soil properties.

3. We calculate the area of each pixel, and the fractional area of the intersections between the grid meshes of the USDA texture map and ORCHIDEE (stored in `soilclass`).

4. Then, we compute `clayfraction` (for output and use in STOMATE), as the weighted area mean of the % of clay particles in the ORCHIDEE grid-cell, based on the areal fraction of each texture in the cell, and the % of clay particles defining

each of the 12 USDA soil texture class. The mean % of sand and silt particles is computed similarly for output.

5. The last step aims at assigning only one soil texture class to each ORCHIDEE grid-cell, further indexed by `njsc(ji)`. To this end, we take the **dominant texture**, i.e. covering the largest fraction, in each ORCHIDEE grid-cell. This is directly performed in `slowproc.f90`, just after the call to `slowproc_soilt`. In this framework, the texture of an ORCHIDEE grid-cell is not given by the mean fractions of clay, sans and silt of the grid-cell.

The main soil properties of the 12 USDA soil textures are given in Table 4 below. They can also be found in `constantes_soil_var.f90`.

In run.def:
HYDROL_CWRR = y
SOILTYPE_CLASSIF = usda
SOILCLASS_FILE = soils_param_usda.nc
SOILALB_FILE = soils_param.nc *(default)*
The file COMP/sechiba.card must also be adapted to include soils_param_usda.nc.

6.3 Zobler map

Here is the related sequence of instructions, mostly in `slowproc_soilt`, under the case `CASE('zobler')`:

1. We read the Zobler texture classes (0 to 7, with 0 and 6 reserved for ocean and ice respectively, and 7=3) at the 1° resolution of the map. By default, the corresponding forcing file is called `soil_param.nc`.

2. Each class is defined by a granulometric composition in `get_soilcorr_zobler`, assuming three main granulometric classes (`ntext=3`), for silt, sand and clay with indices from 1 to 3 respectively. In particular, this defines the % of clay particles for each texture. The tabulated granolometric compositions place the 5 textures in the loamy sand (1), sandy loam (2), loam (3=7), sandy clay loam (4), and clay loam (5), of the 12 USDA soil textural classes (red in Figure 10).

3. Still at the 1° resolution, the 5 above soil textures from the Zobler map are reduced to only three, which are then called the Coarse (holding class 1), Medium (gathering classes 2,3,4) and Fine (class 5) soil textures. The values of the corresponding hydrodynamic parameters have been extracted from the values of Carsel and Parrish (1988) for the 12 USDA texture classes, see the values in d'Orgeval (2006, p80). Given the values found in `constantes_soil_var.f90`, the Coarse, Medium and Fine soil textures respectively correspond to the Sandy loam, Loam, and Clay loam USDA texture classes (blue in Figure 10).

4. We calculate the area of each pixel, and the fractional area of the intersections between the grid meshes of Zobler and ORCHIDEE (stored in `soilclass`)

5. Then, we compute `clayfraction` (for use in STOMATE only), as the mean % of clay particles in the ORCHIDEE grid-cell, based on the % of clay particles defining each of the 5 Zobler soil texture class.

6. The last step aims at assigning only one soil texture class to each ORCHIDEE grid-cell, and is directly performed in `slowproc.f90` (just after the call to `slowproc_soilt`), by taking the dominant texture class as explained for the USDA case.

The main properties of the Coarse, Medium and Fine soil textures are given in Table 5.

In run.def:
HYDROL_CWRR = y
SOILTYPE_CLASSIF = zobler *(default)*
SOILCLASS_FILE = soils_param.nc *(default)*
SOILALB_FILE = soils_param.nc *(default)*

6.4 IMPSOIL

This option is only possible if IMPVEG=TRUE, in 1D configurations (double check this point). Then SOIL_FRACTIONS (nscm-element vector) and CLAY_FRACTION (scalar) must be defined in the `run.def` file:

- SOIL_FRACTIONS will define the variable `soilclass`. Remind that this is not a granulometric composition, but the fraction of each soil texture class (among the three ones that are defined in `constantes_soil_var.f90`: Coarse, Medium and Fine). At the point scale, this vector should be a permutation of (1,0,0), but even if not, the dominant class will be selected as the texture. If you want to use a soil texture that is different from the three above ones, among the 12 soil textures that are provided in Carsel and Parrish (1988), then you should change `constantes_soil_var.f90` and put the suitable values in the column with the largest fraction (`soilclass`).

- if IMPSOIL is true, the `clayfraction` is not deduced from the soil texture class and the corresponding fractions as above, and it needs to be prescribed by means of CLAY_FRACTION. Assuming a point scale study, it should thus be the % of clay particles in the selected soil texture class.

In run.def:
HYDROL_CWRR = y
IMPVEG = y
SOILTYPE_CLASSIF = zobler; SOIL_FRACTIONS with 3 values summing to 1
SOILTYPE_CLASSIF = usda; SOIL_FRACTIONS with 12 values summing to 1

7 Diagnosed soil moisture variables

Some variables are calculated in `hydrol_soil.f90`, `hydrol_diag_soil.f90`, and `hydrol_alma.f90`, for use in `stomate.f90`, `thermosoil.f90`, `diffuco.f90`, or for the output files.

WARNING: The multiplicity of variables with very close meaning increases a lot the risk of bugs.

7.1 Different soil moisture metrics and averages

Soil moisture can be quantified by different variables in ORCHIDEE (see Table 6 for notations):

- the volumetric water contents θ_i, which give the local moisture at the calculation nodes, in $m^3.m^{-3}$ (Figure 2),
- the total water contents W_i of the soil layers defined in Figure 2, and calculated using Eqs 18-20, in $kg.m^{-2}$ or mm,
- the total water content of the soil column: $S = \sum_1^N W_i$, in $kg.m^{-2}$ or mm. It is equivalent to the vertical integration of θ.
- the total water content of litter, defined in ORCHIDEE as the four top soil layers: $L = \sum_1^4 W_i$, in $kg.m^{-2}$ or mm.

All these variables are different in the different soiltiles of one ORCHIDEE grid-cell, and we can define two types of spatial averages across the soiltiles. In the following, we will indicate the simple weighted average across the different soiltiles by an overbar: $\overline{S} = \Sigma_c \, g^c \, S_c$, for the mean total soil moisture for instance. This value gives an average in kg per m^2 of $A_v + A_g = A_L - A_n$ (`vegtot` in the code), and the conversion to kg per m^2 of A_L defines $\widehat{S} = \overline{S}(A_v + A_g)$.

Finally, all these variables can be defined for total, liquid, and solid water, the latter two being identified by the exponents ^{liq} and ^{ice} in this document.

7.2 `hydrol_soil.f90`

- `wtd_ns`: water table depth, defined in each soiltile as the depth of deepest saturated node overlaid by an unsaturated node. It is sought starting at the soil bottom, such that a part of the soil that is saturated but underlaid with unsaturated nodes is not considered as a water table. If the bottom node is not saturated, the water table depth is set to `undef`.
- `wtd`: spatial average of `wtd_ns` over A_{vg}=`vegtot`.

Symbol	SI unit	ORCHIDEE's name	ORCHIDEE's unit
θ_i	-	`mc`	$m^3.m^{-3}$
W_i	$kg.m^{-2}$	no fixed name; sometimes called `soilmoist` or `sm`	$kg.m^{-2}$
θ_s	-	`mcs`	$m^3.m^{-3}$
θ_r	-	`mcr`	$m^3.m^{-3}$
θ_w	-	`mcw`	$m^3.m^{-3}$
θ_c	-	`mcf`	$m^3.m^{-3}$
a_{wet}	-	`mc_awet`	$m^3.m^{-3}$
a_{dry}	-	`mc_adry`	$m^3.m^{-3}$

Table 6: Links between this document's symbols and the soil moisture variable names in `hydrol`.

- `tmc`: defined per soiltile, as the vertical integration of θ, thus $S = \sum_1^N W_i$, **but `tmc` also includes water2infilt!**
- `tmc_litter`: defined per soiltile, from the same vertical integration, but restricted to the top four layers, thus corresponds to L. It does not include water2infilt.
- `soil_wet_litter`: defined per soiltile, as $(L^{\text{liq}} - L_w)/(L_c - L_w)$, where L_c and L_w correspond to critical values of L at the field capacity and wilting point respectively, computed in `hydrol_var_init.f90`.
- `us`: it defines the control of soil moisture onto the transpiration sink in Eq. 21, and is directly used in `diffuco_trans_co2.f90` to define the stress factor onto the stomatal conductance. It is defined for each vegetated PFT and per soil layer, as a function of $n_{\text{root}}(i)$, the mean of the root root density profile $R(z) = \exp(-c_j z)$ within the soil layer i, with $\sum_i n_{\text{root}}(i) = 1$:

$$u_s(1) = 0 \tag{74}$$

$$u_s(i) = n_{\text{root}}(i) \max(0, \min(1, (W_i^{\text{liq}} - W_w)/(W_\% - W_w))) \tag{75}$$

- `humrelv`: it corresponds to $U_s = \sum_i u_s(i)$, and it serves to define β_3 for transpiration. As shown in Figure 7, it is equivalent to the function plotted in De Rosnay (1999, p63), except for the choice of $W_\%$.
- `vegstressv`: it defines the control of soil moisture on the phenology in stomate. It is defined for each PFT as $\sum_i n_{\text{root}}(i) \max(0, \min(1, (W_i - W_w)/(W_c - W_w)))$, thus varies linearly from the wilting point W_w to the field capacity W_c (instead of $W_\%$ for U_s).

7.3 hydrol_diag_soil.f90

This subroutine deals with the transformation of 3D to 2D variables ,and additional diagnostics. Averages are performed across the soiltiles ($\overline{m}$), kept in m^2 of `vegtot` for transmission to stomate, and converted to m^2 of A_L ($\widehat{m}$) for transmission to thermosoil, routing, or output:

- `humtot`: mean of `tmc` at the grid scale, thus corresponding to $\widehat{S}$ in section 7.1. **Note it also includes water2infilt!**

- `humrel`: it is used to compute the water limitation on transpiration in `diffuco.f90`:
  - to compute `vbeta3` in `diffuco_trans.f90` if `control%ok_CO2` is FALSE
  - else to compute `water_lim=humrel` in `diffuco_trans_co2.f90` (default)

  `humrelv` is defined per PFT and soiltile, while `humrel` is defined per PFT only. In the code, we find:

  ```
  humrel(ji,jv) = SUM(humrelv(ji,jv,:))
  ```

  This works because one PFT belongs to one single soiltile, but a simpler way is:

  ```
  humrel(ji,jv) = humrelv(ji,jv,pref_soil_veg(jv))
  ```

- `vegstress`: it is defined per PFT from `vegstressv` per PFT and soiltile:

  ```
  vegstress(ji,jv) = SUM(vegstressv(ji,jv,:))
  ```

  Like for `humrel`, a simpler way would be to rely on `pref_soil_veg(jv)`

- `k_litt`: mean hydraulic conductivity of the litter layer over the entire grid-cell, for use in `routing.f90`, for reinfiltration from floodplains of ponds. The same calculation is performed in `hydrol_diag_soil.f90` and in `hydrol_var_init.f90`. We start by defining the litter hydraulic conductivity in each soiltile, based on the corresponding L^{liq}; the litter wetness is $(L^{\text{liq}} - L_r)/(L_s - L_r)$, and is used to find an index k for the linearized K (see section 3.4).

  `k_litt` is defined in each soiltile as the geometric mean between K_s and K_k, the linearized value of K in the **top** soil layer given the mean wetness in the 4 litter layers (`k_lin(k,1,njsc)`). Finally, a weighted spatial average is performed across the soiltiles, then converted to a grid scale mean ($\widehat{m}$).

  The use of geometric means of K is preferred in d'Orgeval (2006, p78) for diffusion in non saturated soils, following Haverkamp and Vauclin (1979). But why averaging with K_s in the first place ? We can also question the choice of using `k_lin(k)`, instead of Equation 40 which accounts form the effcts of roots on surface permeability.

- `litterhumdiag`: mean of `soil_wet_litter` across soiltiles ($\overline{m}$), for transmission to stomate.

- `dry_soil_frac`: it is used in `condveg` to calculate the albedo of dry soil, excluding the nobio contribution which is further added. It is thus defined as mean fraction of dry litter across soiltiles ($\overline{m}$), based on $(\overline{L_{\text{wet}}} - \overline{L^{\text{liq}}})/(\overline{L_{\text{wet}}} - \overline{L_{\text{dry}}})$, where $\overline{L_{\text{wet}}}$

and $\overline{L_{\rm dry}}$ are wet and dry bounds, outside which albedo is assumed to be constant to its wet/dry value (see section 3.7). Note that this variable is not used when the background albedo is read from a file (possible since [r3171,3618,3740]).

- `soilmoist`: grid-scale mean of the W_i of a given soil layer, thus $\widehat{W_i}$. This variable is computed to feed the "SoilMoist" output in the ALMA standard.
- `shumdiag`: this variable, linked to `vegstressv`, is created for `stomate`, per soil layer (diaglev up to nbdl), as the average across soiltiles ($\overline{m}$) of $\max(0, \min(1, (W_i^{\rm liq} - W_w)/(W_c - W_w)))$, where W_c is the water content at field capacity (section 3.7).
- `shumdiag_perma`: this variable has been created in [r2222-2224], for `thermosoil.f90`, where it is used to make the soil's thermal properties (conductivity and capacity) depend on soil moisture. It is defined per soil layer as the average across all soiltiles of W_i/W_s. Since `thermosoil.f90` works at the grid-scale, the grid-scale average is used here ($\widehat{m}$), but **this would need probably to be changed if the thermal properties of the nobio fraction were explicitely accounted for.**

7.4 `hydrol_alma.f90`

This subroutine defines variables that are required by the ALMA standard. All these variables are grid-scale averages :

- `tot_watsoil_end = humtot`
- `delsoilmoist`: change in `humtot` over the time step
- `soilwet = humtot(ji)/ mx_eau_var(ji)`
- `delintercept`: change in `watveg = SUM(qsintveg(ji,:))` over the time step
- `delswe`: change in `snow(ji)+SUM(snow_nobio(ji,:))` over the time step

7.5 Special output for CMIP

- `humtot_top`: grid-scale mean of soil moisture in the top 10 cm, calculated as the sum of W_i along the top 6 soil layers. It works for the standard vertical discretization, but would deserve to be generalized to any case.

7.6 Water conservation

- `twbr`: this variable has been introduced to monitor the water budget closure in `hydrol.f90`. It gives the total water budget residu of this routine, calculated at each time step as the difference between the total water storage change and the net fluxes. The routine conserves water all the better as this residu is small. **Typical values are around 10^{-4} mm/d** (but `twbr` is exported in mm/s).

8 Areal fractions

8.1 ORCHIDEE's indices (space and texture)

See Table 7.

Symbol	ORCHIDEE's name	Maximum value	Definition
i	`jsl`	`nslm=11`	Soil nodes
k	`i`	`imin=1,imax=51`	Bins to linearize K and D
j	`jv`	`nvmc = 13`	PFTs or MTCs
c	`jst`	`nstm=3`	Soiltiles
	`nsc`	`nscm=3` if Zobler	Texture classes in `hydrol.f90`
		`nscm=12` if USDA	
		`ntext=3`	Granulometric classes,
			to define the granulometric composition
	`jd/jg`	`ngrnd=7`	Soil nodes or soil layers for thermodynamics
	`l/jd/jg`	`nbdl`	Diagnostic soil layers

Table 7: Links between this document's indices and the ones in `hydrol.f90`.

8.2 ORCHIDEE's variables used for areal integrations

The following ORCHIDEE's variables are used to support areal integrations in `hydrol.f90`:

- `frac_nobio`: fractions of A_L covered with either ice, lakes, cities, etc. Several indices are possible for different types on "nobio", but in the trunk, only one is used, supposedly for ice, but it may include the free water bodies ***** to be checked**.
- `totfrac_nobio`: total fraction of "nobio" with respect to A_L, i.e. f_n
- `vegtot`: total fraction of A_L covered by PFTs (bare soil + vegetation) , i.e. f_{vg}
  `vegtot(ji) + totfrac_nobio(ji) = 1`
- `veget_max`: fractions of A_L assigned to the different PFTs, i.e. f^j
  `SUM(veget_max(ji,:))  = vegtot(ji) = 1 - totfrac_nobio(ji)`
- `veget`: fraction of A_L covered by the "dominant surface type" (bare soil for PFT 1, vegetation in other PFTs) in each PFT. It is equal to f_v^j, except for the bare soil PFT (assigned the index $j = 1$), in which `veget` corresponds to f_g^1:
  `veget(ji,1) = veget_max(ji,1)`
  `veget(ji,jv) = veget_max(ji,jv)*(1 - frac_bare(ji,jv))`
- `frac_bare`: evaporating bare soil fraction of `veget_max(jv)` (defined in `slowproc_veget`). It is f_g^j/f^j, and $f_g^1/f^1 = 1$:

```
frac_bare(ji,1) = 1
frac_bare(ji,jv) = 1 - veget(ji,jv)/veget_max(ji,jv) for jv ¿ 1
```

- `tot_bare_soil`: Total evaporating bare soil fraction of A_L, i.e. f_g (does not include nobio)

  ```
  tot_bare_soil(ji) = SUM(veget_max(ji,2:nvm) - veget(ji,:))
                      + veget_max(ji,1)
  ```

  It can also be defined as below, although this is not found in the code:

  ```
  tot_bare_soil(ji) = SUM(frac_bare(ji,:)*veget_max(ji,:))
  ```

- `soiltile`: Fraction of $A_v + A_g$ assigned to each soiltile, i.e. g^c

  ```
  soiltile(ji,1) = veget_max(ji,1) / vegtot(ji)
  SUM(soiltile(ji,:))  = 1
  ```

- `mask_soiltile(ji,jst)= 1` if soitile `jst` exists in grid-cell `ji`

- `pref_soil_veg(jv)=jst`: defines the links between PFTs and soiltiles, in `slowproc _veget.f90`

- `vegetmax_soil` (new name of `corr_veg_soil`): PFT fraction per soiltile, defined as f^j/g^c, knowing that one PFT belongs to a single soiltile by construction:

  ```
  vegetmax_soil(ji,jv,jst) = veget_max(ji,jv) / soiltile(ji,jst)
  ```

  Note that $\sum_c g_c \sum_{j \in c}(f^j/g^c) = f_{vg}$.

- `frac_bare_ns`: Evaporating bare soil fraction per soiltile (defined in `hydrol_vegupd`). This variable is used for the split of `vevapnu` into `ae_ns`, and for the various weightings of bare soil evaporation from the soiltiles to `vegtot` to A_L:

  ```
  frac_bare_ns(ji,jst) = frac_bare_ns(ji,jst)
  + vegetmax_soil(ji,jv,jst) * frac_bare(ji,jv) / vegtot(ji)
  ```

  With the above notations, we find that `frac_bare_ns` equals $\sum_{j \in c}(f_g^j/g^c)/(f_{vg})$. We get that `SUM(frac_bare_ns(ji,jst)*soiltile(ji,:))= tot_bare_soil(ji)/vegtot(ji)` $= f_g/f_{vg}$.

9 Configuration for CMIP6v1

For CMIP6, ORCHIDEE is mostly used coupled to LMDZ (144x142x79), but also in nudged mode (LFMIP) or off-line for LMIP and SP-MIP (Van den Hurk et al., 2016).

Table 8 below summarizes the choices related to `hydrol` for CMIP6v1, for the runs to be launched at the end of December 2017. The corresponding revision is [r4812], and is complemented by specific information in the run.def or orchidee.def files, for the input files and keywords mentioned in Table 8.

Object	CMIP6 Choice	Files and Keywords	Reference
INPUT MAPS			
Soil texture map	Zobler at 1°	SOILTYPE_CLASSIF=zobler SOILCLASS_FILE=soils_param.nc	Sec.6.3, Tab.5
Slope map	ETOPO at 0.25°	cartepente2d_15min.nc	Sec.4.3.2, Eq.57
Land cover, PFTs	CMIP6 maps ESA-LUH2v2 with 15 PFTs	Directory historical/15PFT.v1	Sec.1.2
OPTIONS			
Soil hydrology scheme	Multi-layer diffusive (CWRR)	HYDROL_CWRR=y	This entire note
Vertical discretization	Water : 2m, 11 "geometric" nodes T : 90m and 18 nodes, with the same top 2m	DEPTH_MAX_H=2.0 DEPTH_TOPTHICK≈0.001 DEPTH_MAX_T=90.0 DEPTH_CSTTHICK=90.0	Sect.2.3
Bare soil fraction	Reduced with ext_coeff_vegetfrac_mtc	EXT_COEFF_VEGETFRAC=1	Eq.2
Root profile	Default set of humcste for CWRR		Eqs.32, 42, 47
VG parameters	Default given Zobler soil map		Tab.5
$K_s(z)$	Default, depends PFT via root profile		Eq.33
$\alpha(z)$ and $n(z)$	No dependence to depth z	CWRR_AKS_A0=0. CWRR_AKS_POWER=0. CWRR_NKS_N0=0. CWRR_NKS_POWER=0.	Sect. 3.3
Soil evaporation	No soil resistance	DO_RSOIL=n	Eq.50
Options for other processes with strong link to soil hydrology			
Background albedo	Read from maps based on MODIS	ALB_BG_MODIS=y ALB_BG_FILE=alb_bg.nc	
Throughfall			
Roughness length	Depends on LAI following	ROUGH_DYN=y	Su et al. (2001)
Snow	3-layer snow scheme	OK_EXPLICITSNOW=y	Wang et al. (2013)
Soil freezing	Yes, with attenuation of the frozen profile	OK_FREEZE_CWRR=y OK_THERMODYNAMICAL_FREEZING=y FROZ_FRAC_CORR=1 SMTOT_CORR=2	Sect.5.2, Eq.62
Routing	Yes Based on 0.5° drainage map	STREAM_TCST=0.24 FAST_TCST=3.0 SLOW_TCST=25.0	Ngo-Duc et al. (2007)

Table 8: Specificities of `hydrol` for CMIP6v1.

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