

Laboratoire des Sciences du Climat et de l'Environnement

TECHNICAL NOTE

Description of the energy budgets in ORCHIDEE

Initial author : Julien ALLÉON (julien.alleon@lsce.ipsl.fr) January 4, 2022



Contents

IG	ieneral	introduction	5
11 1	Descrip othe	tion of the current energy budget in ORCHIDEE and interactions with r modules	6
II.1	Introd	uction	6
	II.1.1	Role of this module in ORCHIDEE	6
	II.1.2	Spatial framework for each budgets	6
		II.1.2.1 Photosynthesis and soil water budgets	6
		II.1.2.2 Energy budget	7
	II.1.3	Structure of the note	8
II.2	Mode	l description	9
	II.2.1	Main equations	9
	II.2.2	Turbulent transfer with the atmosphere	11
		II.2.2.1 Louis' model in ORCHIDEE	11
		II.2.2.2 Calculation of the heights	13
	II.2.3	Implicit coupling with the atmosphere model	18
		II.2.3.1 Type of coupling	18
		II.2.3.2 Atmospheric column resolution	18
		II.2.3.3 Surface radiation scheme in an implicit coupling between the GCM	
		and ORHCIDEE	21
11 3	Solitti	ng of the water fluxes	23
11.5	TI 3 1	ß-model concept	2 5 23
	II.3.2	Calculation of the β coefficients	$\frac{20}{25}$
	11.0.2	II 3.2.1 Calculation of β_1	$\frac{20}{25}$
		II 3.2.2. Calculation of β_1 .	26
		II.3.2.3 Calculation of β_3 .	$\frac{20}{27}$
		II.3.2.4 Calculation of β_4	$\frac{2}{29}$
		II.3.2.5 Calculation of β_3	30
II.4	Soil th	nermodynamics	32
	11.4.1	Physical aspects	32
	11.4.2	Thermosoil module	32
	11.4.3	Interaction with water in the layers	36
	11.4.4	Interaction with snow at the surface	37
II.5	Mode	lling in ORCHIDEE	40
	II.5.1	The <i>enerbil</i> module scheme	40
	II.5.2	Subroutine descriptions	41
		II.5.2.1 enerbil_begin subroutine	41
		II.5.2.2 enerbil_surftemp subroutine	42
		II.5.2.3 enerbil_flux subroutine	45
		II.5.2.4 enerbil_evapveg subroutine	48
	II.5.3	thermosoil and explicits now modules	49
		II.5.3.1 <i>thermosoil</i> module	49



II.5.3.2 <i>explicitsnow</i> module	. 51
II.6 Suggestions	54
III Description of the multi-layer energy budget in ORCHIDEE	55
III.1 Introduction III.1.1 Aim and history of this module in ORCHIDEE III.1.2 Current energy budget in ORCHIDEE III.1.3 Notations	55 . 55 . 55 . 55
III.2 Model description III.2.1 General description III.2.2 Energy budget at level i III.2.2 Energy budget at level i III.2.2.1 Leaf energy budget III.2.2.2 Energy transport between layers III.2.3 General energy budget of level i III.2.3 Radiations scheme III.2.3.1 Long Waves radiations scheme III.2.3.2 Short Waves radiations scheme III.2.4 Leaf resistances III.2.4.1 To sensible heat flux III.2.4.2 To latent heat flux	57 57 58 58 59 61 62 62 62 62 62 62 64 5 65
III.3 Implicit resolution III.3.1 Coupling with atmosphere III.3.2 Implicit form of the main equations III.3.3 Resolution of the equations III.3.3.1 Principle of the resolution III.3.3.2 Resolving the system III.3.4 Boundary conditions III.3.4.1 Upper boundary condition III.3.4.2 Lower boundary condition	67 67 69 70 70 70 71 79 79 79 79
III.4 Modelling in ORCHIDEE III.4.1 The mleb module scheme III.4.2 Subroutine descriptions III.4.2 Subroutine descriptions III.4.2 Subroutine descriptions III.4.2.1 The mleb_boxheight subroutine III.4.2.2 The mleb_begin subroutine III.4.2.3 The mleb_profile subroutine III.4.2.4 The mleb_lwrad subroutine III.4.2.5 The mleb_boundarylayer_resistance subroutine III.4.2.6 The mleb_stomatal_resistance subroutine III.4.2.7 The mleb_calc_column subroutine III.4.2.8 The mleb_flux subroutine III.4.2.9 The mleb_evapveg subroutine III.4.3 One-layer case	 86 86 87 88 88 88 89 90 91 92 96 96 97
III.5SuggestionsIII.5.1DebugDebugIII.5.1.1Use of the β sIII.5.1.1	99 . 99 . 99



III.5.1.2 SW radiations scheme \ldots	100
III.5.1.3 Dimensional analysis of the latent heat flux	100
III.5.2 Further improvements	100
III.5.2.1 Multi-tiling necessity	100
III.5.2.2 Remarks on the turbulent transport model	100
III.5.2.3 Link with the new hydraulic architecture scheme	100
III.5.3 Action plan	101
IV Current and future developments	102
IV.1 Multi-layer energy budget	102
IV.2 Multi-tiling energy budget	102



List of Figures

1	Division of the grid-cell into PFTs and soiltiles	7
2	Turbulent diffusion with atmosphere heights and definitions	14
3	Vertical discretization of the atmospheric column.	19
4	Top-Down and Bottom-Up resolution of the atmosphere column temperature	20
5	Soil discretization scheme	33
6	Global resolution scheme of both atmospheric and soil heat diffusion	36
7	Schematic diagram of the snow cover above the ground	38
8	Summary of the main snow processes	39
9	Scheme of the <i>enerbil</i> module	40
10	Scheme of the <i>thermosoil</i> module	50
11	Scheme of the <i>explicitsnow</i> module	52
12	Potential and resistance scheme of the canopy	57
13	Implicit resolution scheme of the current energy budget and soil and atmosphere columns	68
14	Implicit resolution scheme of the multi-layer energy budget and soil and atmosphere columns	69
15	Scheme of the <i>mleb</i> module	86
16	Path of the calculation when $jnlvls = 1$ in $mleb_main$	97



Partie I General introduction

This note is a general description of the way the energy budget is solved in ORCHIDEE. This note is written in January 2021, at the time you read it, some parts of the code may have changed. Moreover, I do not present this note as a gospel, I discovered some parts of the code especially to present them in the note. I may have written some mistakes or misinterpretations of the code. Consequently, if something changed since January 2021 or if something is badly explained, you are kindly invited to update the note by following this link:

https://www.overleaf.com/2942446624wydpjztkzxnw

This link leads to an Overleaf document, you only have to create an account (free) and go through the different documents. This technical note aims at helping everyone understanding ORCHIDEE. The more people help refining and completing the note, the best it would be for the next people involved in the project.

The initial aim of the note was to describe the energy budgets in ORCHIDEE. However, the description of the energy budget leads to the description of all the other processes developed in the model. As the aim was not to make a general technical note of ORCHIDEE, some choices have been made and some parts of the code are maybe not presented or presented shortly. Feel free to ask the persons of the team for more details and add anything you think interesting in the note.

Finally, this note is composed by 2 sub-notes describing the "current" energy budget in ORCHIDEE (*enerbil* module) and the "multi-layer" energy budget in ORCHIDEE (*mleb* module). Initially, the note was divided into those two sub-notes before being merged in only one big technical note. Consequently, some rehearsals may occur between Parts II and III.



Partie II

Description of the current energy budget in ORCHIDEE and interactions with other modules

II.1 Introduction

II.1.1 Role of this module in ORCHIDEE

The *enerbil* module computes the energy budget between the atmosphere and the land surfaces in ORCHIDEE. For each grid-cells at each time step, the module solves the energy budget equations based on the Penmann & Monteith approach[16]. It permits to calculate the sensible and latent heat fluxes exchanged between the land surface and the atmosphere accounting for the various components of the latent heat flux: soil evaporation, transpiration, snow sublimation...

The module is also the key interface of the coupling with the LMDZ model, the Global Circulation Model (GCM) of the IPSL. The implicit coupling between both models is permitted thanks to a subroutine (*enerbil_surftemp*) of the *enerbil* module which computes the values of the static energy, temperature and saturated moisture at the surface at the new time step. This permits a robust coupling at each time step.

The aim of the present note is to focus on the resolution of the energy budget in ORCHIDEE, on the coupling between the GCM and ORCHIDEE and on the parallel calculations which have an impact on the budget (thermosoil, β -model for the latent heat flux splitting...).

II.1.2 Spatial framework for each budgets

At each time step, ORCHIDEE is computing several budgets:

- An energy budget, presented in this technical note.
- A soil hydrology budget, presented in the technical note from Agnès Ducharne [5].
- A photosynthesis budget

II.1.2.1 Photosynthesis and soil water budgets

Each budget is run on a specific framework within each grid cell. The basis of each framework is the concept of Plant Functional Types (PFTs). PFTs are the way land surface model discretize what is in reality a continuous vegetation. They represent different types of vegetation. In ORCHIDEE, PFTs are regrouped in Meta-Classes (MTCs). At the time this note is written, there are 15 PFTs regrouped into 13 MTCs: 1 for bare soil, 8 for forests and 4 for croplands/grasslands (The grasslands PFTs "C3 Boreal", "C3 Temperate" and "C3 tropical" are regrouped into the MTC 10 in ORCHIDEE). Each MTCs is associated to a specific bunch of parameters which permits to differentiate the calculation of the budget according to the MTCs. Because photosynthesis is a plant-associated phenomenon, it has been decided that, for each grid-cell, ORCHIDEE will run 13 different photosynthesis budgets. One for each MTC. (**NB:** As a



simplification, the note will only talk about PFTs from now. This term will, in ORCHIDEE, refer to the 13 MTCs)

As it is described in the related technical note [5], soil water fluxes are computed within "soiltiles" or "soil water columns". On each columns, water input by throughfall and snow melt, water output by total runoff, transpiration and soil evaporation are calculated. The number of soil water columns is reduced to 3: 1 for bare soil, 1 for all the forest PFTs and 1 for all the croplands/grasslands PFTs. However, all the non biological biomes (glaciers, cities, free water...) are regrouped in a "nobio" soiltile. This additional water budget is considered as a simplified glacier with only snow accumulation and melting.

The PFTs and soiltiles are linked in ORCHIDEE's code thanks to a function called *pref_soil_veg* which relates the PFT index to its related soil water column. The 2 different discretizations are described on Figure 1.



Figure 1: On the left: Division of the grid-cell into PFTs On the right: Division of the grid-cell into soiltiles.
"i" corresponds to the indice of the PFT, "j", to the one of the related soil tile (j=pref soil veg(i))

II.1.2.2 Energy budget

Unlike the photosynthesis and soil hydrology budgets, the energy budget is not computed within a sub-grid scale. For now, there is only one energy budget per grid-cell (from ORCHIDEE's point of view). This choice is directed by the coupling between ORCHIDEE and the LMDZ Global Circulation Model. Because both model need to be coupled when running together in the IPSL Earth Model, the energy, carbon and water fluxes from sub-grid scales need to be mixed in order to respect the resolution of LMDz. More precisely, the energy budget which corresponds to a key interface between surface and atmosphere, needs to be seen by LMDz as a only one budget per grid-cell. In order to simplify the energy budget and the interface with the atmosphere, the energy budget has been decided to be computed at the grid cell level. The link between the energy budget at the grid-cell level and the photosynthesis and soil water budgets at a sub-grid scale is made thanks to a β -model which splits the latent heat flux between all the fluxes that compose it (soil evaporation, plant transpiration...). This β -model is described in Section II.3.

(From LMDZ point of view, a grid-cell can have 4 sub-surfaces (ocean, surface, land-ice and sea-ice) which leads to 4 energy budgets and 4 implicit couplings, however, all those sub-surfaces see the same atmosphere : same temperature, humidity and wind)



II.1.3 Structure of the note

Because ORCHIDEE is a complicated model (in terms of number of processes described), describing *enerbil* module calls to describe a lot of other variables calculated in several other parts of the code. In a matter of understanding, I decided to let everything description of *enerbil* code at the end of the note, in Section II.5. However, every variable which is calculated in a specific subroutine in another module has a description of the subroutine just after the description of the calculation. For example, the resolution of the energy budget in *enerbil* needs the calculation of β coefficients. The use of the β coefficients in the calculation of the energy budget is presented in Section II.3. This calculation is done in the subroutine *enerbil_evapveg* which is described in the Section II.5. However, the β coefficient are calculated in the *diffuco* module. The presentation of the subroutines of diffuco are done directly after the presentation of the principles of calculation of the β coefficients in Section II.3.



II.2 Model description

The energy budget computed in the *enerbil* module of ORCHIDEE aims at calculating several variables linked to the energy budget and permit to send other variables to the Global Circulation Model. The module is basically divided into three subroutines:

- The interface with the Global Circulation Model which calculates the variables needed to compute the energy budget.
- The calculation of the fluxes
- The splitting of the latent heat flux into its sub-fluxes.

The module is consequently relying on three different models:

- The surface energy budget
- The implicit coupling
- The β -model that permits the splitting

The aim of the module is to calculate each variable that compose the budget at each time step. In order to help the understanding of the model, the values framed by "{}" are the values of the previous time step. The other ones are the values of the present time step.

II.2.1 Main equations

The general equation that computes the radiation budget relates the net radiation (radiation absorbed by the surface) to the short wave and long wave radiation budgets (respectively $S_n = S \downarrow -S \uparrow$ and $L \downarrow -L \uparrow$). Short wave radiations are coming from the Sun whereas long wave radiations come from the atmosphere. The budget is given by Equation (1).

$$R_n = L \downarrow + S_n - L \uparrow \tag{1}$$

The down-welling short-wave radiations and the down-welling long-wave radiations are computed by the GCM and are inputs of ORCHIDEE's energy module (*enerbil*). The net short-wave radiation (S_n) are obtained by ORCHIDEE thanks to the albedo calculated in the module *albedo surface*.

The up-welling long-wave radiations represents the land surface emission, and can be linked to its temperature by Stefan's law $(L \uparrow = \epsilon \sigma T_{surf}^4)$. Because of the implicit coupling with the atmosphere, the up-welling long-wave radiations cannot rely on the surface temperature of the previous time step. The new surface temperature should then be approximated. This approximation is computed by the interface between the surface and the atmosphere (see Section II.2.3). Because this "new" surface temperature is an intermediate value between the one of the previous time step and the one of the current time step, the up-welling long-wave flux is calculated thanks to a limited Taylor expansion of the surface temperature around the previous value. Finally, the reflected long-wave radiation is added to the flux. The latter is thus given by Equation (2)

$$L \uparrow = \epsilon \sigma \{T_{surf}\}^4 + 4\epsilon \sigma (T_{surf} - \{T_{surf}\})^3 + (1 - \epsilon)L \downarrow$$
(2)



Where ϵ is the emissivity of the surface, σ is Stefan's coefficient and T_{surf} is the surface temperature.

The energy budget equation shows how the net radiation at the surface is used either to heat the soil by conduction (G), evaporate the surface water (F_{lat}) or heat the atmosphere by convection (F_{sens}) . R_n is then linked to the the sensible heat flux (F_{sens}) , the latent heat flux (F_{lat}) , the ground heat flux (G) and the chemical energy stored by photosynthesis $(F_{chem}, neglected here)$. The budget is then expressed as follows:

$$R_n = F_{sens} + F_{lat} + G + F_{chem} \tag{3}$$

In enerbil, the net radiation term is calculated thanks to Equation (1). However, because they are useful for other budgets such has photosynthesis, soil heat convection or soil water diffusion, all the terms of Equation (3) are calculated, F_{sens} and F_{lat} in enerbil and G in thermosoil (see Section II.4).

In *enerbil*, the latent and sensible heat fluxes are calculated respectively thanks to Equations (4) and (5) (in the implicit coupling with atmosphere, their formulae is different and relying on the previous time step, See Section II.2.3).

$$F_{lat} = \lambda.\beta.\rho. |\vec{V}|.C_d.(q_{surf} - q_{air}) \tag{4}$$

$$F_{sens} = \rho. |\vec{V}|.C_d.C_p(T_{surf} - T_{air})$$
(5)

Where, ρ is the air density, $|\vec{V}|$ is the horizontal wind, the norm of the wind vector according to x and y, C_d is the drag coefficient, C_p is the specific heat of air, λ is the latent heat of evaporation (or sublimation), q_{surf} is the saturated surface moisture $(q_{surf} = q_{sat}(T_{surf}))$, q_{air} is the saturated air moisture (at 2m when ORCHIDEE is running alone, in the first atmospheric layer when coupled with LMDZ), T_{surf} is the surface temperature, T_{air} is the air temperature (same as q_{air}) and, finally, β is a resistance coefficient to the potential total evaporation. More details will be given on those fluxes in Section II.2.3 and II.3.

From the latent heat flux, can be deduced the water mass flow along the time step by multiplying F_{lat} by $\Delta t/\lambda$ (in the case of only evaporation or only sublimation). When the resistance coefficient β is equal to 1, this flux represents the potential evaporation of the surface. However, as the potential evaporation represent the evaporation of an hypothetically wet surface (without any resistance), this potential evaporation is over-estimated in some cases because calculated thanks to the surface temperature instead of the surface temperature of the hypothetically wet surface $(T_{s,wet})$ (See more explanations in *Barella-Ortiz et al. (2013)*[2]. This change in the temperature comes from the way the energy budget is computed. T_{surf} is directly computed thanks Equation (3). Calculate the $T_{s,wet}$ would need another energy budget calculation. To avoid this over-estimation or the new calculation, a correction has been introduced in literature by *Milly (1992)*[15]. This correction links the potential evaporation calculated thanks to T_{surf} , $E_p(T_{surf})$ to the potential evaporation calculated thanks to $T_{s,wet}$, $E_p(T_{a,wet})$ thanks to Equation (6).

$$\frac{E_p(T_{surf})}{E_p(T_{s,wet})} = \frac{1+\xi}{1+\beta\xi}$$
(6)

Where ξ is given by Equation (7).



$$\xi = \frac{\lambda \rho |\vec{V}| C_d \frac{\partial q_{sat}}{\partial T} (T_a)}{4\epsilon \sigma T_a^3 + \rho c_{p,air} |\vec{V}| C_d}$$
(7)

And, β is the ratio between the actual evaporation and the potential one as presented in Section II.3. Milly's correction acts directly on the potential evaporation because there is no way to approximate $T_{s,wet}$ instead of solving another energy balance with $T_{s,wet}$ instead of T_{surf} . The expression of the correction is explained in *Milly (1992)*[15], but it mainly relies on a linear analysis of the two different energy balances. Those linearized energy balance permit to access to an equation linking $E_p(T_{surf})$ and $E_p(T_{s,wet})$ to the terms described in Equation (7).

NB: There is one thing I do not understand with this correction. The correction aims at better represent the total potential evaporation flux. This flux is used in a lot of parts of the code (expression of the vbetas, hydrol...). However, in a lot of cases, $E_{pot,tot}$ seems to be used instead of $E_{pot,tot,corr}$. Why this correction is not used everywhere?

II.2.2 Turbulent transfer with the atmosphere

Turbulent transfer of the fluxes between the surface and the atmosphere is represented thanks to the drag coefficient. This coefficient, presented in the Equations (4) and (5) is calculated in two different ways:

- When coupled with LMDZ, C_d is not calculated in ORCHIDEE but in LMDZ. The value is then given to ORCHIDEE at each time-step (but ORCHIDEE computes the roughness heigths which leads to the calculation of the drag coefficient by LMDZ).
- When not coupled to LMDZ, C_d is calculated in the module *diffuco*. This calculation is presented right after.

The calculation of C_d (also expressed as $\frac{1}{r_{ah}.u}$ where u is the wind speed and r_{ah} the aerodynamic resistance) in ORCHIDEE is based on the model developed by Jean-François Louis at ECMWF in 1982 [11]. This model derives from the Monin-Obukhov Similarity Theory (MOST) and permits to express the drag coefficient as a function of Richardson Number and of the roughness heights associated to momentum and heat fluxes.

In ORCHIDEE those calculations take place into two different subroutines. First of all, in the module *condveg*, the roughness heights are calculated in the subroutines *condveg_z0cdrag* and *condveg_z0cdrag_dyn*. This routine computes z_{0m} , the roughness height associated to the momentum, z_{0h} , the roughness height associated to the heat fluxes and d, the displacement height. The difference between both routines is that in the second one, the roughness heights vary dynamically with vegetation. The choice between both calculation is determined thanks to a control parameter *rough_dyn*. Secondly, in the module *diffuco*, the subroutine *diffuco_aero* uses those roughness height to computes the drag coefficients.

II.2.2.1 Louis' model in ORCHIDEE

As presented before, Louis' model derives from the Monin-Obukhov Similarity Theory. It permits to calculate the drag coefficients as functions of the aerodynamic resistance in neutral, stable and unstables conditions thanks to Richardson Number. Richardson Number is expressed as in Equation (8).



$$Ri_b = z_{lev}.g.\frac{\theta_{air} - \theta_{surf}}{\theta_{air}.u^2}$$
(8)

Where θ_{air} and θ_{surf} are the virtual temperatures of the air and the surface, z_{lev} is the height of the first atmospheric layer, g is the gravitational constant and u is the wind speed.

Moreover, the drag coefficient in neutral conditions is expressed thanks to Equation (9).

$$C_{d,neut} = \frac{k^2}{ln(\frac{z_{lev}-d}{z_{0m}}).ln(\frac{z_{lev}-d}{z_{0h}})}$$
(9)

Where k is the Von Karman constant.

Finally, from those two variables, Louis' model has been optimized against observations and the drag coefficient is computed as in Equation (10) for the stable case $(Ri_b > 0)$ and Equation (11) for the unstable case $(Ri_b < 0)$.

$$C_d = \frac{C_{d,neut}}{1 + 3.b.Ri_b.\sqrt{1 + d.Ri_b}}$$
(10)

$$C_d = C_{d,neut} \cdot (1 - \frac{3.b.Ri_b}{1 + 3.C_{d,neut} \cdot b.c. \sqrt{\frac{z_{lev} - d}{z_{0m}} \cdot |Ri_b|}})$$
(11)

diffuco aero subroutine

The subroutine diffuco_aero computes the aerodynamic resistances and the drag coefficients. It started by calculating all the coefficients needed for the calculation of Ri_b after computing $C_{d,neut}$. When the latter is computed, according to the value of Ri_b , C_d is calculated thanks to Equation (10) of (11).



Variable	Name in ORCHIDEE	Description	Unit	\mathbf{Type}
$ \overrightarrow{V} $	speed	Wind speed	$m.s^{-1}$	External input
C_d	$q_c drag$	Surface drag coefficient	_	Output used in enerbil module
z_{lev}	zlev	Height of the first atmospheric layer	m	External input
z_{0m}	z0m	Roughness height for momentum	m	Input from <i>condveg</i> module
z_{0h}	z0h	Roughness height for heat	m	Input from <i>condveg</i> module
d	$\begin{array}{c} 1-roughheight/h\\ \text{where h is the}\\ \text{average height of}\\ \text{the canopy} \end{array}$	Zero-plane displacement height	m	Input from <i>condveg</i> module
k	ct_karman	Von Karman coefficient	—	ORCHIDEE input
$C_{d,neut}$	cd_neut	Surface drag coefficient in neutral conditions	_	Local variable
Ri_b	zri	Richardson number	—	Local variable
$ heta_{air}$	ztvd	Air virtual temperature computed thanks to air and surface temperatures and saturated humidity	K	Local variable
$ heta_{surf}$	ztvs	Surface virtual temperature computed thanks to air and surface temperatures and saturated humidity	K	Local variable

II.2.2.2 Calculation of the heights

As presented in the previous section, the module *condveg* computes the roughness heights needed for the calculation of the drag coefficients. Before explaining the ways the heights are calculated, here are some definitions and the origins used in the different parts of the code.

- Canopy height: The height between the soil and the treetops (it will be noted h here).
- Zero-plane displacement height: The height above the surface at which the mean of the wind velocity is zero *in absence of turbulence* (noted d).
- Roughness height: Difference between d and the effective height at which the mean of the wind velocity stops because of turbulence (noted z0).
- Measures height: When not coupled to LMDZ, ORCHIDEE is forced thanks to meteorological data (mainly, wind at 10m and temperature at 2m). Those data are reanalysed in order to match the heights of measurements to the same height above the canopy, z_{lev} .

The heights are summarized on Figure 2.





Figure 2: Summary of the heights and their definitions

Moreover, the origins from which all the heights are defined defer according to the model, the modules and the use of the model.

- Because it is an atmospheric model, **LMDZ** has as origin the zero-plane height of displacement, *d*.
- In *diffuco*, ORCHIDEE's module, the height called *zlev* is defined above the canopy. The origin is then the height of canopy h.
- In *condveg*, ORCHIDEE's module, the height is defined above the zero-plane height of displacement, *d*.

Those different origins engender several "height conversions" between the ORCHIDEE modules. Because *condveg* is described above d, Equation (9) is reduced to Equation (12).

$$C_{d,neut} = \frac{k^2}{ln(\frac{z_1}{z_{0m}}).ln(\frac{z_1}{z_{0h}})}$$
(12)

Finally, the conversion between *condveg* origin and ORCHIDEE one is made thanks to a variable called *roughheight* which represents... the canopy height minus the zero-plane displacement height!

All those heights are calculated in the module *condveg* in two different subroutines *condveg_z0cdrag* and *condveg_z0cdrag_dyn*. They correspond to two different ways of calculation of the heights. The original one, in *condveg_z0cdrag*, and a new one which takes into account the LAI effects in *condveg_z0cdrag_dyn*.

The **old-fashioned way** of calculation of the heights relies on the inversion of the calculation of the drag coefficients. First of all, the drag coefficients for momentum and heat are approximated for each PFT thanks to Equation (13).



$$C_d = \frac{k^2}{\ln(\frac{z_{lev}}{h_{PFT} * z_0 \text{ over } h})^2} \tag{13}$$

Where h_{PFT} is the height of the canopy of the considered PFT and $z_{0_over_h}$ is a parameter that estimates the roughness height above the canopy.

Because there is one energy budget per grid-cell (See Section II.1.2), all the heights need to be converted from the PFT scale to the grid-cell one. Then, after calculation of all the drag coefficients for each PFT, a mean drag coefficient is calculated thanks to the portion of gridcell occupied by each PFT. To this PFT-mean drag coefficient is added the drag coefficient of the portions of non biological areas of the grid-cell. This gives the global grid-cell mean drag coefficient $C_{d,mean}$.

Finally, from this $C_{d,mean}$, the roughness heights are deduced as in Equation (14) (it is assumed that $z_{0m} = z_{0h} = z_0$). And the conversion variable *roughheight* is given by Equation (15).

$$z_0 = \frac{z_{lev}}{exp(k/\sqrt{C_{d,mean}})} \tag{14}$$

$$roughheight = \overline{h_{PFT}} - d \tag{15}$$

Where $\overline{h_{PFT}}$ is the mean canopy height over the PFTs.

NB: This is exactly the same calculation when the drag coefficient is calculated by the GCM. The roughness heights are calculated following this path but the drag coefficient is calculated in diffuco_aero only when ORCHIDEE is not coupled to ORCHIDEE. Consequently, ORCHIDEE always calculates the C_d and $C_{d,mean}$ in order to get th eroughness heights.

condveg z0cdrag subroutine

The subroutine $condveg_z0cdrag$ computes the heights needed for the calculation of C_d by Louis' model. The first part of the code calculates the mean drag coefficient that will be used for the calculation of the roughness height as in Equation (13). The values of the drag coefficients of each PFT and nobio surface are weighted by the fraction of the grid-cell occupied by the surface (in the code: veget or $veget_max$ for the fraction of each vegetation surface, $frac_nobio$ for the fraction of each nobio surface and tot_bare_soil for the fraction of bare soil. For each type of surface without vegetation (nobio and ground), a specific z0 is used in the calculation of the drag coefficient: $z0_bare$ and $z0_nobio$ (parameters of ORCHIDEE). Finally, a ratio to deduce z_{0m} from z_{0h} is presented ($ratio_z0m_z0h$) but its value is set to 1, so as presented above, $z_{0m} = z_{0h}$. The other variables are the following:



Variable	Name in ORCHIDEE	Description	Unit	Туре
$C_{d,mean}$	dragm = dragh (because $ratio_z0m_z0h \text{ is set}$ to 1)	Surface drag coefficient	_	Local variable
z_{lev}	zlev	Height of the first atmospheric layer	m	External input
z_{0m}	z0m	Roughness height for momentum	m	Output used in <i>diffuco</i> module
z_{0h}	z0h	Roughness height for heat	m	Output used in <i>diffuco</i> module
d	$height_displacement$	Zero plane displacement height (coefficient set to 2/3, to multiply with canopy height h_{PFT})	m	ORCHIDEE input
k	ct_karman	Von Karman coefficient	_	ORCHIDEE input
h_{PFT}	height	Canopy height	m	Input from another module
$z_{0_over_h}$	$z0_over_height$	Parametred value of z0 to calculate the drag coefficients (set to 0.0625m)	m	ORCHIDEE Input

The new way of calculation has been imagined because of a too high sensible heat flow during winter in the deciduous forests. This suggested that the effect of vegetation and LAI was not taken into account in the calculation of the aerodynamic resistance as it should be. Then, instead of adding a vegetation aerodynamic resistance, it has been decided to change the way to calculate the roughness heights and add a dependence to LAI as it is presented in *Su et al. (2001)* [22].

The principle stays the same, the mean over the PFT is made on the drag coefficients but those drag coefficients are now determined thanks to new calculations of z_{0m} and z_{0h} presented in Su's article, as in Equations (16) and (17).

$$z_{0m} = h.(1 - \frac{d}{h}).e^{-\frac{k}{\eta}}$$
(16)

$$z_{0h} = \frac{z_{0m}}{e^{kB^{-1}}} \tag{17}$$

Where, $\eta = c_1 - c_2 exp(-c_3 C_{d,leaf} LAI)$ ($c_1, c_2, c_3, C_{d,leaf}$ are parameters at the PFT level) and kB^{-1} is expressed as in Equation (18).

$$kB^{-1} = \frac{k.C_{d,leaf}}{4.C_t.\eta.(1 - exp(-\frac{C_{d,leaf}.LAI}{2\eta^2}))} \cdot f_c^2 + 2.f_c.f_s.\frac{k.\eta.z_{0m}/h}{C_t^*} + kBs^{-1} \cdot f_s^2$$
(18)

Where, f_c is the fractional canopy coverage, f_s is the bare soil coverage, C_t is the heat transfer of the leaf (PFT parameter), C_t^* is the heat transfer coefficient of the soil ($C_t^* = Pr^{-2/3}.Re^{-1/2}$, with Pr, the Prandtl number and Re, Reynolds number). Finally, kB^{-1} is empirically defined as $kBs^{-1} = 2.46Re^{1/4} - ln(7.4)$. It represents the term for the bare soil.

This new parametrization permits to:

- Take into account the differences between the resistances for the transfer of heat and momentum (i.e. introduction of kB^{-1} parameter)
- Take into account the fact that the roughness depends on the LAI and vary seasonally



NB1: However, this vegetation effect should maybe be integrated in another aerodynamic resistance instead of the drag coefficient. Indeed, for the case of the multi-layer, vegetation effects should probably be calculated during the turbulent transport of the fluxes inside the canopy, not at the drag surface coefficient which should represent the interaction with atmosphere. Thus, it would maybe double count the vegetation effect when running this new parametrization with the multi-layer energy budget. (Needs to be discussed, I maybe missed something)

NB2: Used in LMDZ it leads to screen level values (t2m, q2m) often outside of the [surface-first atmospheric level interval] which is not consistent with the MO laws.

$condveg_z0cdrag_dyn$ subroutine

The subroutine $condveg_z 0cdrag_dyn$

Variable Name in ORCHIDEE		Description	Unit	Туре
z_{0m}	z0m	Roughness height for momentum	m	Output used in <i>diffuco</i> module
z_{0h}	z0h	Roughness height for heat	m	Output used in <i>diffuco</i> module
h	loc_height for the height of each PFT and ave_height for the average over the grid-cell	Canopy height	m	Input from another module / Local variable
d $height_displacement$		Zero plane displacement height. Coefficient set to 0.66, to be multiplied with canopy height	m	ORCHIDEE Input
k	ct_karman	Von karman coefficient	—	ORCHIDEE Input
η	eta	Ratio of friction velocity to the wind speed at the canopy top	_	Local variable
$C_{d,leaf}$	$Cdrag_foliage$	Foliage specific drag coefficient	_	ORCHIDEE Input
LAI	lai	Leaf area Index	_	Input from another module
c_1, c_2, c_3	c1, c2, c3	Parameters	—	ORCHIDEE input
C_t	ct_karman	Von Karman constant	—	ORCHIDEE input
C_t^*	Ct_star	Heat transfer coefficient of the soil	_	Local variable
f_c	$fc = veget/veget_{max}$	Fraction of canopy coverage	—	Local variable
f_s	fs = 1 - fc	Fraction of soil coverage	_	Local variable
kB^{-1}	kb_m1	Coefficient to convert z0m to z0h	_	Local variable
kBs^{-1}	kbs_m1	Coefficient used to calculated kB^{-1}	_	Local variable
Re	Reynolds	Reynolds number	—	ORCHIDEE Input
Pr Prandtl		Prandtl number	_	ORCHIDEE Input



II.2.3 Implicit coupling with the atmosphere model

II.2.3.1 Type of coupling

The ORCHIDEE model can be run following two different ways. The classical one is to run the ORCHIDEE model alone and give it as inputs the meteorological data, the radiation profiles and other parameters at each time step. The second way to run ORCHIDEE is to couple it to the atmosphere model LMDZ.

LMDZ is a general circulation model which calculates the different processes of the atmosphere at each time step. From LMDZ point of view, ORCHIDEE can be seen as a boundary condition at the lower level of the atmosphere. The aim of ORCHIDEE will be to provide the different fluxes (momentum, heat...) which are emitted by the surface towards the atmosphere. However, running both models simultaneously leads to a problem. The surface fluxes are a response to the sun and atmosphere incoming radiations which are coming down to the surface from the atmosphere. Those radiations interact with the atmosphere and change its properties. Moreover, the surface fluxes at a precise time step are also interacting with atmosphere. Consequently, this dynamic system should constantly evolve in response to both solar radiations and incoming surface fluxes.

It is clear from this situation that coupling the radiation scheme between the atmosphere and land surface models is a tricky exercise which needs to be discussed. Several types of coupling exist. As explained above, the radiation scheme implemented is given thanks to Equations (4) and (5). Those two equations can be dicretized as follows in Equations (19) and (20).

$$F_{lat}^{t+1} = \lambda . \beta . \rho . |\overrightarrow{V}| . C_d . (q_{surf}^i - q_{air}^j) = F_{lat}^{t+1} = \lambda . \beta . \rho . |\overrightarrow{V}| . C_d . (q_{surf}(T_{surf}^i) - q_{air}^j)$$
(19)

$$F_{sens}^{t+1} = \rho. |\overrightarrow{V}|.C_d.C_p(T_{surf}^i - T_{air}^j)$$
(20)

Where i and j are time indices. Choosing those time indices is crucial because it will dictate the time in the GCM at which the surface energy balance has to be solved and the approximations that need to be made *Polcher et al. (1998)*[19]. As it has been said several choices can be made:

- Implicit coupling: i = t + 1 and j = t + 1
- Semi-implicit coupling: i = t and j = t + 1
- Explicit coupling: i = t + 1 and j = t
- Open-explicit coupling: i = t and j = t

Every type of coupling has its own advantages and drawbacks. The implicit coupling is the more robust but the harder to implement and the more time consuming. Explicit coupling is the easiest but the less accurate when the frequency of calculation starts to increase.

II.2.3.2 Atmospheric column resolution

The coupling between ORCHIDEE and LMDZ is fully implicit which means that at each time step, all the fluxes are determined. The way this coupling is solved is described in *Dufresne* & *Ghattas (2009)*[6]. In LMDZ, the subroutine in charge of this coupling is *pbl_surface*, in ORCHIDEE, the coupling is done in *enerbil*, in the subroutine *enerbil_surftemp*.



The key variable for the calculation of the surface fluxes is the surface temperature which needs to be determined at the time step t + 1: T_{surf}^{t+1} .

As the surface, the atmosphere is discretized in a precise number of grid cells. To each grid cell is associated a vertical atmosphere column in which the atmospheric properties are calculated. The transport of the properties is diffusing inside the vertical column following a turbulent diffusion scheme. Figure 3 explains the atmospheric discretization and Equations (21) to (23) explain the turbulent transport equations and their discretization.



Figure 3: Vertical discretization of the atmospheric column.

$$\frac{\partial X}{\partial t} = -\frac{1}{\rho} \frac{\partial \Psi^X}{\partial z} = -\frac{\partial \Psi^X}{m_l} \tag{21}$$

$$\Psi_{l-1/2}^X = -\rho k_z \frac{\partial X}{\partial z} \tag{22}$$

$$\Psi_{l-1/2}^X = -K_l \cdot (X_l - X_{l-1}) \tag{23}$$

Where, X is the variable to diffuse (specific humidity, momentum, static energy...), l is the indice of the layer, $K_l = \frac{k_z \cdot \rho^2 \cdot g}{P_{l-1} - P_l} (\delta P = P_{l-1} - P_l = \rho \cdot g \cdot \delta z, k_z$ is the diffusion coefficient, P_l is the pressure at level l and Ψ is the turbulent flux between layer l and l-1.

By discretizing Equation (21) and replacing by the expressions of $\Psi_{l-1/2}^X$, one can get the expression of turbulent transport of Equation (24).

$$(\delta P_l + R_{l+1}^X + R_l^X).X_l = R_l^X.X_{l-1} + R_{l+1}^X.X_{l+1} + \delta P_l\{X_l\}$$
(24)

With $\{X_l\}$ the value of X_l at the previous time step and $R_l^X = g.\delta t.K_l$. Then, at the top of the atmospheric layer, Equation (24) becomes Equation (25) and at the bottom, the interface with surface, Equation (24) becomes Equation (26).

$$(\delta P_n + R_n^X) \cdot X_n = R_n^X \cdot X_{n-1} + \delta P_n \{X_n\}$$

$$\tag{25}$$

$$(\delta P_1 + R_1^X) \cdot X_1 = R_2^X \cdot X_2 + \delta P_1 \{X_1\} - g \cdot \delta t \cdot F_1^X$$
(26)

With F_1^X the flux of X at the bottom layer between the surface and the atmosphere (positive downward).

The resolution scheme is, thus, a tridiagonal system which needs to be solved. This resolution starts from the top of the atmosphere. At layer n, X_n can be rewritten as in Equation (27).



$$X_n = C_n^X + D_n^X X_{n-1} (27)$$

Where, $C_n^X = \frac{\{X_n\} \cdot \delta P_n}{\delta P_n + R_n^X}$ and $D_n^X = \frac{R_n^X}{\delta P_n + R_n^X}$.

Then, the assuming that at a layer l + 1, X_{l+1} can be expressed as $X_{l+1} = C_{l+1}^X + D_{l+1} \cdot X_l$, one can deduce the value of X at the layer l as in equations (28) and (29). Equation (28) is deduced by replacing X_{l+1} by its expression assumed.

$$(\delta P_l + R_{l+1}^X (1 - D_{l+1}) + R_l^X) \cdot X_l = R_l^X \cdot X_{l-1} + R_{l+1}^X \cdot C_{l+1}^X + \delta P_l \{X_l\}$$
(28)

$$X_{l} = \frac{\{X_{l}\}.\delta P_{l} + R_{l+1}^{X}.C_{l+1}^{X}}{\delta P_{l} + R_{l}^{X} + R_{l+1}^{X}(1 - D_{l+1}^{X})} + \frac{R_{l}^{X}}{\delta P_{l} + R_{l}^{X} + R_{l+1}^{X}(1 - D_{l+1}^{X})}.X_{l-1}$$
(29)

Consequently, X_l can be expressed as $X_l = C_l + D_l \cdot X_{l-1}$ with $C_l = \frac{\{X_l\} \cdot \delta P_l + R_{l+1}^X \cdot C_{l+1}^X}{\delta P_l + R_l^X + R_{l+1}^X (1 - D_{l+1}^X)}$ and $D_l = \frac{R_l^X}{\delta P_l + R_l^X + R_{l+1}^X (1 - D_{l+1}^X)}$. Moreover, the coefficients C_l and D_l are expressed only thanks to the properties of the layer above and the variables at the previous time step.

Finally, at layer 1, the interface with the atmosphere, the equations (28) and (29) become equations (30) and (31).

$$(\delta P_1 + R_2^X (1 - D_2)).X_1 = R_2^X . C_2^X + \delta P_1 \{X_1\} - g \delta t F_1^X$$
(30)

$$X_1 = \frac{\{X_1\}.\delta P_1 + R_2^X.C_2^X}{\delta P_1 + R_2^X(1 - D_2^X)} + \frac{-g}{\delta P_1 + R_2^X(1 - D_2^X)}.F_1^X.\delta t$$
(31)

Then, X_1 can be expressed as $X_1 = A_1^X + B_1^X \cdot F_1^X \cdot \delta t$.

From this point, as all the coefficients are described thanks to the properties of the above layer and the state of the layer at the previous time step, the tridiagonal system can be solved following a downhill resolution.

At the beginning of the time step, the properties of the atmosphere column are known from the previous time step. This permits to calculate the coefficients from the top of the atmosphere downward to the bottom layer. Once all the coefficients are known, the surface/atmosphere interface computes the surface temperature calculation and other properties of the surface (the F_1^X fluxes). This leads to the calculation of F_1^X . Once F_1^X is determined, a bottom-up calculation of X_l is started as the algorithm knows all the coefficient and calculates all the properties thanks to their values at the lower layer. This Top-Down and Bottom-Up process can be summarized on Figure 4 (the coupling with the soil resolution is given on Figure 6).

Atmospheric Turbulent Diffusion Top-Down calculation of the atmospheric coefficient A_{atm}^{X} and B_{atm}^{X} . Surface temperature Calculation A_{atm}^{t} , B_{atm}^{t} , H^{t} , λE^{t} , E_{soil}^{t} , Σ_{soil}^{t} , T_{S}^{t} Bottom-Up calculation of the atmospheric temperatures T_{atm}^{t} .

Figure 4: Top-Down and Bottom-Up resolution of the atmosphere column temperature (same for other properties) $(A_{atm}^X \text{ and } B_{atm}^X \text{ correspond to the coefficients } C_l^X \text{ and } D_l^X \text{ in the vertical column and } A_1^X \text{ and } B_1^X \text{ at the bottom layer}$



NB: The equations described here can introduce a counter-gradient which will change the value of the coefficient (see *Dufresne & Ghattas* (2009)[6]).

II.2.3.3 Surface radiation scheme in an implicit coupling between the GCM and ORHCIDEE

All the previous downhill resolution is made in LMDZ. From ORCHIDEE point of view, the result of this calculation is the value of A_1^X and B_1^X (where X will correspond for ORCHIDEE to the saturated air moisture and the surface static energy (which leads to the temperature)). Here, it is needed to be careful, the coefficients in ORCHIDEE have different names than the ones in LMDZ. The conversion is the following:

$$B^{T}(orchidee) = A^{T}(lmdz) \tag{32}$$

$$A^{T}(orchidee) = B^{T}(lmdz).\Delta t$$
(33)

$$B^q(orchidee) = A^q(lmdz) \tag{34}$$

$$A^{q}(orchidee) = B^{q}(lmdz).\Delta t \tag{35}$$

From this point, the coefficient A^T, B^T, A^q, B^q that will be used will be the one of the ORCHIDEE format. Consequently, with this new notation, the surface coupling equation (31) becomes Equation (36).

$$X_1 = B_1^X + A_1^X \cdot F_1^X \tag{36}$$

This equation becomes Equation (37) when expressed in terms of static energy (H_1 being the static energy of the first atmospheric layer) and becomes Equation (38) when expressed in terms of specific humidity.

$$H_1 = C_{p,air} \cdot T_{surf} = B_1^T + A_1^T \cdot F_{sens}^T$$
(37)

$$Q = B_1^q + A_1^q \cdot F_{hum}^q \tag{38}$$

With:

$$F_{sens} = \rho |\vec{V}| C_d \cdot (H_1 - C_{p,air} \cdot T_{surf})$$
(39)

$$F_{hum} = \beta \rho |\vec{V}| C_d (Q - q_{sat}(T_{surf}))$$
(40)

Those two equations are basically Equations (5) and (4).

Equalizing H_1 in Equations (37) and (39) and equalizing Q in Equations (38) and (40), the following Equations (41) and (42).

$$F_{sens} = \frac{B^T - C_{p,air} \cdot T_{surf}}{\frac{1}{\rho |\vec{V}| C_d} - A^T}$$

$$\tag{41}$$

$$F_{lat} = \lambda F_{hum} = \beta \lambda \frac{B^q - q_{sat}(T_{surf})}{\frac{1}{\rho |\vec{\nabla}|C_d} - \beta A^q}$$
(42)

Consequently, we can deduce the latent heat flux and the sensible heat flux from the values of the atmospheric coefficient and the surface temperature.



Those expressions permit to calculate the latent heat and sensible heat fluxes which go to the atmosphere at the beginning of the time step. To deduce the one that will be sent to the atmosphere at the end of the time step, a sensibility analysis is made. This sensibility analysis permit to compute the surface temperature of the new time step and deduce from this temperature all the components of the surface energy budget.

The principle of the sensitivity analysis is to calculate the sensitivities of each part of the energy budget to a change of temperature. Then the change of temperature during the time step duration Δt is computed in order to find the values of the new fluxes.

First of all, the change in surface temperature is given by Equation (43).

$$C_{p,surf} \cdot \frac{\partial T}{\partial t} = R_n + F_{sens} + F_{lat} + G \tag{43}$$

When discretized, this equations becomes Equation (44).

$$C_{p,surf} \cdot \frac{(T_{surf} - \{T_{surf}\})}{\Delta t} = R_n + F_{sens} + F_{lat} + G$$

$$\tag{44}$$

Replacing the fluxes by their expressions permits to arrive to Equation (45).

$$C_{p,surf} \cdot \frac{(T_{surf} - \{T_{surf}\})}{\Delta t} = R_n + \frac{B^T - C_{p,air} \cdot T_{surf}}{\frac{1}{\rho |\overrightarrow{V}|C_d} - A^T} + \beta \lambda \frac{B^q - q_{sat}(T_{surf})}{\frac{1}{\rho |\overrightarrow{V}|C_d} - \beta A^q} + G$$
(45)

Then, by defining the following quantities (with $H = C_{p,air}.T_{surf}$):

$$q_{sat}(T_{surf}) = q_{sat}(\{T_{surf}\}) + \frac{1}{C_{p,air}} \cdot \frac{\partial q_{sat}}{\partial H}|_{C_{p,air} \cdot \{T_{surf}\}}(C_{p,air} \cdot (T_{surf} - \{T_{surf}\}))$$
(46)

$$\frac{\partial F_{sens}}{\partial H} = \frac{1}{\frac{1}{\rho |\vec{V}|C_d} - A^T}$$
(47)

$$\frac{\partial F_{lat}}{\partial H} = \beta \lambda \frac{\frac{1}{C_{p,air}} \cdot \frac{\partial q_{sat}}{\partial H}}{\frac{1}{\rho |\vec{V}| C_d} - \beta A^q}$$
(48)

$$\{F_{sens}\} = F_{sens}(\{T_{surf}\}) \tag{49}$$

$$\{F_{lat}\} = F_{lat}(\{T_{surf}\}) \tag{50}$$

$$\frac{\partial R_n}{\partial H} = \frac{1}{C_{p,air}} \cdot 4.\epsilon. \sigma. (\{T_{surf}\}^3)$$
(51)

The latter equation derives directly from Equations (1) and (2).

$$T_{surf} - \{T_{surf}\} = \frac{\frac{\Delta t}{C_{p,surf}} \cdot (\{R_n\} + G + \{F_{sens}\} + \{F_{lat}\})}{1 - \frac{\Delta t}{C_{p,surf}} (\frac{\partial R_n}{\partial H} + \frac{\partial F_{lat}}{\partial H} + \frac{\partial F_{sens}}{\partial H})}$$
(52)

$$\Delta\theta = C_{p,air} \cdot (T_{surf} - \{T_{surf}\}) = \frac{\Delta t \cdot (\{R_n\} + G + \{F_{sens}\} + \{F_{lat}\})}{\frac{C_{p,surf}}{C_{p,air}} - \frac{\Delta t}{C_{p,air}} (\frac{\partial R_n}{\partial H} + \frac{\partial F_{lat}}{\partial H} + \frac{\partial F_{sens}}{\partial H})}$$
(53)

This last equation permits to access to the new surface static energy and the new surface temperature which will permit to calculate all the other fluxes at the new time step. The implicit coupling between the surface and the atmosphere is closed. The new surface temperature has been calculated thanks to the atmospheric properties at the same time step.



II.3 Splitting of the water fluxes

As it is seen in section II.2.1, the latent heat flux is calculated thanks to the difference between soil and air saturated moisture. However, this latent heat flux is a composed flux which regroups several processes:

- Snow sublimation process
- Canopy interception loss
- Canopy transpiration
- Bare soil evaporation
- Floodplains evaporation

Because they are important variables at the ecosystem scale, they have to be calculated. However, the only way to compute them is to deduce them from the latent heat flux. The method used to estimate those fluxes in ORCHIDEE is called a β -model. It defines the fluxes thanks to the application of a resistance (β) on the potential evaporation.

II.3.1 β -model concept

The β -model consists in associating a resistance coefficient to each process. The β coefficients will be calculated by considering the fraction of the grid-cell which emits the flux and the potential stress applied to this flux. All the coefficients will less or more have the same behaviour and will limitate the latent heat flux in order to approximate the process flux studied as in Equation (54).

$$F_{lat} = \lambda . \rho . |\vec{V}| . C_d . \beta . (q_{soil} - q_{air})$$
(54)

In ORCHIDEE, the β s are associated to the processes as follows:

- Snow sublimation process: β_1
- Canopy interception loss: β_2 (one β_2 per PFT)
- Canopy transpiration: β_3 (one β_3 per PFT)
- Bare soil evaporation: β_4
- Floodplains evaporation: β_5

Other β s can be found in the code, they correspond to:

- $\beta_{2,sum}$: Weighted sum of β_2 over the PFTs
- $\beta_{3,sum}$: Weighted sum of β_3 over the PFTs
- $\beta_{3,pot}$: β associated to the potential transpiration
- β_{23} : β associated to the wetted foliage that will transpire once intercepted water has evaporated.



• β_{bio} : Sum of the β s associated to biologial processes ($\beta_{bio} = \beta_{2,sum} + \beta_{3,sum} + \beta_4$)

The first split between the water fluxes is made in *enerbil* when the latent heat flux is calculated. The latent heat flux is divided between the evaporative processes from the floodplains first, then from the sublimation of the non flooded but snow-covered lands and finally from the non flooded, non snowy lands as in Equation (55).

$$F_{lat} = E_{floodplains} + E_{snow} + E_{other} \tag{55}$$

The split between the sublimation processes and the evaporation ones is made thanks to the resistance coefficients β_1 , β_5 and β . Floodplains evaporation flux is calculated as in equation (56). It is directly a part of the latent heat flux.

$$E_{floodplains} = \lambda_{evaporation}.\beta_5.\rho.|\overrightarrow{V}|.C_d.(q_{soil} - q_{air})$$
(56)

Then, the part of the latent flux coming from the non flooded snowy lands is given by multiplying the flux by $\beta_{1.}(1 - \beta_{5})$ as in Equation (57).

$$E_{snow} = \lambda_{sublimation} \cdot \beta_1 \cdot (1 - \beta_5) \cdot \rho \cdot |\overrightarrow{V}| \cdot C_d \cdot (q_{sol} - q_{air})$$
(57)

And finally, from the non-flooded, non-snowy part of the flux, the evaporation from other processes is deduced as in Equation (58).

$$E_{other} = \lambda_{evaporation} \cdot (1 - \beta_1) \cdot (1 - \beta_5) \cdot \beta_{bio} \cdot \rho \cdot |\overrightarrow{V}| \cdot C_d \cdot (q_{sol} - q_{air})$$
(58)

A second split is then made between the non-snowy, non flooded lands in order to have access to the fluxes coming from bare soil evaporation processes, transpiration, and interception loss evaporation. This split is made thanks to the the resistance coefficients β_4 , $\beta_{2,sum}$ (and β_2 to have the contribution of each PFT) and $\beta_{3,sum}$ (and β_3 to have the contribution of each PFT). The split is deduced from E_{other} as in Equations (60), (61) and (62).

$$E_{other} = E_{interception_loss} + E_{transpiration} + E_{bare_soil_evaporation}$$
(59)

$$E_{interception_loss} = \lambda_{evaporation} \cdot (1 - \beta_1) \cdot (1 - \beta_5) \cdot \beta_2 \cdot \rho \cdot |\overrightarrow{V}| \cdot C_d \cdot (q_{sol} - q_{air})$$
(60)

$$E_{transpiration} = \lambda_{evaporation} \cdot (1 - \beta_1) \cdot (1 - \beta_5) \cdot \beta_3 \cdot \rho \cdot |\vec{V}| \cdot C_d \cdot (q_{sol} - q_{air})$$
(61)

$$E_{bare_soil_evaporation} = \lambda_{evaporation} \cdot (1 - \beta_1) \cdot (1 - \beta_5) \cdot \beta_4 \cdot \rho \cdot |\vec{V}| \cdot C_d \cdot (q_{sol} - q_{air})$$
(62)

Finally, in order to have the actual fluxes of water and not the composition of the latent heat flux, all the previous variables can be multiplied by the factor $\Delta t/\lambda$. Where Δt is the interval of the time step and λ is the related latent heat of sublimation or evaporation.



II.3.2 Calculation of the β coefficients

The β coefficients are calculated in the *diffuco* module, the module that also computes the photosynthesis which will be used in the calculation of the β for transpiration (β_3).

NB: It is important to highlight the fact that the definitions presented right after show that the β s are taking into account effects of stresses **AND** effects of grid partitioning (the fraction of the grid which will be associated to the fluxes). As Agnès Ducharne mentioned in the ticket #350, this behaviour is not really appropriated and leads to problems when calculating the fluxes. Moreover, this behaviour can cause problems in modules such as *mleb* which as been designed for an ecosystem scale and not a grid one.

II.3.2.1 Calculation of β_1

 β_1 is the first resistance coefficient to be calculated in diffuco. It is calculated in the subroutine $diffuco_snow$. β_1 is divided between its part coming from the vegetated lands of the grid-cell, $\beta_{1,bio}$, and the part coming fom non-biological lands of the grid-cell $\beta_{1,nobio}$. Both calculations follow a kind of prediction-correction schemes (stricto sensu). They are first approximated as the fractions of the grid-cell that can sublimate snow as in Equations (63) and (64).

$$\beta_{1,bio} = (1 - f_{nobio,tot}) \cdot f_{snowy_veg} = \beta_{1,bio,predict}$$
(63)

$$\beta_{1,nobio} = f_{nobio} f_{snowy \ nobio} = \beta_{1,nobio,predict} \tag{64}$$

Where, f_{nobio} is the fraction of the grid-cell occupied by non-biological land and f_{snowy_veg} and f_{snowy_nobio} are respectively the parts of biological (vegetated) and non-biological land that are currently snowy.

Once this prediction is made, a verification process is started. The total mass sublimation flux (in $kg.m^{-2}$) engendered by both coefficients is computed following Equation (65).

$$E_{snow_bio/nobio} = \beta_{1,bio/nobio} \cdot E_{pot,tot} = \beta_{1,bio/nobio} \cdot \Delta t \cdot \rho \cdot |\overline{V}| \cdot C_d(q_{sol} - q_{air})$$
(65)

If this mass flux is higher than the current snow mass on biological/non biological lands (calculated in the module *explicitsnow*), then, $\beta_{1,bio}$ and $\beta_{1,nobio}$ are reduced to the fraction of snow mass divided by the total potential water mass evaporation $E_{pot,tot}$ as in Equations (66) and (67).

$$\beta_{1,bio} = \frac{m_{snow,bio}}{E_{pot,tot}} = \beta_{1,bio,predict,corr}$$
(66)

$$\beta_{1,nobio} = \frac{m_{snow,nobio}}{E_{pot,tot}} = \beta_{1,nobio,corr} \tag{67}$$

And,

$$\beta_1 = \beta_{1,bio} + \beta_{1,nobio} \tag{68}$$



diffuco snow subroutine:

The diffuco_snow subroutine is articulated as the precedent description of the calculation. Equations (63) to (68) are performed. However, the calculation of the nobio lands contribution to β_1 is computed as a loop over the nobio surfaces. Consequently, $\beta_{1,nobio}$, $m_{snow,nobio}$, f_{nobio} and $f_{snowy nobio}$ are defined for each nobio surface.

Variable	Name in ORCHIDEE	Description	Unit	Туре
$eta_{1,bio}$	vbeta1	Resistance coefficient to snow sublimation on vegetated lands (vbeta1 is associated to $\beta_{1,bio}$ at the beginning of the subroutine before being updated by adding vbeta1)_add	_	_
$eta_{1,nobio}$	$vbeta1_add$	Resistance coefficient to snow sublimation on non biological lands (lakes, ice, cities)	-	Local variable to the subroutine
β_1	beta1v	total resistance coefficient to snow sublimation	-	Output (used in enerbil module)
$f_{nobio,tot}$	totfrac_nobio	Total fraction of the nobio lands on the grid-cell (sum of the f_{nobio}	_	External input
f_{nobio}	$frac_nobio$	Fraction of each nobio surface	_	External input
f_{snowy_veg}	$frac_snow_veg$	Fraction of vegetated land which is covered by snow	-	Input from condveg module
f_{snowy_nobio}	$frac_snow_nobio$	Fraction of non-biological land covered by snow	_	Input from <i>condveg</i> module
ρ	rau	Air density	$kg.m^{-3}$	Input ORCHIDEE
$ \overrightarrow{V} = \sqrt{u^2 + v^2}$	$speed = \sqrt{u^2 + v^2}$	Wind speed	$m.s^{-1}$	External input
C_d	q_cdrag	Surface drag coefficient	_	Input from diffuco_aero
q_{surf}	qsatt	Surface saturated humidity	$kg.kg^{-1}$	Input from <i>enerbil</i>
q _{air}	qair	Lowest level specific air humidity	$kg.kg^{-1}$	Input from <i>enerbil</i>
m _{snow,bio}	snow	Snow mass on vegetated lands	$kg.m^{-2}$	Input from explicit_snow module
$m_{snow,nobio}$	snow_nobio	Snow mass on non-biological lands	$kg.m^{-2}$	Input from explicit_snow module

II.3.2.2 Calculation of β_5

 β_5 is the resistance coefficient associated to the evaporation of flood plains. As for β_1 , β_5 follows a prediction/correction scheme with the same kind of test.

The subroutine starts by approximating β_5 as the fraction of the grid-cell occupied by floodplains as in Equation (69).

$$\beta_5 = f_{floodplains} = \beta_{5,predict} \tag{69}$$

As for β_1 , the total flood plains evaporation flux engendered by this β_5 is computed as thanks to Equation (70).



$$E_{floodplains,test} = \beta_5.E_{pot,tot} \tag{70}$$

If the predicted flux cannot be supplied by the water reservoir of the flood plains, β_5 is reduced to the evaporation of the mass of water stored inside the flood plains $m_{w,flood}$ thanks to Equation (71).

$$\beta_5 = \frac{m_{w,flood}}{E_{pot,tot}} = \beta_{5,corr} \tag{71}$$

NB: When β_5 is first predicted, it is not directly associated to $f_{floodplains}$ but to $f_{floodplains}$. $\frac{E_{pot,tot,corr}}{E_{pot,tot}}$. I do not really understand why β_5 is the only one to undergo this limitation. Maybe the fact is that $E_{pot,tot,corr}$ is expressed thanks to $T_{s,wet}$ which represents the temperature of air assuming an hypothetically wet surface. Floodplains are saturated wet surfaces so maybe in this case $E_{pot,tot,corr}$ is needed to express the resistance coefficient. Because T_{surf} is unique on the grid-cell, for the floodplains, $T_{s,wet}$ is surely really different from T_{surf} , consequently, Milly's correction is needed is we do not want to underestimate the evaporation of floodplains.

diffuco flood subroutine:

Variable	Name in ORCHIDEE	Description	Unit	Туре
β_5	vbeta5	Resistance coefficient to evaporation of floodplains	_	Output used in enerbil module
$f_{flood plains}$	$totfrac_nobio$	Fraction of grid-cell occupied by floodplains	_	External input
$E_{floodplains,test}$	subtest	Estimated water flux with the β_5 prediction	$kg.m^{-2}$	Local variable
ρ	rau	Air density	$kg.m^{-3}$	Input ORCHIDEE
$ \overrightarrow{V} = \sqrt{u^2 + v^2}$	$speed = \sqrt{u^2 + v^2}$	Wind speed	$m.s^{-1}$	External input
C_d	q_cdrag	Surface drag coefficient	_	Input from diffuco_aero subroutine
q_{surf}	qsatt	Surface saturated humidity	$kg.kg^{-1}$	Input from <i>enerbil</i> module
q_{air}	qair	Lowest level specific air humidity	$kg.kg^{-1}$	Input from <i>enerbil</i> module
$m_{w,flood}$	$flood_r es$	Mass of water in floodplains	$kg.m^{-2}$	Input from <i>hydrol</i> and <i>routing</i> module
$E_{pot,tot}$	evapot	Total potential evaporation	$kg.m^{-2}$	Input from <i>enerbil</i> module

II.3.2.3 Calculation of β_2

 β_2 corresponds to the resistance coefficient of the water intercepted by the vegetation. It is calculated in the subroutine *diffuco_inter*. As for the precedent calculations, β_2 is calculated following a prediction correction scheme. The predicted value of β_2 corresponds to the fraction of intercepted water by the vegetation multiplied by the effective vegetation fraction of each PFT divided by a resistance term which corresponds to the transport across the canopy. The expression used is the one in Equation (72).

$$\beta_2 = f_{veg,eff} \cdot \frac{q_{s,intercepted}}{q_{s,max}} \cdot \frac{1}{1 + |\vec{V}| \cdot C_d \cdot r_{struct}} = \beta_{2,predict}$$
(72)



Where, $f_{veg,eff}$ is the effective vegetation fraction of each PFT (veget in the code), $q_{s,intercepted}$ is the amount of water intercepted by the vegetation per unit of surface, $q_{s,max}$ is the maximum amount of water that can be intercepted by the vegetation per unit of surface, both calculated in the *hydrol* module and r_{struct} is an empirical constant resistance term defined at the PFT level.

As for β_1 and β_5 , a verification is made before a correction. If the water intercepted by vegetation is less than the total water evaporated calculated thanks to $\beta_2.E_{pot,tot}$, then, β_2 is reduced to Equation (73).

$$\beta_2 = \frac{q_{s,intercepted}}{Epot, tot} = \beta_{2,corr} \tag{73}$$

Finally, the subroutine also calculates β_{23} , the resistance coefficient of the wetted foliage which will transpire once the intercepted water has evaporate. If the potential intercepted evaporation ($\beta_{2,predict}.E_{pot,tot}$) is higher than the water intercepted by vegetation, the water stored on vegetation will not be sufficient to answer the climatic demand, then transpiration will occur. Consequently, β_{23} corresponds to the predicted value less the real one as in Equation (74).

$$\beta_{23} = \beta_{2,predict} - \frac{q_{s,intercepted}}{Epot, tot}$$
(74)

diffuco inter subroutine:

The $diffuco_inter$ subroutine computes Equation (72) to (74) for each grid-cell and each PFT.

Variable	Name in ORCHIDEE	Description	Unit	Туре
β_2	vbeta2	Resistance coefficient to evaporation of water intercepted by vegetation	_	Output used in enerbil module
β_{23}	vbeta 23	Resistance coefficient to wetted foliage that will transpire afterwards	_	Output (used in enerbil module)
$f_{veg,eff}$	veget	fraction of surface covered by foliage	_	Input from ORCHIDEE
$q_{s,intercepted}$	qsintveg	Water intercepted by vegetation	$kg.m^{-2}$	Input from <i>hydrol</i> module
$q_{s,max}$	qsintmax	Maximum water that vegetation can intercept	$kg.m^{-2}$	Input from <i>slowproc</i> module
$ \overrightarrow{V} $	speed	Wind speed	$m.s^{-1}$	External input
C_d	q_cdrag	Surface drag coefficient	_	Input from <i>condveg</i> module
r _{struct}	rstruct	Empirical constant coefficient at the PFT level	$s.m^{-1}$	ORCHIDEE input
$E_{pot,tot}$	ziltest * vbeta2	Not explecitly mentioned in the subroutine but corresponds to Equation (54)	$kg.m^{-2}$	Input from <i>enerbil</i>



II.3.2.4 Calculation of β_4

The calculation of β_4 , resistance coefficient for bare soil evaporation is made in the subroutine $diffuco_bare$. However, the key variable used in the calculation of β_4 , E_{bare_lim} , is calculated in the module hydrol. This variable represents the ratio of potential evaporation which is actually made by bare soil evaporation. It consequently corresponds in most of the cases to β_4 . First of all, it is important to understand how E_{bare_lim} is calculated in hydrol. E_{bare_lim} starts by being calculated at the soiltile level (see II.1.2 for the definition of soiltile): $E_{bare_lim,st}$. $F_{bare_lim,st}$, the flux of bare soil evaporation is deduced from the soil total water budget in Equation (75) (written in terms of total moisture content per surface unit of the soiltile ($kg.m^{-2}$)).

$$\frac{\theta_{st} - \{\theta_{st}\}}{\Delta t} = -F_{bare_lim,st} - F_{bottom,st}$$
(75)

Thus, on a time step Δt and weighting it by the effective bare soil fraction of the soiltile which will evaporate $(f_{bare,st})$, the bare soil evaporation per soiltile is given by Equation (76).

$$\Delta t.F_{bare_lim,st} = (\{\theta_{st}\} - \theta_{st} - F_{bottom}.\Delta t).f_{bare,st}$$
(76)

From this flux, the ratio from potential evaporation is deduced as in Equation (77).

$$E_{bare_lim,st} = \frac{\Delta t.F_{bare_lim,st}}{E_{pot,tot}}$$
(77)

And the ratio $E_{bare\ lim}$ is calculated as the sum of the soiltile ones as in Equation (78).

$$E_{bare_lim} = \sum_{st} E_{bare_lim,st}$$
(78)

Now coming back to diffuco_bare, before attributing the value of E_{bare_lim} to β_4 , a test will be done. The sum of bare soil evaporation, intercepted water interception evaporation and transpiration should not be higher than the rate of water flux attributed to those processes $(E_{other} \text{ in Equation (58)})$. This means that $\beta_4 + \beta_{2,sum} + \beta_{3,sum}$ should not exceed 1. So, if the value of E_{bare_lim} is higher than $(1 - \beta_{2,sum} - \beta_{3,sum})$, then:

$$\beta_4 = E_{bare_lim} \tag{79}$$

In the cases where E_{bare_lim} is actually higher than $(1 - \beta_{2,sum} - \beta_{3,sum})$, priority is given to intercepted water evaporation and transpiration and β_4 is reduced to $(1 - \beta_{2,sum} - \beta_{3,sum})$. In those cases, in order to keep a closed water budget, E_{bare_lim} and $E_{bare_lim,st}$ are recalculated as in Equations (80) and (81) (variables between [] correspond to their values before recalculation).

$$E_{bare_lim,st} = \frac{[E_{bare_lim,st}] \cdot (1 - \beta_{2,sum} - \beta_{3,sum})}{[E_{bare_lim}]}$$
(80)

$$\beta_4 = E_{bare_lim} = 1 - \beta_{2,sum} - \beta_{3,sum} \tag{81}$$



$diffuco_bare$ subroutine:

The $diffuco_bare$ subroutine computes Equations (79) to (81) for each grid-cell. Equations (76) to (78) are computed in the hydrol module.

Variable	Name in ORCHIDEE	Description	Unit	Туре
$E_{bare_lim,st}$	evap_bare_lim_ns	Part of total evaporation used for bare soil evaporation for each soiltile	_	Modified variable coming from <i>hydrol</i> module
E_{bare_lim}	$evap_bare_lim$	Part of total evaporation used for bare soil evaporation	_	Modified variable coming from <i>hydrol</i> module
β_4	vbeta4	Resistance coefficient to bare soil evaporation	-	Output used in enerbil module
$\beta_{2,sum}$	vbeta2sum = SUM(vbeta2(ji,:)	Sum over PFTs of the resistance coefficients for the evaporation of water intercepted by vegetation	_	Input from diffuco_inter subroutine
$eta_{3,sum}$	vbeta3sum = SUM(vbeta3(ji,:)	Sum over PFTs of the resistance coefficients for transpiration by vegetation	_	Input from diffuco_trans_co2 subroutine

II.3.2.5 Calculation of β_3

The last resistance coefficient to be calculated is β_3 , the one for transpiration. This resistance coefficient mainly rely on three resistances: the stomatal resistance, the boundary layer resistance and the aerodynamic resistance across the canopy. It is composed by two terms, the effective transpiration coefficient, and the transpiration that occurs after evaporation of the intercepted water as in Equation (82).

$$\beta_3 = \beta_{3,transp} + \beta_{3,transp} \quad after \quad intercept \tag{82}$$

Firstly, $\beta_{3,transp}$ is calculated as the fraction of the canopy that can transpire multiplied by a resistance term as in Equation (83).

$$\beta_{3,transp} = f_{veg,eff}.(1 - \frac{q_{s,intercepted}}{q_{s,max}}).\frac{1}{1 + |\overrightarrow{V}|.C_d.\frac{f_{veg,eff}}{f_{veg,max}}.r_{veg,pft}.r_{veget}}$$
(83)

Where, $f_{veg,eff}$ is the effective fraction of the PFT composed by vegetation, $(1 - \frac{q_{s,intercepted}}{q_{s,max}})$ is the fraction of vegetation per PFT that is not intercepting water, and, finally, $|\vec{V}| \cdot C_d \cdot \frac{f_{veg,eff}}{f_{veg,max}} \cdot r_{veg,pft} \cdot r_{veget}$ is a resistance coefficient for both transport of water within the canopy $(|\vec{V}| \cdot C_d)$ and the stomatal resistance $r_{veget} = 1/g_{s,tot}$ (where $g_{s,tot}$ is the total stomatal conductance) reduced by a vegetation resistance $\frac{f_{veg,eff}}{f_{veg,max}} \cdot r_{veg,pft}$ (a bit more explanation on this choice may be useful).

Concretely, the term correspond to a fraction of an aerodynamic resistance $(R_a = \frac{1}{|\vec{V}|.C_d})$ and a stomatal and boundary layer resistance $(R_{leaf} = \frac{f_{veg,eff}}{f_{veg,max}}.r_{veg,pft}.r_{veget})$. Thus, $\beta_{3,transp}$ corresponds to the reduction induced by the stomatal and boundary layer resistance over the aerodynamic resistance: $\frac{R_a}{R_a + R_{leaf}}$. Indeed, as one can see on Equation (84), the term $\frac{R_a}{R_a + R_{leaf}}$ corresponds to the term implemented in the β_3 coefficient.



$$\frac{R_a}{R_a + R_{leaf}} = \frac{1/(|\overrightarrow{V}|.C_d)}{1/(|\overrightarrow{V}|.C_d) + \frac{f_{veg,eff}}{f_{veg,max}}.r_{veg,pft}.r_{veget}} = \frac{1}{1 + |\overrightarrow{V}|.C_d.\frac{f_{veg,eff}}{f_{veg,max}}.r_{veg,pft}.r_{veget}}$$
(84)

On the other side, the resistance to transpiration after evaporation of intercepted water is calculated with the same expression as in Equation (83) with the ratio of vegetation that have intercepted water $\frac{q_{s,intercepted}}{q_{s,max}}$ instead of $(1 - \frac{q_{s,intercepted}}{q_{s,max}})$. Because the β for transpiration after evaporation of intercepted water has already been calculated with β_{23} in Equation (74), the most restrictive of the two definitions is taken, as in Equation (85).

$$\beta_{3,transp_after_intercept} = MIN(\beta_{23}, f_{veg,eff}, \frac{q_{s,intercepted}}{q_{s,max}}, \frac{1}{1 + |\overrightarrow{V}|.C_d, \frac{f_{veg,eff}}{f_{veg,max}}, r_{veg,pft}, r_{veget}})$$
(85)

diffuco trans co2 subroutine:

The subroutine $diffuco_trans_co2$ also computes the photosynthesis for each PFT. Because photosynthesis is not the subject of the present technical note, the name of the variables cited here are only the one of those needed for the calculation of β_3 . The description of photosynthesis and all the other variables should be the subject of another technical note.

 $\beta_{3,transp}$ and $\beta_{3,transp_after_intercept}$ are not explicitly defined in the module and are only part of the calculation of β_3 . They have been added here in a matter of understanding.

Variable	Name in ORCHIDEE	Description	Unit	Туре
Ba	abota?	Resistance coefficient to		Output used in
ρ_3	000000	transpiration by vegetation		enerbil module
		Resistance coefficient to		Output (used in
β_{23}	vbeta 23	wetted foliage that will	_	enerhil modulo)
		transpire afterwards		enerou module)
f	weget	fraction of surface covered		Input from
Jveg, eff	vegei	by foliage	_	ORCHIDEE
<i>a</i>	qsintveg	Water intercepted by	$kg.m^{-2}$	Input from <i>hydrol</i>
$q_{s,intercepted}$		vegetation		module
<i>a</i>	qsintmax	Maximum water that	$kg.m^{-2}$	Input from <i>slowproc</i>
$q_{s,max}$		vegetation can intercept		module
$ \overrightarrow{V} $	speed	Wind speed	$m.s^{-1}$	External input
C.	q_cdrag	Surface drag coefficient	_	Input from <i>condveg</i>
\cup_d				module
r_{veget}	rveget	Stomatal resistance	$s.m^{-1}$	Local variable
		"Potentiometer to set		
<i>m</i>	range off	vegetation resistance"		ORCHIDEE input
Tveg, pft	Treg_pji	$(r_{veg,pft} = 1 \text{ as a default})$	_	ORCHIDEE input
		value)		
		Sum of the stomatal		Local variable
$g_{s,tot}$	gstot	conductance over PETs	$mol.m^{-2}.s^{-1}.bar^{-1}$	calculated in the
		conductance over PF1s		subroutine



II.4 Soil thermodynamics

As it is presented in Section II.2.1, the surface energy budget can be expressed with 2 approaches. The first one is a radiation flux approach, presented in Equation (1). The second one, relies on the calculation of the convective and conductive fluxes that compose R_n , it is presented in Equation (3). One of those fluxes is the soil heat conduction flux.

Those soil heat conduction aspects are modeled in ORCHIDEE in the module called *thermosoil*. Because the soil temperature and the soil heat flux have direct impacts on the energy budget, this module needs to be presented inside this technical note.

This soil heat conduction will interact with two other processes: the accumulation of snow at the surface, which is computed in the module *explicitsnow* and the changing of its heat properties with the presence of water/ice in the soil layers.

The aim of this part is to present how the soil heat diffusion is solved in a basic setup, without snow at the surface or ice in the layers and then explain how the snow at the surface and the frozen water inside the soil will interact with this diffusion.

II.4.1 Physical aspects

The soil heat conduction modeled in ORCHIDEE is an adaptation of Frédéric Hourdin's thesis in 1992 [10] (See it section 3.3, p39 and Appendix A, p195).

Focusing on the soil heat diffusion, the latter process relies on the description of the temporal variation of temperature in response to a heat flux as presented in Equation (86).

$$\frac{\partial T}{\partial t} = -\frac{1}{C_p} \frac{\partial F_C}{\partial z} \tag{86}$$

 F_C is called heat conductive flux and is calculated as in Equation (87) thanks to the vertical temperature gradient heat conductivity and the soil specific heat. The soil is assumed to be vertically homogeneous across all the grid-cell.

$$F_C = -\lambda \frac{\partial T}{\partial z} \tag{87}$$

Where λ and C_p are respectively the soil thermal conductivity and the soil heat capacity. This leads to a classical Fourier equation as in Equation (88)

$$\frac{\partial T}{\partial t} = \frac{\lambda}{C_p} \frac{\partial^2 T}{\partial z^2} \tag{88}$$

Finally, the heat convective flux described in the energy budget is expressed as follows in Equation (89).

$$G = -\frac{\lambda}{C_p} \frac{\partial T}{\partial z} \tag{89}$$

II.4.2 Thermosoil module

Having two different models for the global atmospheric circulation and the land surface processes is convenient when people are only interested in studying one of those two processes. However,





this shows several problems when the aim of the study is the coupling of both models. As it is demonstrated in Section II.2.3, ORCHIDEE and LMDZ are implicitly coupled. This means that all the variables of the interface are calculated at the same "new" time step. However, this showed several complications for the calculation of energy fluxes in the energy budget. Moreover, because the soil heat flux is a big part of the energy budget, this implicit coupling will also show limitations for the ground heat diffusion model presented here.

The model presented here is coming from Frédéric Hourdin's thesis in 1992 [10]. The model implemented is slightly different as it also introduces snow processes. The objective here is only to provide a example of simple soil heat diffusion model coupled to the LMD Global Circulation Model.

Thanks to a variable change $(z' = z.\sqrt{C_p/\lambda})$, Equation (88) can be simplified as Equation (90) and the heat convective flux is expressed as in Equation (91), where $K = \sqrt{\lambda C_p}$.

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial z'^2} \tag{90}$$

$$G = -K \frac{\partial T}{\partial z'} \tag{91}$$

(From now, z' will be named z).

At the surface interface, the sum of the fluxes can be summarized as in Equation (92) (at the inferior limit, flux is assumed to be 0).

$$L \downarrow +S_n - L \uparrow = F_{sens} + F_{lat} - K \frac{\partial T}{\partial z}$$
(92)

As for the water diffusion module hydrol presented in the technical note by Agnès Ducharne [10], the soil is discretized into several layers, like in Figure 5.



Figure 5: Soil discretization scheme *Hourdin's thesis*[10]

The depth of each node follows a geometrical pattern:



$$z_{k+1} - z_k = \alpha(z_k - z_{k-1}) \tag{93}$$

$$z_k = \frac{\alpha^k - 1}{\alpha - 1} . z_1 \tag{94}$$

Where α is a parameter (set to 2 in the *Hourdin's thesis*[10] where the study deals with Mars).

Temperatures are evaluated at the nodes:

$$z_{k+1/2} = \frac{\alpha^{k+1/2} - 1}{\alpha - 1} . z_1 \tag{95}$$

And the Equation (90) becomes Equation (96).

$$\frac{\partial T_{k+1/2}}{\partial t} = \frac{1}{z_{k+1} - z_k} \cdot \left(\frac{T_{k+3/2} - T_{k+1/2}}{z_{k+3/2} - z_{k+1/2}} - \frac{T_{k+1/2} - T_{k-1/2}}{z_{k+1/2} - z_{k-1/2}}\right)$$
(96)

At the upper layer, the equation becomes Equation (97), at the lower layer, the equation Equation (98).

$$\frac{\partial T_{1/2}}{\partial t} = \frac{1}{z_1 - z_0} \cdot \left(\frac{T_{3/2} - T_{1/2}}{z_{3/2} - z_{1/2}} - \frac{L \downarrow + S_n - L \uparrow - F_{sens} - F_{lat}}{I}\right) \tag{97}$$

$$\frac{\partial T_{N-1/2}}{\partial t} = -\frac{1}{z_N - z_{N-1}} \cdot \left(\frac{T_{N-1/2} - T_{N-3/2}}{z_{N-1/2} - z_{N-3/2}}\right)$$
(98)

Finally, the time discretized heat diffusion equation is given by Equation (99)

$$c_{k+1/2} \cdot (T_{k+1/2}^t - T_{k+1/2}^{t-\delta t}) = d_{k+1} \cdot (T_{k+3/2}^t - T_{k+1/2}^t) - d_k \cdot (T_{k+1/2}^t - T_{k-1/2}^t)$$
(99)

Where,

$$c_{k+1/2} = \frac{z_{k+1} - z_k}{\delta t} \tag{100}$$

$$d_k = \frac{1}{z_{k+1/2} - z_{k-1/2}} \tag{101}$$

At the upper level, this equation becomes:

$$c_{1/2} \cdot (T_{1/2}^t - T_{1/2}^{t-\delta t}) = d_1 \cdot (T_{3/2}^t - T_{1/2}^t) - \frac{L \downarrow + S_n - L \uparrow (T_S^t) - F_{sens} - F_{lat}}{I}$$
(102)

And at the lower level,

$$c_{N-1/2} \cdot (T_{N-1/2}^t - T_{N-1/2}^{t-\delta t}) = -d_{N-1} \cdot (T_{N-1/2}^t - T_{N-3/2}^t)$$
(103)

Just as the atmosphere resolution presented in Section II.2.3, this discretized scheme can be solved by recurrence posing:

$$T_{k+1/2}^t = \alpha_k^t \cdot T_{k-1/2}^t + \beta_k^t \tag{104}$$

Technical note

34



The coefficients α_k^t and β_k^t are deducible thanks to the temperature of the layer at the previous time step $t - \delta t$. At the bottom of the soil column, α_{N-1}^t and β_{N-1}^t are deducible from Equations (103) and (104) as in Equations (105) to (107).

$$\alpha_{N-1}^t = \frac{d_{N-1}}{\Delta_{N-1}^t} \tag{105}$$

$$\beta_{N-1}^{t} = \frac{c_{N-1/2} \cdot T^{t-\delta t}}{\Delta_{N-1}^{t}} \tag{106}$$

With

$$\Delta_{N-1}^t = c_{N-1/2} + d_{N-1} \tag{107}$$

Then, by recurrence and by replacing $T_{k+3/2}$ by its correspondent formula as in Equation (104) $(T_{k+3/2} = \alpha_{k+1}^t \cdot T_{k+1/2}^t + \beta_{k+1}^t)$ in Equation (99), the coefficients α_k^t and β_k^t can be determined as follows:

$$\alpha_k^t = \frac{d_k}{\Delta_k^t} \tag{108}$$

$$\beta_k^t = \frac{c_{k+1/2} \cdot T_{k+1/2}^{t-\delta t} + d_{k+1} \cdot \beta_{k+1}^t}{\Delta_k^t} \tag{109}$$

With

$$\Delta_k^t = c_{k+1/2} + (1 - \alpha_{k+1}^t)d_{k+1} + d_k \tag{110}$$

As for the atmosphere, the coefficients are determined thanks to their values at the previous time step and the values of the layer right below. Consequently, at the beginning of the time step, the temperatures of each layers will be determined thanks to the coupling with atmosphere and other surface processes and the values of the coefficients at the previous time step. Then, once the temperatures are know, the coefficients are recalculated from the top of the soil to the bottom for the next time step.

This step by step process permits to access the surface temperature T_S as presented in Frédéric Hourdin's thesis (p.197)[10].

Implicit coupling with the atmosphere:

As discussed above, this flux needs to be implicitly coupled to the atmosphere. As it is presented in Section II.2.3, the atmospheric model permits to access to the surface temperature T_S at the "new" time step. In parallel, the coefficients α_k and β_k are pre-computed at the previous time step time step. This permits to calculate all the temperatures at the nodes of the soil vertical discretization. Finally, all the new temperatures permit to calculate the new values of the coefficients α_k and β_k which will be needed at the newt time step. The global resolution scheme can be summarized as in Figure 6.




Figure 6: Global resolution scheme of both atmospheric and soil heat diffusion. Adapted from $Hourdin's \ thesis[10]$

II.4.3 Interaction with water in the layers

In parallel of the soil thermal diffusion, an hydrological budget of the soil is computed in the module *hydrol*. This module permits to calculate the amount of water present in each soil layers (in both diffusion scheme, the same layer discretization is used, 11 layers in both cases). This water will interact with the soil thermal budget and the soil thermal properties when it will froze/thaw. It will for example modify the soil thermal conductivity and capacity. The impact of soil freezing has been developed in ORCHIDEE by *Gouttevin et al. (2012)* as shown in *Gouttevin thesis (2012)*[7]. The main equations implemented in ORCHIDEE are explained right after.

The new soil freezing scheme is designed to represent the latent heat exchanges involved in the freezing and melting of soil water, and the changes in thermal and hydrological properties of the ground induced by soil water phase change. The latent heat exchanged during freezing and melting of water acts as a source or a sink term in the Fourier equation (Equation (88)) which becomes Equation (111).

$$C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} (\lambda \frac{\partial T}{\partial z}) + \rho_{ice} L \frac{\partial \theta_{ice}}{\partial t}$$
(111)

Where, L is the latent heat of fusion $(J.kg^{-1})$, ρ_{ice} is the ice density $(kg.m^{-3})$, θ_{ice} is volumetric ice content $(m^3.m^{-3})$.

As explained in *Gouttevin thesis (2012)*[7], in this case, the mechanical effects of soil freezing (expansion of the total volume of soil) are not taken into account. During freeze-up, the latent heat release delays the freezing progression. On the other side, latent heat consumption delays the soil warming. Latent heat term thus systematically opposes to the temperature change. Consequently, it can be seen as a thermal inertia. This lead to the introduction of an apparent heat capacity as in Equation (112).



$$(C_p - \rho_{ice} L \frac{\partial \theta_{ice}}{\partial T}) \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} (\lambda \frac{\partial T}{\partial z})$$
(112)

This permits to define the apparent soil heat capacity C_{app} (soilcap in the code): $C_{app} = C_p - \rho_{ice} L \cdot \frac{\partial \theta_{ice}}{\partial T}$.

Finally, the soil thermal properties also change with the presence of ice and water inside the soil layers. Equation (113) explains the representation of the soil heat capacity as a function of the fraction of water inside the layer. Equation (114) represents the evolution of soil thermal conductivity as a function of the same fraction (revision made by *Wang et al. (2016)*[24].

$$C_p = (f_l \cdot C_{wet} + (1 - f_l) \cdot C_{icy} - C_{dry}) \cdot S + C_{dry}$$
(113)

$$\lambda = (\lambda_s^{1-\theta_i} \cdot \lambda_i^{(1-f_l) \cdot \theta_i} \cdot \lambda_w^{f_l \cdot \theta_i} - \lambda_{dry}) \cdot S + \lambda_{dry}$$
(114)

Where, f_l is the fraction of the liquid soil water, assumed to vary linearly from 1 to 0 between 0°C and -2° C, initially, now, this "freezing window" is set from 1°C to -1° C, λ_s , λ_i and λ_w are the heat conductivities for solid soil, ice and water, respectively, λ_{dry} is the heat conductivity of dry soil $(Wm^{-1}K^{-1})$, S is the total (frozen and unfrozen) soil saturation degree (m^3m^{-3}) and C_{dry} , C_{wet} and C_{icy} are respectively the dry soil, saturated unfrozen and saturated frozen soil heat capacity $(Jm^{-3}K^{-1})$.

All those interactions are directly implemented in the *thermosoil* module (See Section II.5.3.

II.4.4 Interaction with snow at the surface

The aim of this part is to understand the basis of the snow processes and the interactions with the soil and energy budget. More precisions are needed to fully understand what is implemented in the *explicitsnow* module.

As explained, the snow model in ORCHIDEE is based on *Boone et al.* (2001)[3]. This model has been developed for the model ISBA-ES used by Météo-France. It relies on the description of a 3-layer snow cover above the soil and permits to calculate several snow properties and energy and mass transfers such as the snow density, the snow energy balance and heat flow, the snow liquid water content, the impact of snow on the roughness height, melting and freezing...

At each time step, the snow mass balance is given by Equation (115) (this is the snow mass balance in Boone's article, it seems a bit different in ORCHIDEE but I believe that the processes involved are the same).

$$\frac{\partial W_s}{\partial t} = P_n + p_n \cdot P_l - R_{lN} - E_{sn} \tag{115}$$

Where W_s is define as the snow water equivalent (which can be defined as the product between the average snow density and the snow depth), P_n is the snowfall rate, p_n is the fractional snow cover area, P_l is the rainfall rate, so, $p_n P_l$ represents the portion of the total rainfall that is intercepted by the snow surface, R_{lN} is the snow runoff rate (snow that leaves the snow pack from the basis to the soil and E_{sn} is the combined evaporation and sublimation rate.

The snow cover is represented thanks to 3 layers which are added above the soil layers as represented on Figure 7.





Figure 7: Schematic diagram of the snow cover above the ground

The snow cover thickness (D_s) is determined thanks to the snow mass and density and the depth of each sub-layer is calculated following Equation (116), (117) and (118).

$$D_{s1} = \delta 0.25 D_s + (1 - \delta) D_{s1,max} \tag{116}$$

$$D_{s2} = \delta 0.50 D_s + (1 - \delta) [0.34.(D_s - D_{s1,max}) + D_{s1,max}]$$
(117)

$$D_{s3} = D_s - D_{s1} - D_{s2} \tag{118}$$

With the condition $D_{s2} \leq 10D_{s1,max}$ and where $\delta = 1$ if $D_s \leq 0.2m$. This permits to limitate the height of the two first sub-layers in the case of high snow cover.

Once this layering computed, the module will calculate the energy balance inside the snow layers in order to calculate the layers temperature and the heat flux which is going into the soil. This step is essential for the implicit coupling with the atmosphere as the module *explicitsnow* is computed before the soil heat resolution module *thermosoil*. Snow layers temperature and heat flux at the soil/snow cover interface will be sent to the *thermosoil* module.

The heat diffusion inside the snow cover is assumed to be exactly the same as the one in the soil. In the presence of snow, the soil heat resolution module will only take into account three more layers of snow with different properties than the ones of the soil. The snow layer temperatures will, thus, be calculated thanks to the snow coefficients $\alpha_{k,snow}$ and $\beta_{k,snow}$ as presented in Section II.4.2. Then, the coefficients for the next time step will be computed, exactly in the same way as in *thermosoil* module. The only differences between both resolutions are the thermal properties (all the properties are calculated in *explicitsnow* module but it has been decided not to go into deep details in this note).

The snow process resolution can be summarized as on Figure 8.





Figure 8: Summary of the main snow processes calculated and the steps of calculations/interactions with the other modules



II.5 Modelling in ORCHIDEE

All the previous model is developed in ORCHIDEE in the *enerbil* module (except the part explicitly coming from *thermosoil* in Section II.4). This part will now emphasize the architecture of the *enerbil* module and precise a bit its routines.

II.5.1 The *enerbil* module scheme

The scheme of the *enerbil* module can be summarized as in Figure 9.



Figure 9: Scheme of the *enerbil* module

The module is divided into 4 main calculations subroutines: *enerbil_begin, enerbil_surftemp, enerbil_flux* and *enerbil_evapveg.* The description of those subroutines is made in Section II.5.2. The other subroutines *enerbil_initialize, enerbil_finalize, enerbil_clear* and *enerbil_write* are usual subroutines for the good functioning of ORCHIDEE, *enerbil_main* calls the 4 calculation subroutines and, finally, *enerbil_pottemp* is not used or called at all.

The main subroutine *enerbil_main* is calling the 4 calculation subroutines in the following order:

- *enerbil_begin*: in order to calculate preliminary variables, useful for the energy budget.
- *enerbil_surftemp*: in order to calculate the static energy, the saturated surface air moisture, the soil temperature, the air moisture and the air temperature at the "new" time step.



- enerbil_flux: in order to calculate the different fluxes that compose the energy budget.
- enerbil eveapveg: in order to split the water fluxes between its components.

II.5.2 Subroutine descriptions

II.5.2.1 enerbil begin subroutine

The first calculation subroutine to be called by the main one is *enerbil_begin*. The aim of this routine is to calculate preliminary variables useful for the computation of the energy budget. The routine starts by calculating the static energy of the surface (which can be refered as the enthalpy) for the old surface temperature as in Equation (119).

$$\{H_{surf}\} = \{T_{surf}\}.Cp_{air} \tag{119}$$

Then, the routine calls two public routines from the modules *constants_veg* and *qsat_moisture*. Those two routines calculates the surface saturated humidity $q_{surf,sat}(\{T_{surf}\})$ and the derivative of the saturated humidity with respect to the temperature, evaluated at the old temperature, $\frac{\partial q_{surf,sat}}{\partial T}(\{T_{surf}\})$.

Finally, the routine calculates the long-wave radiations absorbed by the surface and the net radiation budget as in Equations (120) and (121).

$$L_{abs} = \epsilon . L \downarrow \tag{120}$$

$$R_n = L \downarrow + S_n - (\epsilon \cdot \sigma \cdot \{T_{surf}\}^4 + (1 - \epsilon) \cdot L \downarrow)$$
(121)

 $R_n, \frac{\partial q_{surf,sat}}{\partial T}(\{T_{surf}\})$ and $q_{surf,sat}(\{T_{surf}\})$ will be used in the subroutine *enerbil_surftemp*, in order to calculate the values at the new time step.

Table of input variables:

Variable	Name in ORCHIDEE	Description	Unit	Input from
$\{T_{surf}\}$	$temp_sol$	Soil temperature at the previous time step	K	Previous time step
$L\downarrow$	lwdown	Down-welling long-wave radiation flux	$W.m^{-2}$	External input (LMDZ or database)
S_n	swnet	Net surface short-wave flux	$W.m^{-2}$	External input (LMDZ or database)
P_b	pb	Lowest level pressure	hPa	External input (LMDZ or database)
ϵ	emis	Emissivity of the surface	_	External input (LMDZ or database)

Table of output variables:



Variable	Name in ORCHIDEE	Description	Unit	Output used in
		Surface dry static		
$\{H_{surf}\}$	psold	energy/potential enthalpy	$J.kg^{-1}$	$enerbil_surftemp$
		at the previous time step		
		Surface saturated humidity		
$\{q_{surf,sat}\}$	$qsol_sat$	at the temperature of the	$kg.kg^{-1}$	$enerbil_surftemp$
		previous time step		
		Derivative of the saturated		
$\partial q ((T, 1))$	pdqsold	humidity estimated at the	$kg.(kg.s)^{-1}$	$enerbil_surftemp$
$\overline{\partial T}(\{I surf\})$		temperature of the previous		
		time step		
R_n	netrad	Net radiation flux	$W.m^{-2}$	$enerbil_surftemp$
L_{abs}	lungha	Long-wave radiation flux	Wm^{-2}	
	iwabs	absorbed by the surface	VV.m -	-

II.5.2.2 enerbil surftemp subroutine

This subroutine is the one that permits the implicit coupling between the surface and the atmosphere. The aim of this routine is to calculate, at the "new" time step, the values of the variables which will permit to compute the energy budget and the diffusion into the atmosphere. As it is precised in Section II.2.3, this implicit scheme relies on *Dufresne & Gattaz (2009)*[6].

The routine is divided into three parts:

- The first one consists in the sensible and latent heat fluxes at the "old" time steps.
- The second one consists in calculating the sensitivities of the fluxes to changes of surface static energy.
- Finally, the change in surface static energy is determined and the "new" surface static energy, "new" surface saturated humidity, "new" surface temperature, "new" potential evaporation and "new" air saturated humidity.

"Old" time step fluxes:

The sensible flux of the old time step is calculated thanks to Equation (41) by replacing T_{surf} by its value at the previous time step $\{T_{surf}\}$. Then the module computes the latent heat flux at the old time step by computing Equation (42) with the same trick with the surface saturated humidity $\{q_{sat,surf}\}$. However, two parts of the latent heat flux are calculated : the part corresponding to the sublimation, using $\beta = \beta_1 \cdot (1 - \beta_5)$ in Equation (42) and using $\beta = (1 - \beta_1) \cdot (1 - \beta_5)\beta_{bio}$ in Equation (42) for the evaporation process.

Sensitivities to changes in surface static energy:

Then, the sensitivities of the fluxes to a change in static energy are computed following Equation (48) to (51). With the same distinction between sublimation and evaporation for the latent heat flux.

"New" time step fluxes:

The first quantity of the new time step to be calculated is the change in surface static energy. This value is given thanks to the Equation (53). From this point, the new surface static energy is determined following Equation (122).

$$H_{surf} = \{H_{surf}\} + \Delta\theta \tag{122}$$

Technical note



The new surface saturated humidity is given by Equation (123).

$$q_{sat}(T_{surf}) = q_{sat}(\{T_{surf}\}) + \frac{1}{C_{p,air}} \frac{\partial q_{sat}}{\partial H} |_{C_{p,air},\{T_{surf}\}} \Delta \theta$$
(123)

Then, the new surface temperature is computed as in Equation (124).

$$T_{surf} = \frac{H_{surf}}{C_{p,air}} \tag{124}$$

The new air potential enthalpy and new latent heat flux (proxy value, the real one is calculated in *enerbil_flux* are given by Equations (125) and (126).

$$H_{air} = \frac{1}{\rho |\vec{V}|C_d} \cdot (\{F_{sens}\} - \frac{\partial F_{sens}}{\partial H} \Delta \theta) + H_{surf}$$
(125)

$$F_{sens,proxy} = \left(\{F_{lat,evap}\} - \frac{\partial F_{lat,evap}}{\partial H}\Delta\theta\right) + \left(\{F_{lat,sub}\} - \frac{\partial F_{lat,sub}}{\partial H}\Delta\theta\right)$$
(126)

Finally, the new saturated humidity of air is calculated as in Equation (127).

$$q_{air} = \frac{1}{\rho |\vec{V}|C_d} \cdot \frac{1}{\lambda_S \cdot \beta_1 \cdot (1 - \beta_5) + \lambda_E \cdot ((1 - \beta_1) \cdot (1 - \beta_5) \cdot \beta_{bio} + \beta_5)} \cdot F_{sens, proxy} + q_{surf, sat} \quad (127)$$

Table of input variables:





Variable	Name in ORCHIDEE	Description	Unit	Input from
ε	emis	Surface emissivity	K	External input (LMDZ or database)
$\{H_{air}\}$	epot_air	Air potential enthalpy at the previous time step	$J.kg^{-1}$	Previous time step
A^T	petAcoef	Coefficient permitting the implicit coupling for Temperature (See Section II.2.3)	_	External input (LMDZ or database)
B^{T}	petAcoef	Coefficient permitting the implicit coupling for Temperature (See Section II.2.3)	$W.m^{-2}$	External input (LMDZ or database)
$\{q_{air}\}$	qair	Lowest level specific humidity at the previous time step	$kg.kg^{-1}$	Previous time step
A^q	petAcoef	Coefficient permitting the implicit coupling for specific humidity (See Section II.2.3)	_	External input (LMDZ or database)
B^q	peqAcoef	Coefficient permitting the implicit coupling for specific humidity (See Section II.2.3)	$kg.kg^{-1}$	External input (LMDZ or database)
$\{G\}$	so il fl x	Soil heat flux at the previous time step	$W.m^{-2}$	thermosoil module (See Section II.4)
ρ	rau	Air density	$kg.m^{-3}$???
(u,v)	u, v	Wind velocity by directional components (u = eastwards, v = northwards)	$m.s^{-1}$	External input (LMDZ or database)
C_d	q_cdrag	Surface drag coefficient	_	condveg module (See Section II.2.2)
β_{bio}	vbeta	Total resistance coefficient for PFT evaporation processes	_	diffuco module (See Section II.3)
β_1	vbeta1	Resistance coefficient for snow sublimation	_	diffuco module (See Section II.3)
β_5	vbeta5	Resistance coefficient for floodplains evaporation	_	diffuco module (See Section II.3)
$C_{p,soil}$	soil cap	Soil calorific capacity	$J.K^{-1}$	thermosoil module (See Section II.4)
$L\downarrow$	lwdown	Down-welling long-wave radiation flux	$W.m^{-2}$	External input (LMDZ or database)
S_n	swnet	Net surface short-wave flux	$W.m^{-2}$	External input (LMDZ or database)
$\{R_n\}$	netrad	Net radiation budget at the previous time step	$W.m^{-2}$	enerbil_begin subroutine

Table of output variables:



Variable	Name in ORCHIDEE	Description	Unit	Output used in
H_{surf}	psnew	Surface dry static energy/potential enthalpy at the new time step	$J.kg^{-1}$	$enerbil_flux$
qsurf, sat	$qsol_sat_new$	Surface saturated humidity at the temperature of the new time step	$kg.kg^{-1}$	$enerbil_flux$
T_{surf}	temp_sol_new	Surface temperature at the new time step	K	enerbil_flux
q_{air}	$qair_new$	Air moisture at the new time step	$kg.kg^{-1}$	$enerbil_flux$
H_{air}	epot_air_new	Air potential enthalpy (epot_air_new = cp_air.T_air)	$J.kg^{-1}$	enerbil_flux

II.5.2.3 enerbil flux subroutine

This subroutine calculates all the fluxes, temperatures and humidities needed for the completion of the energy budget. The routines starts by calculating the upwelling long-wave radiations thanks to Equation (2). Because this flux is calculated thanks to a limited Taylor expansion around the precedent surface temperature, it does not rely on the "new" surface temperature. Then, after the limited Taylor expansion, the radiative surface temperature can be deduced thanks to Equation (128).

$$T_{surf,rad} = \left(\frac{L\uparrow}{\epsilon\sigma}\right)^{\frac{1}{4}} \tag{128}$$

A diagnostic variable used in LMDZ to compute the dependence of the surface layer stability on moisture is calculated according to Equation (129).

$$q_{surf} = q_{air} + (\beta_1 . (1 - \beta_5) + \beta_5) . (q_{surf,sat} - q_{air}) + (1 - \beta_1) . (1 - \beta_5) . \beta_{bio} . (q_{surf,sat} - q_{air})$$
(129)

Once this calculation finished, the calculation of the different fluxes of the energy budget is computed:

- The net radiation, R_n is calculated thanks to Equation (1).
- The total mass water flux, $E_{tot} = \frac{\Delta t}{\lambda} \cdot F_{tot}$, is calculated thanks to the following equation $\frac{\Delta t}{\lambda_{sublimation}} \cdot E_{snow} + \frac{\Delta t}{\lambda_{evaporation}} \cdot (E_{floodplains} + E_{other}).$
- The latent heat flux, F_{lat} , is calculated thanks to Equation (55).
- The sublimation component of the latent heat flux, $F_{sublimation}$, is calculated thanks to (57).
- The sensible heat flux, F_{sens} , is calculated thanks to Equation (5).
- The net long-wave radiation is calculated as the difference between $L \downarrow$ and $L \uparrow$
- The total potential evaporation, $E_{pot,tot}$ is calculated as defined in Equation (65).
- The air temperature, T_{air} , is calculated as the ratio between the new static air energy and the Cp_{air}



This part maybe needs a reviewing:

Once the different fluxes of the energy budget are determined, in order to couple the budget with the snow processes when snow is present at the surface, the subroutine calculates the amount of energy which is injected inside the snow pack ($F_{snow,input}$). To do so, the routine starts by calculating the amount of energy brought by the rainfall (assumed to be at T_{air}):

$$PHPSNOW = \frac{P_W.4.218.10^3.(T_{air} - T_{0^oC})}{\Delta t}$$
(130)

Where P_w is the rainfall rate and $T_{0^oC} = 0^oC$. This amount of energy permits to calculate a the amount of energy sent to the snow pack (by solving a new energy budget for the snowpack):

$$F_{snow,input} = R_n - F_{lat} - F_{sens} + PHPSNOW$$
(131)

Then, the routine recalculates the energy balance by replacing T_{surf} by $T_{0^{\circ}C}$. This permits to calculate another amount of energy transmitted to the snowpack (assuming an air temperature of $0^{\circ}C$). The variable is called $F_{snow,input,0^{\circ}C}$. This permits to access to the change in temperature (additional energy to melt snow for snow ablation case), $T_{surf,add}$ in K:

$$T_{surf,add} = -(F_{snow,input} - F_{snow,input,0^{\circ}C}) \cdot \frac{\Delta t}{C_{p,soil}}$$
(132)

Finally, the net energy into the snow pack is set as:

$$F_{snow,input} = F_{snow,input,0^{\circ}C} \tag{133}$$

End of the part that need to be reviewed

The last step of this subroutine is to computes Milly's correction to potential evaporation presented in Section II.2.1. After computing $E_{pot,tot}$, the correction term is calculated as in Equations (6) and (7). β is computed as $E_{tot}/E_{pot,tot}$.

Once the correction term is calculated, the corrected potential evaporation is computed as in Equation (134).

$$E_{pot,tot,corr} = E_{pot,tot} \cdot \frac{1+\beta\xi}{1+\xi}$$
(134)

NB: Reducing the equations of the code permits effectively to come back to Equation (134). **Table of input variables:**



Variable	Name in ORCHIDEE	Description	Unit	Input from
ε	emis	Surface emissivity	K	External input (LMDZ or database)
$\{T_{surf}\}$	$temp_sol$	Surface temperature at the previous time step	K	Previous time step
T_{surf}	$temp_sol_new$	Surface temperature at the new time step	K	$enerbil_surftemp$
Hair	epot_air	Air potential energy at the new time step	$J.kg^{-1}$	enerbil_surftemp
q_{air}	qair	Lowest level specific humidity at the new time step	$kg.kg^{-1}$	$enerbil_surftemp$
H_{surf}	psnew	Surface dry static energy at the new time step	$J.kg^{-1}$	enerbil_surftemp
$q_{surf,sat}$	$qsol_sat_new$	Surface saturated humidity at the temperature of the new time step	$kg.kg^{-1}$	$enerbil_surftemp$
ρ	rau	Air density	$kg.m^{-3}$???
(u,v)	u, v	Wind velocity by directional components (u = eastwards, v = northwards)	$m.s^{-1}$	External input (LMDZ or database)
C_d	q_cdrag	Surface drag coefficient	_	condveg module (See Section II.2.2)
β_{bio}	vbeta	Total resistance coefficient for PFT evaporation processes	_	<i>diffuco</i> module (See Section II.3)
β_1	vbeta1	Resistance coefficient for snow sublimation	-	diffuco module (See Section II.3)
β_5	vbeta5	Resistance coefficient for floodplains evaporation	-	diffuco module (See Section II.3)
$C_{p,soil}$	soil cap	Soil calorific capacity	$J.K^{-1}$	thermosoil module (See Section II.4)
P_b	pb	Lowest level pressure	hPa	External input (LMDZ or database)
E_{rain}	$precip_rain$	Rainfall	???	External input (LMDZ or database)
h_{snow}	snowdz	Snow depth	m	explicit_snow module
$L\downarrow$	lwdown	Down-welling long-wave radiation flux	$W.m^{-2}$	External input (LMDZ or database)
S_n	swnet	Net surface short-wave flux	$W.m^{-2}$	External input (LMDZ or database)
$\{R_n\}$	netrad	Net radiation budget at the previous time step	$W.m^{-2}$	enerbil_begin subroutine

Table of output variables:



Variable	Name in ORCHIDEE	Description	Unit	Output used in
q_{surf}	qsurf	Surface specific humidity	$kg.kg^{-1}$	LMDZ
F_{sens}	fluxsens	Sensible heat flux	$W.m^{-2}$	ORCHIDEE
Flat	fluxlat	Latent heat flux	$W.m^{-2}$	ORCHIDEE
$F_{sublimation}$	flux subli	Sublimation component of the latent heat flux	$W.m^{-2}$	ORCHIDEE
Etot	vevapp	Total evaporation mass flux	$mm.d^{-1}$	ORCHIDEE
$L\uparrow$	lwup	Up-welling long-wave radiation flux emitted by the surface	$W.m^{-2}$	ORCHIDEE
L_n	lwnet	Net long-wave radiation flux	$W.m^{-2}$	ORCHIDEE
$T_{surf,rad}$	$tsol_rad$	Radiative surface temperature	K	ORCHIDEE
$T_{surf,add}$	$temp_sol_add$	Additional energy to melt snow for the snow ablation case	K	ORCHIDEE

Table of modified variables:

Variable	Name in ORCHIDEE	Description	Unit	Input from / Output used in
R_n	netrad	Net radiation flux	$W.m^{-2}$	$enerbil_begin \ / \\ ORCHIDEE$
$E_{pot,tot}$	evapot	Total potential evaporation	mm/tstep	Previous time step / ORCHIDEE
$E_{pot,tot,corr}$	evapot_corr	Total potential evaporation after Milly's correction	mm/tstep	Previous time step / ORCHIDEE
$F_{snow,input}$	pgflux	Net energy flux into the snowpack	$W.m^{-2}$	$explicit_snow \ / \\ explicit_snow$

II.5.2.4 enerbil_evapveg subroutine

The last routine to be called is *enerbil_evapveg*. This routine computes the splitting of the total evaporation flux into its snow sublimation, floodplains evaporation, bare soil evaporation, intercepted water evaporation and transpiration components:

- Snow sublimation component is calculated thanks to β_1 and Equation (57) multiplied by $\frac{\Delta t}{\lambda_{sublimation}}$.
- Bare soil evaporation component is calculated thanks to β_4 and Equation (62) multiplied by $\frac{\Delta t}{\lambda_{evaporation}}$.
- Floodplains evaporation component is calculated thanks to β_5 and Equation (56) multiplied by $\frac{\Delta t}{\lambda_{evaporation}}$.
- Intercepted water evaporation component is calculated thanks to β_2 and Equation (60) multiplied by $\frac{\Delta t}{\lambda_{evaporation}}$.
- Transpiration component is calculated thanks to β_3 and Equation (61) multiplied by $\frac{\Delta t}{\lambda_{evaporation}}$.



Table of input variables:

Variable	Name in ORCHIDEE	Description	Unit	Input from
q_{air}	qair	Lowest level specific humidity at the new time step	$kg.kg^{-1}$	enerbil_surftemp
qsurf, sat	$qsol_sat_new$	Surface saturated humidity at the temperature of the new time step	$kg.kg^{-1}$	$enerbil_surftemp$
ρ	rau	Air density	$kg.m^{-3}$???
(u,v)	u, v	Wind velocity by directional components (u = eastwards, v = northwards)	$m.s^{-1}$	External input (LMDZ or database)
C_d	q_cdrag	Surface drag coefficient	-	condveg module (See Section II.2.2)
β_2	vbeta2	Resistance coefficient for PFT water interception evaporation	_	diffuco module (See Section II.3)
eta_3	vbeta3	Resistance coefficient for PFT transpiration	_	<i>diffuco</i> module (See Section II.3)
$eta_{3,pot}$	vbeta3pot	Resistance coefficient for PFT potential transpiration	_	diffuco module (See Section II.3)
eta_4	vbeta4	Resistance coefficient for bare soil water evaporation	_	diffuco module (See Section II.3)
β_1	vbeta1	Resistance coefficient for snow sublimation	_	diffuco module (See Section II.3)
β_5	vbeta5	Resistance coefficient for floodplains evaporation	_	diffuco module (See Section II.3)
$E_{pot,tot}$	evapot	Total potential evaporation	mm/tstep	enerbil_flux

Table of output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
E_{snow}	vevaps no	Snow evaporation mass flux	$mm.day^{-1}$	ORCHIDEE
$E_{bare_soil_evaporation}$	vevapnu	Bare soil evaporation mass flux	$mm.day^{-1}$	ORCHIDEE
$E_{floodplains}$	vevapflo	Floodplains evaporation mass flux	$mm.day^{-1}$	ORCHIDEE
$E_{transpiration}$	transpir	Transpiration mass flux	$mm.day^{-1}$	ORCHIDEE
$E_{transpiration,pot}$	transpot	Potential transpiration mass flux	$mm.day^{-1}$	ORCHIDEE
$E_{interception_loss}$	vevapwet	Intercepted water evaporation mass flux	$mm.day^{-1}$	ORCHIDEE

II.5.3 thermosoil and explicitsnow modules

II.5.3.1 thermosoil module

The scheme of the *thermosoil* module can be summarized as in Figure 10.





Figure 10: Scheme of the *thermosoil* module

The *thermosoil* module is computing the heat diffusion resolution presented in Section II.4. It also introduces other processes which are not presented in this note such as heat from organic decomposition, decrease of soil heat conductivity due to soil organic carbon... The



main subroutines for the resolution of the energy budget are:

- thermosoil_coef subroutine: This subroutine computes the calculation of the coefficients α_k and β_k needed for the calculation of the temperature profile inside the soil at the next time step.
- *thermosoil_profile* subroutine: This surboutine solves the tridiagonal system thanks to the coefficient previously determined. It permits to calculate the temperatures at each nodes of the soil.
- thermosoil_cond subroutine: This subroutine computes the soil heat capacity and conductivity according to the soil properties. (The subroutines thermosoil_cond_pft, thermosoil_getdiff, thermosoil_getdiff_pft and thermosoil_getdiff_old_thermix_without_snow are doing the same but for different configurations (with or without taking into account freezing for example).

Because the snow cover is considered as 3 additional layers of soil with different heat properties, the snow coefficient α_k and β_k are calculated in the subroutine *thermosoil_coef*. The snow layer temperatures are calculated in the *explicitsnow* module (See Section II.5.3.2).

Finally, here is a quick table of the main variables described in this note and their names in the code.

Variable	Name in ORCHIDEE	Description	Unit
α_k and β_k	$cgrnd(_snow)$ and $dgrnd(_snow)$	Soil and Snow resolution coefficients	- and K
λ	cnd	Soil heat conductivity	$W.m^{-1}.K^{-1}$
θ	mc_lay and others	Volumetric soil moisture content (for each layer, liquid only, liquid+ice)	$m.s^{-1}$
G	soilflx	Soil heat flux	$W.m^{-2}$
C_{app}	soilcap	Soil apparent heat capacity	$J.m^{-2}.K^{-1}$
T_k	stempdiag	Soil Temperature profile	K

II.5.3.2 *explicitsnow* module

The scheme of the *explicitsnow* module can be summarized as in Figure 11.





Figure 11: Scheme of the *explicitsnow* module

The *explicitsnow* module computes all the snow processes at the Earth surface. Among those processes, the heat diffusion inside the snow cap is calculated. As it has been mentioned, the snow cap is considered as the addition of 3 new soil layers above the ground, with other heat diffusion properties. Thus, the resolution of the snow heat diffusion is divided between the *explicitsnow* module and *thermosoil* module as see in Section II.5.3.1.

The module is divided into several subroutines which compute a precise process:

- *explicitsnow_grain* subroutine: This subroutine calculates the snow grain sizes (process not described here but which has an impact on snow density for example).
- *explicitsnow_compactn* subroutine: This subroutine calculates the snow compaction after the snow fall. It permits to update the heights of the snow layers after the compaction and the value of the snow density.
- *explicitsnow_transf* subroutine: This subroutine computes a mass and heat redistribution (maybe needs more details).
- *explicitsnow_fall* subroutine: This routine computes the snow fall at each time step on the grid cell.
- *explicitsnow levels* subroutine: This routine computes the heights of each snow layers.



- *explicitsnow_profile* subroutine: This routine calculates the snow layers temperatures thanks to the coefficients previously calculated in the *thermosoil* module (See Section II.5.3.1).
- *explicitsnow_melt_refrz* subroutine: This subroutine calculates the snow melt and refreezing processes within the snowpack.
- *explicitsnow_gone* subroutine: This routine checks if snow is gone (maybe needs more details).

All the processes are described in Boone et al. (2001)[3].

Finally, here is a quick table of the main variables described in this note and their names in the code.

Variable	Name in ORCHIDEE	Description	Unit
$\alpha_{k,snow}$ and $\beta_{k,snow}$	$cgrnd_snow ext{ and } \\ dgrnd_snow$	Snow resolution coefficients	- and K
P_n	$precip_snow$	Snow fall	$W.m^{-1}.K^{-1}$
F _{snow,input}	pgflux	Net energy into the snow pack	$W.m^{-2}$
G_{snow}	grndflux	Heat injected in the soil from the snow pack	$W.m^{-2}$
T_{snow}	snowtemp	Snow temperature profile	K
M _{snow}	snow	Snow mass	$kg.m^{-2}$



II.6 Suggestions

This quick part is a list of suggestions in order to improve the understanding of the code.

- Milly's correction of evaporation has two different names in the code. In *enerbil*, the variable of the corrected evaporation is called *evapot_corr* whereas in *sechiba* when the module calls *enerbil*, the variable is called *evapot_penm*. I think that we should be consistent between both names.
- Moreover, it seems that Milly's correction is only used in two different parts of the code: the calculation of *vbeta4* in *diffuco*, β for the evaporation of floodplains, and the calculation of the soil evaporation *evap_soil* in *hydrol*. I think that the evaporation corrected thanks to Milly's correction should be used everywhere.
- In *enerbil*, in the subroutine *enerbil_flux*, the variable defined as *epot_air* and *qair* correspond to the values at the "new" time step. When the routine is called, the variables in arguments are *epot_air_new* and *qair_new*. Maybe that the variables defined in the routine as *epot_air* and *qair_should* be renamed as *epot_air_new* and *qair_new*.
- All the heights in the *diffuco_aero* subroutine and the *condveg* module should be reworded with their proper definition.



Partie III

Description of the multi-layer energy budget in ORCHIDEE

III.1 Introduction

III.1.1 Aim and history of this module in ORCHIDEE

The Multi-layer energy budget has been developed a few years ago by James Ryder during his post-doc at the LSCE. After validating the multi-layer scheme, this module has been implemented in the trunk of ORCHIDEE as the module mleb.

The Multi-layer energy budget has been thought from an ecosystem point of view. This means that the module aims at better representing the exchanges of energy inside the canopy. However, because ORCHIDEE is a global land surface model, the pixels are not always pure canopies. In the cases of several canopies distributed in a specific pixel, the initial aim of the multi-layer energy budget was to represent the pixel as "mean" canopy with several parameters. However, the multi-layer energy budget has never been used on a non pure-pixel.

This choice of point of view has a direct consequence on the results module. When running on pure PFT pixels, the module has strong results which can be compared to the current energy budget module *enerbil*. However, in cases of several PFT on a pixel, the module is currently not working properly.

This is the big difference between *enerbil* and *mleb*:

- *enerbil* has been thought from a pixel/grid-cell point of view. Its aim is to model the energy budget at the pixel level and, then, split those fluxes between the several PFTs that compose the pixel (thanks to the β -model).
- *mleb* has been thought from an ecosystem point of view. It aims at better representing the fluxes inside the canopy. In case of non-pure pixels, if the multi-layer energy budget is used for each canopies of the pixel, a mix has to be made above the canopies (opposite of the β model). However, this case has never been studied as *mleb* run always on pure pixels.

The aim of the present note is to explain how the multi-layer energy budget works and how it is implemented in ORCHIDEE. At the time this note is written (January 2021), several works are made on the multi-layer energy budget. They are summarized in Section IV.1.

III.1.2 Current energy budget in ORCHIDEE

To understand more about the current energy budget in ORCHIDEE, please refer to Part II

III.1.3 Notations

Here is a quick summary of the notations that will be used. Let's consider the following variable:

$$\alpha_{j,i}^k \tag{135}$$

On this variable:



- α is the variable symbol.
- i will always refer to the index of the layer. If there is no first index on the variable, it will refer to the index of the layer too.
- j can be replaced by:
 - A number: it represents an index in the list (ex: $\eta_{3,i}$).
 - *leaf*: this is a leaf variable (ex: $T_{leaf,i}^{t+1}$).
 - a: this is an air variable (ex: $T_{a,i}^{t+1}$).
 - T: the variable is linked to the temperature (ex: $A_{T,i}$).
 - -q: the variable is linked to the humidity (ex: $B_{q,i}$).
 - Other: this is part of the name of the variable (ex: C_p^{air} which represent the air heat capacity).
- k can be replaced by:
 - -t, t+1, t-1: this is the time step at which the variable is calculated (ex: $T_{leaf,i}^{t+1}$).
 - Other: this is part of the name of the variable (ex: C_p^{air} which represent the air heat capacity).



III.2 Model description

III.2.1 General description

The model developed by James Ryder aims at answering to 6 requirements (requirements listed in *Ryder et al.* (2016)[21]:

- 1. Simulate processes that are sufficiently well understood at a canopy level such that they can be parametrised at the global scale through semi-mechanistic techniques.
- 2. Simulate the exposure of each layer of the canopy and the soil layer to Short and Long Waves Radiations and simulate in-canopy gradients.
- 3. Simulate non-standard canopy set-ups (different species in the the same vertical structure for instance).
- 4. Describe directly the interactions between the soil surface and the sub-canopy using an assigned soil resistance rather than a soil-canopy amalgamation.
- 5. Be flexible (stable such as it can be run over 50 or 2 layers).
- 6. Avoid introducing iterative solutions.

As precised in Introduction, it is clear that the model has been developed from an ecosystem point of view in order to well simulates canopy processes.

The model proposes to simulate the canopy as a network of potentials and resistances as on Figure 12.



Figure 12: Potential and resistance scheme of the canopy



At each level, the model will have to calculate the state variables of the layer: the atmospheric humidity and temperature of the level $(q_{a,i} \text{ and } T_{a,i})$ and the leaf temperature $(T_{leaf,i})$. Those state variables are the potentials of the network.

The changes over time of those state variables are governed by the exchanges between layers and between the leaves and the atmosphere of the layer. The exchanges that govern those variations are fluxes of kinds: latent heat flux and sensible heat flux. As precised in the requirements, the model also takes into account the absorption, emission and reflection of radiations at each level by the vegetation and at the soil interface by the soil. Finally, at the extremities, the lower sub-layer interacts with the soil and the upper sub-layer interacts with the atmosphere.

The model can be seen as an electric circuit where the temperatures and humidities are the potentials and the latent and sensible heat fluxes are the current. Those fluxes are interacting with the atmosphere and vegetation through resistances (vegetation resistance for the fluxes coming from leaves and going to the atmosphere and turbulent diffusion resistances for the fluxes coming from the other layers and going at layer i).

The state variables are then determined at each time steps thanks to the energy budgets at each levels (Section III.2.2).

III.2.2 Energy budget at level i

The state variables of each layers are determined mainly thanks to the resolution of three equations:

- The energy balance of the leaves at the layer
- The turbulent transport of sensible heat between layers
- The turbulent transport of latent heat between layers

III.2.2.1 Leaf energy budget

At layer *i*, the vegetation is assumed to form a layer of volume ΔV_i , area ΔA_i and thickness Δh_i . This layer of vegetation is subject to incoming and outgoing fluxes of energy:

- Sensible heat $(H \text{ in } W.m^{-2})$
- Latent heat $(\lambda E \text{ in } W.m^{-2})$
- Short Waves Radiation from the Sun $(R_{SW} \text{ in } W.m^{-2})$
- Long Waves Radiation $(R_{LW} \text{ in } W.m^{-2})$

Consequently, the change in temperature of the vegetation layer can be expressed as follows:

$$\Delta V_i \cdot C_{p,i}^{leaf} \cdot \rho_v \cdot \frac{T_{leaf,i}}{dt} = (R_{SW,i} + R_{LW,i} - H_i - \lambda E_i) \cdot \Delta A_i$$
(136)

Where, ΔV_i is the volume of the box at level i, ΔA_i is the area of vegetation (it can be represented by the Plant Area Density (PAD) in $m^2 \cdot m^{-3}$, where vegetation refers to leaves, stems, grasses...), $C_{p,i}^{leaf}$ is the specific heat of the vegetation layer (assumed to be equal to that



of water and is modulated by the leaf area density $(m^2.m^{-3})$ and ρ_v is the vegetation density $(kg.m^{-3})$.

Equation (136) can be rewritten in terms of the state variables and the resistances shown in Figure 12 as in Equation (137).

$$C_{p,i}^{leaf}.\rho_v.\frac{T_{leaf,i}}{dt} = (R_{SW,i} + R_{LW,i} - C_p^{air}.\rho_a.\frac{T_{leaf,i} - T_{a,i}}{R_i} - \lambda.\rho_a \frac{q_{leaf,i} - q_{a,i}}{R'_i}).\frac{1}{\Delta h_i}$$
(137)

Where, C_p^{air} is the specific heat of air, ρ_a is the air density and R_i and R'_i are respectively the resistances of vegetation to sensible heat flux and latent heat flux (See Section III.2.4 for more details). The expression of sensible and latent heat fluxes correspond to the ones between vegetation and the air of the layer.

III.2.2.2 Energy transport between layers

General transport scheme:

The general transport equation between each layer of the model can be described generally as in Equation (138).

$$\frac{\partial(\rho\chi)}{\partial t} + div(\rho.\chi.\mathbf{u}) = div(\Gamma grad(\chi)) + S_{\chi})$$
(138)

This general equation can be simplified in the case of a vertical transport in Equation (139).

$$\frac{\partial(\chi)}{\partial t} \Delta V = \frac{\partial}{\partial z} (k_*(z) \cdot \frac{\partial \chi}{\partial z}) \Delta V + S(z) \cdot \Delta V$$

$$= -\frac{\partial}{\partial z} (F(z)) \cdot \Delta V + S(z) \cdot \Delta V$$
(139)

Where, χ represents the concentration of the constituent (water vapour, heat, gas...), k(z) represents the vertical eddy diffusivity for the transport of the constituent inside the canopy, F(z) is the flux associated to the transport, S(z) is the source density of the constituent and ΔV is the volume variation.

From this equation, the flux-gradient relationship can be deduced as in Equation (140).

$$F(z) = -k_*(z) \cdot \frac{\partial \chi}{\partial z} \tag{140}$$

As transport in canopies is turbulent, the main challenge here is to describe the eddy diffusivity coefficient k(z). The more physical way to express k(z) has been developed by *Raupach* (1989a) [20]. This model relies on a decomposition of k(z) into a far-field term which represents the purely diffusive transport inside the canopy and a near-field term which represents the effects of persistence inside the canopy. This approach relies on two different assumptions:

- 1. The *far-field* transport can be modeled with a pure gradient-diffusion equation.
- 2. The *near-field* effects can be treated assuming the turbulence to be locally homogeneous.

This model permits to better calculate the transport of constituents inside the canopy and model counter-gradient fluxes which leads to accumulations of constituents in some parts of the



canopy (the curve of concentration of the constituent presents a "belly" in some places of the canopy).

However, Ryder et al. (2016) [21] states that the near-field component of this approach, which relies on a ideally Lagrangian solution, cannot be used in a fully implicit resolution scheme. Consequently, the model implemented in the multi-layer is different from the one developed by Raupach (1989a) [20].

The model used by *Ryder et al.* (2016) [21] relies on an adaptation of the *far-field* results from *Raupach* (1989a) [20]. In the *far-field* theory, the eddy diffusivity coefficient is expressed as in Equation (141).

$$k_*(z) = \sigma_w^2 T_L \tag{141}$$

Where σ_w is the standard deviation in wind vertical velocity along the canopy and T_L is the Lagrangian time-scale, designed as in *Raupach (1989a)* [20].

The standard deviation in wind vertical velocity is calculated following Massman & Weil (1999) [13]. Explaining all the second-order closure model of this article would be too heavy here, you can refer to the article to have more details. The only thing that differs in the multi-layer model of Ryder et al. (2016) [21] from the model of Massman & Weil (1999) [13] is in the calculation of the variable $\eta(z)$ where the factor C_d/P_m is calculated following Wohlfahrt & Cernusca (2002) [25] who express it as $C_{D,eff} = a_1^{-LAD/a_2} + a_3^{-LAD/a_4} + a_5$, where a_1 to a_5 are parameters to be defined and LAD is the leaf area density.

Consequently, by expressing σ_w thanks to Massman & Weil (1999) [13] and T_L thanks to Raupach (1989a) [20], the eddy diffusivity coefficient k(z) for the far-field is known.

However, as Raupach (1989a) [20] demonstrated, the far-field approach only cannot model the real transport of constituents in the canopy, a near-field component has to be involved in the calculation. As it has been explained, Ryder et al. (2016) [21] considers the full Lagrangian solution for the near-field contribution cannot be implemented in an implicit resolution scheme. Consequently, the previous far-field contribution is reviewed in order to introduce a near-field correction term (not considering the near-field term resulted in a bias in the calculation of temperature at nighttime which leads to the necessity of a correction term). This correction has been developed by Makar et al. (1999.) [12] and aims at reducing the eddy diffusivity coefficient in the near-field. This correction is based on a factor R_{nf} . As this factor is relying on the diffusion time of the fluid particle, a similar trick developed by Chen et al. (2016) [4] is implemented in order to link it to the friction velocity $u_* = u(h).(c_1 - c_2.e^{-c_3.\eta(h)})$ (following Massman & Weil (1999) [13], with c_1, c_2 and c_3 parameters, u(z) the wind speed according to the altitude inside the canopy, h the height of the canopy and eta(z) the variable defined above). The aim of the trick is to give R_{nf} a S-shape in function of u_* thanks to the Equation (142).

$$R_{nf} = \frac{1}{1 + e^{-k_{slope}.(u_* - k_{u_*})}}$$
(142)

Where k_{slope} and k_{u_*} are parameters.

Finally, the eddy diffusivity coefficient is expressed as in Equation (143).

$$k_*(z) = R_{nf}(z).\sigma_w^2.T_L \tag{143}$$

This turbulent diffusion scheme is not the more physical way to describe the transfers inside the canopy. This point is discussed in the Section III.5.2.2.



Fluxes of sensible and latent heat between layers:

Rewriting the previous equations in terms of atmospheric temperature and humidity permits to access to the rate of change of the atmospheric temperature and humidity in the layer i. Equation 144 describes the rate of change of temperature.

$$C_p^{air}.\rho_a.\frac{dT_{a,i}}{dt}.\Delta V_i = -\frac{\partial H_{a,i}}{\partial z}.\Delta V_i + \frac{T_{leaf,i} - T_{a,i}}{R_i}.\frac{C_p^{air}.\rho_a}{\Delta h_i}.\Delta V_i$$
(144)

This equation links the change of atmospheric temperature of layer i to the flux of sensible heat between the layers (first term of the right hand side of the equation) and to the source term due to the vegetation (second term of the right hand side of the equation).

By replacing the sensible heat by its formula in Equation (140):

$$H_{a,i} = -\rho_a \cdot C_p^{air} \cdot k_i^* \cdot \frac{\partial T_{a,i}}{\partial z}$$
(145)

The general transport equation of sensible heat is obtained thanks to equation (146).

$$\frac{dT_{a,i}}{dt} \cdot \Delta V_i = -\frac{\partial^2 k_i^* \cdot T_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{T_{leaf,i} - T_{a,i}}{R_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(146)

Following the same approach, the general equation for latent heat flux can be obtained by considering the rate of change of humidity in the atmosphere of the layer i.

$$\lambda . \rho_a. \frac{dq_{a,i}}{dt} . \Delta V_i = -\frac{d(\lambda E)_{a,i}}{dz} . \Delta V_i + \frac{q_{leaf,i} - q_{a,i}}{R'_i} . \frac{\lambda . \rho_a}{\Delta h_i} . \Delta V_i$$
(147)

By replacing the latent heat flux by its formula and by assuming that the leaf cavities are completely saturated (which permits to consider that the vapour pressure of the leaf can be calculated as the saturated vapour pressure at that leaf temperature), the Equations (148) and (149) can be obtained.

$$(\lambda E)_{a,i} = -\lambda . \rho_a . k_i^* . \frac{\partial q_{a,i}}{\partial z}$$
(148)

$$q_{leaf,i}^{t+1} = q_{sat}(T_{leaf,i}^t) + \frac{\partial q_{sat}}{\partial T}|_{T_{leaf,i}^t}(T_{leaf,i}^{t+1} - T_{leaf,i}^t) = \alpha_i \cdot T_{leaf,i}^{t+1} + \beta_i$$
(149)

Where, $\alpha_i = \frac{\partial q_{sat}}{\partial T}|_{T^t_{leaf,i}}$ and $\beta_i = (q_{sat}(T^t_{leaf,i}) - T^t_{leaf,i} \cdot \frac{\partial q_{sat}}{\partial T}|_{T^t_{leaf,i}})$. This permits to access to the general transport equation of latent heat flux as in Equation (150).

$$\frac{dq_{a,i}}{dt} \cdot \Delta V_i = \frac{\partial^2 k_i^* \cdot q_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{(\alpha_i \cdot T_{leaf,i} + \beta_i) - q_{a,i}}{R'_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(150)

III.2.2.3 General energy budget of level *i*

Here is a quick summary of the three main equations that governed the exchanges at the layer *i*:

• Equation (151) balances the energy budget at each canopy air level.



- Equation (152) balances heat fluxes vertically between each atmospheric level and horizontally between each vegetation level and the surrounding air.
- Equation (153) balances latent heat fluxes vertically between each atmospheric level and horizontally between each vegetation level and the surrounding air.

$$C_{p,i}^{leaf}.\rho_v.\frac{T_{leaf,i}}{dt} = (R_{SW,i} + R_{LW,i} - C_p^{air}.\rho_a.\frac{T_{leaf,i} - T_{a,i}}{R_i} - \lambda.\rho_a \frac{q_{leaf,i} - q_{a,i}}{R'_i}).\frac{1}{\Delta h_i}$$
(151)

$$\frac{dT_{a,i}}{dt} \cdot \Delta V_i = -\frac{\partial^2 k_i^* \cdot T_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{T_{leaf,i} - T_{a,i}}{R_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(152)

$$\frac{dq_{a,i}}{dt} \cdot \Delta V_i = \frac{\partial^2 k_i^* \cdot q_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{(\alpha_i \cdot T_{leaf,i} + \beta_i) - q_{a,i}}{R'_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(153)

Resolving each equations at the same time following the implicit scheme imposed by the global circulation model will permit to access to all the data at each layer and each time step (See Section III.3).

III.2.3 Radiations scheme

The radiations scheme used in the multi-layer energy budget aims at determining the value of $R_{SW,i}$ and $R_{LW,i}$ at each layer. The challenge behind the schemes used is to model all the components of both fluxes: scattered flux, reflected fluxes from other layers... in order to obtain the absorb fluxes at each level.

To do so, two different schemes are used to define the Short-Wave radiations and Long-Wave radiations at each layer:

- LW radiations: The model used is the Long-Wave Radiation Transfer Matrix (LRTM) developed by Lianhong Gu in *Gu (1988)* and *Gu et al. (1999)* [8].
- SW radiations: The model used is the Multi-layer Albedo Scheme developed by *McGrath* et al. (2016) [14]

III.2.3.1 Long Waves radiations scheme

The modeling of Long-Wave radiations inside the canopy is a challenge because all the different elements of the canopy (soil, leaves...) are long-waves emitters. Assumptions have to be made to avoid too much calculations or even iteration procedures.

The Long-Wave Radiation Transfer Matrix relies on three different assumptions:

- The scattering coefficients for Long-Wave radiations are very small and can be neglected.
- The resolution process is fully explicit
- Because soil and leaves have often high emissivities, they are assumed to be black bodies.

From those assumptions, to avoid a iteration procedure, the model relies on the definition of a radiation transfer matrix defined as:



$$\begin{pmatrix} R_{LW,surf} \\ R_{LW,1} \\ \vdots \\ R_{LW,i} \\ \vdots \\ R_{LW,i} \\ R_{LW,m} \\ R_{LW,above} \end{pmatrix} = \begin{pmatrix} \alpha_{0,0}^{LW} & \alpha_{0,1}^{LW} & \cdots & \alpha_{0,m}^{LW} & \alpha_{0,m+1}^{LW} \\ \alpha_{1,0}^{LW} & \alpha_{1,1}^{LW} & \cdots & \alpha_{1,m}^{LW} & \alpha_{1,m+1}^{LW} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{i,0}^{LW} & \alpha_{i,1}^{LW} & \cdots & \alpha_{i,m}^{LW} & \alpha_{i,m+1}^{LW} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{m,0}^{LW} & \alpha_{m,1}^{LW} & \cdots & \alpha_{m,m}^{LW} & \alpha_{m,m+1}^{LW} \\ \alpha_{m+1,0}^{LW} & \alpha_{m+1,1}^{LW} & \cdots & \alpha_{m+1,m}^{LW} & \alpha_{m+1,m+1}^{LW} \end{pmatrix} . \begin{pmatrix} \sigma.(T_{surf}^{t})^{4} \\ \sigma.(T_{leaf,i}^{t})^{4} \\ \vdots \\ \sigma.(T_{leaf,i}^{t})^{4} \\ \vdots \\ \sigma.(T_{leaf,i}^{t})^{4} \\ R_{LW} \end{pmatrix}$$

Consequently, at each layers, the Long-Waves radiations absorbed are calculated as:

$$R_{LW,i} = \alpha_{i,m+1}^{LW} \cdot R_{LW} + \sum_{j=1}^{m} \alpha_{i,j}^{LW} \cdot \sigma \cdot (T_{leaf,j}^t)^4 + \alpha_{i,0}^{LW} \cdot \sigma \cdot (T_{surf}^t)^4$$
(154)

Where the $\alpha_{i,j}$ are defined as below:

$$\alpha_{i,j} = \begin{cases} -1 & \text{i=j=0} \\ F(l_t - l_{j-1}) - F(l_t - l_j) & \text{i} = 0, j \in \{1, m\} \\ i = 0, j = m + 1 \\ F(l_j - l_{i-1}) - F(l_{j-1} - l_{i-1}) - F(l_j - l_i) + F(l_{j-1} - l_i) & \text{i} \in \{1, m\}, j \in \{1, i - 1\} \\ 2.F(\Delta l_i) - 2 & \text{i} \in \{1, m\}, i = j \\ F(l_i - l_{j-1}) - F(l_{i-1} - l_{j-1}) - F(l_i - l_j) + F(l_{i-1} - l_j) & \text{i} \in \{1, m\}, j \in \{i + 1, m\} \\ F(l_t) & \text{i} = m + 1, j = 0 \\ F(l_j) - F(l_{j-1}) & \text{i} = 0, j \in \{1, m\} \\ -1 & \text{i} = m + 1, j = m + 1 \\ \end{cases}$$
(155)

Where, l_i represents the cumulative leaf area index when working up to level i from the ground $(l_i = \sum_{i=1}^{i} LAI_i)$ and F(l) simulates the effect of canopy structure on the passage of Long-Wave radiation and is defined as:

$$F(l) = 2 \int_0^1 e^{-\frac{l.G_{leaf}(\mu)}{\mu}.\mu.d\mu}$$
(156)

Where $G_{leaf}(\mu)$ is a function that represents the orientation of the leaves.

However, as presented in Equation (154), the scheme is fully explicit and depends on the leaves temperature at layer at the previous time-step. To make this resolution scheme semi-implicit, James Ryder did a small trick using a truncated Taylor expansion (f(x) = f(a) + f'(a).(x - a)) with $x = T_{leaf,i}^{t+1}$ and $x = T_{leaf,i}^{t}$):

$$\alpha_{i,i}^{LW} \cdot \sigma \cdot (T_{leaf,i}^{t+1})^4 \approx \alpha_{i,i}^{LW} \cdot \sigma \cdot (T_{leaf,i}^t)^4 + 4 \cdot \alpha_{i,i}^{LW} \cdot \sigma \cdot (T_{leaf,i}^t)^3 \cdot (T_{leaf,i}^{t+1} - T_{leaf,i}^t) \\ \approx \alpha_{i,i}^{LW} \cdot \sigma \cdot (4 \cdot (T_{leaf,i}^t)^3 \cdot T_{leaf,i}^{t+1} - 3 \cdot (T_{leaf,i}^t)^4)$$
(157)

Equation (154) thus becomes Equation (158).

$$R_{LW,i} = \alpha_{i,m+1}^{LW} \cdot R_{LW} + \sum_{j=1, j \neq i}^{m} \alpha_{i,j}^{LW} \cdot \sigma \cdot (T_{leaf,j}^t)^4 + \alpha_{i,i}^{LW} \cdot \sigma \cdot (4 \cdot (T_{leaf,i}^t)^3 \cdot T_{leaf,i}^{t+1} - 3 \cdot (T_{leaf,i}^t)^4) + \alpha_{i,0}^{LW} \cdot \sigma \cdot (T_{surf}^t)^4$$
(158)

Technical note

63



This permits to express $R_{LW,i}$ with the following form:

$$R_{LW,i} = \eta_{1,i} \cdot T_{leaf,i}^{t+1} + \eta_{2,i} \tag{159}$$

Indeed, by posing (be careful at the $i \neq j$ below the \sum):

$$R_{LW,i}^{0} = \alpha_{i,m+1}^{LW} \cdot R_{LW} + \sum_{j=1, j \neq i}^{m} \alpha_{i,j}^{LW} \cdot \sigma \cdot (T_{leaf,j}^{t})^{4} + \alpha_{i,0}^{LW} \cdot \sigma \cdot (T_{surf}^{t})^{4}$$
(160)

One can get:

$$\eta_{1,i} = \alpha_{i,i}^{LW} . \sigma . (T_{leaf,i}^t)^3$$
(161)

$$\eta_{2,i} = R^0_{LW,i} - 3.\alpha^{LW}_{i,i} \cdot \sigma \cdot (T^t_{leaf,i})^4 \tag{162}$$

The Long-Wave Radiations at each layers $R_{LW,i}$ are thus determined thanks to Equation (159).

III.2.3.2 Short Waves radiations scheme

The Short-Wave radiations scheme has been developed by $McGrath \ et \ al. \ (2016)[14]$. This model is a development of the Short-Wave radiation model of *Pinty et al.* (2006)[18].

The model relies on a decription of the Short-wave radiations which are divided into several terms at each time-step and layers. All those terms are expressed as a fraction of the total downwelling Short-Wave radiation coming from the Sun. Consequently, at each layer, the absorbed Short Wave radiations $(R_{SW,i})$ are expressed as in Equation (163).

$$R_{SW,i} = \eta_{3,i} \cdot R_{SW}^{down} \tag{163}$$

The main coefficient, $\eta_{3,i}$ is expressed following *McGrath et a. (2016)* [14] resolution. At each layer a (down-welling) flux coming in layer *i* can be either:

- Transmitted to the lower layer without colliding any vegetation. It is noted $T_{veg,i}^{uncoll}$.
- Transmitted to the lower layer after colliding one or several times the vegetation. It is noted $T_{veg,i}^{coll}$.
- Reflected to the upper layer after colliding one or several times the vegetation. It is noted $R_{veg,i}^{coll}$.
- Absorbed by the vegetation. It is note $A_{veg,i}$.

All coefficients are calculated following *Pinty et al. (2006)* [18]. The calculation are based on several key variables:

- The effective Leaf Area Index of the layer LAI_{eff} .
- The single scattering albedo (ω_l) of the layer.
- The scattering phase function for that particular layer.

Technical note



The values of the transmission and reflection quantities are adapted from the two steams model developed in *Pinty et al. (2006)* [18] by *McGrath et al. (2016)*[14] (See articles for more details).

Finally, $A_{veg,i}$ is calculated by taking the difference between all the incoming radiations (collided, uncollided, transmitted...) from above and below layer i and the outgoing radiations of layer i.

Then, $\eta_{3,i} = A_{veg,i}$.

Remark from Sebastiaan: The code for photosynthesis and energy are largely independent but they both make use of Aveg,i. For the moment we have a too low GPP which could be due to the fact that not enough light is being absorbed. If the problem is in the calculation of Aveg (for which we have no indication at the moment) a similar problem would occur in the energy budget calculations. If the problem is in how we apply Aveg the issue could be limited to the diffuco_trans_co2 subroutine. This problem was not present in r2566 (CAN/DOFOCO) so we expect it was introduced during the merge with the N-version. This does not affect the document but it might be worth keeping in it mind for when you start looking into results.

III.2.4 Leaf resistances

The leaf resistances R_i and R'_i presented in Figure 12 and in Equations (151), (152) and (153) correspond to resistances to sensible and latent heat fluxes respectively. When there is no leaf in a layer, those two resistances are set to infinity.

III.2.4.1 To sensible heat flux

The resistance to sensible heat flux corresponds to the resistance of the boundary layer of the leaf surface $R_{b,i}$. The latter resistance can be expressed as in Equation (164).

$$R_i = R_{b,i} = \frac{d_1}{D_{h,air}.N_u} \tag{164}$$

The latter expression is taken from *Monteith and Unsworth (2008)* [17] and $D_{h,air}$ is the thermal diffusivity of air, d_1 is the characteristic leaf length and N_u is the Nusselt number, expressed as follows:

$$N_u = 0.66. Re^{0.5} . Pr^{0.33} \tag{165}$$

Where $Re = \frac{d_{1.u}}{\mu}$ is the Reynolds Number (with μ the kinematic viscosity of air and u the wind speed at level i) and Pr is the Prandtl number (0.7 for air).

III.2.4.2 To latent heat flux

The resistance to latent heat flux R'_i is composed by two different terms: the boudary layer resistance of the leaf $R'_{b,i}$ and the stomatal resistance $R'_{s,i}$.

$$R'_{i} = R'_{b,i} + R'_{s,i} \tag{166}$$

In the case of latent heat flux, still according to *Monteith and Unsworth (2008)* [17], the boudary layer resistance is given by:



$$R'_{b,i} = \frac{d_1}{D_{h,H_2O}.S_h} \tag{167}$$

Where D_{h,H_2O} is the molecular diffusivity of water vapour and S_h is the Sherwood number: $Sh = 0.03.Re^{0.5}.Sc^{0.33}$ (for laminar flows) and $Sh = 0.66.Re^{0.8}.Sc^{0.33}$ (for turbulent flows) (with Sc is the Schmidt Number which is 0.63 for water). The transition from laminar to turbulent occurs when Re = 8000.

Finally, the stomatal resistance at level is expressed according to the Ball-Berry approximation, per level i.

$$R'_{s,i} = \frac{1}{q_{s,i}} = \frac{1}{LAI_i \cdot (g_0 + \frac{a_1 \cdot A \cdot h_s}{C_s})}$$
(168)

Where, g_0 is the residual stomatal conductance, A is the assimilation, h_s is the relative humidity at the leaf surface and C_s is the concentration of CO_2 at the leaf surface.

Consequently, the total resistance to latent heat flux can be expressed as in Equation (169).

$$R'_{i} = \frac{d_{1}}{D_{h,H_{2}O}.S_{h}} + \frac{1}{LAI_{i}.(g_{0} + \frac{a_{1}.A.h_{s}}{C_{s}})}$$
(169)

NB: With the work on the new hydraulic architecture, the stomatal conductance formula as been changed as follows:

$$g_s = g_0 + \frac{a.(A + R_d)}{c_i - c_i^*} \cdot \frac{1 + exp(s_f \cdot \psi_f)}{1 + exp(s_f \cdot (\psi_{leaf} - \psi_f))}$$
(170)

Where R_d is the dark respiration, c_i is the concentration of CO_2 is the stomatal cavities, c_i^* is the CO_2 compensation point, s_f is a sensitivity parameter, ψ_f is a reference water potential and ψ_{leaf} is the leaf water potential (MPa). The objective of this new formulation is to better represent the water status of the vegetation and its behaviour in periods of draughts (See *Tuzet et al. (2003)* [23]).



III.3 Implicit resolution

III.3.1 Coupling with atmosphere

As for the current energy budget (See Part II), the multi-layer energy budget scheme has to be solved following an implicit scheme.

ORCHIDEE has two different types of functioning. ORCHIDEE can be run alone and the atmospheric data will be the inputs of the model or ORCHIDEE can be run in coupled mode with the Global Circulation Model (GCM) called LMDZ. In this coupled mode, the interface between both models has to be precisely studied. In the case of ORCHIDEE-LMDZ, this interface has been chosen implicit which means that all the variables that compose this interface have to be calculated at the same time-step. In the case of the surface energy budget, this means that the latent heat flux and the sensible heat flux are calculated as follows:

$$F_{lat}^{t+1} = \lambda.\beta.\rho.|\overrightarrow{V}|.C_d.(q_{surf}^{t+1} - q_{air}^{t+1}) = F_{lat}^{t+1} = \lambda.\beta.\rho.|\overrightarrow{V}|.C_d.(q_{surf}(T_{surf}^{t+1}) - q_{air}^{t+1})$$
(171)

$$F_{sens}^{t+1} = \rho. |\vec{V}|.C_d.C_p(T_{surf}^{t+1} - T_{air}^{t+1})$$
(172)

The implicit coupling between the surface and the atmosphere permits to have a robust and precise model that can be run over all time-step lengths and pixel areas. However, it engenders complicated atmospheric and surface resolutions for temperature. This resolution is presented in the current energy budget technical note (See Part II). The process of resolution relies on a vertical discretization of the atmosphere and the soil columns. Both discretizations permit to express the temperature at the layer i according to the temperature of the layer below (above for the soil) and to a bunch of coefficients expressed at layer i thanks to the coefficients of the layer above (below for the soil) and the temperature of the previous time-step. The main equation is expressed in Equation (173).

$$X_i = C_i + D_i X_{i-1} (173)$$

This process permits, in the case of the atmospheric column, to first calculate all the coefficients at each layers from the top of the column to the bottom thanks to the temperatures of the previous time step and the coefficients of the above layer. Then, in a second time, the surface temperature is calculated by the current energy budget *enerbil*. Once this surface temperature is known, the calculations of the atmospheric temperature are made from the bottom (the surface) to the top of the atmosphere. This process permits to link the surface and the atmosphere implicitly. The same process is made for humidity. For temperature in the soil, the process is inverted, there is a Top-Down calculation of the temperature which permits to access to a Bottom-Up calculation of the coefficients. The process is summarized on Figure 13.





Figure 13: Implicit resolution scheme of the current energy budget and soil and atmosphere columns

This implicit scheme has to be present in the multi-layer energy budget. This part of the note is dedicated to the derivation of Equations (151), (152) and (153) following the implicit coupling.

Rapidly, the resolution scheme will be a continuity of the one of the atmosphere. A bunch of coefficients will be calculated at each time-step from the top of the canopy to the surface. Once the coefficients will be determined, the model will solve the temperatures thanks to a Bottom-Up calculation. The process can be summarized as in Figure 14.





Figure 14: Implicit resolution scheme of the multi-layer energy budget and soil and atmosphere columns

III.3.2 Implicit form of the main equations

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As a reminder, considering the three main equations of the model with the radiations scheme presented in Section III.2.3, Equations (151), (152) and (153) become respectively Equations (174), (175) and (176).

$$C_{p,i}^{leaf}.\rho_{v}.\frac{T_{leaf,i}}{dt} = (\eta_{1,i}.T_{leaf,i} + \eta_{2,i} + \eta_{3,i}.R_{SW}^{down} - C_{p}^{air}.\rho_{a}.\frac{T_{leaf,i} - T_{a,i}}{R_{i}} - \lambda.\rho_{a}\frac{q_{leaf,i} - q_{a,i}}{R_{i}'}).\frac{1}{\Delta h_{i}}$$
(174)

$$\frac{dT_{a,i}}{dt} \cdot \Delta V_i = -\frac{\partial^2 k_i^* \cdot T_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{T_{leaf,i} - T_{a,i}}{R_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(175)

$$\frac{dq_{a,i}}{dt} \cdot \Delta V_i = \frac{\partial^2 k_i^* \cdot q_{a,i}}{\partial z^2} \cdot \Delta V_i + \frac{(\alpha_i \cdot T_{leaf,i} + \beta_i) - q_{a,i}}{R'_i} \cdot \frac{1}{\Delta h_i} \cdot \Delta V_i$$
(176)

Now, considering the implicit resolution of this system, the 3 previous equations can be discretized as in Equations (177), (178) and (179).

Technical note



$$T_{leaf,i}^{t+1} - T_{leaf,i}^{t} = -\frac{\lambda . \rho_{a}.\Delta t.\beta_{i}}{\rho_{v}.\Delta h_{i}.R_{i}^{\prime}.C_{p,i}^{leaf}} + \frac{\eta_{3}.R_{SW}^{down}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} + T_{leaf,i}^{t+1}.(-C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} - \lambda .\rho_{a}.\frac{\Delta t.\alpha_{i}}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}^{\prime}} + \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}}) + T_{a,i}^{t+1}.C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + q_{a,i}^{t+1}.\lambda .\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}^{\prime}}$$

$$(177)$$

$$\frac{T_{a,i}^{t+1} - T_{a,i}^{t}}{\Delta t} = k_i^* \cdot \frac{T_{a,i+1}^{t+1} - T_{a,i}^{t+1}}{\Delta z_i \cdot \Delta h_i} - k_{i-1}^* \cdot \frac{T_{a,i}^{t+1} - T_{a,i-1}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_i} + \frac{1}{\Delta h_i} \cdot \frac{T_{leaf,i}^{t+1} - T_{a,i}^{t+1}}{R_i}$$
(178)

$$\frac{q_{a,i}^{t+1} - q_{a,i}^{t}}{\Delta t} = k_i^* \cdot \frac{q_{a,i+1}^{t+1} - q_{a,i}^{t+1}}{\Delta z_i \cdot \Delta h_i} - k_{i-1}^* \cdot \frac{q_{a,i}^{t+1} - q_{a,i-1}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_i} + \frac{1}{\Delta h_i} \cdot \frac{\alpha_i \cdot T_{leaf,i}^{t+1} + \beta_i - q_{a,i}^{t+1}}{R_i'}$$
(179)

The implicit system of equation is now properly posed, the next step is the resolution of the system.

III.3.3 Resolution of the equations

The following section will be full of equations taken from the Appendix of *Ryder et al. (2006)* [21]. The first sub-section will be dedicated to a quick explanation of the principle of the resolution, the second sub-section will focus on the equations.

III.3.3.1 Principle of the resolution

The way to solve this implicit system relies on a *proof by induction*. The principle of such a proof is to assume a particular form of solution and prove that this solution can be applies to all the layers. If it is the case, the form of the solution will be the solution of the system.

In the case of the multi-layer, two quantities have to be determined in each layer: the temperature and humidity of the atmosphere at the layer i ($T_{a,i}$ and $q_{a,i}$). As precised on Figure 14, the form of the solution that needs to be found should link the temperature and humidity at layer i with the temperature and humidity of the layer below, in order to permit the Bottom-Up resolution of the system. Consequently, the particular form of the solution assumed are the following:

$$T_{a,i}^{t+1} = A_{T,i} \cdot T_{a,i-1}^{t+1} + B_{T,i} + C_{T,i} \cdot T_{leaf,i}^{t+1} + D_{T,i} \cdot q_{a,i-1}^{t+1}$$
(180)

$$q_{a,i}^{t+1} = A_{q,i} \cdot q_{a,i-1}^{t+1} + B_{q,i} + C_{q,i} \cdot T_{leaf,i}^{t+1} + D_{q,i} \cdot T_{a,i-1}^{t+1}$$
(181)

This particular form of solution permits to rely the state variables to their values at the layer below and the leaf temperature of the layer. The coefficients $A_{T,i}$, $A_{q,i}$, $B_{T,i}$, $B_{q,i}$, $C_{T,i}$, $C_{q,i}$, $D_{T,i}$ and $D_{q,i}$ will have to be determined.

Now that this solution is assumed, the next step is to prove that for each layer, the temperature and humidity of the atmosphere can be expressed as in Equations (180) and (181). To do so, a



proof by recurrence is started. By assuming the form of the equation at layer i+1, we will try to find the same type of solution for the layer *i*. If the same form of equation is found, this proves that the solution can be applied to all the layers.

The objective of the resolution of the system is to determine the formulas of the coefficients. Once those formulas determined, the state variable values in each layers are known simply thanks to Equations (180) and (181). The following part is dedicated to the determination of the coefficients.

III.3.3.2 Resolving the system

Let's start by assuming that $T_{a,i+1}^{t+1}$ and $q_{a,i+1}^{t+1}$ can be expressed as in Equations (180) and (181):

$$T_{a,i+1}^{t+1} = A_{T,i+1} \cdot T_{a,i}^{t+1} + B_{T,i+1} + C_{T,i+1} \cdot T_{leaf,i+1}^{t+1} + D_{T,i+1} \cdot q_{a,i}^{t+1}$$
(182)

$$q_{a,i+1}^{t+1} = A_{q,i+1} \cdot q_{a,i}^{t+1} + B_{q,i+1} + C_{q,i+1} \cdot T_{leaf,i+1}^{t+1} + D_{q,i+1} \cdot T_{a,i}^{t+1}$$
(183)

Leaf energy balance:

The first step is to substitute Equations (180) and (181) in Equation (177):

$$T_{leaf,i}^{t+1} - T_{leaf,i}^{t} = -\frac{\lambda . \rho_{a}.\Delta t.\beta_{i}}{\rho_{v}.\Delta h_{i}.R_{i}'.C_{p,i}^{leaf}} + \frac{\eta_{3}.R_{SW}^{down}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} + T_{leaf,i}^{t+1}.(-C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} - \lambda . \rho_{a}.\frac{\Delta t.\alpha_{i}}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'} + \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}}) + (A_{T,i}.T_{a,i-1}^{t+1} + B_{T,i} + C_{T,i}.T_{leaf,i}^{t+1} + D_{T,i}.q_{a,i-1}^{t+1}).C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + (A_{q,i}.q_{a,i-1}^{t+1} + B_{q,i} + C_{q,i}.T_{leaf,i}^{t+1} + D_{q,i}.T_{a,i-1}^{t+1}).\lambda . \rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}}$$

$$(184)$$

By rearranging the terms in order to have the unknown variables on the left hand side of the equation and the known ones (all variables at time-step t and layer i-1) on the right hand side, one can arrive to the following equation:


$$T_{leaf,i}^{t+1} \cdot \left(1 - \frac{C_{T,i} \cdot C_{p}^{air} \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}} + \frac{C_{p}^{air} \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}} + \frac{\lambda \cdot \rho_{a} \cdot \Delta t \cdot \alpha_{i}}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}'} - \frac{\eta_{1} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf}} - \frac{C_{q,i} \cdot \lambda \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}'}\right)$$

$$= T_{leaf,i}^{t} + q_{a,i-1}^{t+1} \cdot \left(\frac{A_{q,i} \cdot \lambda \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}'} + \frac{D_{T,i} \cdot C_{p}^{air} \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}'}\right)$$

$$+ T_{a,i-1}^{t+1} \cdot \left(\frac{A_{T,i} \cdot C_{p}^{air} \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}} + \frac{D_{q,i} \cdot \lambda \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}'}\right) + \frac{\eta_{2} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf}}$$

$$+ \frac{\eta_{3} \cdot R_{SW}^{down} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}} + \frac{B_{T,i} \cdot C_{p}^{air} \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}} + \frac{B_{q,i} \cdot \lambda \cdot \rho_{a} \cdot \Delta t}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf}} \cdot R_{i}} - \frac{\lambda \cdot \rho_{a} \cdot \Delta t \cdot \beta_{i}}{\rho_{v} \cdot \Delta h_{i} \cdot C_{p,i}^{leaf} \cdot R_{i}}\right)$$

$$(185)$$

Consequently, from Equation (177), we can find out that $T_{leaf,i}^{t+1}$ can be expressed as in Equation (186).

$$T_{leaf,i}^{t+1} = E_i \cdot q_{a,i-1}^{t+1} + F_i \cdot T_{a,i-1}^{t+1} + G_i$$
(186)

With:

$$E_{i} = \frac{\frac{A_{q,i}.\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'} + \frac{D_{T,i}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}}}{1 - \frac{C_{T,i}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{\lambda.\rho_{a}.\Delta t.\alpha_{i}}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'} - \frac{\eta_{i}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}} - \frac{C_{q,i}.\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'}}$$
(187)

$$F_{i} = \frac{\frac{A_{T,i}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{D_{q,i}.\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}}}{1 - \frac{C_{T,i}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{\lambda.\rho_{a}.\Delta t.\alpha_{i}}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} - \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} - \frac{1}{\rho_{v}.\Delta h_{i}.C_{p,i}^{leaf}.R_{i}}$$
(188)

$$G_{i} = \frac{T_{leaf,i}^{t} + \frac{\eta_{2}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}} + \frac{\eta_{3}.R_{SW}^{down}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}} + \frac{B_{T,i}.C_{p}^{air}.\rho_{a}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{B_{q,i}\lambda.\rho_{a}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} - \frac{\lambda.\rho_{a}\Delta t.\beta_{i}}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}}}{1 - \frac{C_{T,i}.C_{p}^{air}.\rho_{a}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{C_{p}^{air}.\rho_{a}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}} + \frac{\lambda.\rho_{a}\Delta t.\alpha_{i}}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'} - \frac{\eta_{1}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}} - \frac{C_{q,i}\lambda.\rho_{a}\Delta t}{\rho_{v}\Delta h_{i}.C_{p,i}^{leaf}.R_{i}'}}$$
(189)

This equation permits to directly link the leaf temperature of the layer i at the time-step t+1 with the atmospheric temperature and humidity at the same time-step but at the layer below.

Latent and sensible heat flux transports:

The goal of the resolution is to find an expression of $T_{a,i}^{t+1}$ and $q_{a,i}^{t+1}$ in the same way as in Equations (180) and (181). Looking at the sensible and latent heat flux transports equations (178) and (179), the objective will be to eliminate the terms $T_{a,i+1}^{t+1}$ and $q_{a,i+1}^{t+1}$ from the equations



(it is not a part of the known variables). Consequently, $T_{a,i+1}^{t+1}$ and $q_{a,i+1}^{t+1}$ are substituted by their expressions (182) and (183).

For the sensible heat flux:

$$\frac{T_{a,i}^{t+1} - T_{a,i}^{t}}{\Delta t} = k_{i}^{*} \cdot \frac{A_{T,i+1} \cdot T_{a,i}^{t+1} + B_{T,i+1} + C_{T,i+1} \cdot T_{leaf,i+1}^{t+1} + D_{T,i+1} \cdot q_{a,i}^{t+1}}{\Delta z_{i} \cdot \Delta h_{i}} - \frac{k_{i}^{*} \cdot T_{a,i}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_{i}} - \frac{k_{i-1}^{*} \cdot T_{a,i}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_{i}} + \frac{k_{i-1}^{*} \cdot T_{a,i-1}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_{i}} + \frac{T_{leaf,i}^{t+1}}{\Delta h_{i} \cdot R_{i}} - \frac{T_{a,i}^{t+1}}{\Delta h_{i} \cdot R_{i}} \tag{190}$$

$$T_{a,i}^{t+1} \cdot (1 - \Delta t \cdot (A_{T,i+1} \cdot \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_{i-1}^*}{\Delta z_{i-1} \cdot \Delta h_i} - \frac{1}{R_i \cdot \Delta h_i}))$$

$$= T_{a,i}^t + \frac{\Delta t \cdot k_i^* \cdot B_{T,i+1}}{\Delta z_i \cdot \Delta h_i} + T_{a,i-1}^{t+1} \cdot \frac{\Delta t \cdot k_{i-1}^*}{\Delta z_{i-1} \cdot \Delta h_i} + q_{a,i}^{t+1} \frac{\Delta t \cdot k_i^* \cdot D_{T,i+1}}{\Delta z_i \cdot \Delta h_i}$$

$$+ T_{leaf,i}^{t+1} \cdot \frac{\Delta t}{\Delta h_i \cdot R_i} + T_{leaf,i+1}^{t+1} \cdot \frac{\Delta t \cdot k_i^* \cdot C_{T,i+1}}{\Delta z_i \cdot \Delta h_i}$$
(191)

For the latent heat flux:

$$\frac{q_{a,i}^{t+1} - q_{a,i}^{t}}{\Delta t} = k_{i}^{*} \cdot \frac{A_{q,i+1} \cdot q_{a,i}^{t+1} + B_{q,i+1} + C_{q,i+1} \cdot T_{leaf,i+1}^{t+1} + D_{q,i+1} \cdot T_{a,i}^{t+1}}{\Delta z_{i} \cdot \Delta h_{i}} - \frac{k_{i}^{*} \cdot q_{a,i}^{t+1}}{\Delta z_{i} \cdot \Delta h_{i}} - \frac{k_{i-1}^{*} \cdot q_{a,i}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_{i}} + \frac{k_{i-1}^{*} \cdot q_{a,i-1}^{t+1}}{\Delta z_{i-1} \cdot \Delta h_{i}} + \frac{\alpha_{i} \cdot T_{leaf,i}^{t+1} + \beta_{i} - q_{a,i}^{t+1}}{\Delta h_{i} R'i} \qquad (192)$$

$$q_{a,i}^{t+1} \cdot (1 - \Delta t \cdot (A_{q,i+1} \cdot \frac{k_{i}^{*}}{\Delta z_{i} \cdot \Delta h_{i}} - \frac{k_{i}^{*}}{\Delta z_{i} \cdot \Delta h_{i}} - \frac{k_{i-1}^{*}}{\Delta z_{i-1} \cdot \Delta h_{i}} - \frac{1}{R_{i}' \cdot \Delta h_{i}}))$$

$$= q_{a,i}^{t} + \frac{\Delta t \cdot k_{i}^{*} \cdot B_{q,i+1}}{\Delta z_{i} \cdot \Delta h_{i}} + \frac{\beta_{i} \cdot \Delta t}{\Delta h_{i} \cdot R_{i}'} + q_{a,i-1}^{t+1} \cdot \frac{\Delta t \cdot k_{i-1}^{*}}{\Delta z_{i-1} \cdot \Delta h_{i}} + T_{a,i}^{t+1} \frac{\Delta t \cdot k_{i}^{*} \cdot D_{q,i+1}}{\Delta z_{i} \cdot \Delta h_{i}} \qquad (193)$$

$$+ T_{leaf,i}^{t+1} \cdot \frac{\alpha_{i} \cdot \Delta t}{\Delta h_{i} \cdot R_{i}'} + T_{leaf,i+1}^{t+1} \cdot \frac{\Delta t \cdot k_{i}^{*} \cdot C_{q,i+1}}{\Delta z_{i} \cdot \Delta h_{i}}$$

Because the objective is to express the temperatures and humidities thanks to the lower layer, the leaf temperature of the layer above $T_{leaf,i+1}^{t+1}$ is substituted by its expression in Equation (186). This leads to the following equations:

$$T_{a,i}^{t+1} \cdot (1 - \Delta t \cdot (A_{T,i+1} \cdot \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_{i-1}^*}{\Delta z_{i-1} \cdot \Delta h_i} - \frac{1}{R_i \cdot \Delta h_i}))$$

$$= T_{a,i}^t + \frac{\Delta t \cdot k_i^* \cdot B_{T,i+1}}{\Delta z_i \cdot \Delta h_i} + T_{a,i-1}^{t+1} \cdot \frac{\Delta t \cdot k_{i-1}^*}{\Delta z_{i-1} \cdot \Delta h_i} + q_{a,i}^{t+1} \frac{\Delta t \cdot k_i^* \cdot D_{T,i+1}}{\Delta z_i \cdot \Delta h_i}$$

$$+ T_{leaf,i}^{t+1} \cdot \frac{\Delta t}{\Delta h_i \cdot R_i} + (E_{i+1} \cdot q_{a,i}^{t+1} + F_{i+1} \cdot T_{a,i}^{t+1} + G_{i+1}) \cdot \frac{\Delta t \cdot k_i^* \cdot C_{T,i+1}}{\Delta z_i \cdot \Delta h_i}$$
(194)

$$q_{a,i}^{t+1} \cdot (1 - \Delta t.(A_{q,i+1}, \frac{k_i^*}{\Delta z_i.\Delta h_i} - \frac{k_i^*}{\Delta z_i.\Delta h_i} - \frac{k_{i-1}^*}{\Delta z_{i-1}.\Delta h_i} - \frac{1}{R_i'.\Delta h_i}))$$

$$= q_{a,i}^t + \frac{\Delta t.k_i^*.B_{q,i+1}}{\Delta z_i.\Delta h_i} + \frac{\beta_i.\Delta t}{\Delta h_i.R_i'} + q_{a,i-1}^{t+1} \cdot \frac{\Delta t.k_{i-1}^*}{\Delta z_{i-1}.\Delta h_i} + T_{a,i}^{t+1} \frac{\Delta t.k_i^*.D_{q,i+1}}{\Delta z_i.\Delta h_i}$$

$$+ T_{leaf,i}^{t+1} \cdot \frac{\alpha_i.\Delta t}{\Delta h_i.R_i'} + (E_{i+1}.q_{a,i}^{t+1} + F_{i+1}.T_{a,i}^{t+1} + G_{i+1}) \cdot \frac{\Delta t.k_i^*.C_{q,i+1}}{\Delta z_i.\Delta h_i}$$
(195)

Technical note



Those equations can be abbreviated as follows:

$$T_{a,i}^{t+1} \cdot X_{1,i} = X_{2,i} + X_{3,i} \cdot T_{a,i-1}^{t+1} + X_{4,i} \cdot q_{a,i}^{t+1} + X_{5,i} \cdot T_{leaf,i}^{t+1}$$
(196)

$$q_{a,i}^{t+1} \cdot Y_{1,i} = Y_{2,i} + Y_{3,i} \cdot q_{a,i-1}^{t+1} + Y_{4,i} \cdot T_{a,i}^{t+1} + Y_{5,i} \cdot T_{leaf,i}^{t+1}$$
(197)

With the following expressions for the coefficients:

$$X_{1,i} = 1 - \Delta t. (A_{T,i+1} \cdot \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_i^*}{\Delta z_i \cdot \Delta h_i} - \frac{k_{i-1}^*}{\Delta z_{i-1} \cdot \Delta h_i} - \frac{1}{R_i \cdot \Delta h_i}) - F_{i+1} \cdot \frac{\Delta t. k_i^* \cdot C_{T,i+1}}{\Delta z_i \cdot \Delta h_i}$$
(198)

$$X_{2,i} = T_{a,i}^{t} + \frac{\Delta t.k_{i}^{*}.B_{T,i+1}}{\Delta z_{i}.\Delta h_{i}} + G_{i+1}.\frac{\Delta t.k_{i}^{*}.C_{T,i+1}}{\Delta z_{i}.\Delta h_{i}}$$
(199)

$$X_{3,i} = \frac{\Delta t.k_{i-1}^*}{\Delta z_{i-1}.\Delta h_i} \tag{200}$$

$$X_{4,i} = \frac{\Delta t.k_i^*.D_{T,i+1}}{\Delta z_i.\Delta h_i} + E_{i+1}.\frac{\Delta t.k_i^*.C_{T,i+1}}{\Delta z_i.\Delta h_i}$$
(201)

$$X_{5,i} = \frac{\Delta t}{\Delta h_i \cdot R_i} \tag{202}$$

$$Y_{1,i} = 1 - \Delta t.(A_{q,i+1}.\frac{k_i^*}{\Delta z_i.\Delta h_i} - \frac{k_i^*}{\Delta z_i.\Delta h_i} - \frac{k_{i-1}^*}{\Delta z_{i-1}.\Delta h_i} - \frac{1}{R_i.\Delta h_i}) - E_{i+1}.\frac{\Delta t.k_i^*.C_{q,i+1}}{\Delta z_i.\Delta h_i}$$
(203)

$$Y_{2,i} = q_{a,i}^t + \frac{\Delta t.k_i^*.B_{q,i+1}}{\Delta z_i.\Delta h_i} + \frac{\beta_i.\Delta t}{\Delta h_i.R_i'} + G_{i+1}.\frac{\Delta t.k_i^*.C_{q,i+1}}{\Delta z_i.\Delta h_i}$$
(204)

$$Y_{3,i} = \frac{\Delta t.k_{i-1}^*}{\Delta z_{i-1}.\Delta h_i}$$
(205)

$$Y_{4,i} = \frac{\Delta t.k_i^*.D_{q,i+1}}{\Delta z_i.\Delta h_i} + F_{i+1}.\frac{\Delta t.k_i^*.C_{q,i+1}}{\Delta z_i.\Delta h_i}$$
(206)

$$Y_{5,i} = \frac{\alpha_i \cdot \Delta t}{\Delta h_i \cdot R'_i} \tag{207}$$

By injecting Equation (197) into Equation (196) in order to replace $q_{air,i}^{t+1}$ by its expression, the expression becomes:

$$T_{a,i}^{t+1} \cdot X_{1,i} = X_{2,i} + X_{3,i} \cdot T_{a,i-1}^{t+1} + X_{4,i} \cdot (\frac{Y_{2,i}}{Y_{1,i}} + \frac{Y_{3,i}}{Y_{1,i}} \cdot q_{a,i-1}^{t+1} + \frac{Y_{4,i}}{Y_{1,i}} \cdot T_{a,i}^{t+1} + \frac{Y_{5,i}}{Y_{1,i}} \cdot T_{leaf,i}^{t+1}) + X_{5,i} \cdot T_{leaf,i}^{t+1}$$

$$(208)$$

Which leads to:

$$T_{a,i}^{t+1} \cdot (X_{1,i} - X_{4,i} \cdot \frac{Y_{4,i}}{Y_{1,i}}) = X_{3,i} \cdot T_{a,i-1}^{t+1} + (X_{2,i} + X_{4,i} \cdot \frac{Y_{2,i}}{Y_{1,i}}) + T_{leaf,i}^{t+1} \cdot (X_{5,i} + X_{4,i} \cdot \frac{Y_{5,i}}{Y_{1,i}}) + q_{a,i-1}^{t+1} \cdot X_{4,i} \cdot \frac{Y_{5,i}}{Y_{1,i}}$$
(209)

Technical note

74



By doing the same process in order to replace $T_{a,i}^{t+1}$ in Equation (196) by its expression in Equation (197), the expression becomes:

$$q_{a,i}^{t+1} \cdot Y_{1,i} = Y_{2,i} + Y_{3,i} \cdot q_{a,i-1}^{t+1} + Y_{4,i} \cdot (\frac{X_{2,i}}{X_{1,i}} + \frac{X_{3,i}}{X_{1,i}} \cdot T_{a,i-1}^{t+1} + \frac{X_{4,i}}{X_{1,i}} \cdot q_{a,i}^{t+1} + \frac{X_{5,i}}{X_{1,i}} \cdot T_{leaf,i}^{t+1}) + Y_{5,i} \cdot T_{leaf,i}^{t+1}$$
(210)

Which leads to:

$$q_{a,i}^{t+1} \cdot (Y_{1,i} - Y_{4,i} \cdot \frac{X_{4,i}}{X_{1,i}}) = q_{a,i-1}^{t+1} \cdot Y_{3,i} + (Y_{2,i} - Y_{4,i} \cdot \frac{X_{2,i}}{X_{1,i}}) + T_{leaf,i}^{t+1} \cdot (Y_{5,i} + Y_{4,i} \cdot \frac{X_{5,i}}{X_{1,i}}) + T_{a,i-1}^{t+1} \cdot Y_{4,i} \cdot \frac{X_{3,i}}{X_{1,i}}$$
(211)

Consequently, $T_{a,i}^{t+1}$ and $q_{a,i}^{t+1}$ can be expressed as follows in Equations (180) and (181). The coefficients can be expressed as:

$$A_{T,i} = \frac{X_{3,i}}{X_{1,i} - X_{4,i} \cdot \frac{Y_{4,i}}{Y_{1,i}}}$$
(212)

$$B_{T,i} = \frac{X_{2,i} + X_{4,i} \cdot \frac{Y_{2,i}}{Y_{1,i}}}{X_{1,i} - X_{4,i} \cdot \frac{Y_{4,i}}{Y_{1,i}}}$$
(213)

$$C_{T,i} = \frac{X_{5,i} - X_{4,i} \cdot \frac{Y_{5,i}}{Y_{1,i}}}{X_{1,i} - X_{4,i} \cdot \frac{Y_{4,i}}{Y_{1,i}}}$$
(214)

$$D_{T,i} = \frac{X_{4,i}}{X_{1,i} - X_{4,i} \cdot \frac{Y_{4,i}}{Y_{1,i}}}$$
(215)

And,

$$A_{q,i} = \frac{Y_{3,i}}{Y_{1,i} - Y_{4,i} \cdot \frac{X_{4,i}}{X_{1,i}}}$$
(216)

$$B_{q,i} = \frac{Y_{2,i} + Y_{4,i} \cdot \frac{X_{2,i}}{X_{1,i}}}{Y_{1,i} - Y_{4,i} \cdot \frac{X_{4,i}}{X_{1,i}}}$$
(217)

$$C_{q,i} = \frac{Y_{5,i} - Y_{4,i} \cdot \frac{X_{5,i}}{X_{1,i}}}{Y_{1,i} - Y_{4,i} \cdot \frac{X_{4,i}}{X_{1,i}}}$$
(218)

$$D_{q,i} = \frac{Y_{4,i}}{Y_{1,i} - Y_{4,i} \cdot \frac{X_{4,i}}{X_{1,i}}}$$
(219)

Finally, this shows that, at each time-step, the temperatures at each layers can effectively be expressed thanks to the values of the temperatures at the previous time-step and in the previous layer. On the other side, the coefficients can all be expressed thanks to their values in the upper layers and thanks to the values of the state variables at the previous time step. At each level of the canopy, the program will calculate the coefficients E_i to G_i which will lead to the calculation of $X_{1,i}$ to $Y_{5,i}$ which will finally lead to the calculation of $A_{T,i}$ to $D_{q,i}$. Once the coefficients



are known in each layers, the temperatures are calculated thanks to equations (180) and (181). The Top-Down resolution of the coefficients and the Bottom-Up resolution of the state variables can, thus, be started at each time-step. The implicit coupling with the atmosphere is achievable. The last step of the resolution is to express the coefficients and state variables at the boundary layers: at the boundary layer with atmosphere, the upper boundary layer at i = n and at the boundary layer with the surface at i = 1.

The resolution of the column can be summarized as in the following Summary chart.

	$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	AtmosphereStand alone : $B_{T,input}$ Top layer (i=n)		1. Top layer (i=n)		Top-Down resolution of the coefficients
Layer i-1 Idem as above	$ \begin{array}{llllllllllllllllllllllllllllllllllll$	Layer i Known variables: $T^t_{leaf,i}$ $q^t_{a,i}$ $\underline{Step 1}$: $\underline{Step 2}$: $\underline{Step 3}$:	Known variables: $A_{T,i+1} B_{T,i+1} C_{T,i+1} D_{T,i+1}$ $A_{q,i+1} B_{q,i+1} C_{q,i+1} D_{q,i+1}$ Layer i+1 $E_{i+1} F_{i+1} G_{i+1}$	2. Intermediate layer i (from n-1 to 2)	Intermediate Soil Infinitesimal surface	Atmosphere Top lay
Soil	$\begin{array}{llllllllllllllllllllllllllllllllllll$	Layer 1 Known variables: $T^{t}_{leaf,j} q^{t}_{a,j} T^{t}_{a,j}$ <u>Step 1:</u> <u>Step 2:</u> <u>Step 3:</u>	Known variables: $A_{T,2} \ B_{T,2} \ C_{T,2} \ D_{T,2}$ $A_{q,2} \ B_{q,2} \ C_{q,2} \ D_{q,2}$ Layer 2 $E_2 \ F_2 \ G_2$	3. Bottom layer (i=1)	layer i er (i=1) e layer	<u>er (i=n)</u>

Bottom-Up resolution of the temperatures

5. Inifini	tesimal surfac	e layer	6. Bottom layer (i=1)	7. Intermediate layer i from 2 to n
Layer 1 Knowr $A_{7,1}$ B $A_{q,1}$ B	variables: $\Gamma_{T_1} C_{\Gamma_{T_1}} D_{\Gamma_{T_1}}$ $\Gamma_{q_1} C_{q_1} D_{q_1}$		See Step 7.	Layer i+1 Idem as below
R_{LW} R_{SW}		u u Surface	Layer 1 Known variables: $T^{t}_{a,1} q^{t}_{a,1} T^{t}_{leaf,1}$ $A_{\tau,1} B_{\tau,1} C_{\tau,1} D_{\tau,1} A_{q,1} B_{q,1} C_{q,1} D_{q,1} E_{1} F_{1} G_{1}$	Layer i Known variables: $T^{t}_{a,i} q^{t}_{a,i} T^{t}_{leaf,i}$ $A_{\tau,i} B_{\tau,i} C_{\tau,i} D_{\tau,i} A_{q,i} B_{q,i} C_{q,i} D_{q,i} E_{i} F_{i} G_{i}$
Soil	J _{soil}		Temperature and humidites: $T^{t+1}_{leof,1} = E_1 \cdot \Phi^{t+1}_{AE} + F_i \cdot \Phi^{t+1}_{H} + G_i$ (Eq.226)	Temperature and humidites:
With: $R_{LW}^{t+1} = \eta_{1,surf} T_{sur}^{t+1}$ $R_{SW}^{t+1} = \eta_{3,surf} R_{SW}$ $\Phi_{AE}^{t+1} = \xi_3 + \xi_4 . T_{AE}^{t+1}$	$f + \eta_{2,surf} \rightarrow \eta_{1,surf} \alpha$ $\downarrow \rightarrow \eta_{3,surf} knowr$ $surf \rightarrow \xi_3 and \xi_4 tc$	nd n _{2,surf} known 1 9 determine	$T^{t+1}_{a,1} = A_{T,1} \cdot \Phi^{t+1}_{H} + B_{T,1} + C_{T,1} \cdot T^{t+1}_{leaf,1} + D_{T,1} \cdot \Phi^{t+1}_{\lambda E} (Eq.223)$ $q^{t+1}_{a,1} = A_{q,1} \cdot \Phi^{t+1}_{\lambda E} + B_{q,1} + C_{q,1} \cdot T^{t+1}_{leaf,1} + D_{q,1} \cdot \Phi^{t+1}_{H} (Eq.224)$	$T^{t+1}_{a,i} = A_{T,i} \cdot T^{t+1}_{a,i-1} + B_{T,i} + C_{T,i} \cdot T^{t+1}_{leof,i} + D_{T,i} \cdot q^{t+1}_{a,i-1} $ (Eq.186)
$\Phi_{J_{oil}}^{t+1} = \xi_1 + \xi_2 . T_{s}^{t+1}$ $J_{soil} = input from th$	$x_f ightarrow \xi_1$ and ξ_2 to ermosoil	determine	O _H O _{λE} Surface	$q_{a,i}^{,i} = A_{q,i} \cdot q_{a,i-1}^{,i-1} + B_{q,i} + C_{q,i} \cdot T_{a,i-1}^{,i-1} + D_{q,i} \cdot T_{a,i-1}^{,i-1} $ (Eq.181)
$\frac{\text{Step 1}}{\Omega_1 \text{ to } \Omega_8} = 1$	<u>Step 2:</u>	<u>Step 3:</u>	Soil Known variables: $\Phi^{t+1}_{\lambda E}, \Phi^{t+1}_{H}$	Layer i-1 Known variables: $T^{t+1} = C^{t+1} = T^{t+1}$
$ \begin{array}{c} f(A_{T,1},B_{T,1},C_{T,1} \\ D_{T,1},A_{q,1},B_{q,1},C_{q,1} \\ ,D_{q,1},E_{1},F_{1},G_{1} \end{array} $	$\boldsymbol{\xi}_1$ to $\boldsymbol{\xi}_4$ = f(Ω_1 to Ω_8)	$\mathbf{T}^{t+1}_{surf} = f(R_{LW}^{t+1}, R_{SW}^{t+1}, \Phi_{SW}^{t+1}, \Phi_{SW}$		1 a,i-1 4 a,i-1 1 leaf,i-1
(Eq. 256 to 263)	(Eq. 270 to 273)	J^{t+1} soil, T^{t} surf)		
		(Eq. 275)		



III.3.4 Boundary conditions

Because the coefficients are expressed thanks to their values at the upper layer and the temperatures and humidity thanks to theirs values at the lower layer, the boundary conditions are restricted to knowing the coefficients at the top of the canopy column (at i = n) and calculating the surface temperature and humidity (at i = 1).

III.3.4.1 Upper boundary condition

The upper boundary condition consists in knowing the value of the coefficients for i = n. As explained before, ORCHIDEE (and, thus, the multi-layer energy budget) can be run alone or coupled with the atmosphere model LMDZ.

When running alone, no implicit coupling is needed so the coefficients at the top of the canopy are restricted to the input temperature and specific humidity of the atmosphere given by the input variables. Consequently, all coefficients are set to zero except $B_{T,n}$ and $B_{q,n}$ that are inputs.

When running coupled with the atmosphere, the atmospheric column inside the canopy can be seen as a continuity of the atmospheric column of LMDZ. Consequently, the atmospheric coefficients of LMDZ are injected directly at the top of the canopy column.

All the values of the coefficients are summarized in Table 1.

Stand-alone model	Coupled model
$A_{T,n}=0$	$A_{T,n} = A_{T,atm}$
$B_{T,n} = B_{T,input}$	$B_{T,n} = B_{T,atm}$
$C_{T,n}=0$	$C_{T,n}=0$
$D_{T,n}=0$	$D_{T,n}=0$
$A_{q,n}=0$	$A_{q,n} = A_{q,atm}$
$B_{q,n} = B_{q,input}$	$B_{q,n} = B_{q,atm}$
$C_{q,n}=0$	$C_{q,n}=0$
$D_{q,n}=0$	$D_{q,n}=0$

Table 1: Values of the coefficients at the top of the canopy when the model is run alone are
coupled with LMDZ

III.3.4.2 Lower boundary condition

The lower boundary layer consists in determining the surface temperature T_{surf} . To do so, the lowest level transport equation has to be solved separately. At i = 1, Equations (177), (178) and (179) become

$$T_{leaf,1}^{t+1} - T_{leaf,1}^{t} = -\frac{\lambda . \rho_{a}.\Delta t.\beta_{1}}{\rho_{v}.\Delta h_{1}.R_{1}'.C_{p,1}^{leaf}} + \frac{\eta_{3}.R_{SW}^{down}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + T_{leaf,1}^{t+1}.(-C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \lambda . \rho_{a}.\frac{\Delta t.\alpha_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} + \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}}) + T_{a,1}^{t+1}.C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + q_{a,1}^{t+1}.\lambda . \rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'}$$

$$(220)$$



$$\frac{T_{a,1}^{t+1} - T_{a,1}^{t}}{\Delta t} = k_1^* \cdot \frac{T_{a,2}^{t+1} - T_{a,1}^{t+1}}{\Delta z_1 \cdot \Delta h_1} - \frac{1}{C_p^{air} \cdot \rho_a} \cdot \frac{\Phi_H^{t+1}}{\Delta h_1} + \frac{1}{\Delta h_1} \cdot \frac{T_{leaf,1}^{t+1} - T_{a,1}^{t+1}}{R_1}$$
(221)

$$\frac{q_{a,1}^{t+1} - q_{a,1}^{t}}{\Delta t} = k_1^* \cdot \frac{q_{a,2}^{t+1} - q_{a,1}^{t+1}}{\Delta z_1 \cdot \Delta h_1} - \frac{1}{\lambda \cdot \rho_a} \cdot \frac{\Phi_{\lambda E}^{t+1}}{\Delta h_1} + \frac{1}{\Delta h_1} \cdot \frac{\alpha_1 \cdot T_{leaf,1}^{t+1} + \beta_1 - q_{a,1}^{t+1}}{R_1'}$$
(222)

As one can see, the transport of sensible and latent heat flux is a bit different between Equations (178)/(179) and (221)/(222). Because i = 1 is the last layer of the atmospheric column, there cannot be a transport of sensible and latent heat flux between the lower layer and layer 1. However, the soil can inject sensible heat and latent heat inside layer 1. This is modelled by imagining the soil as a layer of infinitesimal thickness from which the fluxes are cleared. It will also be at this surface that an energy budget will be solved in order to find out the surface temperature T_{surf} .

As for the other layers inside the column, the temperature and humidity at layer 1 will be assumed equal to a particular form as in Equations (223) and (224). Where the coefficients are determined with the same expression given in Section III.3.3.2 (because the temperature and humidity of the lower layer are not defined, they are replaced by the fluxes of sensible and latent heat flux.

$$T_{a,1}^{t+1} = A_{T,1} \cdot \Phi_H^{t+1} + B_{T,1} + C_{T,1} \cdot T_{leaf,1}^{t+1} + D_{T,1} \cdot \Phi_{\lambda E}^{t+1}$$
(223)

$$q_{a,1}^{t+1} = A_{q,1} \cdot \Phi_{\lambda E}^{t+1} + B_{q,1} + C_{q,1} \cdot T_{leaf,1}^{t+1} + D_{q,1} \cdot \Phi_H^{t+1}$$
(224)

From those assumptions, in a similar approach to the previous section, $T_{leaf,1}^{t+1}$ is tried to be reduced to : $T_{leaf,1}^{t+1} = E_1 \cdot \Phi_{\lambda E}^{t+1} + F_1 \cdot \Phi_H^{t+1} + G_1$. So, from Equation (220), by injecting Equations (223) and (224), the equation becomes:

$$T_{leaf,1}^{t+1} - T_{leaf,1}^{t} = -\frac{\lambda . \rho_{a}.\Delta t. \beta_{1}}{\rho_{v}.\Delta h_{1}.R_{1}'.C_{p,1}^{leaf}} + \frac{\eta_{3}.R_{SW}^{down}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + T_{leaf,1}^{t+1}.(-C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \lambda . \rho_{a}.\frac{\Delta t.\alpha_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} + \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}}) + (A_{T,1}.\Phi_{H}^{t+1} + B_{T,1} + C_{T,1}.T_{leaf,1}^{t+1} + D_{T,1}.\Phi_{\lambda E}^{t+1}).C_{p}^{air}.\rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + (A_{q,1}.\Phi_{\lambda E}^{t+1} + B_{q,1} + C_{q,1}.T_{leaf,1}^{t+1} + D_{q,1}.\Phi_{H}^{t+1}).\lambda . \rho_{a}.\frac{\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'}$$

$$(225)$$



$$T_{leaf,1}^{t+1} \cdot \left(1 + \frac{C_p^{air} \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1} + \frac{\lambda \cdot \rho_a \cdot \Delta t \cdot \alpha_1}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1'} - \frac{\eta_1 \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf}} - \frac{C_{T,1} \cdot C_p^{air} \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1} - \frac{C_{q,1} \lambda \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1'}\right)$$

$$= \Phi_{\lambda E}^{t+1} \cdot \left(\frac{D_{T,1} \cdot C_p^{air} \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1} + \frac{A_{q,1} \lambda \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1'}\right) + \Phi_H^{t+1} \cdot \left(\frac{A_{T,1} \cdot C_p^{air} \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1} + \frac{D_{q,1} \lambda \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1'}\right)$$

$$+ \left(T_{leaf,1}^t + \frac{\eta_3 \cdot R_{SW}^{down} \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf}} + \frac{\eta_2 \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf}}\right)$$

$$+ \frac{B_{T,1} \cdot C_p^{air} \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1} + \frac{B_{q,1} \lambda \cdot \rho_a \cdot \Delta t}{\rho_v \cdot \Delta h_1 \cdot C_{p,1}^{leaf} \cdot R_1'} - \frac{\lambda \cdot \rho_a \cdot \Delta t \cdot \beta_1}{\rho_v \cdot \Delta h_1 \cdot R_1' \cdot C_{p,1}^{leaf}}\right)$$

$$(226)$$

So,

$$E_{1} = \frac{\frac{D_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + \frac{A_{q,1}\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'}}{1 + \frac{C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} - \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \frac{C_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} - \frac{\chi_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \frac{C_{T,1}.C_{p}^{leaf}.R_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{\chi_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \frac{\chi_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{\chi_{1}.\Delta t}{\rho_{v}.\Delta t} - \frac{\chi_{1}.\Delta t}{\varphi_{1}.\Delta t} -$$

$$F_{1} = \frac{\frac{A_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + \frac{D_{q,1}\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}}}{1 + \frac{C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + \frac{\lambda.\rho_{a}.\Delta t.\alpha_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \frac{C_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda.\rho_{a}.\lambda}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{Q_{T,1}^{a}.\lambda}{\rho_{$$

$$G_{1} = \frac{T_{leaf,1}^{t} + \frac{\eta_{3}.R_{SW}^{down}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + \frac{\eta_{2}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} + \frac{B_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + \frac{B_{q,1}\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{\lambda.\rho_{a}.\Delta t.\beta_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}}}{1 + \frac{C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} + \frac{\lambda.\rho_{a}.\Delta t.\alpha_{1}}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} - \frac{\eta_{1}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}} - \frac{C_{T,1}.C_{p}^{air}.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}} - \frac{C_{q,1}\lambda.\rho_{a}.\Delta t}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'} - \frac{(229)}{\rho_{v}.\Delta h_{1}.C_{p,1}^{leaf}.R_{1}'}$$

Now that this simplification is made, let's come back to Equations (221) and (222) where $T_{leaf,2}^{t+1}$, $T_{a,2}^{t+1}$ and $q_{a,2}^{t+1}$ are substituted by their expressions (180), (181) and (186).

$$\frac{T_{a,1}^{t+1} - T_{a,1}^{t}}{\Delta t} = k_{1}^{*} \cdot \frac{A_{T,2} \cdot T_{a,1}^{t+1} + B_{T,2} + C_{T,2} \cdot (E_{2} \cdot q_{a,1}^{t+1} + F_{\cdot} T_{a,1}^{t+1} + G_{2}) + D_{T,2} \cdot q_{a,1}^{t+1} - T_{a,1}^{t+1}}{\Delta z_{1} \cdot \Delta h_{1}} - \frac{1}{C_{p}^{air} \cdot \rho_{a}} \cdot \frac{\Phi_{H}^{t+1}}{\Delta h_{1}} + \frac{1}{\Delta h_{1}} \cdot \frac{T_{leaf,1}^{t+1} - T_{a,1}^{t+1}}{R_{1}} \tag{230}$$

$$\frac{q_{a,1}^{t+1} - q_{a,1}^{t}}{\Delta t} = k_{1}^{*} \cdot \frac{A_{q,2} \cdot q_{a,1}^{t+1} + B_{q,2} + C_{q,2} \cdot (E_{2} \cdot q_{a,1}^{t+1} + F_{\cdot} T_{a,1}^{t+1} + G_{2}) + D_{q,2} \cdot T_{a,1}^{t+1} - q_{a,1}^{t+1}}{\Delta z_{1} \cdot \Delta h_{1}} - \frac{1}{\lambda \cdot \rho_{a}} \cdot \frac{\Phi_{\lambda E}^{t+1}}{\Delta h_{1}} + \frac{1}{\Delta h_{1}} \cdot \frac{\alpha_{1} \cdot T_{leaf,1}^{t+1} + \beta_{1} - q_{a,1}^{t+1}}{R_{1}'} \tag{231}$$

Technical note

81



Which leads to:

$$T_{a,1}^{t+1} \cdot \left(\frac{1}{\Delta t} - \frac{k_1^* \cdot A_{T,2}}{\Delta z_1 \cdot \Delta h_1} - \frac{k_1^* \cdot C_{T,2} \cdot F_2}{\Delta z_1 \cdot \Delta h_1} + \frac{k_1^*}{\Delta z_1 \cdot \Delta h_1} + \frac{1}{R_1 \cdot \Delta h_1}\right) = \frac{T_{a,1}^t}{\Delta t} + q_{a,1}^{t+1} \cdot \frac{k_1^* \cdot C_{T,2} \cdot E_2 + k_1^* \cdot D_{T,2}}{\Delta z_1 \cdot \Delta h_1} + T_{leaf,1}^{t+1} \cdot \frac{1}{R_1 \cdot \Delta h_1} + \frac{k_1^* \cdot C_{T,2} \cdot G_2 + k_1^* \cdot B_{T,2}}{\Delta z_1 \cdot \Delta h_1} - \frac{1}{C_p^{air} \cdot \rho_a} \cdot \frac{\Phi_H^{t+1}}{\Delta h_1}$$
(232)

$$q_{a,1}^{t+1} \cdot \left(\frac{1}{\Delta t} - \frac{k_1^* \cdot A_{q,2}}{\Delta z_1 \cdot \Delta h_1} - \frac{k_1^* \cdot C_{q,2} \cdot E_2}{\Delta z_1 \cdot \Delta h_1} + \frac{k_1^*}{\Delta z_1 \cdot \Delta h_1} + \frac{1}{R_1' \cdot \Delta h_1}\right) \\ = \frac{q_{a,1}^t}{\Delta t} + T_{a,1}^{t+1} \cdot \frac{k_1^* \cdot C_{q,2} \cdot F_2 + k_1^* \cdot D_{q,2}}{\Delta z_1 \cdot \Delta h_1} + T_{leaf,1}^{t+1} \cdot \frac{\alpha_1}{R_1' \cdot \Delta h_1} \\ + \frac{k_1^* \cdot C_{qT,2} \cdot G_2 + k_1^* \cdot B_{q,2}}{\Delta z_1 \cdot \Delta h_1} + \frac{\beta_1}{R_1' \cdot \Delta h_1} - \frac{1}{\lambda \cdot \rho_a} \cdot \frac{\Phi_{\lambda E}^{t+1}}{\Delta h_1}$$
(233)

This proves that $T_{a,1}^{t+1}$ and $q_{a,1}^{t+1}$ can be expressed as follows:

$$T_{a,1}^{t+1}.X_1 = X_2 + \Phi_H^{t+1}.X_3 + q_{a,1}^{t+1}.X_4 + T_{leaf,1}^{t+1}.X_5$$
(234)

$$q_{a,1}^{t+1}.Y_1 = Y_2 + \Phi_{\lambda E}^{t+1}.Y_3 + T_{a,1}^{t+1}.Y_4 + T_{leaf,1}^{t+1}.Y_5$$
(235)

With,

$$X_1 = 1 - \Delta t. \left(\frac{k_1^* \cdot A_{T,2}}{\Delta z_1 \cdot \Delta h_1} - \frac{k_1^* \cdot C_{T,2} \cdot F_2}{\Delta z_1 \cdot \Delta h_1} + \frac{k_1^*}{\Delta z_1 \cdot \Delta h_1} + \frac{1}{R_1 \cdot \Delta h_1}\right)$$
(236)

$$X_2 = T_{a,1}^t + \Delta t. \frac{k_1^* \cdot C_{qT,2} \cdot G_2 + k_1^* \cdot B_{q,2}}{\Delta z_1 \cdot \Delta h_1}$$
(237)

$$X_3 = -\frac{\Delta t}{C_p^{air}.\rho_a.\Delta h_1} \tag{238}$$

$$X_4 = \Delta t. \frac{k_1^* \cdot C_{T,2} \cdot E_2 + k_1^* \cdot D_{T,2}}{\Delta z_1 \cdot \Delta h_1}$$
(239)

$$X_5 = \frac{\Delta t}{R_1 \cdot \Delta h_1} \tag{240}$$

$$Y_1 = 1 - \Delta t. \left(\frac{k_1^* \cdot A_{q,2}}{\Delta z_1 \cdot \Delta h_1} - \frac{k_1^* \cdot C_{q,2} \cdot E_2}{\Delta z_1 \cdot \Delta h_1} + \frac{k_1^*}{\Delta z_1 \cdot \Delta h_1} + \frac{1}{R_1' \cdot \Delta h_1}\right)$$
(241)

$$Y_2 = q_{a,1}^t + \Delta t. \left(\frac{k_1^* \cdot C_{q,2} \cdot G_2 + k_1^* \cdot B_{q,2}}{\Delta z_1 \cdot \Delta h_1} + \frac{\beta_1}{R_1' \cdot \Delta h_1}\right)$$
(242)

$$Y_3 = -\frac{\Delta t}{\lambda . \rho_a . \Delta h_1} \tag{243}$$

$$Y_4 = \Delta t. \frac{k_1^* . C_{q,2} . F_2 + k_1^* . D_{q,2}}{\Delta z_1 . \Delta h_1}$$
(244)

$$Y_5 = \frac{\Delta t.\alpha_1}{R_1'.\Delta h_1} \tag{245}$$

Technical note

82



Finally, by the same process as for layer i (cross-substitution and simplification), the expressions of $A_{T,1}$, $A_{q,1}$, $B_{T,1}$, $B_{q,1}$, $C_{T,1}$, $C_{q,1}$, $D_{T,1}$ and $D_{q,1}$ can be expressed in function of X_1 to Y_5 (Replace $X_{1,i}$ to $Y_{1,i}$ by X_1 to Y_5 in Equations (212) to (219)).

The coefficients are known for the last layer of the atmospheric column. The objective is, now, to determine the surface temperature.

As a reminder, the surface is modelled in the multi-layer scheme as a layer of infinitesimal thickness which receives the heat conduction flux from the soil and transmit sensible and latent heat fluxes to the first layer. By resolving the energy budget of the surface layer, the surface temperature can be deduced. To do so, the first variables to know are the sensible and latent heat fluxes coming from this surface layer. They are expressed as follows:

$$\Phi_{H}^{t+1} = -\rho_{a}.C_{p}^{air}.k_{surf}.\frac{T_{a,1}^{t+1} - T_{surf}^{t+1}}{\Delta z_{surf}}$$
(246)

$$\Phi_{\lambda E}^{t+1} = -\rho_a . \lambda . k_{surf} . \frac{q_{a,1}^{t+1} - q_{surf}^{t+1}}{\Delta z_{surf}}$$
(247)

(**NB**: It is important to notice here that the latent heat flux is defined without the β formulation. This is important for the implementation in the code in Section III.4.)

By replacing $T_{a,1}^{t+1}$ and $q_{a,1}^{t+1}$ by their expression in Equations (223) and (224), the equations become:

$$\Phi_{H}^{t+1} = -\rho_{a}.C_{p}^{air}.k_{surf}.\frac{A_{T,1}.\Phi_{H}^{t+1} + B_{T,1} + C_{T,1}.T_{leaf,1}^{t+1} + D_{T,1}.\Phi_{\lambda E}^{t+1} - T_{surf}^{t+1}}{\Delta z_{surf}}$$
(248)

$$\Phi_{\lambda E}^{t+1} = -\rho_a . \lambda . k_{surf} . \frac{A_{q,1} . \Phi_{\lambda E}^{t+1} + B_{q,1} + C_{q,1} . T_{leaf,1}^{t+1} + D_{q,1} . \Phi_H^{t+1} - q_{surf}^{t+1}}{\Delta z_{surf}}$$
(249)

By replacing $T_{leaf,1}^{t+1}$ by its expression in function of E_1 , F_1 and G_1 , the system becomes:

$$\Phi_{H}^{t+1} = -\rho_{a}.C_{p}^{air}.k_{surf}.\frac{A_{T,1}.\Phi_{H}^{t+1} + B_{T,1} + C_{T,1}.(E_{1}.\Phi_{\lambda E}^{t+1} + F_{1}.\Phi_{H}^{t+1} + G_{1}) + D_{T,1}.\Phi_{\lambda E}^{t+1} - T_{surf}^{t+1}}{\Delta z_{surf}}$$

$$\Phi_{\lambda E}^{t+1} = -\rho_{a}.\lambda.k_{surf}.\frac{A_{q,1}.\Phi_{\lambda E}^{t+1} + B_{q,1} + C_{q,1}.(E_{1}.\Phi_{\lambda E}^{t+1} + F_{1}.\Phi_{H}^{t+1} + G_{1}) + D_{q,1}.\Phi_{H}^{t+1} - q_{surf}^{t+1}}{\Delta z_{surf}}$$

$$(250)$$

$$\Delta z_{surf}$$

$$(251)$$

When simplifying (assuming $q_{surf}^{t+1} = \alpha_{surf} T_{surf}^{t+1} + \beta_{surf}$), this leads to:

$$\Phi_{H}^{t+1}.(1 + \frac{\rho_{a}.C_{p}^{air}.k_{surf}}{\Delta z_{surf}}.(A_{T,1} + C_{T,1}.F_{1})) = -\frac{\rho_{a}.C_{p}^{air}.k_{surf}}{\Delta z_{surf}}.(B_{T,1} + C_{T,1}.G_{1} - T_{surf}^{t+1}) - \frac{\rho_{a}.C_{p}^{air}.k_{surf}}{\Delta z_{surf}}.\Phi_{\lambda E}^{t+1}.(C_{T,1}.F_{1} + D_{T,1})$$
(252)

Technical note



$$\Phi_{\lambda E}^{t+1} \cdot (1 + \frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \cdot (A_{q,1} + C_{q,1} \cdot E_1)) = -\frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \cdot (B_{q,1} + C_{q,1} \cdot G_1 - (\alpha_{surf} \cdot T_{surf}^{t+1} + \beta_{surf})) - \frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \cdot \Phi_H^{t+1} \cdot (C_{q,1} \cdot F_1 + D_{q,1})$$
(253)

Which can be simplified as:

$$\Phi_{H}^{t+1} \cdot \Omega_{1} = \Omega_{2} + \Omega_{3} \cdot T_{surf}^{t+1} + \Omega_{4} \cdot \Phi_{\lambda E}^{t+1}$$
(254)

$$\Phi_{\lambda E}^{t+1} \Omega_5 = \Omega_6 + \Omega_7 T_{surf}^{t+1} + \Omega_8 \Phi_H^{t+1}$$
(255)

Where,

$$\Omega_1 = 1 + \frac{\rho_a \cdot C_p^{air} \cdot k_{surf}}{\Delta z_{surf}} \cdot (A_{T,1} + C_{T,1} \cdot F_1)$$
(256)

$$\Omega_2 = -\frac{\rho_a.C_p^{air}.k_{surf}}{\Delta z_{surf}}.(B_{T,1} + C_{T,1}.G_1)$$
(257)

$$\Omega_3 = \frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \tag{258}$$

$$\Omega_4 = \frac{\rho_a . C_p^{air} . k_{surf}}{\Delta z_{surf}} . (C_{T,1} . F_1 + D_{T,1})$$
(259)

$$\Omega_5 = 1 + \frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \cdot (A_{q,1} + C_{q,1} \cdot E_1)$$
(260)

$$\Omega_6 = -\frac{\rho_a \cdot \lambda \cdot k_{surf}}{\Delta z_{surf}} \cdot (B_{q,1} + C_{q,1} \cdot G_1 - \beta_{surf})$$
(261)

$$\Omega_7 = \frac{\rho_a \cdot \lambda \cdot k_{surf} \cdot \alpha_{surf}}{\Delta z_{surf}} \tag{262}$$

$$\Omega_8 = \frac{\rho_a.\lambda.k_{surf}}{\Delta z_{surf}} (C_{q,1}.F_1 + D_{q,1})$$
(263)

By cross-substituting Equation (255) into (254) and (254) into (255), the fluxes can be expressed in function of T^{t+1}_{surf} .

$$\Phi_H^{t+1} \Omega_1 = \Omega_2 + \Omega_3 T_{surf}^{t+1} + \frac{\Omega_4}{\Omega_5} (\Omega_6 + \Omega_7 T_{surf}^{t+1} + \Omega_8 \Phi_H^{t+1})$$
(264)

$$\Phi_{\lambda E}^{t+1} \cdot \Omega_5 = \Omega_6 + \Omega_7 \cdot T_{surf}^{t+1} + \frac{\Omega_8}{\Omega_1} \cdot (\Omega_2 + \Omega_3 \cdot T_{surf}^{t+1} + \Omega_4 \cdot \Phi_{\lambda E}^{t+1})$$
(265)

Which is simplifies into:

$$\Phi_{H}^{t+1}.(\Omega_{1} - \frac{\Omega_{4}}{\Omega_{5}}.\Omega_{8}) = (\Omega_{2} + \frac{\Omega_{4}}{\Omega_{5}}.\Omega_{6}) + T_{surf}^{t+1}.(\Omega_{3}. + \frac{\Omega_{4}}{\Omega_{5}}.\Omega_{7})$$
(266)

Technical note

84



$$\Phi_{\lambda E}^{t+1}.(\Omega_5 - \frac{\Omega_8}{\Omega_1}.\Omega_4) = (\Omega_6 + \frac{\Omega_8}{\Omega_1}.\Omega_2) + T_{surf}^{t+1}.(\Omega_7. + \frac{\Omega_8}{\Omega_1}.\Omega_3)$$
(267)

The system can be abbreviated as:

$$\Phi_H^{t+1} = \xi_1 + \xi_2 T_{surf}^{t+1} \tag{268}$$

$$\Phi_{\lambda E}^{t+1} = \xi_3 + \xi_4 . T_{surf}^{t+1} \tag{269}$$

Where,

$$\xi_1 = \frac{\Omega_2 + \frac{\Omega_4}{\Omega_5} \cdot \Omega_6}{\Omega_1 - \frac{\Omega_4}{\Omega_5} \cdot \Omega_8} \tag{270}$$

$$\xi_2 = \frac{\Omega_3 + \frac{\Omega_4}{\Omega_5} \cdot \Omega_7}{\Omega_1 - \frac{\Omega_4}{\Omega_5} \cdot \Omega_8} \tag{271}$$

$$\xi_3 = \frac{\Omega_6 + \frac{\Omega_8}{\Omega_1} \cdot \Omega_2}{\Omega_5 - \frac{\Omega_8}{\Omega_1} \cdot \Omega_4} \tag{272}$$

$$\xi_4 = \frac{\Omega_{7.} + \frac{\Omega_8}{\Omega_1} \cdot \Omega_3}{\Omega_5 - \frac{\Omega_8}{\Omega_1} \cdot \Omega_4} \tag{273}$$

Finally, the last step to obtain the surface temperature is to solve the energy budget of the infinitesimal layer (fluxes of latent and sensible heat are supposed negative as in Equations (246) and (247):

$$C_{p}^{surf} \cdot \frac{T_{surf}^{t+1} - T_{surf}^{t}}{\Delta t} = R_{LW,surf} + R_{SW,surf} + \Phi_{H}^{t+1} + \Phi_{\lambda E}^{t+1} + J_{soil}$$
(274)

By replacing the fluxes by their expressions:

$$T_{surf}^{t+1} = T_{surf}^{t} + \frac{\Delta t}{C_{p}^{surf}} \cdot (\eta_{1,surf} \cdot T_{surf}^{t+1} + \eta_{2,surf} + \eta_{3,surf} \cdot R_{SW}^{down} + \xi_{1} + \xi_{2} \cdot T_{surf}^{t+1} + \xi_{3} + \xi_{4} \cdot T_{surf}^{t+1} + J_{soil})$$

$$(275)$$

Which leads to the expression of the surface temperature:

$$T_{surf}^{t+1} = \frac{T_{surf}^t + \frac{\Delta t}{C_p^{surf}} . (\eta_{2,surf} + \eta_{3,surf} . R_{SW}^{down} + \xi_1 + \xi_3 + J_{surf})}{1 - \frac{\Delta t}{C_p^{surf}} . (\xi_2 + \xi_4 + \eta_{1,surf})}$$
(276)

Now that the surface temperature is known, q_{surf}^{t+1} can be determined by $q_{surf}^{t+1} = \alpha_{surf} \cdot T_{surf}^{t+1} + \beta_{surf}$. Thus, the lowest level boundary layer is known and the Bottom-Up calculation of the temperatures inside the column can be computed, as presented in the Summary chart.



III.4 Modelling in ORCHIDEE

All the previous model is developed in ORCHIDEE in the mleb module. This part will now emphasize the architecture of the mleb module and precise a bit its routines.

III.4.1 The *mleb* module scheme

The scheme of the mleb module can be summarized as in Figure 15.





The module is divided into 9 main calculations subroutines: $mleb_begin$, $mleb_profile$, $mleb_lwrad$, $mleb_boudarylayer_resistance$, $mleb_stomatal_resistance$, $mleb_alpha_beta_coeff$, $mleb_calc_column$, $mleb_flux$ and $mleb_evapveg$. The description of those subroutines is made in Section III.4.2. The other subroutines $mleb_initialize$, $mleb_finalize$, $mleb_clear$, $mleb_netcdf$ and $mleb_write$ are usual subroutines for the good functioning of ORCHIDEE, $enerbil_main$ calls the 9 calculation subroutines, $mleb_boxheight$ is a new subroutine in order to clear the code in $mleb_main$ (however this subroutine has to be double-checked) and, finally, $mleb_pottemp$, is not used or called at all.

The main subroutine $mleb_main$ is calling the 9 calculation subroutines in the following order:

- 1. *mleb_boxheight*: in order to calculate the plant area density of each layer of the canopy (the subroutine has to be double-checked, the calculation can also be made directly in *mleb_main* code structure;
- 2. *mleb_begin*: in order to calculate preliminary variables, useful for the energy budget. (I'm not sure that this is really useful, it seems like a copy-paste from the enerbil module which is not needed anymore -> need to be double-checked);
- 3. *mleb_profile*: in order to allocate a Leaf Area Density to each layer and compute the turbulent diffusion profile following *Massman & Weil (1999)* [13] (See Section III.2.2.2);
- mleb_lwrad: in order to compute the Long Wave Radiation scheme following Gu et al. (1999) [8] (See Section III.2.3.1);
- 5. *mleb_boundarylayer_resistance*: in order to compute the leaf boundary layer resistance (See Section III.2.4.2);
- 6. *mleb_stomatal_resistance*: in order to compute the stomatal resistance (See Section III.2.4.2);
- 7. mleb_alpha_beta_coeff: in order to compute the rate of change in saturated humidity at the leaf surface following Monteith & Unsworth (2008) [17];
- 8. *mleb_calc_column*: in order to solve the implicit resolution inside the column (see Section III.3);
- 9. *mleb_flux*: in order to calculate the different fluxes that compose the energy budget as in the *enerbil* module (See Part II);
- 10. *mleb_evapveg*: in order to split the water fluxes between its components as in the *enerbil* module (See Part II);
- 11. Finally, it calls the subroutine *mleb_netcdf* in order to produce an output netcdf file (but the call to this routine blows up the computing time) and it prepares some variables for the next time-step.

III.4.2 Subroutine descriptions

As for the *enerbil* technical note (See Part II), this part aims at explaining the different subroutines of the code. All the main equations have been explained in Section III.2 and III.3. The equations or processes that are not described in the previous sections are added in this part of the technical note.



III.4.2.1 The mleb boxheight subroutine

The aim of this subroutine is to remove a big part of the code that was in the subroutine $mleb_main$. The aim of the subroutine is to calculate the box heights and plant area density as a function of height.

The calculation of the plant area density as a function of height is given thanks to the effective Leaf Area Density LAI_{eff} . Because LAI_{eff} is known at each level of the canopy, Equation (277) permits to access to the PAD as a function of height (**NB**: The following equation is a bit weird).

$$PAD(z) = LAI_{eff}(z).cos(\frac{\pi}{3})$$
(277)

Finally, the heights of each box in the discretization are calculated by separating the cases: below the canopy, inside the canopy and above. The heights are calculated by dividing the difference of heights between each cases by the number of layers needed.

Table of the main input variables:

Variable	Name in ORCHIDEE	Description	Unit	Input from
LAI_{eff}	$laieff_isotrop$	Effective LAI	$m^{-2}.m^{-2}$	$albedo_surface$
z_array_out	z_array_out	Heights of tree levels	m	$mleb_initialize$
ρ	rau	Air density	$kg.m^{-3}$???
max_height_store	max_height_store	Initial maximum canopy height	m	$mleb_initialize$

Table of the main output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
PAD(z)	pad_deltah	Plant Area Density as a function of height	$m^2.m^{-3}$	$mleb_profile$
box_height	vevapnu	Heights of each box edge	m	mleb_profile

III.4.2.2 The mleb begin subroutine

The first calculation subroutine to be called by the main one is *enerbil_begin*. The aim of this routine is to calculate preliminary variables useful for the computation of the energy budget. I think that this subroutine is not useful anymore but it needs to be checked.

To have more information about the calculation that it's computing, please refer to the *enerbil* technical note (Part II).

III.4.2.3 The mleb profile subroutine

The subroutine $mleb_profile$ aims at calculating the turbulent diffusion coefficient $k_*(z)$ following the equations of Massman & Weil (1999) [13], Wohlfahrt & Cernusca (2002) [25] and Chen et al. (2016) [4] in Section III.2.2.2.

Technical note



The first step of the calculation is to use the Plant Area Density as a function of height calculated in the subroutine $mleb_boxheight$ to calculate the leaf area density (cumulative PAD from the top of the canopy). Once the LAD is known, it is used to calculate the coefficient $C_{D,eff}$ presented in Section III.2.2.2. This coefficient (coming from Wohlfahrt & Cernuca (2002) [25]) is then used to calculate the variable $\eta(z)$ which permits to use the model from Massman & Weil (1999) [13] in order to compute the standard deviation in wind vertical velocity σ_w .

Finally, once σ_w is calculated, the routine calculates the *far-field* eddy diffusivity $k_*(z)$ following Equation (141) and using the reducing factor R_{nf} as shown in Equation (142) in order to get the final value of the eddy diffusivity as in Equation (143).

Variable	Name in ORCHIDEE	Description	Unit	Input from
PAD(z)	pad_deltah	Plant Area Density as a function of height	$m^2.m^{-3}$	$mleb_boxheight$
box_height	vevapnu	Heights of each box edge	m	$mleb_boxheight$
k_{slope}	k_eddy_slope	Coefficient used in the calculation of R_{nf}	_	General input
ku*	k_eddy_ustar	Coefficient used in the calculation of R_{nf}	_	General input
$ \overrightarrow{V} $	speed	Wind speed	$m.s^{-1}$	General input

Table of the main input variables:

Table of the main output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
$k_*(z)$	k_eddy	Eddy diffusivity	$m^2.s^{-1}$	$mleb_calc_column$

III.4.2.4 The *mleb lwrad* subroutine

The aim of the subroutine is to compute the Long Wave Radiation Scheme inspired from $Gu \ et$ al. (1999) [8].

The subroutine starts by computing the values of the η above the canopy. Those calculations rely on a variable called *jomega*. **NB:** I do not understand this part of the code at the time I write this note, it should need a double check...

Once those values are calculated, the subroutine is computing the Radiation Transfer Matrix thanks to the system of Equations (155). This matrix is the main output of the subroutine.

Table of the main input variables:





Variable	Name in ORCHIDEE	Description	Unit	Input from
T_{leaf}	$temp_leaf_pres_grid$	Leaf temperature at the present time step	K	Previous time step
T_{surf}	$temp_surf_pres$	Surface temperature at the present time step	K	Previous time step
PAD(z)	pad_deltah	Plant Area Density as a function of height	$m^2.m^{-3}$	$mleb_boxheight$
K_{LW}	big_k_lw	???	???	???
K_{SW}	$big \ k \ lw$???	???	???

Table of the main output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
$jemissivity(_surf)$	$jemissivity(_surf)$???	???	$mleb_calc_column$
$jomega(_sw_surf)$	$jemissivity(_surf)$???	???	$mleb_calc_column$
$eta_{1,above}$	eta_1_above	???	???	$mleb_calc_column$
$eta_{3,above}$	eta_3_above	???	???	$mleb_calc_column$
$lpha_{i,j}$	ngu_alpha	Radiation Transfer Matrix	_	$mleb_calc_column$
$\alpha_{i,i}$	ngu_alpha	Diagonal coefficients of the Radiation Transfer Matrix	_	$mleb_calc_column$

III.4.2.5 The mleb boundarylayer resistance subroutine

This subroutine computes the boundary layer resistance used for the calculation of the resistance to sensible presented in Section III.2.4.1. The calculation order is the following:

- Calculation of the thermal diffusivity of air $D_{h,air} = 1.9.10^{-5} + 1.26.10^{-5} \cdot (T_{air} 273.15)$.
- Calculation of the air viscosity $\mu = 1.35 \cdot 10^{-5} + 10^{-7} \cdot (T_{air} 273 \cdot 15)$
- Calculation of the Reynolds Number $Re = \frac{d_1.u}{\mu}$ where d_1 is the leaf length set to 1cm.
- Calculation of the Nusselt Number in function of the value of the Prandtl number as in Equation (165). (NB: The distinction between the calculations of the Nusselt number is appearing neither in Ryder et al. (2016) [21] nor in Section III.2.4.1, I don't know from where this distinction comes. Moreover, the formula set into the code is not the same as in Equation (165))
- Finally, calculation of the resistance as in Equation (164) (R_i is multiplied by a parametrized factor R_{fac}).

At the top of the canopy, the resistance is set to 1.10^{20} (considering this value to be close to infinity, case when there are no leaves).

Table of the main input variables:



Variable	Name in ORCHIDEE	Description	Unit	Input from
T_{air}	$temp_atmos_pres_grid$	Air temperature at the present time step	K	Previous time step
R_{fac}	br_fac	Multiplication factor to the resistance	—	General Input

Table of the main output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
R_i	big_r	Resistance to sensible heat flux	$s.m^{-1}$	$mleb_calc_column$

III.4.2.6 The mleb stomatal resistance subroutine

This subroutine computes the resistance to latent heat flux presented in Section III.2.4.2. As presented in Equation (169), the resistance to latent heat flux is composed by two different resistance, the stomatal resistance and the boundary layer one.

Unlike what is presented in Section III.2.4.2, the stomatal conductance seems to rely on a formulation taken from *Guimberteau thesis* [9] which relies on the water pressure deficit of the layer and the short waves downwelling radiation. However, I do not have access to the thesis so I could not double check the formula. The formula seems way different than the one described in Section III.2.4.2.

NB: As mentionned by Sebastiaan, the calculation of the stomatal conductance uses the plant area density (which is defined thanks to the effective LAI) instead of the LAI which is weird.

Secondly, the boundary layer resistance is calculated with the following steps:

- Calculation of the molecular diffusivity of water vapour $D_{h,H_2O} = 2.26.10^{-5} + 1.51.10^{-7} \cdot (T_{air} 273.15)$
- Calculation of the air viscosity as for the resistance to sensible heat right above.
- Calculation of the Schmidt Number as the ratio between μ and D_{h,H_2O}
- Calculation of Reynolds number
- Calculation of the Sherwood number according to the Reynolds number
- Calculation of the boundary layer resistance as in Equation (167)

Above the canopy, the resistance is set to infinity (10^{20}) .

Table of the main input variables:



Variable	Name in ORCHIDEE	Description	Unit	Input from
ρ	rau	Air density	$kg.m^{-3}$	General Input
$R_{SW,n}$	swnet	Net short-wave radiations	$W.m^{-2}$	Other module
PAD(z)	pad_deltah	Plant Area Density as a function of height	$m^2.m^{-3}$	$mleb_boxheight$
$R_{LW}\downarrow$	lwdown	Downwelling Long-wave Radiations	$W.m^{-2}$	LMDz
T_{air}	$temp_atmos_pres_grid$	Air temperature at the present time step	K	Previous time step
q_{air}	$q_atmos_pres_grid$	Air saturated humidity at the present time step	$kg.kg^{-1}$	Previous time step

Table of the main output variables:

Variable	Name in ORCHIDEE	Description	Unit	Output used in
R'_i	big_r_prime	Resistance to latent heat flux	$s.m^{-1}$	$mleb_calc_column$

III.4.2.7 The mleb calc column subroutine

This subroutine is the main calculation subroutine. It solves the equations along the canopy column and solves the implicit coupling with the atmosphere. This resolution corresponds to the different results of the Section III.3.3 and III.3.4.

The subroutine starts by initializing some variables. Here, everything is set to 0 except the resistances R_i and R'_i of the last layer which are set to 10^{20} (consider it as infinity).

After this initialization, the subroutines enters into a "convergence loop". The aim of the loop is to equalize the fluxes of water calculated by the module *mleb* and the one calculated by the module *hydraulic_arch*. In *hydraulic_arch*, if the transpiration (calculated thanks to the coefficient β_3 and the energy budget (for more information, see the *enerbil* technical note)) exceeds the amount of water that the soil can provide, the transpiration is reduced to this precise amount of water and the energy budget is recalculated. However, this correction scheme is not adapted to the multi-layer scheme. Because the correction is made for the transpiration of the global canopy, the correction has to be dispatched at each layer which changes the energy budgets of each layer. The multi-layer has, thus, to be recomputed. This correction brings the necessity to compute several times the multi-layer energy budget. This leads to the necessity of this convergence loop when the hydraulic architecture scheme is used and when the soil is stressed. When the classic water scheme is set, the subroutines enters the convergence loop but exit it at the end of the first iteration.

The first calculation which interests this note is the set up of the coefficients at the top of the column. To do so, the upper boundary conditions are set (See Section III.3.4.1) (Note that $B_{T,n} = B_{T,atm}/C_p^{air}$, this is a correction due to the format of the output of LMDz).

Once this set up is finished, the subroutine is defining the coefficients β for the evaporation, sublimation, transpiration in function of the corresponding β . This permits to simplify the equation visualization after.

Once this is done, the subroutine calculates the η_s presented in Section III.2.3. Here, it is important to notice that the definition for the Long-Wave radiation scheme used is different from the one in Section III.2.3.1. Instead of having $R_{LW,i} = \eta_{1,i} \cdot T_{leaf,i}^{t+1} + \eta_{2,i}$, $R_{LW,i}$ is defined as in



Equation (278). Be careful, the $\eta'_{j,i}$ of the next formula are not same as in the previous equation and in Section III.2.3.1. NB: The naming of those $\eta'_{j,i}$ in the code is being reviewed.

$$R_{LW,i} = \eta'_{1,i} \cdot R_{LW}^{down} + \eta'_{2,i} \cdot T_{leaf,i}^{t+1} + \eta'_{3,i}$$
(278)

In practice, $\eta'_{1,i}$ of the previous equation is set to 0 except for the surface layer. Consequently, looking at the code, one should understand that:

mleb module	Technical note
$\eta'_{1,i}$	0
$\eta'_{2,i}$	$\eta_{1,i}$
$\eta'_{3,i}$	$\eta_{2,i}$

Now that this remark is made, the two radiation schemes are computed. The first one, the Long-Wave Radiation scheme is solved first. It uses the results of the subroutine $mleb_lwrad$ which was calculating the coefficients $\alpha_{i,j}^{LW}$. The resolution is divided into two parts, the first one reconstitutes the matrix from Gu et al. (1999) [8] with the formulation of the $\alpha_{i,i}^{LW}$ thanks to the value of the leaf temperature at the previous time step. This part permits to calculate $R_{LW,i}^0$ as in Equation (160). In the second part, $\eta'_{2,i}$ and $\eta'_{3,i}$ are calculated as $\eta_{1,i}$ and $\eta_{2,i}$ in Equations (161) and (162).

Once the Long-Wave Radiation scheme is computed, the subroutine uses the results of the Short-Wave Radiation scheme computed in the module *albedo_surface* in order to compute $\eta'_{4,i}$ (which corresponds to $\eta_{3,i}$ in the present note). **NB:** However, at the time this note is written, the part of the code which uses the results of the Short-Wave Radiation Scheme is commented. Consequently, $\eta'_{4,i}$ is set to 0 except at the layer surface where it is set to 1.

Now that everything is calculated, the subroutine starts by calculating the coefficient thanks to the Top-Down calculation.

The first step is to calculate the coefficients E_i , F_i and G_i at the top of the canopy (**NB**: The calculation starts by a IF condition which distinguishes the case where the number of layer is set to 1. I strongly think that this condition is useless for 2 main reasons. Firstly, if there is only 1 layer, the resolution coefficients are reduced to the ones of the upper boundary condition (See Section III.3.4.1) and the coefficients E_i , F_i and G_i are always multiplied by C_T , D_T , C_q of D_q which are set to 0. Secondly, as soon as the condition is finished, the values of E_1 , F_1 and G_1 are recalculated).

Once the coefficients at the top of the canopy determined, the Top-Down calculation of the coefficients $A_{T,i}$, $B_{T,i}$, $C_{T,i}$, $D_{T,i}$, $A_{q,i}$, $B_{q,i}$, $C_{q,i}$, $D_{q,i}$ is started. The calculation is well following the steps presented in Section III.3.2:

- As the coefficients E_i , F_i and G_i are known (first calculation at the top), the subroutine starts to calculate the coefficients $X_{i,1}$ to $Y_{i,5}$.
- From the coefficients $X_{i,1}$ to $Y_{i,5}$, the coefficients $A_{T,i}$ to $D_{q,i}$ are calculated as in Equations (212) to (219).
- Finally, the coefficients E_i , F_i and G_i are evaluated in order to prepare the calculation for the next layer.

Finally, once all the coefficients are known, the subroutine computes the equations of the surface interface presented in Section III.3.4.2. Thus, it calculates the coefficients $X_{1,1}$ to $Y_{1,5}$



and the resolution coefficients $A_{T,1}$ to $D_{q,1}$. After the calculation of those coefficients, the subroutine calculates the final coefficients E_1 , F_1 and G_1 .

NB: Before finishing the calculation, it is important to notice that all along the previous calculation, an IF condition was separating the cases where the hydrol_flag was set to .TRUE. are not. In the cases where hydrol_flag was set to .TRUE., all the coefficients linked to a change in saturated humidity where set to 0 ($A_{q,i}$ to $D_{q,i}$). I have to look into more details about those cases but I assume that it permits to make the loop converge by not adding more transpiration in each layer and limitate the transpiration in cases of water stress.

Right after those calculations, the surface interface equations are calculated. The subroutine computes the variables Ω_1 to Ω_8 for the cases of evaporation (with $\beta = \beta_{evap}$) and sublimation (with $\beta = \beta_{sub}$). From those variables are calculated the ξ_1 to ξ_4 . ξ_3 and ξ_4 are calculated after a parametrization of the surface evaporation. The evaporation fraction (f_{evap}) is calculated empirically thanks to the values of β_3 and β_4 and two weighting factors ks_weight_1 and ks_weight_2 which are calculated thanks to two parameters: ks_slope and ks_veget . This parametrization relies on the study of *Chen et al. (2016)* [4] which quantifies the resistance coefficient to latent heat according to the over-story phenology (it has been observed that "*In winter, when the under-story is senescent, the characteristics in terms of the evapotranspiration at the interface will closely resemble the evapotranspiration of a bare soil. In summer, however, an under-story will be present and its density relates to the gap fraction of the over-story canopy. Hence, the summertime evapotranspiration of the interface will be closer to the evapotranspiration of a vegetation canopy"). This quantification of the soil evaporation under the canopy permits to evaluate \xi_3 and \xi_4 thanks to the following equations (based on Equations (270) to (273)).*

$$f_{evap} = ks_{weight_1}.\beta_4 + ks_{weight_2}.\sum_{PFT} \frac{1}{\beta_3}$$
(279)

$$\xi_3 = f_{evap} \cdot \frac{\Omega_6 + \frac{\Omega_8}{\Omega_1} \cdot \Omega_2}{\Omega_5 + \frac{\Omega_8}{\Omega_1} \cdot \Omega_4} + \beta_{sub} \cdot \frac{\Omega_{6,sub} + \frac{\Omega_{8,sub}}{\Omega_1} \cdot \Omega_2}{\Omega_{5,sub} + \frac{\Omega_{5,sub}}{\Omega_1} \cdot \Omega_4}$$
(280)

$$\xi_4 = f_{evap} \cdot \frac{\Omega_7 + \frac{\Omega_8}{\Omega_1} \cdot \Omega_3}{\Omega_5 + \frac{\Omega_8}{\Omega_1} \cdot \Omega_4} + \beta_{sub} \cdot \frac{\Omega_{7,sub} + \frac{\Omega_{8,sub}}{\Omega_1} \cdot \Omega_3}{\Omega_{5,sub} + \frac{\Omega_{5,sub}}{\Omega_1} \cdot \Omega_4}$$
(281)

Those expressions permit to add the β -formulation in the multi-layer energy budget and take into account the evaporation of bare soil and snow sublimation. However, as presented in Section III.3.4.2, the variables Ω s have not been defined by considering the latent and sensible heat fluxes with the β -formulation (See "NB" right after the definition of the fluxes). This leads to differences when comparing the model with the module *enerbil*.

NB: As presented in the Section III.5.1.1, I think that the expressions of the Ωs should be revised in order to take into account the β .

Now that all the coefficients are known, the surface temperature and the other quantities of the infinitesimal surface layer can be determined. The surface temperature is defined as in Equation (276). Finally, as for the current energy budget in *enerbil*, other quantities are calculated: $q_{surf,sat}$, H_{surf} , F_{evap} , q_{air} ... (the formulas are exactly the same as in the *enerbil* technical note in Part II).

This last step marks the last calculation of the convergence loop (in the cases where the convergence is needed). The subroutine exits the loop and computes the last calculations:

• Bottom-Up calculation of the temperatures thanks to the coefficients previously determined.



- Calculation of the latent and sensible heat fluxes between each layers
- Calculation of the radiation terms at each layer.
- Calculation of the global latent and sensible heat fluxes (the fluxes between the top layer of the canopy and the atmosphere).
- Calculation of other information inside each layer (source/sink term of each layer thanks to the difference of temperature/humidity between the previous and the new time step, horizontal fluxes at each layers, sums of some fluxes...)

Those last calculations marks the end of the subroutine.

Variable	Name in ORCHIDEE	Description	Unit	Input from
$\{T_{leaf,i}\}$	$temp_leaf_pres_grid$	Leaf temperature at the previous time step	K	Previous time step
$\{q_{air}\}$	$q_atmos_pres_grid$	Sepcific humidity at the previous time step	$kg.kg^{-1}$	Previous time step
$\{T_{air}\}$	$temp_atmos_pres_grid$	Air temperature at the previous time step	K	Previous time step
k_*	k_eddy	Eddy diffusivity between layers	$m^2.s^{-1}$	$mleb_profile$ subroutine
$R_{LW}\downarrow$	lwdown	Long Wave downwelling radiations	$W.m^{-2}$	LMDz
$R_{SW}\downarrow$	swdown	Short Wave downwelling radiations	$W.m^{-2}$	LMDz
$R_{SW,n}$	swnet	Short Wave net radiations	$W.m^{-2}$	albedo_surface module
PAD(z)	pad_deltah	Plant Area Density as a function of height	$m^2.m^{-3}$	$mleb_boxheight$
C_p^{soil}	soilcap	Soil calorific capacity	$J.K^{-1}$	thermosoil module
G	soilflx	Soil heat flux	$W.m^{-2}$	thermosoil module
$\alpha_{i,i}^{LW}$	ngu_alpha	Coefficients of the Long Waver Radiation transfer Matrix	_	mleb_lwrad subroutine
$\begin{array}{c} A_{T,atm}, \\ B_{T,atm}, \\ A_{q,atm}, B_{q,atm} \end{array}$	petAcoef, petBcoef, peqAcoef, peqBcoef	Coefficients for the implicit coupling with LMDz		LMDz
β_1 to β_5	vbeta1 to vbeta5	Resistance coefficients to latent heat flux	_	<i>diffuco</i> module
$\begin{bmatrix} ks_tune, \\ ks_slope, \\ ks_veget \end{bmatrix}$	ks_tune, ks_slope, ks_veget	Empiric coefficients for the tuning of some variables	_	General input

Table of the main input variables:

Table of the main output variables:



Variable	Name in ORCHIDEE	Description	Unit	Output used in
F _{sens}	fluxsens	Sensible heat flux at the grid level	$W.m^{-2}$	General output
F _{lat}	fluxlat	Latent heat flux at the grid level	$W.m^{-2}$	General output
$F_{sens,i}$	$flux_h_grid$	Sensible heat flux between each layers	$W.m^{-2}$	General output
$F_{lat,i}$	$flux_le_grid$	Latent heat flux between each layers	$W.m^{-2}$	General output
$A_{T,i}$ to $D_{q,i}$	a_t to d_q	Implicit coupling coefficients		<i>mleb_calc_column</i> (next time step)
E_i to G_i	big_e to big_g	Implicit coupling coefficients		<i>mleb_calc_column</i> (next time step)
$T_{air,i}$	$t_a_next_grid$	Air temperature at each level of the canopy	K	<i>mleb_calc_column</i> (next time step)
$q_{air,i}$	$q_a_next_grid$	Air specific humidity at each level of the canopy	$kg.kg^{-1}$	<i>mleb_calc_column</i> (next time step)
$T_{leaf,i}$	$temp_leaf_next_grid$	Leaf temperature at each level of the canopy	K	<i>mleb_calc_column</i> (next time step)
T_{surf}	$temp_surf_next$	Surface temperature at the new time step	K	General output / LMDz
F_{Rn}	$flux_netrad$	Net radiation flux between each layers	$W.m^{-2}$	<i>mleb_calc_column</i> (next time step)
F _{Sn}	$flux_netsw$	Short wave net radiation flux between each layers	$W.m^{-2}$	$\frac{mleb_calc_column}{(next time step)}$
F _{Ln}	flux_netrad	Long Wave net radiation flux between each layers	$W.m^{-2}$	<i>mleb_calc_column</i> (next time step)
$\eta'_1 ext{ to } \eta'_4 ext{ and } \eta'_{1,surf} ext{ to } \eta'_{4,surf}$	eta_1 to eta_4_surf	Coefficients for the Radiation schemes		mleb_calc_column (next time step)

Table of the main local variables:

Variable	Name in ORCHIDEE	Description	Unit
_	big_e_top to big_g top	Numerator of the coefficients E_i to G_i (big e to big g)	
_	big_efg_bottom	Denominator of the coefficients E_i to $G_i \ (big_e \text{ to } big_g)$	
Ω_1 to $\Omega_{8,sub}$	big_omega_1 to big_omega_8_sub	Coefficients for the surface interface	
ξ_1 to ξ_4	xi_1 to xi_4	Coefficients for the surface interface	
f_{evap}	$evap_fraction$	β equivalent coefficients for the soil evaporation	

III.4.2.8 The *mleb_flux* subroutine

This subroutine calculates all the fluxes, temperatures and humidities needed for the completion of the energy budget. The only difference with the current energy budget computed in *enerbil* is the fact that the sensible and latent heat fluxes are calculated in the subroutine *mleb_calc_column*. For everything else, please refer to the *enerbil* technical note in Part II.

III.4.2.9 The *mleb_evapveg* subroutine

This routine computes the splitting of the total evaporation flux into its snow sublimation, floodplains evaporation, bare soil evaporation, intercepted water evaporation and transpiration components.



To have more details about the use of the β s and how they permit to split the evaporatino flux, please refer to the *enerbil* technical note in Part II.

III.4.3 One-layer case

The multi-layer energy budget presented in the *mleb* module is configurable in order to reduce the number of layers to only one layer. The objective behind the development of the *mleb* module is to come back to the *enerbil* equations when running the *mleb* module with only one layer. At the time this note is written, the equations from both modules (*enerbil* and *mleb* when reduced to one layer) are a bit different. A precise description of the equations is given in the technical note *Collapse of the calculations of mleb (with jnlvls* = 1) and *enerbil*, Julien ALLÉON (2021) [1]. The path of the calculation when the case jnlvls = 1 is set is presented in Figure 16.



Figure 16: Path of the calculation when jnlvls = 1 in $mleb_main$



The conclusion of the collapse of the equations were the following:

- There is a mistake in the definition of the ξ_i at the surface interface. The β has to be present at the denominators of the ξ_i . The β s have to be re-thought in the multi-layer energy budget.
- There is a factor ρ. |V|.C_d which differs for the latent heat flux expressions between both modules. (NB: As presented in Section III.5.1.3, this should be an error from the note because this difference seems not to appear in the code)
- The part of the code related to the Short Wave Radiation Scheme has been commented which leads to differences in the calculation of the surface temperature.



III.5 Suggestions

III.5.1 Debug

III.5.1.1 Use of the βs

The β coefficients are resistance coefficients to the potential total evaporation. As the total evaporation of the canopy regroups a lot of different processes such as snow sublimation, soil evaporation or transpiration, it is needed in the code to separate those different fluxes from the evaporation fluxes. This is the role of the β coefficients. β coefficients are representing two different processes:

- As the total potential evaporation is expressed at the grid cell level, the β are representing the fraction of the grid cell which emits the evaporation/sublimation flux.
- As the total potential evaporation expresses a kind of demand from the atmosphere (a "potential" evaporation), the β coefficients are also expressing the stresses applied to this potential evaporation (especially for the transpiration).

In the multi-layer energy budget, the β are used at the surface interface level. The aim of the β here is clearly to represent the fraction of the soil behind the canopy which will evaporate. This fraction of the soil can be covered by snow. Thus, two evaporation fluxes are modelled: snow sublimation of the soil behind the canopy and soil evaporation. As there is no stress, β are just representing here the fraction of the soil which evaporates.

From this reflection, several remarks can be made:

- 1. As the latent heat flux from the soil is chosen to take into account the β coefficients, Equation (247) should be reviewed into $\Phi_{\lambda E}^{t+1} = -\beta . \rho_a . \lambda . k_{surf} . \frac{q_{a,1}^{t+1} - q_{surf}^{t+1}}{\Delta z_{surf}}$. From this new equation, a new expression for the Ω will be found which will take into account those β coefficients. Finally, the expression of ξ_3 and ξ_4 will be changed and will directly take into account the β . Thus, we will not have to multiply the expressions by f_{evap} and β_{sub} in Equations (280) and (281).
- 2. Currently, the soil latent heat flux is taking into account two different processes: soil evaporation (represented by β_4 and snow sublimation β_1 . However, if I understand well, a part of the soil below the canopy can also be flooded and this part is represented by the floodplains fraction β_5 . Consequently, I think that a third flux should be taken into account: the floodplain evaporation below the canopy.
- 3. As expressed in Equation (279), f_{evap} is only taking into account β_4 and the β_3 of each PFT. However, in the current energy budget module *enerbil* (See Part II), the evaporation flux is always weighted by the fraction of the grid which is not sublimating snow $(1 - \beta_1)$. This is not the case here which could lead to differences between both codes. Moreover, collapsing *mleb* to 1 layer will not make appear the same factor as in *enerbil* $(1 - \beta_1).(1 - \beta_5).\beta$ but f_{evap} which will lead to differences.
- 4. Finally, as presented in Section III.5.2.1, the multi-layer energy budget has been thought from an ecosystem point of view. This is in contradiction with the necessity to have one energy budget per grid in grid-cells with several PFTs. The multi-layer energy budget should be used at the PFT level.



NB: In the document of the collapse of the equations of both modules [1], the conclusion with the β is different from this one. The module uses f_{evap} instead of β_{evap} . This difference is due to a misunderstanding in the flag ok_impose_can_structure. The good version of the reflection is the one presented here.

III.5.1.2 SW radiations scheme

As presented in the Section III.4.2.7, the part of the code linked to the Short-Wave Radiation Scheme has been commented which leads to one of the problems mentioned in the document about the collapse of both module [1]. This part should be debugged and uncommented in order to make the model works.

III.5.1.3 Dimensional analysis of the latent heat flux

The document about the collapse of both module equations [1] was citing a difference of a factor $\rho . |\vec{V}| . C_d$ between the formulas of the latent heat flux in both modules. It seems to be an error, the factor appears in both modules.

III.5.2 Further improvements

III.5.2.1 Multi-tiling necessity

As presented above, the multi-layer energy budget has been thought at the ecosystem level which is incoherent with the necessity to have one energy budget per grid cell as for now with the *enerbil* module (See Part II).

This thought leads to 2 necessities:

- Review the β model in order to separate the stresses from the fraction of grid-cell.
- Couple the multi-layer approach with a multi-tiling one in order to use the multi-layer energy budget only for the PFT.

To do so, I started to think about a multi-tiling approach which we should talk about.

III.5.2.2 Remarks on the turbulent transport model

As presented in Section III.2.2.2, the turbulent transport diffusion model implemented currently in the model corresponds to an adapted *far-field* model whereas a real *near-field/far-field* model. This is a clearly empirical model. The justification behind was that the *near-field/far-field* model would be impossible with an implicit coupling with the atmosphere.

According to Jérôme Ogée, this should be possible but would need more development in order to have a really physical model. This thought is under investigation.

III.5.2.3 Link with the new hydraulic architecture scheme

As presented in Section III.4.2.7, coupling the multi-layer energy budget with the current hydraulic architecture correction scheme leads to the necessity of having a convergence loop. This loop is due to the correction made in period of stresses.



A new hydraulic architecture scheme has been developed, following *Tuzet et al. (2003)* [23]. This hydraulic architecture links the stomatal conductance to the leaf water status which is linked to a plant water budget directly linked to the soil water status. This new model doesn't need any correction and is modelling more physically the water transport inside the plants. Consequently, coupling this new scheme with the multi-layer energy budget could really improve the transfer of water between the the leaves and the atmosphere at each level. This would permit to model:

- The water available at each layer thanks to the gravity resistance and the plant water transport at each level.
- Couple the stomatal conductance at each level with the soil water content and thus avoid iterations

However, the implicit coupling with atmosphere and the parametrized number of layers (from 1 to 50) will lead to difficult development. But I think the project exciting.

III.5.3 Action plan

Here is a quick summary of the action plan that, according to me, should be followed in order to debug/improve the multi-layer energy budget scheme:

- 1. *Review:* Review the conclusions of the notes.
- 2. *Debug:* Uncomment and Debug what needs to be debugged in the Short Wave Radiation Scheme
- 3. Debug: Review the formulation of the Ω in order to introduce the β and add an IF condition in order to make the *mleb* module collapsed to one layer exactly the same as *enerbil*.
- 4. Improvement: Review and Discuss about the use of the β s and the multi-tiling approach
- 5. Improvement: Review the turbulent diffusion scheme
- 6. *Improvement:* Better coupling between the new hydraulic architecture and the multi-layer energy budget.



Partie IV

Current and future developments

Two different projects are in phase of development: a multi-layer energy budget and a multi-tiling approach of the energy budget.

IV.1 Multi-layer energy budget

The energy budget presented in this Part II assumes the surface to be a big leaf of infinitesimal thickness. This approach is interesting in order to simplify the energy budget and permits to have pretty good results.

The aim of the multi-layer energy budget presented in Part III is to provide a way to model the diffusion of each fluxes inside the canopy. The canopy has now a finite thickness and is divided into several layers between which turbulent flux exchanges will occur. This more physical permits to increase the accuracy of the energy budget. The transport within the canopy is now modeled thanks to a turbulent diffusion scheme.

This project started several years ago thanks to James Ryder[21]. The result of the project is the so called *mleb* module which computes the multi-layer energy budget. However, several problems occurred and the project has been left on side. The major problems of the current multi-layer energy budget are the following:

- The model can only be run at the site level, no global simulation can be computed with the current multi-layer energy budget.
- Even if the module has been developed in order to choose the number of layers, collapsing the multi-layer energy budget to only one layer does not permit to have the same results as the model presented here.

The project has, then, be abandoned. However, a new discussion about this project has been started and its development is back on the table.

At the time this note is written (January 2021), several works are currently being done on the multi-layer energy budget:

- Debug the module for the one-layer case
- Improve the turbulent diffusion transport inside the canopy
- Improve and Debug the use of the multi-layer scheme in mixed pixels.

IV.2 Multi-tiling energy budget

The multi-layer energy budget presented before is still running at the grid-cell level. However, studies has shown that running the energy budget at the PFT level permit to increase the accuracy of the model. On the other hand, new discussions have started inside the scientific community about the way to define the different sub-grid frameworks. Even if the PFT approach has now been implemented in most of the land surface models, new approaches seem to be interesting. Among them, the concept of Surface Functional Type (SFT) is becoming important.



A Surface Functional Type corresponds to a bunch of component (soil type, PFT...) regrouped under a same set of parameters. This new way to define the sub-grids frameworks permits to avoid several conversion problems. A grid-cell would then be divided into several SFTs only, and all the processes would be running on the SFTs.

This discussion started last year thanks to two initiatives:

- One from James Ryder, who started the following report: Link
- One from a group of interested among the ORCHIDEE team: Link

This project started again but will need more discussion than the multi-layer one.





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