S1 Canopy model SiLCan

S1.1 General

SiLCan stands for Simplified Layered Canopy. In our accompanying manuscript this model is coupled to the (slightly modified) CLASS model (Vilà-Guerau de Arellano et al., 2015), and to a model that calculates soil COS uptake, see our accompanying manuscript. The canopy model simulates 4 different tracers in the canopy: temperature, specific humidity, CO_2 and carbonyl sulphide (COS). These tracers are calculated in each canopy layer, i.e. each layer has an air temperature and a CO_2 concentration. Exchange between the air and vegetation is simulated, but atmospheric chemistry is not included. The model distinguishes 4 categories of leaves: sunlit-dry, sunlit-wet, shaded-dry and shaded-wet leaves. For each of these categories, variables such as skin temperature (T_s) and stomatal conductance are calculated. At each time step, there are two iterations in which skin temperatures, longwave radiation, stomatal conductances and leaf fluxes are recalculated. In this document we refer a few times to the MLC-CHEM model, this is the Multi-Layer Canopy CHemistry and Exchange Modelling system, Ganzeveld et al. (2002) (Visser et al., 2022, for a recent application), the code of MLC-CHEM is available at https://github.com/ganzeveld/MLC-CHEM.

S1.2 Numerical discretisation in space

The numerical discretisation follows a similar approach as Sun et al. (2015), but note that the direction of the vertical axis is swapped. We have a 1-dimensional model, we use a finite-volume grid to discretise the canopy, in N layers. The bottom of the model is located at z = 0 m and the top at z = z_{toc}. A node is placed in each control volume. The user can specify the location of the nodes, but for every node the following should hold: 0.01 < z_{node} < z_{toc}. The location of the $N+1$ control volume edges (interfaces) are calculated as follows [m]:

$$z_{\text{int},i} = \begin{cases} z_{\text{toc}}, \quad i = N \\ z_{\text{node},i} - (z_{\text{node},i} - z_{\text{node},i-1})/2, \quad 0 < i < N \\ 0, \quad i = 0 \end{cases} \tag{S1}$$

Thus, the location of the interfaces (except top and bottom) is in the middle between each two neighbouring nodes. The thicknesses [m] of the N control volumes are given by:

$$\Delta z_i = \begin{cases} (z_{\text{toc}} - z_{\text{node},i}) + (z_{\text{node},i} - z_{\text{node},i-1})/2, \quad i = N-1 \\ (z_{\text{node},i+1} - z_{\text{node},i-1})/2, \quad 0 < i < N-1 \\ (z_{\text{node},i} + z_{\text{node},i+1})/2, \quad i = 0 \end{cases} \tag{S2}$$

We calculate the pressure at the ith node [Pa] as follows:

$$P_i = P_{\text{s}} - \rho_{\text{air}}\, g\, z_{\text{node},i} \tag{S3}$$

wherein g is the (constant) gravitational acceleration $[\mathrm{m\,s^{-2}}]$ and ρ_{air} is a constant representing air density $[\mathrm{kg\,m^{-3}}]$. P_{s} is the pressure at the soil surface [Pa], calculated as follows:

$$P_{\text{s}} = P_{\text{toc}} + \rho_{\text{air}}\, g\, z_{\text{toc}} \tag{S4}$$

wherein P_{toc} is the pressure at the top of the canopy [Pa], provided by the user.

S1.3 Shortwave radiation

The incoming shortwave radiation at the top of the canopy ($\text{SW}_{\text{in,top}}$,$[\mathrm{W\,m^{-2}}]$) is calculated by the CLASS model (Vilà-Guerau de Arellano et al., 2015). We calculate photosynthetically active radiation (PAR, $[\mathrm{W\,m^{-2}}]$) from this shortwave radiation:

$$\text{PAR}_{\text{top}} = \text{fr}_{\text{PAR}}\text{SW}_{\text{in,top}} \tag{S5}$$

wherein $\mathrm{fr_{PAR}}$ $[-]$ is the fraction of shortwave radiation that is within the range of PAR, with a default value of 0.5 (the user can provide a constant value as model input). $\mathrm{PAR_{top}}$ is split into direct and diffuse PAR. For this we follow the approach of Weiss and Norman (1985), with a few small adaptions. The calculation of optical air mass m $[-]$ has been changed into (as in MLC-CHEM):

$$m = \frac{35}{(1224(\cos(\mathrm{sza}))^2 + 1)^{0.5}} \tag{S6}$$

wherein 'sza' is the solar zenith angle. Equations 1 and 4 From Weiss and Norman (1985) are slightly simplified by neglecting the P/P0 term. Constant B used in eq 11 of Weiss and Norman was set to 7.0 instead of 0.7 (as in MLC-CHEM). In equation 11 in the paper of Weiss and Norman, variable 'RATIO' is set equal to 0.9 when it exceeds 0.9. Instead, we set RATIO equal to 0.89999999 when the variable exceeds the value of 0.89999999. This is done to avoid problems for the adjoint of the model (undefined derivative of model equation when RATIO equals 0.9).

Equation 3 From Weiss and Norman (1985) has been changed into:

$$R_{dV} = 0.4 * (600 * \cos(\mathrm{sza}) - R_{DV}) \tag{S7}$$

Equation 5 From Weiss and Norman (1985) has been changed into:

$$R_{dN} = 0.6 * (720 * \cos(\mathrm{sza}) - R_{DN} - w * \cos(\mathrm{sza})) \tag{S8}$$

We give here the equations for PAR used in our model, together with some equations that are not themselves implemented in the model, but are insightful to derive the equations in the model. The absorbed PAR is calculated separately for sunlit and shaded leaves, and differs between canopy layers. For radiation extinction through the canopy, we generally follow the approach of Spitters (1986). Similar to Eq. 7 of Spitters (1986), we introduce an extinction coefficient for perfectly absorbing black leaves (k_{bl}) $[\mathrm{m^2_{ground}\,m^{-2}_{leaf}}]$. This is the extinction coefficient for direct radiation, wherein direct radiation that transforms into diffuse radiation is considered 'lost'. Because we use all-sided leaf area index in contrast to the one-sided leaf area index in Spitters (1986), Eq. 7 from Spitters (1986) slightly changes:

$$k_{\mathrm{bl}} = \frac{0.5}{2\sin(\beta)} \tag{S9}$$

wherein β is the solar elevation angle $[-]$. Furthermore, as in Launiainen et al. (2011), we introduce a clumping factor clf $[-]$ to account for the shading effect by other leaves. The scattering coefficient for leaves (and other plant material) σ $[-]$ is set to 0.2 (Hikosaka et al., 2016b). Additionally, we introduce for each vegetation layer a factor that defines the fraction of plant material that consists of green photosynthesising leaves ($\mathrm{fr_{green}}$ $[-]$). The extinction coefficient for direct PAR radiation is given by (supplementary material Pedruzo-Bagazgoitia et al. (2017)) $[\mathrm{m^2_{ground}\,m^{-2}_{leaf}}]$:

$$k_{\mathrm{dir,sca}} = k_{\mathrm{bl}} * \sqrt{1-\sigma} \tag{S10}$$

$k_{\mathrm{dir,sca}}$ is smaller than k_{bl}, since direct PAR radiation can also be transformed into diffuse radiation, which can still be absorbed by plants. $k_{\mathrm{dir,sca}}$ is not the true extinction coefficient for direct radiation, but an extinction coefficient to calculate the radiation flux density resulting from direct radiation at the top of the canopy (see also supplementary material Pedruzo-Bagazgoitia et al. (2017)). This radiation ($\mathrm{PAR_{from\,dir\,top}}$) can be calculated as follows $[\mathrm{W\,m^{-2}_{horizontal\,surface}}$, or simply $\mathrm{W\,m^{-2}_{ground}}]$:

$$\mathrm{PAR_{from\,dir\,top}} = \mathrm{PAR_{dir,top}}\,\tau_{\mathrm{dir,sca}} = \mathrm{PAR_{dir,top}} \exp(-k_{\mathrm{dir,sca}} * \mathrm{LAI_{above}}\,\mathrm{clf}) \tag{S11}$$

in which $\mathrm{LAI_{above}}$ $[\mathrm{m^2_{plant\,surface}\,m^{-2}_{ground}}]$ is the amount of plant material above the level (height of node) we look at (including branches etc.). $\mathrm{PAR_{dir,top}}$ is the direct PAR radiation at the top of the canopy $[\mathrm{W\,m^{-2}_{horizontal\,surface}}]$. The quantity $\tau_{\mathrm{dir,sca}}$ is dimensionless.

The radiation resulting from diffuse PAR radiation at the top of the canopy can similarly be calculated by multiplying the diffuse radiation at the top of the canopy ($\mathrm{PAR_{dif,top}}$) with the following quantity $[-]$:

$$\tau_{\mathrm{dif}} = \exp(-k_{\mathrm{dif}} * \mathrm{LAI_{above}}\,\mathrm{clf}) \tag{S12}$$

Note that k_{dif} $[\mathrm{m}^2_{\mathrm{ground}}\mathrm{m}^{-2}_{\mathrm{leaf}}]$ (or more generally $[\mathrm{m}^2_{\mathrm{ground}}\mathrm{m}^{-2}_{\mathrm{plant\,surface}}]$) is not modelled by an equation, but instead is taken from user input. The direct PAR radiation in the canopy resulting from direct PAR radiation at the top of the canopy can be calculated by multiplying the direct PAR radiation at the canopy top with the following quantity $[-]$:

$$\tau_{\mathrm{dir}} = \mathrm{fr}_{\mathrm{sun}} = \exp(-k_{\mathrm{bl}} * \mathrm{LAI}_{\mathrm{above}}\,\mathrm{clf}) \tag{S13}$$

Note that τ_{dir} is also the fraction of leaves at a certain level that is sunlit (Hikosaka et al., 2016b; Launiainen et al., 2011). The reflection coefficient for diffuse radiation is calculated as follows (supplementary material Pedruzo-Bagazgoitia et al. (2017), Hikosaka et al. (2016b, eq 1.21)) $[-]$:

$$\rho_{\mathrm{dif}} = \frac{1-\sqrt{1-\sigma}}{1+\sqrt{1-\sigma}} \tag{S14}$$

In the equation above, a horizontal leaf distribution is used due to the assumed isotropy of diffuse light (supplementary material Pedruzo-Bagazgoitia et al. (2017)). For direct radiation, the reflection coefficient is given by (supplementary material Pedruzo-Bagazgoitia et al. (2017)) $[-]$:

$$\rho_{\mathrm{dir}} = \rho_{\mathrm{dif}} \frac{2}{1+1.6\sin(\beta)} \tag{S15}$$

The PAR falling on a shaded leaf can be calculated as follows $[\mathrm{Wm}^{-2}_{\mathrm{shaded\,leaf}}]$:

$$\mathrm{PAR}_{\mathrm{sha}} = \mathrm{PAR}_{\mathrm{dif,top}} * \tau_{\mathrm{dif}} + (\mathrm{PAR}_{\mathrm{dir,top}} * \tau_{\mathrm{dir,sca}} - \mathrm{PAR}_{\mathrm{dir,top}} * \tau_{\mathrm{dir}}) \tag{S16}$$

wherein the term between brackets contains the secondary diffuse radiation resulting from direct radiation at the top of the canopy (See also Eq. 6 and Eq. 13 of Spitters (1986)). The PAR falling on a horizontally oriented sunlit leaf can be calculated as follows $[\mathrm{Wm}^{-2}_{\mathrm{horizontal\,sunlit\,leaf}}]$:

$$\mathrm{PAR}_{\mathrm{sun}} = \mathrm{PAR}_{\mathrm{dir,top}} + \mathrm{PAR}_{\mathrm{sha}} \tag{S17}$$

as it assumed that the intensity of the direct beam hitting a leaf does not decrease with height. The direct PAR that is absorbed per square meter of sunlit green (photosynthesising) leaves, excluding direct radiation that is scattered and turned into diffuse, can be calculated using the following equation $[\mathrm{Wm}^{-2}_{\mathrm{sunlit\,green\,leaf}}]$:

$$\mathrm{PAR}_{\mathrm{dirdir,abs}} = -1\frac{d\mathrm{PAR}_{\mathrm{dir}}}{d\mathrm{LAI}_{\mathrm{above}}}\frac{1}{\mathrm{fr}_{\mathrm{sun}}}(1-\sigma) \tag{S18}$$

Wherein $\mathrm{fr}_{\mathrm{sun}}$ is the fraction of sunlit leaves ($= \tau_{\mathrm{dir}}$). This factor is necessary to obtain the correct units, we calculate absorption per m^{-2} of sunlit leaf area, in contrast to Eq. 9 of Spitters (1986), where m^{-2} leaf area is used. $\mathrm{PAR}_{\mathrm{dir}}$ $[\mathrm{W\,m}^2_{\mathrm{ground}}]$, the direct radiation remaining from direct radiation at the top of the canopy is defined as follows:

$$\mathrm{PAR}_{\mathrm{dir}} = \mathrm{PAR}_{\mathrm{dir,top}}\,\tau_{\mathrm{dir}} = \mathrm{PAR}_{\mathrm{dir,top}}\exp(-k_{\mathrm{bl}}\mathrm{LAI}_{\mathrm{above}}\,\mathrm{clf}) \tag{S19}$$

Using this equation in equation S18 we get:

$$\mathrm{PAR}_{\mathrm{dirdir,abs}} = k_{\mathrm{bl}} * \mathrm{clf} * (1-\sigma) * \tau_{\mathrm{dir}} * \frac{\mathrm{PAR}_{\mathrm{dir,top}}}{\tau_{\mathrm{dir}}} \tag{S20}$$

wherein τ_{dir} thus cancels out. Note that in Eq. S18, we assume that non-photosynthesising plant material (branches etc.) absorbs the same amount of PAR per m^2 of surface area. The (non-secondary) diffuse PAR (originating from diffuse radiation at the top of the canopy) that is absorbed per square meter leaf, can be calculated using the following equation (See also Pedruzo-Bagazgoitia et al. (2017, supplemantary material eq. 16)):

$$\mathrm{PAR}_{\mathrm{dif,abs}} = -1\frac{d\mathrm{PAR}_{\mathrm{dif}}}{d\mathrm{LAI}_{\mathrm{above}}}(1-\rho_{\mathrm{dif}}) \tag{S21}$$

wherein PAR$_{\text{dif}}$, the radiation resulting from diffuse radiation at the top of the canopy is calculated as follows $[\mathrm{W\,m^2_{ground}}]$:

$$\text{PAR}_{\text{dif}} = \text{PAR}_{\text{dif,top}}\,\tau_{\text{dif}} = \text{PAR}_{\text{dif,top}}\exp(-k_{\text{dif}} * \text{LAI}_{\text{above}}\,\text{clf}) \tag{S22}$$

Using this equation in eq. S21 (See also eq. 10 of Spitters, 1986):

$$\text{PAR}_{\text{dif,abs}} = (1-\rho_{\text{dif}}) * \text{PAR}_{\text{dif,top}} * k_{\text{dif}} * \text{clf} * \tau_{\text{dif}} \tag{S23}$$

Wherein PAR$_{\text{dif,abs}}$ has the units of $[\mathrm{W\,m^2_{leaf}}]$, or more generally $[\mathrm{W\,m^2_{plant\,surface\,area}}]$. We can calculate the fraction of PAR, originating from direct PAR radiation at the top of the canopy, that arrives as direct radiation at a certain height level $[-]$:

$$\text{fr}_{\text{dir,dir}} = \frac{\tau_{\text{dir}}\,\text{PAR}_{\text{dir,top}}}{\text{PAR}_{\text{dir,top}}\,\tau_{\text{dir,sca}}} \tag{S24}$$

One minus this fraction gives the fraction that arrives as diffuse radiation. The reflection coefficient $[-]$ present in the equations for absorbed PAR originating from direct radiation (Eq. S26, Eq. S27) is calculated as a weighted average:

$$\rho_{\text{PARdirabs}} = \text{fr}_{\text{dir,dir}}\rho_{\text{dir}} + (1-\text{fr}_{\text{dir,dir}})\rho_{\text{dif}} \tag{S25}$$

And absorbed PAR originating from direct radiation at the top of the canopy is calculated as (similar to eq. S21) $[\mathrm{Wm^{-2}_{green\,leaf}}]$:

$$\text{PAR}_{\text{dir,abs}} = \frac{-d\text{PAR}_{\text{from dir top}}}{d\text{LAI}_{\text{above}}}(1-\rho_{\text{PARdirabs}}) \tag{S26}$$

Elaborating this equation using Eq. S11, we obtain an equation similar to eq. S23 $[\mathrm{Wm^{-2}_{green\,leaf}}]$:

$$\text{PAR}_{\text{dir,abs}} = (1-\rho_{\text{PARdirabs}}) * \text{PAR}_{\text{dir,top}} * k_{\text{dir,sca}} * \text{clf} * \tau_{\text{dir,sca}} \tag{S27}$$

The equation above is similar to Eq. 11 of Spitters (1986). Absorbed secondary diffuse radiation (diffuse radiation originating from direct radiation at the top of canopy) is calculated as (similar to the second term in the RHS of eq.13 of Spitters, 1986) $[\mathrm{Wm^{-2}_{green\,leaf}}]$:

$$\text{PAR}_{\text{dif,sec,abs}} = \text{PAR}_{\text{dir,abs}} - \text{PAR}_{\text{dirdir,abs}}\,\tau_{\text{dir}} \tag{S28}$$

The factor τ_{dir} is necessary to convert PAR$_{\text{dirdir,abs}}$ from $[\mathrm{Wm^{-2}_{sunlit\,green\,leaf}}]$ to $[\mathrm{Wm^{-2}_{green\,leaf}}]$. Absorbed radiation by shaded green leaves $[\mathrm{Wm^{-2}_{green\,shaded\,leaf}}]$:

$$\text{PAR}_{\text{sha,abs}} = \text{PAR}_{\text{dif,abs}} + \text{PAR}_{\text{dif,sec,abs}} \tag{S29}$$

Absorbed radiation by sunlit leaves $[\mathrm{Wm^{-2}_{green\,sunlit\,leaf}}]$ is the sum of direct radiation at the top of the canopy (as the direct beam itself does not change) and the PAR absorbed by shaded leaves:

$$\text{PAR}_{\text{sun,abs}} = \text{PAR}_{\text{sha,abs}} + \text{PAR}_{\text{dirdir,abs}} \tag{S30}$$

which is similar to eq. 14 of Spitters (1986). Note that, when the upper side of (part of) a leaf is sunlit, we assume the whole leaf area of (that part of) the leaf to be sunlit, we assume the absorbed PAR to be divided over all sides of the (part of the) leaf.

S1.4 Longwave radiation

We do not take the orientation of the leaf into account in the longwave radiation calculations, we assume the flux density per $\mathrm{m^2_{leaf}}$ to be the same as the flux density per $\mathrm{m^2_{ground}}$. Outgoing longwave radiation is calculated using the Stefan–Boltzmann law, separately for each leaf category $[\mathrm{Wm}^{-2}_{\mathrm{leaf}}]$. For example, for sunlit dry leaves in the ith layer we have the following equation:

$$\mathrm{LW}_{\text{out,sun,dry},i} = \varepsilon_{\mathrm{i}}\, 5.67 \times 10^{-8}\, T^4_{\text{s,dry,sun},i} \tag{S31}$$

in which ε_i $[-]$ is the emissivity (=absorptivity) of the leaves, taken identical for each layer. $T_{\text{s,dry,sun},i}$ is the skin temperature of sunlit dry leaves (or leaf parts) in the ith layer. Note that we calculate the outgoing longwave radiation per m^2 of all-sided (sunlit dry) leaf area. Outgoing soil longwave radiation is also calculated, e.g. for sunlit soil:

$$\mathrm{LW}_{\text{out,soil,sun}} = \varepsilon_{\text{soil}}\, 5.67 \times 10^{-8}\, T^4_{\text{s,soil,sun}} \tag{S32}$$

In the above equation $\varepsilon_{\text{soil}}$ $[-]$ is the emissivity of the soil. The units of $\mathrm{LW}_{\text{out,soil,sun}}$ are $[\mathrm{Wm}^{-2}_{\text{sunlit soil}}]$. A weighted average for the soil is calculated $[\mathrm{Wm}^{-2}_{\text{soil}}]$:

$$\mathrm{LW}_{\text{out,soil}} = \mathrm{fr}_{\text{sun,soil}}\, \mathrm{LW}_{\text{out,soil,sun}} + (1 - \mathrm{fr}_{\text{sun,soil}})\, \mathrm{LW}_{\text{out,soil,sha}} \tag{S33}$$

wherein $\mathrm{fr}_{\text{sun,soil}}$ $[-]$ is the fraction of the soil that is sunlit. Incoming longwave radiation flux density $[\mathrm{Wm}^{-2}_{\text{leaf or ground}}]$ is calculated either as the incoming longwave radiation flux density at the top of the canopy $[\mathrm{Wm}^{-2}_{\text{ground}}]$ multiplied with a factor, or based on the outgoing longwave radiation in nearby layers. In the first case (the configuration we recommend for our model) we have the following equation for a leaf in the ith layer $[\mathrm{Wm}^{-2}_{\text{leaf}}]$:

$$\mathrm{LW}_{\text{in,abs},i} = s_{\text{LWin},i}\, \varepsilon_i * \mathrm{LW}_{\text{in,atm}} \tag{S34}$$

In which $s_{\text{LWin},i}$ $[-]$ is a scaling factor (fixed in time, but allowed to vary between layers) that can be optimised, and $\mathrm{LW}_{\text{in,atm}}$ is the incoming longwave radiation at the canopy top $[\mathrm{Wm}^{-2}_{\text{ground}}]$, calculated by CLASS. Note that we calculate the incoming longwave radiation per m^2 of all-sided (sunlit dry) leaf area. The absorbed longwave radiation for the soil $[\mathrm{Wm}^{-2}_{\text{ground}}]$ is (in the first case mentioned above) calculated as:

$$\mathrm{LW}_{\text{in,abs,soil}} = s_{\text{LWin,soil}}\, \varepsilon_{\text{soil}} * \mathrm{LW}_{\text{in,atm}} \tag{S35}$$

In the second case we first roughly estimate the outgoing longwave radiation flux density of all layers. To estimate the outgoing longwave radiation flux density of the ith layer $[\mathrm{Wm}^{-2}_{\text{ground}}]$, we calculate a weighted average:

$$\mathrm{LW}_{\text{out},i} = (1 - \mathrm{fr}_{\text{wet},i}) * (\mathrm{fr}_{\text{sun},i}\mathrm{LW}_{\text{out,sun,dry},i} + (1 - \mathrm{fr}_{\text{sun},i})\mathrm{LW}_{\text{out,sha,dry},i}) + \mathrm{fr}_{\text{wet},i} * (\mathrm{fr}_{\text{sun},i}\mathrm{LW}_{\text{out,sun,wet},i} + (1 - \mathrm{fr}_{\text{sun},i})\mathrm{LW}_{\text{out,sha,wet},i}) \tag{S36}$$

wherein $\mathrm{fr}_{\text{wet},i}$ is the fraction of plant material that is wet in the ith layer, and $\mathrm{fr}_{\text{sun},i}$ is the fraction of plant material that is sunlit in the ith layer (See Eq. S13). Note that leaf area index of the layer is not directly used in the above rough estimation. For the incoming longwave radiation (in the second case), we have the following equation for a layer with index i, that is not the top or bottom layer $[\mathrm{Wm}^{-2}_{\text{leaf}}]$:

$$\mathrm{LW}_{\text{in,abs},i} = s_{\text{LWin},i}\, \frac{\varepsilon_i * (\mathrm{LW}_{\text{out},i-1} + \mathrm{LW}_{\text{out},i+1})}{2} \tag{S37}$$

And for a leaf in the top and bottom layer respectively (with index i) $[\mathrm{Wm}^{-2}_{\text{leaf}}]$:

$$\mathrm{LW}_{\text{in,abs,top layer}} = s_{\text{LWin},i}\, \frac{\varepsilon_i * (\mathrm{LW}_{\text{out},i-1} + \mathrm{LW}_{\text{in,atm}})}{2} \tag{S38}$$

$$\mathrm{LW}_{\text{in,abs,bot layer}} = s_{\text{LWin},i}\, \frac{\varepsilon_i * (\mathrm{LW}_{\text{out,soil}} + \mathrm{LW}_{\text{out},i+1})}{2} \tag{S39}$$

The factor 1/2 arises because we calculate the radiation per m^2 of all-sided leaf area, we average the radiation over both the upper and lower sides of the leaf. In this second case we have the following equation for the soil $[\mathrm{Wm}^{-2}_{\text{ground}}]$:

$$\mathrm{LW}_{\text{in,abs,soil}} = s_{\text{LWin,soil}}\, \varepsilon_{\text{soil}} * \mathrm{LW}_{\text{out,0}} \tag{S40}$$

wherein $\mathrm{LW}_{\text{out,0}}$ is the outgoing longwave radiation flux density of the bottom layer $[\mathrm{Wm}^{-2}_{\text{ground}}]$.

S1.5 Heat and H_2O fluxes vegetation

The vegetative fluxes are calculated separately for each category of leaves in each layer. For calculating the H_2O fluxes we first calculate a few additional quantities. First the resistance for transpiration of water $[\mathrm{s\,m^{-1}}]$, for a sunlit dry leaf and shaded dry leaf respectively, in the ith layer:

$$r_{\text{H2O,sun,dry},i} = r_{\text{b,H2O},i} + \left(\frac{\text{SF}}{r_{\text{cut,H2O}}} + \frac{1}{r_{\text{s,H2O,sun,dry},i}}\right)^{-1} \tag{S41}$$

$$r_{\text{H2O,sha,dry},i} = r_{\text{b,H2O},i} + \left(\frac{\text{SF}}{r_{\text{cut,H2O}}} + \frac{1}{r_{\text{s,H2O,sha,dry},i}}\right)^{-1} \tag{S42}$$

wherein $r_{\text{b,H2O},i}$ is the leaf boundary layer resistance for water vapour in the ith layer, $r_{\text{cut,H2O}}$ is a constant representing the cuticular resistance for H_2O $[\mathrm{s\,m^{-1}}]$, and $r_{\text{s,H2O,sun,dry},i}$ is the stomatal resistance for water vapour for sunlit dry leaves in the ith layer. SF $[-]$ stands for 'sides factor' and is defined as follows:

$$\text{SF} = \begin{cases} 1, & \text{if stomata on all sides of leaf} \\ 2, & \text{if stomata on only one side of leaf (assuming two-sided leaf with equal area on both sides)} \end{cases} \tag{S43}$$

The presence of stomata on one or on all sides of the leaves is controlled by a switch than can be set by the user. A sketch of the resistance schemes for dry leaf area for both cases is shown in Fig. S1. The stomatal resistance for water vapour (for e.g. sunlit dry leaves in the ith layer) is calculated as $[\mathrm{s\,m^{-1}}]$ (See also Eq. 3.8 Jacobs, 1994):

$$r_{\text{s,H2O,sun,dry},i} = \frac{1}{1.6\, g_{\text{s,CO2,sun,dry},i}} \tag{S44}$$

wherein $g_{\text{s,CO2,sun,dry},i}$ (stomatal conductance for CO_2 for sunlit dry leaves in ith layer) is calculated with Eq. S99. The boundary layer resistance for H_2O $[\mathrm{s\,m^{-1}}]$ in layer i is only a function of wind speed and is calculated as (similar to MLC-CHEM, see also Meyers et al. (1989) Eq. 7a and Eckert and (translator) Gross (1963), as cited by Meyers et al. (1989)):

$$r_{\text{b,H2O},i} = 180\left(\frac{0.07}{\max[10^{-10}, U_i]}\right)^{0.5} \tag{S45}$$

wherein U_i is the wind speed in layer i $[\mathrm{m\,s^{-1}}]$. The saturated water water vapour pressure inside the substomatal cavity of a (sunlit dry) leaf in a layer with index i, $e_{\text{sat}}(T_{\text{s,sun,dry}})_{\text{L},i}$, is calculated by linearising the e_{sat} function around $T = T_{\text{a}}$ (air temperature, [K]), for reasons explained in section S1.7:

$$e_{\text{sat}}(T_{\text{s,sun,dry}})_{\text{L},i} = e_{\text{sat}}(T_{\text{a},i}) + \left.\frac{de_{\text{sat}}}{dT}\right|_{T=T_{\text{a},i}} (T_{\text{s,sun,dry},i} - T_{\text{a},i}) \tag{S46}$$

wherein the subscript L indicates 'linearised'. The saturated water water vapour pressures in this equation have the units [Pa]. For the e_{sat} function we use Tetens formula. The saturated water molar concentration inside the substomatal cavity of a (sunlit dry) leaf $[\mathrm{mol_{H2O}\,m^{-3}}]$:

$$C_{\text{H2Osat}}(T_{\text{s,sun,dry},i})_{\text{L},i} = e_{\text{sat}}(T_{\text{s,sun,dry},i})_{\text{L}} \frac{1}{P_i}\, \rho_{\text{air}} \frac{1000}{M_{\text{air}}} \tag{S47}$$

wherein ρ_{air} is air density $[\mathrm{kg\,m^{-3}}]$ and M_{air} is the molar mass of air $[\mathrm{g\,mol^{-1}}]$, both are constant in the model, both in space and time. P_i is the air pressure at the canopy node we do the calculation for (Eq. S3). Using the previous equations, the water vapour flux of a sunlit dry leaf with layer index i $[\mathrm{mol\,m_{leaf}^{-2}\,s^{-1}}]$ is given by:

$$F_{\text{H2O,sun,dry},i} = \frac{C_{\text{H2Osat}}(T_{\text{s,sun,dry},i})_{\text{L},i} - C_{\text{H2O,a},i}}{r_{\text{H2O,sun,dry},i}} \tag{S48}$$

wherein $C_{\mathrm{H2O,a},i}$ is the H_2O concentration in the air in the canopy layer with index i $[\mathrm{mol_{H2O}\,m^{-3}}]$. In case of stomata on all sides of the leaf, the equation above represents the flux per m^2 of all-sided leaf area. In the other case (SF=2), the flux differs between both sides of the leaf and the equation above represents the total flux per m^2 of one-sided leaf area. See however Sect. S1.14 for a critical note. For a wet leaf (e.g sunlit wet), the resistance is less since the water does not need to pass through the stomata or cuticle:

$$F_{\mathrm{H2O,sun,wet}} = \frac{C_{\mathrm{H2Osat}}(T_{\mathrm{s,sun,wet}})_{\mathrm{L}} - C_{\mathrm{H2O,a}}}{r_{\mathrm{b,H2O}}} \tag{S49}$$

The H_2O flux from the dry vegetation in layer i $[\mathrm{mol\,m_{ground}^{-2}\,s^{-1}}]$ is calculated as a weighted average:

$$F_{\mathrm{H2O,veg,dry},i} = \frac{1}{\mathrm{SF}}\left(F_{\mathrm{H2O,sun,dry},i}\,\mathrm{LAI}_{\mathrm{sun,dry},i} + F_{\mathrm{H2O,sha,dry},i}\,\mathrm{LAI}_{\mathrm{sha,dry},i}\right) \tag{S50}$$

Division by SF is necessary in case the stomata are located on only one side of the leaf. Note that also in that case, we account for the cuticular pathway being present on both sides of the leaf, via Eq. S41 and Eq. S42. $\mathrm{LAI}_{\mathrm{sun,dry},i}$ represents the amount of all-sided leaf area that is dry and sunlit in the ith layer $[\mathrm{m^2_{sunlit\ dry\ leaf}\,m^{-2}_{ground}}]$. It is calculated as follows:

$$\mathrm{LAI}_{\mathrm{sun,dry},i} = \mathrm{LAI}_i\,\mathrm{fr}_{\mathrm{sun},i}(1-\mathrm{fr}_{\mathrm{wet},i}) \tag{S51}$$

wherein $\mathrm{fr}_{\mathrm{sun},i}$ is the fraction of sunlit leaves in the ith layer (Eq. S13) and $\mathrm{fr}_{\mathrm{wet},i}$ is the fraction of vegetation area that is wet in the ith layer (Eq. S130). Note that both quantities can also vary in time. The LAI of the other three leaf categories is calculated in a similar way. The H_2O flux from the wet vegetation in layer i $[\mathrm{mol\,m_{ground}^{-2}\,s^{-1}}]$ is calculated as follows:

$$F_{\mathrm{H2O,veg,wet},i} = \frac{1}{\mathrm{fr}_{\mathrm{green},i}}\left(F_{\mathrm{H2O,sun,wet},i}\,\mathrm{LAI}_{\mathrm{sun,wet},i} + F_{\mathrm{H2O,sha,wet},i}\,\mathrm{LAI}_{\mathrm{sha,wet},i}\right) \tag{S52}$$

Note that division by $\mathrm{fr}_{\mathrm{green},i}$ $[-]$ is necessary to include the evaporation flux from branches etc. For the sensible heat flux, we first calculate the boundary layer resistance for heat $[\mathrm{s\,m^{-1}}]$ in layer i as (Martin et al., 1999; Monteith and Unsworth, 1990):

$$r_{\mathrm{b,Heat},i} = \frac{r_{\mathrm{b,H2O},i}}{0.93} \tag{S53}$$

The sensible heat flux from a sunlit dry leaf $[\mathrm{W\,m^{-2}_{sunlit\ dry\ leaf}}]$ is given by:

$$H_{\mathrm{sun,dry}} = \rho_{\mathrm{air}}\,c_{\mathrm{p}}\,\frac{T_{\mathrm{s,sun,dry}} - T_{\mathrm{a}}}{r_{\mathrm{b,heat}}} \tag{S54}$$

wherein ρ_{air} $[\mathrm{kg\,m^{-3}}]$ is air density and c_{p} is the specific heat of dry air at constant pressure $[\mathrm{J\,kg^{-1}\,K^{-1}}]$. The sensible heat flux for the other leaf categories is calculated similarly, e.g. for shaded wet leaf area:

$$H_{\mathrm{sha,wet}} = \rho_{\mathrm{air}}\,c_{\mathrm{p}}\,\frac{T_{\mathrm{s,sha,wet}} - T_{\mathrm{a}}}{r_{\mathrm{b,heat}}} \tag{S55}$$

The total sensible heat flux from the vegetation in layer i $[\mathrm{W\,m^{-2}_{ground}}]$ is calculated as a weighted average:

$$H_{\mathrm{veg},i} = \frac{1}{\mathrm{fr}_{\mathrm{green},i}}\left(H_{\mathrm{sun,dry},i}\,\mathrm{LAI}_{\mathrm{sun,dry},i} + H_{\mathrm{sha,dry},i}\,\mathrm{LAI}_{\mathrm{sha,dry},i} + H_{\mathrm{sun,wet},i}\,\mathrm{LAI}_{\mathrm{sun,wet},i} + H_{\mathrm{sha,wet},i}\,\mathrm{LAI}_{\mathrm{sha,wet},i}\right) \tag{S56}$$

Note that division by $\mathrm{fr}_{\mathrm{green},i}$ is necessary to include the heat flux from branches etc.

S1.6 Heat and H_2O fluxes soil

We first calculate the air temperature at 0 m height above the soil [K]:

$$T_{\mathrm{a,0m}} = T_{\mathrm{a,0}} \left(\frac{P_{\mathrm{s}}}{P_0} \right)^{\frac{R_{\mathrm{d}}}{c_{\mathrm{p}}}} \tag{S57}$$

wherein $T_{\mathrm{a,0}}$ [K] and P_0 [Pa] are the air temperature and pressure respectively at the node in the lowest layer of the canopy. P_{s} [Pa] is the air pressure at the soil surface. R_{d} is the gas constant for dry air with units $\mathrm{J\,kg^{-1}\,K^{-1}}$. The soil sensible heat flux (sunlit) $[\mathrm{W\,m^{-2}}]$ is calculated as:

$$H_{\mathrm{soil,sun}} = \rho_{\mathrm{air}}\, c_{\mathrm{p}} \frac{T_{\mathrm{s,soil,sun}} - T_{\mathrm{a,0m}}}{r_{\mathrm{a,soil,heat}}} \tag{S58}$$

wherein $r_{\mathrm{a,soil,heat}}$ $[\mathrm{s\,m^{-1}}]$ is the aerodynamic resistance for heat transport between the soil surface and the first vegetation layer. It is calculated as (Bonan et al., 2018):

$$r_{\mathrm{a,soil,heat}} = \frac{1}{0.4^2\, U_0} \log\left(\frac{z_0}{0.01}\right) \log\left(\frac{z_0}{0.001}\right) \tag{S59}$$

wherein z_0 is the height at which the node in the first vegetation layer is placed [m], and U_0 is the wind speed in the lowest vegetation layer $[\mathrm{m\,s^{-1}}]$. The shaded soil flux is calculated similarly. The total soil sensible heat flux $[\mathrm{W\,m^{-2}}]$ is a weighted average between sunlit and shaded soil:

$$H = \mathrm{fr}_{\mathrm{sun,soil}}\, H_{\mathrm{soil,sun}} + (1 - \mathrm{fr}_{\mathrm{sun,soil}}) H_{\mathrm{soil,sha}} \tag{S60}$$

The (sunlit) soil H_2O flux $[\mathrm{mol\,m^{-2}\,s^{-1}}]$ is calculated as:

$$F_{\mathrm{H2O,sun,soil}} = \frac{\mathrm{RH}_{\mathrm{soil}}\, C_{\mathrm{H2Osat}}(T_{\mathrm{s,sun,soil}})_{\mathrm{L}} - C_{\mathrm{H2O,0}}}{r_{\mathrm{soil,H2O}} + r_{\mathrm{a,soil,heat}}} \tag{S61}$$

wherein $\mathrm{RH}_{\mathrm{soil}}$ $[-]$ is the fractional humidity in the soil air (Ma and Liu, 2019; Bonan et al., 2018) at the location where T = $T_{\mathrm{s,sun,soil}}$, the user should provide the constant value of $\mathrm{RH}_{\mathrm{soil}}$. $r_{\mathrm{soil,H2O}}$ is the part of the resistance that accounts for the transport inside the soil, for this we use the variable 'rssoil' calculated by CLASS. Note that we use $r_{\mathrm{a,soil,heat}}$ both for heat and water vapour. $C_{\mathrm{H2O,0}}$ $[\mathrm{mol\,m^{-3}}]$ is the water vapour molar concentration in the lowest vegetation layer. Note that we linearise (indicated by subscript L) $C_{\mathrm{H2Osat}}(T)$ around T = $T_{\mathrm{a,0m}}$, for reasons explained in Sect. S1.7. The total soil H_2O flux $[\mathrm{mol\,m^{-2}\,s^{-1}}]$ is calculated as:

$$F_{\mathrm{H2O,soil}} = \mathrm{fr}_{\mathrm{sun,soil}}\, F_{\mathrm{H2O,soil,sun}} + (1 - \mathrm{fr}_{\mathrm{sun,soil}}) F_{\mathrm{H2O,soil,sha}} \tag{S62}$$

Besides the soil sensible heat and soil H_2O fluxes, we also calculate the soil heat flux (positive if heat flows into the soil), seperately for sunlit and shaded soil $[\mathrm{W\,m^{-2}_{sunlit\,or\,shaded\,soil}}]$:

$$G_{\mathrm{soil,sun}} = \lambda\,(T_{\mathrm{s,soil,sun}} - T_{\mathrm{soil}}) \tag{S63}$$

$$G_{\mathrm{soil,sha}} = \lambda\,(T_{\mathrm{s,soil,sha}} - T_{\mathrm{soil}}) \tag{S64}$$

wherein T_{soil} [K] is the soil temperature of the upper soil layer, calculated by CLASS. λ is a thermal diffusivity $[\mathrm{W\,m^{-2}K^{-1}}]$. The total soil heat flux $[\mathrm{W\,m^{-2}_{ground}}]$ is calculated as follows:

$$G_{\mathrm{soil}} = \mathrm{fr}_{\mathrm{sun,soil}}\, G_{\mathrm{soil,sun}} + (1 - \mathrm{fr}_{\mathrm{sun,soil}}) G_{\mathrm{soil,sha}} \tag{S65}$$

Note that $\mathrm{fr}_{\mathrm{sun,soil}}$ $[-]$ is calculated by using Eq. S13, with $\mathrm{LAI}_{\mathrm{above}}$ equal to the total LAI of the canopy (and including branches etc.).

S1.7 Energy balance

The energy balance on a leaf surface in a vegetation layer is given by the following equation $[\mathrm{W\,m_{leaf}^{-2}}]$:

$$\mathrm{SW_{in,abs}} + \mathrm{LW_{in,abs}} - \mathrm{LW_{out}} = H + LE + S_{\mathrm{Heat}} \tag{S66}$$

wherein the LHS contains radiation terms and the RHS consists respectively of the sensible heat flux, latent heat flux and heat storage inside the leaf. The absorbed shortwave radiation for a leaf surface ($\mathrm{SW_{in,abs}}$) is calculated as follows:

$$\mathrm{SW_{in,abs}} = \frac{1}{\mathrm{fr_{PAR}}} \mathrm{PAR_{abs}} \tag{S67}$$

wherein $\mathrm{fr_{PAR}}$ $[-]$ is the fraction of shortwave radiation that is within the range of PAR (see Eq. S5), and the calculation of $\mathrm{PAR_{abs}}$ is shown in Sect. S1.3 (Eq. S30 for sunlit leaf area, Eq. S29 for shaded leaf area). Note that we assume $\mathrm{fr_{PAR}}$ to be fixed within the canopy, and we assume no preferential absorption of PAR compared to $\mathrm{SW_{in}}$. For the longwave radiation terms in Eq. S66, see Sect. S1.4. The skin temperature follows from elaborating and rewriting the energy balance. In the energy balance equation, H and LE are in our model a linear function of T_{s}, while $\mathrm{LW_{out}}$ is a non-linear function of T_{s}. To more easily solve the energy balance equation for T_{s}, we take $\mathrm{LW_{out}}$ from the previous iteration/time step, so its dependence on the current T_{s} is removed. Additionally, note that we linearised $LE(T_{\mathrm{s}})$ around the air temperature, so that LE is a linear function of T_{s} (Sect. S1.5). The latent heat flux $[\mathrm{W\,m_{leaf}^{-2}}]$ can be obtained from the $\mathrm{H_2O}$ flux $[\mathrm{mol\,m_{leaf}^{-2}\,s^{-1}}]$ as follows:

$$LE = \frac{M_{\mathrm{H2O}}\, L_{\mathrm{v}}\, F_{\mathrm{H2O}}}{1000} \tag{S68}$$

wherein M_{H2O} is the molar mass of water $[\mathrm{g\,mol^{-1}}]$ and L_{v} the latent heat of vaporisation $[\mathrm{J\,kg^{-1}}]$. Heat storage S_{Heat} $[\mathrm{W\,m_{leaf}^{-2}}]$ is defined as a fraction $\mathrm{fr_{Hsto}}$ $[-]$ of the absorbed net radiation:

$$S_{\mathrm{Heat}} = \mathrm{fr_{Hsto}}\, (\mathrm{SW_{in,abs}} + \mathrm{LW_{in,abs}} - \mathrm{LW_{out}}) \tag{S69}$$

This is somewhat similar to Ma and Liu (2019), who define it as a fraction of the sensible heat flux. Our choice is a pragmatic choice, as this term is difficult to model. The energy balance equation is calculated for all four categories of leaves. For a sunlit dry leaf it becomes $[\mathrm{W\,m_{leaf}^{-2}}]$ (using Eq. S54 and Eq. S48):

$$\mathrm{SW_{in,abs}} + \mathrm{LW_{in,abs}} - \mathrm{LW_{out}} = \frac{\rho_{\mathrm{air}} c_{\mathrm{p}} (T_{\mathrm{s}} - T_{\mathrm{a}})}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000} \frac{1}{\mathrm{SF}} \left(\frac{C_{\mathrm{H2Osat}}(T_{\mathrm{s}})_{\mathrm{L}} - C_{\mathrm{H2O,a}}}{r_{\mathrm{H2O,sun,dry}}} \right) + S_{\mathrm{Heat}} \tag{S70}$$

wherein $r_{\mathrm{H2O,sun\ dry}}$ is defined in Eq. S41. The factor $\frac{1}{\mathrm{SF}}$ is added for the case that stomata are present on only one side of the leaf. This factor is only applied to LE, as the other terms do not include a stomatal resistance. As also e.g. incoming shortwave radiation is averaged over all sides of a leaf (Sect. S1.3), we thus calculate a skin temperature based on fluxes averaged over the two sides of the leaf. Implementing Eq. S47 and Eq. S46 from Sect. S1.5 into the equation above we get:

$$\mathrm{SW_{in,abs}} + \mathrm{LW_{in,abs}} - \mathrm{LW_{out}} = \frac{\rho_{\mathrm{air}} c_{\mathrm{p}} (T_{\mathrm{s}} - T_{\mathrm{a}})}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} \left(C_{\mathrm{H2Osat}}(T_{\mathrm{a}}) + \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}} (T_{\mathrm{s}} - T_{\mathrm{a}}) - C_{\mathrm{H2O,a}} \right) + S_{\mathrm{Heat}} \tag{S71}$$

wherein P is the pressure at the node of the vegetation layer we consider. An explicit expression for $T_{\mathrm{s,sun,dry}}$ (shortened to T_s) can be obtained from this equation. Rewriting the equation above:

$$\begin{aligned} &\left(\frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}} \right) T_{\mathrm{s}} = \mathrm{SW_{in,abs}} + \mathrm{LW_{in,abs}} - \mathrm{LW_{out}} - S_{\mathrm{Heat}} + \\ &\frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}\, T_{\mathrm{a}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}} T_{\mathrm{a}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} (C_{\mathrm{H2O,a}} - C_{\mathrm{H2Osat}}(T_{\mathrm{a}})) \end{aligned} \tag{S72}$$

And thus:

$$T_{\mathrm{s,sun,dry}} = \frac{\mathrm{SW}_{\mathrm{in,abs}} + \mathrm{LW}_{\mathrm{in,abs}} - \mathrm{LW}_{\mathrm{out}} - S_{\mathrm{Heat}} + \frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}\, T_{\mathrm{a}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} \left(\left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}\, T_{\mathrm{a}}}{P M_{\mathrm{air}}} - C_{\mathrm{H2Osat}}(T_{\mathrm{a}}) + C_{\mathrm{H2O,a}} \right)}{\frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{H2O,sun,dry}}} \frac{1}{\mathrm{SF}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}}} \tag{S73}$$

A very similar equation applies to a shaded dry leaf, but variables $\mathrm{LW}_{\mathrm{out}}$, $\mathrm{SW}_{\mathrm{in,abs}}$ and S_{Heat} differ between sunlit and shaded leaves, and $r_{\mathrm{H2O,sha,dry}}$ should be used instead of $r_{\mathrm{H2O,sun,dry}}$. We give here also the equation for a wet leaf:

$$T_{\mathrm{s,wet}} = \frac{\mathrm{SW}_{\mathrm{in,abs}} + \mathrm{LW}_{\mathrm{in,abs}} - \mathrm{LW}_{\mathrm{out}} - S_{\mathrm{Heat}} + \frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}\, T_{\mathrm{a}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{b,H2O}}} \left(\left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}\, T_{\mathrm{a}}}{P M_{\mathrm{air}}} - C_{\mathrm{H2Osat}}(T_{\mathrm{a}}) + C_{\mathrm{H2O,a}} \right)}{\frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}}{r_{\mathrm{b,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 r_{\mathrm{b,H2O}}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}}} \tag{S74}$$

Again, $\mathrm{LW}_{\mathrm{out}}$, $\mathrm{SW}_{\mathrm{in,abs}}$ and S_{Heat} differ between sunlit and shaded leaf area. Note that we assume that wet leaf area can occur on all sides of the leaf (Sect. S1.10). For the soil surface we have a slightly different energy balance (we leave out the subscript soil in the radiation terms, for brevity):

$$\mathrm{SW}_{\mathrm{in,abs}} + \mathrm{LW}_{\mathrm{in,abs}} - \mathrm{LW}_{\mathrm{out}} = \frac{\rho_{\mathrm{air}} c_{\mathrm{p}} (T_{\mathrm{s}} - T_{\mathrm{a,0m}})}{r_{\mathrm{a,soil,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000} \left(\frac{\mathrm{RH}_{\mathrm{soil}}\, C_{\mathrm{H2Osat}}(T_{\mathrm{s}})_{\mathrm{L}} - C_{\mathrm{H2O,a}}}{r_{\mathrm{soil,H2O}} + r_{\mathrm{a,soil,heat}}} \right) + G \tag{S75}$$

wherein the terms have the units $\mathrm{W\,m^{-2}_{sunlit\,soil}}$ when considering sunlit soil or $\mathrm{W\,m^{-2}_{shaded\,soil}}$ when considering shaded soil. See Sect. S1.6 for more information on the terms in the right hand side of the equation. G is given by Eq. S63 or Eq. S64. $C_{\mathrm{H2Osat}}(T_{\mathrm{s}})$ was linearised around $T_{\mathrm{s}} = T_{\mathrm{a,0m}}$, the temperature at 0 m height above the soil (Sect. S1.6), to make the relation between soil evaporation and T_{s} linear, which simplifies the skin temperature calculation. The absorbed shortwave radiation for a soil surface ($\mathrm{SW}_{\mathrm{in,abs}}$ $[\mathrm{W\,m^{-2}_{ground}}]$) is calculated as follows:

$$\mathrm{SW}_{\mathrm{in,abs,soil}} = (1 - \mathrm{alb}_{\mathrm{soil}}) \frac{1}{\mathrm{fr}_{\mathrm{PAR}}} \mathrm{PAR}_{\mathrm{soil}} \tag{S76}$$

wherein $\mathrm{PAR}_{\mathrm{soil}}$ $[\mathrm{W\,m^{-2}_{ground}}]$ is the amount of PAR reaching the soil (differs between sunlit and shaded soil surface area), and $\mathrm{alb}_{\mathrm{soil}}$ $[-]$ is the soil albedo. $\mathrm{fr}_{\mathrm{PAR}}$ is a constant in the model, introduced in Eq. S5. Expanding the soil surface energy balance equation:

$$\mathrm{SW}_{\mathrm{in,abs}} + \mathrm{LW}_{\mathrm{in,abs}} - \mathrm{LW}_{\mathrm{out}} = \frac{\rho_{\mathrm{air}} c_{\mathrm{p}} (T_{\mathrm{s}} - T_{\mathrm{a,0m}})}{r_{\mathrm{a,soil,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000} \left(\frac{\mathrm{RH}_{\mathrm{soil}}\, C_{\mathrm{H2Osat}}(T_{\mathrm{a,0m}}) + \mathrm{RH}_{\mathrm{soil}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a,0m}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}} (T_{\mathrm{s}} - T_{\mathrm{a,0m}}) - C_{\mathrm{H2O,a}}}{r_{\mathrm{soil,H2O}} + r_{\mathrm{a,soil,heat}}} \right) + \lambda\,(T_{\mathrm{s}} - T_{\mathrm{soil}}) \tag{S77}$$

When defining $Q = \mathrm{SW}_{\mathrm{in,abs}} + \mathrm{LW}_{\mathrm{in,abs}} - \mathrm{LW}_{\mathrm{out}}$, the resulting skin temperature [K] becomes (given here for sunlit soil):

$$T_{\mathrm{s,soil,sun}} = \frac{Q + \frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}\, T_{\mathrm{a,0m}}}{r_{\mathrm{a,soil,heat}}} + \lambda\, T_{\mathrm{soil}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 (r_{\mathrm{soil,H2O}} + r_{\mathrm{a,soil,heat}})} \left(\mathrm{RH}_{\mathrm{soil}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a,0m}}} \frac{1000 \rho_{\mathrm{air}}\, T_{\mathrm{a,0m}}}{P M_{\mathrm{air}}} - \mathrm{RH}_{\mathrm{soil}}\, C_{\mathrm{H2Osat}}(T_{\mathrm{a,0m}}) + C_{\mathrm{H2O,a}} \right)}{\frac{\rho_{\mathrm{air}}\, c_{\mathrm{p}}}{r_{\mathrm{a,soil,heat}}} + \frac{M_{\mathrm{H2O}} L_{\mathrm{v}}}{1000 (r_{\mathrm{soil,H2O}} + r_{\mathrm{a,soil,heat}})} \mathrm{RH}_{\mathrm{soil}} \left.\frac{de_{\mathrm{sat}}}{dT}\right|_{T=T_{\mathrm{a,0m}}} \frac{1000 \rho_{\mathrm{air}}}{P M_{\mathrm{air}}} + \lambda}$$

(S78)

For shaded soil, the same equation is used, only the variables $\mathrm{SW_{in,abs}}$ and $\mathrm{LW_{out}}$ differ compared to sunlit soil in the equation above.

S1.8 Photosynthesis and COS exchange vegetation

S1.8.1 Photosynthesis

For calculating stomatal conductance and photosynthesis, we follow the A-gs approach (Jacobs, 1994; Ronda et al., 2001), but our method of integrating over the canopy differs. We assume all conditions for each leaf category inside a layer to be constant, thus for upscaling from leaf to layer level, a simple weighted average multiplication with leaf area index of each leaf category in the considered layer suffices. We give here the equations we use in our model and some extra information, for more details on A-gs, see Jacobs (1994). We first calculate the $\mathrm{CO_2}$ compensation point $[\mathrm{mg_{CO2}\,m_{air}^{-3}}]$:

$$[\mathrm{CO_2}]_{\mathrm{comp}} = \rho_{\mathrm{air}}\,[\mathrm{CO_2}]_{\mathrm{comp,ref}}\,{Q_{10,\mathrm{CO2}}}^{0.1(T_{\mathrm{a}}-298)} \tag{S79}$$

Which is consistent with equation 3.14 of Jacobs (1994) (rounding 298 K to 25 degrees Celcius, and taking T in equation 3.14 of Jacobs (1994) as air temperature). The units of $[\mathrm{CO_2}]_{\mathrm{comp,ref}}$ are $[\mathrm{mg_{CO2}\,kg_{air}^{-1}}]$ and $Q_{10,\mathrm{CO2}}$ is dimensionless. Mesophyll conductance $[\mathrm{m\,s^{-1}}]$ is calculated consistent with equation 3.15 of Jacobs (1994) (rounding 25 degrees Celcius to 298 K, and taking T in equation 3.15 of Jacobs (1994) as air temperature):

$$g_{\mathrm{m}} = \frac{g_{\mathrm{m,ref}}\,{Q_{10,\mathrm{gm}}}^{0.1(T_{\mathrm{a}}-298)}}{1000(1+\exp[0.3*(T_{1,gm}-T_{\mathrm{a}})])(1+\exp[0.3*(T_{\mathrm{a}}-T_{2,gm})])} \tag{S80}$$

In the equation above, $g_{\mathrm{m,ref}}$ has the units $[\mathrm{mm\,s^{-1}}]$ (there is a factor 1000 in the denominator of the equation above) and $Q_{10,\mathrm{gm}}$ is dimensionless. $T_{1,gm}$ and $T_{2,gm}$ are constant reference temperatures [K]. We use equation A9 From Ronda et al. (2001) (with 1/9 $\approx$ 0.11) to calculate a variable f_{min} $[-]$:

$$f_{\mathrm{min}} = \frac{-(\frac{g_{\mathrm{min,H2O}}}{1.6}-\frac{g_{\mathrm{m}}}{9})+\sqrt{(\frac{g_{\mathrm{min,H2O}}}{1.6}-\frac{g_{\mathrm{m}}}{9})^2+\frac{4g_{\mathrm{min,H2O}}\,g_{\mathrm{m}}}{1.6}}}{2g_{\mathrm{m}}} \tag{S81}$$

Note that we use (as in Ronda et al., 2001) the value of 1.6 (ratio of molecular diffusivities of water and $\mathrm{CO_2}$ in air). In case $g_{\mathrm{min,H2O}}$ $[\mathrm{m\,s^{-1}}]$ represents a minimum stomatal conductance (for water vapour), this will be the most appropriate value. If however $g_{\mathrm{min,H2O}}$ represents a cuticular conductance, the value of 30 (Eq. S101) might be more appropriate. For simplicity, we stick with the number from Ronda et al. (2001). The vapour pressure deficit [kPa]:

$$D_{\mathrm{s}} = \frac{e_{\mathrm{sat}}(T_{\mathrm{s}})-e}{1000} \tag{S82}$$

wherein e [Pa] is the water vapor pressure in the air of the considered canopy layer, for e_{sat} see Sect. S1.5. In case D_{s} is negative, we force it to be 0 in the A-gs equations. We calculate D_0 [kPa], the value of D_{s} at which the stomata close (Eq. 13 of Ronda et al., 2001):

$$D_0 = \frac{f_0 - f_{\mathrm{min}}}{a_{\mathrm{d}}} \tag{S83}$$

wherein f_0 $[-]$ and a_{d} $[\mathrm{kPa^{-1}}]$ are constants, more information can be found in Ronda et al. (2001). In the equation below we calculate a variable C_{frac} $[-]$, used in our later Eq.S86 to calculate the internal $\mathrm{CO_2}$ concentration inside the substomatal cavity (See also Eq. 3.25 Jacobs, 1994):

$$C_{\mathrm{frac}} = f_0\left(1-\frac{D_{\mathrm{s}}}{D_0}\right)+f_{\mathrm{min}}\frac{D_{\mathrm{s}}}{D_0} \tag{S84}$$

The variable C_{frac} corresponds to variable f in Jacobs (1994), which is defined in Equation 3.20 of Jacobs (1994). Note that, when $D_{\text{s}} = D_0$, C_{frac} equals f_{min}, and when $D_{\text{s}} = 0$, C_{frac} equals f_0. Note also that, when using Eq. S83, the equation above could actually also be written as:

$$C_{\text{frac}} = f_0 - D_{\text{s}} a_{\text{d}} \tag{S85}$$

which shows that f_{min} is here not the minimum value of C_{frac}, as for an infinitely large D_{s}, C_{frac} goes to minus infinity. The internal CO$_2$ concentration $[\text{mg}_{\text{CO2}}\,\text{m}^{-3}]$ is calculated using Eq. 3.21 (or equivalently 3.20) of Jacobs (1994):

$$[\text{CO}_2]_{\text{int}} = C_{\text{frac}}([\text{CO}_2] - [\text{CO}_2]_{\text{comp}}) + [\text{CO}_2]_{\text{comp}} \tag{S86}$$

wherein $[\text{CO}_2]$ is the CO$_2$ concentration $[\text{mg}_{\text{CO2}}\,\text{m}^{-3}]$ in the air outside the leaf boundary layer. The maximal assimilation rate without CO$_2$, soil moisture or light limitation $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$ (triose-phosphate-utilisation-limited net rate of photosynthesis, Van Diepen et al. (2022)) is calculated consistent with equation 3.15 of Jacobs (1994) (rounding 25 degrees Celcius to 298 K, and taking T in equation 3.15 of Jacobs (1994) as air temperature):

$$A_{\text{m,max}} = \frac{A_{\text{m,max,ref}}\, {Q_{10,\text{Am}}}^{0.1(T_{\text{a}}-298)}}{(1+\exp[0.3*(T_{1,Am} - T_{\text{a}})])(1+\exp[0.3*(T_{\text{a}} - T_{2,Am})])} \tag{S87}$$

wherein $A_{\text{m,max,ref}}$ has the units $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$, $Q_{10,\text{Am}}$ is dimensionless and $T_{1,Am}$ and $T_{2,Am}$ are constants expressed in [K]. In contrast to other A-gs parameters such as $Q_{10,\text{Am}}$, we allow $A_{\text{m,max,ref}}$ to differ among canopy layers. We assume $A_{\text{m,max,ref}}$ in each layer to be linearly related to the total and photosynthetic nitrogen content in the leaves in that layer (Hikosaka et al., 2016a), i.e., in terms of the variables used in Eq. 2 of Hikosaka et al. (2016a), we assume the following:

$$A_{\text{m,max,ref}} \propto N_{\text{area}} - N_{\text{b}} = (N_0 - N_{\text{b}})\exp(-K_{\text{b}}F) \tag{S88}$$

The equation above leads to the following equation for $A_{\text{m,max,ref}}$ in each model layer:

$$A_{\text{m,max,ref}} = A_{\text{m,max,ref,toc}} \exp(-K_{\text{b}} \text{LAI}_{\text{above}}) \tag{S89}$$

wherein $\text{LAI}_{\text{above}}$ $[\text{m}^2_{\text{plant surface}}\text{m}^{-2}_{\text{ground}}]$ is the amount of plant material above the level (height of node) we look at (including branches etc.), K_{b} $[\text{m}^2_{\text{ground}}\text{m}^{-2}_{\text{plant surface}}]$ is an extinction coefficient for $A_{\text{m,max,ref}}$ and $A_{\text{m,max,ref,toc}}$ $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$ is the value of $A_{\text{m,max,ref}}$ at the top of the canopy.

To take the effect of soil moisture stress into account, we define a variable β_{w} $[-]$ (approximately eq. 16 Ronda et al., 2001):

$$\beta_{\text{w}} = \max\left(10^{-3}, \min\left(1, \frac{w_2 - w_{\text{wilt}}}{w_{\text{fc}} - w_{\text{wilt}}}\right)\right) \tag{S90}$$

wherein w_2 $[-]$ is the volumetric soil moisture content of the deeper soil layer, w_{fc} $[-]$ is the volumetric soil water content at field capacity and w_{wilt} $[-]$ is the volumetric soil water content at wilting point (all as in CLASS). Depending on user input variable c_β, there are multiple options for the soil moisture stress factor f_{str} $[-]$:

$$f_{\text{str}} = \begin{cases} \beta_{\text{w}} & \text{, in case } c_\beta = 0 \\ \frac{1-\exp(-P_{\text{fstr}}\,\beta_{\text{w}})}{1-\exp(-P_{\text{fstr}})} & \text{, in case } c_\beta \neq 0 \end{cases} \tag{S91}$$

In case $c_\beta \neq 0$, we need to calculate P_{fstr} $[-]$, which again depends on user input variable c_β:

$$P_{\text{fstr}} = \begin{cases} 6.4c_\beta & \text{, in case } c_\beta < 0.25 \text{ and } c_\beta \neq 0 \\ 7.6c_\beta - 0.3 & \text{, in case } 0.25 \geq c_\beta < 0.5 \\ 2^{3.66c_\beta + 0.34} - 1 & \text{, in case } c_\beta \geq 0.5 \end{cases} \tag{S92}$$

The above approach for the soil moisture stress is the same as in CLASS. We now define a quantity $A_{\text{m,exp}}$ $[-]$:

$$A_{\text{m,exp}} = -\frac{g_{\text{m}}([\text{CO}_2]_{\text{int}} - [\text{CO}_2]_{\text{comp}})}{A_{\text{m,max}}} \tag{S93}$$

In case the above quantity is greater than 0, it is set to -1×10^{-15}. The maximal assimilation rate without light or soil moisture limitation $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$ (Eq. 3.13 Jacobs, 1994):

$$A_{\text{m}} = A_{\text{m,max}} * (1 - \exp(A_{\text{m,exp}})) \tag{S94}$$

Note that A_{m} is per m^2 one-sided leaf area, as we assume $A_{\text{m,max,ref,toc}}$ to be given per m^2 one-sided leaf area. Dark respiration $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$:

$$R_{\text{dark}} = \frac{1}{9} A_{\text{m}} \tag{S95}$$

This dark respiration formulation is the same as in Jacobs (1994), who based himself on Van Heemst (1986, p16). The formulation as in Jacobs (1994) might however lead to an incorrect relation between dark respiration and atmospheric CO_2, see discussion in Van Diepen et al. (2022). The initial quantum use efficiency ε $[\text{mg}_{\text{CO2}}\,\text{J}^{-1}]$ (Eq. 3.10 Jacobs, 1994):

$$\varepsilon = \varepsilon_0 \frac{[\text{CO}_2] - [\text{CO}_2]_{\text{comp}}}{[\text{CO}_2] + 2[\text{CO}_2]_{\text{comp}}} \tag{S96}$$

wherein ε_0 (maximum initial quantum use efficiency, Van Diepen et al., 2022) has the units $[\text{mg}_{\text{CO2}}\,\text{J}^{-1}]$. The gross assimilation at the leaf scale $[\text{mg}_{\text{CO2}}\,\text{m}^{-2}\text{s}^{-1}]$ is calculated as (note that this is not our calculation of CO_2 uptake by the plants):

$$A_{\text{g}} = f_{\text{str}}\,(A_{\text{m}} + R_{\text{dark}})\left(1 - \exp\left(\frac{-1\,\varepsilon\,2\text{PAR}_{\text{abs}}}{A_{\text{m}} + R_{\text{dark}}}\right)\right) \tag{S97}$$

whereby we make use of Eq. 3.12 of Jacobs (1994). Note that the factor 2 is added to account for the fact that absorbed PAR was averaged over the upper and lower sides of the leaf (as A_{m} is a flux per m^2 one-sided leaf area, PAR_{abs} should be per m^2 one-sided leaf area as well). We make the assumption that light falling on top of the leaf can also be used for the photosynthesis flux at the lower side of the leaf. We define a variable D_* [kPa] (different from formulation given in Ronda et al., 2001):

$$D_* = \frac{D_0}{(f_0 - f_{\text{min}})\frac{1}{1-f_0}} \tag{S98}$$

The stomatal conductance at leaf scale $[\text{m}\,\text{s}^{-1}]$ is calculated as (large similarity to Eq. 11 Ronda et al., 2001):

$$g_{\text{s,CO2}} = \alpha_{\text{sto}} \frac{\frac{1}{1-f_0} A_{\text{g}}}{2([\text{CO}_2] - [\text{CO}_2]_{\text{comp}})(1 + \frac{D_{\text{s}}}{D_*})} \tag{S99}$$

wherein α_{sto} $[-]$ is a scaling factor for the stomatal conductance. If this factor is set to a value of 1, it does not play a role. Note that the factor 1/2 in the formula above is added since the conductance is defined per m^2 two-sided leaf area, just as for the net CO_2 assimilation at the leaf scale (Eq. S105). Note that the units of the stomatal conductance can also be written as $[\text{m}^3\,\text{m}^{-2}_{\text{two-sided leaf area}}\,\text{s}^{-1}]$. We define a leaf conductance for CO_2 $[\text{m}\,\text{s}^{-1}]$ (not yet including boundary layer conductance), the equation differs between dry (Eq. S100) and wet (Eq. S102) leaves. Note that $g_{\text{s,CO2}}$ and thus also e.g. $g_{\text{leaf,CO2,dry}}$ differs between sunlit and shaded leaves.

$$g_{\text{leaf,CO2,dry}} = \frac{\text{SF}}{r_{\text{cut,CO2}}} + g_{\text{s,CO2}} \tag{S100}$$

The factor SF accounts for the case in which stomata are only present on one side of the leaf. In that case, there are two cuticular conductance pathways and only one stomatal conductance pathway. See Sect. S1.14 for a critical note. $r_{\text{cut,CO2}}$ is the cuticular resistance for CO_2, a constant given by:

$$r_{\text{cut,CO2}} = 30\, r_{\text{cut,H2O}} = \frac{30}{g_{\text{min,H2O}}} \tag{S101}$$

in which the factor 30 (average of 20 and 40) is based on Boyer (2015) and Márquez et al. (2021). $g_{\text{min,H2O}}$ is the cuticular conductance for water vapour (see also Eq. S81 and text below that equation). For a wet leaf we have the following equation for leaf conductance for CO_2:

$$g_{\text{leaf,CO2,wet}} = \frac{\text{SF}}{r_{\text{cut,CO2}} + r_{\text{ws,CO2}}} + g_{\text{s,CO2}} \tag{S102}$$

In the latter equation it is assumed that the stomata are not covered by water. In case variable 'stomblock' is changed from 0 to 1, this assumption is removed and the equation becomes instead:

$$g_{\text{leaf,CO2,wet}} = \frac{\text{SF}}{r_{\text{cut,CO2}} + r_{\text{ws,CO2}}} + \frac{1}{r_{\text{ws,CO2}} + \frac{1}{g_{\text{s,CO2}}}} \tag{S103}$$

Variable $r_{\text{ws,CO2}}$ $[\text{s}\,\text{m}^{-1}]$ is the wet skin (water layer) resistance for CO_2, a constant provided by the user. We still need to account for the boundary layer resistance for CO_2 $[\text{s}\,\text{m}^{-1}]$, which is (for the ith layer) obtained by the following equation (see also our Eq. S45 and Eq. 3.7 Jacobs, 1994):

$$r_{\text{b,CO2},i} = 1.37 \times 180 \left(\frac{0.07}{\text{max}[10^{-10}, U_i]} \right)^{0.5} = 1.37\, r_{\text{b,H2O},i} \tag{S104}$$

The net CO_2 assimilation at the leaf scale is given by:

$$A_{\text{n,leaf}} = -\frac{[\text{CO}_2] - [\text{CO}_2]_{\text{int}}}{r_{\text{b,CO2}} + \frac{1}{g_{\text{leaf,CO2}}}} \tag{S105}$$

A negative value for $A_{\text{n,leaf}}$ means net uptake. The units of this flux are $[\text{mg}_{\text{CO2}}\,\text{m}_{\text{leaf}}^{-2}\,\text{s}^{-1}]$, note that in case of stomata on only one side of the leaf, there is only a cuticular flux (no stomatal flux) on half of the leaf. In this case, to obtain the total mass of CO_2 coming out of a leaf each second, the flux needs to be multiplied with the one-sided leaf area of the leaf. In case of stomata on both sides, the equation above represents the CO_2 uptake per m^2 two-sided-leaf area, the total mass of CO_2 coming out of a leaf each second is obtained by multiplication with the two-sided leaf area of the leaf. Scaling up from leaf to layer scale (for both cases), for a layer i $[\text{mg}_{\text{CO2}}\,\text{m}_{\text{ground}}^{-2}\,\text{s}^{-1}]$:

$$A_{\text{n},i} = \frac{1}{\text{SF}} \left(A_{\text{n,leaf,sun,dry},i}\, \text{LAI}_{\text{sun,dry},i} + A_{\text{n,leaf,sun,wet},i}\, \text{LAI}_{\text{sun,wet},i} + A_{\text{n,leaf,sha,dry},i}\, \text{LAI}_{\text{sha,dry},i} + A_{\text{n,leaf,sha,wet},i}\, \text{LAI}_{\text{sha,wet},i} \right) \tag{S106}$$

Finally, this is converted into a molar flux $[\text{mol}_{\text{CO2}}\,\text{m}_{\text{ground}}^{-2}\,\text{s}^{-1}]$:

$$F_{\text{CO2,veg},i} = A_{\text{n},i} \frac{0.001}{M_{\text{CO2}}} \tag{S107}$$

wherein M_{CO2} is the molar mass of CO_2 $[\text{g}_{\text{CO2}}\,\text{mol}_{\text{CO2}}^{-1}]$.

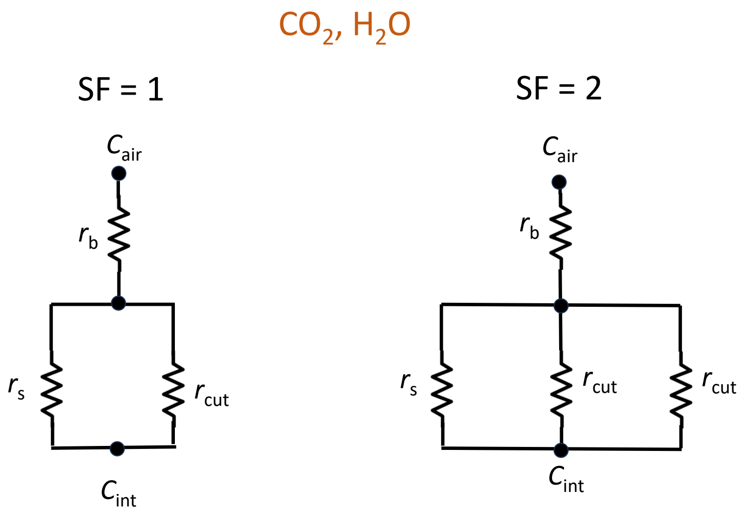

Figure S1. Sketch of the used resistance schemes for a dry leaf for CO_2 and H_2O. SF=1 is the case with stomata on all sides of the leaf, while the case SF=2 corresponds to stomata on only one side of the leaf. Note that for CO_2 a mesophyll resistance g_{m} is calculated as well (Eq. S80), which is used in Eq. S81 and Eq. S93, it is however not an explicit component in the resistance scheme. In the case of CO_2, C_{int} corresponds to $[CO_2]_{\text{int}}$ $[\mathrm{mg_{CO2}\,m^{-3}}]$, in the case of H_2O it corresponds to $C_{\text{H2Osat}}(T_{\text{s}})_{\text{L}}$ $[\mathrm{mol_{H2O}\,m^{-3}}]$. Note that also the quantities r_{s}, C_{air}, r_{b} and r_{cut} differ between CO_2 and H_2O. C_{int} and r_{s} are calculated separately for sunlit and for shaded leaf area (we calculate separate fluxes for sunlit and shaded leaf area, see text).

S1.8.2 COS exchange vegetation

For COS, we use a different 'endpoint' in the uptake than for CO_2, namely the point where the COS concentration becomes negligibly small. The internal conductance for COS is assumed to account for two conductances, namely mesophyll conductance and a conductance related to carbonic anhydrase activity (Berry et al., 2013; Sun et al., 2024; Cho et al., 2023). We calculate an internal conductance for COS $[\mathrm{m\,s^{-1}}]$ for each category of leaves and for each layer (Cho et al., 2023, with some adaptions):

$$g_{\text{int,COS}} = \frac{0.001 M_{\text{air}}}{\rho_{\text{air}}} \alpha_{\text{giCOS}}\, V_{\text{max,giCOS}}\, F_{\text{rz,giCOS}} \frac{\frac{2}{T_{\text{eq,giCOS}} \exp\left(\frac{-\Delta_{\text{Ha,giCOS}}}{R\,T_{\text{eq,giCOS}}}\right)}\, T_{\text{s}} \exp\left(\frac{-\Delta_{\text{Ha,giCOS}}}{R\,T_{\text{s}}}\right)}{1+\exp\left(\frac{-\Delta_{\text{Heq,giCOS}}}{R}\left(\frac{1}{T_{\text{s}}}-\frac{1}{T_{\text{eq,giCOS}}}\right)\right)} \tag{S108}$$

wherein α_{giCOS} and $F_{\text{rz,giCOS}}$ are dimensionless, $V_{\text{max,giCOS}}$ has the units $[\mathrm{mol_{air}\,m^{-2}\,s^{-1}}]$, $T_{\text{eq,giCOS}}$ has units [K], R is the universal gas constant $[\mathrm{J\,K^{-1}\,mol^{-1}}]$ and $\Delta_{\text{Ha,giCOS}}$ and $\Delta_{\text{Heq,giCOS}}$ have the units $[\mathrm{J\,mol^{-1}}]$. The factor $\frac{0.001 M_{\text{air}}}{\rho_{\text{air}}}$ converts the conductance from $[\mathrm{mol_{air}\,m^{-2}\,s^{-1}}]$ to $[\mathrm{m\,s^{-1}}]$. Before the mentioned unit conversion, the model checks whether the internal conductance is smaller than $1\times10^{-100}\ \mathrm{mol_{air}\,m^{-2}\,s^{-1}}$, in that case it is set to $1\times10^{-100}\ \mathrm{mol_{air}\,m^{-2}\,s^{-1}}$ before converting. The resistance $[\mathrm{s\,m^{-1}}]$ is easily obtained from the conductance $[\mathrm{m\,s^{-1}}]$:

$$r_{\text{int,COS}} = \frac{1}{g_{\text{int,COS}}} \tag{S109}$$

The stomatal resistance $[\mathrm{s\,m^{-1}}]$ for COS is obtained from the stomatal conductance for CO_2 (Seibt et al., 2010):

$$r_{\text{s,COS}} = 1.21 \frac{1}{g_{\text{s,CO2}}} \tag{S110}$$

Note that the stomatal resistance can differ between all four leaf categories, and is thus calculated separately for all leaf categories (sun-dry, shaded-dry, sun-wet, shaded-wet). We relate the cuticular conductance for COS to that of water by the following equation:

$$g_{\text{cut,COS}} = \frac{g_{\text{min,H2O}}}{30} \tag{S111}$$

For simplicity we have assumed the ratio of the cuticular conductance of COS and H_2O equal to that of CO_2 and H_2O (Eq. S101). The boundary layer resistance for COS (in the ith layer) is calculated as (See also Eq. 2 of Stimler et al., 2010):

$$r_{\text{b,COS},i} = 1.56\, r_{\text{b,H2O},i} \tag{S112}$$

The resistance for a dry leaf $[\mathrm{s\,m^{-1}}]$ is given by:

$$r_{\text{COS,leaf,dry}} = r_{\text{b,COS}} + \frac{1}{\frac{1}{r_{\text{s,COS}}+r_{\text{int,COS}}} + \text{SF}\, g_{\text{cut,COS}}} \tag{S113}$$

The factor SF is explained in Sect. S1.5. A sketch of the resistance schemes for dry leaf area for COS is shown in Fig. S2. For a wet leaf the resistance depends on the choice of the 'stomblock' variable. In case of non-water covered stomata ('stomblock' = 0):

$$r_{\text{COS,leaf,wet}} = r_{\text{b,COS}} + \frac{1}{\frac{1}{r_{\text{s,COS}}+r_{\text{int,COS}}} + \text{SF}\,\frac{1}{\frac{1}{g_{\text{cut,COS}}}+r_{\text{ws,COS}}}} \tag{S114}$$

And in the other case:

$$r_{\text{COS,leaf,wet}} = r_{\text{b,COS}} + \frac{1}{\text{SF}\,\frac{1}{\frac{1}{g_{\text{cut,COS}}}+r_{\text{ws,COS}}} + \frac{1}{r_{\text{ws,COS}}+r_{\text{s,COS}}+r_{\text{int,COS}}}} \tag{S115}$$

Variable $r_{\text{ws,COS}}$ $[\mathrm{s\,m^{-1}}]$ is the wet skin (water layer) resistance for COS, a constant provided by the user. We calculate leaf-scale fluxes of COS, e.g. for sunlit dry leaves in layer i $[\text{mol m}_{\text{leaf}}^{-2}\text{s}^{-1}]$:

$$F_{\text{COS,leaf,sun,dry},i} = -\frac{[\text{COS}]_i}{r_{\text{COS,leaf,sun,dry},i}} \tag{S116}$$

wherein $[\text{COS}]_i$ is the molar concentration of COS in layer i $[\mathrm{mol\,m^{-3}}]$. We scale up from the leaf to the layer scale as follows $[\text{mol m}_{\text{ground}}^{-2}\text{s}^{-1}]$:

$$F_{\text{COS,veg},i} = \frac{1}{\text{SF}}(\text{LAI}_{\text{sun,dry},i}\, F_{\text{COS,sun,dry},i} + \text{LAI}_{\text{sha,dry},i}\, F_{\text{COS,sha,dry},i} + \text{LAI}_{\text{sun,wet},i}\, F_{\text{COS,sun,wet},i} + \text{LAI}_{\text{sha,wet},i}\, F_{\text{COS,sha,wet},i}) \tag{S117}$$

See also Eq. S106 and the text above it. See Sect. S1.14 for a critical note.

S1.9 Canopy wind speeds

The calculation of wind speeds inside the canopy is based on the theory of Cionco (1965) and the equations of the MLC-CHEM model, with some adaptions. First, some parameters are set based on canopy height and (all-sided) leaf area index (LAI, $[\mathrm{m^2\,m^{-2}}]$). For simplicity, we do not account for branches or dead leaves, only green (photosynthesising) leaves.

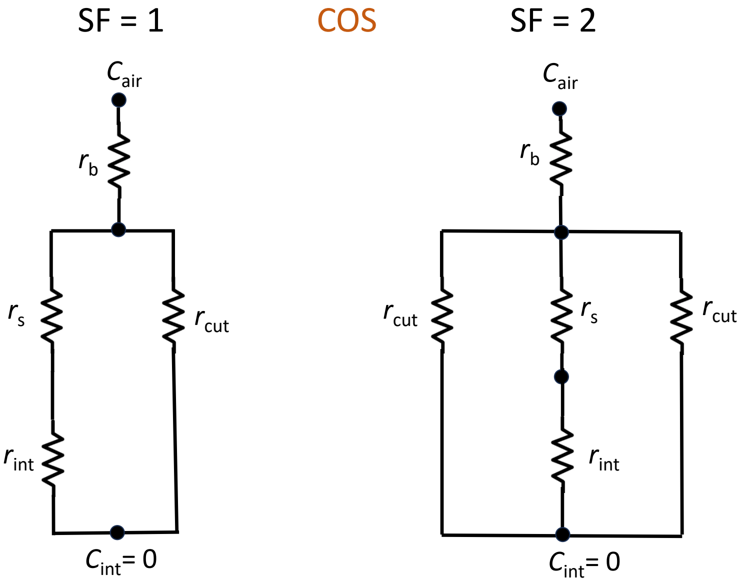

Figure S2. Sketch of the used resistance schemes for a dry leaf for COS. SF=1 is the case with stomata on all sides of the leaf, while the case SF=2 corresponds to stomata on only one side of the leaf. r_{int} and r_{s} are calculated separately for sunlit and for shaded leaf area (we calculate separate fluxes for sunlit and shaded leaf area, see text).

We first determine the extinction coefficient α_{wind} $[-]$ and a coefficient β_{wind} $[-]$. We distinguish three cases depending on canopy height. The first case is when the canopy is smaller than 2.5 m:

$$\alpha_{\mathrm{wind}} = \min\left(0.65\frac{\mathrm{LAI}}{2}, 3\right) \tag{S118}$$

$$\beta_{\mathrm{wind}} = 0.25 \tag{S119}$$

The second case is when the canopy is larger than 10 m:

$$\alpha_{\mathrm{wind}} = \min\left(\frac{\mathrm{LAI}}{2}, 4\right) \tag{S120}$$

$$\beta_{\mathrm{wind}} = 0.75 \tag{S121}$$

The third case is when the canopy is between 2.5 and 10 m (including 2.5 and 10):

$$\alpha_{\mathrm{wind}} = \min\left(0.65\frac{\mathrm{LAI}}{2}, 3\right) \tag{S122}$$

$$\beta_{\mathrm{wind}} = 0.75 \tag{S123}$$

For calculating wind speeds in the layers, we have two options of calculating, depending on a switch called 'lad_dependence_u'. This switch controls whether to make the wind extinction between two nodes directly dependent on leaf area density between these nodes (besides the potential indirect link via α_{wind}). If the switch is set to True, we have the following equation for the top layer $[\mathrm{m\,s^{-1}}]$:

$$U_{\text{top layer}} = U_{\text{toc}}\,\text{Exp}\left(-\alpha_{\text{wind}}\,\alpha_{\text{wind scale}}\frac{\text{lad}_{\text{top layer}}}{\text{lad}_{\text{mean}}}\left(1-\frac{z_{\text{top layer}}}{z_{\text{toc}}}\right)^{\beta_{\text{wind}}}\right) \tag{S124}$$

wherein U_{toc} (Sect. S1.11) is the wind speed at the top of the canopy $[\mathrm{m\,s^{-1}}]$, $z_{\text{top layer}}$ is the height of the node of the top layer [m], and z_{toc} is canopy height [m]. $\alpha_{\text{wind scale}}$ $[-]$ is a scaling factor for α_{wind}. $\text{lad}_{\text{top layer}}$ is (all-sided) leaf area density $[\mathrm{m^2\,m^{-3}}]$ in the top layer. lad_{mean} is the layer-averaged leaf area density, calculated as:

$$\text{lad}_{\text{mean}} = \frac{\sum_{i=0}^{N-1}\text{lad}_i}{N} \tag{S125}$$

wherein lad_i is the leaf area density of the layer with index i, and N is the number of layers. Besides the top layer, the wind speed in any other layer (with index i) is calculated as $[\mathrm{m\,s^{-1}}]$:

$$U_i = U_{i+1}\,\text{Exp}\left(-\alpha_{\text{wind}}\,\alpha_{\text{wind scale}}\frac{\text{lad}_i+\text{lad}_{i+1}}{2\,\text{lad}_{\text{mean}}}\left(\left(1-\frac{z_i}{z_{\text{toc}}}\right)^{\beta_{\text{wind}}}-\left(1-\frac{z_{i+1}}{z_{\text{toc}}}\right)^{\beta_{\text{wind}}}\right)\right) \tag{S126}$$

wherein U_{i+1} is the wind speed in the layer above. In case the switch 'lad_dependence_u' is set to False, we have the following equation for each layer (including top layer):

$$U_i = U_{\text{toc}}\,\text{Exp}\left(-\alpha_{\text{wind}}\,\alpha_{\text{wind scale}}\left(1-\frac{z_i}{z_{\text{toc}}}\right)^{\beta_{\text{wind}}}\right) \tag{S127}$$

In the equations above, z_i is the height of the node in the ith layer.

S1.10 Liquid water vegetation

We calculate the amount of liquid water present on top of the vegetation (or e.g. at the lower side of a leaf), in a simplified way. Hereto, we make use of an equivalent water depth on the vegetation, in each canopy model layer. The tendency in equivalent water layer depth in a layer i is calculated as $[\mathrm{m\,s^{-1}}, \mathrm{m^3_{water} m^{-2}_{ground}\,s^{-1}}]$:

$$\frac{dW_{\text{l},i}}{dt} = \frac{-F_{\text{H2O,veg,wet},i}\,M_{\text{H2O}}}{1000\,\rho_{\text{w}}} \tag{S128}$$

The flux $F_{\text{H2O,veg,wet},i}$ is given by Eq. S52. The equivalent water layer $[\mathrm{m}, \mathrm{m^3_{water} m^{-2}_{ground}}]$ in layer i at time index $t+1$ is calculated as:

$$W_{\text{l},i,t+1} = W_{\text{l},i,t} + \Delta t\frac{dW_{\text{l},i}}{dt} \tag{S129}$$

wherein Δt is the time step of the canopy model. We do not allow $W_{\text{l},i,t+1}$ to become negative, by forcing it to zero in case the equation above leads to a negative number. The equivalent liquid water layer is used to determine the fraction of vegetation surface area that is wet in a layer i at time index t $[-]$:

$$\text{fr}_{\text{wet},i,t} = \min\left(1, \frac{W_{\text{l},i,t}}{W_{\text{l,max},i}}\right) \tag{S130}$$

And $W_{\text{l,max},i}$ $[\mathrm{m}, \mathrm{m^3_{water} m^{-2}_{ground}}]$ is calculated as:

$$W_{\text{l,max},i} = \frac{\text{LAI}_i * W_{\text{l,max height}}}{\text{fr}_{\text{green},i}} \tag{S131}$$

wherein $W_{\text{l,max height}}$ $[\mathrm{m}, \mathrm{m^3_{water} m^{-2}_{veg\,surface}}]$ is the maximum depth of water anywhere at a leaf (or branch etc.) surface. This value is constant in time and throughout the canopy, and is provided by the user. LAI_i represents the amount of all-sided leaf area (without branches) in the ith layer $[\mathrm{m^2_{leaf}\,m^{-2}_{ground}}]$.

S1.11 Boundary conditions canopy model

We give here the time-varying boundary conditions for the canopy model as they are when the canopy model is coupled to the CLASS model. In principle, the canopy model can also be run stand-alone, forced with different boundary conditions. We have already mentioned some boundary conditions calculated by CLASS: Incoming shortwave radiation at the top of the canopy ($\mathrm{SW}_{\mathrm{in,top}}$, Sect. S1.3), incoming longwave radiation at the top of the canopy ($\mathrm{LW}_{\mathrm{in,atm}}$, Sect. S1.4), $r_{\mathrm{soil,H2O}}$ (Sect. S1.6), and T_{soil} (Sect. S1.6). The sine of the solar elevation angle ($\sin(\beta)$) is also calculated by CLASS and used by the canopy model (Sect. S1.3). Soil respiration is as in the CLASS code $[\mathrm{mg_{CO2}\ m_{ground}^{-2} s^{-1}}]$:

$$\mathrm{Resp} = R_{10}\left(1-\frac{C_{\mathrm{w}}\,w_{\mathrm{max}}}{w_{\mathrm{g}}+w_{\mathrm{min}}}\right)\exp\left(\frac{E_0}{283.15*8.314}\left(1-\frac{283.15}{T_{\mathrm{soil}}}\right)\right) \tag{S132}$$

See Vilà-Guerau de Arellano et al. (2015, Appendix F). In this formulation, soil respiration is a function of the soil water content of the upper soil layer (w_{g}, $[-]$) and of the temperature of this soil layer (T_{soil}, [K]). Both are calculated by CLASS. Soil respiration from the equation above is transformed to a flux with the correct units for the canopy model $[\mathrm{mol_{CO2}\, m_{ground}^{-2} s^{-1}}]$:

$$F_{\mathrm{CO2,soil}} = \frac{\mathrm{Resp}}{1000 M_{\mathrm{CO2}}} \tag{S133}$$

This respiration flux ends up in the lowest canopy layer (See also Sect. S1.13). We assume the flux to account both for root respiration, and soil (including litter) heterotrophic respiration. A soil carbonyl sulphide flux $[\mathrm{mol_{COS}\, m_{ground}^{-2} s^{-1}}]$ should also be given as boundary condition to the canopy model. The wind speed at the top of the canopy is calculated as $[\mathrm{m\,s^{-1}}]$:

$$U_{\mathrm{toc}} = \sqrt{u^2+v^2} \tag{S134}$$

wherein u and v are the zonal and meridional wind speeds in the mixed layer respectively, calculated by CLASS. The water mole fraction (amount fraction, ratio H_2O and air) at the top of the canopy $[\mathrm{cmol_{H2O}\,mol_{air}^{-1}}]$ is calculated as:

$$\mathrm{rat}_{\mathrm{H2O,toc}} = \frac{100\,e}{P_{\mathrm{toc}}} = \frac{100\,q}{0.622} \tag{S135}$$

wherein mixed-layer specific humidity q $[\mathrm{kg_{H2O}\,kg_{air}^{-1}}]$ is calculated by CLASS, 0.622 is approximately the ratio of the molar masses of water and air, and P_{toc} is the top-of-canopy air pressure [Pa]. e [Pa] is a vapour pressure calculated by CLASS. The canopy model converts $\mathrm{rat}_{\mathrm{H2O,toc}}$ into a molar concentration $[\mathrm{mol_{H2O}\,m^{-3}}]$:

$$[\mathrm{H_2O}]_{\mathrm{toc}} = \frac{\mathrm{rat}_{\mathrm{H2O,toc}} 1000 \rho_{\mathrm{air}}}{100 M_{\mathrm{air}}} \tag{S136}$$

wherein ρ_{air} is air density $[\mathrm{kg\,m^{-3}}]$ and M_{air} is the molar density of air $[\mathrm{g\,mol^{-1}}]$, both constant in the model.

The top-of-canopy mole fractions of CO_2 ($\mathrm{rat}_{\mathrm{CO2,toc}}$ [ppm]) and COS ($\mathrm{rat}_{\mathrm{COS,toc}}$ [ppb]) also need to be provided as boundary conditions for the SiLCan model. For these we use the mixed-layer mole fractions calculated by CLASS. The values are converted into molar concentrations $[\mathrm{mol\,m^{-3}}]$ by the canopy model, using formulas similar to the one above:

$$[\mathrm{CO_2}]_{\mathrm{toc}} = \frac{\mathrm{rat}_{\mathrm{CO2,toc}} 1000 \rho_{\mathrm{air}}}{10^6 M_{\mathrm{air}}} \tag{S137}$$

$$[\mathrm{COS}]_{\mathrm{toc}} = \frac{\mathrm{rat}_{\mathrm{COS,toc}} 1000 \rho_{\mathrm{air}}}{10^9 M_{\mathrm{air}}} \tag{S138}$$

The potential temperature at the top of the canopy is also a boundary condition, we use the potential temperature in the mixed layer (θ [K], calculated by CLASS) for this. This potential temperature is converted by the canopy model into a 'heat concentration' at the top of the canopy $[\mathrm{J\,m^{-3}}]$:

$$[\mathrm{heat}]_{\mathrm{toc}} = \rho_{\mathrm{air}}\, c_{\mathrm{p}} \theta \tag{S139}$$

wherein c_p is the specific heat of dry air at constant pressure $[\mathrm{J\,kg^{-1}\,K^{-1}}]$. The 'heat concentration' at the top of the canopy is used in equations S154 and S160 (in case the considered scalar is heat).

Note that we use mixed-layer values for our top-of-canopy boundary conditions. Instead of subscript 'toc' we use subscript 'mixed layer' in e.g. Eq. S160. Given that we calculate exchanges with the mixed layer, we include a resistance between the top of the canopy and the mixed layer. We use the variable 'ra' from CLASS for this purpose, see also later in Eq. S152.

Note that it is also possible to prescribe time series of PAR at the top of the canopy ($\mathrm{PAR_{top}}$), as well as of COS, CO_2, H_2O and temperature in the canopy layers.

S1.12 Turbulent fluxes, exchange coefficients and turbulent conductance

Exchange of mass and heat between vegetation layers in the model happens by means of turbulent fluxes. For simplicity we use first-order closure of the turbulent fluxes. We use the following differential equation for a flux of scalar s:

$$F_\mathrm{s} = -K\frac{\partial C_\mathrm{s}}{\partial z} \tag{S140}$$

To calculate the fluxes,we calculate exchange coefficients K $[\mathrm{m^2\,s^{-1}}]$, at all the interfaces of the layers except for the soil interface. We take the exchange coefficients to be identical for all scalars. To calculate the K, we base ourselves on Launiainen et al. (2011). We first calculate a displacement height [m]:

$$d = 0.7 z_\mathrm{toc} \tag{S141}$$

We define a variable $\alpha^{'}$ $[-]$:

$$\alpha^{'} = k\left(1 - \frac{d}{z_\mathrm{toc}}\right) \tag{S142}$$

wherein k is the von Karman constant and z_toc is the canopy height. We calculate a mixing length [m] at the top of the canopy:

$$l_\mathrm{toc} = k\left(z_\mathrm{toc} - d\right) \tag{S143}$$

We also calculate a mixing length [m] for each of the interfaces between canopy layers. Here we distinguish two cases, in the first case $z_{\mathrm{int},i} < \alpha^{'} z_\mathrm{toc}/k$, wherein $z_{\mathrm{int},i}$ [m] is the height level of the interface with index i. In this case the mixing length of the interface with index i is given by:

$$l_i = k\, z_{\mathrm{int},i} \tag{S144}$$

and in the other case:

$$l_i = \alpha^{'} z_\mathrm{toc} \tag{S145}$$

We calculate the derivative of wind speed with height at the canopy top $[\mathrm{s^{-1}}]$:

$$\frac{\partial U}{\partial z}_\mathrm{toc} = \frac{U_\mathrm{toc} - U_\mathrm{top\ layer}}{z_\mathrm{toc} - z_\mathrm{top\ layer}} \tag{S146}$$

And for the interfaces between canopy layers $[\mathrm{s^{-1}}]$:

$$\frac{\partial U}{\partial z}_i = \frac{U_i - U_{i-1}}{z_i - z_{i-1}} \tag{S147}$$

wherein z_i and U_i are the height of the node of the layer with index i, and the wind speed in the layer with index i respectively (thus, we consider the wind speeds in the layers above and below the interface). Finally the exchange coefficients $[\mathrm{m^2\,s^{-1}}]$, first for the canopy top:

$$K_\mathrm{toc} = K_\mathrm{scale,toc}\, l_\mathrm{toc}^2 \left|\frac{\partial U}{\partial z}_\mathrm{toc}\right| + K_\mathrm{add,toc} \tag{S148}$$

And for an interface with index i, between canopy layers:

$$K_i = K_{\text{scale},i}\, l_i^2 \left|\frac{\partial U}{\partial z}_i\right| + K_{\text{add},i} \tag{S149}$$

wherein the vertical bars indicate 'absolute value of'. In those equations, K_{scale} is a scaling factor $[-]$, which defaults to unity. It can be used for inverse modelling purposes, or to manually adapt the K values. The term K_{add} $[\mathrm{m^2\,s^{-1}}]$ can also be used for inverse modelling or manual adaption, it defaults to 0. The exchange coefficients are actually for momentum. However, as in Launiainen et al. (2011), we set exchange coefficients for scalars to be identical. Also, K_{scale} could be used to modify the exchange coefficients from momentum to values appropriate for scalars (using turbulent Schmidt number, Launiainen et al. (2011)). Now we use the exchange coefficient of an interface with index i (except top and bottom interfaces) to calculate the turbulent conductance G_i $[\mathrm{m\,s^{-1}}]$ of that interface:

$$G_i = \frac{K_i}{z_i - z_{i-1}} \tag{S150}$$

wherein z_i is the height of the node in the ith layer. For the canopy top we have the following conductance $[\mathrm{m\,s^{-1}}]$, when taking only the in-canopy part of the exchange path into account:

$$G_{\text{toc,ic}} = \frac{K_{\text{toc}}}{z_{\text{toc}} - z_{\text{top layer}}} \tag{S151}$$

Given that we want to calculate the flux between the top canopy layer and the mixed layer, we need to account for an additional resistance. The conductance we use for transport between these layers is given by the following equation:

$$G_{\text{top lay to ML}} = \frac{1}{\frac{1}{G_{\text{toc,ic}}} + r_{\text{a,toc to ML}}} \tag{S152}$$

wherein $r_{\text{a,toc to ML}}$ $[\mathrm{s\,m^{-1}}]$ is the resistance between canopy top and mixed layer, we use the variable 'ra' from CLASS for this purpose. Using the conductances, the turbulent flux of a scalar s between canopy layers $i-1$ and i can be calculated as:

$$F_{\text{s},i-1\to i} = -1\, G_i\, (C_{\text{s},i} - C_{\text{s},i-1}) \tag{S153}$$

And for the flux between the top canopy layer and the mixed layer:

$$F_{\text{s,top layer}\to\text{mixed layer}} = -1\, G_{\text{top lay to ML}}\, (C_{\text{s,mixed layer}} - C_{\text{s,top layer}}) \tag{S154}$$

In these equations, e.g. $C_{\text{s},i}$ is the concentration of scalar s in the ith layer. In case of CO_2, COS or H_2O, $C_{\text{s},i}$ and $F_{\text{s},i-1\to i}$ have the units of $[\mathrm{mol\,m^{-3}}]$ and $[\mathrm{mol\,m^{-2}\,s^{-1}}]$ respectively, in case of heat (temperature) they have the units of $[\mathrm{J\,m^{-3}}]$ and $[\mathrm{J\,m^{-2}\,s^{-1}}]$ respectively.

S1.13 Updating concentrations in time

The discretisation in time follows a very similar approach to Sun et al. (2015). The governing differential equation for the concentration of a scalar s $[\mathrm{mol\,m^{-3}}$ or $\mathrm{J\,m^{-3}}]$ is given by (using Fick's law for diffusion in one dimension, and Eq. S140):

$$\frac{\partial C_{\text{s}}}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial C_{\text{s}}}{\partial z}\right) + S = -\frac{\partial}{\partial z}(F_{\text{s}}) + S \tag{S155}$$

wherein S contains the source-sink terms $[\mathrm{mol\,m^{-3}\,s^{-1}}$ or $\mathrm{J\,m^{-3}\,s^{-1}}]$. We discretise the equation above in space by integrating over height in each control volume (canopy layer):

$$\Delta z_i \frac{\partial C_{\text{s},i}}{\partial t} = \begin{cases} -(F_{\text{s},i\to\text{mixed layer}} - F_{\text{s},i-1\to i}) + S_i\,\Delta z_i, & i = N-1 \\ -(F_{\text{s},i\to i+1} - F_{\text{s},i-1\to i}) + S_i\,\Delta z_i, & 0 < i < N-1 \\ -(F_{\text{s},i\to i+1} - F_{\text{s,soil}\to i}) + S_i\,\Delta z_i, & i = 0 \end{cases} \tag{S156}$$

See Sect. S1.2 for N and Δz_i. The above can also be written as:

$$\Delta z_i \frac{\partial C_{\mathrm{s},i}}{\partial t} = \begin{cases} F_{\mathrm{s},i-1\to i} - F_{\mathrm{s},i\to \text{mixed layer}} + S_i\,\Delta z_i, & i = N-1 \\ F_{\mathrm{s},i-1\to i} - F_{\mathrm{s},i\to i+1} + S_i\,\Delta z_i, & 0 < i < N-1 \\ F_{\mathrm{s},\text{soil}\to i} - F_{\mathrm{s},i\to i+1} + S_i\,\Delta z_i, & i = 0 \end{cases} \tag{S157}$$

We can rewrite the equation above in matrix form:

$$\mathbf{A}\frac{d}{dt}\boldsymbol{C}_\mathrm{s} = \mathbf{B}\boldsymbol{C}_\mathrm{s} + \boldsymbol{E} \tag{S158}$$

wherein diagonal matrix $\mathbf{A}$ = diag($\Delta z_0, \Delta z_1, ..., \Delta z_{N-1}$), vector $\boldsymbol{C}_\mathrm{s}$ = $(C_{\mathrm{s},0}, C_{\mathrm{s},1}, ..., C_{\mathrm{s},N-1})$,

$$\mathbf{B} = \begin{bmatrix} -G_1 & G_1 & 0 & ... & 0 & 0 & 0 & 0 \\ G_1 & -(G_1+G_{1+1}) & G_2 & ... & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & ... & G_{N-3} & -(G_{N-3}+G_{N-3+1}) & G_{N-2} & 0 \\ 0 & 0 & 0 & ... & 0 & G_{N-2} & -(G_{N-2}+G_{N-2+1}) & G_{N-1} \\ 0 & 0 & 0 & ... & 0 & 0 & G_{N-1} & -(G_{N-1}+G_N) \end{bmatrix} \tag{S159}$$

(unless the number of canopy layers is less than the number of columns shown here). Matrix $\mathbf{B}$ has the dimensions $N \times N$, i.e. the number of rows and columns is equal to the number of canopy layers, and

$$\boldsymbol{E} = (F_{\mathrm{s,veg},0} + F_{\mathrm{s,soil}}, F_{\mathrm{s,veg},1}, ..., F_{\mathrm{s,veg},N-2}, F_{\mathrm{s,veg},N-1} + G_N\, C_{\mathrm{s,mixed\ layer}}) \tag{S160}$$

wherein $F_{\mathrm{s,veg},i}$ $[\mathrm{mol\,m^{-2}\,s^{-1}}$ or $\mathrm{J\,m^{-2}\,s^{-1}}]$ is given by either Eq. S107 (CO_2), Eq. S117 (COS), Eq. S56 (Heat) or the sum of Eq. S50 and Eq. S52 (H_2O). $F_{\mathrm{s,soil}}$ is given by Eq. S60 in case of heat, Eq. S62 in case of water, Eq. S133 in case of CO_2, and for COS it is calculated by a separate model (or can be chosen to be zero). $C_{\mathrm{s,mixed\ layer}}$ $[\mathrm{mol\,m^{-3}}$ or $\mathrm{J\,m^{-3}}]$ is obtained by making use of variables calculated by CLASS (See Sect. S1.11). It is given by Eq. S136 in case of water, Eq. S137 in case of CO_2, Eq. S138 in case of COS, and given by Eq. S139 in case of heat. Note that G_1 up to G_{N-1} is calculated with Eq. S150, and G_N is calculated with Eq. S152. Vector $\boldsymbol{E}$ is of size N.

For the time integration, a Crank-Nicolson method is used. Equation S158 is discretised at times $t = (n+1/2)\Delta t$:

$$\mathbf{A}\frac{\boldsymbol{C}_{\mathrm{s},\boldsymbol{n+1}} - \boldsymbol{C}_{\mathrm{s},\boldsymbol{n}}}{\Delta t} = \mathbf{B}\frac{\boldsymbol{C}_{\mathrm{s},\boldsymbol{n+1}} + \boldsymbol{C}_{\mathrm{s},\boldsymbol{n}}}{2} + \boldsymbol{E} \tag{S161}$$

Rewriting the equation above:

$$\boldsymbol{C}_{\mathrm{s},\boldsymbol{n+1}} = (2\mathbf{A} - \Delta t\mathbf{B})^{-1}[(2\mathbf{A} + \Delta t\mathbf{B})\boldsymbol{C}_{\mathrm{s},\boldsymbol{n}} + 2\Delta t\boldsymbol{E}] \tag{S162}$$

wherein Δt is the time step of the canopy model. If any of the resulting concentrations is negative, the negative concentration is set to zero. The canopy air temperatures [K] are derived from the heat concentrations. For the ith layer, the following equation is used:

$$T_i = \frac{C_{\mathrm{heat},i}}{\rho_\mathrm{air}\, c_\mathrm{p}}\left(\frac{100000}{P_i}\right)^{-R_\mathrm{d}/c_\mathrm{p}} \tag{S163}$$

wherein the factor containing pressure is used to convert potential temperature into temperature. Note that, by defining heat concentrations based on potential temperature, there is a zero-flux between layers of equal potential temperature, while there is a small flux between layers of equal temperature (as there is a zero-flux between layers of equal concentrations). For the other scalars besides temperature, we do not account for the effect of pressure differences between layers on the fluxes between layers. Concentrations in units of $[\mathrm{mol\,m^{-3}}]$ depend on air density $[\mathrm{kg_{air}\,m^{-3}}]$, but air density is constant in the model. Note that for the exchange of sensible heat between vegetation (or soil) and canopy air (Eq. S54 for sunlit dry leaf area, Eq. S55 for shaded wet leaf area, Eq. S58 for sunlit soil), we do not convert the temperatures in the equations to potential temperatures.

S1.14 Note on resistances

Note that the resistance calculations (for H_2O, CO_2 and COS) are not fully consistent between the case with stomata on one side of the leaf (SF = 2) and the case with stomata on all sides of the leaf (SF = 1). This is clear from the following: in the case where the stomatal resistance is infinitely large, this pathway does not play a role. The cases for SF = 1 and SF = 2 should then lead to an identical layer scale flux, as everything passes through the cuticle. When for simplicity assuming there are only dry sunlit leaves in a layer, the layer scale flux (we take CO_2 for a layer with index i as example) becomes:

$$A_{\mathrm{n},i} = \frac{1}{\mathrm{SF}} A_{\mathrm{n,leaf,sun,dry},i}\, \mathrm{LAI}_{\mathrm{sun,dry},i} = -\frac{\mathrm{LAI}_{\mathrm{sun,dry},i}}{\mathrm{SF}} \frac{[\mathrm{CO_2}]_i - [\mathrm{CO_2}]_{\mathrm{int},i}}{r_{\mathrm{b,CO2},i} + \frac{1}{g_{\mathrm{leaf,CO2},i}}} = -\frac{\mathrm{LAI}_{\mathrm{sun,dry},i}}{\mathrm{SF}} \frac{[\mathrm{CO_2}]_i - [\mathrm{CO_2}]_{\mathrm{int},i}}{r_{\mathrm{b,CO2},i} + \frac{1}{\frac{\mathrm{SF}}{r_{\mathrm{cut,CO2}}} + g_{\mathrm{s,CO2},i}}} \tag{S164}$$

Given that we look at a situation with infinite stomatal resistance, $g_{\mathrm{s,CO2},i} = 0$, and the equation becomes:

$$A_{\mathrm{n},i} = -\frac{\mathrm{LAI}_{\mathrm{sun,dry},i}}{\mathrm{SF}} \frac{[\mathrm{CO_2}]_i - [\mathrm{CO_2}]_{\mathrm{int},i}}{r_{\mathrm{b,CO2},i} + \frac{r_{\mathrm{cut,CO2}}}{\mathrm{SF}}} \tag{S165}$$

which is not independent of SF. The reason for this can be found in how the leaf boundary layer resistance (r_b) is added. If instead of the resistance scheme shown in Fig. S1, the pathways would be taken completely parallel, then the total resistance for CO_2 would be given by the following equation (now again more general as the case $g_{\mathrm{s,CO2},i} = 0$):

$$r_{\mathrm{CO2},i} = \frac{1}{\frac{\mathrm{SF}}{r_{\mathrm{b,CO2},i} + r_{\mathrm{cut,CO2}}} + \frac{1}{r_{\mathrm{b,CO2},i} + r_{\mathrm{s,CO2},i}}} \tag{S166}$$

And thus the flux would be given by:

$$A_{\mathrm{n},i} = -\frac{\mathrm{LAI}_{\mathrm{sun,dry},i}}{\mathrm{SF}} \frac{[\mathrm{CO_2}]_i - [\mathrm{CO_2}]_{\mathrm{int},i}}{\frac{1}{\frac{\mathrm{SF}}{r_{\mathrm{b,CO2},i} + r_{\mathrm{cut,CO2}}} + \frac{1}{r_{\mathrm{b,CO2},i} + r_{\mathrm{s,CO2},i}}}} = -\frac{\mathrm{LAI}_{\mathrm{sun,dry},i}}{\mathrm{SF}} \left([\mathrm{CO_2}]_i - [\mathrm{CO_2}]_{\mathrm{int},i}\right) \left(\frac{\mathrm{SF}}{r_{\mathrm{b,CO2},i} + r_{\mathrm{cut,CO2}}} + \frac{1}{r_{\mathrm{b,CO2},i} + r_{\mathrm{s,CO2},i}}\right) \tag{S167}$$

In this equation, in case of an infinite stomatal resistance, there would be no difference between SF = 1 and SF = 2. Also, in case of an infinite cuticular resistance (and no infinite stomatal resistance), the flux (that is (averaged) per m^2 of all-sided leaf area) would differ by a factor 2 between the cases SF = 1 and SF = 2, as would be expected. The calculation of r_b should be chosen appropriate for the used resistance scheme. Given the uncertainty in the calculation of the boundary layer resistance (Meyers et al., 1989), the variation that is likely present between leaves and tree species, and the generally relatively limited importance of r_b and the cuticular pathway in our canopy model (with default parameters and common boundary conditions), we keep the resistance schemes as shown in Fig. S1 and Fig. S2.

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