Appendix 10.3

The stomata-photosynthesis model and the sunlit-shadow radiation model in Daisy

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1 Introduction

Photosynthesis is the conversion of CO_2 to organic compounds in the presence of light. The chloroplasts of a plant cell are the seat of photosynthesis, and they are present only in the cells of the green parts of the plant. Photosynthesis can be conveniently treated as three separate components: 1) light reactions, in which radiant energy is absorbed and used to generate the high energy compounds ATP and NADPH; 2) dark reactions, which include the biochemical reduction of CO_2 to sugars using high energy compounds generated in the light reactions; and 3) supply of CO_2 from the ambient air to the site of reduction in the chloroplast.

Plants can be classified into at least three major groups based on the biochemical pathway by which they fix CO_2: the C_3, C_4, and CAM (Crassulacean acid metabolism, which is a pathway adapted to arid conditions, allowing photosynthesis during the day but only gas exchange at night). The latter is not implemented in Daisy and will not be described in this context. The C_4 photosynthesis differs from C_3 in several biochemical and physiological properties, and C_4 plants lack several features of C_3 plants that are associated to photorespiration. Both C_3 and C_4 plants use the enzyme ribulose biphosphate carboxylase (RuBP or Rubisco) for the primary fixation of CO_2; however, the Rubisco reaction is compartmented differently. Most plants use the C_3 pathway, including all the temperate cereals (wheat, barley, etc), root crops (e.g. potato and sugar beet), and leguminous species (beans, etc.), while C_4-photosynthesis is associated with a warm climate where reduction of photorespiration is beneficial. The C_4 pathway, is important for agricultural crops like maize, sugarcane, sorghum, pearl millet, and certain grasses for pasture as Sudan grass.

The sun/shade radiation model in Daisy (sun-shade-open canopy, abbreviated SSOC) is inspired by the sun/shade model of de Pury and Farquhar (1997). The sun/shade model of de Pury and Farquhar (1997) is a single-layer model which describes the sunlit and shaded leaves separately. In the sun/shade model of de Pury and Farquhar (1997) the angle of incidence (incoming radiation) on leaves is not considered. Instead, the partitioning between the sunlit and shaded fractions of the canopies is changed every time step. As described in Ch. 10, section 10.5.3, the canopy in Daisy is divided in several layers (n, by default 30) with equal leaf area index. The cumulative absorbed irradiance (from the top of the canopy) is calculated for each canopy layer in the SSOC-model.

A number of widely used mechanistic models of photosynthesis and stomata conductance at the leaf level (e.g. Boegh et al. (2002); Leuning (1995); Collatz et al. (1991); Sellers et al. (1996)) are derived from the C_3 photosynthesis model of Farquhar et al. (1980) and the empirical stomatal conductance model of Ball et al. (1987). Boegh et al. (1987) and Collatz et al. (1991) have implemented these two models combined with the leaf energy balances for both C_3 and C_4 plants, as is required for the SSOC-model. These interacting models are solved by a numerical method, the Newton Raphson method.

Two models, based on the Farquhar-Ball-Collatz models, are implemented in the DAISY code. They are named the *FC-C3* and the *FC-C4* model, for C_3 and C_4 plants, respectively.

The content of this Appendix

The description of the Farquhar photosynthesis is complex, as it includes calculation of the light absorbed by the leaves as the potential driver of photosynthesis (Section 4), estimation of the Rubisco capacity to carry out the fixation (Section 5), and estimation of the CO_2-transport across the stomata allowing carbon fixation (Section 6). All these factors may limit the photosynthesis. Section 7 summarizes the temperature correction models applied, and Section 8 outlines the calculation procedure for the photosynthesis conductance model.

The calculation of the absorbed light is also an integral part of the energy calculation of the SSOC-SVAT model. Here, the calculations are described for PAR only, but in the SSOC-SVAT-model, similar calculations are carried out for Near Infrared light (NIR). NIR and PAR are treated in the same way with respect to energy calculations for the SSOC-model calculations, considering their different optical properties. Also, the transport of water vapour across the stomata links this photosynthesis model to the sensible heat calculations of the SSOC.

2 Radiation types and calculations

Shortwave radiation comprises photosynthetically active radiation (PAR) and near infrared radiation (NIR). In the model PAR contributes 50 % and NIR contributes 47% of the global radiation (Ross, 1975). Only PAR contributes to photosynthesis, while both types are relevant for energy calculations.

The types of irradiances considered in the model is irradiance directly from the sun hitting the leaves (beam, $I_{(b,i)}$) and diffuse irradiance, $I_{(d,i)}$, but in addition irradiance scattered when hitting a leaf may be absorbed by other leaves. This is named scattered beam, $I_{(bs,i)}$, and scattered diffuse irradiance, $I_{(ds,i)}$.

The total amount of irradiance absorbed by sunlit leaves is calculated as absorbed beam plus absorbed diffuse and absorbed scattered beam irradiance, e.g. absorbed $I_{(b,i)} + I_{(d,i)} + I_{(bs,i)}$. The irradiance absorbed by shaded leaves is calculated as absorbed diffuse and absorbed scattered beam, e.g. absorbed $I_{(d,i)} + I_{(bs,i)}$. Diffuse and scattered radiations are assumed isotropic, and beam radiation is unidirectional.

3 Calculation of PAR

The photosynthetic quantum flux, I, (eq. 10.3.1) is often the major factor determining the rate of carbon dioxide (CO_2) assimilation of individual leaves. As mentioned above, only about 50% of global radiation is PAR. This fraction is hard coded in the model.

$$I_{(Total,0)} = \omega \cdot f_{PAR} \cdot S_i \qquad (10.3.1)$$

where

f_{PAR} = the fraction of radiation, which is PAR (0.5).

ω = conversion factor to convert daylight from [W m^{-2}] to [mol m^{-2} s^{-1}] (ω = 4.6·10^{-6} [mol s^{-1} W^{-1}] (McCree, 1981)),

S_i = Global radiation [W m^{-2}], and

$I_{(Total,0)}$ = Total PAR per unit ground area above the canopy [mol m^{-2} s^{-1}]

If global diffuse radiation is climate input:

If the global diffuse radiation is given in the weather input file, the diffuse PAR above the canopy, $I_{(d,0)}$, is given by:

$$I_{(d,0)} = \omega \cdot f_{PAR} \cdot R_d \quad (10.3.2)$$

where

R_d = Global diffuse radiation [W m^{-2}], and

$I_{(d,0)}$ = Diffuse PAR per unit ground area above the canopy [mol m^{-2} s^{-1}]

and the photosynthetic quantum flux, I, for beam PAR above the canopy, $I_{(b,0)}$, is given by:

$$I_{(b,0)} = \omega \cdot f_{PAR} \cdot (S_i - R_d) \quad (10.3.3)$$

If global diffuse radiation must be calculated:

If the global diffuse radiation is not given as an input driving variable, the diffuse radiation model (*difrad*) in DAISY calculates the fraction of the total PAR that is diffuse PAR by the principles described by de Pury and Farquhar (1997). This model was originally developed for short wave radiation, which has different scattering and absorption properties than PAR but de Pury and Farquhar (1997) assumed that the process is similar for PAR. It is furthermore assumed, that the diffuse fraction of the total PAR equals the fraction of total global radiation that is diffuse. Direct beam PAR calculated from extra-terrestrial PAR is given by:

$$I_{(b\_optimal)} = \alpha^m \cdot S_{io} \cdot sin(\beta) \quad (10.3.4)$$

where

$I_{b\_optimal}$ = Direct beam PAR under a cloudless sky [W m^{-2}]

α = Atmospheric transmission coefficient of PAR (by default 0.72 [ ] (de Pury and Farquhar, 1997). Values range from 0.6-0.9 depending on dust particles.

m = optical air mass [ ], calculated in eq. (10.3.5),

S_{io} = Extraterrestrial radiation [W m^{-2}] (eq. (2.13), see Chapter 2), and

β = the solar elevation angle [radian] (eq. (2.16)). If $sin(\beta)<0.01$, $sin(\beta)=1$.

The optical air mass is given by:

$$m = \frac{P}{P_0 \cdot sin(\beta)} \quad (10.3.5)$$

where

P = the atmospheric pressure [Pa], see. Eq. (2.6) in Chapter 2.

P_0 =the atmospheric pressure at sea level ($1.013 \cdot 10^5$ [Pa])

The diffuse PAR ($I_{d\_optimal}$) under a cloudless sky is given by eq. (10.3.6):

$$I_{(d\_optimal)} = f_a \cdot (1 - \alpha^m) \cdot S_{io} \cdot sin(\beta) \quad (10.3.6)$$

where

$I_{d\_optimal}$ = Diffuse PAR under a cloudless sky [W m^{-2}]

f_a = forward scattering coefficient of PAR in the atmosphere (0.426 [ ]).

The fraction of diffuse radiation (f_d) of the total attenuated radiation for cloudless skies can then be expressed as:

$$f_d = \frac{I_{d\_optimal}}{I_{d\_optimal} + I_{b\_optimal}} \quad (10.3.7)$$

where

f_d = fraction of diffuse radiation under a cloudless sky [ ]

The expression for f_d can be reduced to a function of a^m and f_a:

$$f_d = \frac{f_a \cdot (1 - \alpha^m) \cdot S_{io} \cdot sin(\beta)}{\alpha^m \cdot S_{io} \cdot sin(\beta) + f_a \cdot (1 - \alpha^m) \cdot S_{io} \cdot sin(\beta)}$$

$$f_d = \frac{(1 - \alpha^m)}{\frac{1}{f_a}\alpha^m + (1 - \alpha^m)}$$

$$f_d = \frac{(1 - \alpha^m)}{1 + \alpha^m \left(\frac{1}{f_a} - 1\right)} \quad (10.3.8)$$

Early morning and late evening, the sinus function of the solar elevation angle, $sin(\beta)$, becomes negative while there is still light and then it is assumed that all radiation is diffuse by setting $f_d = 1.0$. The global diffuse radiation is then given by eq. (10.3.8). The diffuse (eq. (10.3.2)) and direct beam PAR (eq. (10.3.3), ($I_{(b,0)}=0$) can then be calculated.

$$R_d = f_d \cdot S_i \quad (10.3.9)$$

4 Distribution of irradiance in the canopy

Each plant community has a unique spatial leaf pattern for displaying photosynthetic surfaces and to capture photosynthetic active radiation (PAR). Absorption of photosynthetic quantum flux, I, depends on leaf orientation, leaf arrangement in the canopy, sun elevation in the sky, changes in spectral distribution of I through the canopy, and multiple reflections of I within the canopy. To describe the penetration of diffuse, beam and scattered PAR in the canopy, it is assumed that the decrease of I down into a canopy is analogous to

absorption of light by chlorophyll or other pigments in a solution, which is described by Beer's law (Nobel, 1991). In the following, the subscript $_{(f,i)}$) refers to the sunlit or shaded fraction, f, of the leaves, and canopy layer, i.

4.1 Calculation of sunny and shaded fractions of LAI

Sun fleck penetration, sunlit leaf area fraction

The sunlit leaf area fraction (or the sun fleck penetration), $f_{(sun,\ i)}$ [ ], of canopy layer, i, is given by:

$$f_{(sun,i)} = exp(-k_b \cdot L_i) \tag{10.3.10}$$

where

L_i = The cumulative leaf area index from top of the canopy down to layer i [m^2 m^{-2}]. ($L=0$ for $i=0$ (top), $L=L_c$ for $i=n$ (bottom)).

k_b = Extinction coefficient of beam radiation for black leaves [ ].

The extinction coefficient of beam radiation is calculated as:

$$k_b = \begin{cases} \dfrac{0.5}{sin(\beta)} & sin(\beta) > 0.0625 \\ 8.0 & sin(\beta) \leq 0.0625 \end{cases} \tag{10.3.11}$$

where β is the solar elevation angle [radians]

A maximum value of 8.0 is set, as k_b reaches unrealistic values when the solar elevation goes towards 0 (and for negative values). The boundary of 0.0625 radians corresponds to about 3.6°.

The penetration of sun flecks in the canopy at two different development stages with different leaf area index is shown in Figure 1. Increasing leaf area index through the canopy layers decreases the penetration of sun flecks.

The sunlit leaf area fraction, $L_{(sun,i)}$ [m^2 m^{-2}], of canopy layer *i* is then calculated as the difference between sun fleck penetration (eq. (10.3.10) to layer $(i\text{-}1)$ and layer i, divided by k_b:

$$L_{(sun,i)} = [exp(-k_b L_{i-1}) - exp(-k_b L_i)]/k_b \tag{10.3.12}$$

while the shaded leaf area index, $L_{(sh,i)}$ [m^2 m^{-2}] in the canopy layer is:

$$L_{(sh,i)} = L_i - L_{(sun,i)} \tag{10.3.13}$$

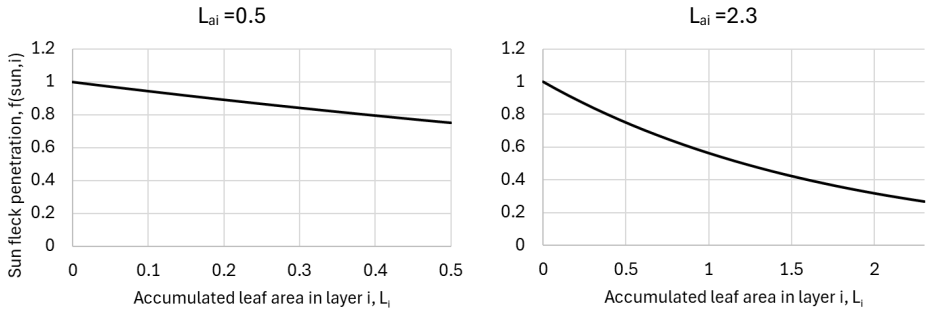

Figure 1.The sun fleck penetration in the canopy layers given by eq. (10.3.10) and (10.3.11) (using sin(β)=0.87) at two different leaf area index values for the total canopy (L_c). (L_c = 0.5, L_c = 2.3).

The cumulative sunlit and total leaf area indices in the canopy layers, at two leaf area index values of the canopy, are shown in Figure 2. In the early stage of crop development, where the total leaf area index is low (left, Figure 2) all the leaves in the canopy are mainly sunlit. However, at the later development stage, where the total leaf area index is increased, the shaded fraction of the leaves increases (right, Figure 2.

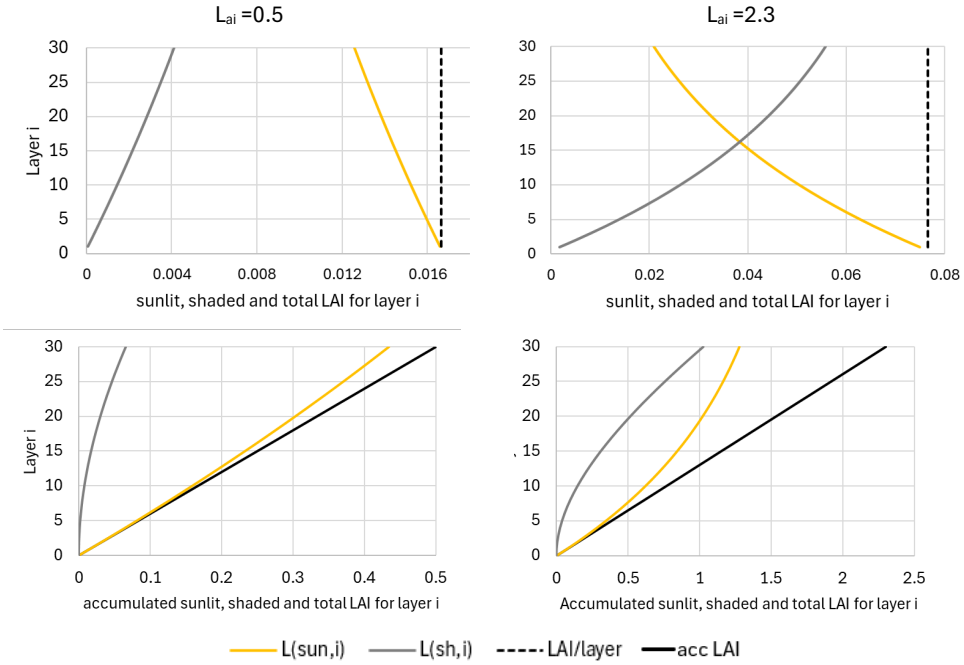

Figure 2. Top: Total LAI per calculation layer, as well as the sunlit and shaded fraction of each calculation layer for two values of total L_{ai} (0.5 and 2.3). Bottom: Accumulated LAI, accumulated sunlit LAI, and accumulated shaded LAI for each calculation layer for two values of total L_{ai} (0.5 and 2.3).

4.2 General equations for light penetration (de Pury and Farquhar (1997))

Although the Daisy implementation does not follow all aspects of de Pury and Farquhar (1997), their governing equations for light penetration (A2-A8 in the article) are listed in Table 1. This is done to ease the understanding of the calculations for sunlit and shaded leaves in the following sections. The equations A2, A3 and A5 in Table 1 describe light penetration similarly to Beer's law.

Table 1. Equations for radiation absorption in a multi-layer model (de Pury and Farquhar, 1997). The equations A2, A3 and A5 calculate light penetration rather than absorption, in parallel to Beer's law.

$I_{(b,i)} = I_{(b,0)}\left(1-\rho_{b,c}\right)\cdot k_b.exp(-k_b L_i)$	Beam irradiance – without scattering, average for all leaves.	A2
$I_{(b,i)} = I_{(b,0)}\left[\left(1-\rho_{b,c}\right)\cdot k_b'\cdot exp(-(k_b')L_i)\right]$	Beam irradiance – with scattering, average for all leaves	A3
$k' = k\sqrt{(1-\sigma)}$	Modified extinction coefficients to account for scattering by leaves	A4
$I_{(d,i)} = I_{(d,0)}\left(1-\rho_{d,c}\right)\cdot k_d'\cdot exp(-k_d' L_i)$	Diffuse irradiance	A5
$I_{total,i} = I_{b,i} + I_{d,i}$	Total irradiance	A6
$I_{sh,i} = I_{d,i} + I_{bs,i}$	Irradiance absorbed by shaded leaves	A7
$I_{(bs,i)} = I_{(b,0)}\left[\left(1-\rho_{b,c}\right)\cdot k_b'\cdot exp(-(k_b')L_i) - (1-\sigma)\cdot k_b\cdot exp(k_b L_i)\right]$	Scattered beam irradiance. Note: this equation is (A3-A2), where $\rho_{b,c}$ in A2 is exchanged with the leaf scattering coefficient for PAR.	A8
σ	Leaf scattering coefficient of PAR [ ]	
$\rho_{b,c}$	Canopy reflection coefficient for beam PAR [ ]	
$\rho_{d,c}$	Canopy reflection coefficient for diffuse PAR [ ]	

4.3 Light absorption in sunlit leaves

The total absorbed irradiance for the sunlit leaf fraction is the sum of absorbed direct beam irradiance, the diffuse irradiance and the scattered beam irradiance.

Absorbed direct beam irradiance

The cumulative (from top of the canopy to the actual layer, layer i), absorbed direct beam (without scattering) irradiance, $I_{(b,i)}$, is given by (Boegh et al. (2002), Plauborg et al. (2010)):

$$I_{(b,i)} = I_{(b,0)}(1-\sigma)[1-exp(-k_b L_i)] \quad (10.3.14)$$

where

σ = Leaf scattering coefficient of PAR [ ], (σ = 0.15 for wheat (de Pury and Farquhar, 1997)).

$I_{(b,0)}$ = Beam quantum flux per unit ground area above the canopy [mol m^{-2} s^{-1}], calculated by Eq. (10.3.3).

L_i = The cumulative leaf area index from top of the canopy to layer i [m^2 m^{-2}]. ($L=0$ for $i=0$ (top), $L=L_{ai}$ for $i=n$ (bottom)).

Note, that by using [$1-exp(-k_b L_i)$], this equation differs from eq. (A2) in Table 1 because it describes light absorption rather than light penetration.

Absorbed scattered beam irradiance

The cumulative (integrated) (from top of the canopy to the actual layer, layer i) quantum flux of scattered beam irradiance, $I_{(bs,i)}$, is given in eq. A8 in Table 1 above. However, in Daisy, the canopy reflection coefficient, $\rho_{b,c}$ is substituted by the canopy-soil reflection coefficient, $\rho_{b,c-s}$ (Plauborg et al., 2010).

$$I_{(bs,i)} = I_{(b,0)}\Big[(1-\rho_{b,c-s})k'_b[1-exp(-(k'_b)L_i)] - (1-\sigma)k_b[1-exp(k_b L_i)]\Big] \quad (10.3.15)$$

where

k'_b = Modified extinction coefficient of beam radiation due to leaf scattering [ ], calculated in eq. (10.3.16), and

$\rho_{b,c-s}$ = Canopy -soil reflection coefficient for beam PAR, calculated in eq. (10.3.18) (Plauborg et al., 2010)). It should be noted that de Pury and Farquhar, (1997) use another parameter, namely the canopy reflection coefficient for beam PAR, $\rho_{b,c}$ (see eq. (10.3.17)), in equation (10.3.15) without taking into account the soil surface reflectance.

The modified extinction coefficient is calculated as:

$$k'_b = k_b\sqrt{(1-\sigma)} \quad (10.3.16)$$

The canopy -soil reflection coefficient for beam PAR ($\rho_{b,c-s}$) requires two additional parameters, the direct beam canopy reflectance, $\rho_{b,c}$, and the soil surface reflectance of PAR, ρ_s, which is an input parameter. $\rho_{b,c}$ is calculated in eq. (10.3.17). ρ_s has a default value of 0.1 [ ] (Houborg, 2006). It can be modified using the plf *Ps_PAR_SWE* [pF→ <none>], which describes the effect of soil water on ρ_s.

The canopy reflection coefficient for beam PAR is calculated as:

$$\rho_{b,c} = 1 - exp\left(-2\frac{k_b}{(1+k_b)}\frac{\left(1-\sqrt{(1-\sigma)}\right)}{\left(1+\sqrt{(1-\sigma)}\right)}\right) \quad (10.3.17)$$

and the canopy-soil reflection coefficient for beam PAR is given by:

$$\rho_{b,c-s} = \frac{\rho_{b,c} + \frac{\rho_{b,c}-\rho_s}{\rho_{b,c}\cdot\rho_s - 1}exp(-2k'_b L_{ai})}{1 + \rho_{b,c}\frac{\rho_{b,c}-\rho_s}{\rho_{b,c}\cdot\rho_s - 1}exp(-2k'_b L_{ai})} \quad (10.3.18)$$

where L_{ai} is the total leaf area.

Eq. (10.3.15) must be considered for each layer, i, and combined with the area of sun fleck penetration, eq. (10.3.10), to describe the cumulative quantum flux of scattered beam irradiance for the sunlit part of the leaves of layer i, resulting in eq. (10.3.19):

$$I_{(bs,i)} = I_{(b,0)}\left[\left(1-\rho_{b,c-s}\right)[1-exp(-(k'_b+k_b)L_i)]\frac{k'_b}{(k'_b+k_b)} - (1-\sigma)\frac{[1-exp(-2k_bL_i)]}{2}\right] \quad (10.3.19)$$

Absorbed diffuse irradiance

Similarly, the cumulative (from top of the canopy to the actual layer, layer i) quantum flux of diffuse irradiance, $I_{(d,i)}$, is calculated by combining the equation for diffuse irradiance (A5 in Table 1) with eq. (10.3.10) for sun fleck penetration, and substituting the canopy reflection coefficient for diffuse light with a canopy-soil reflection coefficient, resulting in eq. (10.3.20).

$$I_{(d,i)} = I_{(d,0)}\left(1-\rho_{d,c-s}\right)[1-exp(-(k'_d+k_b)L_i)]\frac{k'_d}{(k'_d+k_b)} \quad (10.3.20)$$

where

$I_{(d,0)}$ = Diffuse quantum flux per unit ground area above the canopy [mol m^{-2} s^{-1}].

k'_d = Extinction coefficient of diffuse and scattered PAR radiation [ ], calculated in eq. (10.3.21) (de Pury and Farquhar, 1997),

$\rho_{d,c-s}$ = Canopy-soil reflection coefficient for diffuse PAR calculated in eq. (10.3.24). This is different from the $\rho_{d,c}$ used by de Pury and Farquhar (1997), which is shown in eq. (10.3.25) for information.

$$k'_d = k_d\sqrt{(1-\sigma)} \quad (10.3.21)$$

where k_d is given by (Plauborg et al., 2010):

$$k_d = \frac{-ln(\tau_d)}{L_{ai}} \quad (10.3.22)$$

where L_{ai} is the total leaf area and τ_d is calculated below by integrating over the hemisphere (ψ [radians]):

$$\tau_d = 2\int_0^{\pi/2} exp(-k_b L_{ai}) sin(\psi)\, cos(\psi)\, d\psi \qquad (10.3.23)$$

The canopy-soil reflection coefficient for diffuse PAR, $\rho_{d,c\text{-}s}$, is calculated similarly to $\rho_{b,c\text{-}s}$ (Plauborg et al., 2010), except k_b' is exchanged with k_d':

$$\rho_{d,c-s} = \frac{\rho_{b,c} + \frac{\rho_{b,c} - \rho_s}{\rho_{b,c} \cdot \rho_s - 1} exp(-2k'_d L_{ai})}{1 + \rho_{b,c} \frac{\rho_{b,c} - \rho_s}{\rho_{b,c} \cdot \rho_s - 1} exp(-2k'_d L_{ai})} \qquad (10.3.24)$$

The reflection coefficient used by (de Pury and Farquhar, 1997) for diffuse irradiance was calculated by numerical integration of $\rho_{b,c}$ and sky radiance over the hemisphere of the sky, as shown below for comparison:

$$\rho_{d,c} = \frac{1}{I_d(0)} \int_0^{\pi/2} N_d(\alpha)\, \rho_{b,c}(\alpha) d\alpha \qquad (10.3.25)$$

where

N_d = diffuse photon radiance of the sky, $I_d(0)/(2\pi)$ [µmol $m^{-2}s^{-1}$ $radian^{-1}$],

α = angle of beam irradiance to the leaf normal [radians].

The total quantum flux received by sunlit leaves

The cumulative (from top of the canopy to the actual layer) quantum flux of irradiance absorbed by sunlit leaves, $I_{(sun,i)}$,in each canopy layer is calculated as the sum of eq. (10.3.14), eq. (10.3.19), and eq. (10.3.20):

$$I_{(sun,i)} = I_{(b,i)} + I_{(bs,i)} + I_{(d,i)} \qquad (10.3.26)$$

The absorbed irradiances of the sunlit fractions in the canopy layers, at two different leaf area index values of the canopy, L_c, are shown in Figure 3. It is seen that for the sunlit fraction of the leaves, the most dominating type of irradiance which is absorbed is the direct beam fraction even at high leaf area index-values. However, the sunlit leaf area fraction decreases through the canopy layers which is not shown in Figure 3. The diffuse and scattered radiation remains relatively small through the canopy in this example. If the shaded fraction increases, for example during cloudy conditions, then the diffuse and scattered radiation also increases for sunlit leaves.

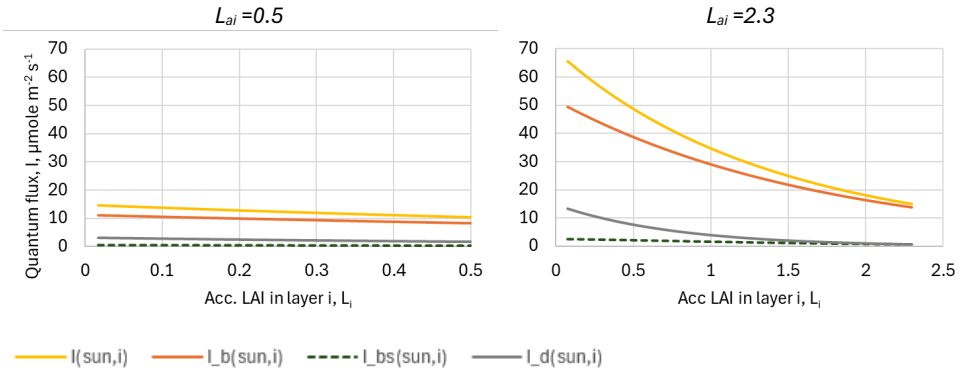

Figure 3. The absorbed quantum flux of the sunlit fractions, $I_{(sun,i)}$, as a function of the cumulative leaf area index, L_{ai}) in the canopy layers given by eq. (10.3.14), (10.3.19-20) and (10.3.26) at two different leaf area index values for the total canopy (L_c). Left: L_c = 0.5. Right: L_c = 2.3. S_i was set to 700 [W m^{-2}] and β = 60 degrees.

4.4 Light absorption in shaded leaves

The irradiance absorbed by the shaded leaf area of the canopy is calculated as the difference between the total irradiance absorbed by the canopy, $I_{(total,i)}$, (eq. 10.3.27) and the irradiance absorbed by the sunlit leaf area, $I_{(sun,i)}$ (eq. 10.3.26).

The total quantum flux absorbed by the canopy, $I_{(total,i)}$ (see eq. A2, A5 and A6 in Table 1), is given by:

$$I_{(total,i)} = \left(I - \rho_{b,c-soil}\right)I_{(b,0)}\left(1 - exp(-k'_b L_i)\right) + \left(I - \rho_{d,c-soil}\right)I_{(d,0)}\left(1 - exp(-k'_d L_i)\right) \quad (10.3.27)$$

The quantum flux absorbed by the shaded leaf area, $I_{(sh,i)}$ is then calculated as a difference:

$$I_{sh,i} = I_{(total,i)} - I_{(sun,i)} \quad (10.3.28)$$

The absorbed quantum flux of the total, sunlit and shaded parts are shown in Figure 4.

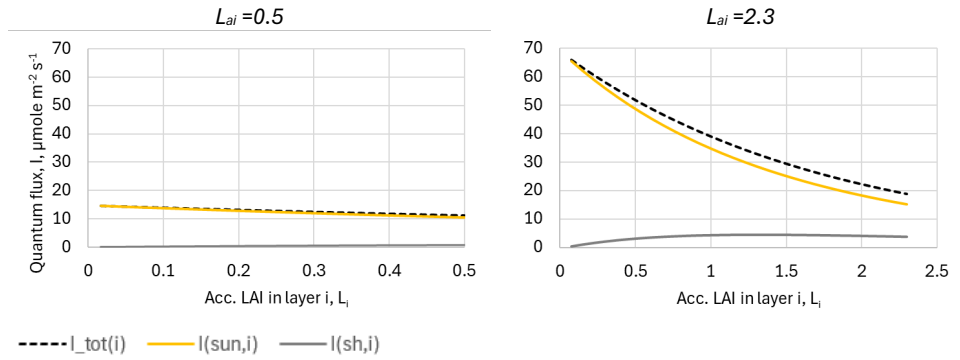

Figure 4. The actual quantum flux of absorbed irradiances (total, sunlit and shaded) as a function of the total leaf area index in each canopy layer, L_i, at two different leaf area index values of the total canopy (L_{ai}). Top: L_c = 0.5. Bottom: L_c = 2.3. S_i was set to 700 [W m^{-2}] and β = 60 degrees.

5 Photosynthetic capacity

5.1 Rubisco-N in leaves

Rubisco is the most abundant protein in leaves of C_3 plants, constituting up to half the total leaf protein. For this reason, it plays a crucial role in the nitrogen economy of plants.

The *rubiscoN* sub-model estimates, by default, the amount of photosynthetically active N in leaves to be 75 % of the total N (Boegh et al., 2002). This amount is specified using the parameter *fraction* [ ]. This option is chosen as default, as many of the parameters used in the SSOC/Farquhar-models stem from the work by Boegh et al. (2002). A certain amount of N per LAI can be deducted before multiplying with the fraction, if required, using the parameter *offset* [g N m^{-2}].

It is, however, also possible to describe the amount of photosynthetically active N using the N-limits defined for the plant, that is the non-functional and critical limits of N. The non-functional N is considered to be structural N, and thus not used in photosynthesis. The N content above the critical content is considered luxury N uptake, that is also not used in photosynthesis. Hence, the photosynthetic active Rubisco nitrogen, N_P, could also be given by:

$$N_R = \begin{cases} N_a - N_n, & 0 < (N_a - N_n) \leq (N_c - N_n) \\ N_c - N_n, & (N_a - N_n) > (N_c - N_n) \\ 0, & 0 \geq (N_a - N_n) \end{cases} \qquad (10.3.29)$$

where

N_R = The photosynthetically active Rubisco associated nitrogen [mol m^{-2}],

N_a = The actual leaf nitrogen content [mol m^{-2}],

N_c = The critical limit for leaf nitrogen above which the uptake is luxury [mol m^{-2}],

N_n = the non-functional (structural leaf nitrogen) [mol m^{-2}].

The crop production component in Daisy calculates the actual leaf nitrogen content in the canopy, N_a. The *CropN*-component in Daisy calculates the critical, N_c, and non-functional, N_n, limits based on specified concentrations and the dry matter weight of the leaves. To apply this approach, the two Boolean parameters *subtract_Nf* and *subtract_Pt* should be set to *true* (default is *false*), and in that case, the fraction must be set to 1.0.

Boegh et al. (2002) recalculated the N-content [g N $(g\ DM)^{-1}$] by dividing by specific leaf area [$m^2\ g^{-1}$] and molar weight [$g\ mol^{-1}$], resulting in mol m^{-2}. They used a specific leaf area of 1/54.08 [$m^2\ g^{-1}$]. In Daisy, specific leaf area is specified in the crop files.

The Rubisco N distribution with depth in the canopy layer, $N_{R(f,i)}$, can be defined by two different functions (*exp*, or *uniform*). These functions are described in section 5.2.

5.2 Canopy nitrogen distribution sub-models (*RubiscoN-dist*)

The maximum leaf Rubisco capacity in each layer is defined as function of photosynthetic active nitrogen. The distribution of photosynthetic active nitrogen in the canopy can be described by two different functions (*exp* or *uniform)*.

Exponential distribution (exp)

The exponential model is described by (Boegh et al., 2002). The photosynthetically active Rubisco associated nitrogen in the sunny or shaded part of the i'th layer can be calculated as:

$$N_{R(f,i)} = N_{R(f,0)} exp\left(\frac{-k_n L_{(f,i)}}{L_{ai}}\right) \quad (10.3.30)$$

where

k_n = Coefficient of leaf nitrogen allocation in a canopy (0.713 [ ] (Boegh et al., 2002)

$L_{(f,i)}$ = Cumulative leaf area index [m^2 m^{-2}] for layer i.

L_{ai} = The total leaf area.

$N_{R(f,i)}$ = The photosynthetically active Rubisco-associated nitrogen in the sunny or shaded part of layer i, [mol m^{-2}].

$N_{R(f,0)}$ = The photosynthetically active Rubisco-associated nitrogen in the top of the canopy [mol m^{-2}].

The photosynthetic active nitrogen (Rubisco N) in the top of the canopy, $N_{R(f,0)}$, is found by integrating eq. (10.3.30) and isolating $N_{R(f,0)}$:

$$\begin{aligned} N_{R(f,i)} &= N_{R(f,0)}\left(1 - \exp\left(-k'_n L_{(f,i)}\right)\right)/k'_n \\ N_{R(f,0)} &= \frac{k_n N_R}{1 - exp(-k'_n L_{ai})} \end{aligned} \quad (10.3.31)$$

where N_R is the total amount of photosynthetically active Rubisco associated nitrogen [mol m^{-2}] given by eq. (10.3.29) and $k'_n = k_n/L_{ai}$..

Figure 5 shows the distribution of photosynthetically active nitrogen (Rubisco N) according to eq. (10.3.30) (blue line) and (10.3.31) (orange line), assuming that $N_{R(f,0)}$ = 150.8 [mmol m^{-2}] for two values of L_{ai}. This corresponds to N_R = 53.9 and 248 mmol m^{-2} for the total canopy with L_{ai} = 0.5 and 2.3, respectively. Note, that although the units appear to be identical, $N_{R(f,i)}$ is mmol m^{-2} leaf, while the accumulated value is in mmol m^{-2} soil surface. Thus, the end point of the orange line is the total N-content per m^2 soil.

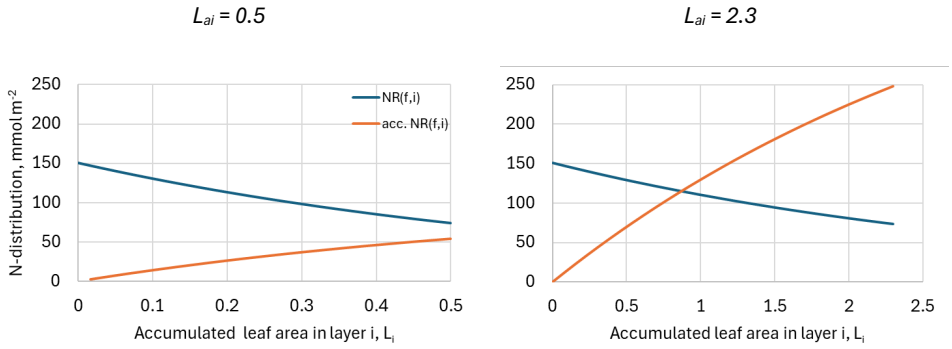

Figure 5. The nitrogen distribution of Rubisco N as a function of the cumulative leaf area index in the canopy layers (L_i) with $N_{R(f,0)}$ equal to 219.4 mmol m^{-2}. This corresponds to N_R = 92.3 and 248 mmol m^{-2} for the total canopy with L_{ai} = 0.5 and 2.3, respectively. The blue line is calculated according to eq. (10.3.30), while the orange line is the integrated value from eq. (10.3.31-top). Note that $N_{R(f,i)}$ is mmol m^{-2} leaf, while the accumulated value is in mmol m^{-2} soil surface.

Option 4: uniform

The option *uniform* assumes a uniform distribution of Rubisco-N in the canopy for photosynthesis. The concentration used is thus the N-content of the crop divided by molar weight of N and by L_{ai} [mol m^{-2} leaf]. In this case, the blue line in Figure 5 will be a horizontal line of constant value, and the accumulated $N_{R(f,i)}$ will be a straight line from 0 to the total N-content in [mol m^{-2} soil].

The options allow specification of the fraction of photosynthetically active N in the canopy (*f_photo*, default = 1 []). According to (Boegh et al., 2002), the value of this fraction is 0.75. However, non-functional N is already subtracted from the leaf-N in the *cropN* module. Therefore, the parameter has be set to 1 as default.

5.3 Conversion from Rubisco-N to photosynthetic capacity

The maximum leaf Rubisco capacity in each layer, $V_{max25,i}$, determined at 25 °C is described as:

$$V_{max25(f,i)} = \chi_n N_{R(f,i)} \qquad (10.3.32)$$

where

$V_{max25(f,i)}$ = The maximum leaf Rubisco capacity at 25 °C [mol m^{-2} s^{-1}]

χ_n = The ratio of measured Rubisco capacity to leaf nitrogen (default = 1.16·10^{-3} [mol mol^{-1} s^{-1}] for wheat (Boegh et al., 2002)).

In fact, both the N-content per leaf area and the accumulated N-content per m^2 soil are proportional to the respective V_{max25}-values, using this factor.

The partitioning of leaves into sunlit and shaded fractions is continually changing throughout the day. The calculation of the photosynthetic capacity is affected by these separate fractions.

5.4 Sunlit leaves

The fraction of $V_{m(sun,i)}$ per leaf area (the rubisco capacity of each layer, i) is calculated simply by multiplying the value for the leaf ($V_{max25(f,i)}$)with the sun fleck penetration calculated in eq.(10.3.10) and correcting for leaf temperature.

$$V_{m(sun,i)} = L_{(sun,i)} \cdot V_{\max 25(f,i)} \cdot f_{V_{max}}^{CX}(T_l) \qquad (10.3.33)$$

The temperature functions, $f_{V_{max}}^{CX}(T_l)$, differ between C_3 and C_4-photosynthesis, see eq. (10.3.71) and (10.3.72) [mol m^{-2} s^{-1}], section 7. T_l is the leaf temperature, in this case of the sunlit leaves.

Assuming the default option for N-distribution in the canopy (*exp*), the accumulated photosynthetic capacity of the sunlit leaf fraction, $V_{mSun,i}$, of each canopy layers is, given by:

$$V_{m(sun,i)}^{acc} = L_i \cdot V_{\max(f,0)}^{T} \left[\frac{1 - exp(-k'_n - k_b L_i)}{k'_n + k_b L_{,i}} \right] \qquad (10.3.34)$$

where

k_b = Extinction coefficient of beam radiation ([ ], given by eq. (10.3.10).

k'_n = Coefficient of leaf nitrogen allocation in a canopy (0.713 in *rubiscoNdist*-option *exp*(de Pury and Farquhar, 1997)), divided by L_{ai}.

$V_{m(sun,i)}^{acc}$ = The accumulated canopy photosynthetic capacity in sunlit leaves for layer 1 to *i* [mol m^{-2} s^{-1}].

$V^{T}_{max(f,0)}$ = The maximum leaf Rubisco capacity in sunlit leaves at temperature T_l [mol m^{-2} s^{-1}], calculated as $N_{R(f,0)}$ (eq. (10.3.31) $\cdot \chi_n \cdot f_{V_{max}}^{CX}(T_l)$.

5.5 Shaded leaves

Photosynthetic capacity of the shaded leaf fraction, $V_{m,(sh,i)}$, [mol m^{-2} s^{-1}],of each canopy layers is given by:

$$V_{m(sh,i)} = L_{(sh,i)} \cdot V_{\max 25(f,i)} \cdot f_{V_{max}}^{CX}(T_l) \qquad (10.3.35)$$

In this case, the maximum leaf rubisco capacity is multiplied by the shaded fraction of the leaf layer and the temperature correction based on the temperature of the shaded leaf.

Figure 6 shows the different fractions of the photosynthetic capacity in the canopy together with the nitrogen distribution.

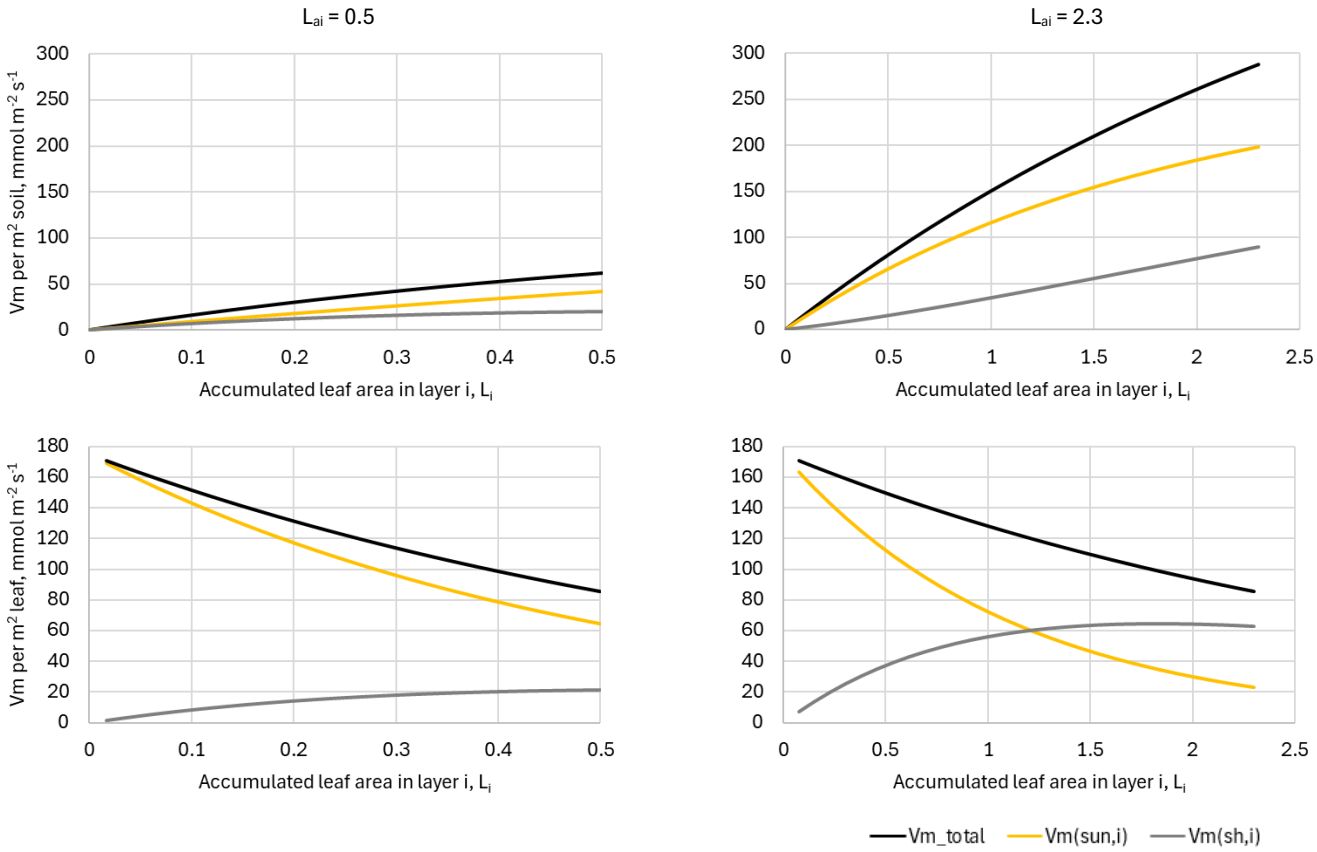

Figure 6. Top panel: Accumulated photosynthetic capacity (Vm_{total}) per m² soil surface, divided in accumulated values for the sunny ($Vm_{(sun,i)}$) and shaded ($Vm_{(sh,i)}$) parts, at 25 °C. Note, that axes differ between figures. Bottom panel: The same variables per m² leaf. The total values differ from the respective curves in Figure 5 by the factor χ_n.

6 Photosynthesis and stomata conductance model

As for the calculation of absorbed PAR and Rubisco-distribution in the canopy layers, the photosynthesis model considers the sunlit and shaded leaves separately. Temperature and humidity are calculated by the *SSOC* SVAT model above and inside the canopy. The two compartments are separated by the aerodynamic resistance, r_a. Temperature is also calculated inside the stomata of sunlit and shaded leaves. Between the inside of the stomata and the leaf surface, there is a resistance, r_s, and between the leaf surface and the general canopy, there is a boundary resistance, r_b, both of which may differ between sunlit and shaded leaves. Resistance and conductance are inversely related. See the description of the SSOC-model in Appendix 2.4 for further details.

6.1 Stomatal sub-model

The stomata conductance model

Complex physiological mechanisms adjust the opening of stomata in response to changes in environmental conditions which affect the stomatal conductance of leaves and the canopy. In the Daisy component *stomatacon*, six submodels are listed, each of which are attempts to describe the stomata conductance of water vapour. Each of these are described below. The default choice is *Leuning*.

wsf

The *wsf*-function only describes the effect of abscisic acid (ABA) on stomata closure. This function is described in section 6.4, together with generation of ABA due to water stress. The calculated water stress effect is applied in all the following equations, if the function is parameterised. The default is no effect of ABA ($wsf = 1$ [ ]).

The BB and BB_base model

The *BB* model builds on *BB_base* and does not have any additional parameters; thus, it applies the default values supplied in BB_base. In this case, the stomatal response to environmental and physiological factors is modelled according to the empirical model developed by Ball et al. (1987). The model describes stomatal conductance for water, g^w_s [mol m^{-2} s^{-1}] as linearly related to CO_2 assimilation rate, A, and relative humidity, h_s, and inversely related to the CO_2 partial pressure, ρ_s, at the leaf surface. The stomatal conductance, g^w_s, for the sunlit or shaded fraction, f, of the leaves, and canopy layer, i, is given by:

$$g^w_{s(f,i)} = \begin{cases} w_{sf} \cdot m \dfrac{A_{(f,i)} \cdot P \cdot h_{s(f,i)}}{\rho_{s(f,i)}} + b_{(f,i)} & A_{(f,i)} > 0 \\ b_{(f,i)} & A_{(f,i)} \le 0 \end{cases} \qquad (10.3.36)$$

where

w_{sf} = water stress factor [ ] (section 6.4). $wsf = 1$ for no water stress.

m = Empirical vegetation constant [ ]. ($m = 9$ for wheat, $m = 11$ for soybean).

$b_{(f,i)}$ = Stomatal intercept factor. $b_{(f,i)} = b \cdot L_{(f,i)}$, where $b = 0.01$ [mol m^{-2} s^{-1}].

$L_{(f,i)}$ = Cumulative leaf area index [ ].

h_s = Relative humidity at the leaf surface calculated by eq. (10.3.41) [ ].

$A_{(f,i)}$ = The net photosynthesis rate [mol m^{-2} s^{-1}].

$\rho_{s(f,i)}$ = Partial CO_2 pressure at the leaf surface [Pa].

P = Atmospheric pressure [Pa]), calculated in eq. (2.6), Chapter 2.

The stomata conductance for the influx of CO_2 and the simultaneous efflux of water are directly linked to two vegetation-dependent coefficients (m, b). The two vegetation-dependent coefficients, m and b, have been parameterized by Wang and Leuning (1998) and Ball and Berry (1982) for wheat and soybean, respectively, but may be changed by the user in the BB_base-option.

Leuning

Leuning (Leuning, 1995) is the default option used by the *Farquhar* photosynthesis option. To improve the description of stomatal behaviour at low CO_2 concentrations, ρ_s is replaced with (ρ_s minus the CO_2 compensation point, Γ^*). Also, an additional term is introduced: $(1+D_s/D_0)$, where D_s is the moisture deficit [Pa] and D_0 is an empirical constant [Pa], by default 1500 [Pa].

In this case, the stomatal conductance, $g^w{}_s$, for the sunlit or shaded fraction, f, of the leaves, and canopy layer, i, is given by:

$$g^w_{s(f,i)} = \begin{cases} w_{sf} \cdot m \dfrac{A_{(f,i)} \cdot P \cdot h_{s(f,i)}}{\left(\rho_{s(f,i)} - \Gamma^{*T}_{(f)}\right)\left(1 + {}^{D_s}/_{D_0}\right)} + b_{(f,i)} & A_{(f,i)} > 0 \\ b_{(f,i)} & A_{(f,i)} \leq 0 \end{cases} \qquad (10.3.37)$$

where

w_{sf}, m, $b_{(f,i)}$, $L_{(f,i)}$, $A_{(f,i)}$, $\rho_{s(f,i)}$, and P, are defined above, and

h_s = Relative humidity at the leaf surface calculated analogous to eq. (10.3.41) [ ].

$\Gamma^{*T}_{(f)}$ = Temperature corrected CO_2 compensation point of photosynthesis (default = 3.69 [Pa] at 25 °C (de Pury and Farquhar, 1997)), see eq. (10.3.66).

D_s = The humidity deficit [Pa].

D_0 = An empirical constant, by default 1500 [Pa].

For the last two options, the units are slightly different. Here, $\rho_{s(f,i)}$ is recalculated to [ppm] ($c_s(f,i) = \rho_{s(f,i)}/P_{tot} \cdot 10^6$), and the net photosynthesis rate, $A_{(f,i)}$ is specified in [µmol m^{-2} s^{-1}]: $A^*_{(f,i)} = A_{(f,i)} \cdot 10^6$.The options *SHA12* and *SHA14* in combination with ABA-effects (*wsf*) were tested on measured data by Ahmadi et al. (2009) and could be parameterised to provide good fits (R^2 between 0.82 and 0.92).

SHA12

The SHA12 sub-model is identical to eq. 12 in Ahmadi et al. (2009):

$$g^w_{s(f,i)} = w_{sf} \cdot m \frac{\left(A^*_{(f,i)}\right)^{\lambda} \cdot \left(h_{s(f,i)}\right)^{\alpha}}{c_{s(f,i)}} \qquad (10.3.38)$$

where

α and λ are empirical constants given as input representing a humidity effect and a net photosynthesis effect, respectively. m is still a slope parameter, but its dimension depends on α and λ.

In addition, the minimum conductivity is an optional parameter (min [mol H_2O/m^2 leaf s^{-1}] that can be given as input. $g_{s(f,i)}$ is set to min if the calculated value is smaller than min.

SHA14

The SHA14 sub-model is identical to eq. 14 in Ahmadi et al. (2009):

$$g^w_{s(f,i)} = w_{sf} \cdot m \frac{exp\left(\lambda \cdot A^*_{(f,i)}\right) \cdot exp\left(\alpha \cdot h_{s(f,i)}\right)}{c_{s(f,i)}} \quad (10.3.39)$$

where

α and λ are empirical constants given as input representing a humidity effect and a net photosynthesis effect, respectively. m is a conductivity factor [mol H_2O m^{-2} leaf s^{-1}].

In addition, the maximum conductivity is an optional parameter (max [mol H_2O/m^2 leaf s^{-1}] that can be given as input. By default, there is no maximum. If a max value is defined, $g^w_{s(f,i)}$ is set to max if the calculated value is larger than max.

Finding humidity at the leaf surface, h_s

The stomatal model is merged with diffusion equations for water vapor flux through leaf boundary layer and stomata. The humidity at the leaf surface, h_s, is derived, according to Collatz et al. (1991), by solving the following quadratic equation (eq. 10.3.40) by the second root, illustrated for the BB_option:

$$\frac{w_{sf} \cdot m \cdot A_{(f,i)} \cdot P}{\rho_{s(f,i)}} {h_{s(f,i)}}^2 + \left(b_{(f,i)} + g^w_{b(f,i)} - \frac{w_{sf} \cdot m \cdot A_{(f,i)} \cdot P}{\rho_{s(f,i)}}\right) h_{s(f,i)} + \left(\frac{-e_a}{e_{l\_sat}} g^w_{b(f,i)} - b_{(f,i)}\right) = 0$$

where

$g^w_{b(f,i)}$ = Leaf boundary -layer conductance of water [mol m^{-2} s^{-1}].

e_a = Actual vapor pressure in the air [Pa].

e_{l_sat} = Saturated vapor pressure at the leaf surface given by eq. (10.3.42) [Pa].

Actual vapour pressure

The actual air vapour pressure, e_a, is calculated from the relative humidity and the saturated vapor pressure, e_{sat}:

$$e_a = h_a e_{a\_sat} \quad (10.3.41)$$

where h_a is the relative humidity of the air [mol mol^{-1}] and the saturated vapour pressure, e_{sat}, at the leaf surface or in the air is calculated as shown in eq. (10.3.43)

$$e_{sat}(T) = \Big(\big((a \cdot T + b) \cdot T + c\big)T + d\Big)T + e \quad (10.3.42)$$

where T is the temperature [°C], and the constants are defined as a = $5.818 \cdot 10^{-4}$; b = $1.408 \cdot 10^{-2}$; c = 1.675; d = $4.222 \cdot 10^{1}$; and e = $6.174 \cdot 10^{2}$.

The combined boundary- and stomata resistance for CO_2

The total boundary and stomata resistance to CO_2-movement ($r_t^{CO_2}$) can be described as:

$$r_t^{CO_2} = 1.4 \cdot r_b^w + 1.6 \cdot r_s^w = \frac{1.4}{g_b^w} + \frac{1.6}{g_s^w} = \frac{1.4 g_s^w + 1.6 g_b^w}{g_s^w \cdot g_b^w} \qquad (10.3.43)$$

The corresponding conductance for CO_2, $g_t^{CO_2}$equals $1/r_t^{CO_2}$.

CO_2 partial pressure inside stomata

The CO_2 partial pressure in the leaf interior, ρ_i, for C_3 and C_4 plants, are given by Collatz et al. (1991) and Collatz et al. (1992), respectively:

$$\rho_{i(f,i)} = \rho_a - P \cdot A_{(f,i)} \frac{1.6 \cdot g^w_{b(f,i)} + 1.4 \cdot g^w_{s(f,i)}}{g^w_{b(f,i)} \cdot g^w_{s(f,i)}} \quad \text{For } C_3$$

$$\rho_{i(f,i)} = \rho_a - P_{tot} A_{(f,i)} \frac{1.6}{g^w_{s(f,i)}} \quad \text{For } C_4 \qquad (10.3.44)$$

where

$\rho_{i(f,i)}$ = CO_2 partial pressure in the interior of the leaf [Pa].

$A_{(f,i)}$ = The net rate of photosynthesis [mol m^{-2} s^{-1}].

$g^w_{s(f,i)}$ = Stomatal conductance of leaves given by eq. (10.3.36-39), [mol m^{-2} s^{-1}].

$g^w_{b(f,i)}$ = leaf boundary-layer conductance [mol m^{-2} s^{-1}], calculated by the SSOC-model, Appendix 2.4, section 3.

ρ_a = The partial CO_2-pressure in the air (35 [Pa]). The atmospheric CO2-level can be specified in the weather files as a fraction.

6.2 Photosynthesis of C_3 leaves

Leaf assimilation (or gross photosynthetic rate) of C_3-leaves is described as the minimum of two limiting rates, w_c and w_e, which are functions that describe the assimilation rates as limited by the efficiency of the photosynthetic Rubisco capacity, w_c, and the amount of PAR absorbed, w_e, respectively.

Rubisco-limited assimilation rate, w_c

The assimilation rate limited by the efficiency of the photosynthetic Rubisco capacity, w_c, is given by (10.3.45):

$$w_{c(f,i)} = V_{m(f,i)} \frac{\rho_{i(f,i)} - \Gamma^{*T}_{(f)}}{\rho_{i(f,i)} + K_{cl}} \qquad (10.3.45)$$

where

$V_{m(f,i)}$ =Photosynthetic Rubisco capacity [mol m^{-2} s^{-1}]. V_m is the maximum catalytic capacity of Rubisco per unit leaf area (Farquhar et al., 1980), calculated in eq. (10.3. 33 or 35).

$\rho_{i(f,i)}$ = CO_2 partial pressure in leaf interior [Pa].

$\Gamma^{*T}_{(f)}$ = Temperature corrected (eq. (10.3.66)) CO_2 compensation point of photosynthesis (default = 3.69 [Pa] at 25 °C (de Pury and Farquhar, 1997)),

and K_{cl} is given by eq. (10.3.29):

$$K_{cl} = K_c^T \left(1 + \frac{O_2}{K_O^T}\right) \quad (10.3.46)$$

where

K_c^T = Temperature corrected (eq. (10.3.66)) Michaelis-Menten constant of Rubisco for CO_2 (default = 40.4 [Pa] at 25 °C (de Pury and Farquhar, 1997)),

K_O^T = Temperature corrected (eq. (10.3.66)) Michaelis-Menten constant of Rubisco for O_2 (default = 24800 [Pa] at 25 °C (de Pury and Farquhar, 1997)),

O_2 = O_2 partial pressure in leaf interior (20.5 ·10^3 [Pa] (de Pury and Farquhar, 1997).

The light limited rate of photosynthesis, w_e

The light limited rate of photosynthesis, w_e, is given by eq. (10.3.47):

$$w_{e(f,i)} = J_{(f,i)} \frac{\rho_{i(f,i)} - \Gamma_{(f)}^{*T}}{4 \cdot \left(\rho_{i(f,i)} + 2\Gamma_{(f)}^{*T}\right)} \quad (10.3.47)$$

where $J_{(f,i)}$ is the rate of electron transport [mol m^{-2} s^{-1}].

The rate of electron transport, J, depends on the absorbed irradiance, I_{le}, and an empirical constant, θ. The constant, θ, describes the non-linear curvature of leaf electron transport response to irradiance (Farquhar et al., 1980). The rate of electron transport, $J_{(f,i)}$, is estimated by solving the following quadratic equation (eq. 10.3.48) by the small root:

$$\theta \cdot J_{(f,i)}{}^2 - \left(I_{le(f,i)} + J_{m(f,i)}\right) J_{(f,i)} + I_{le(f,i)} \cdot J_{m(f,i)} = 0 \quad (10.3.48)$$

where

$I_{le(f,i)}$ = effectively absorbed PAR [mol m^{-2} s^{-1}], see below.

$J_{(f,i)}$ = Rate of electron transport [mol m^{-2} s^{-1}],

$J_{m(f,i)}$ = Potential rate of electron transport [mol m^{-2} s^{-1}], see below, and

θ = Empirical constant, curvature of leaf response to irradiance (default = 0.7 [ ] (de Pury and Farquhar, 1997).

The potential rate of electron transport, $J_{m(f,i)}$, is given calculated based on V_{max25}:

$$J_{max25(f,i)} = 2.1\, V_{max25(f,i)}$$
$$J_{m(f,i)} = J_{max25(f,i)} \cdot f_{Vmax(f,i)}(T_l) \cdot f_{eff}(T_l) \quad (10.3.49)$$

where

$V_{max25(f,i)}$ = The maximum leaf Rubisco capacity at 25°C [mol m^{-2} s^{-1}], calculated in eq. (10.3.32),

$f_{\mathrm{Jmax}(f,i)}^T(T_l)$ = the temperature corrected J_{max25} defined in eq. (10.3.69), and

$f_{eff}(T_l)$ = user defined correction (*TempEff* [°C-> <none>, see below].

$f_{eff}(T_l)$ was introduced to be able to avoid excessive growth for early crops in cold climate. In the original documentation, D3.2, a function was suggested that was 0 up to 4°C, 1 from 10 °C and linear between those two points. The function does not have a default value and should thus be defined by the user. The function has no impact on the calculations if defined as: *(TempEff (0 1) (100 1)))*.

The photosynthetic active radiation (PAR) effectively absorbed by the leaf, I_{le}, is given by Collatz et al. (1991) as:

$$I_{le(f,i)} = I_{(f,i)} \cdot \alpha \qquad (10.3.50)$$

where

α = The fraction of PAR effectively absorbed (default = 0.08 [ ] (Collatz et al., 1991),

$I_{(f,i)}$ = Absorbed irradiance given by eq. (10.3.26) and (10.3.28) [mol m^{-2} s^{-1}]

Net photosynthetic rate of C$_3$ leaves

Thus, the net leaf photosynthetic rate, A, is given by:

$$A_{(f,i)} = min\{w_{c(f,i)}; w_{e(f,i)}\} - R^{C3}_{(f,i)} \qquad (10.3.51)$$

where

$A_{(f,i)}$ = Net photosynthesis [mol m^{-2} s^{-1}]

$R^{C3}_{(f,i)}$ = Leaf respiration [mol m^{-2} s^{-1}] given by eq. (10.3.54)

$w_{c(f,i)}$ = Rubisco-limited rate of assimilation [mol m^{-2} s^{-1}], and

$w_{e(f,i)}$ = Light-limited rate of assimilation [mol m^{-2} s^{-1}].

In reality, the transition from one limitation to another appears to be somewhat gradual. Thus, following (Collatz et al., 1991) A is estimated in the *FC-C3* sub-model by solving the following quadratic equation (eq. 10.3.52) by the first root (Collatz et al., 1991):

$$\beta \cdot \left(A_{(f,i)}\right)^2 - \left(w_{c(f,i)} + w_{e(f,i)}\right)A_{(f,i)} + w_{c(f,i)} \cdot w_{e(f,i)} = 0 \qquad (10.3.52)$$

where β is an empirical curvature constant, by default = 0.95 [ ].

β is an empirical constants that describes the transition between limitations, and its value is typical close to one (Collatz et al., 1991). Solving eq. (10.3.52), the net photosynthetic rate is given by eq. (10.3.53):

$$A_{(f,i)} = \frac{\left(w_{c(f,i)} + w_{e(f,i)}\right) - \sqrt{\left(w_{c(f,i)} + w_{e(f,i)}\right)^2 - 4\beta w_{c(f,i)} \cdot w_{e(f,i)}}}{2\beta} - R^{C3}_{(f,i)}$$

Figure 7 shows the relation between the light limited rate, w_e, and the Rubisco limited rate, w_c, as a function of the overall photosynthesis. When the quantum light flux is high, w_c limits the photosynthesis at low CO_2 partial pressure (Figure 7,

left). On the contrary, when the quantum light flux is low, w_e limits the photosynthesis over the entire range(Figure 7, right).

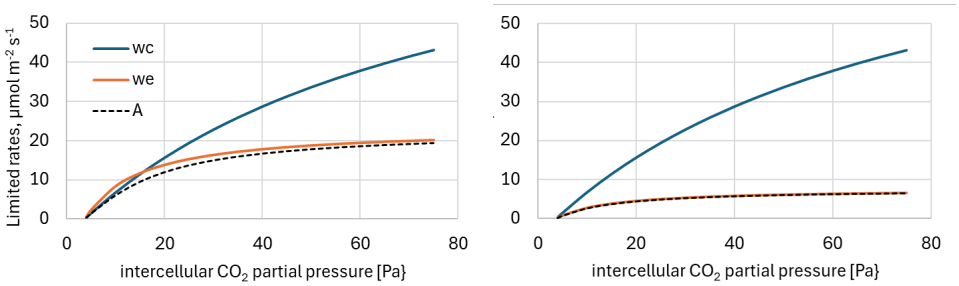

Figure 7. Relation between the light limited rate, w_e, and the Rubisco limited rate, w_c, as a function of the overall photosynthesis ($A+R$) with the parameter settings: T_a = 25 °C, and V_{max25} = 90 µmol m^{-2} s^{-1}. Left: $I_{total,i}$ = 1500 µmol m^{-2} s^{-1}. Right: $I_{total,i}$ = 400 µmol m^{-2} s^{-1}. Both curves are generated as functions of ρ_i. and overall photosynthesis is a function of w_e and w_c (eq. (10.3.53)).

In Figure 8, photosynthesis is plotted against the intercellular partial pressure of CO_2 in the absence of stomata limitations, and against the absorbed quantum flux density.

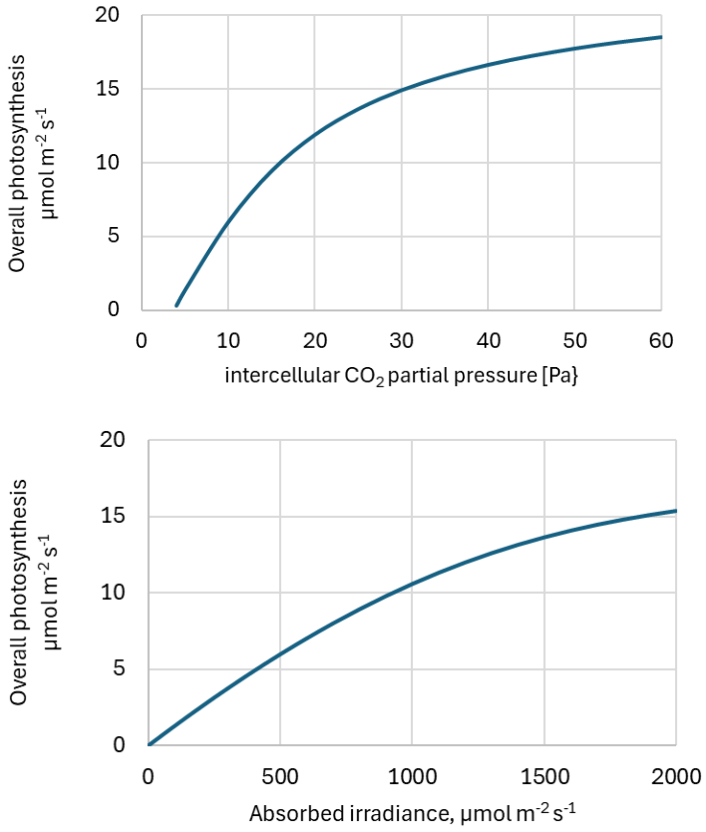

*Figure 8. The effect of a) the intercellular partial pressure of CO_2 and b) the absorbed quantum flux of leaf C_3 photosynthesis. The parameter settings used are: The temperature T = 25 °C, and V_{max25} = 90 µmol m^{-2} s^{-1} in eq. (10.3.45**)**. In a): The absorbed irradiance (quantum flux density) by the leaf $I_{total,0}$ = 1500 µmol m^{-2} s^{-1}, in b): The intercellular partial pressure of CO_2, ρ_i = 25 Pa.*

Respiration rate of C_3-leaves

A central process in cellular metabolism is respiration, the oxidation of sugar to CO_2 and water. With respiration, cells obtain the useful chemical energy, adenosine triphosphate (ATP) from sugar, in order to maintain life and growth. The leaf respiration rate, $R_{(f,i)}$, is proportional to the photosynthetic Rubisco capacity (de Pury and Farquhar, 1997):

$$R^{C3}_{25(f,i)} = 0.0089 \cdot V_{max25(f,i)}$$
$$R^{C3}_{(f,i)} = R^{C3}_{25(f,i)} \cdot f^{C3}_{R25}(T) \quad (10.3.54)$$

where $R^{C3}_{(f,i)}$ is the leaf respiration per unit leaf area [mol m^{-2} s^{-1}], $V_{max25(f,i)}$ is calculated in eq. (10.3.32), and $f^{C3}_{R25}(T)$ is a factor for temperature correction described in eq. (10.3.66).

In Figure 9 the Farquhar leaf respiration calculated by eq. (10.3.54) is compared with the overall respiration calculated in Daisy for different crop components. In Daisy the respiration is divided into maintenance and growth respiration. The overall respiration calculated by eq. (10.3.54) is comparable to the total growth and maintenance respiration for all organs in Daisy. To avoid counting the losses twice, the net photosynthesis based on stomata conductance is calculated by eq. (10.3.51). The net photosynthesis is thereafter re-calculated by adding the respiration given by eq. (10.3.54) and subtracting the overall respiration which is the sum of growth and maintenance respiration for root, storage organ, leaf and stem compartment.

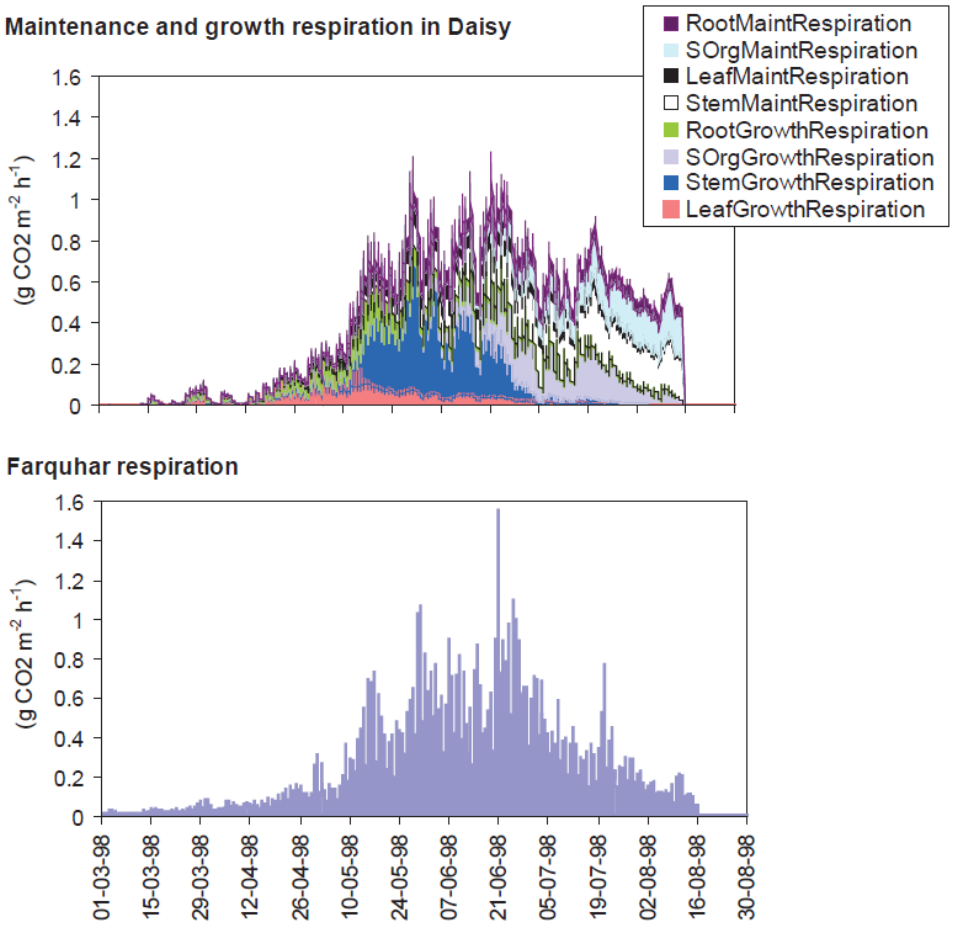

Figure 9. Top: The maintenance and growth respiration calculated by different crop components in Daisy. Bottom: Farquhar "leaf respiration" calculated by eq. (10.3.54).

6.3 Photosynthesis of C4 leaves

The photosynthetic model of C_4 plants is based on the model developed by Collatz et al. (1992) and predicts photosynthesis as a function of temperature, photosynthetic active quantum flux density, CO_2 pressure and relative humidity at the leaf surface. The important adjustable parameters in the C_4 model are the capacities of Rubisco and PEP carboxylase to fix CO_2 which can be estimated from leaf photosynthetic responses to light and CO_2. The C_4 photosynthesis model links the C_3 photosynthesis in the bundle sheath chloroplast with a carbon pump driven by the activity of PEP carboxylase in the mesophyll leaf cells. Carbon derived from intercellular CO_2 is fixed into C_4 acids in the mesophyll, transported to the bundle sheath cells and released as CO_2. Leakage of inorganic carbon from the bundle sheath cells to the intercellular spaces occurs because there is a large gradient in CO_2 concentration created by the pump.

The light limited rate of photosynthesis, w_e

At rate limiting light intensities, the efficiency of CO_2 fixation with respect to absorbed light (quantum yield) determines the rate of photosynthesis. The light dependent rate is given by:

$$w_{e(f,i)} = a_{abs} \cdot \alpha_{C4} \cdot I_{(f,i)} \quad (10.3.55)$$

where

a_{abs} = Leaf absorptivity to PAR (by default, a_{abs} = 0.86 (Collatz et al., 1992),

α_{C4} = Initial slope of photosynthetic light response (by default, α_{C4} = 0.04 [mol mol^{-1}] (Collatz et al., 1992),

$I_{(f,i)}$ = Absorbed irradiance given by eq. (10.3.17) and (10.3.19) [mol m^{-2} s^{-1}].

At low CO_2 concentrations, empirical studies show that net photosynthesis, A, increases linearly from the compensation point (near zero Pa) to rate saturation which occurs at an intercellular CO_2 partial pressure of about 10 Pa. Thus, the CO_2 limited flux given by Collatz et al. (1992) can be calculated as:

$$w_{c(f,i)} = k_T \frac{\rho_{i(f,i)}}{P} \quad (10.3.56)$$

where

k_T = Temperature-corrected (eq. (10.3.68)) initial slope of photosynthetic CO_2 response (by default 0.6 [mol m^{-2} s^{-1}] at 25 °C (Collatz et al., 1992).

$\rho_{i(f,i)}$ = CO_2 partial pressure in leaf interior [Pa].

P = The atmospheric pressure [Pa], see eq. (2.6) in Chapter 2).

The Rubisco limited rate of photosynthesis, w_s

Empirical observations show that when w_c and w_e are not limiting, then the rate of assimilation approaches a rate, w_s, that is largely independent of CO_2 and light. The rate under these conditions is controlled by the capacity for CO_2 fixation by Rubisco:

$$w_{s(f,i)} = V_{m(f,i)} \quad (10.5.57)$$

where $V_{m(f,i)}$ is the photosynthetic capacity per unit leaf area given by eq. (10.3.33) and 10.3.35) [mol m^{-2} s^{-1}].

The net photosynthetic rate of C4 leaves

The steady state balance of these transport processes, the net leaf photosynthetic rate, A, is given by:

$$A_{(f,i)} = min\{w_{c(f,i)}; w_{e(f,i)}; w_{s(f,i)}\} - R^{C4}_{(f,i)} \quad (10.3.58)$$

where

$A_{(f,i)}$ = Net photosynthesis [mol m^{-2} s^{-1}],

$R^{C4}_{(f,i)}$ = Leaf respiration [mol m^{-2} s^{-1}] given by eq. (10.3.61),

$w_{c(f,i)}$ = CO_2-limited rate of assimilation [mol m^{-2} s^{-1}], eq.(10.3.57).

$w_{e(f,i)}$ = Light-limited rate of assimilation [mol m^{-2} s^{-1}], eq.(10.3.56)and

$w_{s(f,i)}$ = Rubisco-limited rate of assimilation [mol m^{-2} s^{-1}], eq.(10.3.58).

The transition from one limitation to another appears to be somewhat gradual and therefore the photosynthesis is estimated by solving the following quadratic equations (eq. (10.3.39) and eq. (10.3.40) by the first root:

$$\theta \cdot \left(M_{(f,i)}\right)^2 - \left(w_{s(f,i)} + w_{e(f,i)}\right)M_{(f,i)} + w_{s(f,i)} \cdot w_{e(f,i)} = 0 \qquad (10.3.59)$$

where

$M_{(f,i)}$ = The flux determined by Rubisco and light [mol m^{-2} s^{-1}].

θ = Curvature parameter (by default, 0.83 [ ] (Collatz et al., 1992).

The curvature parameter, θ, gives a gradual transition between the light limited and Rubisco limited flux. The limitation on the overall rate, M, and the CO_2 limited flux, w_c, is likewise expressed by a quadratic equation:

$$\beta \cdot \left(A_{(f,i)}\right)^2 - \left(M_{(f,i)} + w_{c(f,i)}\right)A_{(f,i)} + M_{(f,i)} \cdot w_{c(f,i)} = 0 \qquad (10.3.60)$$

where

$A_{(f,i)}$ = The flux determined by M and CO_2 [mol m^{-2} s^{-1}].

β = Curvature parameter (by default, 0.93 [ ] (Collatz et al., 1992).

The curvature parameter, β, gives a gradual transition between M and the CO_2-limited flux.

Respiration rate for C4 leaves

The respiration rate for C4-plants is also calculated differently from C3-plants. Both the relationship to V_{max25} and the temperature relationship is different:

$$R^{C4}_{25(f,i)} = 0.015 \cdot V_{max25(f,i)}$$
$$R^{C4}_{(f,i)} = R^{C4}_{25(f,i)} \cdot f^{C4}_{R25}(T) \qquad (10.3.61)$$

where V_{max25} is calculated in eq. (10.3.32) and the temperature correction is found in eq. (10.3.71).

6.4 The water stress factor

The water stress factor account for the effect of abscisic acid (ABA) in plants. It is assumed that ABA is generated in the root tips in response to soil drying and is transported to the leaves through the xylem system with the transpiration stream (Plauborg et al., 2010). In addition, it is assumed that the ABA concentration in the leaf apoplast is identical to the ABA concentration in the xylem sap. Storage, degradation, and transportation time are ignored. The user has different options to describe the formation of ABA as a rate or concentration (see below). For example, using the *uptake* option, the ABA production in the roots is assumed to be a function of the water potential in the soil surrounding the roots. Since the soil water potential varies within the root zone, the ABA concentration in the xylem, c_{ABA} [ng cm^{-3}] is estimated as

$$c_{ABA} = \frac{\int_\Omega P_{ABA} d\Omega}{\int_\Omega S d\Omega} \qquad (10.3.62)$$

where Ω represents the root zone, P_{ABA} is the ABA production [ng cm^{-3} s^{-1}], and S is the actual water uptake from a specific point in the root zone [L s^{-1}]

The ABA-production is estimated as:

$$P_{ABA} = S \cdot f_{ABA}(h_p) \quad (10.3.63)$$

where h_p is the soil water potential and $f_{ABA}(h_p)$ is a function linking the relationship between c_{ABA} and h_p. In Plauborg et al. (2010), $f_{ABA}(h_p)$ is parameterized as:

$$f_{ABA}(h_p) = 30.45 - 690 \cdot h_p \quad (10.3.64)$$

where the first number is in [ng cm^{-3}] and the second is in [ng cm^{-3} MPa^{-1}].

Options for production of ABA

The options available to describe the ABA-production are *none, root, soil,* and *uptake*.

none

none is default and translates to no ABA production.

root

The option *root* considers ABA production in the roots. The assumptions are that each length of root will produce ABA with a rate that depends solely on the water pressure in the cell where the root length is located, and that all the ABA will be included in the water uptake. The user must write an expression that specifies the $f_{ABA}(h_p)$ ABA production per root length [g cm^{-1} h^{-1}]. The symbol "h" will be bound to water pressure [cm].

soil

The *soil* option considers ABA production based on soil location. The user must write an expression to evaluate the ABA uptake [g cm^{-3} h^{-1}]. The symbols "h", "L" and "S" represent water pressure [cm], root density [cm cm^{-3}] and water uptake [cm^3 cm^{-3} h^{-1}], respectively.

uptake

The *uptake* option considers ABA production based on concentration in water uptake. The assumption is that water uptake from roots in a specific region of the soil comes with a specific ABA concentration, which depends solely on the water pressure in that region. The user must write an expression that quantifies the ABA concentration in water uptake [g cm^{-3}]. The symbol "h" represents the water pressure [cm].

When ABA is produced, it may influence the stomatal conductance through the *wsf* parameter in the equations in section 6.1. The *wsf*-parameter is calculated as:

$$wsf = exp\left(-\beta\left(c_{ABA} - c_{ABA}^{min}\right)\right) \cdot exp(-\delta|\psi_c|) \quad (10.3.65)$$

where

β = an empirical constant describing the effect of ABA, by default = 0 [cm^3 g^{-1}]

c_{ABA} = The calculated ABA concentration in the xylem [g cm^{-3}],

c_{ABA}^{min} = Level of ABA in unstressed plants [g cm^{-3}],

δ = an empirical constant describing the effect of crown water potential. By default = 0 [MPa^{-1}]

ψ_c = Crown water potential calculated by the model [MPa]

7 Temperature dependencies

Several of the photosynthetic- and stomatal-parameters depend on the temperature of the leaf. For C3 plants this includes the parameters K_c, K_O, Γ^*, V_m, J_m and R. For C4 plants it concerns the parameters Γ^*, k_T, V_m and R.

Arrhenius fuction for K_c, K_O, Γ^* and respiration of C3-plants

For the C3 photosynthesis model, the parameters $K_{c,25}$, $K_{O,25}$, Γ^*_{25}, and R^{C3} are adjusted for the effect of temperature by the Arrhenius function (de Pury and Farquhar, 1997). For the C4 photosynthesis model, only the Γ^* is used in the model and adjusted by the Arrhenius function:

$$X_T = X_{25} exp\left(\frac{E_{a,x}(T_l - 25)}{298 \cdot R \cdot (T_l + 273)}\right) \quad (10.3.66)$$

where

X_T = Parameter X at T [°C], X = K_c, K_O, Γ^* and R^{C3}.

X_{25} = Parameter X at 25 [°C].

$E_{a,x}$ = Activation energy for parameter X [J mol^{-1}].

R =Universal gas constant (8.314 [J m^{-1} K^{-1}]

T_l =Leaf temperature [°C] (for sunny or shaded leaves).

Activation energies of the model parameters adjusted for temperature dependencies by eq. (10.3.66) and parameter values at 25 °C are listed in Table 2. These values are default values in the respective photosynthesis models in Daisy.

Table 2. Activation energies and values at 25 °C of the model parameters adjusted for temperature dependencies by eq. (10.3.66) listed in (de Pury and Farquhar, 1997). These parameters are given as default values in the model and can be changed by the user.

Parameter X	E_a [J mol^{-1}]	X_{25} [Pa]
Γ^*	29000	3.69
K_O	36000	24800
K_c	59400	40.4
R^{C3}	66400	Calculated

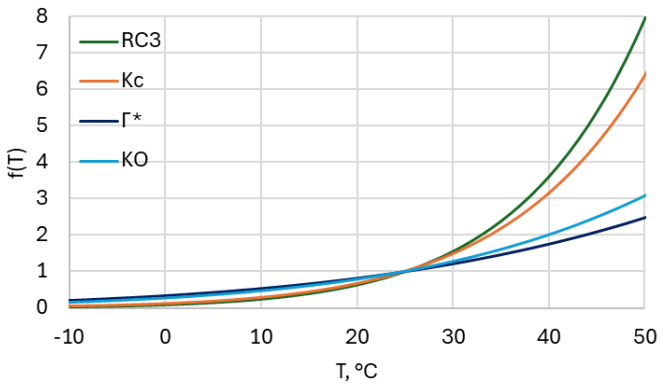

Figure 10. Temperature functions for Γ^*, K_c, K_O and respiration of C3-plants. All temperature functions are 1 at 25 °C.

Respiration of C4-plants

The temperature correction for respiration of C4-plants is described by Collatz et al. (1992) as

$$f_{R25}^{C4}(T_l) = \frac{Q_{10,R,C4}^{\left({}^{(T_l-25)}/_{10}\right)}}{\left(1 + exp\left(1.3 \cdot (T_l - 55)\right)\right)} \quad (10.3.67)$$

where

$Q_{10,R,C4}$ = The Q_{10}-parameter for C4-respiration (by default = 2.0; (Collatz et al., 1992).

The function increases until 55°C and then drops steeply till around 60°C, see Figure 11.

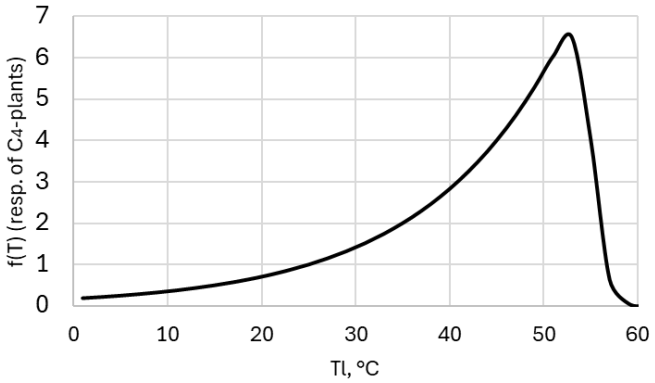

Figure 11. Temperature factor for respiration for C4-plants.

k_T (C4-plants)

The pseudo-first order rate constant with respect to CO_2, k_T, for C4-plants is given by Collatz et al. (1992) as:

$$k_T = k \cdot Q_{10,k}^{\left({}^{(T_l-25)}/_{10}\right)} \quad (10.3.68)$$

where

T_l = The leaf temperature [°C],

k_T = The pseudo-first order rate constant with respect to CO_2 [mol m^{-2} s^{-1}]

k = Rate constant (by default = 0.6 [mol m^{-2} s^{-1}], and

$Q_{10,k}$ = The Q_{10}-parameter of k (by default =1.8 [ ]).

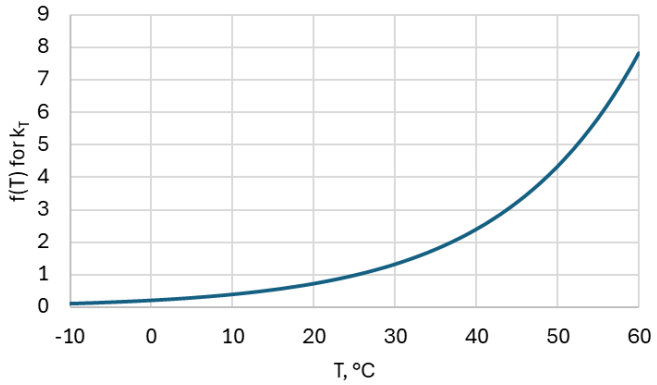

Figure 12. Temperature function for K_T.

J_m (C_3 and C_4-plants)

The parameter J_m, for calculation of the electron-transport limited rate of photosynthesis, is also adjusted by temperature according to (de Pury and Farquhar, 1997). However, for temperatures below 10 °C the temperature function is reduced with a linear function. Below 4 C° J_m = 0. The air temperature in °K (T_l^K) is calculated as $T_l + 273.15$.

$$f_{J\max(f,i)}(T_l) = exp\left[\frac{(T_l^K - 298)\cdot E_{a,Jm}}{R\cdot T_l^K \cdot 298}\right]\frac{\left[1+exp\left(\frac{S\cdot 298 - H}{R\cdot 298}\right)\right]}{\left[1+exp\left(\frac{S\cdot T_l^K - H}{R\cdot T_l^K}\right)\right]} \quad (10.3.69)$$

where

T_l = Leaf temperature [°C]. T_l^K is leaf temperature in [°K]

R =Universal gas constant (8.314 [J m^{-1} K^{-1}],

H = Curvature parameter of J_m (by default = 220000 [J mol^{-1}] (de Pury and Farquhar, 1997))

S = Electron transport temperature response parameter (by default = 710 [J mol^{-1} K^{-1}] de Pury and Farquhar (1997)).

$E_{a,Jm}$ = Activation energy for J_m (by default = 37000 [J mol^{-1}] (de Pury and Farquhar, 1997)).

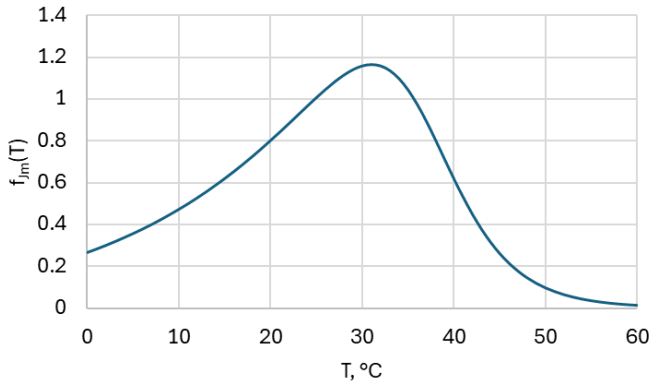

Figure 13. Temperature function for J_m.

V_m, C_3-plants

In the C_3 photosynthesis model, the maximum photosynthetic Rubisco capacity is adjusted for the temperature dependency by a function defined by (Harley et al., 1992) and partly by (Bernacchi et al., 2001), see eq. (10.3.71). As above, the air temperature in °K (T_l^K) is calculated as $(T_l + 273.15)$.

$$f_{vmax}^{C3}(T_l) = \frac{exp\left(C_{Vmax} - \frac{E_{a,Vmax}}{R \cdot T_l^K}\right)}{\left[1 + exp\left(\frac{S_v \cdot T_l^K - E_{da,Vmax}}{R \cdot T_l^K}\right)\right]} \quad (10.3.70)$$

where

$f_{vmax}^{C3}(T_l)$ = The temperature correction factor,

$E_{a,Vmax}$ = Activation energy for V_{max} (by default = 65330 [J mol^{-1}] (Bernacchi et al., 2001)),

$E_{da,Vmax}$ = Deactivation energy for V_{max} (by default = 202900 [J mol^{-1}] (Harley et al., 1992))

C_{Vmax} = Temperature scaling constant for V_{max} (by default = 26.35 [ ] (Bernacchi et al., 2001))

S_v = Entropy term for V_{max} (by default = 650 [J mol^{-1} K^{-1}] (Harley et al., 1992))

Vm, C_4-plants

In the C_4 photosynthesis model, the effect of temperature on the photosynthetic Rubisco capacity is given by (Collatz et al., 1992):

$$f_{vmax}^{C4}(T_l) = \frac{Q_{10Vm}^{\left((T_a-25)/10\right)}}{\left[1 + exp\left(0.3(T_l - 40)\right)\right]\left[1 + exp\left(0.2425(15 - T_l)\right)\right]} \quad (10.3.71)$$

where

T_l = The leaf temperature [°C]

$f_{vmax}^{C4}(T_l)$ = The temperature correction factor [ ]

Q_{10Vm} = The Q_{10} parameter of V_m (by default = 2.4 [ ]).

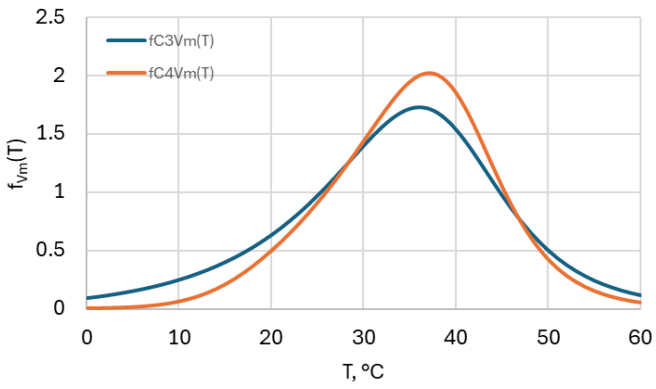

Figure 14. Temperature functions for V_m^{C3} and V_m^{C4}. For lower temperatures the temperature correction on photosynthesis will be higher for C_3-plants, while from 29-47°C, the temperature correction photosynthesis will be higher for C_4-plants.

Graphic comparison of the parameters

The effects of temperature on the leaf C_3 parameters are shown in Figure 15 together with the effect of temperature on the overall photosynthesis.

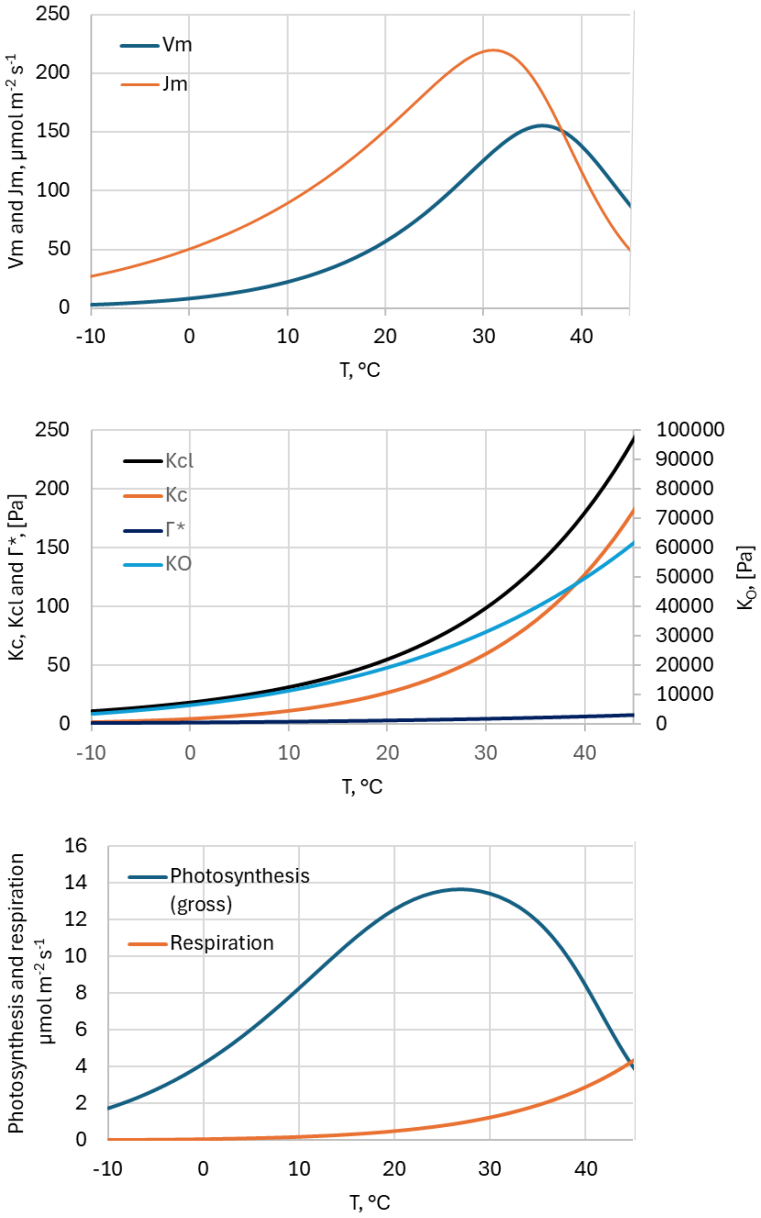

Figure 15. The effect of temperature on leaf C_3 photosynthesis parameters: a) J_m and V_m, b) K_c, K_O, Γ^* given by eq. (10.3.66), and K_{cl} calculated from eq. (10.3.46), c) the overall photosynthesis and respiration calculated by Farquhar. The intercellular partial pressure of CO_2 is 25 Pa, the absorbed irradiance (quantum flux density) by the leaf is 1500 µmol m^{-2} s^{-1} and V_{max25} is 90 µmol m^{-2} s^{-1}.

8 Calculation procedure of the photosynthesis-conductance model

The general method

There is a strong interaction between the photosynthesis submodel and the stomatal sub-model in this system. The Daisy code is constructed to obtain a numerical solution, using an initial guess for the stomatal conductance ($g^w_s = (L_{i-1} - L_i)/5$ [mol m^{-2} s^{-1}]), and the CO_2 partial pressure in the leaf interior (ρ_i = 0.5 ρ_a = 17.5 [Pa]). The code calculates the leaf temperature, photosynthesis, g^w_s and ρ_i by iterations using the Newton-Raphson method until ρ_i is stable. The Newton-Raphson Method states that if $x = r$ is an approximation to $f(x) = 0$, then a better solution is given by:

$$r^{new} = r - \frac{f(r)}{f'(r)} \tag{10.3.72}$$

When estimating ρ_i, the function $f(x)$ is given by:

$$f(x) = \rho_{i(f,i)}(t) - \rho_{i(f,i)}(t-1) \tag{10.3.73}$$

where

$\rho_{i(f,i)}$ = CO_2 partial pressure in leaf interior in the sunlit or shaded fraction, f, in canopy layer i [Pa], and

t = time step (h).

Calculation for C3-plants

For C3-plants, ρ_i is calculated using eq. (10.3.44). The derivative of $f(x)$ can be written as:

$$f'(x) = -P_{tot}\left(1.6\frac{1}{g^w_{s(f,i)}(t)} + 1.4\frac{1}{g^w_{b(f,i)}(t)}\right)dx - 1 \tag{10.3.74}$$

where

$g^w_{s(f,i)}$ = Stomatal conductance of leaves [mol m^{-2} s^{-1}],

$g^w_{b(f,i)}$ = Leaf boundary-layer conductance [mol m^{-2} s^{-1}], and

dx for C3-plants is given by eq. (10.3.75):

$$dx = \begin{cases} V_{m(f,i)}\dfrac{K_{cl} + \Gamma^{*T}_{(f)}}{\left(\rho_{i(f,i)} + K_{cl}\right)} & w_c < w_e \\ V_{m(f,i)}\dfrac{K_{cl} + \Gamma^{*T}_{(f)}}{4 \cdot \left(\rho_{i(f,i)} + 2\Gamma^{*T}_{(f)}\right)} & w_c \geq w_e \end{cases} \tag{10.3.75}$$

where

$V_{m(f,i)}$ = Photosynthetic capacity per unit leaf area in the sunlit or shaded fraction, f, in canopy layer i [mol m^{-2} s^{-1}], eq. (10.3.33-35).

$\rho_{i(f,i)}$ = CO_2 partial pressure in leaf interior in the sunlit or shaded fraction, f, in canopy layer i [Pa], eq. (10.3.36-39).

K_{cl} = The effective Michaelis-Menten coefficient CO_2 [Pa], eq. (10.3.46).

$\Gamma_{(f)}^{*T}$ = The temperature-corrected CO_2 compensation point of photosynthesis [Pa].

The Newton-Raphson solution to $\rho_{i(f,i)}(t)$ is then given by eq. (10.3.76):

$$\rho_{i(f,i)}(t) = \rho_{i(f,i)}(t-1) - \frac{\left(\rho_{i(f,i)}(t) - \rho_{i(f,i)}(t-1)\right)}{\left[-P_{tot}\left(1.6\frac{1}{g^{w}_{s(f,i)}(t)} + 1.4\frac{1}{g^{w}_{b(f,i)}(t)}\right)dx(t) - 1\right]}$$

Eq. (10.3.76) is used to calculate the partial pressure of CO_2 in stomata.

Calculation for C4-plants

For C4 plants, the same considerations can be made, resulting in eq. (10.3.77):

$$\rho_{i(f,i)}(t) = \rho_{i(f,i)}(t-1) - \frac{\left(\rho_{i(f,i)}(t) - \rho_{i(f,i)}(t-1)\right)}{\left[-P_{tot}\left(1.6\frac{1}{g^{w}_{s(f,i)}(t)}\right)dx(t) - 1\right]} \qquad (10.3.77)$$

dx for C4-plants is given by:

$$dx(t) = \frac{k_T\left(A_{(f,i)}M_{(f,i)}\right)}{\left(2\beta \cdot A_{(f,i)}\right) - M_{(f,i)} - wc_{(f,i)}} \qquad (10.3.78)$$

9 Parameter overview

Table 3. Related Parameter names in Daisy.

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
f_{PAR}	The fraction of radiation which is PAR	Raddist_DPF	*PARinSi*	0.5, hardcoded	[]
S_i	Global radiation	weather	*GlobRad*	User specified	[W m^{-2}]
R_d	Diffuse radiation	weather or difrad, eq. (10.3.8)	*DiffRad*	Optional parameter, the value may be calculated in *difrad, DPF.*	[W m^{-2}]
α	Atmospheric transmission coefficient of PAR (0.72 [ ] in de Pury and Farquhar (1997)), eq. (10.3.4). The value lies in the interval 0.6-0.9 depending on dust particles.	difrad, DPF	*a*	Default = 0.84	[]
R_{ex} *or* S_{io}	Extra-terrestrial radiation, see Ch.2, eq. (2.13).			Calculated	[W m^{-2}]
β	Solar elevation angle			Calculated	[radian]
P	Atmospheric pressure	weather	*air_pressure*	Calculated, eq. (2.6)	[Pa]
f_a	Forward scattering coefficient of PAR in the atmosphere, eq. (10.3.6).	difrad, DPF	*fa*	0.426	[ ]
σ	Leaf scattering coefficient of PAR, eq. (10.3.16).	raddist, sun-shade	*Sigma_PAR*	0.15	[ ]
ρ_s	Soil reflection coefficient of PAR, eq. (10.3.24).	raddist, sun-shade	*Ps_PAR*	0.1	[ ]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
	Effect of soil water (pF) on ρ_s.	raddist, sun-shade	*Ps_PAR_SWE*	plf, default is a constant value of 1	[pF -><none>]
χ_n	The ratio of measured Rubisco capacity to leaf nitrogen (default = $1.16 \cdot 10^{-3}$ [mol mol^{-1} s^{-1}] for wheat (Boegh et al., 2002)), eq. (10.3.32)	photosynthesis, Farquhar	*Xn*	0.00116	[mol mol^{-1} s^{-1}]
	Fraction of N in leaves that is RuBisCo-N. First, structural and luxury N may be subtracted, see the following parameters.	rubiscoN	*fraction*	0.75	[ ]
	Subtract this amount of N per LAI	rubiscoN	*offset*	0	[g N m^{-2}]
	Subtract N corresponding to the non-functional concentration in leaves	rubiscoN	*Subtract_Nf*	false	
	Subtract N above the critical concentration in leaves.	rubiscoN	*Subtract_Pt*	false	
k_n	Extinction coefficient of nitrogen in the canopy, eq. (10.3.30)	rubiscoNdist, exp	*kn*	0.713	[ ]
f_photo	Fraction of photosynthetically active N in canopy.	rubiscoNdist, uniform	*f_photo*	1	[ ]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
Γ^*_{25}	CO_2 compensation point of photosynthesis at 25°C	photosynthesis, Farquhar	*Gamma25*	3.69	[Pa]
E_{a,Γ^*}	Activation energy for Γ^*	photosynthesis, Farquhar	*Ea_Gamma*	29000	[J mol^{-1}]
m	Stomatal slope factor, eq. (10.3.36-39)	stomatacon, BB_base, Leuning.	*m*	m = 9 for soyabean, 11 for wheat	[ ]
b	Constant required to calculate the stomatal intercept $b_{(f,i)}$, eq. (10.3.36-37)	stomatacon, BB_base, Leuning, MNA.	*b*	0.01	[mol m^{-2} s^{-1}]
D_0	Empirical coefficient, eq. (10.3.37)	stomatacon, Leuning	*Do*	1500	[Pa]
max	Maximal conductivity	stomatacon, SHA14	*max*	By default, there is no maximum.	[mol H_2O m^{-2} leaf s^{-1}]
min	Minimal conductivity	stomatacon, SHA12	*min*	Optional parameter. By default, there is no minimum.	[mol H_2O m^{-2} leaf s^{-1}]
m	Slope parameter, depends on α and λ., eq. (10.3.38)	stomatacon, SHA12	*m*	User defined	Dimension depends on α and λ
α	Humidity effect	stomatacon, SHA12,	*alpha*	1	[ ]
λ	Net photosynthesis effect	stomatacon, SHA12,	*lambda*	1	[ ]
m	Slope parameter, depends on α and λ, eq. (10.3.39)	stomatacon, SHA14	*m*	User defined	[mol H_2O m^{-2} leaf s^{-1}]
α	Humidity effect	stomatacon, SHA14	*alpha*	User defined	[ ]
λ	Net photosynthesis effect	stomatacon, SHA14	*lambda*	User defined	[ ]
$K_{c,25}$	Michaelis-Menten constant for Rubisco for CO_2 at 25°C.	photosynthesis, FC_C3	*Kc25*	40.4 (the value for wheat (Collatz et al., 1991))	[Pa]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
$K_{O,25}$	Michaelis-Menten constant of Rubisco for O_2 at 25°C.	photosynthesis, FC_C3	*Ko25*	24800 (the value for wheat (Collatz et al., 1991))	[Pa]
θ	Curvature of leaf response of electron transport to irradiance, eq. (10.3.48)	photosynthesis, FC_C3	*theta*	0.7	[ ]
$f_{eff}(T)$	Temperature factor for assimilate production, eq. (10.3.49)	photosynthesis, FC_C3	*TempEff*	User defined. NB: there is no default, it must be defined.	[°C-><none>]
α	The fraction of PAR effectively absorbed, eq. (10.3.50).	photosynthesis, FC_C3	*alfa*	0.08	[ ]
β	Curvature parameter, eq. (10.3.52)	photosynthesis, FC_C3	*beta*	0.95	[ ]
α_{C4}	Initial slope of the photosynthetic light response, eq. (10.3.55).	photosynthesis, FC_C4	*alpha*	0.04	{mol mol^{-1}]
a_{abs}	Leaf absorptivity to PAR, eq. (10.3.55).	photosynthesis, FC_C4	*paab*	0.86	Not specified.
k_{25}	Initial slope of photosynthetic CO2-response at 25 °C.	photosynthesis, FC_C4	*kj*	0.6	[mol m^{-2} s^{-1}]
θ	Curvature parameter, eq. (10.3.59).	photosynthesis, FC_C4	*theta*	0.83	[ ]
β	Curvature parameter, eq. (10.3.60)	photosynthesis, FC_C4	*beta*	0.93	[ ]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
$\boldsymbol{\beta}$	An empirical constant describing the effect of ABA, eq. (10.3.65).	stomatacon, WSF	*beta*	0	[cm g^{-1}]
$\boldsymbol{c_{ABA}^{min}}$	Level of ABA in unstressed plants, eq. (10.3.65).	stomatacon, WSF	*ABA_min*	0	[g cm^{-3}]
$\boldsymbol{\delta}$	An empirical constant describing the effect of crown water potential, eq. (10.3.65).	stomatacon, WSF	*delta*	0	[MPa^{-1}]
$\boldsymbol{Q_{10,k}}$	The Q10-parameter of k, eq. (10.3.68).	photosynthesis, FC_C4	*Q10k*	1.8	[ ]
$\boldsymbol{E_{a,k0}}$	Activation energy for k_O, eq. (10.3.66).	photosynthesis, FC_C3	*Ea_ko*	36000	[J mol^{-1}]
$\boldsymbol{E_{a,kc}}$	Activation energy for k_c, eq. (10.3.65)	photosynthesis, FC_C3	*Ea_kc*	59400	[J mol^{-1}]
$\boldsymbol{E_{a,Rd}}$	Activation energy for R_d, eq. (10.3.65)	photosynthesis, FC_C3	*Ea_rd*	66400	[J mol^{-1}]
$\boldsymbol{Q_{10,R,C4}}$	The Q_{10}-parameter for C_4-respiration, eq. (10.3.67)	photosynthesis, FC_C4	*Q10rd*	2	[ ]
$\boldsymbol{H}$	Curvature parameter of J_m, eq. (10.3.69).	photosynthesis, FC_C3	*H*	220000	[J mol^{-1}]
$\boldsymbol{S}$	Electron transport temperature response parameter, eq. (10.3.69).	photosynthesis, FC_C3	*S*	710	[J mol^{-1} K^{-1}]
$\boldsymbol{E_{a,Jm}}$	Activation energy for J_m, eq. (10.3.69).	photosynthesis, FC_C3	*Ea_Jm*	37000	[J mol^{-1}]

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default	Default unit
$E_{a,Vmax}$	Activation energy for V_{max}, eq. (10.3.70).	photosynthesis, FC_C3	Ea_Vm	65330	[J mol^{-1}]
$E_{da,Vmax}$	Deactivation energy for V_{max}, eq. (10.3.70).	photosynthesis, FC_C3	Eda_vm	202900	[J mol^{-1}]
S_v	Entrophy term, eq. (10.3.70).	photosynthesis, FC_C3	Sv	650	[J mol^{-1} K^{-1}]
C_{Vmax}	Temperature scaling constant for V_{max}, eq. (10.3.70).	photosynthesis, FC_C3	C_Vm	26.35	[ ]
Q_{10Vm}	The Q_{10} parameter of V_m, eq. (10.3.65) , eq. (10.3.71).	photosynthesis, FC_C4	$Q10vm$	2.4	[ ]

Original text from	D3_2 (Safir), (Plauborg et al., 2010)	
Updated by	date	For Daisy version
Styczen, M	2025 04 09	7.0.7

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