

The equations used to simulate the leaf gas exchange are presented below and are similar to what is presented in (von Caemmerer *et al.*, 2009; Yin & Struik, 2009; Duursma, 2015; Bonan, 2019).

Photosynthesis model

We used the FCB photosynthesis model (Farquhar *et al.*, 1980), which represents the net CO₂ assimilation rate as:

$$A_n = \min(A_c, A_j, A_p) - R_d \quad \text{Eqn 1}$$

where A_c is the rate of maximum carboxylation, A_j is the maximum rate of RuBp regeneration (or electron transport) and A_p is the export limited assimilation rate also know as the rate of triose phosphate utilization. R_d is the daytime respiration rate that is not attributable to the photorespiratory pathway.

A_c , A_j and A_p are given by:

$$A_c = \frac{(c_i - \Gamma^*) V_{cmax}}{c_i + K_c \left(1 + \frac{O_2}{K_o}\right)} \quad \text{Eqn 2}$$

$$A_j = \frac{(c_i - \Gamma^*) \frac{J}{4}}{c_i + 2\Gamma^*} \quad \text{Eqn 3}$$

$$A_p = 3T_p \quad \text{Eqn 4}$$

where Γ^* is the photorespiratory CO₂ compensation point, c_i is the intercellular CO₂ concentration, V_{cmax} is the maximum carboxylation velocity, K_c and K_o are the Michaelis–Menten coefficients of rubisco activity for CO₂ and O₂, respectively. J is the potential electron transport rate, given by:

$$J = \frac{I_2 + J_{max} - \sqrt{(I_2 + J_{max})^2 - 4\theta I_2 J_{max}}}{2\theta} \quad \text{Eqn 5}$$

where I_2 is the photosynthetically active irradiance absorbed by photosystem II, J_{max} is the maximum electron transport rate and θ is an empirical curvature factor (usually estimated as 0.7). T_p is the Triose phosphate utilization rate.

Note that Eqn 2, 3 and 4 are in the form:

$$A_n = \frac{(c_i - \Gamma^*) x}{c_i + y} - R_d \quad \text{Eqn 6}$$

where x and y take different meaning depending on the limitation on A_n . When A_n is limited by A_c , x is V_{cmax} , and y is $K_c \left(1 + \frac{O_2}{K_o}\right)$. When A_n is limited by A_j x is $J/4$ and y is $2\Gamma^*$. When A_n is limited by A_p x is $3T_p$ and y is $-\Gamma^*$.

A smoothing function is sometimes used in place of the minimum in Eqn 1 (Collatz *et al.*, 1991).

$$\theta_{cj} A_i^2 - A_i (A_j + A_c) + A_j A_c = 0 \quad \text{Eqn 7}$$

$$\theta_{ip}A^2 - A(A_i + A_p) + A_iA_p = 0 \quad \text{Eqn 8}$$

where θ_{cj} and θ_{ip} are empirical smoothing constants describing the transition between limitations. Note than in those equations, A_i is an intermediate variable that is first calculated and used in Eqn 8. A is the resulting gross CO₂ assimilation rate which can be used in place of $\min(A_c, A_j, A_p)$. Careful consideration must be used when applying this smoothing approach, as it can significantly reduce A_n in some conditions (Rogers *et al.*, 2021).

Gas transport between the leaf and the atmosphere

The diffusion of the CO₂ from the leaf surface to the intercellular environment can be described by Fick's law of diffusion (Fick, 1855):

$$C_i = CO_{2s} - 1.6 \frac{A_n}{g_{sw}} \quad \text{Eqn 9}$$

where CO_{2s} is the concentration of CO₂ at the leaf surface, g_{sw} is the stomatal conductance for H₂O vapor, and 1.6 is the ratio of diffusivity of H₂O and CO₂ through the stomata (Jarvis, 1971).

Stomatal conductance model

Several empirical models of stomatal conductance can be used:

The USO model (Medlyn *et al.*, 2011):

$$g_{sw} = g_0 + 1.6 \left(1 + \frac{g_1}{\sqrt{VPD_{leaf}}}\right) \frac{A_n}{CO_{2s}} \quad \text{Eqn 10}$$

where g_0 and g_1 are two parameters of the model and VPD_{leaf} is the leaf to air vapor pressure deficit.

The simplified form of the USO model (Medlyn *et al.*, 2011):

$$g_{sw} = g_0 + 1.6g_1 \frac{A_n}{CO_{2s}\sqrt{VPD_{leaf}}} \quad \text{Eqn 11}$$

The BBW model (Ball *et al.*, 1987):

$$g_{sw} = g_0 + g_1 \frac{A_n}{CO_{2s}RH} \quad \text{Eqn 12}$$

Where RH is the relative humidity of the air expressed as a fraction.

Note that all these models can be rewritten in the linear form:

$$g_{sw} = g_0 + m \frac{A_n}{CO_{2s}} \quad \text{Eqn 13}$$

Coupling the photosynthesis, gas transport and stomatal conductance models

The system of equations {Eqn 6, Eqn 9, Eqn 13} can be solved analytically. C_i corresponds to the larger root of a degree 2 polynomial (below) and can be used to calculate A_n and g_{sw} (Bonan, 2019).

$$\begin{cases} A_n = \frac{(c_i - \Gamma^*)x}{c_i + y} - R_d \\ C_i = CO_{2s} - 1.6 \frac{A_n}{g_{sw}} \\ g_{sw} = g_0 + m \frac{A_n}{CO_{2s}} \end{cases} \quad \text{Eqn 14}$$

$$aC_i^2 + bC_i + c = 0 \quad \text{Eqn 15}$$

where :

$$a = g_0 + \frac{m}{CO_{2s}}(x - R_d) \quad \text{Eqn 16}$$

$$b = yg_0 + \frac{m}{CO_{2s}}(-\Gamma^*x - R_dy) - CO_{2s}g_0 + (x - R_d)(1.6 - m) \quad \text{Eqn 17}$$

$$c = -yCO_{2s}g_0 + (1.6 - m)(-\Gamma^*x - R_dy) \quad \text{Eqn 18}$$

Temperature effects on model parameters

The parameters of the photosynthesis model (V_{cmax} , J_{max} , T_p , R_d , Γ^* , K_c and K_o) are temperature dependent, and are often given at a reference temperature of 25 °C (Bernacchi *et al.*, 2001, 2003; Leuning, 2002). An Arrhenius function (Eqn 19) or a modified Arrhenius function (Eqn 20) can be used to correct for the temperature effect:

$$P(T_{leaf}) = P_{ref} e^{\frac{H_a}{RT_{ref}} - \frac{H_a}{RT_{leaf}}} \quad \text{Eqn 19}$$

$$P(T_{leaf}) = \frac{P_{Ref} \left(1 + e^{\frac{sT_{ref} - H_d}{RT_{ref}}} \right) e^{\frac{H_a}{RT_{Ref}} \left(1 - \frac{T_{ref}}{T_{leaf}} \right)}}{1 + e^{\frac{sT_{leaf} - H_d}{RT_{leaf}}}} \quad \text{Eqn 20}$$

where P is the value of the parameter at T_{leaf} , P_{ref} is the value of the parameter at the reference temperature, H_a is the energy of activation in $J \text{ mol}^{-1}$, H_d is the energy of deactivation in $J \text{ mol}^{-1}$ and s is an entropy term. R is the ideal gas constant. In this equation, the temperature T_{ref} and T_{leaf} are in Kelvin.

Coupling the gas exchange model with a leaf energy balance model

The system of equations 14 represents leaf gas exchange and is driven by an estimation of conditions at the leaf surface. In order to properly account for environmental effects on leaf surface conditions a leaf energy budget has to be considered and allows to calculate the value of the boundary layer conductance (g_{bw}) and the leaf temperature (T_{leaf}). We used a leaf energy budget model published by (Muir, 2019) and followed the numerical approach by (Bonan, 2019) which uses an iterative solving function to estimate T_{leaf} and g_{bw} .

In brief, the numerical approach uses an initial estimate of leaf temperature ($T_{leaf} = T_{air} + 1$), CO_{2s} ($CO_{2s} = CO_{2a}$) and RH_s ($RH_s = RH_a$). Using these initial values, the system of equation 14 is solved by accounting for the leaf temperature effect on the photosynthetic parameters (Eqn 19 and 20). The leaf energy budget is then evaluated (Muir, 2019) and produces an estimate of a new T_{leaf} and g_{bw} . These values are used to calculate a new CO_{2s} and a new RH_s using Eqn 21 and Eqn 22, respectively.

$$CO_{2s} = CO_{2a} - \frac{1.37A_n}{g_{bw}} \quad \text{Eqn 21}$$

$$RH_s = \frac{e_s}{e_{sat}(T_{leaf})} 100 \quad \text{Eqn 22}$$

$$e_s = \frac{e_a g_{bw} + e_i g_{sw}}{g_{bw} + g_{sw}} \quad \text{Eqn 23}$$

e_i is the vapor pressure (kPa) at the temperature of the leaf and is assumed to be at saturation ($RH = 100\%$). $e_{sat}(T_{leaf})$ can be calculated using an approximation formula such as (Tetens, 1930) equation (Eqn 24).

$$e_{sat}(T_{leaf}) = 0.6108 e^{\frac{17.27 T_{leaf}}{T_{leaf} + 237.3}} \quad \text{Eqn 24}$$

Note that in this equation, the leaf temperature is in degree Celsius.

If the new T_{leaf} solution is within a user specified margin of the initial value (by default less than 0.05 degree of difference), we consider that the numerical solution has converged. If the difference is high (e.g., > 0.05), the initial values are replaced by the new values and the calculations are repeated until the numerical solution reaches convergence.

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