Leaf gas exchange equations

The equations used to simulate 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 CO_2 assimilation rate as:

$$A_n = \min\left(A_c, A_j, A_p\right) - R_{day} \quad \text{Eqn 1}$$

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 known as the rate of triose phosphate utilization. R_{day} 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 CO_2 compensation point, c_i is the intercellular CO_2 concentration, V_{cmax} is the maximum carboxylation velocity, K_c and K_o are the Michaelis−Menten coefficients of rubisco activity for CO_2 and O_2, 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.

$$I_2 = Abso\phi Q \quad \text{Eqn 6}$$

Where *Abso* is the leaf absorptance in the visible (400 to 700 nm), Q is the visible irradiance at the leaf surface in mol m^{-2} s^{-1} and ϕ is the maximum quantum yield of electron transport of absorbed light.

ϕ can be further described by Eqn 4 where f is the fraction of irradiance not used for photochemistry, often fixed as 0.15 (von Caemmerer et al., 2009; Yin et al., 2021). The 2 in the denominator accounts for the absorption of half of the irradiance by each photosystem.

$$\phi = (1 - f)/2 \quad \text{Eqn 7}$$

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

$$A_n = \frac{(c_i - \Gamma^*)\,x}{c_i + y} - R_d \quad \text{Eqn 8}$$

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).

$$\theta_{cj} A_i^2 - A_i\left(A_j + A_c\right) + A_j A_c = 0 \quad \text{Eqn 9}$$

$$\theta_{ip} A^2 - A\left(A_i + A_p\right) + A_i A_p = 0 \quad \text{Eqn 10}$$

where θ_{cj} and θ_{ip} are empirical smoothing constants describing the transition between limitations. Note that in those equations, A_i is an intermediate variable that is first calculated and used in Eqn 10. A is the resulting gross CO_2 assimilation rate which can be used in place of $\min\left(A_c, A_j, A_p\right)$. Careful consideration must be used when applying this smoothing approach, as it can significantly reduce A_n in some conditions (Rogers *et al.*, 2021).

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 11) or a modified Arrhenius function (Eqn 12) can be used to scale the parameters from 25°C to the leaf temperature:

$$P(T_{leaf}) = P_{ref} e^{\frac{H_a}{RT_{ref}} - \frac{H_a}{RT_{leaf}}} \quad \text{Eqn 11}$$

$$P(T_{leaf}) = \frac{P_{Ref}\left(1 + e^{\frac{sT_{ref} - H_d}{RT_{ref}}}\right) e^{\frac{H_a}{RT_{Ref}}\left(1 - \frac{T_{ref}}{T_{leaf}}\right)}}{1 + e^{\frac{sT_{leaf} - H_d}{RT_{leaf}}}} \quad \text{Eqn 12}$$

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 mol^{-1}, H_d is the energy of deactivation in J 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.

Parameters

The parameters of the different equations as well as their units are given in Table 1. They derive from the Community Land Model 4.5 (Oleson *et al.*, 2013).

Note that the absorptance of the leaf is derived from the radiation interception model parameters, which are variable in CLM4.5 depending on the biome and plant functional types. We chose to set the leaf absorptance to 0.85 which is used for several plant functional types and is close enough to the values 0.84 and 0.88 which are used for other plant functional types (See Table 3.1 within Oleson *et al.*, 2013).

Table 1 Parameters of the FvCB model as used in CLM4.5 (Oleson *et al.*, 2013, Tables 3.1, 8.2 and paragraph 8.2), see Tables

Parameter	Definition	Value at 25°C	Unit	Activation energy (J mol^{-1})	Deactivation energy (J mol^{-1})	Entropy term (J mol^{-1} K−1)
V_{cmax}	Maximum rate of carboxylation	-	µmol m^{-2} s^{-1}	65330	149250	485
J_{max}	Maximum rate of electron transport	-	µmol m^{-2} s^{-1}	43540	152040	495
T_p	Triose phosphate utilization	-	µmol m^{-2} s^{-1}	65330	149250	485
R_{day}	Mitochondrial respiration in the light		µmol m^{-2} s^{-1}	46390	150650	490
K_c	Michaelis-Menten constant, CO2	404.9	µmol mol^{-1}	79430	-	-
K_o	Michaelis-Menten constant, O2	278.4	mmol mol^{-1}	36380	-	-
Γ^*	CO2 compensation point	42.75	µmol mol^{-1}	37830	-	-
Abso	Absorptance of the leaf	0.85	-	-	-	-
ϕ	Apparent quantum yield	0.425	-	-	-	-
θ	Empirical curvature factor	0.7	-	-	-	-
θ_{cj}	Collatz smooting factor between Vcmax and Jmax	0.999	-	-	-	-
θ_{jt}	Collatz smooting factor between Jmax and TPU	0.999	-	-	-	-

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