# **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 CO2 assimilation rate as:

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:

Eqn 2

Eqn 3

Eqn 4

where 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:

Eqn 5

where 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.

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.

Eqn 7

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

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 . When *A*n is limited by *A*j *x* is *J*/4 and *y* is When *A*n is limited by *A*p, *x* is 3*T*p and *y* is -.

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

Eqn 9

Eqn 10

where and 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 CO2 assimilation rate which can be used in place of . 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, , *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:

Eqn 11

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℃ | 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 | - | - | - | - |
| θcj | Collatz smooting factor between Vcmax and Jmax | 0.999 | - | - | - | - |
| θjt | Collatz smooting factor between Jmax and TPU | 0.999 | - | - | - | - |

**Fitting procedure**

Gilles?

**References**

**Bernacchi CJ, Pimentel C, Long SP**. **2003**. In vivo temperature response functions of parameters required to model RuBP-limited photosynthesis. *Plant, Cell & Environment* **26**: 1419–1430.

**Bernacchi CJ, Singsaas EL, Pimentel C, Jr ARP, Long SP**. **2001**. Improved temperature response functions for models of Rubisco-limited photosynthesis. *Plant, Cell & Environment* **24**: 253–259.

**Bonan G (Ed.)**. **2019**. Stomatal Conductance. In: Climate Change and Terrestrial Ecosystem Modeling. Cambridge: Cambridge University Press, 189–212.

**von Caemmerer S, Farquhar GD, Berry JA**. **2009**. *Biochemical model of C3 photosynthesis In Photosynthesis in Silico. Understanding Complexity from Molecules to Ecosystemns. Edited by Laisk, A., Nedbal, L. and Govindjee*. Springer, Dordrecht, The Netherlands.

**Collatz GJ, Ball JT, Grivet C, Berry JA**. **1991**. Physiological and environmental regulation of stomatal conductance, photosynthesis and transpiration: a model that includes a laminar boundary layer. *Agricultural and Forest Meteorology* **54**: 107–136.

**Duursma RA**. **2015**. Plantecophys - An R Package for Analysing and Modelling Leaf Gas Exchange Data (PC Struik, Ed.). *PLOS ONE* **10**: e0143346.

**Farquhar GD, Caemmerer S von, Berry JA**. **1980**. A biochemical model of photosynthetic CO2 assimilation in leaves of C3 species. *Planta* **149**: 78–90.

**Leuning R**. **2002**. Temperature dependence of two parameters in a photosynthesis model. *Plant, Cell & Environment* **25**: 1205–1210.

**Oleson K, Lawrence D, Bonan G, Drewniak B, Huang M, Koven C, Levis S, Li F, Riley W, Subin Z, *et al.*** **2013**. Technical description of version 4.5 of the Community Land Model (CLM)(No. NCAR/TN-503+ STR). *UCAR: Boulder, CO, USA*.

**Rogers A, Kumarathunge DP, Lombardozzi DL, Medlyn BE, Serbin SP, Walker AP**. **2021**. Triose phosphate utilization limitation: an unnecessary complexity in terrestrial biosphere model representation of photosynthesis. *New Phytologist* **230**: 17–22.

**Yin X, Struik PC**. **2009**. C3 and C4 photosynthesis models: An overview from the perspective of crop modelling. *NJAS - Wageningen Journal of Life Sciences* **57**: 27–38.