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:

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:

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.

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

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 . 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 7

Eqn 8

where and 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 . 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):

Eqn 9

where CO2s 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):

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):

Eqn 11

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

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:

Eqn 13

**Coupling the photosynthesis, gas transport and stomatal conductance models**

The system of equations 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).

Eqn 14

Eqn 15

where :

Eqn 16

Eqn 17

Eqn 18

**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 19) or a modified Arrhenius function (Eqn 20) can be used to correct for the temperature effect:

Eqn 19

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 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.

**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 a 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 = *CO2*a) 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 *CO2*s and a new *RH*s using Eqn 21 and Eqn 22, respectively.

Eqn 21

Eqn 22

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).

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.

**References**

**Ball JT, Woodrow IE, Berry JA**. **1987**. A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: Progress in photosynthesis research. Springer, 221–224.

**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.

**Fick A**. **1855**. Ueber Diffusion. *Annalen der Physik* **170**: 59–86.

**Jarvis P**. **1971**. The estimation of resistances to carbon dioxide transfer. In: Plant photosynthetic production. Manual of methods. The Hague, Netherlands: Dr. W. Junk NV, 566–631.

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

**Medlyn BE, Duursma RA, Eamus D, Ellsworth DS, Prentice IC, Barton CVM, Crous KY, Angelis PD, Freeman M, Wingate L**. **2011**. Reconciling the optimal and empirical approaches to modelling stomatal conductance. *Global Change Biology* **17**: 2134–2144.

**Muir CD**. **2019**. tealeaves: an R package for modelling leaf temperature using energy budgets. *AoB PLANTS* **11**.

**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.

**Tetens O**. **1930**. Uber einige meteorologische Begriffe. *Z. geophys* **6**: 297–309.

**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.