

The equations used to simulate the leaf gas exchange are presented below.

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

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

where A_c is the rate of maximum carboxylation and A_j is the maximum rate of RuBp regeneration (or electron transport) and R_d is the daytime respiration rate that is not attributable to the photorespiratory pathway.

A_c and A_j are given by:

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

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

where Γ^* is 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, and J is the potential electron transport rate, given by:

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

where I_2 is the photosynthetic irradiance absorbed by the photosystem II, J_{max} is the maximum electron transport rate and θ is an empirical curvature factor (usually around 0.7).

Note that Eqn A2 and A3 are in the form:

$$A_n = \frac{(c_i - \Gamma^*) x}{c_i + y} - R_d \quad \text{Eqn 5}$$

where x and y equal V_{cmax} and $K_c \left(1 + \frac{O_2}{K_o}\right)$, respectively, when A_n is limited by A_c , and equal $J/4$ and $2\Gamma^*$, respectively, when A_n is limited by A_j .

The diffusion of the CO₂ from the leaf surface to the intercellular environment can be described by the MSWF theory:

$$C_i = \frac{C_s \left(g_{sc} + g_{cc} - \frac{E_s}{2} \right) - A_n}{g_{sc} + g_{cc} + \frac{E_s}{2}} \quad \text{Eqn 6}$$

where C_s is the CO₂ concentration at the leaf surface (ppm), g_{sc} and g_{cc} are the stomatal and cuticular conductance to CO₂, respectively, E_s is the transpiration through the stomata.

$$E_s = \frac{g_{sw} (w_i - w_s)}{1 - \frac{w_i + w_s}{2}}$$

where g_{sw} is the stomatal conductance to water, w_i and w_s are the water vapour concentration inside and on the surface of the leaf, respectively, in mol mol⁻¹.

$$w_i = 0.61365 \frac{e^{\frac{17.502 * T_{leaf}}{240.97 + T_{leaf}}}}{P_{atm}}$$

$$w_s = 0.61365 \frac{e^{\frac{17.502 * T_s}{240.97 + T_s}}}{P_{atm}} RH_s$$

$$g_{sc} = g_{sw}/1.6$$

$$g_{cc} = \frac{g_{cw}}{20}$$

And finally, the leaf conductance to water vapor is modeled using the USO model:

$$g_{lw} = g_0 + 1.6(1 + g_1 \frac{g_1}{\sqrt{VPD_{leaf}}}) \frac{A_n}{C_s} \quad \text{Eqn 7}$$

where g_0 corresponds to g_{lw} for $A_n = 0$. Note that Eqn 7 gives the leaf water conductance (g_{lw}) and not the stomatal conductance (g_{sw}) as g_0 is assumed to be the sum of the cuticular conductance (g_{cw}) and the conductance of the stomata which are imperfectly closed ($g_{sw,min}$).

The system of equations {Eqn 5, Eqn 6, Eqn 7} corresponds to:

$$\left\{ \begin{array}{l} A_n = \frac{(C_i - \Gamma^*) x}{C_i + y} - R_d \\ g_{sw} = g_0 - g_{cw} + 1.6(1 + g_1 \frac{g_1}{\sqrt{VPD_{leaf}}}) \frac{A_n}{C_s} \\ C_i = \frac{C_s (\frac{g_{sw}}{1.6} + l - g_{sw}k) - A_n}{\frac{g_{sw}}{1.6} + l + g_{sw}k} \end{array} \right\} = \left\{ \begin{array}{l} A_n = \frac{(C_i - \Gamma^*) x}{C_i + y} - R_d \\ g_{sw} = g_0 - g_{cw} + m \frac{A_n}{C_s} \\ C_i = \frac{C_s (\frac{g_{sw}}{1.6} + l - g_{sw}k) - A_n}{\frac{g_{sw}}{1.6} + l + g_{sw}k} \end{array} \right\}$$

$$\text{where } l = \frac{g_{cw}}{20} \text{ and } k = \frac{(w_i - w_s)}{2 - w_i - w_s}$$

The solution for C_i corresponds to the root of a polynomial of degree 2.

