The equations used to simulate the leaf gas exchange are presented below. Note that in this model we consider that the leaf surface conditions are known, in particular, the gas concentration and temperature.

Photosynthesis model

We used the FvCB photosynthesis model (Farquhar *et al.*, 1980), which represents the net CO_2 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 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, 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 2 and 3 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.

Transport of water and carbon dioxide between the leaf surface and the interior of the leaf

The diffusion of the CO_2 from the leaf surface to the intercellular environment can be described by the MSWF theory (Eqn 13 in Márquez *et al.*, 2021):

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

where C_s is the CO_2 concentration at the leaf surface, g_{sc} and g_{cc} are the stomatal and cuticular conductance to CO_2, respectively, E_s is the transpiration through the stomata (Eqn 10 and supplementary note 3 in Márquez *et al.*, 2021).

$$E_s = \frac{g_{sw}\,(w_i-w_s)}{1-\frac{w_i+w_s}{2}} \qquad \text{Eqn 7}$$

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

$$w_i = 0.61365\,\frac{e^{17.502*\frac{T_{leaf}}{240.97+T_{leaf}}}}{P_{atm}} \qquad \text{Eqn 8}$$

$$w_s = 0.61365\,\frac{e^{17.502*\frac{T_s}{240.97+T_s}}}{P_{atm}}\,RH_s \qquad \text{Eqn 9}$$

$$g_{sc} = g_{sw}/1.6 \qquad \text{Eqn 10}$$

$$g_{cc} = \frac{g_{cw}}{20} \qquad \text{Eqn 11}$$

Note that the total leaf transpiration E_T is the sum of the leaf transpiration through the stomata and the cuticular transpiration E_c (Eqn 10 and supplementary note 3 in Márquez *et al.*, 2021).

$$E_c = g_{cw}(w_i - w_s) \qquad \text{Eqn 12}$$

Eqn 6 can be rewritten using Eqn 7, 10 and 11:

$$C_i = \frac{C_s\left(g_{sc} + g_{cc} - \frac{g_{sw}\,(w_i - w_s)}{2 - w_i + w_s}\right) - A_n}{g_{sc} + g_{cc} + \frac{g_{sw}\,(w_i - w_s)}{2 - w_i + w_s}}$$

which is equivalent to:

$$C_i = \frac{C_s\left(\frac{g_{sw}}{1.6} + \frac{g_{cw}}{20} - \frac{g_{sw}\,(w_i - w_s)}{2 - w_i + w_s}\right) - A_n}{\frac{g_{sw}}{1.6} + \frac{g_{cw}}{20} + \frac{g_{sw}\,(w_i - w_s)}{2 - w_i + w_s}}$$

and to:

$$C_i = \frac{C_s\left[g_{sw}\left(\frac{1}{1.6} - k\right) + l\right] - A_n}{g_{sw}\left(\frac{1}{1.6} + k\right) + l} \qquad \text{Eqn 13}$$

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

20 is the ratio of CO_2 to H_2O cuticular conductance (Márquez *et al.*, 2021).

Model of leaf conductance

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

$$g_{\mathrm{lw}} = g_0 + 1.6\left(1 + \frac{g_1}{\sqrt{VPD_{\mathrm{leaf}}}}\right)\frac{A_n}{C_s} \qquad \text{Eqn 14}$$

where g_0 corresponds to g_{lw} for $A_n = 0$, g_1 is a conductance parameter, and VPD_{leaf} is the leaf to air vapor deficit in kPa. Note that Eqn 14 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 ($g_{sw,min}$). Therefore:

$$g_{\mathrm{sw}} = g_0 - g_{cw} + 1.6\left(1 + \frac{g_1}{\sqrt{VPD_{\mathrm{leaf}}}}\right)\frac{A_n}{C_s} \qquad \text{Eqn 15}$$

Eqn 15 can be rewritten as

$$g_{\mathrm{sw}} = \mathrm{q} + m\mathrm{A_n} \qquad \text{Eqn 16}$$

where q = $g_0 - g_{cw}$ and $m = 1.6\left(1 + \frac{g_1}{\sqrt{VPD_{\mathrm{leaf}}}}\right)\frac{1}{C_s}$

Solving the three models together

Eqns 5, 13 and 16 depend on each other as A_n depends on C_i, g_{sw} depends on A_n and C_i depends on both g_{sw} and A_n. Such system of equations $\{Eqn\ 5, Eqn\ 13, Eqn\ 16\}$ is either solved numerically or analytically.

This system can be rewritten as:

$$\begin{cases} A_n = \dfrac{(C_i - \Gamma^*)\, x}{C_i + y} - R_d \\ g_{sw} = q + m\mathrm{A_n} \\ C_i = \dfrac{C_s\left[g_{sw}\left(\frac{1}{1.6} - k\right) + l\right] - A_n}{g_{sw}\left(\frac{1}{1.6} + k\right) + l} \end{cases}$$

Analytically, the solutions for C_i correspond to the roots of a polynomial of degree 2:

$$aC_i^2 + bC_i + c = 0$$

where

$$a = \frac{1}{1.6}\mathrm{R_d\, m} + \mathrm{R_d\, k\, m} - \frac{1}{1.6}\mathrm{m\, x} - \mathrm{k\, m\, x} - \frac{1}{1.6}\mathrm{q} - \mathrm{k\, q} - \mathrm{l}$$

$$b = \frac{1}{1.6}\Gamma^*\, m\, x + \Gamma^*\, k\, m\, x - \frac{1}{1.6}R_d\, C_s\, m + R_d\, C_s\, k\, m + \frac{1}{1.6}R_d\, m\, y + R_d\, k\, m\, y + \frac{1}{1.6}C_s\, m\, x - C_s\, k\, m\, x + \frac{1}{1.6}C_s\, q - C_s\, k\, q - \frac{1}{1.6}q\, y - k\, q\, y + C_s\, l - l\, y + R_d - x$$

$$c = -\frac{1}{1.6}\Gamma^*\, C_s\, m\, x + \Gamma^*\, C_s\, k\, m\, x - \frac{1}{1.6}R_d\, C_s\, m\, y + R_d\, C_s\, k\, m\, y + \frac{1}{1.6}C_s\, q\, y - C_s\, k\, q\, y + C_s\, l\, y + x\,\Gamma^* + R_d\, y$$

In our simulations, the larger root was the solution kept for C_i. It was used to solve A_n which can then be used to calculate g_{sw}.

Note that if the vCF1981 model of gas transport is used instead of the M2021 model, $g_{cw} = 0$. Note also that if the Fick's law of diffusion is used, then $g_{cw} = 0$ and k = 0.