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 CO2 assimilation rate as:

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:

Eqn 2

Eqn 3

where 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:

Eqn 4

where 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:

Eqn 5

where *x* and *y* equal *V*cmax and , respectively, when *A*n is limited by *A*c, and equal *J*/4 and , 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 CO2 from the leaf surface to the intercellular environment can be described by the MSWF theory (Eqn 13 in Márquez *et al.*, 2021):

Eqn 6

where *C*s is the CO2 concentration at the leaf surface, and are the stomatal and cuticular conductance to CO2, respectively, *E*s is the transpiration through the stomata (Eqn 10 and supplementary note 3 in Márquez *et al.*, 2021).

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.

Eqn 8

Eqn 9

Eqn 10

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).

) Eqn 12

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

which is equivalent to:

and to:

Eqn 13

where k = and l =

20 is the ratio of CO2 to H2O cuticular conductance (Márquez *et al.*, 2021).

**Model of leaf conductance**

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

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:

Eqn 15

Eqn 15 can be rewritten as

Eqn 16

where q = and

**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 is either solved numerically or analytically.

This system can be rewritten as:

Analytically, the solutions for *C*i correspond to the roots of a polynomial of degree 2:

where

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.