# 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 CO<sub>2</sub> assimilation rate as:

$$A_n = \min(A_c, A_i, A_p) - R_d$$
 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:

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

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

$$A_p = 3T_p$$
 Eqn 4

where  $\Gamma^*$  is the photorespiratory CO<sub>2</sub> compensation point,  $c_i$  is the intercellular CO<sub>2</sub> concentration,  $V_{\text{cmax}}$  is the maximum carboxylation velocity,  $K_c$  and  $K_o$  are the Michaelis-Menten coefficients of rubisco activity for CO<sub>2</sub> and O<sub>2</sub>, respectively. J is the potential electron transport rate, given by:

$$J = \frac{I_2 + J_{max} - \sqrt{(I_2 + J_{max})^2 - 4\theta I_2 J_{max}}}{2\theta}$$
 Eqn 5

where  $I_2$  is the photosynthetically active irradiance absorbed by photosystem II,  $J_{\text{max}}$  is the maximum electron transport rate and  $\theta$  is an empirical curvature factor (usually estimated as 0.7).  $T_p$  is the Triose phosphate utilization rate.

$$I_2 = Abso\phi Q$$
 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<sup>-2</sup> s<sup>-1</sup> and  $\phi$  is the maximum quantum yield of electron transport of absorbed light.

 $\phi$  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.

$$\phi = (1 - f)/2$$
 Eqn 7

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

$$A_n = \frac{(c_i - \Gamma^*) x}{c_i + y} - R_d$$
 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  $K_c \left(1 + \frac{o_2}{K_o}\right)$ . When  $A_n$  is limited by  $A_j$  x is J/4 and y is  $2\Gamma^*$ . When  $A_n$  is limited by  $A_p$  x is  $3T_p$  and y is  $-\Gamma^*$ .

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

$$\theta_{cj}A_i^2 - A_i(A_j + A_c) + A_jA_c = 0$$
 Eqn 9

$$\theta_{in}A^2 - A(A_i + A_n) + A_iA_n = 0$$
 Eqn 10

where  $\theta_{cj}$  and  $\theta_{ip}$  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 CO<sub>2</sub> assimilation rate which can be used in place of min( $A_c$ ,  $A_j$ ,  $A_p$ ). 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

Diffusion of CO<sub>2</sub> from the leaf surface to the intercellular environment can be described by Fick's law of diffusion (Fick, 1855):

$$C_{\rm i} = CO_{\rm 2s} - 1.6 \frac{A_{\rm n}}{g_{\rm sw}}$$
 Eqn 11

where  $CO_{2s}$  is the concentration of  $CO_2$  at the leaf surface,  $g_{sw}$  is the stomatal conductance for  $H_2O$  vapor, and 1.6 is the ratio of diffusivity of  $H_2O$  and  $CO_2$  through the stomata (Jarvis, 1971). See (Lamour *et al.*, 2021) for more details on this equation.

## Stomatal conductance model

Several empirical models of stomatal conductance can be used:

The USO model (Medlyn et al., 2011):

$$g_{\text{sw}} = g_0 + 1.6(1 + \frac{g_1}{\sqrt{VPD_{\text{leaf}}}}) \frac{A_n}{\text{co}_{2\text{s}}}$$
 Eqn 12

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):

$$g_{\text{sw}} = g_0 + 1.6g_1 \frac{A_n}{\text{CO}_{2\text{s}}\sqrt{VPD_{\text{leaf}}}}$$
 Eqn 13

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

$$g_{\text{sw}} = g_0 + g_1 \frac{A_n}{\text{CO}_{2S}RH}$$
 Eqn 14

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:

$$g_{\text{sw}} = g_0 + m \frac{A_n}{\text{CO}_{2s}}$$
 Eqn 15

(Lamour et al., 2022) model of conductance is also implemented:

$$g_{\text{sw}} = g_0 + 1.6 \frac{g_1}{\sqrt{VPD_{\text{leaf}}}} \frac{A_g^2}{\text{CO}_{2S}}$$
 Eqn 16

where  $A_g = A_n + R_d$ .

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

The system of equations  $\{Eqn\ 8, Eqn\ 11, Eqn\ 15\}$  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).

$$\begin{cases} A_n = \frac{(c_i - \Gamma^*) x}{c_i + y} - R_d \\ C_i = CO_{2s} - 1.6 \frac{A_n}{g_{sw}} \\ g_{sw} = g_0 + m \frac{A_n}{CO_{2s}} \end{cases}$$
 Eqn 16

$$aC_i^2 + bC_i + c = 0 Eqn 17$$

where:

$$a = g_0 + \frac{m}{co_{2s}}(x - R_d)$$
 Eqn 18

$$b = yg_0 + \frac{m}{co_{2s}}(-\Gamma^*x - R_dy) - CO_{2s}g_0 + (x - R_d)(1.6 - m)$$
 Eqn 19

$$c = -yCO_{2s}g_0 + (1.6 - m)(-\Gamma^*x - R_dy)$$
 Eqn 20

For the Lamour et al. 2022 conductance model, the solutions of the system of equations  $\{Eqn\ 8, Eqn\ 11, Eqn\ 16\}$  for  $C_i$  corresponds to the roots of a degree 3 polynomial (below). Among the three solutions two are imaginary and one is real. The real solution is used and allow the calculation of  $A_n$  and  $g_{sw}$ :

$$aC_i^3 + bC_i^2 + cC_i + d = 0$$
 Eqn 21

where:

$$\begin{split} a &= 5g_{0}CO_{2s}\sqrt{VPD_{leaf}} + 8g_{1}x^{2} \\ b &= -16\Gamma^{*}g_{1}x^{2} - 5\sqrt{VPD_{leaf}}CO_{2s}^{2}g_{0} + 10\sqrt{VPD_{leaf}}CO_{2s}g_{0}y - 8CO_{2s}g_{1}x^{2} \\ &- 8\sqrt{VPD_{leaf}}R_{dark}CO_{2s} + 8\sqrt{VPD_{leaf}}CO_{2s}x \\ c &= 8\Gamma^{*2}g_{1}x^{2} + 16\Gamma^{*}CO_{2s}g_{1}x^{2} - 10\sqrt{VPD_{leaf}}CO_{2s}^{2}g_{0}y + 5\sqrt{VPD_{leaf}}CO_{2s}g_{0}y^{2} \\ &- 8\Gamma^{*}\sqrt{VPD_{leaf}}CO_{2s}x - 16\sqrt{VPD_{leaf}}R_{dark}CO_{2s}y + 8\sqrt{VPD_{leaf}}CO_{2s}xy \\ d &= -8\Gamma^{*2}CO_{2s}g_{1}x^{2} - 5\sqrt{VPD_{leaf}}CO_{2s}^{2}g_{0}y^{2} - 8\Gamma^{*}\sqrt{VPD_{leaf}}CO_{2s}xy \\ &- 8\sqrt{VPD_{leaf}}R_{dark}CO_{2s}y^{2} \end{split}$$

#### **Temperature effects on model parameters**

The parameters of the photosynthesis model ( $V_{\rm cmax}$ ,  $J_{\rm max}$ ,  $T_{\rm p}$ ,  $R_{\rm d}$ ,  $\Gamma^*$ ,  $K_{\rm c}$  and  $K_{\rm o}$ ) 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:

$$P(T_{leaf}) = P_{ref}e^{\frac{H_a}{RT_{ref}} - \frac{H_a}{RT_{leaf}}}$$
 Eqn 22

$$P(T_{leaf}) = \frac{P_{Ref}\left(1 + e^{\frac{sT_{ref} - H_d}{RT_{ref}}}\right) e^{\frac{H_a}{RT_{Ref}}\left(1 - \frac{T_{ref}}{T_{leaf}}\right)}}{\frac{sT_{leaf} - H_d}{RT_{leaf}}}$$
Eqn 23

where P is the value of the parameter at  $T_{\text{leaf}}$ ,  $P_{\text{ref}}$  is the value of the parameter at the reference temperature,  $H_{\text{a}}$  is the energy of activation in J mol<sup>-1</sup>,  $H_{\text{d}}$  is the energy of deactivation in J mol<sup>-1</sup> and s is an entropy term. R is the ideal gas constant. In this equation, the temperature  $T_{\text{ref}}$  and  $T_{\text{leaf}}$  are in Kelvin.

## Coupling the gas exchange model with a leaf energy balance model

The system of equations 16 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), called tealeave. It needs several input parameters such as d the characteristic leaf dimension defined as the diameter of the largest circle that can be inscribed within the margin of the leaf. It also uses the stomatal conductance ( $g_{sw}$ , Eqn 14 to 16) and the cuticular conductance. Here, we assumed that the cuticular conductance was equal to  $g_0$ , as FATES assume that the minimum conductance is  $g_0$ . Note that the photosynthesis model uses Q, the leaf photosynthetically active radiation in the wavelengths 400 to 700 nm in  $\mu$  mol m<sup>-2</sup> s<sup>-1</sup>. For its calculations, tealeave uses the shortwave  $S_{sw}$  solar radiation in the wavelengths 300 to 4000 nm, in W m<sup>-2</sup>. The relation between Q and  $S_{sw}$  is  $Q = 4.57 * 0.45 * S_{sw}$ , where 4.57 converts watt.m-2 in  $\mu$  mol m<sup>-2</sup> s<sup>-1</sup> and 0.45 accounts for the difference in wavelengths (see Yun *et al.*, (2020) for an example).

We followed the numerical approach by (Bonan, 2019) to couple the leaf gas exchange equations (Eqn 16) with the leaf energy budget. In brief, the numerical approach uses an initial estimate of leaf temperature ( $T_{\text{leaf}} = T_{\text{air}} + 1$ ),  $CO_{2s}$  ( $CO_{2s} = CO_{2a}$ ) and  $RH_s$  ( $RH_s = RH_a$ ). Using these initial values, the system of equation 16 is solved by accounting for the leaf temperature effect on the photosynthetic parameters (Eqn 22 and 23). The leaf energy budget is then evaluated (Muir, 2019) and produces an estimate of a new  $T_{\text{leaf}}$  and  $g_{\text{bw}}$ . These values are used to calculate a new  $CO_{2s}$  and a new  $RH_s$  using Eqn 24 and Eqn 25, respectively.

$$CO_{2s} = CO_{2a} - \frac{1.37A_n}{g_{hw}}$$
 Eqn 24

$$RH_S = \frac{e_S}{e_{Sat}(T_{leaf})} 100$$
 Eqn 25

$$e_S = \frac{e_a g_{bw} + e_i g_{sw}}{g_{bw} + g_{sw}}$$
 Eqn 26

 $e_i$  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 27).

$$e_{sat}(T_{leaf}) = 0.6108e^{\frac{17.27T_{leaf}}{T_{leaf} + 237.3}}$$
 Eqn 27

Note that in this equation, the leaf temperature is in degree Celsius.

If the new  $T_{\text{leaf}}$  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 converge.

## Parameters used in FATES for broadleaf evergreen tropical species

The parameters of the equations can be chosen by the package user, the values for the parameters used in FATES are synthetized in Table 1. More info and updated values can be found here: <a href="https://github.com/NGEET/fates/blob/master/parameter\_files/fates\_params\_default.cdl">https://github.com/NGEET/fates/blob/master/parameter\_files/fates\_params\_default.cdl</a>,

https://fates-users-guide.readthedocs.io/projects/tech-doc/en/latest/fates\_tech\_note.html#fundamental-photosynthetic-physiology-theory

Table 1 Parameters used in FATES terrestrial biosphere model to simulate leaf gas exchange of broadleaf evergreen tropical species

Parameter	Definition	Value at 25°C	Unit	Activation energy (J mol <sup>-1</sup> )	Deactivation energy (J mol <sup>-1</sup> )	Entropy term (J mol <sup>-1</sup> K-1)
V <sub>cmax</sub>	Maximum rate of carboxylation	50	μmol m-2 s-1	65330	149250	485
$J_{ m max}$	Maximum rate of electron transport	$1.67 \ V_{\rm cmax} = 83.5$	μmol m-2 s-1	43540	152040	495
$T_{ m p}$	Triose phosphate utilization	$V_{\rm cmax} / 6 = 8.33$	μmol m-2 s-1	53100	150650	490
$R_{ m dark}$	Dark adapted respiration	$0.0142 \ V_{\rm cmax} = 0.71$	μmol m-2 s-1	46390	150650	490
K <sub>c</sub>	Michaelis-Menten constant, CO2	404.9	μmol mol <sup>-1</sup>	36380	-	-
K <sub>o</sub>	Michaelis-Menten constant, O2	278.4	mmol mol <sup>-1</sup>	79430	-	-

Γ*	CO2 compensation point	42.75	μmol mol <sup>-1</sup>	37830	-	-
Abso	Absorptance of the leaf	0.831	-	-	-	-
ф	Apparent quantum yield	0.425	-	-	-	-
θ	Empirical curvature factor	0.7	-	-	-	-
$\theta_{cj}$	Collatz smooting factor between Vcmax and Jmax	0.999	-	-	-	-
$\theta_{jt}$	Collatz smooting factor between Jmax and TPU	0.999	-	-	-	-
<i>g</i> <sub>1</sub>	Slope parameter of the USO conductance model (Eqn 12)	4.1	kPa <sup>0.5</sup>			
g <sub>0</sub>	Intercept parameter of the USO conductance model (Eqn 12)	0.01	mol m <sup>-</sup> 2 s <sup>-1</sup>			
d	Leaf characteristic dimension (leaf energy budget)	0.04	m			

 $<sup>^{1}</sup>$ In FATES, the visible leaf reflectance and transmittance are 0.11 and 0.06, respectively, so the leaf absorptance is 1-0.11-0.06=0.83, see Table 2

## Scaling gas exchanges from leaf to canopy

The equations presented before describe gas exchanges at the leaf scale. Scaling from leaf to canopy is done similarly as in FATES. The gas exchange equations are at the leaf scale but several assumptions are used to describe the vegetation and the environment within the canopy.

## **Biophysical constant**

The air temperature,  $CO_2$ , and humidity are considered constant within the vegetation (however, the leaf temperature,  $CO_2$  at the leaf surface and humidity at the leaf surface may change, due to the leaf energy balance and boundary layer, see Coupling the gas exchange model with a leaf energy balance model).

Wind speed, used in the leaf energy budget to calculate  $g_{bw}$ , is assumed to follow an exponential decrease with *LAI* within the canopy (Buckley *et al.*, 2014).

$$wd(LAI) = wd_0e^{-0.5LAI}$$
 Eqn C1

where wd is the wind speed in m s<sup>-1</sup> and  $wd_0$  is the wind speed at the top of the canopy.

The light intercepted by the leaves within the canopy is calculated using Norman (1979) radiation model, as implemented by Bonan (2019), and used in FATES. The detail of the equations can be found in his book, or in FATES documentation (https://fates-users-guide.readthedocs.io/projects/tech-doc/en/latest/fates\_tech\_note.html#fundamental-radiation-

transfer-theory). The code used in the package is the one from Bonan (2019), converted from matlab to R.

(https://github.com/gbonan/bonanmodeling/blob/master/sp\_14\_03/NormanRadiation.m).

The direct photosynthetic light  $Q_{\text{dir}}$  at the top of the canopy as well as the diffuse light  $Q_{\text{dif}}$  are an input of the radiation interception model. Since the proportion of direct to total light  $R_{\text{dir}}$  is rarely measured, we use the same empirical approximation as in CLM4.5 and FATES when those models are used without coupling with an atmospheric model (Offline mode, Eqn 26. 7 in

https://opensky.ucar.edu/islandora/object/technotes%3A515/datastream/PDF/view Eqn 26.7, p 400).

$$R_{dir} = a_0 + a_1 Q_W + a_2 Q_W^2 + a_3 Q_W^3$$

where  $R_{dir}$  is the ratio of direct visible radiation to the total visible solar radiation  $Q_W$  (Watt m<sup>-2</sup>), the empirical constant  $a_0$ ,  $a_1$ ,  $a_2$  and  $a_3$  are 0.17639, 0.00380, -9.0039 10<sup>-6</sup> and 8.1351 10<sup>-9</sup>, respectively. The conversion from watt m<sup>-2</sup> to  $\mu$ mol m<sup>-2</sup> s<sup>-1</sup> is done using Q=Qw4.57 where Q is the total visible radiation in  $\mu$ mol m<sup>-2</sup> s<sup>-1</sup>.

A similar method is used to estimate the diffuse and direct NIR.

$$R_{dir,NIR} = b_0 + b_1 NIR + b_2 NIR^2 + b_3 NIR^3$$

where the empirical constant  $b_0$ ,  $b_1$ ,  $b_2$  and  $b_3$  are 0.29548, 0.00504, - 1.4957  $10^{-5}$  and 1.4881  $10^{-8}$ , respectively, and NIR is the near infrared (700 to 4000 nm) estimated as Q/4.57.

The radiation model also uses the cosinus of the solar zenith angle (cosz) calculated as (Miguez *et al.*, 2009):

$$cosz = sin\varphi sin\delta + cos\varphi cos\delta cos h$$

where h is the solar hour angle in radians,  $\delta$  is the solar declination angle in radians, and  $\phi$  is latitude (radians).

$$\delta = -23.5\cos\left(\frac{360(D_j + 10)}{365} \frac{\pi}{180}\right) \frac{\pi}{180}$$

where  $D_i$  is the day of year

$$h = 15(t - 12) \frac{\pi}{180}$$

where *t* is the time during the day in hour.

Note that the canopy is assumed to be made of leaves only to compute the radiation interception model. The effect of the branches and stems is not considered. Note also that the soil abedo is modeled in FATES and depends on the color and water saturation. Here, since a model of soil is

not considered, we used fixed value of 0.1 for the soil albedo of direct and diffuse visible radiation and 0.2 for direct and diffuse NIR radiation.

Table 2 Parameters of the radiation interception model used in FATES for tropical broadleaf species

CI	Leaf clumping index	0.85
χ	Index of departure of the leaf angles from a spherical distribution	0.32
$ ho_{vis}$	Leaf reflectance in the visible	0.11
$ au_{vis}$	Leaf transmittance in the visible	0.06
ρνis_soil	Soil reflectance in the visible	0.201
$ ho_{NIR}$	Leaf reflectance in the NIR	0.46
$ au_{NIR}$	Leaf transmittance in the NIR (radiation interception model)	0.33
PNIR_soil	Soil reflectance in the NIR (radiation interception model)	0.331

<sup>&</sup>lt;sup>1</sup>The calculation of the soil albedo is more complex in FATES and depend on the soil class as well as on its humidity. Here we used an average value for the albedo in the visible and the NIR.

#### Leaf traits

 $V_{\rm cmax25}$  decreases exponentially from the top of the canopy to the ground with the leaf area index (LAI)

$$V_{cmax25}(LAI) = V_{cmax25,top}e^{-k_nLAI}$$
 Eqn C1

where  $V_{\text{cmax25,top}}$  is the value of  $V_{\text{cmax25}}$  at the top of the canopy and  $k_n$  is the exponential decrease coefficient.

 $k_{\rm n}$  depends to  $V_{\rm cmax25,top}$  in FATES and is calculated according to Lloyd et al. 2010 empirical relationship (Fig. 10 within the paper)

$$k_n = e^{0.00963V_{cmax25,top}-2.43}$$
 Eqn C2

For a  $V_{\rm cmax25,top}$  of 50 used in FATES for broadleaf tropical evergreen species,  $k_{\rm n}$  is 0.142

 $J_{\text{max25}}$ ,  $T_{\text{p25}}$  and  $R_{\text{dark25}}$  are scaled based on  $V_{\text{cmax25}}$  within the canopy:

$$J_{max25}(LAI) = 1.67V_{cmax25}(LAI)$$
 Eqn C3
$$T_{p25}(LAI) = 1/6V_{cmax25}(LAI)$$
 Eqn C4

All the other traits of Table 1 are assumed to be constant within the canopy.

The vegetation is represented by a fixed number of vertical layers nlayers. It is assumed that the LAI of each layer is constant.

## Calculation of the carbon assimilated and the water transpired by the canopy

The radiation interception model calculates  $Q_{\rm dir}$  and  $Q_{\rm dif}$  absorbed by sun and shade leaves for each layer of the canopy as well as the proportion of shade and sun leaves. It also calculates  $NIR_{\rm dir}$  and  $NIR_{\rm dif}$  that are used by tealeave (leaf energy budget) to calculate Tleaf. The leaf gas exchange model is run independently for each type of leaf (sun and shade, by canopy layer). The gas exchange by all the leaves of the canopy corresponds then to the sum of gas exchanged by each type of leaf and scaled to their surface area.

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