



Supplement of

Impact of canopy environmental variables on the diurnal dynamics of water and carbon dioxide exchange at leaf and canopy level

Raquel González-Armas et al.

Correspondence to: Raquel González-Armas (raquel.gonzalezarmas@wur.nl)

The copyright of individual parts of the supplement might differ from the article licence.

S1 Tendencies of the leaf gas exchange

This section contains instructions to calculate the tendency equations for the A- g_s model as implemented in CLASS model (details of A- g_s in CLASS are in appendix E of Vilà-Guerau de Arellano et al. 2015). We do not write the equations of the A- g_s model here but we used the same formulation than vapor pressure deficit is referred as VPD instead of D_S . The code needed for calculating the budget tendency equation for CLASS model output is in a Github repository (https://github.com/Rglezarm/LIAISE_manuscript). This repository also contains the code needed to reproduce all the figures and analysis of the manuscript.

S1.1 General approaches to calculate tendencies

The tendency equations have been computed with respect to two different set of environmental drivers. The first set is the one used in the present manuscript and has been termed (1) process-based tendencies. Here the set of environmental variables are PAR, T, VPD, C_a and soil water content at the rootzone (w_2). The second set of environmental variables is PAR, T, air water vapor pressure (e), C_a and w_2 . The tendency equations derived with respect to this set has been termed (2) model-based tendencies.

S1.1.1 Process-based tendencies

With this approach, partial tendencies are computed with respect to environmental variables that are known to directly control the plant photosynthesis and the dynamic stomatal movements. However, the environmental variables are not completely independent from each other. Specifically, VPD is known to depend on T, through the following expression:

$$VPD = e_{sat}(T) - e \quad (S1)$$

Here, we are assuming that water vapor is saturated inside the sub-stomatal cavities, and that the temperature inside those cavities is equal to the atmospheric temperature. A partial derivative with respect to a variable x_i ($x_i = \text{PAR}, C_a, \text{VPD}, T$ or w_2) is calculated by leaving all the other variables from the set constant. Because of the tight relation between T and VPD, eq. (S1), we highlight this fact of partial derivative by explicitly indicating in the tendency with respect to T (VPD) that VPD (T) has been kept constant by adding it as a sub-index. To keep VPD constant when T changes, the atmospheric vapor pressure, e , must balance the temperature change. According to this approach and to our formulation, we write the process-based tendency equation for a general variable Y (e.g., g_s , A_n , or TR_{leaf}) with the following mathematical expression.

$$\frac{dY}{dt} = \frac{\partial Y}{\partial \text{PAR}} \frac{d\text{PAR}}{dt} + \left(\frac{\partial Y}{\partial T} \right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial Y}{\partial VPD} \right)_T \frac{dVPD}{dt} + \frac{\partial Y}{\partial C_a} \frac{dC_a}{dt} + \frac{\partial Y}{\partial w_2} \frac{dw_2}{dt} \quad (S2)$$

S1.1.2 Model-based tendencies

In a similar fashion to the previous approach, the model-based tendency equation for a general variable Y can be mathematically written as:

$$\frac{dY}{dt} = \frac{\partial Y}{\partial \text{PAR}} \frac{d\text{PAR}}{dt} + \frac{\partial Y}{\partial T} \frac{dT}{dt} + \frac{\partial Y}{\partial e} \frac{de}{dt} + \frac{\partial Y}{\partial C_a} \frac{dC_a}{dt} + \frac{\partial Y}{\partial w_2} \frac{dw_2}{dt} \quad (S3)$$

Although these two approaches view the tendencies through different lens, they are directly linked to each other.

S1.1.3 Relation between process-based and model-based tendencies

Because we know that VPD is a function of T and e , a direct link between process-based and model-based budget tendency equations can be obtained. The following equations depict the relation between the partial tendency terms of the two approaches.

$$\frac{\partial Y}{\partial T} = \left(\frac{\partial Y}{\partial T} \right)_{VPD} + \left(\frac{\partial Y}{\partial VPD} \right)_T \frac{\partial VPD}{\partial T} \quad (S4)$$

$$\frac{\partial Y}{\partial e} = \left(\frac{\partial Y}{\partial VPD} \right)_T \frac{\partial VPD}{\partial e} \quad (S5)$$

Because the functional form of VPD is known (eq. (S1)), its partial derivative with respect to T and e can be computed.

$$\frac{\partial VPD}{\partial T} = \frac{de_{sat}}{dT} \quad (S6)$$

$$\frac{\partial VPD}{\partial e} = -1 \quad (S7)$$

Considering all the concepts of this section we can construct the following final expression to calculate the model-based tendency equations from the process-based ones.

$$\frac{dY}{dt} = \frac{\partial Y}{\partial PAR} \frac{dPAR}{dt} + \left[\left(\frac{\partial Y}{\partial T} \right)_{VPD} + \left(\frac{\partial Y}{\partial VPD} \right)_T \frac{\partial e_{sat}}{\partial T} \right] \frac{dT}{dt} - \left(\frac{\partial Y}{\partial VPD} \right)_T \frac{de}{dt} + \frac{\partial Y}{\partial C_a} \frac{dC_a}{dt} + \frac{\partial Y}{\partial w_2} \frac{dw_2}{dt} \quad (S8)$$

S1.2 Strategy to calculate the budget tendency equations for A- g_s model

Now that we have described the connection between the process-based and model-based budget tendency equations, we will focus on deriving the process-based ones, eq. (S2), for the A- g_s scheme. The tendency equations can be computed for any intermediate variable of the leaf gas exchange. Note that in the previous section we have denoted such generic variable as Y . This fact implies that we can quantify the effect that changes of the environmental variables have in any variable of the leaf gas exchange. Our final goal is to do that for the stomatal conductance to water vapor (g_s), the net assimilation rate (A_n) and the leaf transpiration (TR_{leaf}).

In leaf gas exchange models, these variables are generally linked to each other. Their dependency varies from one model (or even implementation of a model) to another. A- g_s model structure can be summarized as follows. The first step of the model is to calculate the variables that depend solely on temperature. After that, C_i is computed through several equations that capture its dependency with T , VPD and C_a . These variables allow the calculation of CO_2 primary productivity (A_m). Subsequently, gross primary productivity is calculated for a soil at field capacity (A_g^*). This means that the plant is completely unstressed in terms of soil water content. At this step, the dependency on PAR is also included. The fourth step is to include the soil water content dependency of gross primary productivity. This is done by applying a soil water stress function ($f(w_2)$) that factorize the gross primary productivity at field capacity. At this point, both the stomatal conductance to water vapor, net assimilation rate of CO_2 and leaf transpiration can be computed. Table S1 defines A- g_s variables that may not have been introduced before. The A- g_s parameters can be found in Table 3 of the manuscript.

Taking advantage of this structure, we calculate the tendency equations as follows:

1. **Calculate the total temporal derivatives of the environmental variables.** $\frac{dPAR}{dt}$, $\frac{dT}{dt}$, $\frac{dVPD}{dt}$, $\frac{dC_a}{dt}$ and $\frac{dw_2}{dt}$ are calculated using a numerical technique called symmetric difference quotient applied to the output of the numerical experiments performed with CLASS.

2. Calculate the tendency equation of the CO₂ primary productivity (A_m). Equations in Sect. S1.3.
3. Calculate tendency equation of the gross primary productivity under unstressed water situations (A_g^*). Equations in Sect. S1.4.
4. Calculate the tendency equation of the gross primary productivity at a particular soil water content in the root zone (A_g). Equations in Sect. S1.5.
5. Calculate the tendency equation of the net leaf assimilation rate (A_n). Equations in Sect. S1.6.
6. Calculate the tendency equation of the stomatal conductance to water vapor (g_{sw}). Equations in Sect. S1.7.
7. Calculate the tendency equation of the leaf transpiration (TR_{leaf}). Equations in Sect. S1.8.

Table S1. List of variables used in the A-g_s model that may have not been introduced before.

Variables	
Symbol	Definition
α (mg J ⁻¹)	Light use efficiency
A_g (mg m _{leaf} ⁻² s ⁻¹)	CO ₂ gross primary productivity at leaf level
A_g^* (mg m _{leaf} ⁻² s ⁻¹)	Unstressed CO ₂ gross primary productivity at leaf level
A_m (mg m _{leaf} ⁻² s ⁻¹)	CO ₂ primary productivity
$A_{m,max}$ (mg m _{leaf} ⁻² s ⁻¹)	CO ₂ maximal primary productivity
A_n (mg m _{leaf} ⁻² s ⁻¹)	Net CO ₂ assimilated rate
R_d (mg m _{leaf} ⁻² s ⁻¹)	Dark respiration
Γ (ppmv)	CO ₂ compensation point
C_{frac} (-)	Fraction of the concentration ($C_i - \Gamma$)/($C_a - \Gamma$)
D_0 (kPa)	Water vapor pressure deficit when stomata close
g_m (mm s ⁻¹)	Mesophyll conductance

S1.3 The tendency equation of A_m

A_m depends on C_a , T and VPD. Its tendency equation can be described as follows:

$$\frac{dA_m}{dt} = \frac{\partial A_m}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial A_m}{\partial T} \right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial A_m}{\partial VPD} \right)_T \frac{dVPD}{dt} \quad (S9)$$

S1.3.1 Dependency on C_a

$$\frac{\partial A_m}{\partial C_a} = g_m C_{frac} \left(1 - \frac{A_m}{A_{m,max}} \right) \quad (S10)$$

S1.3.2 Dependency on VPD at constant T

$$\left(\frac{\partial A_m}{\partial VPD}\right)_T = \frac{\partial A_m}{\partial C_i} \frac{\partial C_i}{\partial C_{frac}} \left(\frac{\partial C_{frac}}{\partial VPD}\right)_T \quad (S11)$$

To calculate the above expression, some additional terms are needed:

$$\frac{\partial A_m}{\partial C_i} = g_m \left(1 - \frac{A_m}{A_{mmax}}\right) \quad (S12)$$

$$\frac{\partial C_i}{\partial C_{frac}} = C_a - \Gamma \quad (S13)$$

$$\left(\frac{\partial C_{frac}}{\partial VPD}\right)_T = -a_d \quad (S14)$$

S1.3.3 Dependency on T at constant VPD

$$\begin{aligned} \left(\frac{dA_m}{dT}\right)_{VPD} &= \frac{\partial A_m}{\partial A_{mmax}} \frac{dA_{mmax}}{dT} + \frac{\partial A_m}{\partial g_m} \frac{dg_m}{dT} + \frac{\partial A_m}{\partial \Gamma} \frac{d\Gamma}{dt} \\ &+ \frac{\partial A_m}{\partial C_i} \left[\frac{\partial C_i}{\partial \Gamma} \frac{d\Gamma}{dT} + \frac{\partial C_i}{\partial C_{frac}} \left(\frac{\partial C_{frac}}{f_{min}} + \frac{\partial C_{frac}}{\partial D_0} \frac{\partial D_0}{f_{min}} \right) \left(\frac{\partial f_{min}}{\partial f_{min0}} \frac{\partial f_{min0}}{\partial g_m} + \frac{\partial f_{min}}{\partial g_m} \right) \frac{dg_m}{dT} \right] \end{aligned} \quad (S15)$$

To calculate the above expression, some temperature dependent functions are needed:

$$\frac{\partial \Gamma}{\partial T} = 0.1 \cdot \Gamma \cdot \log Q_{10\Gamma} \quad (S16)$$

$$\frac{\partial A_{mmax}}{\partial T} = 0.1 \cdot A_{mmax} \left[\log Q_{10Am} + 3 \cdot \frac{e^{0.3(T_{1Am}-T)} - e^{0.3(T-T_{2Am})}}{(1 + e^{0.3(T_{1Am}-T)})(1 + e^{0.3(T-T_{2Am})})} \right] \quad (S17)$$

$$\frac{\partial g_m}{\partial T} = 0.1 \cdot g_m \left[\log Q_{10gm} + 3 \cdot \frac{e^{0.3(T_{1gm}-T)} - e^{0.3(T-T_{2gm})}}{(1 + e^{0.3(T_{1gm}-T)})(1 + e^{0.3(T-T_{2gm})})} \right] ; \quad (S18)$$

together with other terms

$$\frac{\partial A_m}{\partial A_{mmax}} = \frac{A_m}{A_{mmax}} - \frac{g_m C_{frac} (C_a - \Gamma)}{A_{mmax}} \left(1 - \frac{A_m}{A_{mmax}}\right) \quad (S19)$$

$$\frac{\partial A_m}{\partial g_m} = C_{frac} (C_a - \Gamma) \left(1 - \frac{A_m}{A_{mmax}}\right) \quad (S20)$$

$$\frac{\partial A_m}{\partial \Gamma} = -g_m C_{frac} \left(1 - \frac{A_m}{A_{mmax}} \right) \quad (\text{S21})$$

$$\frac{dA_m}{dC_i} = g_m \left(1 - \frac{A_m}{A_{mmax}} \right) \quad (\text{S22})$$

$$\frac{dC_i}{d\Gamma} = 1 - C_{frac} \quad (\text{S23})$$

$$\frac{dC_i}{dC_{frac}} = C_a - \Gamma \quad (\text{S24})$$

$$\frac{\partial C_{frac}}{\partial f_{min}} = \frac{VPD}{D_0} \quad (\text{S25})$$

$$\frac{\partial C_{frac}}{\partial D_0} = (f_0 - f_{min}) \frac{VPD}{D_0^2} \quad (\text{S26})$$

$$\frac{\partial D_0}{\partial f_{min}} = -\frac{1}{a_d} \quad (\text{S27})$$

$$\frac{\partial f_{min}}{\partial g_m} = \frac{g_{minw}}{1.6 \cdot g_m} \frac{1}{\sqrt{f_{min0}^2 + \frac{4 \cdot g_{minw}}{1.6} g_m}} - \frac{f_{min}}{g_m} \quad (\text{S28})$$

$$\frac{\partial f_{min}}{\partial f_{min0}} = -\frac{f_{min}}{2 \cdot g_m f_{min} + f_{min0}} \quad (\text{S29})$$

$$\frac{\partial f_{min0}}{\partial g_m} = -\frac{1}{9} \quad (\text{S30})$$

S1.4 The tendency equation of A_g^*

$$\frac{dA_g^*}{dt} = \frac{\partial A_g^*}{\partial PAR} \frac{dPAR}{dt} + \frac{\partial A_g^*}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial A_g^*}{\partial T} \right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial A_g^*}{\partial VPD} \right)_T \frac{dVPD}{dt} ; \quad (\text{S31})$$

with

S1.4.1 Dependency on PAR

$$\frac{\partial A_g^*}{\partial PAR} = \alpha \left(1 - \frac{A_g^*}{A_m + R_{dark}} \right) \quad (S32)$$

S1.4.2 Dependency on C_a

$$\frac{\partial A_g^*}{\partial C_a} = \left(\frac{\partial A_g^*}{\partial R_{dark}} \frac{\partial R_{dark}}{\partial A_m} + \frac{\partial A_g^*}{\partial A_m} \right) \frac{\partial A_m}{\partial C_a} + \frac{\partial A_g^*}{\partial \alpha} \frac{\partial \alpha}{\partial C_a} \quad (S33)$$

To calculate the above expression some additional terms are needed:

$$\frac{\partial A_g^*}{\partial R_{dark}} = \frac{A_g^*}{A_m + R_{dark}} - \frac{\alpha PAR}{A_m + R_{dark}} \left(1 - \frac{A_g^*}{A_m + R_{dark}} \right) \quad (S34)$$

$$\frac{\partial R_{dark}}{\partial A_m} = \frac{1}{9} \quad (S35)$$

$$\frac{\partial A_g^*}{\partial A_m} = \frac{\partial A_g^*}{\partial R_{dark}} \quad (S36)$$

$$\frac{\partial A_g^*}{\partial \alpha} = PAR \left(1 - \frac{A_g^*}{A_m + R_{dark}} \right) \quad (S37)$$

$$\frac{\partial \alpha}{\partial C_a} = \frac{3 \cdot \alpha_0 \Gamma}{(C_a + 2\Gamma)^2} \quad (S38)$$

S1.4.3 Dependency on VPD at constant T

$$\left(\frac{\partial A_g^*}{\partial VPD} \right)_T = \left(\frac{\partial A_g^*}{\partial R_{dark}} \frac{\partial R_{dark}}{\partial A_m} + \frac{\partial A_g^*}{\partial A_m} \right) \left(\frac{\partial A_m}{\partial VPD} \right)_T \quad (S39)$$

S1.4.4 Dependency on T at constant VPD

$$\left(\frac{\partial A_g^*}{\partial T}\right)_{VPD} = \left(\frac{\partial A_g^*}{\partial R_{dark}} \frac{\partial R_{dark}}{\partial A_m} + \frac{\partial A_g^*}{\partial A_m}\right) \left(\frac{\partial A_m}{\partial T}\right)_{VPD} + \frac{\partial A_g^*}{\partial \alpha} \frac{\partial \alpha}{\partial T} \frac{d\Gamma}{dT} \quad (S40)$$

$$\frac{\partial \alpha}{\partial \Gamma} = -\frac{3 \cdot \alpha_0 C_a}{(C_a + 2\Gamma)^2} \quad (S41)$$

S1.5 The tendency equation of A_g

$$\frac{dA_g}{dt} = \frac{\partial A_g}{\partial PAR} \frac{dPAR}{dt} + \frac{\partial A_g}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial A_g}{\partial T}\right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial A_g}{\partial VPD}\right)_T \frac{dVPD}{dt} + \frac{\partial A_g}{\partial w_2} \frac{dw_2}{dt} \quad (S42)$$

As mentioned previously, the gross primary productivity (A_g) is calculated from that under unstressed water situations (A_g^*) and a soil water stress function ($\beta(w_2)$), $A_g = A_g^* \cdot \beta(w_2)$. Similarly the tendency equation of A_g can be computed from that of A_g^* and an additional term:

$$\frac{dA_g}{dt} = \beta \frac{dA_g^*}{dt} + A_g^* \frac{d\beta(w_2)}{dw_2} \frac{dw_2}{dt} \quad (S43)$$

S1.5.1 Dependency on PAR

$$\frac{\partial A_g}{\partial PAR} = \frac{\partial A_g^*}{\partial PAR} \cdot \beta \quad (S44)$$

S1.5.2 Dependency on C_a

$$\frac{\partial A_g}{\partial C_a} = \frac{\partial A_g^*}{\partial C_a} \cdot \beta \quad (S45)$$

S1.5.3 Dependency on VPD at constant T

$$\left(\frac{\partial A_g}{\partial VPD}\right)_T = \left(\frac{\partial A_g^*}{\partial VPD}\right)_T \cdot \beta \quad (S46)$$

S1.5.4 Dependency on T at constant VPD

$$\left(\frac{\partial A_g}{\partial T}\right)_{VPD} = \left(\frac{\partial A_g^*}{\partial T}\right)_{VPD} \cdot \beta \quad (S47)$$

S1.5.5 Dependency on w_2

$$\frac{\partial A_g}{\partial w_2} = A_g^* \frac{d\beta(w_2)}{dw_2} \quad (S48)$$

A_g^* is given by the model and as a consequence, the only term we analytically solve in this section is $\frac{d\beta(w_2)}{dw_2}$.

The functional form of the water-stress function β implemented in CLASS model is the one presented by Combe et al. (2016). The following equations govern the functional form and were proposed in the cited manuscript (see equations (13) and (14) of the manuscript).

$$SMI = \frac{w_2 - w_{wp}}{w_{fc} - w_{wp}} \quad (S49)$$

$$\beta = \frac{1 - e^{-P(C_\beta)SMI}}{1 - e^{-P(C_\beta)}} \quad (S50)$$

$$P(C_\beta) = \begin{cases} 6.4 \cdot C_\beta & \text{if } 0 \% \leq C_\beta < 25 \% , \\ 7.6 \cdot C_\beta - 0.3 & \text{if } 25 \% \leq C_\beta < 50 \% , \\ 2^{3.66 \cdot C_\beta + 0.34} - 1 & \text{if } 50 \% \leq C_\beta \leq 100 \% . \end{cases} \quad (S51)$$

Taking into account that functional form, the analytical derivative of β with respect to w_2 is:

$$\frac{d\beta}{dw_2} = \frac{1}{w_{fc} - w_{wp}} \frac{P(C_\beta)e^{-P(C_\beta)SMI}}{1 - e^{-P(C_\beta)}} \quad (S52)$$

S1.6 The tendency equation of A_n

A_n is the difference between the gross primary productivity and the dark respiration.

$$A_n = A_g - R_{dark} \quad (S53)$$

The budget tendency equation of A_n is:

$$\frac{dA_n}{dt} = \frac{\partial A_n}{\partial PAR} \frac{dPAR}{dt} + \frac{\partial A_n}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial A_n}{\partial T}\right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial A_n}{\partial VPD}\right)_T \frac{dVPD}{dt} + \frac{\partial A_n}{\partial w_2} \frac{dw_2}{dt} \quad (S54)$$

which can be related to that of A_g

$$\frac{dA_n}{dt} = \frac{dA_g}{dt} - \frac{dR_{dark}}{dA_m} \frac{dA_m}{dt} \quad (\text{S55})$$

S1.7 The budget tendency equation of g_s and g_{sc}

The stomatal conductance to carbon dioxide g_{sc} is calculated through the following equation:

$$g_{sc} = g_{min,c} + \frac{a_1 A_g}{(C_a - \Gamma) \left(1 - \frac{VPD}{D_*}\right)} \quad (\text{S56})$$

The total temporal derivatives of g_s and g_{sc} are related, eq. (S57). Therefore, we only need to calculate the budget tendency equation for one of the two.

$$\frac{dg_s}{dt} = \mu \cdot \frac{dg_{sc}}{dt} \quad (\text{S57})$$

where μ is the ratio of the molecular diffusivities between water vapor and carbon dioxide and is approximately 1.6.

The tendency equation for g_{sc} is:

$$\frac{dg_{sc}}{dt} = \frac{\partial g_{sc}}{\partial PAR} \frac{dPAR}{dt} + \frac{\partial g_{sc}}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial g_{sc}}{\partial T}\right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial g_{sc}}{\partial VPD}\right)_T \frac{dVPD}{dt} + \frac{\partial g_{sc}}{\partial w_2} \frac{dw_2}{dt} \quad (\text{S58})$$

S1.7.1 Dependency on PAR

$$\frac{\partial g_{sc}}{\partial PAR} = \frac{\partial g_{sc}}{\partial A_g} \frac{\partial A_g}{\partial PAR} \quad (\text{S59})$$

$$\frac{\partial g_{sc}}{\partial A_g} = \frac{a_1}{(C_a - \Gamma) \left(1 - \frac{VPD}{D_*}\right)} \quad (\text{S60})$$

S1.7.2 Dependency on C_a

$$\frac{\partial g_{sc}}{\partial C_a} = \left(\frac{\partial g_{sc}}{\partial C_a}\right)_{A_g} + \frac{\partial g_{sc}}{\partial A_g} \frac{\partial A_g}{\partial C_a} \quad (\text{S61})$$

$$\left(\frac{\partial g_{sc}}{\partial C_a}\right)_{A_g} = -\frac{g_{sc} - g_{minc}}{C_a - \Gamma} \quad (\text{S62})$$

$$\frac{\partial g_{sc}}{\partial A_g} = \frac{g_{sc} - g_{minc}}{A_g} \quad (\text{S63})$$

S1.7.3 Dependency on VPD at constant T

$$\left(\frac{\partial g_{sc}}{\partial VPD}\right)_T = \left(\frac{\partial g_{sc}}{\partial VPD}\right)_{A_g, T} + \frac{\partial g_{sc}}{\partial A_g} \left(\frac{\partial A_g}{\partial VPD}\right)_T \quad (\text{S64})$$

$$\left(\frac{\partial g_{sc}}{\partial VPD}\right)_{A_g, T} = -\frac{g_{sc} - g_{minc}}{D_* + VPD} \quad (\text{S65})$$

S1.7.4 Dependency on T at constant VPD

$$\left(\frac{\partial g_{sc}}{\partial T}\right)_{VPD} = \left(\frac{\partial g_{sc}}{\partial \Gamma}\right)_{A_g} \frac{d\Gamma}{dT} + \frac{\partial g_{sc}}{\partial A_g} \left(\frac{\partial A_g}{\partial T}\right)_{VPD} \quad (\text{S66})$$

$$\left(\frac{\partial g_{sc}}{\partial \Gamma}\right)_{A_g, T} = \frac{g_{sc} - g_{minc}}{C_a - \Gamma} \quad (\text{S67})$$

S1.8 Tendency equation for TR_{leaf}

In this research, we have estimated TR_{leaf} as:

$$TR_{leaf} = g_s \rho \frac{0.622}{P_s} VPD \quad (\text{S68})$$

where ρ is the air density and P_s the surface pressure taken as 101300 Pa. The tendency equation of TR_{leaf} has the following form

$$\frac{dTR_{leaf}}{dt} = \frac{\partial TR_{leaf}}{\partial PAR} \frac{dPAR}{dt} + \frac{\partial TR_{leaf}}{\partial C_a} \frac{dC_a}{dt} + \left(\frac{\partial TR_{leaf}}{\partial T}\right)_{VPD} \frac{dT}{dt} + \left(\frac{\partial TR_{leaf}}{\partial VPD}\right)_T \frac{dVPD}{dt} + \frac{\partial TR_{leaf}}{\partial w_2} \frac{dw_2}{dt} \quad (\text{S69})$$

S1.8.1 Dependency on PAR

$$\frac{\partial TR_{leaf}}{\partial PAR} = \frac{dTR_{leaf}}{dg_s} \frac{dg_s}{dPAR} \quad (S70)$$

$$\frac{dTR_{leaf}}{dg_s} = \rho \frac{0.622}{P_s} VPD \quad (S71)$$

S1.8.2 Dependency on C_a

$$\frac{\partial TR_{leaf}}{\partial C_a} = \frac{dTR_{leaf}}{dg_s} \frac{\partial g_s}{\partial C_a} \quad (S72)$$

S1.8.3 Dependency on VPD at constant T

$$\left(\frac{\partial TR_{leaf}}{\partial VPD} \right)_T = \frac{dTR_{leaf}}{dg_s} \left(\frac{\partial g_s}{\partial VPD} \right)_T + g_s \rho \frac{0.622}{P_s} \quad (S73)$$

S1.8.4 Dependency on T at constant VPD

$$\left(\frac{\partial TR_{leaf}}{\partial T} \right)_{VPD} = \frac{dTR_{leaf}}{dg_s} \left(\frac{\partial g_s}{\partial T} \right)_{VPD} \quad (S74)$$

S1.8.5 Dependency on w_2

$$\frac{\partial TR_{leaf}}{\partial w_2} = \frac{dTR_{leaf}}{dg_s} \frac{\partial g_s}{\partial w_2} \quad (S75)$$

S2 Observed direct and diffuse components of shortwave radiation

Fig. S1 and Fig. S2 show the radiation components for the studied day and for a cloudy day occurred during LIAISE Field Campaign.

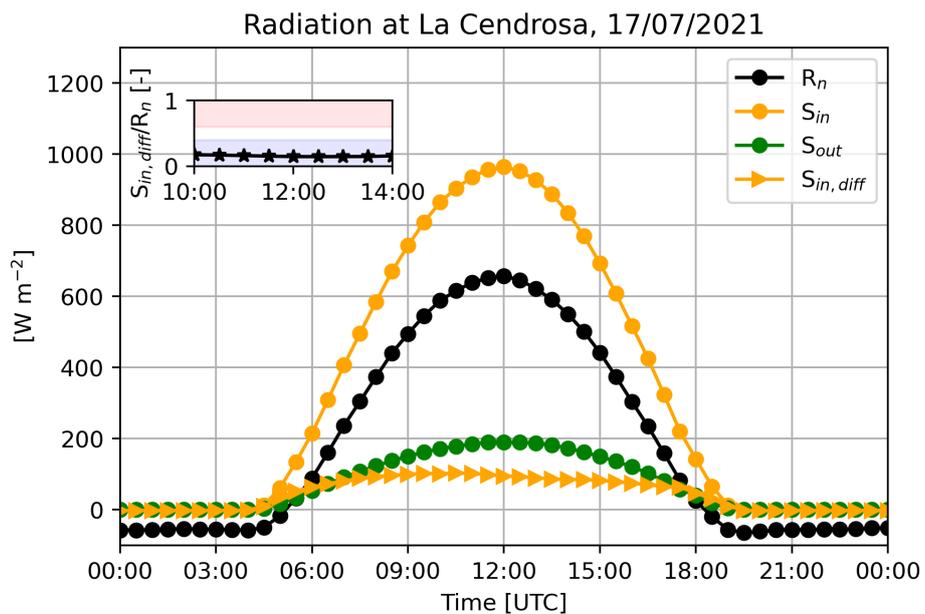


Figure S1. Radiation components at La Cendrosa during the studied day. The inset figure depicts the ratio of diffuse radiation ($S_{in,diff}$) to net radiation (R_n). The blue shaded area depicts a low diffusive regime whereas the red shaded area depicts a high diffusive regime according to the classification used by Niyogi et al. (2004).

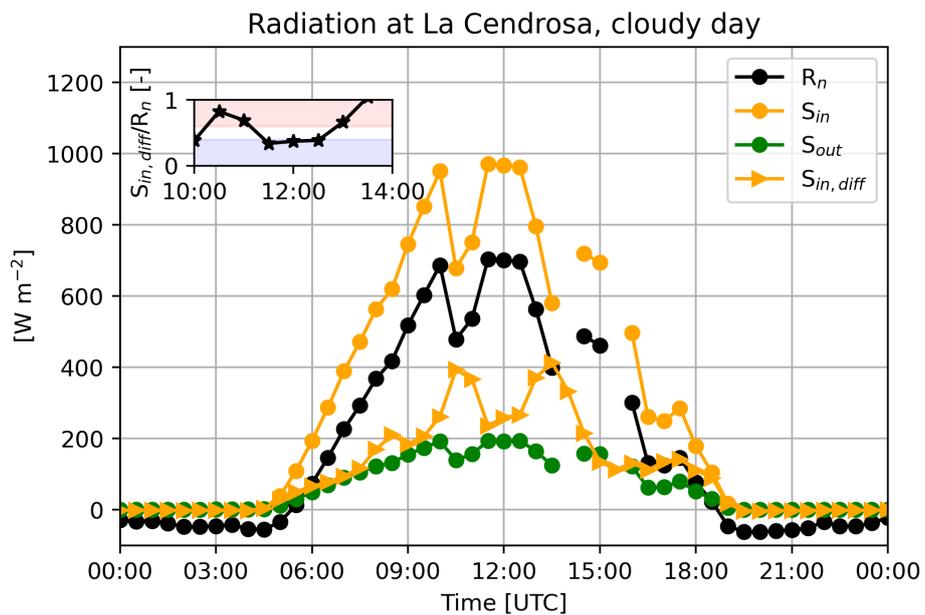


Figure S2. Same as Fig. S1 but for a cloudy day occurred during the LIAISE field campaign.

S3 Additional numerical experiment with modelled C_a similar to observed C_a

To explore the implications of the mismatch between modelled and observed C_a , we carried out a new numerical experiment called IMP-CO2. In IMP-CO2, we forced C_a at 3 m to be similar to the C_a measured by the eddy-covariance system at La Cendrosa (Fig. S3). In that way, C_a was lower for IMP-CO2 than for CONTROL throughout the day with the largest differences occurring in the morning. IMP-CO2 resulted in larger stomatal conductance values (approximately 5 % more than Control averaged over the numerical experiment time), slightly lower leaf net CO_2 assimilation rate (approximately -2%) and slightly larger leaf transpiration (approximately 2%). The diurnal shape of the fluxes and the tendencies remained similar between IMP-CO2 and Control. Focusing on comparing the tendency terms of IMP-CO2 (Fig. S4) and Control (Fig. 6 in the manuscript), all the terms remained similar except for the C_a terms. The C_a terms of the tendencies of IMP-CO2 had the same magnitude than the C_a terms of Control. The main difference of the C_a terms was that they peaked earlier for IMP-CO2 than for CONTROL. That means that the leaf gas exchange variables were affected earlier by the CO_2 temporal changes which is logical since the large drop in CO_2 occurs before in IMP-CO2 than in Control. Despite these differences, IMP-CO2 results led to the same conclusions of the study. For instance, like in Control, in IMP-CO2 the CO_2 diurnal variability contributes the least to the diurnal dynamics of $g_{s,w}$, A_n and TR_{leaf} .

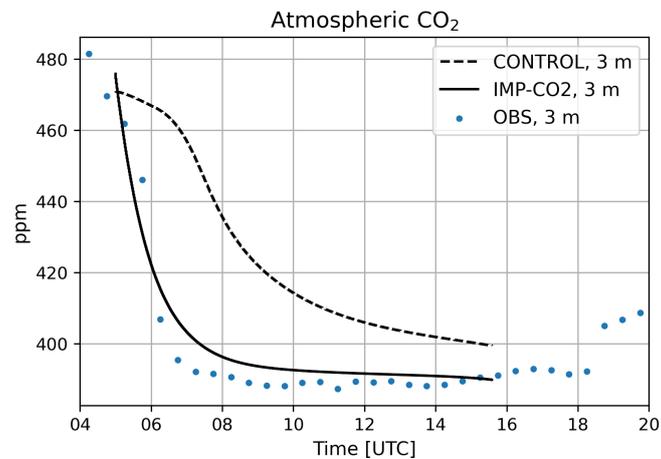


Figure S3. Diurnal time series of C_a for the studied day. Blue dots depict observations at La Cendrosa measured with an Eddy covariance system at 3 meter height whereas the black lines show the model results for Control (dashed line) and IMP-CO2 (solid line) experiments.

S4 Comparing observed and modelled leaf gas exchange

To compliment the comparison between the modelled and the observed leaf gas exchange, we show the modelled leaf variables against the observations and post-processed observations (Fig. S5). Additionally, we provide the slope and intercept of a linear regression fitted through the model results and observations.

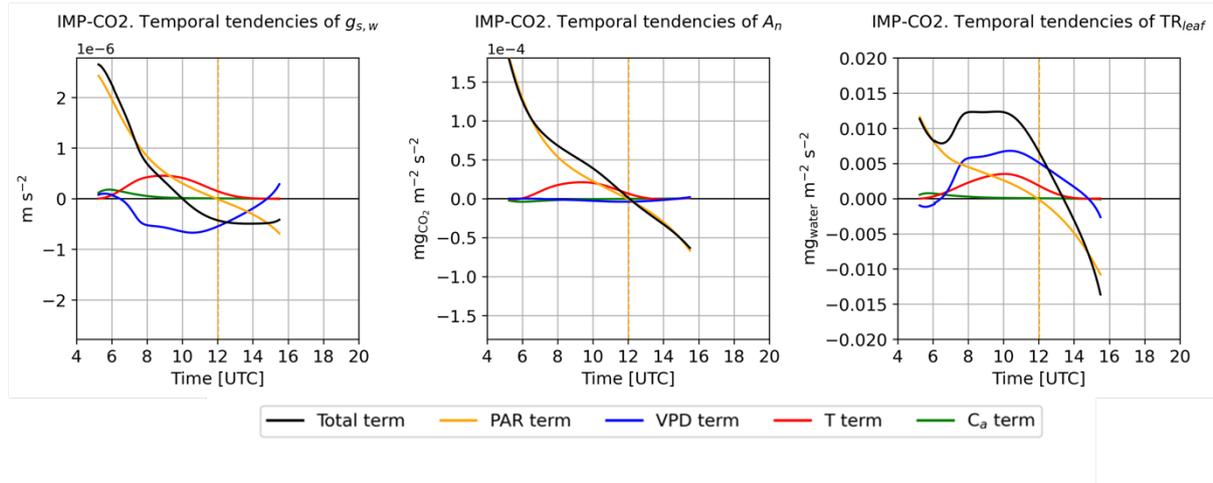


Figure S4. Temporal evolution of the tendencies of: (6a) $g_{s,w}$, (6b) A_n and (6c) TR_{leaf} for IMP-CO2 numerical experiment. Black lines depict the total tendency terms, grey dashed lines depict the sum of the partial terms and the other solid coloured lines depict the partial tendency terms due to temporal changes of PAR (orange lines), VPD (blue lines), T (red lines) and C_a (green lines). The vertical dashed orange lines depict solar noon.

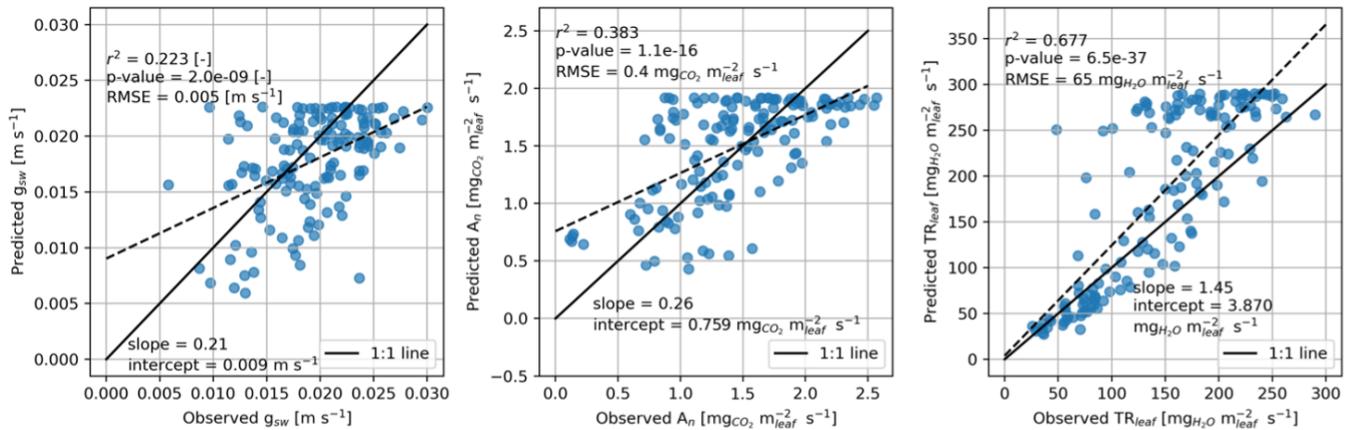


Figure S5. Modelled leaf gas exchange variables against observations and post-processed observations of $g_{s,w}$, A_n and TR_{leaf} . The solid black lines depict the line with slope = 1 and intercept = 0, where model and observations are equal. The dashed black lines depict the linear regression fitted through the data. Intercepts, slopes, root mean squared errors (RMSE), r^2 and p-values are provided inside the figures.

References

- Combe, M., de Arellano, J. V.-G., Ouwensloot, H. G., and Peters, W.: Plant water-stress parameterization determines the strength of land-atmosphere coupling, *Agricultural and forest meteorology*, 217, 61–73, 2016.
- Niyogi, D., Chang, H.-I., Saxena, V., Holt, T., Alapaty, K., Booker, F., Chen, F., Davis, K. J., Holben, B., Matsui, T., et al.: Direct observations of the effects of aerosol loading on net ecosystem CO₂ exchanges over different landscapes, *Geophysical Research Letters*, 31, 2004.
- Vilà-Guerau de Arellano, J., Van Heerwaarden, C., Van Stratum, B., and Van Den Dries, K.: Atmospheric boundary layer: Integrating air chemistry and land interactions, 2015.