Consistent responses of vegetation gas exchange to elevated atmospheric CO₂ emerge from heuristic and optimization models

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Abstract. Elevated atmospheric CO₂ concentration is expected to increase leaf CO₂ assimilation rates, thus promoting plant growth and increasing leaf area. It also decreases stomatal conductance, allowing water savings that have been hypothesized to drive large-scale greening, in particular in arid and semiarid climates. However, the increase in leaf area could reduce the ameliorating effect of elevated CO₂ concentration on soil water depletion. The net effect of elevated CO₂ on leaf- and canopy-level gas exchange thus remains unclear. To address this question, a heuristic model based on the Partitioning of Equilibrium Transpiration and Assimilation (PETA) hypothesis and a model based on stomatal optimization theory are used and their outcomes compared. Predicted relative changes in leaf- and canopy-level gas exchange rates are used as a metric of responses to changes in atmospheric CO₂ concentration. Both models predict reductions of leaf-level transpiration rate due to decreased stomatal conductance under elevated CO₂, but negligible (PETA) or no (optimization) changes in canopy-level transpiration due to the compensatory effect of increased leaf area. Leaf- and canopy-level CO₂ assimilation are predicted to increase, with an amplification of the CO₂ fertilization effect at the canopy-level due to the enhanced leaf area. The expected increase in vapor pressure deficit (VPD) under warmer conditions is predicted to decrease the sensitivity of gas exchange to atmospheric CO₂ concentration in both models except at growth temperatures lower than the photosynthetic thermal optimum. The consistent predictions by different models that canopy-level transpiration varies little under elevated CO₂ due to combined stomatal conductance reduction and leaf area increase highlights the coordination of physiological and morphological characteristics in vegetation to maximize resource use (here water) under altered atmospheric conditions.

1   Introduction

Elevated atmospheric CO_2 causes stomatal closure and reduces leaf-level transpiration while increasing net CO_2 assimilation (Medlyn et al., 2001). These leaf-level observations led to the hypothesis that whole plant-, stand-, or catchment-scale

35   transpiration would also be reduced as a consequence of increasing atmospheric CO_2 concentrations. Results from Earth system models (Fowler et al., 2019; Mankin et al., 2019; Betts et al., 2007; Swann et al., 2016) seem to support this hypothesis. Nevertheless, Earth system models do not always include all the indirect effects of elevated CO_2 on plants (De Kauwe et al., 2021) and empirical evidence of decreased transpiration based on runoff measurements is limited (Ukkola et al., 2016). Elevated CO_2 also stimulates plant growth and thus increases leaf area (Pan et al., 2022; Norby et al., 1999).

40   Higher growth is also in part stimulated indirectly via reduced transpiration rate and hence less frequent water stress. Leaf area is expected to increase the most in water-limited ecosystems (Donohue et al., 2013) and in open canopies (Bader et al., 2013; Duursma et al., 2016), but it increased also in mesic forests (McCarthy et al., 2006; Norby et al., 1999), as well as in crops and herbaceous natural vegetation (Pritchard et al., 1999). This increase in the canopy-level evaporating surface area could counterbalance the reduction in transpiration caused by stomatal closure at the leaf level, but it is not clear if and under

45   which conditions these two effects balance out.

There is both empirical and theoretical evidence of this balancing effect. In water-limited ecosystems, where total evapotranspiration is already at its upper limit, leaf-level water savings under elevated atmospheric CO_2 tend to be compensated for by increased leaf area (Donohue et al., 2013; Schymanski et al., 2015). However, also transpiration in mesic forests can be insensitive to atmospheric CO_2 (Tor-ngern et al., 2015; Schäfer et al., 2002). More generally, canopy

50   transpiration rates are not affected or even increase under elevated atmospheric CO_2 when the canopy is relatively open (leaf area index, LAI<5 m^2 m^{-2}, Donohue et al. (2017)). At the catchment scale, evapotranspiration also has not varied significantly with increasing CO_2 concentrations, as indicated by minor variations in runoff attributed to trends in atmospheric CO_2 (Knauer et al., 2017; Yang et al., 2021). Therefore, the net effect of increasing atmospheric CO_2 concentration on canopy transpiration appears lower than the effect at the leaf level.

55   In line with these empirical results, a detailed process-based model predicted that the direct effect of elevated CO_2 on stomatal conductance is likely to be compensated for by indirect effects mediated by higher evaporative demand by the larger leaf area, especially in dry and semi-arid regions (Fatichi et al., 2016, 2021). In particular, elevated CO_2 did not affect evapotranspiration at dry sites, and caused a small decline (-4 to -7%) at wet or intermediately wet sites where further increases in leaf area would not significantly improve light capture (Fatichi et al., 2016). Similarly, an optimality-based

60   model showed that reduced stomatal conductance in response to elevated CO_2 was offset by increasing leaf area mainly in water-limited environments with low canopy coverage, whereas such a compensatory effect did not emerge in energy-limited environments (Schymanski et al., 2015). When considering plant acclimation using the same model, transpiration in water-limited ecosystems even increased because of deepening roots and reduced bare soil evaporation due to shading. While empirical and modelling results point to some compensation of leaf-level stomatal downregulation by increased leaf

65 area, at least in water limited systems and in young stands, the question remains as to how the net effect of elevated CO_2 on canopy-level gas exchange varies across ecosystems when CO_2 concentrations change in concert with increasing vapor pressure deficit (VPD, or D) and soil aridity.

Process-based models can help disentangle the effects of these confounded drivers, but simpler, analytical models can provide more immediate insights into this question from a theoretical perspective. Analytical models of plant gas exchange

70 have been premised on different assumptions, ranging from heuristic approaches to those based on eco-evolutionary theory. An example of the first type is the heuristic Partitioning of Equilibrium Transpiration and Assimilation (PETA) model, which describes how leaf area index (LAI), canopy and leaf transpiration, and CO_2 assimilation are expected to vary in response to elevated atmospheric CO_2 concentrations (Donohue et al., 2017, 2013). This model is based on the observation that leaf-level water use efficiency increases linearly with atmospheric CO_2 concentration, and leads to a set of relations

75 between the relative changes in CO_2 assimilation and transpiration rates, and the relative changes in climatic conditions and in leaf area caused by increasing atmospheric CO_2 concentrations. An alternative approach is to consider plant responses to changes in environmental conditions as optimized by natural selection (Harrison et al., 2021). Along these lines, optimal stomatal conductance models were developed on the assumption that net CO_2 assimilation is maximized due to stomatal regulation of gas exchange (Cowan and Farquhar, 1977; Mencuccini et al., 2019). Both approaches are appealing as they

80 provide closed-form solutions for gas exchange rates as a function of environmental conditions and plant characteristics, allowing to disentangle in a transparent way the compound effects of atmospheric CO_2 concentrations and other climatic conditions. However, predictions from these two analytical models have never been compared.

The optimal stomatal conductance models can be more or less sensitive to changes in atmospheric CO_2 depending on how the net CO_2 assimilation rate is represented and how the Lagrange multiplier for the optimization problem (λ, interpreted as

85 marginal water use efficiency) is set (Katul et al., 2010; Medlyn et al., 2011; Buckley and Schymanski, 2014). A key limitation of these optimization approaches is that λ remained unspecified and was thus regarded as a fitting parameter, because changes in soil water availability during dry periods were not considered. This is equivalent to performing an 'instantaneous' optimization without considering the dynamics of soil water or changes in leaf area that can alter leaf-gas exchange, albeit at longer time scales (i.e., time scales much longer than the opening and closure of stomata in response to

90 environmental stimuli). Considering λ as a fitting parameter allows capturing some trends in the data with respect to environmental stimuli such as vapor pressure deficit, temperature, or photosynthetically active radiation, but does not provide insights into stomatal responses to elevated CO_2 from a theoretical perspective. A more theoretically sound approach is formulating the stomatal optimization problem to explicitly consider the dynamic nature of soil water—utilizing water quickly today necessarily reduces its availability tomorrow (Lu et al., in review). With this 'dynamic feedback' approach to

95 stomatal optimization, λ becomes an internal variable to be solved for in the optimization (Manzoni et al., 2013; Mrad et al., 2019). This 'dynamic feedback' approach considers soil water as a limited resource, but it can be further improved by also considering limitations on the transpiration rate caused by reduced water transport from the soil to the leaves. These three variants of the stomatal optimization model have not been compared with regard to combined stomatal and leaf area

responses to atmospheric CO_2 concentrations: i) 'instantaneous' optimization (OPT1); ii) 'dynamic feedback' optimization
100 with no effect of water limitation in dry conditions (OPT2); and iii) 'dynamic feedback' optimization including the effect of
water limitation in dry conditions (OPT3).

In this contribution, we compared the PETA model and the three optimization model variants, providing a set of predictions
in the form of compact analytical equations. These equations, in turn, quantify the sensitivity of gas exchange rates
(especially transpiration) to changing climatic conditions, and thus allow addressing the following questions:

105 1. How do leaf and canopy gas exchange rates respond to atmospheric CO_2 concentrations according to these different
models?

2. How does gas exchange respond to combined changes in CO_2 concentration and atmospheric or soil drought?

2 Theory

Both PETA and optimization models describe leaf and canopy exchanges of water vapor and CO_2. They rest on three key
110 simplifications. First, the entire canopy is subject to the same conditions and well-coupled to the atmosphere; i.e., the 'big
leaf' approximation is used (Sect. 2.1). Second, plants are assumed to have reached an equilibrium at yearly to decadal time
scales; i.e., they have acclimated to the atmospheric conditions by varying their growing season LAI and stomatal
conductance. At the shorter time scale of a dry-down, plants are assumed to maintain static leaf area, while they can still
adjust stomatal conductance in response to variations in soil water. Third, photosynthetic capacity and vapour pressure
115 deficit are considered fixed over the dry-down duration, but allowed to vary at climatic time scales (in this way, they are
treated as simple model parameters instead of dynamic variables).

The models differ in the way stomatal responses are modelled, and in their predicted responses of net CO_2 assimilation rates
(Figure 1; Sect. 2.2 and 2.3). Conversely, to facilitate the model inter-comparison, the same dependence of LAI to
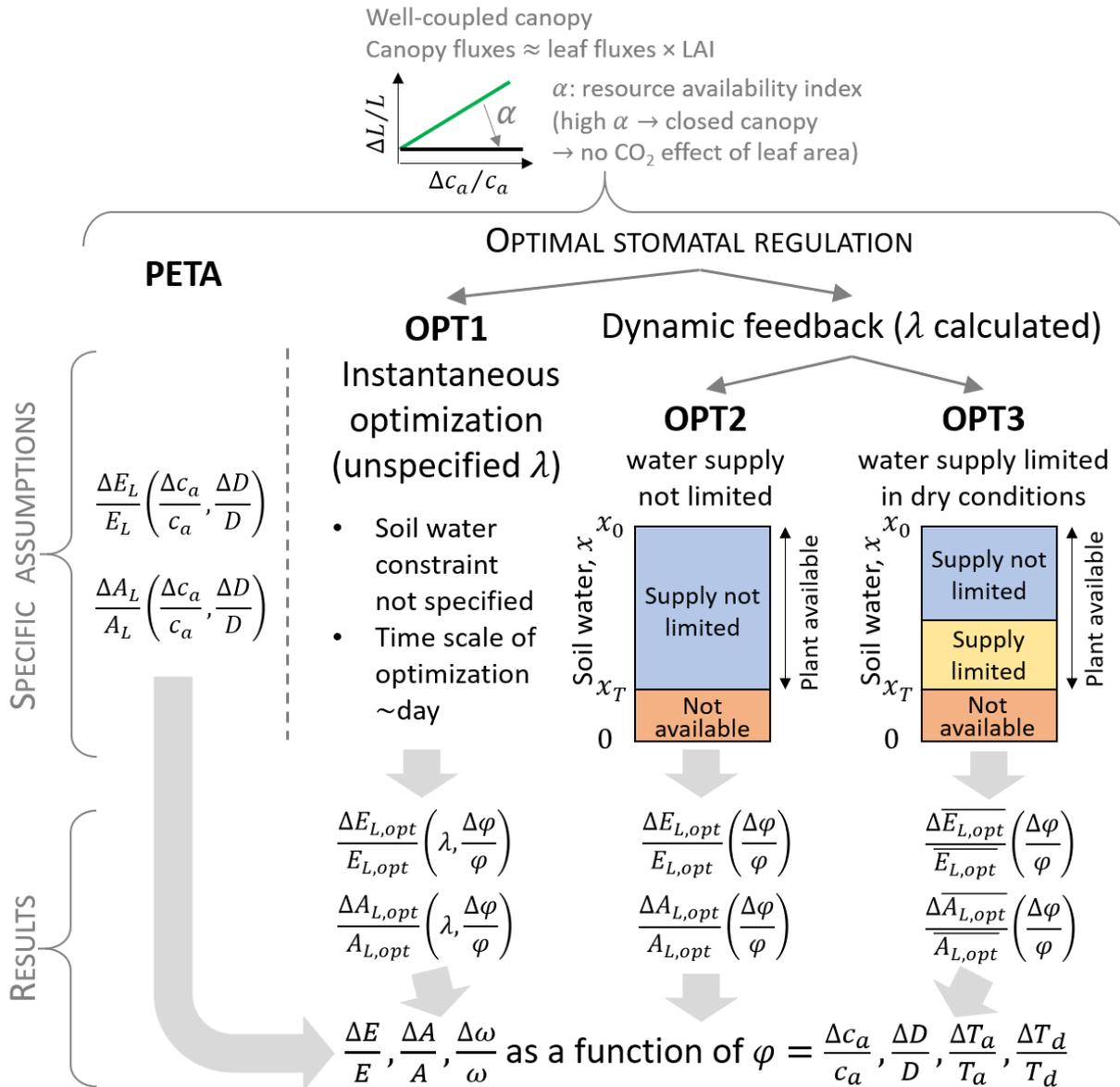atmospheric CO_2 concentration was considered (Sect. 2.1). All symbols are defined in Table 1.

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Table 1. Definitions of symbols (including units), and subscripts and superscripts.

Symbol	Definition	Units
a	Ratio of the diffusivities of H_2O and CO_2 (a=1.6)	-
a_1	Maximum Rubisco carboxylation capacity	μmol CO_2 (m^2 leaf)$^{-1}$ s^{-1}
a_2	Half saturation constant for net CO_2 assimilation	μmol CO_2 (mol air)$^{-1}$
A	Net canopy CO_2 assimilation rate	μmol CO_2 (m^2 ground)$^{-1}$ s^{-1}
A_L	Net leaf CO_2 assimilation rate	μmol CO_2 (m^2 leaf)$^{-1}$ s^{-1}
c_a	CO_2 concentration in the atmosphere	μmol CO_2 (mol air)$^{-1}$
D	Vapor pressure deficit	mol H_2O (mol air)$^{-1}$

E	Canopy transpiration rate	mol H_2O (m^2 ground)$^{-1}$ s^{-1}
E_L	Leaf transpiration rate	mol H_2O (m^2 leaf)$^{-1}$ s^{-1}
g	Stomatal conductance to CO_2	mol air (m^2 leaf)$^{-1}$ s^{-1}
H	Hamiltonian ($H = A - \lambda E$)	µmol CO_2 (m^2 ground)$^{-1}$ s^{-1}
J	Canopy C gain over the period T (objective function)	µmol CO_2 (m^2 ground)$^{-1}$
k	Carboxylation capacity ($= a_1/(a_2 + \chi c_a)$)	mol air (m^2 leaf)$^{-1}$ s^{-1}
L	Leaf area index	m^2 leaf (m^2 ground)$^{-1}$
M_w	Molecular weight of water (M_w=18 g (mol H_2O)$^{-1}$)	g (mol H_2O)$^{-1}$
x	Relative volumetric soil moisture (saturation normalized between wilting point and field capacity so $0 \leq x \leq 1$)	-
x_0	Initial relative volumetric soil moisture	-
x_T	Final relative volumetric soil moisture	-
T_a	Air temperature (assumed equal to canopy temperature)	°C
T_d	Mean length of dry-down	d
T_{day}	Daylight time conversion factor (T_{day} =3600×12 s d^{-1})	s d^{-1}
w_0	Root zone storage capacity	m
α	Resource availability index	-
χ	Ratio of internal to atmospheric CO_2 concentrations	-
$\Delta\varphi$	Finite variation of the generic quantity φ between future and current values	Same units as φ
κ	Proportionality constant in the $E_{SR}(x)$ relation	d^{-1}
λ	Lagrange multiplier	µmol CO_2 (mol H_2O)$^{-1}$
ν	Unit conversion factor ($\nu = T_{day}M_w/\rho_w$)	m^3 s (mol H_2O)$^{-1}$ d^{-1}
ρ_w	Density of liquid water (ρ_w =10^6 g m^{-3})	g m^{-3}
ω	Leaf or canopy water use efficiency ($\omega = A_L/E_L = A/E$)	µmol CO_2 (mol H_2O)$^{-1}$
ω_i	Intrinsic leaf or canopy water use efficiency ($\omega_i = \omega D$)	µmol CO_2 (mol air)$^{-1}$
Subscripts and superscripts		
t	Subscript indicating future conditions at a generic time t	
opt	Subscript indicating optimal stomatal conductance, transpiration rate, assimilation rate, or water use efficiency	
w	Subscript indicating water-limited conditions	
$*$	Superscript indicating the transition point between well-watered and water-limited conditions	
$\bar{\varphi}$	Overbar indicates temporal averaging of the generic quantity φ (Eq. 1)a)i)(25))	

Fig. 1. Conceptual representation of the models used to assess gas exchange responses (transpiration E and net CO_2 assimilation A) to changes in atmospheric CO_2 concentrations c_a, vapor pressure deficit D (either independent of or caused by changes in air temperature T_a), and length of a representative dry-down T_d (during which soil moisture x decreases from the initial value x_0 to x_T). Three variants of the stomatal optimization model are considered: i) 'instantaneous' optimization (OPT1, where the marginal water use efficiency λ is unspecified), ii) 'dynamic feedback' optimization with no effect of water limitation in dry conditions (OPT2), and iii) 'dynamic feedback' optimization including the effect of water limitation in the 'supply limited' regime (OPT3). Leaf-level gas exchange responses (subscript L) are assumed in the heuristic PETA model, whereas they are results of optimal stomatal regulation in the optimization models (subscript opt). Water use efficiency is denoted by $\omega = A/E$. Overbar indicates temporal averaging over the length of a representative dry-down period; φ indicates a generic climatic variable (c_a, D, T_a, or T_d).

2.1   Leaf- and canopy-level transpiration and assimilation rates

135   Leaf-level transpiration rate E_L (mol H_2O (m^2 leaf)$^{-1}$ s^{-1}) is described as an isothermal diffusion-driven process with negligible leaf boundary layer resistance,

$$E_L = agD, \tag{1}$$

where a=1.6 is the ratio between the diffusivities of water vapour and CO_2 (nondimensional), g is the stomatal conductance to CO_2 (mol air (m^2 leaf)$^{-1}$ s^{-1}), and D is the atmospheric vapor pressure deficit expressed as a molar fraction (mol H_2O (mol air)$^{-1}$).

140   The leaf CO_2 uptake rate A_L (μmol CO_2 (m^2 leaf)$^{-1}$ s^{-1}) is similarly described as a carbon flux mediated by stomatal conductance and driven by the difference between atmospheric and leaf internal CO_2 concentrations (respectively c_a and c_i, expressed in μmol CO_2 (mol air)$^{-1}$). Mass conservation further implies that the rate of CO_2 uptake into the leaf must equal the net CO_2 assimilation rate. This is modelled as a function of internal CO_2 concentration as

$$A_L = \frac{a_1 c_i}{a_2 + c_i} \approx \frac{a_1 c_i}{a_2 + \chi c_a} = k c_i, \tag{2}$$

where a_1 and a_2 are temperature-dependent kinetic constants that we assume are independent of c_a as a first approximation,

145   and k is the maximum Rubisco carboxylation capacity (mol air (m^2 leaf)$^{-1}$ s^{-1}). The parameters defining k can be related to light availability and temperature, but we assume here that light is fixed and long-term mean temperature is varied as a model parameter. Following Katul et al. (2010), c_i in the denominator of the second term is approximated as $c_i \approx \chi c_a$, where χ is the long-term ratio of leaf internal to atmospheric CO_2 concentration, so that $k = a_1/(a_2 + \chi c_a)$. This assumption is reasonable when a_2 is commensurate to or larger than c_i (expected for Rubisco limited assimilation) so that variations in c_i

150   can be ignored when summed to a_2. As a result, A_L is a linear function of c_i but with a declining slope at high CO_2 concentration. Equating the rates of CO_2 uptake and assimilation yields a relation between A_L and g (e.g., Hari et al., 1986),

$$A_L = \frac{gk}{g+k} c_a. \tag{3}$$

Therefore, increasing atmospheric CO_2 concentration affects the net CO_2 assimilation rate via two direct effects—it increases the available CO_2 in the leaf (through c_a) and it decreases the marginal return on CO_2 fixation at high CO_2 concentrations (through k). Temperature effects on k are considered using the temperature response functions for Rubisco-limited

155   assimilation of Medlyn et al. (2002). While in the three variants of the optimization model A_L is described by Eq. (3), in the PETA model, the emerging response of A_L to environmental variations are described based on heuristic arguments (Sect. 2.2).

Nonlinear models of assimilation accounting for Rubisco or RuBP regeneration limitation (Farquhar et al., 1980; Vico et al., 2013; Katul et al., 2010) would yield a more complex relation between A_L and g. These complex relations allow exploring

160   short-term responses of gas exchange to variations in temperature, VPD, and photosynthetically active radiation (Medlyn et al., 2011; Katul et al., 2010; Vico et al., 2013). However, we focus on long-term responses to CO_2 concentration—which are

not affected by the specific choice of assimilation kinetics, as demonstrated in the following—and select the simplest model for A_L for the sake of mathematical tractability.

Further assuming that a big-leaf approximation and that the canopy is well-coupled with the atmosphere, the canopy-level
165 transpiration (E) and CO_2 assimilation rates (A), respectively can be estimated as the leaf-level exchange scaled up by the LAI (L)

$$E = E_L L,$$
$$A = A_L L. \qquad (4)$$

Hence, by promoting plant growth and larger LAI, elevated atmospheric CO_2 levels can have an indirect effect on gas exchange mediated by L—in addition to any effect on g or A_L. This linear scaling does not capture nonlinear effects of leaf area on CO_2 uptake, such as decreasing returns of higher LAI due to self-shading and redistribution of nitrogen (dePury and
170 Farquhar, 1997). It also neglects the effect of aerodynamic resistance on canopy gas exchange, which can be large in dense canopies (Juang et al., 2008). However, this simplification does not strongly affect the sensitivity of gas exchange rates to changes in atmospheric CO_2 concentrations (Donohue et al., 2017). Therefore, we expect that the consequences of increasing LAI on gas exchange could be slightly magnified at high LAI values with this model.

Knowing transpiration and CO_2 assimilation rates, the instantaneous water use efficiency (WUE) is given as $\omega = A_L/E_L =$
175 A/E. The intrinsic water use efficiency (i.e., the ratio of net CO_2 assimilation rate and stomatal conductance) is linked to ω as $\omega_i = \omega D$. Due to the linear scaling from leaf- to canopy-levels, both WUE and intrinsic WUE are numerically the same at these two spatial scales.

Neglecting evaporation from the soil surface, the soil water balance during a dry-down with negligible precipitation can be written as (in units of m d^{-1}),

$$w_0 \frac{dx}{dt} = -\nu E, \text{ with initial condition } x(0) = x_0, \qquad (5)$$

180 where x is the plant-available relative soil moisture (i.e., the saturation level rescaled between 0 at the wilting point and 1 at field capacity, as in Porporato et al., 2004), w_0 is the root zone water storage capacity (m), ν is a unit conversion factor to make the units of E in Eq. (4) (mol H_2O (m^2 ground)$^{-1}$ s^{-1}) consistent with typical units used in water balance equations (m d^{-1}): $\nu = T_d M_w/\rho_w$ (m^3 s (mol H_2O)$^{-1}$ d^{-1}), with $T_d = 3600 \times 12$ s d^{-1}: active transpiration period in a day, $M_w = 18$ g (mol H_2O)$^{-1}$: molecular weight of water; $\rho_w = 10^6$ g m^{-3}: density of liquid water. The dry-down starts at a soil moisture x_0 below
185 field capacity, so that the only water loss from the soil in Eq. (5) is E, and lasts for a period T, leaving a residual amount of water x_T at the end.

2.2 Partitioning of Equilibrium Transpiration and Assimilation (PETA) model

The PETA model is formulated as a set of relations between the relative changes of variables related to leaf gas exchange and the relative change in VPD and atmospheric CO_2 concentration. Following Donohue et al. (2013, 2017), the premise of

190 PETA is that leaf-level WUE (ω) scales linearly with c_a (see also Lavergne et al., 2019), and inversely with the square root of VPD. This relation can be explained by the definition of WUE, $\omega = A_L/E_L \sim c_a(1 - \chi)/D$, where χ decreases with increasing D as a result of stomatal closure while photosynthesis continues, leading to $\omega \sim c_a/\sqrt{D}$ (Donohue et al., 2013 and references therein). The relative change in ω depends, by definition, on A_L and E_L, and thus also on c_a and D according to the following relations (Donohue et al., 2017),

$$\frac{\Delta\omega}{\omega} = \frac{1+\frac{\Delta A_L}{A_L}}{1+\frac{\Delta E_L}{E_L}} - 1 \approx \frac{1+\frac{\Delta c_a}{c_a}}{1+\frac{\Delta\sqrt{D}}{\sqrt{D}}} - 1 = \frac{1+\frac{\Delta c_a}{c_a}}{\sqrt{1+\frac{\Delta D}{D}}} - 1. \tag{6}$$

195 In Eq. (6) and in the following, the symbol Δ indicates a finite (not infinitesimal) variation; i.e., the value at a future time t minus the current time value (e.g., $\Delta c_a = c_{a,t} - c_a$). The equality on the far right-hand side of Eq. (6) is obtained by noting that $\Delta\sqrt{D}/\sqrt{D} = \sqrt{1 + \Delta D/D} - 1$, which allows expressing the variation in ω as a function of the relative variation in D rather than the variation of its square root. The PETA model then links heuristically the expected relative changes in L, A_L, and E_L to changes in ω as driven by c_a and D, and to resource availability as quantified by an index α ($0 \leq \alpha \leq 1$). This

200 index represents how far vegetation is from closed-canopy conditions—high α indicates high resource availability and thus a closed canopy that cannot allow additional leaf area increases (see also Sect. 2.5). With these premises, the relative changes are expressed in the PETA model as (Donohue et al., 2017),

$$\frac{\Delta L}{L} = \frac{\Delta\omega}{\omega}(1 - \alpha)^2,$$

$$\frac{\Delta A_L}{A_L} = \frac{\Delta\omega}{\omega}\alpha, \tag{7}$$

$$\frac{\Delta E_L}{E_L} = \left(\frac{1}{1+\frac{\Delta\omega}{\omega}} - 1\right)(1 - \alpha).$$

When changes in D are small, and variations in WUE are mostly driven by c_a, Eq. (6) reduces to $\Delta\omega/\omega \approx \Delta c_a/c_a$, and the variations in L, A_L, and E_L can be recalculated accordingly. The relations between leaf area and gas exchange rates with c_a

205 implicit in Eq. (7) can be explained as follows:

- Under conditions of low resource availability (i.e., $\alpha \to 0$), increases in c_a allow higher leaf area ($\Delta L/L \to \Delta\omega/\omega$), while CO_2 assimilation rate per leaf area remains unchanged ($\Delta A_L/A_L \to 0$), and transpiration rate per leaf area decreases (i.e., c_a causes a structural response compensated for by stomatal closure at the leaf level).

- Under conditions of high resource availability (i.e., $\alpha \to 1$), increases in c_a do not cause changes in leaf area, which is

210 already large thanks to the available resources ($\Delta L/L \to 0$); however, net assimilation rate per leaf area increases ($\Delta A_L/A_L \to \Delta\omega/\omega$), while transpiration rate per leaf area remains unchanged ($\Delta E_L/E_L \to 0$).

The relations between relative changes in canopy transpiration and photosynthesis and changes in c_a are found by multiplying the leaf-level fluxes by L (Eq. (4)), obtaining,

$$\frac{\Delta A}{A} = \left(1 + \frac{\Delta A_L}{A_L}\right)\left(1 + \frac{\Delta L}{L}\right) - 1, \tag{8}$$

$$\frac{\Delta E}{E} = \left(1 + \frac{\Delta E_L}{E_L}\right)\left(1 + \frac{\Delta L}{L}\right) - 1.$$

Equations (7) and (8) thus link gas exchange changes to atmospheric CO_2 concentration changes for a given resource

215   availability α. Finally, we can calculate the variation in intrinsic WUE ($\omega_i = \omega/D$),

$$\frac{\Delta \omega_i}{\omega_i} = \left(1 + \frac{\Delta \omega}{\omega}\right)\left(1 + \frac{\Delta D}{D}\right) - 1. \tag{9}$$

A simplified version of the PETA model is described in Appendix A.

2.3 Optimal stomatal control models

The optimal stomatal conductance model is formulated as an optimal control problem with the objective to maximize net CO_2 assimilation at the canopy level over a set time interval T_d (duration of a representative dry period),

$$J = \int_0^{T_d} A(g(t), x(t), t)dt, \tag{10}$$

220   subject to the constraint that soil moisture x is limited. Maximizing CO_2 assimilation at the leaf level would be mathematically equivalent (see Eq. (4)), since leaf area is not treated as a control variable, but as a time-invariant parameter during a dry-down (as in e.g., Manzoni et al., 2013). However, plants can still alter allocation and thus leaf area in response to atmospheric CO_2 concentration at climatic time scales (years to decades), which are much longer than the daily to weekly scales at which the optimization problem is formulated. In Eq. (10), the leaf net CO_2 assimilation rate is explicitly written as

225   a function of stomatal conductance (g) and soil moisture (x) to emphasize the dependence of both on the control variable (g) and the state variable representing the constraint (x). This optimal control problem can be solved by using the Euler-Lagrange formulation that reduces to maximizing the Hamiltonian (H) with respect to g. That is, defining the Hamiltonian as $H = A + \lambda(-E)$, we obtain,

$$\frac{d}{dt}\left(\frac{\partial H}{\partial \dot{g}}\right) - \frac{\partial H}{\partial g} = 0 \Rightarrow \frac{\partial H}{\partial g} = 0 = \frac{\partial A}{\partial g} - \lambda \frac{\partial E}{\partial g}, \tag{11}$$

where the first term on the left-hand side of Eq. (11) is ignored because H is independent of $\dot{g} = \partial g/\partial t$; λ is the Lagrange

230   multiplier, and in the second term E is the sum of all fluxes of water lost from the soil (in this case, only the transpiration rate), expressed in mol H_2O (m^2 ground)$^{-1}$ s^{-1}. With this choice of units for the water loss term, λ is expressed in µmol CO_2 (mol H_2O)$^{-1}$. Other choices for the units of A and E would not affect the results of the following calculations, except for the numerical value of λ.

Three variants of the optimization model can now be described: i) instantaneous optimization where λ is treated as a fitting

235   parameter (OPT1), ii) dynamic feedback optimization where λ is derived mathematically before obtaining the optimal stomatal conductance, but where transpiration is independent of soil moisture until the available water has been consumed (OPT2), and iii) dynamic feedback optimization where transpiration is reduced as soil dries (OPT3).

2.3.1 OPT1: instantaneous stomatal optimization

If stomatal conductance is allowed to vary through time but independently of soil moisture, the Lagrange multiplier of the
240 optimization is time-invariant. Substituting Eq. (1) and (3) in Eq. (11) and solving for g yields (Hari et al., 1986; Katul et al., 2010; Lloyd and Farquhar, 1994; Palmroth et al., 1999)

$$g_{opt} = k \left(\sqrt{\frac{c_a}{a\lambda D}} - 1 \right), \tag{12}$$

where λ is regarded as an adjustable parameter. Because the effects of soil moisture dynamics on stomatal conductance are neglected, this approach is termed 'instantaneous' optimization. For a set value of λ, Eq. (12) describes the short-term responses of stomatal conductance to c_a, D, and any environmental condition affecting k. However, this equation neglects the
245 fact that soil water is limited, which imposes a constraint on how much water can be transpired in a given time interval.

2.3.2 OPT2: dynamic feedback optimization with transpiration rate independent of soil moisture

A more realistic approach that overcomes the limitation of a freely adjustable λ is determining the value of λ by imposing the constraint that the initial soil moisture x_0 is depleted, leaving only x_T at the end of the time interval T_d. This means that we impose $x(t = T_d) = x_T$ as the soil moisture at the end of the dry-down described by Eq. (5), where transpiration depends
250 on $g_{opt}(\lambda)$ from Eq. (12); i.e., $\int_0^{T_d} vE(t)dt = \int_0^{T_d} vag_{opt}(\lambda)DLdt = w_0(x_0 - x_T)$. With this constraint in place, the only unknown is λ, which is found as (Manzoni et al., 2013),

$$\lambda = c_a aD \left[\frac{w_0(x_0 - x_T)}{kLT_d v} + aD \right]^{-2}. \tag{13}$$

The linear scaling of λ with c_a in Eq. (13) is not externally imposed (as in Katul et al., 2010), but is an emergent property of the optimization with limited water availability. In this sense, λ is not simply an adjustable parameter (as it has been treated previously), but rather a clearly defined property of the coupled soil-plant system, including the ending soil moisture.
255 Substituting Eq. (13) into Eq. (12) and (3), the values of optimal stomatal conductance and optimal leaf-level CO_2 assimilation rate are found as (solid line in Fig. 2a),

$$g_{opt} = \frac{w_0(x_0 - x_T)}{vaDLT_d}, \tag{14}$$

$$A_{L,opt} = c_a \left(\frac{1}{k} + \frac{vaDLT_d}{w_0(x_0 - x_T)} \right)^{-1}. \tag{15}$$

These equations represent the long-term response of leaf gas exchange rates to c_a, D, and any other environmental condition and soil parameter.

Equations (14) and (15) show that optimal stomatal conductance (and thus transpiration rate) and net CO_2 assimilation rate
260 are independent of time or soil moisture but vary with soil water storage capacity, $w_0(x_0 - x_T)$, and other environmental conditions (recall that c_a, D, and k are time invariant during the dry-down, but allowed to vary at longer time scales over

which climatic changes occur). Even without a direct dependence of gas exchange on soil moisture (which is explored in OPT3), this solution accounts for soil moisture dynamics, because faster transpiration reduces soil water storage more rapidly. In this sense, this approach is denoted 'dynamic feedback' optimization.

265 Equation (14) could be also found by simply imposing that the time invariant stomatal conductance adjusts to use all the water in the allotted time (details are shown in Sect. 3.1). Therefore, assuming optimal stomatal control and a limited amount of plant-available water results in a stomatal conductance equation that is independent of the atmospheric CO_2 concentration (no direct control), but that is inversely proportional to LAI. This implies an inverse, indirect control of atmospheric CO_2 concentration on leaf-level stomatal conductance. In contrast, leaf-level net CO_2 assimilation rate increases with atmospheric

270 CO_2 concentration (direct control), even though this effect decreases at high c_a due to the dependence of k on c_a (in Eq. (2)). The canopy-level optimal stomatal conductance and CO_2 assimilation rate are simply obtained from the leaf-level quantities using Eq. (4).
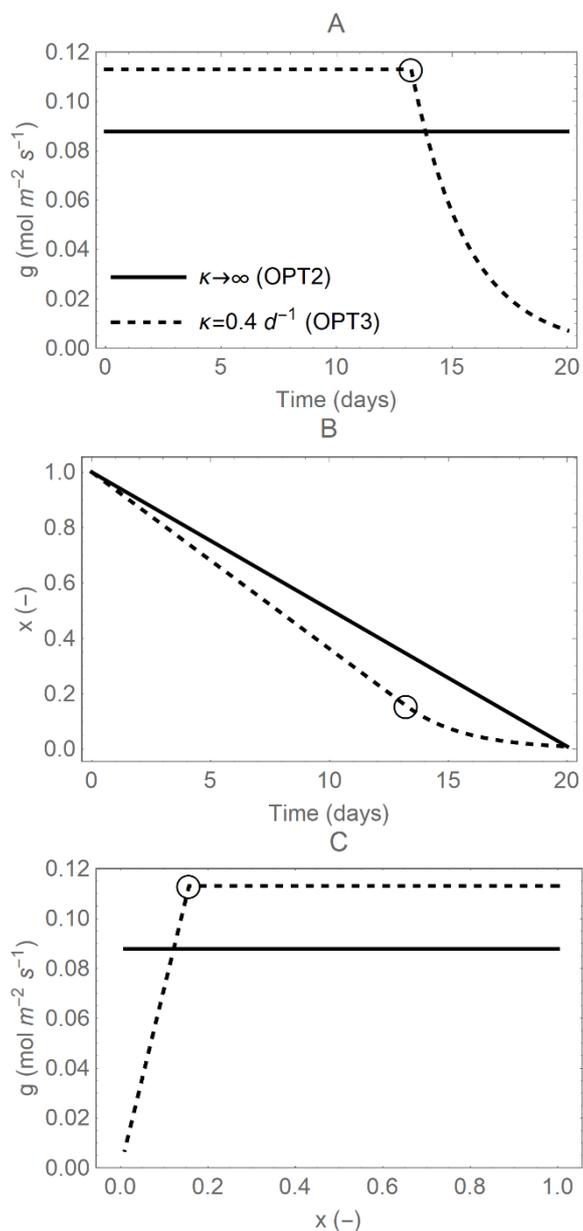
Finally, using the optimal stomatal conductance in Eq. (14), the soil water balance of Eq. (5) can be solved to obtain the time trajectory of soil moisture during the dry-down (solid line in Fig. 2b),

$$x = x_0 - va g_{opt} DLt = x_0 - (x_0 - x_T)\frac{t}{T_d}, \qquad (16)$$

275 where, on the right-hand side, it is clear that the optimal solution leads to a linear decrease in soil moisture from the initial soil moisture x_0 to the final value x_T. When limited soil moisture constrains water flows, optimal stomatal conductance deviates from the time-invariant value of Eq. (14), leading to a nonlinear decrease in x during a dry period, as explained in OPT3.

The equations of OPT2 can be used in two ways. Environmental conditions and soil parameters can be set to the long-term

280 mean values and λ determined accordingly with Eq. (13); the same mean conditions can be used in Eq. (14)-(15) to study the responses of gas exchange to long-term climatic changes. This is the approach we will follow in this contribution. Alternatively, one can calculate λ based on the long-term mean environmental conditions and soil parameters, insert that specific value in Eq. (12), and then study the short-term responses of stomatal conductance to changes in c_a, D, and k for given λ. This solution still accounts for the dynamic feedback mechanism, but allows studying responses to fluctuations

285 around the long-term mean conditions as captured by the value of λ.

Fig. 2. Temporal trajectories of A) plant available soil moisture (x) and B) leaf-level stomatal conductance (g), and C) relations between g and x (with time increasing from right to left), during a single dry period of duration T_d=20 d. Line styles indicate when water supply from the soil is unlimited (OPT2: solid line, infinite κ; Eq. (14) and (16)) or limited in dry conditions (OPT3: dashed line, finite κ; Eq. (18)-(22)). Open circles indicate the transition points to water limited conditions (x^* and g^*_{opt} at time t^*). Parameter values are as in Table 2.

2.3.3   OPT3: dynamic feedback optimization with transpiration rate limited by soil moisture

Different from OPT1 and OPT2, we now consider soil moisture limitations on gas exchange (dashed lines in Fig. 2).
295   Stomatal conductance is reduced as soil moisture decreases during a dry period, because of the combined effect of lowered water pressures along the soil-plant system and reduced conductance to water transport in the soil and plant xylem (Cruiziat et al., 2002; Klein, 2014). As a result, transpiration rate proceeds at a high and stable rate in well-watered conditions, but decreases approximately linearly as soil moisture declines due to stomatal closure and limited water supply from the soil (Sadras and Milroy, 1996). Mathematically, in well-watered conditions, stomatal conductance is calculated with Eq. (12)
300   after finding the Lagrange multiplier specific for model OPT3, denoted by λ^*. This Lagrange must in fact be recalculated because the boundary conditions of the optimization have changed compared with those in OPT2.

The decrease in transpiration during drying is often included in soil-plant-atmosphere models through a piecewise linear function, representing water stress-induced reductions in E (Federer, 1979; Sloan et al., 2021). These observations motivate the inclusion of a further constraint in the optimization, with respect to OPT1 and OPT2, in the form of a soil moisture-
305   limited transpiration rate under dry conditions that effectively constrains the allowable range of stomatal conductance (Manzoni et al., 2013),

$$E_w = \frac{w_0 \kappa}{v} x. \tag{17}$$

Here, the subscript 'w' refers to water-limited conditions, v adjusts the units so that E_w has the same units as E (i.e., mol H_2O (m^2 ground)$^{-1}$ s^{-1}), and κ is a coefficient with units of d^{-1} that captures the effect of limited rate of water supply from the bulk soil to the roots (which can be approximated as the saturated hydraulic conductivity (m d^{-1}) divided by the soil water storage
310   capacity w_0 (m)). This approximation implies that E_w scales linearly with soil moisture, thus neglecting the nonlinear effect of soil moisture on hydraulic conductivity under unsaturated conditions (Mualem, 1986). Therefore, we expect slower reductions in transpiration as soil dries compared to using a nonlinear relation between E_w and x.

Since $E = E_L L = agDL$ (Eq. (1) and (4)) and the water flux through the soil-plant-atmosphere continuum is conserved at the daily (or longer) time scale, we can equate water supply from the soil (E_w) and demand by the canopy (E), and obtain $E_w = agDL$, where g is different from the optimal value due to the limited water supply from the soil. Solving for g yields the
315   $agDL$, where g is different from the optimal value due to the limited water supply from the soil. Solving for g yields the stomatal conductance under water limited conditions (dashed line at low x in Fig. 2c),

$$g_w = \frac{w_0 \kappa}{vaDL} x. \tag{18}$$

This value of stomatal conductance represents a so-called 'boundary' for the optimization problem. Because the transpiration rate is a linear function of soil moisture (Eq. (17)), the time trajectory of x in water-limited conditions is found by solving Eq. (5) as (dashed line at $t > t^*$ in Fig. 2b),

$$x_w(t) = x^* e^{-\kappa(t-t^*)}, \tag{19}$$

320 where t is measured since the beginning of the dry period, and x^* and t^* are respectively the soil moisture and the time at the transition between well-watered and water-limited regimes (open circles in Fig. 2). The stomatal conductance at the transition point is also found by substituting $x = x^*$ in Eq. (18).

Next, we can obtain x^*, t^*, and λ^*. Three equations are set up to match the optimal solution under well-watered conditions and the water-limited solution in dry conditions: i) a continuity condition for stomatal conductance; ii) a continuity condition

325 for soil moisture; and iii) a constraint on the amount of soil water left at the end of the dry-period (set at x_T as in OPT2):

$$\text{i)} \qquad g_{opt}(t^*) = g^*_{opt} = k\left(\sqrt{\frac{c_a}{a\lambda^* D}} - 1\right) = \frac{w_0\kappa}{vaDL}x^*, \qquad (20)$$

$$\text{ii)} \qquad x(t^*) = x^* = x_0 - \frac{vaDL}{w_0}g^*_{opt}t^* \qquad (21)$$

$$\text{iii)} \qquad x_w(T_d) = x_T = x^* e^{-\kappa(T_d - t^*)}. \qquad (22)$$

The system of Eq. (20)-(22) can be solved to obtain the unknowns x^*, t^*, and λ^* (and thus also g_{opt} for the initial phase at $t < t^*$). To this aim, Eq. (20) and (21) are solved as a function of t^*,

$$x^* = \frac{x_0}{1 + \kappa t^*}, \qquad (23)$$

$$g^*_{opt} = \frac{x_0 w_0 \kappa}{vaDL(1 + \kappa t^*)}, \qquad (24)$$

whereas the remaining condition in Eq. (22) can be solved numerically for t^* for a given x^* (open circles in Fig. 2). This solution of the optimization problem based on the continuity equations at the boundary between well-watered and water

330 limited regimes leads to the same result obtained by adding a Lagrange multiplier within the Hamiltonian to account for the constraint of Eq. (18) (Manzoni et al., 2013).

To summarize the solution of the OPT3 model (dashed lines in Fig. 2), optimal stomatal conductance is initially constant and equal to g^*_{opt} (Eq. (24)), until soil moisture becomes limiting at x^*. At this point, stomatal conductance is constrained by water supply from the soil and is given by g_w (Eq. (18)). The more limiting the water supply, the longer the time under water

335 limitation and the higher g^*_{opt} in the initial phase of the dry-down to ensure that all the soil water is used. After calculating stomatal conductance, transpiration and net CO_2 assimilation rates are obtained using Eq. (1) and (3) as before.

Predictions of the OPT3 model must be interpreted as time trajectories, different from the time-invariant gas exchange rates of the other models (OPT1, OPT2, and PETA). Thus, to compare results to those from the other models, the time-averaged gas exchange rates are calculated as,

$$\bar{\varphi} = \frac{\int_0^{T_d} \varphi(t)dt}{T_d}, \qquad (25)$$

340 where the averaging operator is applied to any time-dependent leaf- or canopy-level gas exchange rate $\varphi(t)$ ($\varphi = E_L, A_L, E, A$).

15

2.4 Comparing the results of optimization and PETA models

To compare the results of the optimization models with those of the PETA model, we calculate the relative changes in leaf transpiration and assimilation rates

$$\frac{\Delta E_{L,opt}}{E_{L,opt}} = \frac{E_{L,opt,t}}{E_{L,opt}} - 1,$$

$$\frac{\Delta A_{L,opt}}{A_{L,opt}} = \frac{A_{L,opt,t}}{A_{L,opt}} - 1,$$

(26)

345   where $E_{L,opt}$ and $A_{L,opt}$ are evaluated at baseline (current) environmental conditions, and subscript t indicates conditions at a future time. To make the equations of the PETA and optimization models comparable, the future values of c_a, D, L, and T_d appearing in the equations for the optimal gas exchange rates are expressed as $c_{a,t} = (\Delta c_a / c_a + 1)c_a$, $D_t = (\Delta D / D + 1)D$, $L_t = (\Delta L / L + 1)L$, and $T_{d,t} = (\Delta T_d / T_d + 1)T_d$. Furthermore, LAI changes are consistently included in PETA and optimization models by combining Eq. (6) and (7) to determine $\Delta L / L$. Leaf-level rates in the optimization model variants are

350   scaled up to the canopy-level as in the PETA model (Eq. (8)), thus including the additional indirect effect of atmospheric CO_2 concentration on LAI.

The relative changes for transpiration can be re-written in a compact form at both the leaf and canopy levels for OPT2 and OPT3 (after some algebraic manipulation of Eq. (1), (4), and (14)),

$$\frac{\Delta E_{L,opt}}{E_{L,opt}} = \frac{1}{\left(\frac{\Delta L}{L}+1\right)\left(\frac{\Delta T_d}{T_d}+1\right)} - 1,$$

$$\frac{\Delta E_{opt}}{E_{opt}} = \frac{1}{\frac{\Delta T_d}{T_d}+1} - 1.$$

(27)

While in the PETA model the water use efficiency ω is prescribed (Eq. (6)), in the optimization model ω is obtained as a

355   result of the optimization, $\omega_{opt} = \frac{A_{L,opt}}{E_{L,opt}} = \frac{A_{opt}}{E_{opt}}$. Accordingly, variations in ω induced by changing CO_2 concentration and VPD are calculated as,

$$\frac{\Delta \omega_{opt}}{\omega_{opt}} = \frac{\omega_{opt,t}}{\omega_{opt}} - 1.$$

(28)

Similarly, the variations in intrinsic water use efficiency are found using the definition $\omega_i = \omega D$ as,

$$\frac{\Delta \omega_{i,opt}}{\omega_{i,opt}} = \frac{\omega_{opt,t} D_t}{\omega_{opt} D} - 1.$$

(29)

In scenarios in which VPD does not change in the future (i.e., $D_t = D$), the variations in WUE and intrinsic WUE are the same.

2.5 Model parameters and climate change scenarios

360   We parameterized the models for a generic vegetation type and a baseline climate (Table 2), based on which variations in gas exchanges for a wide range of future climate conditions are evaluated. In both the PETA and optimization models, LAI varies with atmospheric CO_2 concentration and VPD in the same manner (Fig. 1). Growth chamber and FACE experiments

showed that LAI generally increases in open canopies and young stands with increasing atmospheric CO_2 concentration across plant functional types (symbols in Fig. 3). However, the rate of increase varies depending on growth conditions, with

365 the LAI of closed-canopy and older plant communities responding less to increasing CO_2 levels than those of younger communities (Bader et al., 2013; Duursma et al., 2016). We test these effects by varying the resource availability parameter α (Donohue et al., 2017, 2013), which increases from zero when leaf area responds the most to increasing CO_2 concentration (low resource availability that sustains small leaf area and/or young plants) to one when leaf area is unresponsive (high resource availability and/or older plants). The intermediate value α =0.5 is selected for the analyses involving simultaneous

370 changes of atmospheric CO_2 concentration, VPD, and length of the dry period.

In the PETA model, α is the only adjustable parameter, so no further parameter selection is necessary. In the optimization model, we selected parameter values representative of A-c_i curves for C_3 plants (Table 2). Soil parameters determining the water storage capacity w_0 refer to a loam soil and intermediate rooting depth (Table 2.1 in Rodriguez-Iturbe and Porporato, 2004). The baseline values of c_a, D and T_d represent current climatic conditions under a mild temperature regime. The dry-

375 down length of T_d=20 d corresponds to dry spell lengths for which vegetation is adapted; i.e., between the length of the average dry period and that of an actual drought. The baseline L=2 m^2 m^{-2} is reasonable for a relatively open canopy, meeting the assumption of well coupled conditions.

The c_a, T_d, and D are allowed to vary in the ranges expected under future climatic conditions. We explore a range in c_a from 400 to 800 µmol CO_2 (mol air)$^{-1}$ (maximum $\Delta c_a/c_a$ =1), in line with atmospheric CO_2 concentration being expected to

380 approximately double from 2016 to 2100 according to a high-emission scenario (SSP3-7.0, IPCC, 2021).

The VPD is changed by letting relative humidity vary at constant temperature or by letting temperature vary at constant relative humidity. The first scenario allows isolating the effect of VPD on stomatal conductance and transpiration alone. In the second scenario, VPD affects both water and CO_2 exchanges because of direct effects on the former and indirect effects on the latter via photosynthetic capacity (Medlyn et al., 2002), which in turn also affects gas exchange in the optimization

385 models (again via k). To allow a comparison between the two scenarios, VPD is varied in the same range, even though projected variations in VPD are mostly attributed to warming (relative humidity variations are expected to be moderate). Taking the United States as an example, VPD increases are expected to range between ~40 and ~65% by the end of the century, depending on the general circulation model used for the projections, with a median of ~50% (Ficklin and Novick, 2017; Yuan et al., 2019). While this value is probably higher than the global average, we use it as an upper bound for our

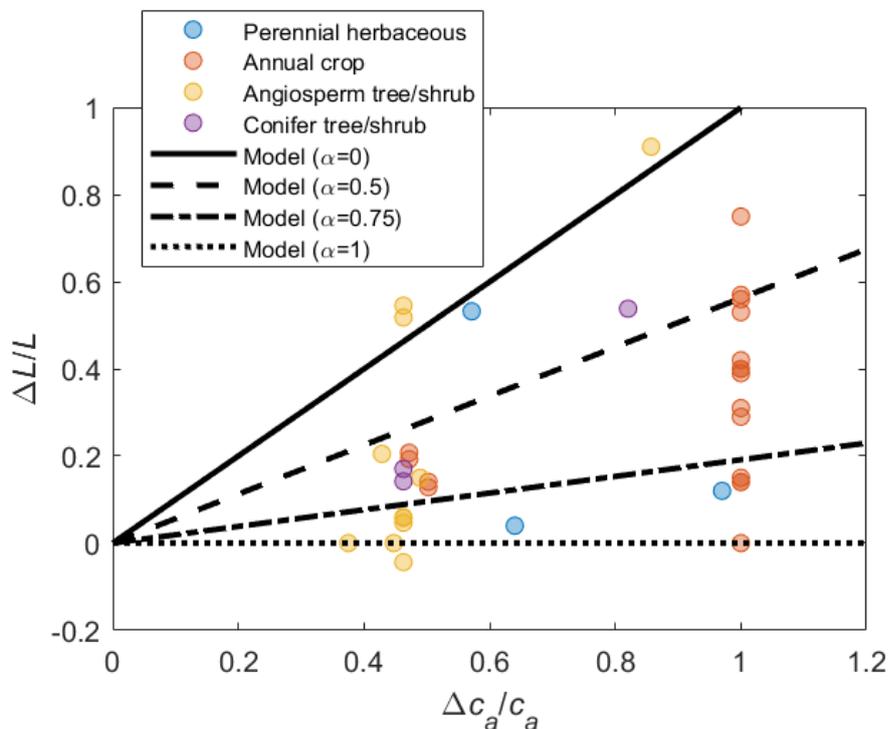390 sensitivity analyses (maximum $\Delta D/D$ =0.5).

Dry period lengths during the growing season have been shifting towards either longer or shorter lengths depending on location, with historical variations up to ~±10% per decade (Breinl et al., 2020). Because of this large variability in historical times, and the large uncertainty in projected dry period durations, we consider T_d variations between ±50% ($\Delta T_d/T_d$ ranges from -0.5 to +0.5).

395

Table 2. Baseline parameter values (relative variations in c_a, D, T_a, and L are calculated with respect to the values reported here).
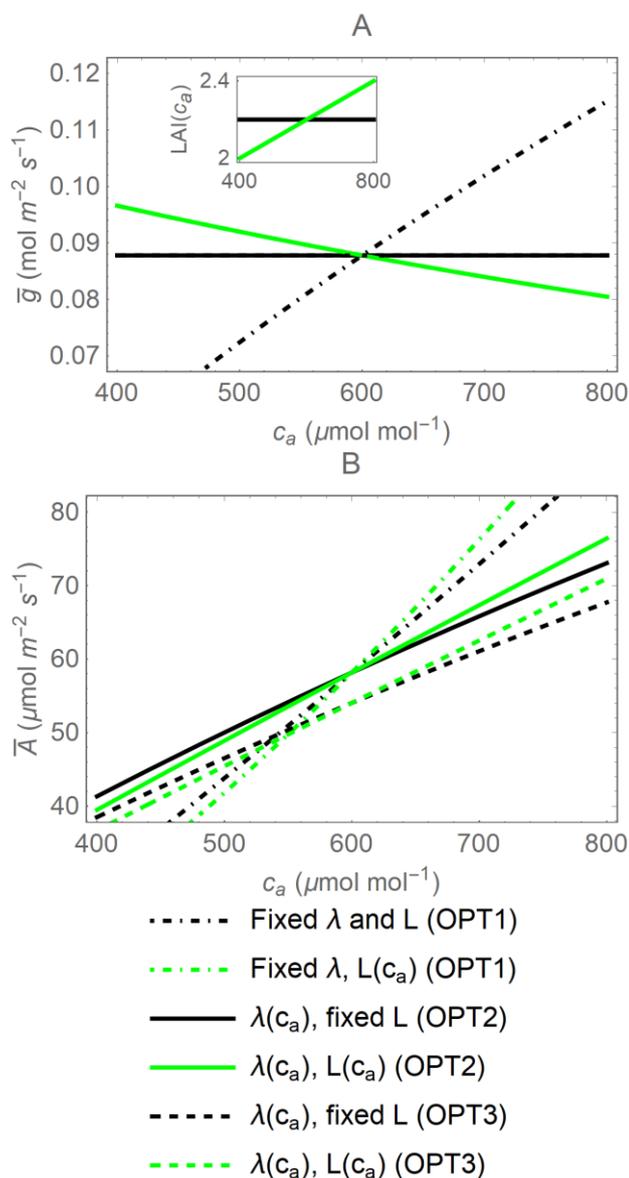
Symbol	Value	Units	Notes and sources
a_1	100	μmol CO_2 m^{-2} s^{-1}	Typical of C3 plants (Campbell and Norman, 1998)
a_2	710	μmol CO_2 (mol air)$^{-1}$	Typical of C3 plants (calculated after Medlyn et al., 2002)
c_a	410	μmol CO_2 (mol air)$^{-1}$	Ambient atmospheric CO_2 concentration in 2013
D	0.015	mol H_2O (mol air)$^{-1}$	Calculated at T_a=20 °C with 35% relative humidity
L	2	m^2 m^{-2}	Chosen value
x_0	1	-	Equivalent to the field capacity
x_T	0.01	-	Equivalent to the wilting point
T_a	20	°C	Chosen value
T_d	20	d	Chosen value
w_0	0.09	m	Product of porosity (0.45 m^3 m^{-3}), rooting depth (0.4 m), and difference in saturation between field capacity and wilting point (0.41 m^3 m^{-3}) for a loam soil (Table 2.1 in Rodriguez-Iturbe and Porporato, 2004)
α	0.5	-	Chosen value (intermediate resource availability)
χ	0.7	-	Typical of C3 plants (Campbell and Norman, 1998)
κ	0.4	d^{-1}	Chosen value

Fig. 3. Relative change in leaf area ($\Delta L/L$) as a function of relative change in atmospheric CO₂ concentration ($\Delta c_a/c_a$), across plant functional types (colours); lines show how the change in leaf area is modelled depending on resource availability α (higher availability implies larger leaf area under ambient conditions and therefore lower sensitivity to changes in c_a, Eq. (7)). The effect of variations in vapor pressure deficit on leaf area are not considered in this figure, so that $\Delta L/L = \Delta c_a/c_a (1-\alpha)^2$. The same variations in L due to c_a (for given α) are prescribed in both PETA and optimization models. Data points represent temporal averages of leaf area changes in response to elevated c_a at plant to stand scales, shown to illustrate the range of observed responses (data and sources are reported in the Supplementary Information).

3 Results

We start by comparing the effects of atmospheric CO₂ concentration on gas exchange in the three variants of the optimization model (Fig. 4). Next, the CO₂ effects are assessed in both the PETA and optimization models at fixed VPD, but with different values of α (Fig. 5). Finally, the combined effects of CO₂ concentration and VPD (Fig. 6-7), and CO₂ concentration and dry period length (Fig. 8) are assessed in both models.

Fig. 4. Effect of relative plant available soil moisture (x) and atmospheric CO_2 concentration (c_a) on gas exchange as predicted by three variants of the stomatal optimization model (identified by different line dashing). A) Mean stomatal conductance ($\bar{g}$) and B) mean canopy net CO_2 assimilation rate ($\bar{A}$) during a dry period of T_d=20 d as a function of c_a, when transpiration is either independent of soil moisture (OPT2, solid lines) or water limited in dry conditions (OPT3, dashed lines), and with leaf area index (L) acclimating with increasing c_a or fixed (green *vs.* black lines, respectively). The dot-dashed lines refer to the 'instantaneous' optimal stomatal conductance (OPT1), obtained from Eq. (12) with λ set to a constant value (Eq. (13) at c_a=600 μmol CO_2 (mol air)[-1]). The inset in panel A shows how L varies with c_a; to make visual comparisons easier, L variations are centred around a common value for all model variants at c_a=600 μmol CO_2 (mol air)[-1]. Parameter values are as in Table 2.

3.1 Optimal stomatal conductance under varying atmospheric CO_2 concentration

425 Different variants of the optimization model predict contrasting responses to atmospheric CO_2 concentration. The instantaneous optimization OPT1 (in which λ is a fixed parameter, Eq. (12)) predicts increasing stomatal conductance with increasing c_a regardless of LAI (black and green dot dashed lines in Fig. 4A are overlapping). Conversely, with increasing c_a, the dynamic feedback optimization OPT2 (Eq. (14)) predicts that stomatal conductance is stable when LAI is fixed or decreasing when LAI acclimates with c_a (solid black and green lines in Fig. 4A, respectively).

430 When soil moisture limitations are imposed in dry conditions and for given c_a, the optimal stomatal conductance obtained from OPT3 (Eq. (24)) is higher in well-watered conditions, but decreases at low soil moisture (dashed line in Fig. 2C) compared with the model variant without soil moisture limitations (solid line in Fig. 2C). However, the mean stomatal conductance ($\bar{g}$) over the dry-down is independent of whether soil water becomes limiting or not, because $\bar{g}$ is only a function of the total available soil water (solid and dashed lines in Fig. 4A are overlapping). This result can be derived

435 analytically by formulating the constraint that soil water is limited as a relation between total transpiration amount and available soil water,

$$\int_0^{T_d} \nu E(t)dt = w_0(x_0 - x_T). \tag{30}$$

Using the definition of temporal average, Eq. (30) can be written as,

$$\bar{E} = \frac{\int_0^{T_d} E(t)dt}{T_d} = \frac{w_0(x_0 - x_T)}{\nu T_d}. \tag{31}$$

Recalling Eq. (1) and (4), the mean stomatal conductance can thus be expressed as,

$$\bar{g} = \frac{\int_0^{T_d} g(t)dt}{T_d} = \frac{\int_0^{T_d} E(t)dt}{aDLT_d} = \frac{w_0(x_0 - x_T)}{\nu aDLT_d}, \tag{32}$$

which is independent of the specific trajectory $g(t)$, but it is indirectly dependent on c_a via L.

440 Canopy-level net CO_2 assimilation rate increases with c_a in all optimization models due to the direct CO_2 fertilization effect, but more so when leaf area acclimates (green *vs.* black lines in Fig. 4B), and at a higher rate with the instantaneous optimization approach (dot-dashed *vs.* solid lines in Fig. 4B). In contrast to the mean stomatal conductance, the mean net CO_2 assimilation rate depends on whether soil water is limiting or not (i.e., the specific $g(t)$ matters), due to the nonlinear nature of the $A_L(g)$ relation (Eq. (3)). In particular, diminishing returns at high g cause $\bar{A}$ to be lower when optimal g from

445 OPT3 is higher under well-watered conditions and lower in dry conditions, compared to OPT2 with time-invariant g. This explains why the dashed lines in Fig. 4B are lower than the corresponding solid lines.
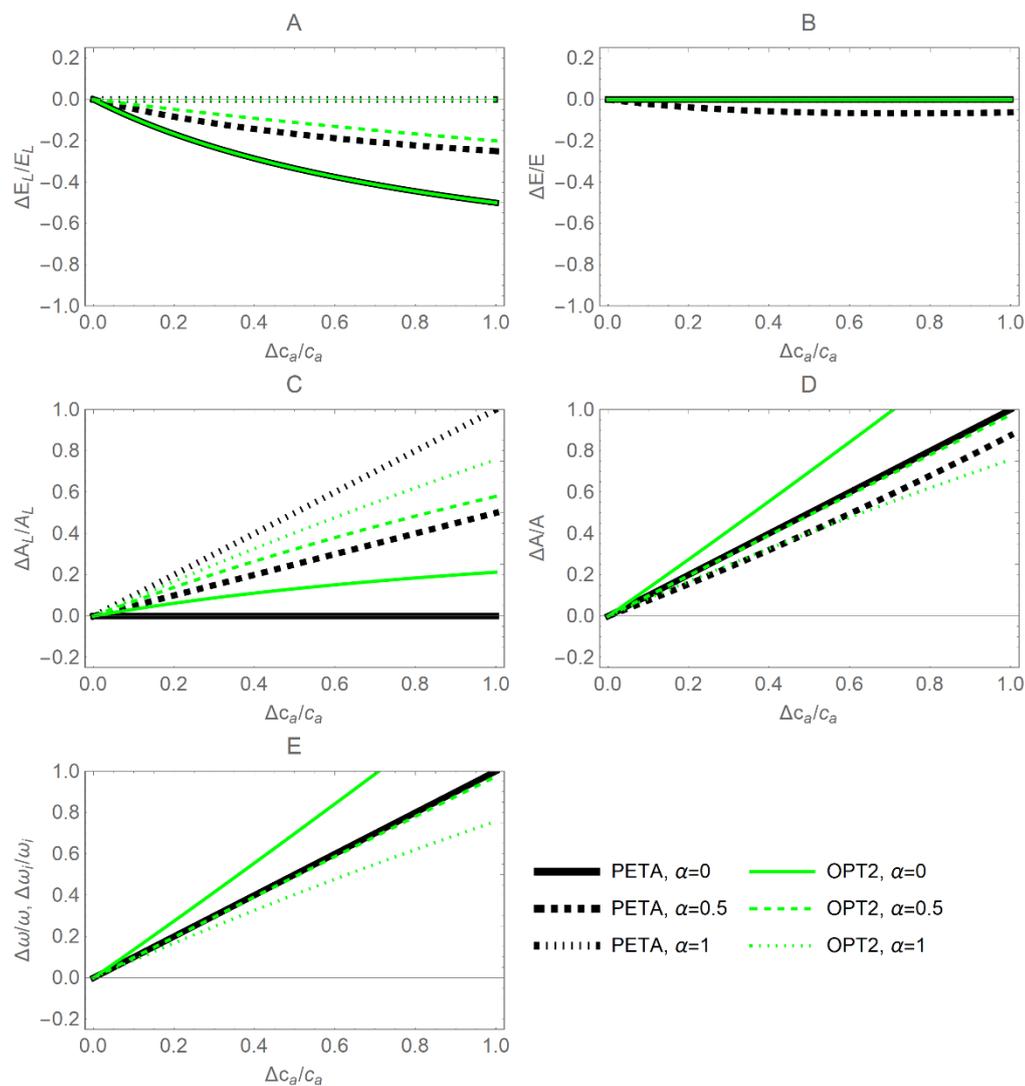
Based on the results in Fig. 4, we can say that inclusion of the dynamic feedback (OPT2 and OPT3) in the stomatal optimization model produces plausible responses to elevated c_a. The dynamic feedback variants are also more suitable given our focus on long-term responses of gas exchange. Conversely, the stomatal response to elevated CO_2 of OPT1 is not

450 realistic because λ is independent of c_a (Fig. 4A; see also Sect. 4.4). This unrealistic response was among the first hints that λ must increase with c_a irrespective of whether Rubisco or RuBP regeneration limits net assimilation (Katul et al., 2009, 2010).

In contrast, the responses of both dynamic feedback approaches are plausible. In the following comparisons with the PETA model, we consider only the optimization model without any water limitation effect (OPT2), because the relative changes in gas exchange rates are essentially the same when including water limitation (OPT3; results not shown), despite variations in the absolute rates.

Fig. 5. Relative changes in leaf-level (A, C) and canopy-level (B, D) gas exchange rates as a function of relative change in atmospheric CO_2 concentration c_a, as predicted by the PETA model (black lines) and the optimal stomatal control model OPT2 (green lines): A) leaf-level transpiration rate (E_L), B) canopy-level transpiration rate (E), C) leaf-level assimilation rate (A_L), D) canopy-level assimilation rate (A), and E) water use efficiency (ω, equivalent to intrinsic WUE at constant VPD). Changes in c_a have both direct and indirect effects on the CO_2 and water vapor exchange rates; the indirect effects are mediated by changes in leaf area that also depend on resource availability, indicated by α (Fig. 3): lower values of α refer to low-resource, open-canopy conditions with largest leaf area stimulation by elevated c_a; for $\alpha = 1$ leaf area is constant. Vapor pressure deficit and dry period length are assumed to be constant and equal to the baseline values (Table 2).
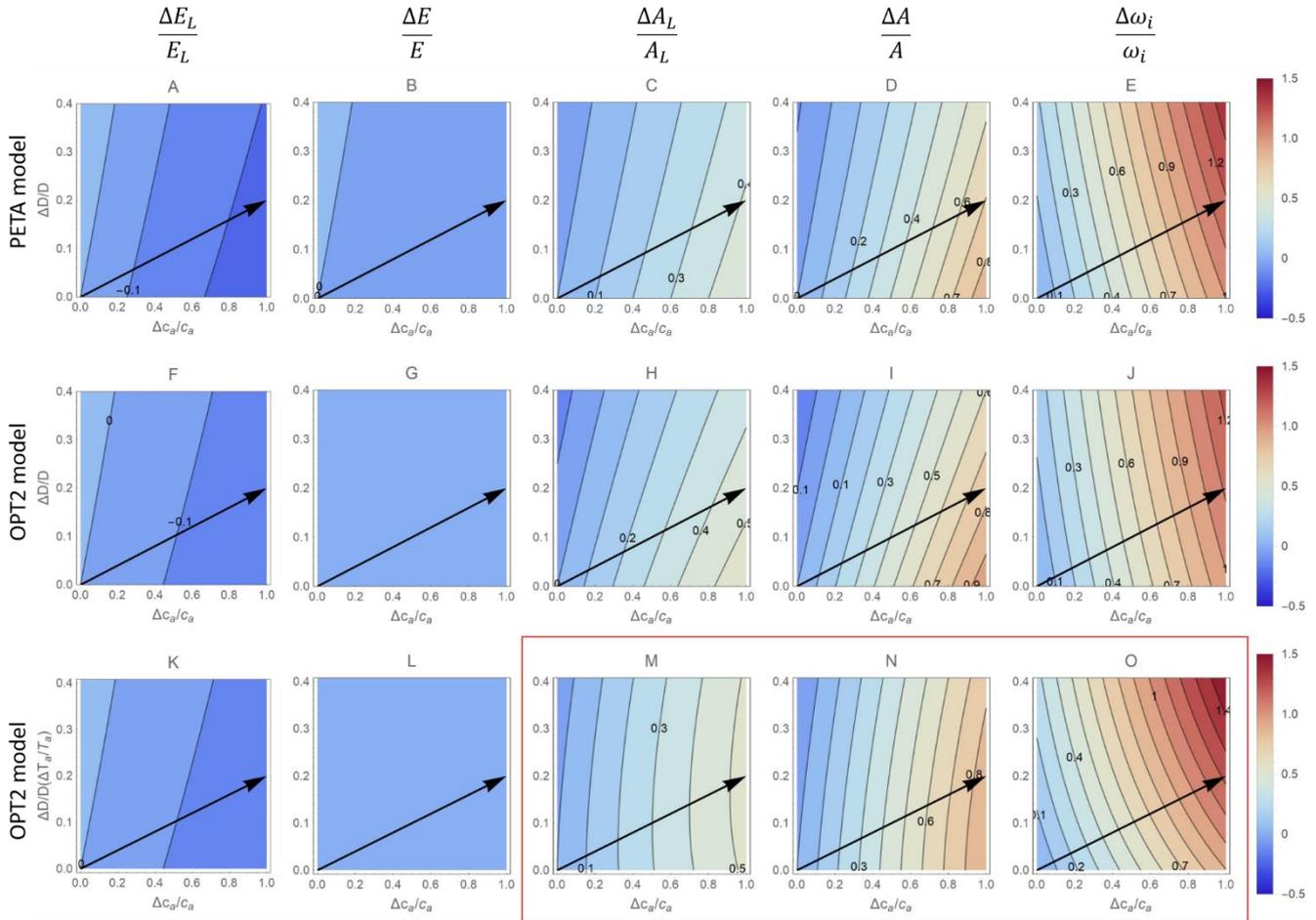
3.2 Gas exchange responses to changes in atmospheric CO₂ concentration

The relative variations of gas exchange rates and water use efficiency predicted under elevated CO_2 concentration by the PETA and optimization model with dynamic feedback but no water limitation (OPT2) are broadly consistent (Fig. 5). As CO_2 concentration increases, both models predict decreasing leaf-level (Fig. 5A, except for $\alpha = 0$), but stable canopy-level

470 transpiration rates (Fig. 5B), and increasing net CO_2 assimilation rates at both leaf- and canopy-levels (Fig. 5C, D). As a consequence, water use efficiency (ω) increases with increasing atmospheric CO_2 concentration (Fig. 5E). In the PETA model, the increase in ω is linear with CO_2 by definition (Eq. (6)), while it is slightly nonlinear for the optimization models. The predicted sensitivity of the gas exchange responses varies between PETA and optimization models, depending on the resource availability index α, in particular for the rate of net CO_2 assimilation (Fig. 5C, D). At the leaf level, higher α

475 reduces the sensitivity of transpiration rates, but increases that of net CO_2 assimilation rates to increasing CO_2 concentration in both models (compare dotted and solid lines in Fig. 5A, C). In contrast, at the canopy-level, higher α reduces the net CO_2 assimilation responses to CO_2 concentration in the PETA model (Fig. 5D). Conversely, by construction, canopy-level transpiration is independent of atmospheric CO_2 according to the optimality model (Eq. (31); all green lines overlap on the $\Delta E/E = 0$ axis in Fig. 5B). By definition, ω is independent of resource availability in the PETA model (all black lines are

480 overlapping in Fig. 5E), whereas lower resource availability (higher α) decreases the sensitivity of ω to increasing CO_2 concentration according to the optimality model. In the following analyses, we prescribed an intermediate value of resource availability ($\alpha = 0.5$).

3.3 Gas exchange responses to combined changes in atmospheric CO₂ concentration, VPD, and dry period length

The gas exchange patterns driven by c_a and D are largely consistent between the PETA and optimization models. In both

485 PETA and OPT2 models, at a given c_a, higher VPD slightly increases leaf-level transpiration (Fig. 6A, F, K), but has no effect on canopy-level transpiration (Fig. 6B, G, L) because leaf area decreases with increasing VPD (Eq. (6) and (7)). The decrease in stomatal conductance at higher VPD in both models, and irrespective of how the change in VPD is imposed, causes the intrinsic water use efficiency to increase (Fig. 6E, J, O). Moreover, higher VPD decreases leaf- and canopy-level net CO_2 assimilation when VPD is varied at fixed temperature (Fig. 6C-D for PETA, H-I for OPT2). However, when VPD is

490 varied because of changing temperature (which also affects photosynthetic parameters; bottom row), leaf-level net CO_2 assimilation increases and then decreases slightly as VPD is increased, whereas canopy-level net CO_2 assimilation decreases (Fig. 6M, N). Following a hypothetical trajectory of a simultaneous increase in c_a and D (arrows in Fig. 6), increasing VPD reduces the improvement in canopy-level net CO_2 assimilation rate caused by elevated CO_2 alone, while leading to a greater improvement in intrinsic water use efficiency.
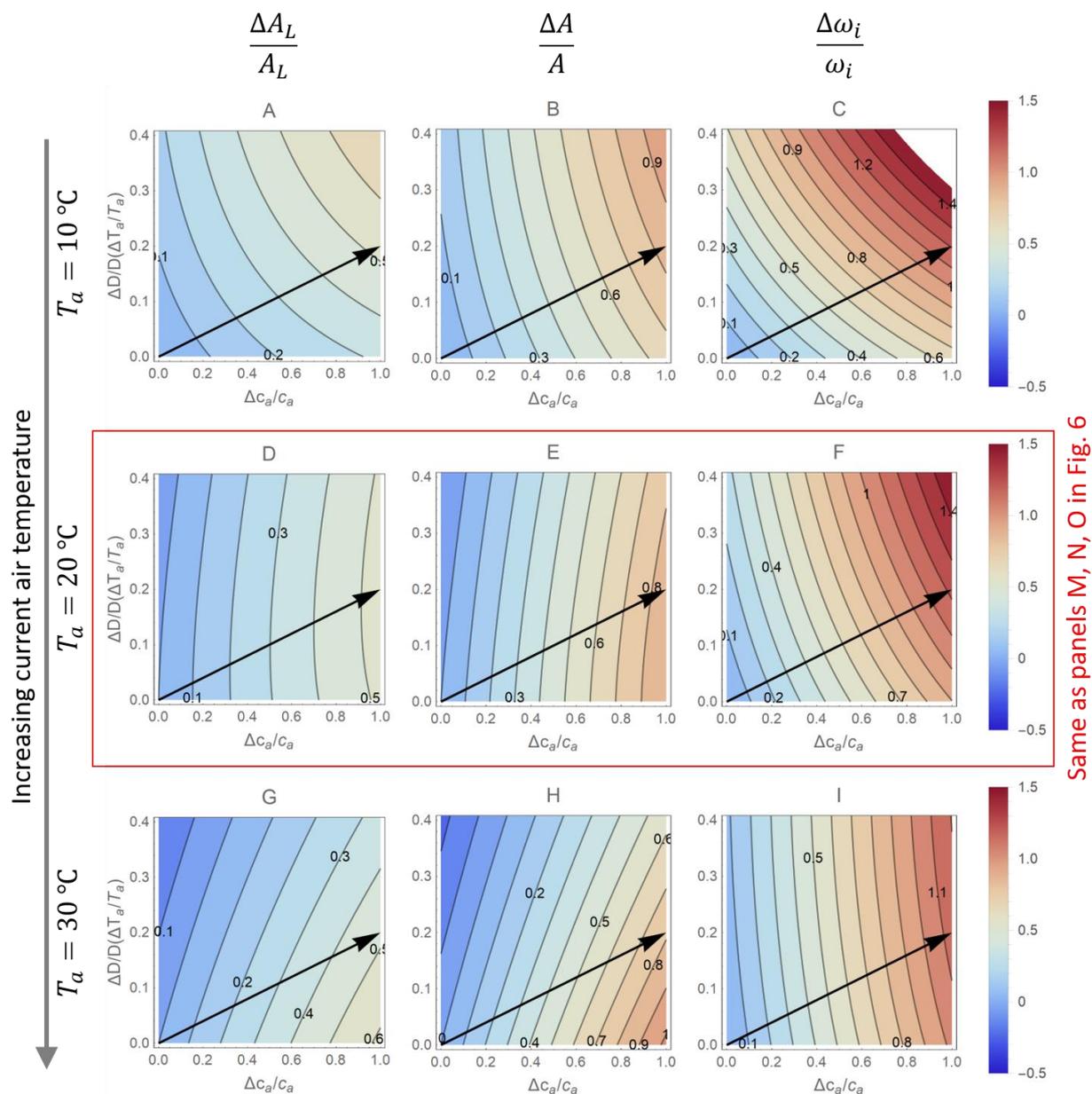
Same as panels D, E, F in Fig. 7

Fig. 6. Contour plots of relative changes in leaf-level (A, C, F, H, K, M) and canopy-level (B, D, G, I, L, N) gas exchange rates as a function of relative changes in atmospheric CO_2 concentration c_a (x-axis), and vapor pressure deficit D (y-axis), as predicted by the PETA model (top panels) and the optimal stomatal control model OPT2 (centre and bottom panels): A, F, K) leaf-level transpiration rate (E_L); B, G, L) canopy-level transpiration rate (E); C, H, M) leaf-level assimilation rate (A_L); D, I, N) canopy-level assimilation rate (A); and E, J, O) intrinsic water use efficiency (ω_i). In F-J, D is varied by letting the relative humidity change at constant temperature T_a (i.e., the assimilation rate constants do not co-vary with D); in K-O, D is varied by letting the T_a change at constant relative humidity, set at 50% (i.e., the assimilation rate constants co-vary with D due to the effect of T_a). Leaf area index varies with c_a and D according to Eq. (7) with α =0.5. Black arrows indicate hypothetical temporal trends in D and c_a assuming a CO_2 concentration doubling and associated T_a increase. The dry period length is assumed to be constant and equal to the baseline value (Table 2).
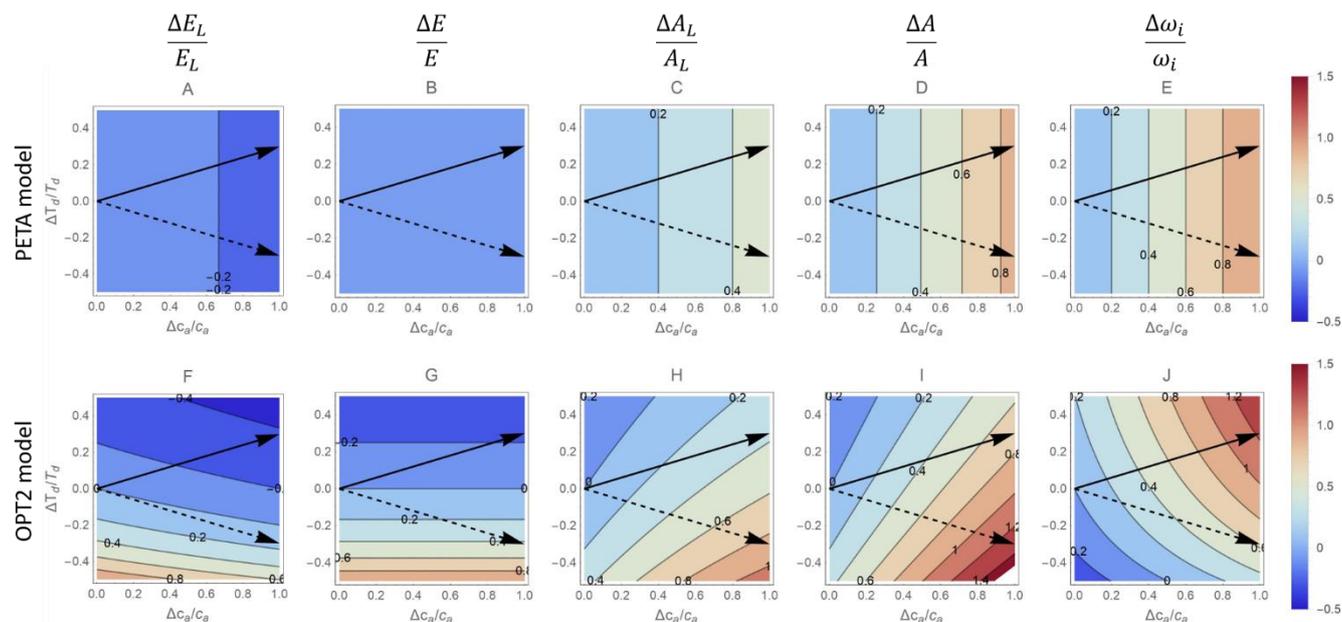
While the responses of transpiration rates are the same regardless of how the variation in VPD is produced, patterns in net
510 CO_2 assimilation rates (and thus also water use efficiency) depend strongly on the selected baseline temperature in the
optimization model, as shown in Fig. 7. Here, only results from the optimization model (OPT2) are shown, because the
PETA model cannot attribute variations in VPD to relative humidity or temperature. At low baseline T_a (top row), higher
VPD enhances net CO_2 assimilation because changes in VPD are driven by temperature increases that also promote
photosynthesis (i.e., the baseline T_a is below the photosynthetic thermal optimum). In contrast, at high baseline T_a (bottom
515 row), temperature increases driving VPD inhibit photosynthesis (i.e., the baseline T_a is above the photosynthetic thermal
optimum). The case shown in the central row (same as in Fig. 6) is intermediate between these two extremes. As a result,
simultaneously increasing VPD and c_a along the arrows in Fig. 7 causes a faster or slower increase in net CO_2 assimilation
than would occur due to changes in c_a alone, depending on whether the baseline temperature is lower or higher than the
thermal optimum, respectively. Accordingly, with increasing baseline T_a, the c_a-driven enhancement of intrinsic water use
520 efficiency also decreases (Fig. 7C, F, I).

Changing the length of the mean dry period leads to contrasting responses of the PETA and optimization models (Fig. 8),
mostly because PETA does not include any effect of soil moisture on the CO_2 responses (i.e., predicted responses are
independent of T_d; see Fig. 8A-E). In the optimization model, for a given c_a, longer dry periods lower all gas exchange rates
(Fig. 8F-I), while increasing the intrinsic water use efficiency (Fig. 8J). Following a hypothetical trajectory of increasing c_a
525 and T_d (solid arrows in Fig. 8F-J), the lengthening of the dry periods—similar to increasing VPD—reduces the positive
effect of elevated CO_2 on net CO_2 assimilation compared to a scenario where only c_a is increased. The opposite pattern
occurs if we assume wetting (shorter T_d) is associated with elevated CO_2 (dashed arrows in Fig. 8F-J).

Fig. 7. Contour plots of relative changes in leaf- (A_L; A, D, G) and canopy-level (A; B, E, H) net CO_2 assimilation rates, as well as intrinsic water use efficiency (ω; C, F, I) as a function of relative changes in atmospheric CO_2 concentration c_a (x-axis), and vapor pressure deficit D (y-axis), as predicted by the optimal stomatal control model OPT2. The baseline temperature used to calculate relative changes is increased from top (T_a=10 °C) to bottom (30 °C), with the central panels corresponding to panels M, N and O in Fig. 6 (T_a=20 °C). Changes in VPD are driven by temperature T_a at constant relative humidity (increasing from top to bottom to keep the same baseline VPD). Other parameters are as in Fig. 6.

Fig. 8. Contour plots of relative changes in leaf-level (A, C, F, H) and canopy-level (B, D, G, I) gas exchange rates as a function of relative chances in atmospheric CO_2 concentration c_a (x-axis) and dry period length T_d (y-axis), as predicted by the PETA model (top panels) and the optimal stomatal control model OPT2 (bottom panels): A, F) leaf-level transpiration rate (E_L); B, G) canopy-level transpiration rate (E); C, H) leaf-level assimilation rate (A_L); D, I) canopy-level assimilation rate (A); and E, J) intrinsic water use efficiency (ω_i). Leaf area index varies with c_a and D according to Eq. (7) with α =0.5. Black arrows indicate hypothetical temporal trends in T_d and c_a in locations where T_d will lengthen (solid arrow) or shorten (dashed arrow) as c_a increases. The vapor pressure deficit is assumed to be constant and equal to the baseline value (Table 2).

4 Discussion

4.1 Water availability constrains leaf and canopy transpiration responses to atmospheric CO_2 (question 1)

Vegetation acclimates and adapts to increasing atmospheric CO_2 concentration by adjusting tissue-level traits, biomass allocation and, ultimately, community composition. Even in a CO_2-fertilized world, several other resources might limit vegetation growth, including light, nutrients, and water. It is therefore reasonable to expect that growth patterns will adjust so that the available resources are used effectively. These adjustments might occur at different biological levels and temporal scales (organ, whole plant, community) and can be large and possibly of opposite sign. However, we can expect that their net effects converge towards an effective use of any limiting resource in addition to carbon. As a result, despite potentially large variations in individual plant traits, limiting resources would be utilized to the maximum extent possible. In other words, quoting out of context, "Se vogliamo che tutto rimanga com'è bisogna che tutto cambi." [For everything to remain as it is, everything must change.] (di Lampedusa G. T., 1958, "Il Gattopardo").

Both PETA and dynamic feedback optimization models predict that in fully acclimated plants and for a given soil water availability and VPD, increasing atmospheric CO_2 concentration will cause a decrease in leaf-level transpiration and have no

560 effect on transpiration at the canopy level. This is in contrast to observed reductions in stomatal conductance and thus leaf-level transpiration at elevated CO_2 concentrations in the short-term, when plants are not fully acclimated. However, PETA and optimization model predictions are consistent with both long-term observations in presumably fully acclimated plants (Schäfer et al., 2002) and results from more detailed models (Fatichi et al., 2016). The decreased sensitivity of transpiration rate to elevated CO_2 is expected in the long-term when allowing plant or community-averaged traits besides stomatal

565 conductance to optimally acclimate (or adapt), because constraints in resources other than CO_2 become important and ultimately determine gas exchange and plant growth (Schymanski et al., 2015). Predicting long-term gas exchange under elevated CO_2 thus requires considering the full spectrum of plant adjustments, in particular in ecosystems where water is a known limiting factor.

Our argument that plants are ultimately constrained by water availability, at least in semiarid or seasonally dry ecosystems,

570 should be reflected by stable soil moisture values in long-term CO_2 enrichment experiments. However, soil moisture can be higher under elevated CO_2 conditions, contradicting the assumption of the optimization model (Lu et al., 2016a; Fay et al., 2012). This increased water availability might occur only in the short-term because CO_2 enrichment had not been running long enough for plants and communities to fully acclimate. Moreover, our simplified model does not include intra- or inter-specific competition occurring in response to elevated CO_2 (e.g., Fay et al., 2012), which can alter water use strategies by

575 intensifying water consumption at high soil moisture (Manzoni et al., 2013), and therefore cause a deviation from the optimal stomatal conductance behaviour we derived here. Other empirical evidence instead support the assumption that soil water is a main constraint for transpiration—especially in water-limited ecosystems where atmospheric demand is high, evapotranspiration tends to match precipitation on an annual basis (Williams et al., 2012), or even exceed it during the growing season due to soil water storage.

580 Both PETA and optimization models predict increasing leaf- and canopy-level net CO_2 assimilation rates with increasing c_a—a well-known response (Ainsworth and Long, 2005; Norby et al., 1999). As a consequence of combined changes in transpiration and net CO_2 assimilation, WUE and iWUE also increase. Indeed, changes in WUE estimated from flux-towers and isotope composition of tree rings can be more than proportional (Keenan et al., 2013; Mastrotheodoros et al., 2017) or almost proportional to changes in c_a (Dekker et al., 2016; Frank et al., 2015; Lavergne et al., 2019). Our results suggest

585 relative changes in iWUE between 0.15 and 0.29 % ppm[-1] with the lower values when VPD is assumed fixed and higher values when it increases together with CO_2 concentration (Fig. 6 and 7). Values reported in previous studies tend to overlap to this range or be higher: 0.22-0.35 % ppm[-1] (for broadleaf and conifers, respectively, Frank et al., 2015), 0.3-0.75 % ppm[-1] (with variation between angiosperms and conifers, and among climates, Adams et al., 2020), 0.41 % ppm[-1] (Penuelas et al., 2011), 0.44 % ppm[-1] (Saurer et al., 2014), 0.52 % ppm[-1] (Dekker et al., 2016). Our estimates were obtained without any

590 parameter adjustment (for the PETA model, only α could be adjusted; for the optimization model, physiological and soil

parameters could be varied within reasonable ranges). Therefore, we consider the predictions of iWUE sensitivity reasonable, given the simplicity of our approach.

4.2 Atmospheric CO_2 and vapor pressure deficit interact in defining gas exchange responses (question 2)

The effect of elevated atmospheric CO_2 is mediated by changes in other environmental variables related to water availability,
595 such as VPD and the duration of dry periods. For a given c_a, increasing VPD has little or no effect on transpiration rates because, in the PETA model, relative changes in VPD have small effects on WUE (they appear under the square root of Eq. (6)), and hence on E_L (Eq. (7)). If gas exchanges were only controlled by diffusion (without leaf internal CO_2 drawdown by photosynthesis), VPD would have a stronger effect on transpiration rates, as shown in Appendix A for the case of PETA model. Similarly, minor VPD effects in the optimization model are due to soil water constraining transpiration, with stomatal
600 conductance adjusting accordingly. Indeed, because of this constraint, $g \sim D^{-1}$, where D is interpreted as the long-term mean VPD (Eq. (32)). Had we calculated λ from long-term environmental conditions (so that λ is constant), and then let VPD vary for given c_a, LAI and other conditions, to simulate short-term VPD responses, we would have instead obtained $g \sim D^{-1/2}$, consistent with observations in short-term measurements. In fact, the declines of stomatal and canopy conductance with increasing D when all other environmental conditions are fixed was well-captured by $g \sim 1 - m \log(D)$ with $m = 0.5\text{-}0.6$
605 (Oren et al., 1999). This logarithmic relation can be approximated by $g \sim D^{-1/2}$ (Katul et al., 2009). Confirming these results, in a recent meta-analysis, increasing VPD decreased g and net CO_2 assimilation rate, but increased leaf transpiration rate (Lopez et al., 2021). However, in the same study, plant-level transpiration rate also increased with VPD, with a saturating effect, which is in contrast with the model-predicted small increase (according to PETA) or no change (according to optimization) of E as VPD increases (Fig. 6). Structural adjustments not considered here—e.g., rooting depth—might allow
610 plants accessing more water when the evaporative demand is higher, explaining higher than predicted plant-level transpiration in that meta-analysis.

Reductions in g cause less than proportional reductions in net CO_2 assimilation rates (Eq. (3)), implying increasing iWUE with increasing VPD for given c_a. Such a response was observed at the ecosystem level, regardless of changes in soil moisture, leading to the projection (under RCP 8.5) that iWUE could increase by 10% to 35% by 2100 because of the
615 increase in VPD alone (Zhang et al., 2019), in line with results in Fig. 6.

Increasing VPD (driven by either temperature or relative humidity) in conjunction with c_a has limited effects on transpiration rates and increases the sensitivity of iWUE to c_a in both models (Fig. 6), whereas the sensitivity of net CO_2 assimilation varies with temperature in the optimization model (Fig. 7). This temperature effect is caused by the direct temperature dependence of photosynthetic kinetics (Medlyn et al., 2002) and the indirect effect via VPD. As the growth temperature is
620 increased (i.e., moving towards lower latitudes), the optimization model predicts decreasing sensitivity of net CO_2 assimilation to changes in c_a when VPD variations are driven by warming. Lower sensitivities at high growth temperatures are due to negative effects of warming on photosynthesis implemented in the model, as the growth temperature moves

beyond the thermal optimum of photosynthesis. Accounting for thermal acclimation and different thermal optima depending on growth conditions (Vico et al., 2019; Smith et al., 2020) could compensate for this decline in sensitivity, but warming

625   could also have other consequences that are not considered here. For example, warming can lengthen the growing season, and change nutrient availability and biomass allocation to leaves *vs.* roots (Way and Oren, 2010), which in turn might affect the equilibrium LAI and photosynthetic capacity. Considering all these factors is beyond the scope here, where we restricted temperature effects to the kinetics of photosynthesis and warming-induced air drying.

4.3 Atmospheric CO₂ and dry-down duration interact in defining gas exchange responses (question 2)

630   The dry-down duration affects the gas exchange response to elevated c_a only in the optimization model OPT2, where T_d appears explicitly in the equations. Not surprisingly, longer dry periods cause stomatal conductance to be downregulated, resulting in decreased gas exchange rates, while shorter ones increase them. This result is perhaps best understood by considering Eq. (32), where, all else being equal, $\bar{g} \sim T_d^{-1}$. This prediction is a consequence of the assumption that plants have evolved to use all soil water during the hypothetical dry-down of duration T_d, and that the total water storage during the

635   dry period is fixed regardless of its duration. If longer T_d were instead associated with incomplete recharge resulting in lowered initial soil moisture x_0, the exponent of the $\bar{g}$ *vs.* T_d relation would be even more negative. As a result, all gas exchange rates would decrease with lengthening of T_d faster than in Fig. 8. Notably, longer dry periods increase WUE because as stomata close, the slope of the $A_L(g)$ relation in our simple model steepens (Eq. (3)). In fact, Eq. (2) suggests that for $g/k \gg 1$, $A_L(g) \approx k\,c_a$, $\partial A_L/\partial g \approx 0$ (a minimum corresponding to no stomatal limitation). Conversely, when $0 <$

640    $g/k \ll 1$, $A_L(g) \approx g\,c_a$, $\partial A_L/\partial g \approx c_a$, which is the maximum attainable slope when all CO₂ taken up is also assimilated. While typical rain exclusion experiments alter rewetting intensities more than dry period durations, rainfall manipulations where the same amount of water is concentrated into fewer, more intense events could provide a suitable testing ground for these predictions. The advantage of these experiments compared to observations along a natural climatic gradient is that all conditions except rainfall timing and amount are the same, as in our numerical experiments where we let one or two factors

645   vary at a time. Consistent with model results, both net CO₂ assimilation rates and stomatal conductance decrease when rainfall frequency is reduced in a grassland ecosystem (Knapp et al., 2002; Fay et al., 2002). These reduced gas exchanges lower plant productivity, but also promote allocation to roots when rainfall frequency is reduced (Fay et al., 2003), suggesting that flexible allocation to belowground tissues might complement the stomatal conductance and leaf area adjustments that are the focus of the simple models used here. Lower rainfall frequency (for given total precipitation) can

650   also increase productivity in semi-arid ecosystems where fewer larger events promote soil moisture thanks to higher infiltration and lower evaporation from the soil surface (Heisler-White et al., 2008). These factors in the water balance were not explicitly considered here, but can be important to determine the amount of available water, which in turn is the key constraint for stomatal responses to elevated atmospheric CO₂.

4.4 Model assumptions and limitations

655 The choice of the specific limiting factor for photosynthesis leads to a range of optimal stomatal conductance solutions as a function of the Lagrange multiplier λ and other environmental conditions. Equation (3) assumes that the net CO_2 assimilation rate depends linearly on leaf internal CO_2 concentration, but it saturates at high atmospheric CO_2 concentration (thus partly capturing the nonlinear nature of the A-c_i curve). Other assumptions can be imposed, including light-limited (Medlyn et al., 2011) or CO_2 and light co-limited photosynthesis (Vico et al., 2013; Dewar et al., 2018). The resulting

660 stomatal conductance can be mathematically similar to or different from Eq. (12), and in particular with contrasting dependencies on atmospheric CO_2 concentration. For example, the optimization model OPT2 that we selected for its mathematical simplicity does not correctly predict the short-term stomatal closure observed when atmospheric CO_2 concentration is increased (Fig. 4A). This is a known pathology of this formulation (Medlyn et al., 2011; Katul et al., 2010; Buckley and Schymanski, 2014), but assuming RuBP-limited photosynthesis or co-limitation also leads to the same issue,

665 even though it appears at lower c_a (Vico et al., 2013; Dewar et al., 2018). These erroneous responses appear when λ is fixed (i.e., using the instantaneous optimization approach without acclimation), instead of being determined while solving the optimization problem or being heuristically increased at higher CO_2 concentration (Katul et al., 2010; Manzoni et al., 2011).

As long as the Hamiltonian of the optimization problem is independent of soil moisture, the Lagrange multiplier is time invariant because a necessary condition for the optimization is $d\lambda/dt = -\partial(A - \lambda E)/\partial x$ (Manzoni et al., 2013). The

670 numerical value of this time invariant λ can be determined by imposing the condition that all available water is used by the end of the dry period. Accounting for this constraint and thus calculating λ in Eq. (12) (or any analogous formulations based on other assumptions) leads to an optimal stomatal conductance value that essentially reflects the constraint imposed on water availability (Eq. (14) or (24))—regardless of the assumed kinetics of photosynthesis. In turn, this means that any assumption on the factor limiting photosynthesis will lead to the same optimal stomatal conductance value as long as the

675 Lagrange multiplier is solved for within the optimization problem. Therefore, the predictions of the optimization model after imposing the constraint of limited water availability are expected to be similar for any choice of the net CO_2 assimilation model.

Other models based on instantaneous maximization of C gains for given costs offer alternative frameworks to predict responses to atmospheric CO_2 concentrations and other environmental changes (Sperry et al., 2017; Mencuccini et al., 2019;

680 Huang et al., 2018; Bassiouni and Vico, 2021). While these approaches are more physiologically accurate and their predictions compare well with observed trends, they do not guarantee that the water use is optimal over the whole optimization period. Therefore, there remains a gap between approaches based on optimal control over a specified time interval, and those evaluating an instantaneous balance of gains and costs.

In more complex models, it was assumed that not only stomatal conductance, but also LAI or rooting depth were optimized

685 to reach a certain objective (typically maximize long-term productivity) (Schymanski et al., 2015). Here instead, LAI was prescribed—not optimized—as a function of c_a and environmental conditions as reflected by α. Combining stomatal and leaf

area optimization would have resulted in a more complex model that would have been difficult to compare to the PETA model. Rooting depth or root density were also not optimized, nor were they varied here, as they are not included as parameters in the PETA model. However, we can speculate that deeper or more dense roots might allow access to a larger
690 soil water store. If elevated CO_2 increases leaf area and plant size overall, allometric relations would predict a corresponding increase in root biomass and spatial extent (see Chapter 6 in Hunt and Manzoni, 2015; Niklas and Enquist, 2002). Consistent with this expectation, an optimality model predicted deeper roots and higher root area indices under elevated CO_2, which supplied water to support higher transpiration rates than seen under ambient CO_2 (Schymanski et al., 2015). In the analytical optimality model, transpiration rate scales linearly with the soil water storage capacity w_0 (Eq. (14) or (24)), which is in turn
695 a linear function of rooting depth. Therefore, in this model that only optimizes stomatal conductance, deeper roots under elevated CO_2 would also have a positive effect on transpiration.

Besides root allocation, we also neglected evaporation from the soil surface. Changes in LAI do not affect strongly the partitioning of evapotranspiration into transpiration and evaporation, thanks to two compensating mechanisms—with increasing LAI, interception and subsequent evaporation from leaf surfaces increase, while heating of the soil surface is
700 reduced, thus also reducing evaporation (Fatichi and Pappas, 2017; Paschalis et al., 2018). Therefore, even without explicitly modelling evaporation from the soil, the relative changes in gas exchange (as presented here) should be correctly predicted.

For simplicity, we restricted our analysis to deterministic conditions—a single 'representative' dry-down with prescribed initial and final soil moisture states, and duration. Clearly, all these features of dry periods should be treated as stochastic, because rainfall timing and amounts are inherently stochastic (Rodriguez-Iturbe and Porporato, 2004). Stomatal optimization
705 can be studied also in a stochastic rainfall scenario consisting of consecutive dry-downs of random initial states and durations, where rainfall is characterized by a constant mean event frequency and daily intensity. Under long-term steady state conditions, the optimization of CO_2 assimilation integrated over an infinite time period (as was done in Eq. (10)) can be replaced by the integral over all possible states of the stochastic processes (i.e., over all values of stochastic soil moisture) (Lu et al., 2016b, 2020). The resulting solution reflects the expected stomatal behaviour under the probabilistic (in contrast to
710 deterministic) evolution of soil moisture. Stomatal conductance and transpiration rate were predicted to increase with mean annual precipitation (especially so with high rainfall frequency for given total precipitation), with a saturation effect at high precipitation. Similarly, plants should evolve towards more intensive use of water when rainfall frequency or amount per event increase, at lease in recruitment limited plant communities (Lindh and Manzoni, 2021). This effect is qualitatively similar to our prediction of higher transpiration with increasing water storage capacity. Moreover—and consistent with our
715 results—optimal water use under stochastic rainfall was not predicted to change under elevated atmospheric CO_2.

5 Conclusions

Despite increasing atmospheric CO_2 concentration and VPD, only small changes in canopy-scale evapotranspiration have been observed or predicted (Fatichi et al., 2016; Knauer et al., 2017; Yang et al., 2021). That long-term transpiration is a

720 'conserved' hydrological quantity had been already noted when comparing forests under current climatic conditions (Roberts, 1983), suggesting that vegetation acclimates in such a way as to maintain stable transpiration under a given climate. This behaviour could be the result of a number of compensatory feedback mechanisms, including acclimation of leaf area together with stomatal conductance. We quantified the consequences of simultaneous changes in stomatal conductance and leaf area on gas exchange by means of two analytical models of stomatal conductance: PETA and stomatal

725 optimization. Both models predict low sensitivity of canopy transpiration rates to a changing climate, but for different reasons. In the PETA model this was the result of a set of heuristic assumptions on how gas exchange varies with leaf area and water use efficiency, whereas, in the optimization model, this stemmed from water availability setting constraints on canopy transpiration. Moreover, when leaf area increases in response to elevated CO_2, stomata close according to the optimization model, regardless of the chosen formulation for net CO_2 assimilation. With stable transpiration and predicted increases in net CO_2 assimilation rates in both models, intrinsic water use efficiency is also predicted to increase under

730 elevated CO_2. Finally, the sensitivity of net CO_2 assimilation, and to some degree of intrinsic water use efficiency, to changes in CO_2 concentration are mediated by warming-induced increases in VPD. Drier air is expected to enhance the positive effect of elevated CO_2 concentrations on net CO_2 assimilation and water use efficiency, but only at growth temperatures lower than the photosynthetic thermal optimum, whereas the effect of rising CO_2 concentration is reduced at high growth temperature. Increases of VPD, air temperature and dry-down durations may have all contributed to the

735 observation that the rate of intrinsic water use efficiency has increased more than proportionally to the current rise in atmospheric CO_2 levels. Overall, these results imply that physiological and morphological traits acclimate to changing environmental conditions in a coordinated manner to ensure that limiting resources such as water are used efficiently.

Appendix A: Separating diffusion and biochemical limitations to net assimilation using a simplified PETA model

A simplified version of the PETA model can be derived considering that, in free air CO_2 enrichment experiments, $\chi = c_i/c_a$

740 is roughly constant at a fixed VPD (Ainsworth and Long, 2005). This leads to $\omega \sim c_a/D$ instead of $\omega \sim c_a/\sqrt{D}$ as postulated above to derive Eq. (6). This simplification is equivalent to ignoring the dependence of the intercellular to ambient CO_2 concentration on D (i.e., $1 - \chi$ is constant), and allows tracking the sensitivity to D only due to diffusion through the stomata. With this assumption, a simplified PETA model is obtained in which,

$$\frac{\Delta\omega}{\omega} = \frac{1+\frac{\Delta c_a}{c_a}}{1+\frac{\Delta D}{D}} - 1. \tag{33}$$

This simplified model can be used to separate the effects of diffusion limitations to gas exchange from the combined

745 diffusion and biochemical limitations (full PETA model with ω calculated from Eq. (6); Fig. 6). By promoting CO_2 transport from the atmosphere to the leaf, biochemical demand lowers the negative effect of stomatal closure at high VPD. Therefore, including biochemical limitations that draw down leaf internal CO_2 concentrations with stomatal closure reduces the sensitivity of leaf and canopy transpiration and net CO_2 assimilation to higher VPD at a fixed c_a. In fact, combining Eq. (33)

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with Eq. (7), we find $\Delta E_L/E_L \sim (1 + \Delta D/D)(1 + \Delta c_a/c_a)^{-1}$, suggesting a stronger increase in E_L with increasing VPD

750   compared to the case of compound diffusion and biochemical demand (i.e., $\Delta E_L/E_L \sim (1 + \Delta D/D)^{-1/2}(1 + \Delta c_a/c_a)^{-1}$).

The relative change in leaf net assimilation ($\Delta A_L/A_L \sim \Delta\omega/\omega$, Eq. (7)) scales as $(1 + \Delta c_a/c_a)(1 + \Delta D/D)^{-1/2}$ when biochemical demand is accounted for (Eq. (6)) and as $(1 + \Delta c_a/c_a)(1 + \Delta D/D)^{-1}$ when it is not included (Eq. (33)). Taking the ratio, we find that biochemical demand changes $\Delta A_L/A_L$ by a factor $(1 + \Delta D/D)^{-1/2}$ and $\Delta E_L/E_L$ by a factor of $(1 + \Delta D/D)^{1/2}$ compared to the case of simple gas diffusion, indicating higher sensitivities of gas exchange when

755   increasing VPD.

Data availability

Data shown in Fig. 3 are reported in the Supplementary Information.

Author contributions

SM, GGK, and GV designed the study, with feedback from all co-authors. SM developed the model, produced the results

760   and drafted the manuscript. All co-authors commented on the draft and contributed to the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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765   soil interface".

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