Instantaneous stomatal optimization results in suboptimal carbon gain due to legacy effects

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ABSTRACT

Stomatal optimization has been a common phenomenological approach to represent plant stomatal regulation for decades. Recent studies that maximize the instantaneous net carbon gain reproduce empirical stomatal conductance variations in relation to fast environmental stimuli such as photosynthetically active radiation and vapor pressure deficit. However, this instantaneous stomatal optimization framework lacks the ability to account for 'legacy effects' associated with plant-environment feedbacks. Here, the solutions of two stomatal optimization models that do and do not account for these legacy effects are compared. The comparisons focus on stomatal conductance, transpiration rates, net carbon gain rates, and permanent xylem damage over time under different rainfall regimes and in the presence and absence of competition. It is shown that the optimal solution resulting from the instantaneous stomatal optimization is significantly less productive in most scenarios and not viable when xylem embolism cannot be fully repaired. Accounting for legacy effects improves plant productivity and therefore is essential to understanding stomatal regulation based on the optimality principle. These model comparisons demonstrate that legacy effects are significant to shape vegetation acclimation and adaptation responses to climate and environmental change, and thus must be resolved in future stomatal optimization schemes.

Key words: instantaneous carbon maximization, legacy effect, permanent xylem embolism, stochastic rainfall, stomatal optimization, water competition

1. INTRODUCTION

Stomatal regulation is a cornerstone process that links the exchange of carbon and water between vegetation and atmosphere and how it is affected by plant water stress. Its significance to plant physiology and evolution is not in dispute and has motivated centuries of research (Hetherington & Woodward, 2003). Stomatal regulation has also been recognized for its key role in global environmental change, by coupling the terrestrial water, carbon, and energy cycles at the ecosystem level (Gentine *et al.*, 2019) and defining the risk of plant vulnerability to and mortality from drought (Martin-StPaul *et al.*, 2017; Anderegg *et al.*, 2018; Hochberg *et al.*, 2018; Blackman *et al.*, 2019; Feng *et al.*, 2019).

An important contribution to the understanding of stomatal regulation is the theory of stomatal optimization, which was first proposed by Cowan & Troughton (1971) and later expanded upon by Cowan & Farquhar (1977) and many others (Buckley *et al.*, 2017; Harrison *et al.*, 2021). In the process of gaseous CO_2 uptake, water vapor molecules are inevitably lost through the stomata and must be replenished from the soil reservoir. Inspired by this observation, Cowan & Troughton (1971), Givnish & Vermeij (1976), Cowan & Farquhar, (1977), and Hari *et al.* (1986) cast stomatal regulation as an economic problem of leaf-level plant gas exchange: plants, constrained by a fixed water supply in the soil, regulate stomatal conductance in response to environmental cues to achieve maximum carbon gain over a prescribed time period (presumed to be much longer than the timescale at which guard cells open or close). Under certain restricted conditions (usually when the resource constraint is not severe), the solutions based on stomatal optimization provide a means to predict how stomatal conductance varies with environmental cues (e.g., vapor pressure deficit, light, CO_2 concentration, and to a lesser extent soil moisture availability). Since then, various 'off-shoots' and modifications to this optimization framework have emerged, with different goals (e.g., minimize water loss; Sperry & Love, 2015; Sperry *et al.*, 2017) and constraints (e.g., water limitation is prescribed instantaneously through "profit maximization", Wolf *et al.*, 2016) associated with stomatal regulation. Stomatal optimization has since then complemented empirical (e.g., Jarvis, 1976; Ball *et al.*, 1987; Leuning, 1995) and mechanistic models (e.g., Hills *et al.*, 2012) as a top-down, goal-oriented approach to study stomatal regulation. Some of these solutions have been incorporated into vegetation productivity (e.g., Stocker *et al.*, 2020) and land surface models (e.g., Medlyn *et al.*, 2011; Eller *et al.*, 2020). In short, stomatal optimization theory is at the basis of several recent formulations and is increasingly adopted into a wide range of models. There is also unprecedented opportunity to evaluate their predictions from in situ measurements, observation networks, and remote sensing products. The time is thus ripe to revisit the

premises of the stomatal optimization theory and how they relate to fundamental conceptualizations of plant water use, for a better-informed application of this phenomenological approach.

The goal at the heart of stomatal optimization is the maximization of cumulative carbon gain over some period as a proxy of ecological fitness and reproductive success. Yet, plants' current water use affects their future carbon gain, by using resources now that would then not be available in the future or incurring in damage that would jeopardize future carbon gains – which we label as "legacy effects". In fact, this temporal tradeoff between current water use and future carbon gain is implicit in Cowan and Farquhar's original formulations of the stomatal optimization problem: how can plants optimally distribute a *fixed* amount of water over a specified period of time? Because cumulative carbon gain is the result of continuous investment of carbon and other resources by plants over time, legacy effects decouple the optimal strategy from instantaneous environmental cues. That is, maximizing instantaneous carbon gain would trivially result in maximum stomatal conductance until soil water is completely depleted. To achieve more realistic predictions through instantaneous optimization (and to bypass issues related to the interpretation of the Lagrange multiplier-parameter in Cowan and Farquhar's formulation), various cost functions related to transpirations rates or plant water potential have been introduced (as reviewed in Wang *et al.*, 2020). How these cost functions can, at a single point in time, approximate the time-integrated legacy effects remains an open question (Buckley & Schymanski, 2014).

The central question concerning the role of legacy effects is this: can plants maximize their cumulative net carbon gain over time by maximizing their net carbon gain at every single moment? We hypothesize that this is not the case because legacy effects will incur opportunity costs on plants' current water use in the form of reduced future carbon gain. A strategy that maximizes net carbon gain at every moment, in the presence of legacy effects, will inevitably reduce the highest possible net carbon gain in the future and thus the cumulative net carbon gain over time.

Here we test this hypothesis by comparing the optimal stomatal strategies that account for legacy effects against representative stomatal optimization models developed in recent years that do not account for legacy effects. Especially, we consider their ability to account for legacy effects associated with plant-environment feedback and co-evolution and how these legacy effects affect plant performance under varying drought conditions. We anticipate these legacy effects to play an important role in shaping vegetation acclimation and adaptation responses to climate and environmental change.

2. THEORY

2.1. Legacy effects

Amongst the many possible types of legacy effects, previous studies have explored the role of soil-plant feedback and permanent or irrecoverable xylem embolism. The first type, the soil-plant feedback, is a temporal tradeoff between plants' current water consumption and their future soil water availability (Manzoni *et al.*, 2013; Mrad *et al.*, 2019). Amongst all the environmental cues relevant to plant gas exchange, soil water stands out as the only one strongly regulated by plants themselves. That is, the more water plants consume now, the less water will be left for them in the future during a single dry-down (Cowan & Farquhar, 1977; Cowan, 1986). In contrast, other environmental variables can effectively be considered to be external conditions – i.e., be independent of plant influence – at the intermediate timescale of drought-induced water stress, although plants do have the ability to partially regulate vapor pressure deficit or CO_2 concentrations in the atmosphere at multiple time scales spanning boundary layer dynamics to multi-decadal (Lebrija-Trejos *et al.*, 2010). At low soil moisture levels, plants may be forced to give up CO_2 uptake partially or completely due to the elevated risk of desiccation. It follows that any optimal behavior by plants should account for the fact that the increase in current carbon gain due to increased water consumption comes at the cost of reduced future carbon gain due to decreased water availability. Under certain conditions, the plant's ability to partially adjust atmospheric vapor pressure deficit and air temperature can impact predisposition to rainfall (Siqueira *et al.*, 2009; Konings *et al.*, 2010), but this effect will not be explicitly considered here.

The second type of legacy effect is permanent or irrecoverable xylem embolism. Xylem embolism is incurred when the growing mismatch between water supply and demand reduces the plant's capacity for xylem water transport. If not fully repaired, an embolized xylem will limit the water supply from the soil to the leaves (even if soil water becomes abundant again). In turn, this will potentially induce stomatal closure that reduces CO_2 uptake for photosynthesis (Hubbard *et al.*, 2001; Sperry *et al.*, 2002; Anderegg *et al.*, 2014). Thus, this effect of permanent xylem embolism can also be regarded as an opportunity cost of reduced future carbon gain (Wolf *et al.*, 2016). In the extreme case of hydraulic failure, plants are forced to stop photosynthesis completely. Therefore, permanent xylem damage complicates stomatal optimization by introducing a tradeoff between plants' current water use and their future water transport capacity. Similar arguments can be extended to the phloem system, though the focus here is maintained on the xylem for illustration purposes (Konrad *et al.*, 2018).

2.2. The "Dynamic-Feedback" Approach

Relevant to the consideration of legacy effects, recent advances in stomatal optimization can be grouped into two broad categories (Table 1): (i) an "instantaneous" approach that achieves maximum net carbon gain based on given environmental inputs at every instant, and (ii) a time-explicit, "dynamic feedback" approach that optimizes stomatal conductance over time to maximize *cumulative* carbon gain. Both approaches can respond to changing environmental conditions. The key difference is that the instantaneous approach determines the optimal stomatal conductance based on the current information only, including current environmental conditions and plant water status (e.g., xylem hydraulic damage), whereas the dynamical feedback approach characterizes the optimal stomatal conductance behavior based on current and future information. Here, the difference between instantaneous and dynamic-feedback approaches should be distinguished from the idea that plants may encode past information through genetic memory resulting from natural selection (e.g., functional traits that characterize xylem vulnerability curves). That is, plants may adapt to past and future environmental conditions through functional traits that define their water use strategies, but these traits are treated as being static within both instantaneous and dynamic-feedback approaches. Therefore, it is reasonable to expect instantaneous approaches to account for past information through parameterized traits, but this type of past information can be similarly accounted for by dynamic-feedback approaches. In contrast, the defining difference between instantaneous and dynamic-feedback approaches lies in their ability to account for the implications on future resource availability or acquisition (i.e., legacy effects) in the process of finding the optimal behavior.

In practice, the instantaneous optimization approach has shown an extraordinary capacity to reproduce empirical patterns (Sperry *et al.*, 2017a; Venturas *et al.*, 2018; Bassiouni & Vico, 2021), especially in relation to high frequency (e.g., diurnal) vapor pressure deficit responses (Katul *et al.*, 2009, 2010). However, the fundamental premise of the instantaneous approach is that plants should trade as much future carbon gain as possible for the current carbon gain. This tradeoff does not always make sense as plants undergo soil water stress over time, as plant water-use efficiency (WUE) increases with moderate soil water stress (DeLucia & Heckathorn, 1989) and thus water (on a per carbon basis) becomes less costly.

Table 1: Examples of instantaneous and dynamic-feedback stomatal optimization models, including optimization methodology and the definitions for their objective functions, costs Θ, and constraints. ESS refers to the evolutionarily stable strategy under competitive environments.

Models	Optimization approach	Objective function	Cost function, Θ	Legacy effects considered (Feedback constraints)
Instantaneous				
Prentice et al. (2014)	Instantaneous	$\min \Theta$	$\frac{jE}{A} + \frac{mV_{c,max}}{A}$	None
Wolf et al. (2016)	Instantaneous, ESS	$\max(A - \Theta)$	$uP^2 + vP + w$	None
Sperry et al. (2017)	Instantaneous, ESS	$\max(A - \Theta)$	$A_{max}\left(1 - \frac{k}{k_{max}}\right)$	None
Eller et al. (2018)	Instantaneous, ESS	$\max(A - \Theta)$	$A\left(1 - \frac{k}{k_{max}}\right)$	None
Dynamic feedback within a single dry down				
Cowan & Farquhar (1977)	Dynamic feedback	$\max \int_0^T A\ dt$	None	$\int_0^\infty E\ dt \leq W_0,\ \frac{dW}{dt} = -E$
Mäkelä et al. (1996)	Dynamic feedback	$\max \int_0^\infty e^{-\lambda t} A\ dt$	None	$\int_0^\infty E\ dt \leq W_0,\ \frac{dW}{dt} = -E$ (rainfall is stochastic)
Manzoni et al. (2013)	Dynamic feedback	$\max \int_0^T A\ dt + J_T$	None	$\frac{dW}{dt} = -(E + L)$
Mrad et al. (2019)	Dynamic feedback	$\max \int_0^T A\ dt + J_T$	None	$\frac{dW}{dt} = -(E + L)$ (E also specified by plant hydraulics)
Dynamic feedback over consecutive dry downs				
Lu et al. (2016)	Dynamic feedback	$\max \int_0^\infty \bar{A}\ dt$	None	$\frac{dW}{dt} = R - E - L$ (rainfall R is stochastic)
Lu et al. (2020)	Dynamic feedback, ESS	$\max \int_0^\infty \overline{A - \Theta}\ dt$	$\beta\ (1 - \frac{k}{k_{max}})$	$\frac{dW}{dt} = R - E - L$ (rainfall R is stochastic) Permanent xylem embolism

Abbreviations. A: net photosynthetic rate, *T*: dry down duration, λ: rainfall frequency per day, *P:* absolute value of leaf xylem pressure, J_T: carbon value of terminal soil moisture, $V_{c,max}$: maximum carboxylation rate, *j,m,u,v,w*: fitting parameters, *k*: soil-plant hydraulic conductance, k_{max}: maximum hydraulic conductance with no transpiration or no xylem cavitation, β: carbon cost per unit of recovered *k, W*: soil water storage in the rooting zone, W_0: soil water available at beginning of dry down, *R:* rainfall, *E*: evapotranspiration, *L*: leakage below the rooting zone. Overbar on $\bar{A}$ and $\overline{A - \Theta}$ indicates temporal averages due to random nature of rainfall.

The dynamic feedback approach incorporates an explicit time component into the description of the optimal trajectory of stomatal aperture. This addition provides a feedback related to temporal tradeoffs in water use and carbon uptake. The temporal characterization provides a necessary (but not sufficient) basis to account for legacy effects – not only of soil-water feedback and permanent xylem embolism, but also of others related to plant physiology and conservation of resources. In the last decade, it has become increasingly clear that leaf-level gas exchange is closely connected with many other plant physiological processes and thus should not be autonomously optimized. For example, efforts have been made to couple plant hydraulic and sucrose transport constraints (Huang *et al.*, 2018), soil salinity (Perri *et al.*, 2019), leaf phenology (Konrad *et al.*, 2017), belowground allocation (Schymanski *et al.*, 2009), and soil-to-leaf nutrient regulation (Buckley *et al.*, 2002; Palmroth *et al.*, 2013) into stomatal optimization, all of which effectively reformulate the original stomatal optimization problem from leaf-level to whole-plant level (Buckley, 2021).

Finally, recent work has also expanded on the idea that stomatal regulation can be formulated as either a carbon maximizing, ecological strategy problem (e.g., Cowan & Farquhar, 1977) or a competition-driven, evolutionary strategy problem (e.g., Wolf et al., 2016) (Table 1). These alternative formulations diverge fundamentally in the conceptualization of an "optimal" solution, requiring different mathematical tools. The carbon maximization paradigm maximizes the carbon gain of individual plants, and its solutions are derived using optimal control theory (e.g., Mäkelä *et al.*, 1996). Soil evaporation and drainage are seen as processes "competing" with plants for soil water, reducing the benefit of leaving water for later use and thus affecting the optimal stomatal response (Cowan 1982). In contrast, the competition paradigm stems from game theory and searches for an evolutionarily stable strategy (ESS, Maynard Smith, 1974) for stomatal response to environmental cues, with which plants can guarantee a higher or equal carbon gain against competitors with any alternative stomatal strategy when competing for water (i.e., when neighboring plants share access to a local soil water pool). Both paradigms are theoretically sound, and both can be formulated in a time-explicit or an instantaneous manner, but caution should be used when comparing their predictions given their differing premises for stomatal optimization. In practice, the presence of competition has often been used as justification for neglecting temporal effects through the instantaneous approach (Wolf et al. 2016). However, the compensatory effect of competition is never absolute. Even for plants subject to competition, some of the water saved by a more conservative water use strategy can be used later by the same plant. In addition, excessive water use may impair plants' future ability to take up water in a way that has no

influence on a competitor's current water uptake ability. Thus, it is possible to subject plants simultaneously to competition as well as time explicit legacy effects (Lu *et al.*, 2020).

The conjecture to be explored here is that the time-explicit, dynamic feedback approach is more appropriate (i.e., results in higher cumulative carbon gain) in the presence of legacy effects than the instantaneous approach. To this end, we compare calculations from the dynamic feedback approach against the instantaneous approach. In this comparison, we consider the two types of legacy effects (i.e., soil-plant feedback and permanent xylem damage) and two 'end-member' timescales of soil moisture variability: (i) during a single dry-down (no precipitation, so that water availability is dictated by the initial root-zone soil moisture content), and (ii) stochastic rainfall (equivalent to a sequence of consecutive dry-downs after random rainfall inputs). We demonstrate that by accounting for these legacy effects, the optimal solution from the dynamic feedback approach results in greater cumulative net carbon gain for plants than that based on the instantaneous carbon gain rate.

3. METHODS

We directly compare the instantaneous and dynamic feedback stomatal optimization strategies. These two strategies are derived under the same modeling conditions (see the *Plant gas exchange model* section), including the legacy effects of soil-plant feedback and permanent xylem embolism (see Table S1), but under different optimization goals (see the *Optimization goals* section), resulting in different quantitative responses of stomatal conductance to environmental conditions. To illustrate their differences, we compare them in two dry-down scenarios (*i.e.,* the single dry-down and stochastic rainfall scenarios), which are defined in the *Dry-down scenarios* section. Soil water availability is treated as the only dynamic resource, while all the other environmental cues (*e.g.,* vapor pressure deficit) are externally supplied (as constants for ease of comparisons). All the symbols and their definitions are given in Table 2.

3.1. Plant gas exchange model

To allow for a direct comparison, we use the same model to calculate the dynamic feedback and instantaneous optimal stomatal strategies following the setup from Eller *et al.* (2018). The associated parameter values are also kept the same (see Table 1 in Eller *et al.*, 2018). The model by Eller *et al.* (2018) describes how plant photosynthesis and transpiration rates depend on stomatal conductance. Transpiration rate are also regulated by xylem hydraulic conductance and depend on plant hydraulic

229 traits as well as soil and plant water potentials. Finally, following Wolf *et al.* (2016), we assume the
230 existence of an instantaneous carbon cost of plant water use and define its dependence on
231 instantaneous plant water potential. In Table S1, we summarize the model equations and the references
232 in the original paper.

233 The model by Eller *et al.* (2018) does not have a component of permanent xylem embolism, so we use
234 the definition given by Lu *et al.* (2020) for both the instantaneous and dynamic feedback optimal
235 stomatal strategies. Briefly, permanent embolism changes the vulnerability curve of the xylem over
236 time. The extent to which xylem embolism can recover after embolism is defined as a prescribed
237 percentage, p_k, of the recovered vs unimpaired xylem conductance at a given water potential. Recovery
238 is assumed to take place instantaneously as soon as rewatering occurs. A p_k of 100% corresponds to
239 perfectly recoverable embolisms and indicates that the xylem vulnerability curve does not change with
240 successive embolisms. In contrast, a p_k of 0% corresponds to zero recovery, so plant hydraulic
241 conductance at any given time is determined by the lowest plant water potential yet experienced by the
242 plant up to that time. For intermediate cases ($0\% < p_k < 100\%$), the percentage loss of hydraulic
243 conductivity (PLC) is repaired only to a fraction p_k of the original, unimpaired xylem conductance at any
244 given water potential. Any percentage loss represented by $p_k < 100\%$ represents a legacy effect (the
245 lower the p_k, the larger the legacy effect) that irreversibly reduces plant hydraulic capacity as the soil
246 becomes progressively drier. More details on this scheme can be found in Lu *et al.* (2020) (e.g., Fig. 1,
247 Eqs. 4 & 5).

248 **3.2. Optimization goals**

249 There are two basic differences between the instantaneous and dynamic feedback stomatal
250 optimization strategies. First, instantaneous stomatal optimization strategies are presumed to be able to
251 competitively exclude all others (Wolf *et al.*, 2016), while different dynamic feedback stomatal
252 optimization strategies can be constructed in ways that do or do not account for competition for water
253 (Lu *et al.*, 2016, 2020) (Table 1). To compare these approaches, the performance of the same
254 instantaneous stomatal optimization strategy are examined and compared with the corresponding
255 dynamic feedback strategies, both in the absence or presence of competition for water, using the same
256 net carbon gain function.

Second, the instantaneous stomatal optimization strategy optimizes the instantaneous value of stomatal conductance, g_s, given all atmospheric and soil moisture variables as external conditions. Conceptually, this means that atmospheric or soil moisture conditions are not treated as internal variables, and their temporal dynamics are not factored into the optimal stomatal strategy (which exerts "open loop control"). In contrast, the dynamic feedback strategy optimizes the stomatal conductance including its response to soil water availability, i.e., $g_s(s)$, where s represents the relative soil water content or degree of saturation. Thus, the dynamic feedback strategy optimization results in a functional relation to soil moisture, with only the atmospheric variables acting as external input. This is how the dynamic feedback strategy can account for the ability of plants to dynamically regulate their own soil water supply (*i.e.,* the local soil moisture dynamics) and thus the legacy effect of soil-plant feedback (a "closed loop control" with respect to soil water). It is possible to extend both approaches to include interactive effects between plants and their micrometeorological states (Katul *et al.*, 2012; Manoli *et al.*, 2016), but this extension is not considered here.

The instantaneous stomatal optimization strategy maximizes the instantaneous net carbon gain by adjusting g_s, given the current atmospheric and soil conditions

$$\max_{g_s} B(g_s, s) \tag{1}$$

where B is the instantaneous net carbon gain rate (see Table S1 or Eqs. 2.8 & 2.9 in Eller *et al.* (2018)). Note that B is typically expressed as the difference between carbon assimilation A and a cost function θ, which can be related to transpiration or decline in water potential (see Table 1 for a selection of different cost functions). For convenience, we only show explicitly the dependence of B on s (i.e., relative soil water content, which is a state variable that ranges between 0 and 1) and g_s (the control variable), but not on the atmospheric forcings (e.g., vapor pressure deficit, light) or static parameters (e.g., photosynthetic capacity, hydraulic traits). The effect of g_s on whole-plant net carbon gain rate is derived assuming a constant leaf area and well-coupled conditions between the plant and atmosphere so that air temperature reasonably approximates surface temperature. These approximations are imposed on both model formulations for the purposes of their comparison.

In the absence of competition for water, the dynamic feedback stomatal optimization strategy maximizes the long-term average net carbon gain rate (equivalent to cumulative carbon gain) over a specified time horizon by adjusting $g_s(s)$. Then, the corresponding objective function is

$$\max_{g_s(s)} \bar{B}(g_s(s), s) \tag{2}$$

where $\bar{B}(g_s(s), s)$ is the long-term average net carbon gain rate given the stomatal response to relative soil water availability $g_s(s)$,

$$\bar{B}(g_s(s), s) = \frac{1}{T}\int_0^T B\left(g_s\big(s(t)\big), s(t)\right) dt \tag{3}$$

where T marks the end of the optimization period. For example, in a simple single dry-down scenario, T is the prescribed length of the dry-down.

The maximization in Eq. 2 is subject to the water availability constraint – the cumulative transpiration at any given time cannot exceed the cumulative water supply, for any time τ from 0 to T. Mathematically, this constraint abides by

$$\int_0^\tau E\left(g_s\big(s(t)\big)\right) dt \le W(\tau), \forall \tau \in [0, T], \tag{4}$$

where $W(\tau)$ is the cumulative water supply up until time τ. In the case of a single dry-down scenario, $W(\tau)$ is equal to $W(0)$, the initial soil water availability, for any τ between 0 and T.

In the presence of competition for water, the dynamic feedback stomatal optimization searches for the evolutionarily stable strategy (ESS, Maynard Smith, 1974) that can guarantee a higher or equal long-term average net carbon gain rate than that of any alternative strategy of the competitors. Mathematically, the ESS condition implies

$$\bar{B}_{ESS}\big(g_{s,ESS}(s), s_{ESS}\big) \ge \bar{B}_I\big(g_{s,I}(s), s_{ESS}\big) \tag{5}$$

where $\bar{B}_{ESS}$ and $\bar{B}_I$ are the long-term average net carbon gain rates of the ESS and any alternative strategy in the competition, respectively, and $g_{s,ESS}(s)$ and $g_{s,I}(s)$ are the corresponding stomata response of the ESS and any alternate strategy of an invader (subscript I). The soil moisture conditions in both cases, designated by s_{ESS}, are set by feedback from the ESS stomatal response, as the ESS was first formulated based on the idea that no competitor can benefit from switching to a strategy other than the ESS.

Eq. 5 can be used to find the ESS for both full and partial xylem recovery. In the case of full xylem recovery, the ESS can be found from applying Eq. 5 instantaneously, since any difference in legacy effects between strategies imposed by soil-plant feedback has been effectively eliminated by imposing

the same soil moisture condition, s_{ESS}, for all strategies. In the case of partial recovery, the legacy effect due to permanent xylem damage remains, and the ESS can no longer be found from instantaneous optimization. Rather, the ESS must first account for how the extent of xylem recovery might affect stomatal conductance through reduced xylem hydraulic conductance, through a two-step process. The full details of the derivation can be found in Lu *et al.* (2020).

3.3. Dry-down scenarios

A total of eight scenarios are explored to compare the performance of instantaneous *vs.* dynamic feedback optimization with different conditions of water supply (see *Water Supply* section below), competition, and permanent xylem damage (Table 3). In each scenario, both instantaneous and dynamic feedback optimization with the same net carbon gain function *B* from Eller *et al.* (2018) (Table S1) is implemented to find the optimal stomatal strategy. We examine five state variables within the plant gas exchange model: relative soil water availability, transpiration rate, net carbon gain rate, stomatal conductance, and permanent percentage loss of xylem hydraulic conductivity.

Soil water balance

The dynamics of the relative soil water availability is defined at the daily scale by

$$nZ\frac{ds}{dt} = R - E(g_s) \tag{6}$$

where *t* is the time; *R* is the throughfall input defined by the specific water supply condition (see below); and *E* is the stomata-controlled transpiration rate (see Table S1 or Eq. 2.2 in Eller *et al.* (2018)). The product of soil porosity *n* and rooting depth *Z* converts the relative soil moisture to a soil water depth, consistent with the dimensions of the water fluxes; i.e., water volumes per unit ground area and time. For convenience, drainage losses below the rooting zone and lateral losses are ignored. The *s* can be converted into soil water potential, Ψ_s, based on a soil water retention curve (Campbell, 1974):

$$\Psi_s(s) = \Psi_e s^{-q} \tag{7}$$

where *q* is the curvature parameter presumed to vary with soil texture and Ψ_e (MPa) is a reference soil water potential near saturation. Then, stomatal conductance is determined according to the stomatal strategy under consideration. The other three state variables (*i.e.,* transpiration rate, net carbon gain rate, and permanent percentage loss of xylem hydraulic conductivity) are determined based on their

dependence on $\Psi_s(s)$ and stomatal conductance defined by the plant gas exchange model (see Table S1).

Water supply conditions

Plant carbon uptake under two water supply conditions with different rainfall input are modeled: (i) during a single dry-down and (ii) under stochastic rainfall. During a single dry-down, both the initial soil water availability and the length of the dry-down are prescribed. There is no additional water supply till the end of the dry-down. Under this condition, the water constraint defined with Eq. 4 can be simplified to

$$\int_0^T E\left(g_s\left(s(t)\right)\right) dt \leq nZs_0 \tag{8}$$

where s_0 and T are the prescribed initial relative soil water availability and dry-down duration, respectively. The same single dry-down condition has also been first proposed by Cowan & Farquhar (1977). In their derivations, the constraint in Eq. (8) was not formally included leaving the optimization formulation with one adjustable parameter: the marginal profit that measures how much carbon is gained per unit of transpired water, or "marginal carbon product of water" (Buckley & Schymanski, 2014).

The single dry-down condition lacks the key components of natural rainfall – the main source of soil water supply and its variability. Cowan recognized that "Because replenishment of the reserves by rainfall is irregular and unpredictable, the course plants follow in growing and using water cannot be invariably successful" (Cowan, 1982). Thus, we consider also the more realistic condition where plants take up carbon under stochastic rainfall, during a period equivalent to an infinite number of consecutive dry downs. Under stochastic rainfall, every dry-down lasts for a random period. The soil water availability at the beginning of every dry-down, expressed as water depth, is the sum of the random rainfall input, and the amount of water left over from the previous dry-down.

To represent stochastic rainfall, one may concatenate a large number of consecutive dry downs (*e.g.,* > 100). This brute-force approach may be accurate enough for any practical purpose but is too computationally intensive to implement. Alternatively, we can invoke the probabilistic model of soil water balance under stochastic rainfall developed by Rodriguez-Iturbe *et al.* (1999) and Laio *et al.*, (2001). There, stochastic steady state conditions are assumed, and rainfall is idealized as a marked

Poisson process characterized by the mean rainfall event depth and rainfall frequency (the product of which is the mean rainfall rate). Given the stomatal response to the relative soil water availability, $g_s(s)$, and hence its role on the transpiration rate, the probability density function of the relative soil water availability, $p(s, g_s(s))$, can be derived from a stochastic form of the soil water differential Eq. 6 (the full derivation can be found in Rodriguez-Iturbe *et al.* (1999); a simplified form can be found in Porporato *et al.* (2004), Eq. 2) as

$$p(g_s(s), s) = \frac{C}{E(g_s(s))} e^{-\frac{n Z}{\alpha} s + \lambda \int_0^s \frac{n Z}{E(g_s(u))} du} \quad (9)$$

where C is a constant of integration defined by the normalizing condition that $p(g_s(s), s)$ must integrate to unity as s varies from 0 to 1, representing the lower and upper bounds of the relative soil water availability; α (m) is the mean depth of rainfall events; λ (day^{-1}) is mean rainfall frequency; n (-) is the soil porosity; and Z (m) is the effective plant rooting depth. Optionally, the transpiration term in this probabilistic model of soil water balance can be replaced with a more general soil water loss term that accounts for both plant transpiration and other means of soil water loss (*e.g.,* deep infiltration, surface evaporation, *etc.*). In this stochastic rainfall scenario, we can exchange the long-term average in eq 3 with the ensemble average so that the long-term mean net carbon gain rate defined with Eq. 3 becomes (Lu *et al.*, 2016)

$$\bar{B}(g_s(s)) = \int_0^1 B(g_s(s), s) p(g_s(s), s) ds. \quad (10)$$

Implementation

In the single dry-down scenario (but not in the stochastic rainfall scenario), the simulations were run in discrete time with all the state variables updated daily. In the stochastic scenario, optimal solutions are found by maximizing Eq. 10. In the search for the dynamic feedback stomatal optimization strategy without competition for water, we take a simplified approach by requiring the stomatal response to soil water potential to take on the following functional form for both single-dry down and stochastic scenarios:

$$g_s(\Psi_s) = a \cdot e^{-\left(\frac{\Psi_s}{c}\right)^b} \quad (11)$$

where a, b, and c are fitting parameters. This approach only approximates the theoretical solution by Lu *et al.* (2016) due to the additional numerical constraint defined with Eq. 11, but can largely reduce the

computation time. The three fitting parameters are optimized using Bayesian optimization (Mockus, 2012), an optimization algorithm for expensive-to-evaluate functions as is the case here. Care should be taken to either numerically eliminate or explicitly account for the atom of probability (Rodriguez-Iturbe *et al.*, 1999) that appears in the probability distribution at the lower bound of the domain of the stomatal response function. In the instantaneous optimization scenario, Eq. 11 is substituted with the solution from Eller *et al.* (2018) (Table S1) that relates stomatal response to plant and soil water potential.

In the presence of competition for water, we derive the dynamic feedback stomatal optimization strategy following the approach by Lu *et al.* (2020).

The model was written in Python and all the subsequent analyses were also conducted in Python. The Bayesian optimization was implemented using the 'bayesian-optimization' package (Nogueira, 2014). The code, including documentation, input data, and example output, can currently be found at https://github.com/feng-ecohydro/stomatal-optimization and will be published upon manuscript acceptance.

The model results for the single dry down case are also compared to experimental data collected in Venturas *et al.* (2018) from aspen (*Populus tremuloides*) saplings subjected to a "severe drought" treatment. The 4-yr-old saplings were planted in 0.8 m x 0.8 m grid and irrigated to field capacity at the start of the experiment. The "severe drought" treatment, one of four treatments, received limited irrigation during the experiment. The experiment lasted for more than two months, but we used data only during the initial dry down before the onset of a large rainstorm that rewetted the soil. The soil, atmospheric, and plant parameters adopt values published from the study. The maximum whole-plant hydraulic conductance (0.01 mol m^{-2} s^{-1} MPa^{-1}) and maximum Rubisco carboxylation rate at 25°C (120 µmol m^{-2} s^{-1}) are based on the measured values at the beginning of the "severe drought" treatment, and the leaf area index (0.17 m^2 m^{-2}) is set to the average value measured for saplings across the "severe drought" treatment. The water potential at 50% loss in hydraulic conductivity (-1.22 MPa) is the corresponding value measured at the leaves. Other parameter values used in the simulations are summarized in Table 2.

Table 2. Description of symbols, definitions, values, and units of measurement. † and ‡ refer to values informed by Venturas *et al.* (2018) and Eller *et al.* (2018), respectively.

Symbol	Description	Value	Unit
Soil properties			
q	Curvature parameter for soil water retention curve	3.1	unitless
n	Soil porosity	0.38†	$m^3\ m^{-3}$
Z	Effective plant rooting depth	0.1	m
Ψ_e	Soil water potential near saturation	-1.5e-3	MPa
Plant hydraulic & photosynthetic parameters			
a	Parameter for stomatal response to soil water potential	(0.02, 1)	$mol\ m^{-2}\ s^{-1}$
b	Parameter for stomatal response to soil water potential	(0.1, 10)	-
c	Parameter for stomatal response to soil water potential	(-1, -0.01)	MPa
LAI	Leaf area index	0.17†	$m^2\ m^{-2}$
k_{max}	Maximum root to leaf hydraulic conductance	0.01†	$mol\ m^{-2}\ s^{-1}\ MPa^{-1}$
Ψ_{50}	Plant water potential at 50% loss in hydraulic conductivity	-1.22†	MPa
p_k	Percentage of recovered vs. unimpaired xylem conductance at a given water potential	Varies	-
$V_{cmax,25}$	Maximum Rubisco carboxylation rate at 25°C	0.00012†	$mol\ m^{-2}\ s^{-1}$
ϕ	Quantum efficiency of photosynthesis	0.1‡	$mol\ mol^{-1}$
ω	Leaf scattering coefficient	0.15‡	-
T_{upp}, T_{low}	Upper and lower range of optimal temperature for Rubisco activity	40, 10‡	°C
Environmental inputs			
α	Mean depth of rain events	Varies	m
λ	Rainfall frequency	Varies	day^{-1}
T	Dry down duration	Varies	day
T_a	Air temperature	28.7†	°C
I_{PAR}	Incident photosynthetically active radiation	0.002†	$mol\ m^{-2}\ s^{-1}$
D	Vapor pressure deficit	0.03†	$mol\ mol^{-1}$
P_{atm}	Atmospheric pressure	90,000†	Pa
c_a	Partial pressure of CO_2	40‡	Pa
O_a	Partial pressure of O_2	21,000‡	Pa
I	Photosynthetically active period during the day	36,000	$s\ day^{-1}$
Model state variables			
B	Net carbon gain rate	-	$\mu mol\ m^{-2}\ s^{-1}$
A	Carbon assimilation	-	$\mu mol\ m^{-2}\ s^{-1}$
θ	Carbon cost of water	-	$\mu mol\ m^{-2}\ s^{-1}$
c_i	Intercellular CO_2 pressure	-	Pa
J_c, J_l, J_e	Rubisco, light, and transport limited photosynthesis	-	$\mu mol\ m^{-2}\ s^{-1}$
K_c, K_o	Michaelis-Menten onstant for CO_2 and O_2	-	-
PLC_0	Percent loss of conductance for the undamaged xylem	-	-
E	Transpiration rate normalized by soil water storage	-	day^{-1}

g_s	Stomatal conductance to CO_2	-	mmol m^{-2} s^{-1}
$g_s(s)$	Stomatal response to drought	-	mmol m^{-2} s^{-1}
k	Plant hydraulic conductivity	-	mol m^{-2} s^{-1} MPa^{-1}
s	Relative soil moisture, $\in [0, 1]$	-	m^3 m^{-3}
W	Soil water storage (= n Z s)	-	m
Ψ_s	Soil water potential	-	MPa
Ψ_p	Plant water potential	-	MPa

4. RESULTS

4.1. Effect of soil-plant feedback on optimal stomatal conductance

The results from the single dry-down scenario (Table 3, Scenario 1) show that, in the absence of competition and permanent embolism, the dynamic feedback strategy results in a much less aggressive stomatal behavior with lower stomata conductance (and thus lower net carbon gain rate) in well-watered conditions compared to the instantaneous strategy (Fig. 1a). In turn, the more aggressive stomatal strategy predicted by the instantaneous optimization results initially in a high net carbon gain rate (Fig. 1b). Because this causes faster soil water depletion (Fig. 1c), plants are forced to slow down gas exchange over time. In contrast, plants adopting the dynamic feedback strategy maintain a relatively stable gas exchange rate during the entire dry-down period. Their net carbon gain rate is lower than that of plants adopting the instantaneous strategy only at the beginning, but exceeds the latter quickly, leading to a higher total net carbon gain over the whole dry-down period. Results from both the instantaneous and dynamic feedback strategies are consistent with the range of values measured during a dry down experiment from Venturas *et al.* (2018) (Fig. 1, gray dots).

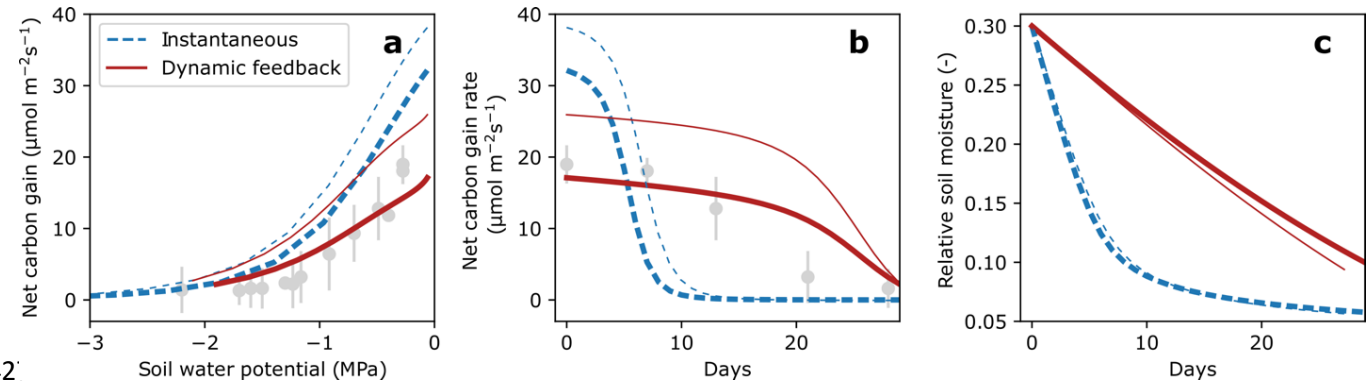

Figure 1. Contrasting behaviors of instantaneous and dynamic feedback strategies are shown for (a) net carbon gain rate as function of soil water potential, (b) net carbon gain rate during a single dry-down, and (c) the resulting relative soil moisture over time, in the absence of competition for water and permanent xylem embolism. Color indicates the strategy: the dynamic feedback (red solid) and

instantaneous (blue dashed) stomatal optimization strategies. Thick lines correspond to a scenario with I_{PAR} = 2000 µmol m^{-2} s^{-1} and D=0.03 mol mol^{-1}, and thin lines with I_{PAR} = 1000 µmol m^{-2} s^{-1} and D=0.015 mol mol^{-1}. The gray dots indicate corresponding measured values from aspen saplings in the severe drought experiment from Venturas et al. (2018), with grey lines showing the confidence intervals. The initial relative soil water availability is s_0 = 0.3 and the duration of the dry-down is 30 days. Soil parameters are b = 3.1, Ψ_s = -0.0015 MPa, with porosity n = 0.38 and effective plant rooting depth Z = 0.1 m. All other parameter values are as listed in Table 2.

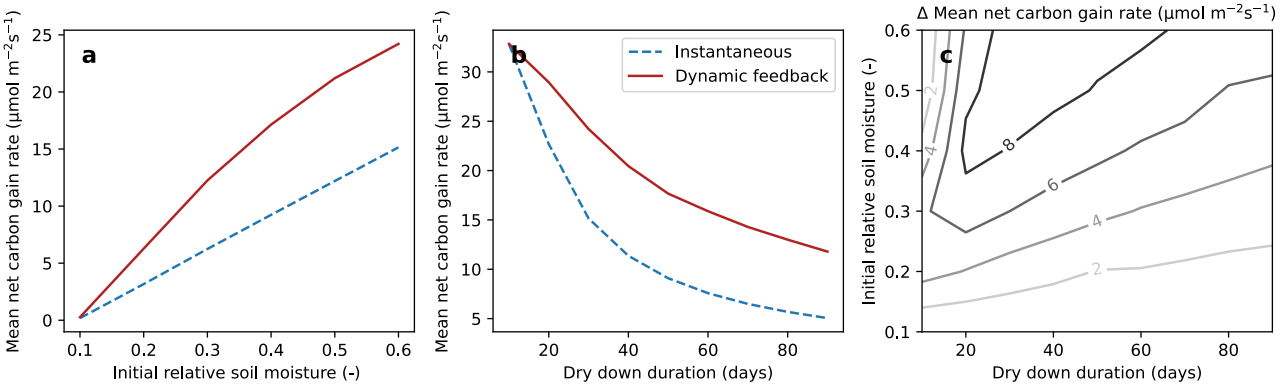

Figure 2. Total net carbon gain during a single dry-down for both the dynamic feedback and instantaneous strategies under varying (a) initial relative soil water availability and (b) dry down duration. The difference in net carbon gain between the dynamic feedback strategy and the instantaneous strategy are shown in (c) under a combination of dry down duration and initial soil moisture conditions. All parameter values are the same as listed in Table 2.

The advantage of dynamic feedback strategy over the instantaneous strategy during a single dry down varies under different dry down durations and initial soil water availabilities. The difference in the cumulative net carbon gain between the dynamic feedback strategy and the instantaneous strategy increases with increasing initial soil water availability at an intermediate dry down duration (Fig. 2c).

The same pattern between the instantaneous and dynamic feedback strategies emerges in the stochastic rainfall scenario (Table 3, Scenario 2). Here, the stochastic rainfall scenario can be represented by a consecutive series of dry downs (Fig. 3). Like the single dry down case, the instantaneous strategy tends to exhibit more aggressive water uptake that results temporarily in higher stomatal conductance and carbon gain at the beginning of each dry down (Fig. 3b, c), but more quickly depletes available soil moisture (Fig. 3a). As a result, the dynamic feedback stomatal optimization

strategy results in higher expected carbon gain than the instantaneous one across gradients of rainfall frequency and mean annual precipitation (Fig. 4). Also, the relative advantage of the dynamic feedback optimization strategy increases in drier climates, as the difference in net carbon gain rate between the dynamic feedback and the instantaneous strategy increases with more drought-like conditions represented by decrease in mean annual precipitation and rainfall frequency (Fig. 4b).

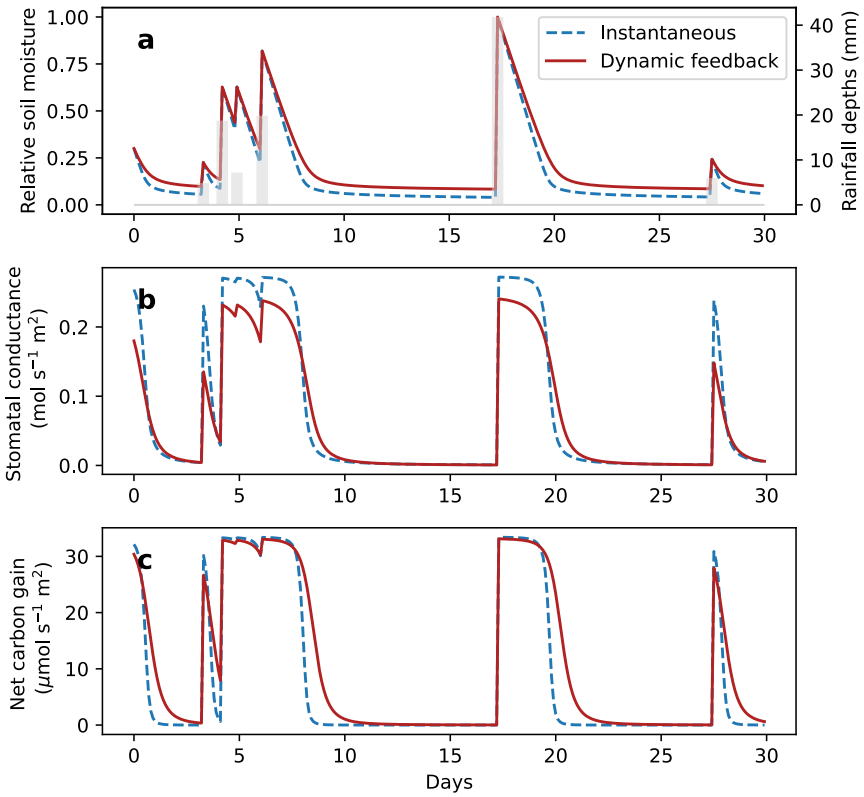

Figure 3: The relative moisture (a), stomatal conductance (b), and and net carbon gain (c) of instantaneous versus dynamic feedback strategies simulated over an arbitrary 30 day period over a stochastic rainfall scenario. Frequency of rainfall is set to λ = 0.15 d^{-1} with mean annual precipitation of 1000 mm (i.e., α = 18.3 mm). Light grey bars in (a) show rainfall events. All other parameters are as listed in Table 2.

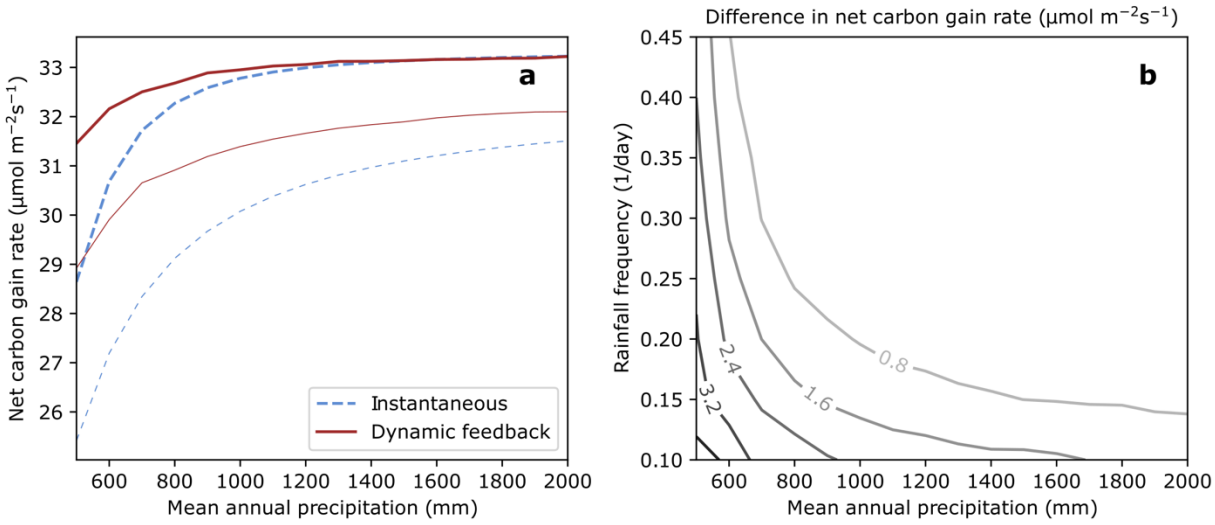

Figure 4. (a) The expected value of net carbon gain rates under stochastic rainfall for the instantaneous (blue dashed) and dynamic feedback (red solid) stomatal optimization strategies and (b) their difference for a range of mean annual precipitation and rainfall frequencies. These simulations are produced in the absence of competition for water and permanent xylem embolism. Line width in panel (a) indicates the rainfall frequency: λ = 0.15 d^{-1} (thin) and 0.30 d^{-1} (thick). All other parameters are same as listed in Table 2.

4.2. Effect of combined soil-plant feedback and permanent xylem damage on optimal stomatal conductance

Considering permanent xylem embolism as an additional legacy effect on top of soil-plant feedback shows an even larger advantage of the dynamic feedback strategy over the instantaneous strategy, because the aggressive water uptake adopted by the instantaneous strategy always leads to 100% xylem embolism in the simulations. In the single dry-down scenario (Table 3, Scenario 5; Fig. 5), we consider that plants can only refill 50% of the embolized xylem. In this case, the instantaneous stomatal optimization strategy – in the absence of other physiological or phenological adjustments (e.g., leaf area) – leads to a complete loss of xylem hydraulic conductivity toward the end of the dry-down period (Fig. 5c, blue dashed lines). This potentially fatal consequence results from the lack of considering the legacy effects of permanent xylem embolism in the optimization. That is, this strategy maximizes the current net carbon gain rate without considering how resulting damage to the xylem hydraulic conductivity can reduce future carbon gain. In contrast, by accounting for the legacy effect of

permanent xylem damage, the dynamic feedback strategy keeps the permanent xylem damage at very low levels by restraining excessive water consumption (Fig. 5c, red solid lines). By doing so, the dynamic feedback strategy also manages to maintain higher soil water availability (Fig. 5b) and relatively high net carbon gain rate (Fig. 5a) throughout the whole dry-down period, resulting in cumulatively higher net carbon gain.

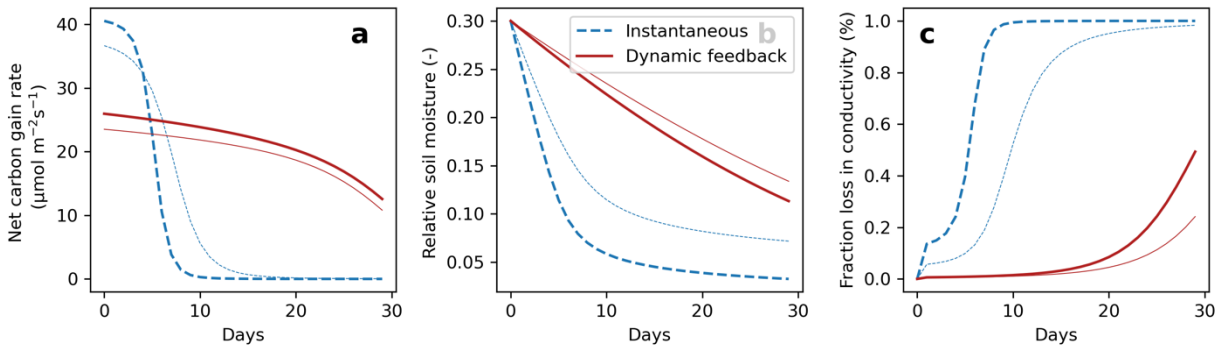

Figure 5. The dynamics of net carbon gain rate (a), relative soil moisture (b), and fraction loss in conductivity (c) during a single dry-down in the absence of competition for water. Color indicates the strategy: the dynamic feedback (red) and instantaneous (blue) stomatal optimization strategies. Line width indicates different values of water potential at 50% xylem cavitation: -1 MPa (thin) and -2 MPa (thick). In this simulation, we consider plants can refill 50% of the embolized xylem. The simulation lasts for 30 days and the initial relative soil water availability is 0.3 m^3 m^{-3}. All other parameter values are as listed in Table 2.

Because the instantaneous stomatal optimization strategy will eventually reach complete hydraulic failure when including the legacy effect imposed by (partially or completely) irreparable xylem embolism, any viable strategy will win against this strategy under competition. This is the case both during a single dry-down and under stochastic rainfall (Table 3, Scenarios 7 & 8). We have verified that the dynamic feedback stomatal optimization strategy does exist and manages to control the permanent xylem embolism with or without competition for water. In Fig. S1, we show how the expected net carbon gain rate of the dynamic feedback strategy changes with the local rainfall regime. However, when plants can always completely refill the embolized xylem, the instantaneous and dynamic feedback stomatal optimization strategies become identical under competition (Scenarios 3 & 4; Wolf *et al.*, 2016; Lu *et al.*, 2020).

In Table 3, we summarize the main conclusion in each of the comparisons that we have conducted. As mentioned above, the instantaneous stomatal optimization is either less productive or not viable in most comparisons with only one exception: in the presence of competition for water, the instantaneous and dynamic feedback stomatal optimization strategies are identical when plants can instantaneously and completely refill the embolized xylem (Wolf *et al.*, 2016; Lu *et al.*, 2020) (Table 3, Scenarios 3 & 4), which implies that plants can entirely eliminate the legacy effects of xylem embolism.

Table 3. A summary of the simulation results. In this table, the instantaneous and dynamic feedback stomatal optimization strategies are denoted by 'IS' and 'DS', respectively. EES refers to evolutionarily stable strategy. Lu *et al.* (2020)

No.	Permanent embolism	Competition	Dry-down scenario	Outcome	Support
1	No	No	Single dry-down	IS is less productive.	Figure 1 & 2
2			Stochastic rainfall	IS is less productive.	Figure 3 & 4
3		Yes	Single dry-down	IS and DS are identical and evolutionarily stable.	Lu *et al.* (2020)
4			Stochastic rainfall	IS and DS are identical and evolutionarily stable.	Lu *et al.* (2020)
5	Yes	No	Single dry-down	IS will reach 100% loss of hydraulic conductivity.* DS is optimal.	Figure 5
6			Stochastic rainfall	IS will reach 100% loss of hydraulic conductivity. DS is optimal.	Figure S1
7		Yes	Single dry-down	IS will reach 100% loss of hydraulic conductivity.*	Lu *et al.* (2020)
8			Stochastic rainfall	IS will reach 100% loss of hydraulic conductivity. DS is ESS.	Figure S1 Lu *et al.* (2020)

*During a single dry-down, the instantaneous stomatal optimization strategy may not reach 100% loss of hydraulic conductivity if the dry-down ends soon enough.

5. DISCUSSION

Although both the instantaneous and the dynamic feedback strategy can produce predictions that are comparable to measurements (Figure 1), the sensitivity of these model results to prescribed parameters (and the uncertainties associated with measuring those parameters) means that the validity of the assumptions embedded in these strategies cannot be established based on existing empirical evidence alone. Instead, we demonstrate the implications of those assumptions by 'pushing' drydowns to extended periods either deterministically (in the case of a single drydown) or statistically (in the case of stochastic simulations through λ). We have shown that, due to legacy effects, the instantaneous strategy (maximizing instantaneous carbon gain) is neither optimal in the absence of competition nor evolutionarily stable. The legacy effects that render the instantaneous strategy suboptimal are represented in our analysis by soil-plant feedback and permanent xylem embolism. Each of them effectively introduces a temporal tradeoff between the current and future carbon gain that encourages plants to leave some water for future use when it is abundant or, equivalently, discourages excessive instantaneous water consumption. In the absence of plant competition for water, these temporal tradeoffs explain why maximizing instantaneous carbon gain lowers the cumulative carbon gain over time. In long-term, stochastic rainfall scenarios, the advantages of the dynamic feedback strategy over the instantaneous strategy increases under drought-like conditions, with lower mean annual precipitation or rainfall frequency (Figure 4). In these scenarios we have set other environmental variables like vapor pressure deficit and temperature to be constant because they do not impose legacy effects on plants. However, the sensitivity of the results to variations in these external forcings remains to be investigated.

For plants with shared access to water, water competition motivates plants adopt an instantaneous strategy even under a limited water supply – they must use up water quickly so that the water will not be used by their neighbors. Indeed, we have shown that the ESS framework effectively eliminates the legacy effects of soil-plant feedback (Eq. 5). Consequently, although the instantaneous and dynamic feedback stomatal optimization strategies still differ in the objective function used for stomatal optimization, they arrive at the same mathematical results (Lu *et al.*, 2020) and provide the rationale for the instantaneous stomatal optimization model by Wolf *et al.*, (2016). Nevertheless, competition cannot eliminate the influence of other legacy effects (such as permanent xylem damage) on the optimal stomatal strategy. In a scenario where the xylem is only partially (i.e., not completely) recoverable, we have also shown that the instantaneous stomatal optimization strategy will inevitably lead to hydraulic failure (Fig. 5) due to its aggressive water use. In contrast, the dynamic feedback stomatal optimization

552 strategy is not only viable but also evolutionarily stable. The dynamically optimal strategy is achieved by
553 controlling the soil water availability at a level that is both too high for any more conservative strategy
554 (with lower stomatal conductance and less damage in the xylem) and too low for any more aggressive
555 strategy (with higher stomatal conductance and more damage in the xylem) to be more productive (Lu
556 *et al.*, 2020).

557 In addition to the legacy effects related soil-plant feedback and permanent xylem embolism examined
558 here, there exist other legacy effects that may also play a significant role in stomatal optimization. Each
559 of these legacy effects can be associated with a different state variable that is dynamically regulated by
560 plants themselves and, in turn, affects plants' carbon gain over time. These state variables may be
561 internal to the plant, such as xylem vulnerability incurred due to water stress, or external to the plant,
562 such as the soil water availability that is subject to soil-plant feedback. Here we discuss three examples
563 of potential legacy effects due to: 1) leaf growth (constrained by plant carbon balance), 2) leaf aging
564 (constrained by RuBisCo synthesis and degradation), and 3) decline in plant hydraulic capacity due to
565 salinity (constrained by soil salt balance). By coordinating its carbon stores with water balance, plants
566 can allocate carbon toward leaf growth over time (Schymanski *et al.*, 2009). Because total leaf area also
567 influences the total transpiration rate (and thus future water availability), this allows plants to adopt a
568 dynamic feedback carbon maximization strategy that can be scaled from the leaf level (by considering
569 stomatal regulation only) to the whole-plant level (by considering stomatal regulation simultaneously
570 with leaf area; Bassiouni & Vico, 2021). By coordinating the temporal tradeoff in carbon investments
571 towards leaf growth or maintenance, plants can increase mean WUE over the course of leaf life span.
572 However, this process can be complicated by the decline in leaf photosynthetic capacity due to leaf
573 ageing (Kikuzawa, 1991; Kitajima *et al.*, 2002), which can introduce additional constraints to carbon
574 maximization. Detto & Xu (2020) shows that given the tradeoffs between total costs of RuBisCO
575 synthesis and degradation, as well as other chemical and mechanical defenses, plants can optimize the
576 control of the maximum carboxylation velocity, V_{cmax}, for the maximum cumulative photosynthesis and
577 total carbon gain over the leaf's lifespan. Finally, salinity limits water movement from the soil to the leaf
578 and thus gas exchange (Perri *et al.*, 2019; Qiu & Katul, 2020), similarly to the effect of xylem embolism.
579 Thus, we can expect stomatal regulation to also influence the plant's ambient salinity by controlling the
580 chemical equilibrium between leaf and soil salt concentrations through transpiration (which decreases
581 soil water and increases salinity).

All these legacy effects indicate that a modeling framework that can accommodate both the current and future impacts of plants' behavior is essential to understand stomatal regulation, and more generally, the whole-plant water use strategy, based on the optimality principle. However, due to its modeling framework, the instantaneous stomatal optimization approach fundamentally lacks the ability to incorporate these dynamical feedbacks. Competition can eliminate the legacy effects on optimal stomatal response when the legacy effects are caused by variables external to the plant (such as soil water availability in the case of soil-plant feedback). In this case, competition will remove any water 'saved' for future use. However, when the legacy effects occur internally (such as in the case of permanent xylem damage), competition with neighbors will no longer compensate for the influence of legacy effects on the optimal stomatal response. That is, competition will not mitigate the impacts of reduced long-term hydraulic conductance caused by aggressive current water use. In those cases, the more aggressive stomatal strategy resulting from the instantaneous optimization will no longer coincide with the ESS.

6. CONCLUSIONS

In conclusion, legacy effects – the reduction in future carbon gain due to excessive current water use – will always render instantaneous stomatal optimization suboptimal in terms of long-term carbon gain. The presence of water competition may mitigate the impacts of some, but not all, types of legacy effects. This means that the instantaneously optimal stomatal strategy is equivalent to the ESS only under limited scenarios and is by no means a general result (Wolf *et al.*, 2016). Legacy effects are likely ubiquitous in nature, most commonly introduced through conserved quantities like soil water supply (e.g., the more water used now the less will be available for later) but also through long-term reduction in water uptake capacity due to xylem damage (e.g., the more water used now the less water can be acquired later). Given its success in reproducing empirical land surface fluxes (Eller *et al.*, 2020; Sabot *et al.*, 2020; Bassiouni & Vico, 2021; Harrison *et al.*, 2021), the instantaneous stomatal optimization models provide a phenomenological, 'macroscopic' representation of complex biological phenomena, aggregating numerous 'microscopic' processes involved in stomatal aperture adjustments, from genetic coding to physical and chemical signaling between roots and leaf. However, instantaneous stomatal optimization does not offer any finality to the dynamics of g_s. So while it has been shown to capture observed stomatal responses to short-term atmospheric forcing, it also has known limitations in representing long-term stomatal responses, especially with respect to elevated CO_2 concentrations (Katul *et al.*, 2009, 2010; Medlyn *et al.*, 2011; Buckley & Schymanski, 2014).

What is needed to bridge the practicality and ease of use of instantaneous models and their theoretical grounding is a means for understanding the timescales over which sacrificing short-term gain for long-term fitness may provide a selective advantage for plants. Such reconciliation between instantaneous and time-integrated optimization has also been previously explored using the marginal carbon profit and cost of water, while emphasizing the role of whole plant carbon balance (Buckley & Schymanski, 2014). Here, if we compare the instantaneous solutions against the dynamic feedback solution derived using the same instantaneous cost function (say, designated by θ) then we have shown here that the dynamic feedback solution derived from the same cost function will always outperform the instantaneous solution in the absence of competition. Then, a related and open question is this: what is the "effective" cost function – denoted θ' – that mimics the long-term effects of θ? We can surmise that θ' cannot simply be a linear function of θ, as simply scaling the cost function will not yield a different optimal value (but only increase or decrease the carbon gain associated with that optimal value). Therefore, the ratio of θ' to θ must necessarily be a function of water availability or plant water potential. This makes intuitive sense, as the ratio of θ' to θ represents a tradeoff between the current and future cost of water, which should theoretically vary due to water availability and plant hydraulic state. Future work can attempt to resolve the form of this exchange ratio and how it can be informed by the various timescales of environmental variabilities and the degree to which plant stomatal regulation are coupled to those variabilities.

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AUTHOR CONTRIBUTIONS

Y.L. and X.F. conceptualized, designed, and performed the research; X.F. and Y.L. wrote the manuscript. All other authors, listed alphabetically, contributed to refining the ideas presented in this paper, interpreting the data, and editing the manuscript.

REFERENCES

Anderegg WRL, Anderegg LDL, Berry JA, Field CB. **2014**. Loss of whole-tree hydraulic conductance during severe drought and multi-year forest die-off. *Oecologia* **175**: 11–23.

Anderegg WRL, Wolf A, Arango-Velez A, Choat B, Chmura DJ, Jansen S, Kolb T, Li S, Meinzer FC, Pita P, *et al.* 2018. Woody plants optimise stomatal behaviour relative to hydraulic risk. *Ecology Letters* **21**: 968–977.

Ball JT, Woodrow IE, Berry JA. **1987**. A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: Progress in photosynthesis research. Springer, 221–224.

Bassiouni M, Vico G. **2021**. Parsimony vs predictive and functional performance of three stomatal optimization principles in a big-leaf framework. *New Phytologist* **231**: 586–600.

Blackman CJ, Creek D, Maier C, Aspinwall MJ, Drake JE, Pfautsch S, O'grady A, Delzon S, Medlyn BE, Tissue DT. **2019**. Drought response strategies and hydraulic traits contribute to mechanistic understanding of plant dry-down to hydraulic failure. *Tree Physiology* **39**: 910–924.

Buckley TN. **2021**. Optimal carbon partitioning helps reconcile the apparent divergence between optimal and observed canopy profiles of photosynthetic capacity. *New Phytologist* **230**: 2246–2260.

Buckley TN, Miller JM, Farquhar GD. **2002**. The mathematics of linked optimisation for water and nitrogen use in a canopy. *Silva Fennica* **36**: 639–669.

Buckley TN, Sack L, Farquhar GD. **2017**. Optimal plant water economy. *Plant Cell and Environment* **40**: 881–896.

Buckley TN, Schymanski SJ. **2014**. Stomatal optimisation in relation to atmospheric CO2. *New Phytologist* **201**: 372–377.

Campbell GS. **1974**. A simple method for determining unsaturated conductivity from moisture retention data. *Soil science* **117**: 311–314.

Cowan IR. **1982**. Regulation of water use in relation to carbon gain in higher plants. In: Physiological plant ecology II. Springer, 589–613.

Cowan I. **1986**. Economics of carbon fixation in higher plants. *On the economy of plant form and function:*

Cowan IR, Farquhar GD. **1977**. Stomatal function in relation to leaf metabolism and environment. *Symposia of the Society for Experimental Biology* **31**: 471–505.

Cowan IR, Troughton JH. **1971**. The relative role of stomata in transpiration and assimilation. *Planta* **97**: 325–336.

DeLucia EH, Heckathorn SA. **1989**. The effect of soil drought on water-use efficiency in a contrasting Great Basin desert and Sierran montane species. *Plant, Cell & Environment* **12**: 935–940.

Detto M, Xu X. **2020**. Optimal leaf life strategies determine Vc,max dynamic during ontogeny. *New Phytologist* **228**: 361–375.

Eller CB, Rowland L, Mencuccini M, Rosas T, Williams K, Harper A, Medlyn BE, Wagner Y, Klein T, Teodoro GS, *et al.* 2020. Stomatal optimization based on xylem hydraulics (SOX) improves land surface model simulation of vegetation responses to climate. *New Phytologist* **226**: 1622–1637.

Eller CB, Rowland L, Oliveira RS, Bittencourt PRL, Barros F V., Da Costa ACL, Meir P, Friend AD, Mencuccini M, Sitch S, *et al.* 2018. Modelling tropical forest responses to drought and El Niño with a stomatal optimization model based on xylem hydraulics. *Philosophical Transactions of the Royal Society B: Biological Sciences* **373**.

Feng X, Ackerly DD, Dawson TE, Manzoni S, McLaughlin B, Skelton RP, Vico G, Weitz AP, Thompson SE. **2019**. Beyond isohydricity: The role of environmental variability in determining plant drought responses. *Plant Cell and Environment* **42**: 1104–1111.

Gentine P, Green JK, Guérin M, Humphrey V, Seneviratne SI, Zhang Y, Zhou S. **2019**. Coupling between the terrestrial carbon and water cycles - A review. *Environmental Research Letters* **14**.

Givnish TJ, Vermeij GJ. **1976**. Sizes and shapes of liane leaves. *The American Naturalist* **110**: 743–778.

Hari P, Mäkelä A, Korpilahti E, Holmberg M. **1986**. Optimal control of gas exchange. *Tree Physiology* **2**: 169–175.

Harrison SP, Cramer W, Franklin O, Prentice IC, Wang H, Brännström Å, de Boer H, Dieckmann U, Joshi J, Keenan TF, *et al.* 2021. Eco-evolutionary optimality as a means to improve vegetation and land-surface models. *New Phytologist* **231**: 2125–2141.

Hetherington AM, Woodward FI. **2003**. The role of stomata in sensing and driving environmental change. *Nature* **424**: 901–908.

Hills A, Chen ZH, Amtmann A, Blatt MR, Lew VL. **2012**. Onguard, a computational platform for quantitative kinetic modeling of guard cell physiology. *Plant Physiology* **159**: 1026–1042.

Hochberg U, Rockwell FE, Holbrook NM, Cochard H. **2018**. Iso/Anisohydry: A Plant–Environment Interaction Rather Than a Simple Hydraulic Trait. *Trends in Plant Science* **23**: 112–120.

Huang C-W, Domec J-C, Palmroth S, Pockman WT, Litvak ME, Katul GG. **2018**. Transport in a coordinated soil-root-xylem-phloem leaf system. *Advances in water resources* **119**: 1–16.

Hubbard RM, Ryan MG, Stiller V, Sperry JS. **2001**. Stomatal conductance and photosynthesis vary linearly with plant hydraulic conductance in ponderosa pine. *Plant, Cell and Environment* **24**: 113–121.

Jarvis PG. **1976**. The interpretation of the variations in leaf water potential and stomatal conductance found in canopies in the field. *Philosophical Transactions of the Royal Society of London. B, Biological*

Sciences **273**: 593–610.

Katul G, Manzoni S, Palmroth S, Oren R. **2010**. A stomatal optimization theory to describe the effects of atmospheric CO2 on leaf photosynthesis and transpiration. *Annals of botany* **105**: 431–442.

Katul GG, Oren R, Manzoni S, Higgins C, Parlange MB. **2012**. Evapotranspiration: a process driving mass transport and energy exchange in the soil-plant-atmosphere-climate system. *Reviews of Geophysics* **50**.

Katul GG, Palmroth S, Oren R. **2009**. Leaf stomatal responses to vapour pressure deficit under current and CO2-enriched atmosphere explained by the economics of gas exchange. *Plant, Cell and Environment* **32**: 968–979.

Kikuzawa K. **1991**. A Cost-Benefit Analysis of Leaf Habit and Leaf Longevity of Trees and Their Geographical. *The American Naturalist* **138**: 1250–1263.

Kitajima K, Mulkey SS, Samaniego M, Joseph Wright S. **2002**. Decline of photosynthetic capacity with leaf age and position in two tropical pioneer tree species. *American Journal of Botany* **89**: 1925–1932.

Konings AG, Katul GG, Porporato A. **2010**. The rainfall-no rainfall transition in a coupled land-convective atmosphere system. *Geophysical Research Letters* **37**: 1–5.

Konrad W, Katul G, Roth-Nebelsick A, Grein M. **2017**. A reduced order model to analytically infer atmospheric CO2 concentration from stomatal and climate data. *Advances in Water Resources* **104**: 145–157.

Konrad W, Katul G, Roth-Nebelsick A, Jensen KH. **2018**. Xylem functioning, dysfunction and repair: A physical perspective and implications for phloem transport. *Tree Physiology* **39**: 243–261.

Laio F, Porporato A, Ridol L, Rodriguez-iturbe I. **2001**. Plants in water-controlled ecosystems: active role in hydrologic processes and response to water stress II. Probabilistic soil moisture dynamics. *Advances in Water Resources* **24**: 707–723.

Lebrija-Trejos E, Pérez-García EA, Meave JA, Bongers F, Poorter L. **2010**. Functional traits and environmental filtering drive community assembly in a species-rich tropical system. *Ecology* **91**: 386–398.

Leuning R. **1995**. A critical appraisal of a combined stomatal-photosynthesis model for C3 plants. *Plant, Cell & Environment* **18**: 339–355.

Lu Y, Duursma RA, Farrior CE, Medlyn BE, Feng X. **2020**. Optimal stomatal drought response shaped by competition for water and hydraulic risk can explain plant trait covariation. *New Phytologist* **225**: 1206–1217.

Lu Y, Duursma RA, Medlyn BE. **2016**. Optimal stomatal behaviour under stochastic rainfall. *Journal of Theoretical Biology* **394**: 160–171.

Mäkelä A, Berninger F, Hari P. **1996**. Optimal control of gas exchange during drought: Theoretical analysis. *Annals of Botany* **77**: 461–468.

Manoli G, Domec J, Novick K, Oishi AC, Noormets A, Marani M, Katul G. **2016**. Soil–plant–atmosphere conditions regulating convective cloud formation above southeastern US pine plantations. *Global change biology* **22**: 2238–2254.

Manzoni S, Vico G, Palmroth S, Porporato A, Katul G. **2013**. Optimization of stomatal conductance for

maximum carbon gain under dynamic soil moisture. *Advances in Water Resources* **62**: 90–105.

Martin-StPaul N, Delzon S, Cochard H. **2017**. Plant resistance to drought depends on timely stomatal closure. *Ecology Letters* **20**: 1437–1447.

Maynard Smith J. **1974**. The theory of games and the evolution of animal conflicts. *Journal of Theoretical Biology* **47**: 209–221.

Medlyn BE, Duursma RA, Eamus D, Ellsworth DS, Prentice IC, Barton CVM, Crous KY, De Angelis P, Freeman M, Wingate L. **2011**. Reconciling the optimal and empirical approaches to modelling stomatal conductance. *Global Change Biology* **17**: 2134–2144.

Mockus J. **2012**. *Bayesian approach to global optimization: theory and applications*. Springer Science & Business Media.

Mrad A, Sevanto S, Domec J-C, Liu Y, Nakad M, Katul G. **2019**. A Dynamic Optimality Principle for Water Use Strategies Explains Isohydric to Anisohydric Plant Responses to Drought. *Frontiers in Forests and Global Change* **2**.

Nogueira F. **2014**. Bayesian Optimization: Open source constrained global optimization tool for Python. *GitHub. See https://github. com/fmfn/BayesianOptimization*.

Palmroth S, Katul GG, Maier CA, Ward E, Manzoni S, Vico G. **2013**. On the complementary relationship between marginal nitrogen and water-use efficiencies among Pinus taeda leaves grown under ambient and CO 2-enriched environments. *Annals of Botany* **111**: 467–477.

Perri S, Katul GG, Molini A. **2019**. Xylem–phloem hydraulic coupling explains multiple osmoregulatory responses to salt stress. *New Phytologist* **224**: 644–662.

Porporato A, Daly E, Rodriguez-iturbe I. **2004**. Soil water balance and ecosystem response to climate change. *The American naturalist* **164**: 625–632.

Prentice IC, Dong N, Gleason SM, Maire V, Wright IJ. **2014**. Balancing the costs of carbon gain and water transport: Testing a new theoretical framework for plant functional ecology. *Ecology Letters* **17**: 82–91.

Qiu R, Katul GG. **2020**. Maximizing leaf carbon gain in varying saline conditions: an optimization model with dynamic mesophyll conductance. *The Plant Journal* **101**: 543–554.

Rodriguez-Iturbe I, Porporato A, Ridolfi L, Isham V, Cox DR, Coxi DR. **1999**. Probabilistic modelling of water balance at a point: the role of climate , soil and vegetation. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **455**: 3789–3805.

Sabot MEB, De Kauwe MG, Pitman AJ, Medlyn BE, Verhoef A, Ukkola AM, Abramowitz G. **2020**. Plant profit maximization improves predictions of European forest responses to drought. *New Phytologist* **226**: 1638–1655.

Schymanski SJ, Sivapalan M, Roderick ML, Hutley LB, Beringer J. **2009**. An optimality-based model of the dynamic feedbacks between natural vegetation and the water balance. *Water Resources Research* **45**: 1–18.

Siqueira M, Katul G, Porporato A. **2009**. Soil moisture feedbacks on convection triggers: The role of soil–plant hydrodynamics. *Journal of Hydrometeorology* **10**: 96–112.

Sperry JS, Hacke UG, Oren R, Comstock JP. **2002**. Water deficits and hydraulic limits to leaf water

supply. *Plant, Cell and Environment* **25**: 251–263.

Sperry JS, Love DM. **2015**. What plant hydraulics can tell us about responses to climate-change droughts. *New Phytologist* **207**: 14–27.

Sperry JS, Venturas MD, Anderegg WRL, Mencuccini M, Mackay DS, Wang Y, Love DM. **2017a**. Predicting stomatal responses to the environment from the optimization of photosynthetic gain and hydraulic cost. *Plant Cell and Environment* **40**: 816–830.

Sperry JS, Venturas MD, Anderegg WRL, Mencuccini M, Mackay DS, Wang Y, Love DM. **2017b**. Predicting stomatal responses to the environment from the optimization of photosynthetic gain and hydraulic cost. *Plant Cell and Environment* **40**: 816–830.

Stocker BD, Wang H, Smith NG, Harrison SP, Keenan TF, Sandoval D, Davis T, Prentice IC. **2020**. P-model v1.0: An optimality-based light use efficiency model for simulating ecosystem gross primary production. *Geoscientific Model Development* **13**: 1545–1581.

Venturas MD, Sperry JS, Love DM, Frehner EH, Allred MG, Wang Y, Anderegg WRL. **2018**. A stomatal control model based on optimization of carbon gain versus hydraulic risk predicts aspen sapling responses to drought. *New Phytologist* **220**: 836–850.

Wang Y, Sperry JS, Anderegg WRL, Venturas MD, Trugman AT. **2020**. A theoretical and empirical assessment of stomatal optimization modeling. *New Phytologist*: 311–325.

Wolf A, Anderegg WRL, Pacala SW. **2016**. Optimal stomatal behavior with competition for water and risk of hydraulic impairment. *Proceedings of the National Academy of Sciences of the United States of America* **113**: E7222–E7230.