Historical changes in the stomatal limitation of photosynthesis: empirical support for an optimality principle

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- The ratio of leaf-internal (c_i) to ambient (c_a) partial pressure of CO_2, defined here as χ, is an index of adjustments in both leaf stomatal conductance and photosynthetic rate to environmental conditions. Measurements and proxies of this ratio can be used to constrain vegetation models uncertainties for predicting terrestrial carbon uptake and water use.
- We test a theory based on the least-cost optimality hypothesis for modelling historical changes in χ over the 1951-2014 period, across different tree species and environmental conditions, as reconstructed from stable carbon isotopic measurements across a global network of 103 absolutely-dated tree-ring chronologies. The theory predicts optimal χ as a function of air temperature, vapour pressure deficit, c_a and atmospheric pressure.

- The theoretical model predicts 39% of the variance in χ values across sites and years, but underestimates the inter-site variability in the reconstructed χ trends, resulting in only 8% of the variance in χ trends across years explained by the model.
- Overall, our results support theoretical predictions that variations in χ are tightly regulated by the four environmental drivers. They also suggest that explicitly accounting for the effects of plant-available soil water and other site-specific characteristics might improve the predictions.

Keywords: leaf-internal CO_2 concentration, stable carbon isotopes, tree rings, optimality, least-cost hypothesis, water use efficiency

1. Introduction

The net uptake of atmospheric CO_2 by the terrestrial biosphere, which acts as a sink for about 30% of anthropogenic CO_2 emissions, has helped to reduce the increase in atmospheric CO_2 concentration – and therefore has dampened climate change – since the beginning of the industrial era (Le Quéré *et al.*, 2018). However, it is still unclear how atmospheric CO_2, climate, and other environmental changes will influence the future strength of the terrestrial carbon sink (Ciais *et al.*, 2013; Ballantyne *et al.*, 2015; Schimel *et al.*, 2015). It has been suggested that the magnitude of net terrestrial carbon uptake is likely to decline in the future as a result of various mechanisms including resource limitations on the CO_2 'fertilization' effect due to nitrogen availability (Reich *et al.*, 2006; Reich & Hobbie, 2013), reduced water availability due to changes in the hydrological cycle (Zhao & Running, 2010; Humphrey *et al.*, 2018; Green *et al.*, 2019), or enhanced turnover of soil carbon due to warming (Knorr *et al.*, 2005; Li *et al.*, 2018). Yet, the extent to which these processes might affect the terrestrial carbon sink is still largely unknown, especially when considering the real possibility of plant adaptation and acclimation that may occur over decadal to longer timescales. Current models of the terrestrial biosphere incorporate different formulations of the underlying processes, including photosynthesis and leaf gas exchanges responses to varying CO_2 concentrations (Rogers *et al.*, 2017), the impact of soil moisture stress on photosynthesis and stomatal conductance (De Kauwe *et al.*, 2013), and carbon allocation and turnover (De Kauwe *et al.*, 2014) – leading to large differences in simulated terrestrial CO_2 uptake and future climate change. New metrics and proxies of key biological processes are thus needed to improve and reduce uncertainties in terrestrial models.

The ratio (hereafter termed χ) of leaf-internal (c_i) to ambient (c_a) partial pressure of CO_2 is a key metric of physiological function in plant leaves being determined by both stomatal conductance on the short term and photosynthetic biochemical capacity on longer time scales (Farquhar *et al.*, 1982). Thus, χ is the key variable for the study of carbon uptake. Under some conditions it can also provide insights into changes in intrinsic water-use efficiency (iWUE), i.e. the ratio of photosynthesis to stomatal conductance, defined as iWUE = c_a (1-χ)/1.6 (Ehleringer *et al.*, 1993). As there are many other definitions of water use efficiency by plants, each with different meanings (Lavergne *et al.*, 2019), analysis of data directly in terms of χ is preferred here. Plants assimilate the heavier $^{13}CO_2$ molecules less readily than $^{12}CO_2$ because of their slower diffusion through the stomata and preferential fixation of $^{12}CO_2$ by Rubisco, resulting in a discrimination against ^{13}C compared to ^{12}C, defined as $\Delta^{13}C$ (Park & Epstein, 1960). In C_3 plants, $\Delta^{13}C$ is principally determined by χ. Thus, reconstructing long-term effective values of χ from $\Delta^{13}C$ derived from stable isotope $^{13}C/^{12}C$ ratio ($\delta^{13}C$) measured in plant materials (including tree rings), or even in atmospheric CO_2, can offer valuable insights into stomatal and photosynthetic adjustments to environmental conditions. As air masses are transported and mixed rapidly in the turbulent lower atmosphere, $\Delta^{13}C$ values inferred from atmospheric $\delta^{13}CO_2$ are representative of processes occurring at regional (Ballantyne *et al.*, 2010; Peters *et al.*, 2018) or global (Keeling *et al.*, 2017) scales, while values derived from tree rings reflect ecophysiological processes at the individual plant level. Thus, $\delta^{13}C$ data from different sources can in principle be used to evaluate and improve the representation of stomatal and photosynthetic behaviour in models at different spatial scales. However, atmospheric $\delta^{13}CO_2$ is also influenced by many other processes, such as ocean-atmosphere gas exchange and isotope disequilibrium fluxes (Keeling *et al.*, 2017), complicating the derivation of long-term changes in χ using atmospheric data.

Formulations for $\Delta^{13}C$ have been included in vegetation models (Saurer *et al.*, 2014; Frank *et al.*, 2015; Raczka *et al.*, 2016; Keller *et al.*, 2017) and evaluated using existing observations as recommended by the Coupled Model Intercomparison Project Phase 6 (CMIP6), which coordinates current Earth System modelling activities internationally (Eyring *et al.*, 2016; Jones *et al.*, 2016). Yet some recent studies have shown that current models overestimate the decrease in $\Delta^{13}C$ (and the associated increase in water-use efficiency) over the 20^{th} century (Keller *et al.*, 2017) or simulate an increase in both $\Delta^{13}C$ and water-use efficiency at leaf level, which is inconsistent with biological theory (Raczka *et al.*, 2016). These studies demonstrate that $\Delta^{13}C$ can reveal explicit biases within the models. Errors in the simulation of $\Delta^{13}C$ can, however, be difficult to attribute to particular processes. Incomplete, empirical descriptions of the processes determining χ in vegetation models and incorrect assumptions about key parameters in the model of photosynthesis may cause discrepancies between observed and predicted $\Delta^{13}C$. Many models assign fixed parameter values to different plant functional types (PFTs) (Rogers *et al.*, 2017), but this approach overlooks the ability of plants (within any one PFT) to acclimate or adapt to environmental changes (Wullschleger *et al.*, 2014; Martínez-Sancho *et al.*, 2018; Dorado-Liñán *et al.*, 2019). Also, some of the processes linking c_i to $\Delta^{13}C$ have been neglected. The potential impact of fractionations during the transport of CO_2 from the intercellular space to the chloroplasts, and during photorespiration have been described

(Ubierna & Farquhar, 2014), and may be important to include when analysing historical trends (Seibt *et al.*, 2008; Keeling *et al.*, 2017; Schubert & Jahren, 2018; Lavergne *et al.*, 2019). Accordingly, there is a need to probe the assumptions about leaf gas exchange incorporated in such models, to include the known physiological and environmental processes influencing $\Delta^{13}C$, and to evaluate the resulting simulations with long-term carbon isotope data.

Simpler analytical models can provide an integrative approach to understand whole-plant responses to environmental changes via the general hypothesis that plants optimize their physiology towards maximizing fitness (Medlyn *et al.*, 2013; Dewar *et al.*, 2018). However, the trade-off between the benefits and costs of stomatal opening (carbon gain at the expense of water loss) and investments in photosynthetic biochemistry (requiring nitrogen and energy) is still not completely understood; in particular, the specific nature of the costs remains an open question. Different optimization hypotheses for the control of stomatal conductance have been proposed – reviewed in Buckley (2017) and Dewar *et al.* (2018) – that make different predictions of stomatal responses to the environment. The Cowan-Farquhar optimality hypothesis states that leaves maximize the difference between photosynthesis and the carbon cost of transpiration, i.e. $A - E/\lambda$, where A is the photosynthesis rate, E is the rate of transpiration and λ is an 'exchange rate' between carbon and water (Cowan & Farquhar, 1977; Katul *et al.*, 2010; Buckley & Schymanski, 2014; Sperry *et al.*, 2017). λ has usually been determined as a function of soil moisture (Manzoni *et al.*, 2013) and of xylem water potential (Wolf *et al.*, 2016; Sperry *et al.*, 2017). The Cowan-Farquhar optimality hypothesis, however, does not account for the costs of maintaining both water flow and photosynthetic capacity (Givnish, 1986). Following the least-cost optimality hypothesis proposed by Wright *et al.* (2003), Prentice *et al.* (2014) introduced the alternative criterion that leaves minimize the summed unit costs of transpiration and carboxylation, i.e. $(a_E E + b_V.V_{cmax})/A$, where a_E is the sapwood maintenance cost per unit of transpiration capacity and b_V is the cost associated with the maintenance of photosynthetic (carboxylation) capacity (V_{cmax}) (Rogers, 2014). Dewar *et al.* (2018) analysed another criterion, following Givnish (1986), whereby the cost of stomatal opening arises from nonstomatal reductions in photosynthesis induced by leaf water stress. The authors explored different hypotheses in which reduced leaf water potential leads to a reduction either in V_{cmax} or in mesophyll conductance. Predicted stomatal responses were broadly similar to those derived from the least-cost optimality hypothesis (Dewar *et al.*, 2018), although the reduction of V_{cmax} rather than mesophyll conductance provided a better fit across different PFTs (Gimeno *et al.*, 2019).

Here we test the theoretical framework implied by the least-cost optimality hypothesis for predicting long-term changes in χ across the globe, during a period of steadily increasing c_a (around 85 ppm over 1951–2014). Spatial patterns of χ predicted by the least-cost hypothesis have been supported by analyses of leaf $\delta^{13}C$ data at the regional (Bloomfield *et al.*, 2019) and global (Wang *et al.*, 2017b) scales. However, simulations of χ and its trends over the past decades using this model still await evaluation against long-term observations. Here we first reconstruct changes in χ over 1951-2014 using a global tree-ring $\delta^{13}C$ ($\delta^{13}C_{TR}$) network of 103 sites. We then compare model predictions and reconstructions for their spatial and temporal patterns and examine the sensitivity of predicted and isotope-derived χ to the environmental drivers of the model and other constraints. Our aim is to address the following questions: (1) Can temporal variations in χ – as indexed by long-term $\delta^{13}C_{TR}$ measurements – be predicted by the least-cost hypothesis? (2) How well do these predictions of χ reproduce the ratio's observed dependency on environmental drivers? Finally, (3) are there any other potential environmental controls on χ that should be considered in order to improve these predictions?

2. Material and methods

a. Observational dataset of χ

We compiled 103 absolutely-dated $\delta^{13}C_{TR}$ chronologies from published and unpublished materials representing different PFTs (DBF: deciduous broadleaf forest (*n* = 29) and ENF: evergreen needleleaf forest (*n* = 74)) and environmental contexts in the temperate and boreal zones, with at least 30 years of records over the 1951-2014 period when most data were available (Fig. 1; Table S1). $\delta^{13}C_{TR}$, i.e. the ratio of ^{13}C to ^{12}C of the wood component compared to an internationally accepted standard material, was derived from cellulose (with just two exceptions where bulk wood was used) and from either the whole ring (WR, *n* = 65; including both earlywood and latewood) or only latewood (LW, *n* = 38; Table S1). The analytical error in the $\delta^{13}C_{TR}$ measurements was typically ± 0.15‰. $\Delta^{13}C$ for each series was calculated as:

$$\Delta^{13}\mathrm{C} = \frac{\delta^{13}CO_2-(\delta^{13}C_{TR}-d)}{1+(\delta^{13}C_{TR}-d)/1000} \qquad \text{Eqn 1}$$

where $\delta^{13}CO_2$ is the stable isotopic composition of atmospheric CO_2 in the year of ring formation, and *d* (‰) quantifies the sum of discriminations beyond those associated with the production of the primary photosynthetic assimilates: 1.9‰ between leaf organic matter and bulk wood (Badeck *et al.*, 2005), and 2.1 ± 1.2‰ between leaf organic matter and α-cellulose (Frank *et al.*, 2015). For each year, $\Delta^{13}C$ was used to derive χ_{iso} (i.e. the isotope-derived χ) with the model from Farquhar *et al.* (1982) including an explicit fractionation term for photorespiration as recommended by several studies (e.g. Ubierna & Farquhar, 2014; Schubert & Jahren, 2018; Lavergne *et al.*, 2019) but assuming effectively infinite boundary layer and mesophyll conductances, and negligible fractionation during mitochondrial respiration (Ghashghaie *et al.*, 2003; Evans & Von Caemmerer, 2013):

$$\Delta^{13}\mathrm{C} = a + (b - a)\chi_{iso} - f\frac{\Gamma^*}{c_\mathrm{a}} \qquad \text{Eqn 2}$$

where *a*, *b* and *f* represent in turn: isotope fractionations due to CO_2 diffusion in air (4.4‰: Craig, 1953), effective Rubisco carboxylation (26-30‰) and photorespiration (8-16‰; Ubierna & Farquhar, 2014), respectively. Γ^* (Pa) is the CO_2 compensation point in the absence of mitochondrial respiration, i.e. the value of c_i at which the rate of photosynthetic CO_2 uptake equals that of photorespiratory CO_2 evolution, calculated from the temperature and pressure response: $\Gamma^* = \Gamma^*_{25}\ P_{atm}/P_0\ \exp[\Delta H_a.(T - 298)/(R.T.298)]$, with Γ^*_{25} the photorespiratory compensation point at 25°C, ΔH_a the activation energy for Γ^* (Bernacchi *et al.*, 2001), *T* the temperature, *R* the universal gas constant (Moldover *et al.*, 1988), and P_{atm} and P_0 the ambient and sea-level atmospheric pressures. Note that we did not consider mesophyll conductance (g_m) in our calculations because information on g_m, which is highly variable between species (von Caemmerer & Evans, 2015) and may fluctuate over long time periods (Flexas *et al.*, 2008), is generally lacking. Nevertheless, given the influence of g_m in the full discrimination model, we provide a sensitivity analysis in the Supporting Information (Text S1 and Fig. S1).

From Eqns 1 and 2, χ_{iso} can be written as:

$$\chi_{\mathrm{iso}} = \frac{\left(\frac{\delta^{13}CO_2 - (\delta^{13}C_{TR} - d)}{1 + (\delta^{13}C_{TR} - d)/1000}\right) - a + f\frac{\Gamma^*}{c_\mathrm{a}}}{b - a} \qquad \text{Eqn 3}$$

The choice of the values in Eqn 3 for the fractionation factors related to Rubisco carboxylation (*b*), photorespiration (*f*) and post-photosynthetic processes (*d*) does not affect the trend estimates of χ_{iso} but only modulates the mean χ_{iso} levels (Fig. S1). In the following, we have used the mean values from their range of uncertainties of *b* = 28‰ and *f* = 12‰ (Ubierna & Farquhar, 2014). Post-photosynthetic fractionations were assumed equal for all species (*d* = 2.1‰ for cellulose and 1.9‰ for bulk wood) because information quantifying these effects for individual species is sparse (Seibt *et al.*, 2008; Wingate *et al.*, 2008; Bowling *et al.*, 2008; Gessler *et al.*, 2014). Thus, we inevitably made some approximations that may have contributed to uncertainty in the reconstructed χ_{iso} values. Finally, to minimize the potential effect of mixing and turnover of non-structural carbohydrate pools of different ages and metabolic history in $\delta^{13}C_{TR}$ (Gessler *et al.*, 2014), we have aggregated the resulting χ_{iso} series into boxcar averages over a five-year period.

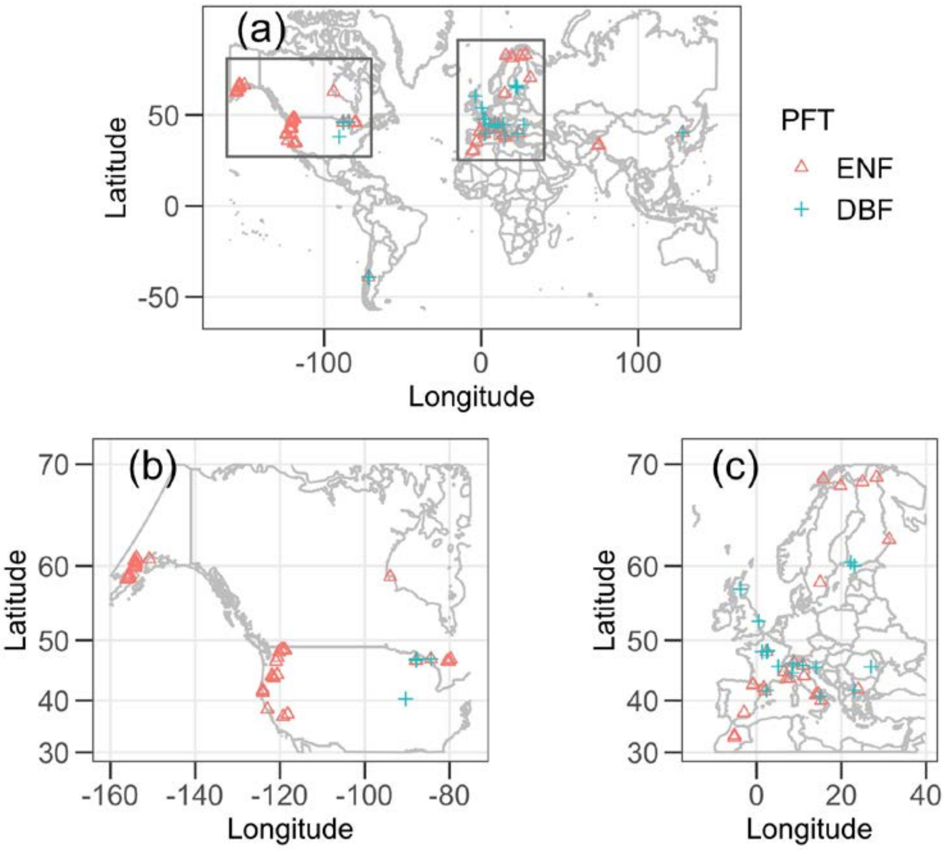

Fig. 1 (a) Location of the selected 103 tree-ring sites with carbon isotopic measurements (see Table S1 for details). Zoom over North America (b) and Europe (c) where the network is denser. PFT: plant functional type (DBF: deciduous broadleaf forest (n = 29) and ENF: evergreen needleleaf forest (n = 74)).

b. Prediction of χ following the optimality hypothesis

i. The theoretical model

The theory to predict χ (χ_{pred}, hereafter) following the least-cost optimality hypothesis has been introduced (Prentice *et al.*, 2014; Wang *et al.*, 2017b; Stocker *et al.*, 2019a) and applied in several recent studies (Dong *et al.*, 2017; Wang *et al.*, 2017a; Togashi *et al.*, 2018; Bloomfield *et al.*, 2019; Smith *et al.*, 2019). One of the strengths of the model is that there is no distinction among PFTs and biomes, except for the well-established differences between C_3 and C_4 plants, and therefore no fixed parameter defines the behaviour of the vegetation as in most current models (Rogers *et al.*, 2017). Thus, vegetation functions are allowed to evolve freely with environmental changes. The model is driven by P_{atm}, observed air temperature (T), vapour pressure deficit (D) and c_{a} at the selected time step (here, monthly) as follows:

$$\chi_{\mathrm{pred}} = \frac{c_{\mathrm{i}}}{c_{\mathrm{a}}} = \frac{\Gamma^*}{c_{\mathrm{a}}} + \left(1 - \frac{\Gamma^*}{c_{\mathrm{a}}}\right)\frac{\xi}{\xi + \sqrt{D}} \qquad \text{Eqn 4a}$$

where

$$\xi = \sqrt{\beta \frac{K+\Gamma^*}{1.6\eta^*}} \qquad \text{Eqn 4b}$$

ξ modulates the sensitivity of χ_{pred} to D, β (unitless) is the ratio of cost factors for carboxylation and transpiration ($b_{\mathrm{V}}/a_{\mathrm{E}}$) at 25°C, η^* is the viscosity of water relative to its value at 25°C, and K (Pa) is the effective Michaelis constant for Rubisco-limited photosynthesis at ambient partial pressure of O_2 (O, Pa) given by:

$$K = K_C\left(1 + \frac{O}{K_O}\right) \qquad \text{Eqn 5}$$

where K_{C} (Pa) and K_{O} (Pa) are the Michaelis constants of Rubisco for carboxylation and oxygenation, respectively. K and η^* are known functions of T and P_{atm}, and can be estimated following Bernacchi *et al.* (2001) and Huber *et al.* (2009), respectively. P_{atm} is calculated from elevation (z) following Allen *et al.* (1998). Only one free parameter is used here, i.e. β, whose values were estimated independently for ENF and DBF based on the tree-ring network of $\delta^{13}C$ data using Eqn 4 under the mean environmental conditions over the studied period (see Text S2; $\beta_{\mathrm{ENF}} = 176$ and $\beta_{\mathrm{DBF}} = 191$). Note that our assumption of a constant β is a practical approximation based on environmental conditions as β may vary over time, e.g., due to changes in soil moisture content (Stocker *et al.*, 2018, 2019b). Thus, the theoretical model does not explicitly account for potential effects of changes in soil moisture on χ (the potential impacts of soil moisture limitation on χ are discussed further below). Also, as $c_{\mathrm{a}} > \Gamma^*$ under field conditions, the theory predicts that χ is only slightly dependent on c_{a}. Overall, optimal χ

following the theory is expected to increase with increasing T but to decrease with increasing D and c_a, and decreasing P_{atm} (i.e. increasing z) (Wang *et al.*, 2017a).

ii. Driving data

Latitude and longitude were used to extract minimum and maximum temperatures (T_{min} and T_{max}, °C) and actual vapour pressure (e_a, hPa) for each site from monthly 0.5° resolution data provided by the Climatic Research Unit (CRU TS4.01; Harris *et al.*, 2014). When not provided by the authors (Table S1), z (km) used to infer P_{atm} were obtained from the WATCH Forcing Data methodology applied to ERA-Interim data (WFDEI) with 0.5° resolution (Weedon *et al.*, 2014) using the latitude and longitude of the site. Estimated z values from WFDEI dataset were in reasonably good agreement with those provided by authors, when available ($r^2 = 0.77$, $p < 0.001$; Fig. S2). Monthly atmospheric CO_2 concentrations (in ppm) for the 1958-2014 period were derived from in-situ direct measurements provided by the Scripps Institution of Oceanography (http://scrippsco2.ucsd.edu/data/atmospheric_co2/). For the 1951-1958 period, we interpolated the monthly CO_2 values using the mean seasonal cycle recorded over 1958-2014 and the yearly CO_2 values from a merged product based on ice core data and in-situ direct measurements (Fig. S3). The c_a dataset was first corrected for the elevation effect and converted into Pascals prior to being used for the analyses, as: c_a (Pa) = 10^{-6} $[CO_2]_{ppm}$ P_{atm}. Atmospheric $\delta^{13}CO_2$ data for the historical period of interest were extracted from a recent compilation by Graven *et al.* (2017).

We calculated the monthly mean daytime air T ($T_{daytime}$, °C) to consider only the part of the day when photosynthesis occurs, as:

$$T_{\text{daytime}} = T_{max}\left\{\frac{1}{2} + \frac{[\sqrt{(1-x^2)}]}{2arccosx}\right\} + T_{min}\left\{\frac{1}{2} - \frac{[\sqrt{(1-x^2)}]}{2arccosx}\right\} \quad \text{Eqn 6a}$$

where

$$x = -\tan\phi \tan\delta \quad \text{Eqn 6b}$$

with ϕ the latitude (°) and δ the average solar declination for the month (Jones, 2013).

Given our hypothesis of infinite boundary layer conductance in Eqn 3, we assumed equality of leaf and air temperatures. Monthly mean daytime D ($D_{daytime}$, kPa) was calculated following Allen *et al.* (1998) using $T_{daytime}$, monthly mean e_a and P_{atm} as:

$$D_{\text{daytime}} = 0.611e^{\left|\frac{8.635 \cdot T_{daytime}}{237.3+T_{daytime}}\right|} - 0.10e_a \frac{P_{atm}}{P_0}$$ Eqn 7

c. Model evaluation

For evaluating model predictions against reconstructions, the monthly χ_{pred} values initially calculated following Eqn 4 using the monthly mean daytime values of climate predictors (i.e. T_{daytime}, D_{daytime}) and c_{a} were aggregated as medians over the most productive months of the growing season to produce the growing-season χ_{pred} series. At each site the peak growing-season months, when most of the carbon to build the tree ring is fixed, were estimated based on a literature review (see Table S1). When no information was available, we assumed a growing season centred over summer months, i.e. June-August for the Northern hemisphere. We then aggregated the resulting yearly χ_{pred} series as five-year boxcar averages before comparing them with independently estimated, also five-year averaged χ_{iso}.

All statistical analyses were conducted in the open-source statistical environment R (R Core Team & R Development Core Team, 2018). We first compared the spatial and temporal patterns of χ between reconstructions and predictions before investigating potential biases in the predictions. The agreement between χ_{pred} and χ_{iso} values was assessed using the adjusted *R*-squared (R^2_{adj}), the root mean square error (RMSE), the Akaike information criterion (AIC; Akaike, 1973) and the Bayesian information criterion (BIC) using the R package performance (Lüdecke *et al.*, 2019); overall, lower RMSE, AIC and BIC values indicating greater explanatory power. The temporal changes in χ at each site for both reconstructions and predictions were quantified using the Theil-Sen estimator from the R package trend (Pohlert, 2018), which calculates a trend as the median of the slopes of all lines through pairs of points (Sen, 1968). Before estimating Theil-Sen trends, χ_{pred} and χ_{iso} values were converted into percentages of changes in χ relative to the site mean, in order to make the trends more comparable with each other:

$$\chi\ (\%) = \frac{\chi_t - \chi_{mean}}{\chi_{mean}} \times 100$$ Eqn 8

where χ_{t} and χ_{mean} are the values for χ at the time resolution considered (five years) and for the whole 1951-2014 period, respectively. The resulting χ trend estimates were compared between reconstructions and predictions using different linear regression models. We first applied the ordinary least squares (OLS) method for reducing the residuals in the linear regression and then applied the M-estimators method to perform robust linear regressions (RLM) using the R package MASS (Venables & Ripley, 2002). The M-estimators method is generally less sensitive to outliers than the OLS method. To assess the effect of temporal changes in growing-season mean T_{daytime} and D_{daytime} (hereafter T_g and D_g, respectively) on χ trends, we additionally calculated T_g and D_g trends following the same approach as described above.

As a further examination of the skill of the least-cost hypothesis, we investigated the relative dependencies of χ_{pred} and χ_{iso} values on the four drivers of the model using multiple linear regression. To do so, we first calculated the logit-transformed χ_{iso} and χ_{pred} values as: logit $\chi = \ln[\chi/(1-\chi)]$. Logit transformation stabilizes variance in quantities with a (0,1) range and also simplifies the comparison of the sensitivity of χ to environmental variables. We also estimated the model bias (B) in χ predictions at each site as:

$$B = \frac{\chi_{pred} - \chi_{iso}}{\chi_{iso}} \times 100 \qquad \text{Eqn 9}$$

Linear regressions of logit χ_{iso}, logit χ_{pred} and B against the four primary drivers (T_g, natural log-transformed D_g, c_a and z) as predictors were applied using OLS. The variance explained by each of the fixed effects was calculated via commonality analyses using the R package yhat (Nimon *et al.*, 2013). We also tested two linear mixed-effect models (Bolker *et al.*, 2009; Zuur *et al.*, 2009) using the R package lme4 (Bates *et al.*, 2015) that included the four above-mentioned fixed-effects but also a random effect related to site to account for site grouping on variance partitioning. One model included only random intercepts, while another included both random intercepts and slopes. The variance explained by the fixed effects and that explained by the entire models, including both fixed and random effects, were also calculated.

Finally, to investigate the potential influences of soil water availability on χ, we tested different multiple linear models of logit χ_{iso} and B that included the primary drivers of the least-cost hypothesis and one index of plant-available soil water as predictors. Three alternative indices of drought severity or soil water availability were tried: 1) a drought index based on climate water balance (the Standardized Precipitation-Evapotranspiration Index, SPEI) inferred from the 0.5° gridded monthly SPEIbase dataset (Beguería *et al.*, 2010); 2) the surface soil moisture content (θ, m^3 m^{-3}) data extracted at each site from the 0.25° resolution product of the European Space Agency Climate Change Initiative (Dorigo *et al.*, 2017); and 3) an estimate of the ratio of actual evapotranspiration to equilibrium evapotranspiration (Priestley-Taylor coefficient, α)

calculated at each site using the SPLASH model (Davis *et al.*, 2017) (see Text S3 for more details).

All linear models were compared using analysis of variance (ANOVA), RMSE, AIC and BIC. The partial residuals of most models were computed using the R package effects (Fox *et al.*, 2018) and the respective residual plots were visually examined against environmental variables.

3. Results

Model-data comparison of χ values

Over the studied 1951–2014 period, χ_{pred} and χ_{iso} values were in reasonable agreement (R^2_{adj} = 0.39, RMSE = 0.062, AIC = –3015, BIC = –3000, $p < 0.001$; Fig. 2b), but were more consistent for ENF than DBF sites (R^2_{adj} = 0.38, RMSE = 0.063, AIC = –2140, BIC = –2126 for ENF versus R^2_{adj} = 0.21, RMSE = 0.054, AIC = –907, BIC = –896 for DBF, $p < 0.001$; Fig. 2a). χ_{pred} values from high-elevation sites (i.e. with low P_{atm}) tended to be lower than those from low-elevation sites (i.e. high P_{atm}), although the reconstructed values did not show this distinction as clearly as the predicted values (Fig. 2b).

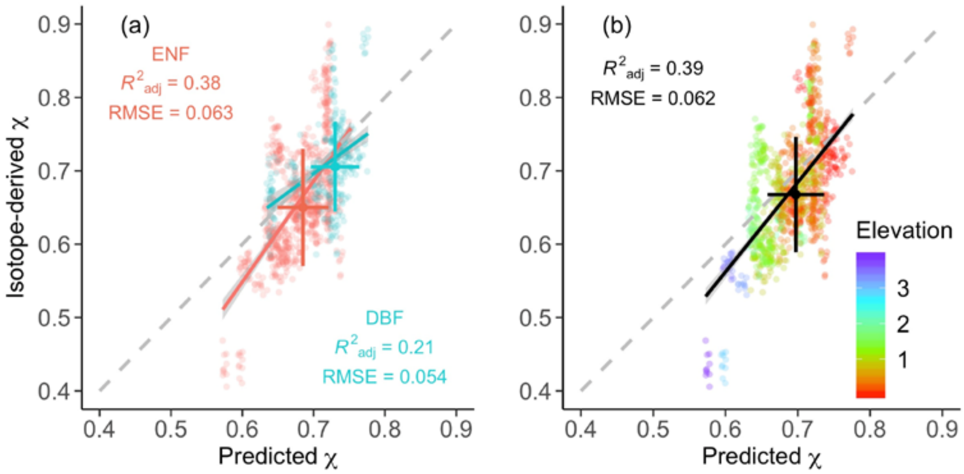

Fig. 2 Predicted versus isotope-derived five-year boxcar averages of χ over 1951-2014. Median and standard deviations are shown for each PFT (a) or for all PFTs (b). The bold lines are the ordinary least-squares (OLS) regressions for each PFT (a) or combined (b). The dashed grey line is the 1:1 line. DBF: deciduous broadleaf forests (n = 29), ENF: evergreen needleleaf

forests (n = 74). R^2_{adj}, adjusted r-squared ($p < 0.001$); RMSE, root mean square error of the predictions. Elevation is in km.

Model-data comparison of long-term trends in χ

The median χ trends across sites were not significantly different from zero, either for the isotope-based reconstructions (ranging across sites between -1.41 and 1.89% 5yr^{-1}) or for the model predictions (ranging across sites between –0.27 and 0.27% 5yr^{-1}) ($p > 0.20$; Student's t test; Fig. 3a). These results indicate that on average across sites, both χ_{iso} and χ_{pred} stayed nearly constant while c_a increased by 2.05% 5yr^{-1}. Reconstructed and predicted χ trends were not significantly different ($p = 0.906$; Student's t test). However, the variability of χ trends between sites was larger in χ_{iso} than in χ_{pred} (interquartile range IQR = 0.60 versus 0.12; $p < 0.001$; F test). No significant differences in χ_{iso} trends were detected between ENF and DBF series or between latewood and whole ring series ($p > 0.40$; Student's t test). χ trends tended to be lower at sites with increase in T_g and D_g, but these differences were only significant for the predicted trends (Fig. 3c-d). Predicted and isotope-derived historical χ trends were only slightly related to each other for all sites (R^2_{adj} = 0.08, RMSE = 0.507, AIC = 159, BIC = 166), as shown using either OLS or RLM ($p < 0.003$; Fig. 3b). The relationship between χ_{iso} and χ_{pred} trends was mainly driven by ENF sites (R^2_{adj} = 0.11, RMSE = 0.135, AIC = -78, BIC = -73, $p = 0.003$ for ENF versus R^2_{adj} = 0.03, RMSE = 0.069, AIC = -67, BIC = -63, $p = 0.199$ for DBF).

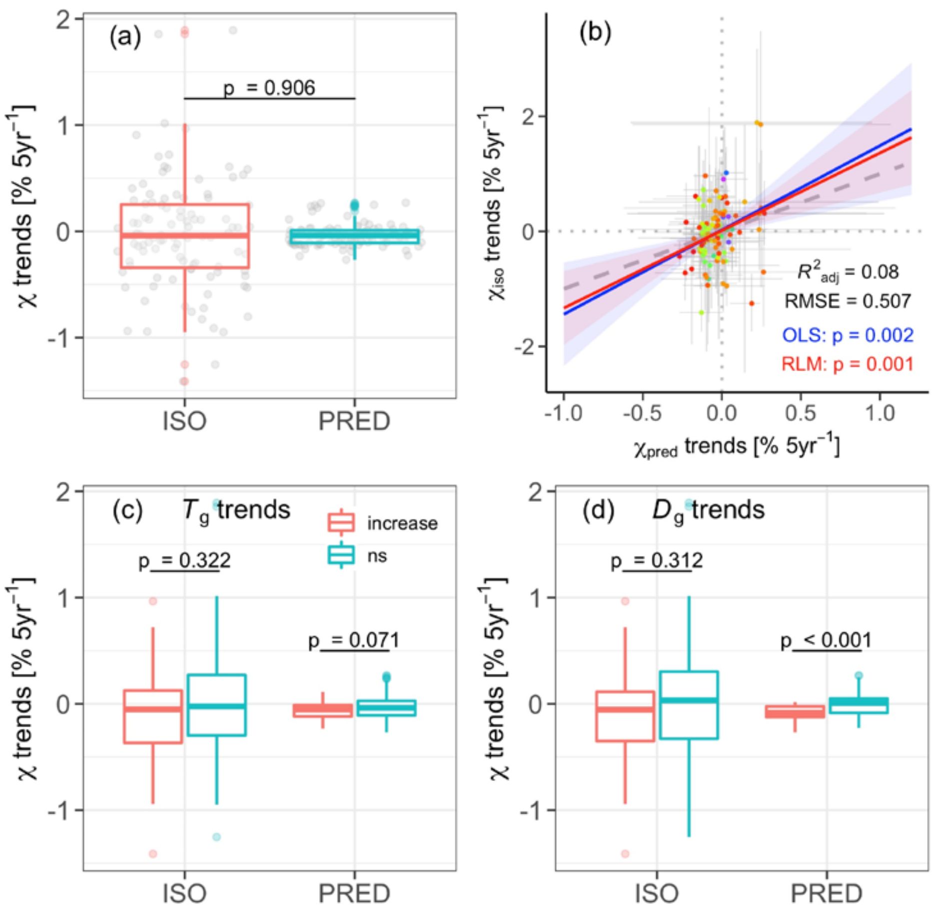

Fig. 3 Temporal changes in isotope-derived (ISO) and predicted (PRED) χ over 1951-2014 for the selected 103 tree-ring sites (see Table S1). The Theil-Sen trends of the % of changes relative to the site mean (% $5yr^{-1}$) are presented considering all sites (a-b), or at each site depending on the historical trends in T_g (c) or D_g (d) (ns: non-significant trend, increase: positive trend). In (a), (c) and (d), the p-values from the Student's *t* tests performed between the different groups of trends are indicated. In (b), the 95% confidence intervals of the Theil-Sen trends are shown in light grey. The dashed grey line is the 1:1 line. The coloured lines with associated 95% confidence intervals are for different regression models: ordinary least squares (OLS) and robust (RLM) linear models. The p-value for these models are indicated. R^2_{adj}, adjusted r-squared; RMSE, root mean square error of the predictions.

Model-data comparisons against environmental drivers

The partial residuals of logit χ_{iso} values increased with increasing T_g but decreased with increasing ln D_g, c_a and z (i.e. decreasing P_{atm}) consistent with those of logit χ_{pred} (Table 1 and Fig. 4). When ignoring c_a as environmental driver of χ_{iso}, the variance explained by the statistical model was similar to the one including c_a (R^2_{adj} = 0.37; see Table S2), the second model being only slightly improved (ANOVA test, p = 0.036). The relatively small contribution to the explained variance of the unique effect of c_a compared to the other drivers (Table 1) suggests that c_a had only a minor effect on χ_{iso}. When significant, the logit χ_{iso} responses to changing T_g, ln D_g and c_a varied and diverged from the general pattern at some sites (Figs 4a-c), however no clear pattern for these discrepancies emerged.

The linear mixed-effects models for logit χ_{iso} with T_g, ln D_g, c_a and z (indexing P_{atm}) as fixed effects, and site as a random effect, performed better than the model considering only fixed effects (lower AIC and BIC, significant ANOVA test, $p < 0.001$; R^2_{cond} = 0.94 versus R^2_{adj} = 0.39; Tables 1 and S2a). The model with random intercepts and slopes yielded lower AIC and BIC values than the one with only random intercepts. Both models, however, tended to assign most of the variance in logit χ_{iso} to the random effects (around 64%), whereas the fixed effects only contributed around 30% of the variance (Table S2a).

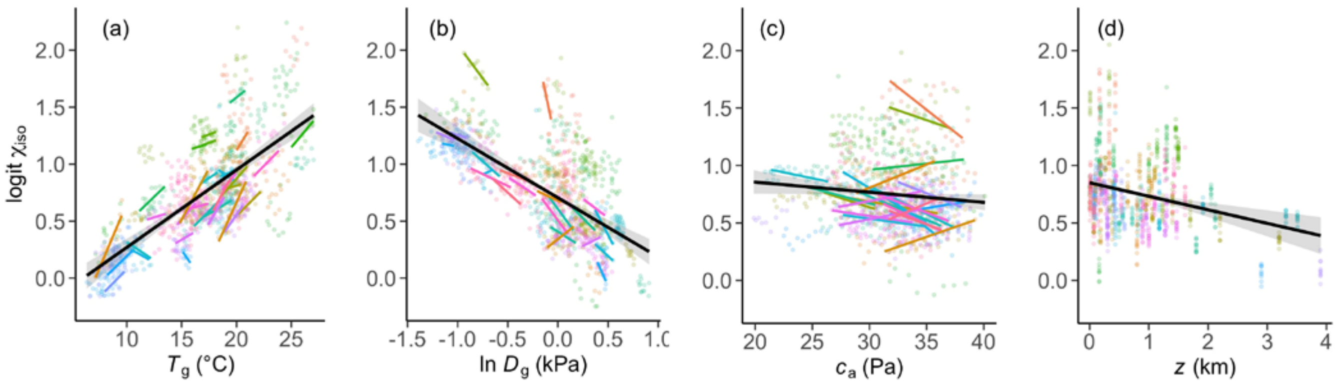

Fig. 4 Partial residual plots showing temporal and spatial variations in the five-year boxcar average of logit χ derived from tree-ring stable carbon isotope data as a function of growing-season average climate variables (a, daytime temperature T_g; b, natural log-transformed vapour pressure deficit D_g), c, partial pressure of CO_2 corrected for elevation effect (c_a) and d, elevation (z) indexing P_{atm} during 1951-2014. The colours correspond to sites. The solid colour lines indicate the modelled response from the multiple linear regression models for each site, while the solid black lines are those for all sites combined (see Table 1 for statistics). The grey shaded area represents the 95% confidence interval of the regression. Only significant trends at 95% ($p < 0.05$) are shown.

Table 1. Summary statistics for the environmental dependencies of reconstructed and predicted logit χ. ΔT_g is the difference between growing-season mean temperature T_g and 25˚C. Standard error (SE), Student's *t* test (t-value), contributions to the explained variance (R^2) of unique effect (Unique) and both unique and common effects (Total) for each environmental driver (in % of R^2), adjusted r-squared (R^2_{adj}), root mean square error (RMSE), Akaike information criterion (AIC) and Bayesian information criterion (BIC). The statistical significance of the models is indicated ($p < 0.001$, *** and $p < 0.05$, *).

	Predictor	Estimate	SE	t-value	Unique	Total	R^2_{adj}	RMSE	AIC	BIC
Recons-truction	ΔT_g	0.068***	0.005	12.745	24.65	14.63	0.37***	0.306	522	552
	ln D_g	–0.520***	0.056	–9.202	12.85	6.03				
	z	–0.118***	0.026	–4.458	3.02	67.93				
	c_a	–0.009*	0.004	–2.096	0.67	36.28				
	Intercept	1.625***	0.145	10.924						
Prediction	ΔT_g	0.061***	<0.001	153.40	33.04	13.15	0.98***	0.023	–5208	–5178
	ln D_g	–0.504***	0.004	–119.95	20.20	7.08				
	z	–0.040***	0.002	–20.17	0.57	62.33				
	c_a	–0.004***	<0.001	–11.71	0.19	35.39				
	Intercept	1.401***	0.011	126.39						

Model biases versus environmental constraints

Overall, the theoretical model for χ showed a significant positive bias with increasing z (decreasing P_{atm}) mainly due to two sites (p < 0.001; Fig. 5c) but no bias related to T_g, ln D_g or c_a were detected (Figs 5a-b). Nevertheless, there were significant biases with changing T_g, ln D_g or c_a at some individual sites (Figs 5a-b) but the magnitudes and signs of these biases varied among sites.

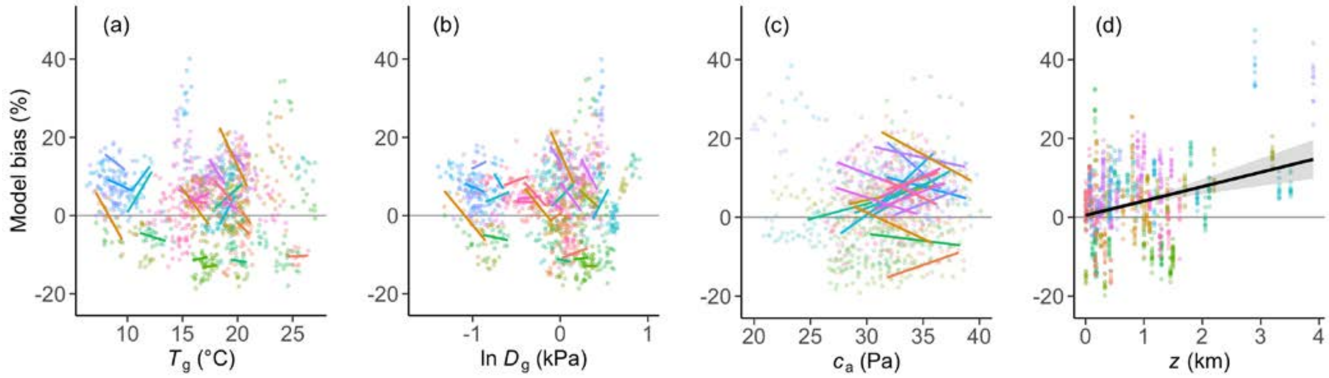

Fig. 5 Partial residual of the model bias (%) in χ predicted by the theoretical model plotted against growing-season mean daytime climate variables (a, temperature T_g; b, natural log-transformed vapour pressure deficit D_g), c, partial pressure of CO_2 corrected for elevation effect (c_a) and d, elevation (z) during 1951-2014. The solid black line is the regression line for all sites. The grey-shaded area represents the 95% confidence interval for the regression line. Only significant trends ($p < 0.05$) are shown. Colours are as in Fig. 4, i.e. representing the different sites.

Including one of the indices of soil water availability, i.e. θ or α, as additional driver of logit χ_{iso} in the linear regression model slightly improved the model fits (lower AIC and BIC, significant ANOVA test, $p < 0.05$) but both the dependencies of logit χ_{iso} on z and on c_a were then no longer significant (Table S2b). The model showed a significant negative bias with increasing θ and α (Fig. 6b-c), indicating an overestimation of χ at low soil-moisture sites and underestimation of χ at high soil-moisture sites at least over the 1979-2014 period. Note that model biases related to these additional drivers diverged from the general responses at some individual sites.

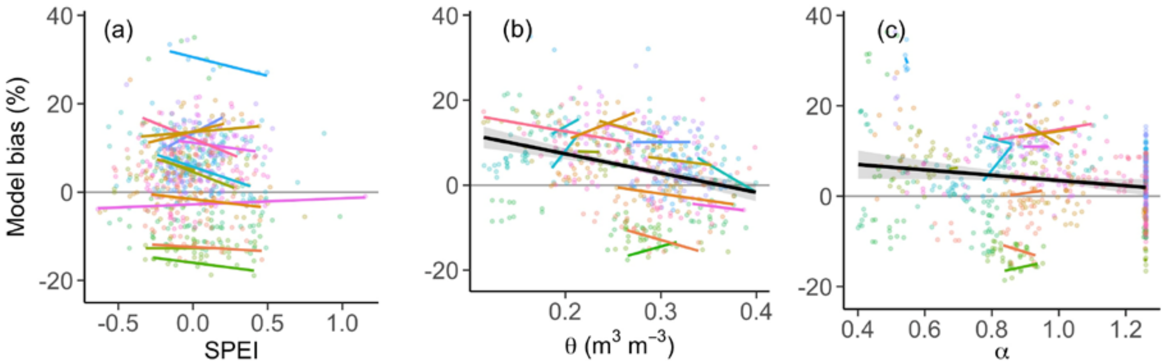

Fig. 6 Partial residual plots of the model bias (%) in χ predicted by the theoretical model plotted against growing-season average water availability or drought indices over 1979-2014 (a, Standardized Precipitation-Evapotranspiration Index, SPEI; b, surface soil moisture content, θ; c, Priestley-Taylor coefficient, α) (see Table S2b). The solid colour lines indicate the modelled response from the multiple linear regression models for each site, while the solid black lines are those for all sites combined. The grey-shaded area represents the 95% confidence interval for the regression line. Only significant trends at 95% ($p < 0.05$) are shown. Colours are as in Fig. 5, i.e. representing the different sites.

4. Discussion

The aim of our study was to evaluate long-term values and trends of χ as predicted by the least-cost hypothesis against a large network of stable carbon isotope-derived χ series from tree rings. Our results are compelling as they demonstrate that despite uncertainties related to the use of tree-ring $\delta^{13}C$ data as proxy of leaf-gas exchanges (see also Text S4), the model predicted 39% of the variance in χ across sites and years. However, only 8% of the variance in χ trends across years was explained by the model, in part due to the larger site-to-site variability in χ trends reported in the tree-ring dataset compared to the predictions. In the following sections, we address both the skills and limitations of the model for predicting plant stomatal and photosynthetic adjustments to environmental conditions. We also discuss potential additional drivers of χ to consider in future studies.

Main drivers influencing χ and biases in the model

Rising T_g increases photosynthetic costs by increasing the Michaelis constant of Rubisco (K), whilst reducing water transport costs due to the reduced viscosity of water (η^*). Both effects combined with the increase in the photorespiratory compensation point (Γ^*) with higher T_g are expected to lead to higher ξ (Eqn 4). However, D_g tends to increase with rising T_g, so the effect of temperature on χ, being influenced in opposite ways by ξ and D_g (Wang *et al.*, 2017a), is not straightforward to predict. Increasing D_g tends to increase the water transport required per mole of carbon fixed, and thus the transpiration costs, leading to lower χ. Decreasing P_{atm} decreases K, due to the reduced partial pressure of O_2, thereby increasing the affinity of Rubisco for CO_2 and reducing the carboxylation capacity required per mole of carbon fixed. At the same time, (all else equal) the actual vapour pressure declines while the saturated vapour pressure remains constant, implying an increase in D_g. Thus, as P_{atm} decreases (z increases), both effects preferentially enhance Rubisco capacity relative to water transport capacity, favouring a lower χ (Körner & Diemer, 1987; Körner *et al.*, 1991; Terashima *et al.*, 1995; Wang *et al.*, 2017a). Finally, elevated c_a increases photosynthesis by increasing the carboxylation rate, while also increasing the transpiration efficiency of plants via a decrease in stomatal conductance. As a result, the direct effect of c_a on χ is difficult to assess at first glance.

In general, rising T_g tended to cause an increase of logit χ_{iso}, suggesting that the temperature dependencies of K, Γ* and η* had a stronger impact on χ than that of D_g (Fig. 5a). As expected, lower χ_{iso} values were observed with increasing D_g and z (Fig. 5b-c), consistent with previous studies (Körner & Diemer, 1987; Körner, Farquhar, & Wong, 1991; Zhu, Siegwolf, Durka, & Korner, 2010). Overall, the slight decrease in logit χ_{iso} with rising c_a implies that c_i increases less than proportionally to increase in c_a. The stronger unique effects of T_g and D_g relative to P_{atm} and c_a on logit χ_{iso} (Table 1) suggests that both T_g and D_g are the dominant drivers of change in χ at many sites. The apparently divergent responses (relative to the general pattern) of logit χ_{iso} to T_g, D_g and c_a at some sites may be indicative of site-specific characteristics not included in the model that also contributed to changes in χ_{iso}. It is also plausible that both T_g and D_g data inferred from the 0.5° resolution CRU dataset, or even the c_a data mainly derived from the Mauna Loa Observatory (Hawaii), were not fully capturing microclimatic differences between or within sites.

The environmental dependencies of χ were for the most part captured correctly by the theoretical model (Table 1). Nonetheless, the model tended to underestimate the negative impact of decreasing P_{atm} (increasing z) on χ values (Table 1 and Fig. 6c), suggesting that the observational data were more sensitive to lower P_{atm} (higher z) than predicted by the theory. The positive bias in predicted χ at high-elevation sites was mainly due to two ENF sites both located in the mountains of Kashmir (Table S1; Treydte *et al.*, 2009) and thus could also be an artefact of site selection. These sites were characterised by the lowest mean T_g and D_g values and wettest conditions in the network for the sites located above 2.5 km. It is thus plausible that the combined effects of relatively low T_g and low D_g on χ have dampened the negative effect of low P_{atm} (high z) on predicted χ values. It is worth noting that the dependency of χ on z depends on the relative humidity and the actual vapour pressure. As a result, the predicted coefficient for the elevational dependency of χ in the linear regression (here –0.040; Table 1) is not expected to be of same magnitude as the theoretical coefficient estimated under standard conditions (T = 25°C and relative humidity = 50%) in the former study (i.e. Wang *et al.*, 2017b; –0.0815, see Text S5).

Other potential controls on χ

The large variability in the magnitude of χ_{iso} trends among sites (Fig. 3) and the different dependences of χ_{iso} to the environmental constraints at some sites (Fig. 5) suggest that other controls on χ not captured by the model are operating and may explain part of the remaining variance in χ_{iso} that was mostly assigned to random effects by the linear mixed-effects models (Table S2a). For instance, the least-cost hypothesis considers the influence of atmospheric demand for water on χ but does not predict how dry soils further influence χ (Verhoef & Egea, 2014; Rogers *et al.*, 2017). Here we found that, independent of the individual effects of T_g, D_g, c_a and z on χ, the model tended to underestimate χ values at high soil moisture and to overestimate χ values at low soil moisture (Fig. 7b-c). In a meta-analysis of drying experiments, Zhou *et al.* (2013) demonstrated that the parameter g_1 of the Medlyn *et al.* (2011) model, based on the Cowan-Farquhar optimality hypothesis – mathematically equivalent to ξ in the least-cost model – is reduced by low soil moisture, and that this occurs at a less negative pre-dawn water potential than the decline in V_{cmax} that occurs in very dry soils. Thus, under drying conditions with reduced soil water availability, χ is expected to decrease via a reduction of ξ. Nonetheless, because D_g and soil moisture are tightly coupled at weekly to monthly timescales (Sulman *et al.*, 2016; Gentine *et al.*, 2019), their relative contributions on changes in χ may be difficult to disentangle (Buckley, 2017; Zhou *et al.*, 2019; Yi *et al.*, 2019), complicating the inclusion of soil water limitation in the framework of the least-cost optimality hypothesis. Recent research testing empirical parameterizations of the effect of soil moisture on gross primary production suggests that the value for β, held constant here, should in fact decline with decreasing soil moisture content (Stocker *et al.*, 2018, 2019b). Further research at sites with different soil water availability and different evaporative demand should help in implementing soil moisture effect in the model through a theoretically motivated reduction of β.

Some studies have suggested that increases in leaf N content with fossil fuel combustion and agricultural emissions (Galloway *et al.*, 2008) might stimulate photosynthetic capacity (Walker *et al.*, 2014) and increase stomatal conductance, resulting in changes in $\Delta^{13}C$ and χ. Based on experiments where N and S fertilizers were applied directly to tree canopies, Guerrieri *et al.*

(2011) found strong effects of both on $\Delta^{13}C$ and χ, with the magnitude of changes related to the element and the time since application or cessation. Their results generally agreed with previous work demonstrating that the effect of N fertilization on tree-ring $\Delta^{13}C$ is short-lived (Brooks & Coulombe, 2009). Nevertheless, the causal mechanisms underlying $\Delta^{13}C$ responses to both climate and N deposition are not well established (Leonardi *et al.*, 2012). Based on an observational global dataset of V_{cmax}, Smith *et al.* (2019) showed that the dependence of V_{cmax} on leaf N was overestimated in vegetation models, as also suggested by Rogers (2014) – and that V_{cmax} can be predicted well from T_g, D_g, z and light availability alone. These findings suggest that leaf N deposition is not a primary driver of photosynthetic capacity, but rather that the photosynthetic demand itself constrains leaf N content (Dong *et al.*, 2017). Thus, even though changes in leaf N concentrations accompanying changes in V_{cmax} can affect both $\Delta^{13}C$ and χ, we suggest that the environmental drivers of such variations are implicitly included in the least-cost model.

Even though some processes influencing χ may be missing, our compilation of 103 tree-ring $\delta^{13}C$ records supports the theoretical optimal responses of χ to a combination of T_g, D_g, P_{atm} and c_a over the period 1951–2014 as predicted by the least-cost hypothesis (Prentice *et al.*, 2014; Wang *et al.*, 2017b). Crucially, the theory predicts χ to be only slightly dependent on c_a, implying that rising c_a leads to a quasi-proportional increase in c_i and an increase in the biochemical rate of carbon uptake (Farquhar *et al.*, 1980). As c_a rises, the ratio of Γ^* to c_a declines and the average responses of χ to c_a converges to zero (Eqn 4). This response is supported by experimental studies showing no change or a small decrease in χ, on average, with sustained CO_2 enrichment (Ainsworth & Long, 2005), and by historical studies (Keeling *et al.*, 2017; Schubert & Jahren, 2018). This response, however, also contrasts with several studies using leaf and wood $\delta^{13}C$ measurements from CO_2 enrichment experiments and/or palaeorecords apparently showing an increase of χ with rising c_a at c_a levels ranging from 200 to 600 ppm (Voelker *et al.*, 2016; Hare *et al.*, 2018), or even a large decrease of χ with sustained CO_2 enrichment (Battipaglia *et al.*, 2013). It is worth noting that these studies did not include the photorespiration term in the discrimination model. The apparent strong influence of rising c_a on χ in these studies might be an artefact caused by disregarding this effect, as was also indicated by Schubert & Jahren (2018) and Lavergne *et al.* (2019). Our analysis of partial residuals of logit χ_{iso} suggests that, across geographically and phylogenetically diverse trees, the average response of χ_{iso} to c_a is weak (Table 1 and Fig. 5) – as predicted by the least-cost hypothesis.

Our results have strong implications for the understanding of the coupled terrestrial carbon and water cycles, because they indicate that the increase in intrinsic water-use efficiency (iWUE) expected with rising atmospheric CO_2 can be offset by increasing T_g (or, potentially, by decreasing D_g and/or increasing soil moisture availability). Also, for the same increase in atmospheric CO_2, iWUE may increase with decreasing P_{atm} (increasing z). Our research complements recent attempts to quantify the relative contributions of environmental drivers to changes in plant water use (Frank *et al.*, 2015; Dekker *et al.*, 2016; Adams *et al.*, 2019) by highlighting eco-evolutionary optimality mechanisms underlying these changes.

Current vegetation and land-surface models suffer from large uncertainties, mainly due to incomplete or inaccurate representations of the fundamental processes governing not only leaf-level gas exchange (Raczka *et al.*, 2018), but also competition, carbon allocation, demography and responses to disturbances such as wildfires and insects attacks. Improving the representation of ecophysiological responses to the environment is only part of a much bigger problem with current terrestrial models. It is a central part nonetheless, and our research suggests a way forward – based on optimality theory – for the representation of the coupled terrestrial carbon and water cycles in next-generation Earth System models.

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Author contributions

A.L and I.C.P. designed the research. S.V., A.C, H.J.deB., V.D., I.R., I.D-L., E.M-S., G.B., F.C.M., J.J.C., R.C., Y.F., A.M., C.J.S., R.M.K., J.S.R. and T.E.D. provided tree-ring carbon isotopic data. A.L. compiled and analysed the data. A.L. and K.J.B. computed the linear mixed-effect models. A.L. wrote the paper with input and revisions from all co-authors.

Code and data availability

The implementation of the model in R is available via the R package rpmodel (https://github.com/stineb/rpmodel; Stocker *et al.*, 2019a). The R code used for all the numerical analyses presented here is available through https://github.com/Alielav/NP_Lavergneetal2019. The isotope-derived and predicted χ data over the 1951-2014 period are provided in the Supporting Information. Except for data explicitly specified as available upon request in Table S1, all the tree-ring $\delta^{13}C$ data are available in the Supporting Information.

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