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Final version
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Published in: New Phytologist

The response of ecosystem water-use efficiency to rising atmospheric CO2 concentrations: sensitivity and large-scale biogeochemical implications

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Received: 16 July 2016
Accepted: 17 September 2016
doi: 10.1111/nph.14288

Key words: continental discharge, evapotranspiration, leaf to ecosystem scaling, rising atmospheric CO2 concentration, seasonal CO2 exchange, water-use efficiency (WUE).
Summary

- Ecosystem water-use efficiency (WUE) is an important metric linking the global land carbon and water cycles. Eddy covariance-based estimates of WUE in temperate/boreal forests have recently been found to show a strong and unexpected increase over the 1992–2010 period, which has been attributed to the effects of rising atmospheric CO₂ concentrations on plant physiology.
- To test this hypothesis, we forced the observed trend in the process-based land surface model JSBACH by increasing the sensitivity of stomatal conductance ($g_s$) to atmospheric CO₂ concentration. We compared the simulated continental discharge, evapotranspiration (ET), and the seasonal CO₂ exchange with observations across the extratropical northern hemisphere.
- The increased simulated WUE led to substantial changes in surface hydrology at the continental scale, including a significant decrease in ET and a significant increase in continental runoff, both of which are inconsistent with large-scale observations. The simulated seasonal amplitude of atmospheric CO₂ decreased over time, in contrast to the observed upward trend across ground-based measurement sites.
- Our results provide strong indications that the recent, large-scale WUE trend is considerably smaller than that estimated for these forest ecosystems. They emphasize the decreasing CO₂ sensitivity of WUE with increasing scale, which affects the physiological interpretation of changes in ecosystem WUE.

Introduction

The ongoing rise in atmospheric CO₂ concentration ($c_a$) affects gas exchange between the vegetation and the atmosphere. Plants respond directly to rising $c_a$ through increased net carbon assimilation ($A_n$) and reduced stomatal conductance ($g_s$) (Morison, 1987; Field et al., 1995; Ainsworth & Rogers, 2007). These fundamental physiological responses lead to increased intrinsic water-use efficiency ($iWUE = A_n/g_s$) and reduced transpiration ($T$) at the leaf level, with potential implications for the terrestrial hydrological cycle and global climate (Sellers et al., 1996; Betts et al., 2007; Doutriaux-Boucher et al., 2009; Andrews et al., 2011). Current theory predicts a moderate decrease in $g_s$ as CO₂ concentrations rise, which results in an approximately proportional increase of $iWUE$ with $c_a$, and a constant ratio of intercellular ($c_i$) to ambient CO₂ concentrations ($c_i/c_a$) (Ball et al., 1987; Leuning, 1995; Katul et al., 2010; Medlyn et al., 2011). These theoretical considerations are strongly supported by multiple lines of experimental and observational evidence at the leaf, plant, and stand level. Reconstructed long-term records of $c_i$ using tree-ring carbon isotope ($δ^{13}C$) measurements suggest a moderate increase in $iWUE$ of 20.5% from the 1960s to the early 2000s with a consistent response among climate zones and biomes (Peñuelas et al., 2011). The same method applied to temperate and boreal forests over the 20th century has similarly shown an approximately proportional increase of $iWUE$ and $c_a$ (Feng, 1999; Saurer et al., 2014; Frank et al., 2015), with some sites showing a weakened $iWUE$ response to $c_a$ towards the end of the 20th century (Waterhouse et al., 2004; Gagen et al., 2011). Exposing plants to elevated CO₂ concentrations yields similar physiological responses. Results from three free-air CO₂ enrichment (FACE) experiments demonstrated that C3 plants growing in CO₂-enriched air (ambient CO₂ + 200 ppm; c. 50% increase in $c_a$) showed...
concurrent significant reductions in $g_s$ and increases in photosynthesis, which resulted in an increase of 68% in iWUE, and an unchanged $c_i/c_a$ (Ainsworth & Long, 2005). Intrinsic WUE is an important metric at leaf level, characterizing plant physiological properties irrespective of atmospheric water demand (Ehleringer et al., 1993). At the ecosystem level, WUE can be approximated by the ratio of gross primary production (GPP) to evapotranspiration (ET) under conditions of low nonbiotic components of the evaporation flux, such as soil or interception evaporation. As ecosystem WUE is strongly modulated by climatic factors, in particular vapor pressure deficit (VPD), an ‘inherent’ WUE metric (IWUE = (GPP × VPD)/ET) was defined to facilitate the comparison of ecosystems with different atmospheric demand and to provide an approximation of iWUE at the ecosystem level (Beer et al., 2009). IWUE, as all other WUE metrics at the ecosystem level, is subject to environmental feedbacks, which tend to strengthen as scale is increased (Field et al., 1995; Wilson et al., 1999). In particular, the partial decoupling of canopies from the atmosphere makes stand transpiration become increasingly insensitive to changes in canopy conductance ($G_c$) (Jarvis & McNaughton, 1986), and a given decrease in $G_c$ has been shown to translate into a weaker response of transpiration, even in relatively well coupled forests (e.g. Wullschleger et al., 2002). Elevated $c_a$ further has structural effects on plant canopies through increasing leaf area index (LAI) (Norby & Zak, 2011), which has been surmised to reduce or even offset the physiological effects of $c_a$ on vegetation water use (Piao et al., 2007; Gerten et al., 2008). Consequently, transpiration and WUE at the ecosystem level are less responsive to changes in $c_a$ than their leaf-level equivalents (Wilson et al., 1999; Wullschleger et al., 2002; De Kauwe et al., 2013). Notwithstanding these expectations, a recent analysis of eddy covariance data from 21 flux tower sites across temperate and boreal forests from 1992 to 2010 (Keenan et al., 2013; henceforth ‘K13’) showed a strong increase in ecosystem IWUE. This study attributed the trend in IWUE to vegetation responses to rising atmospheric CO2 concentrations, but the observed increase was substantially stronger than predicted by current theory and found by previous empirical evidence. The hypothesis put forward was that plant gas exchange is regulated in a way to keep $c_i$ constant despite continuously increasing $c_a$, which suggests that the most likely underlying physiological mechanism for the IWUE trend is a strong decrease in $G_c$ as $c_a$ rises. This finding challenges our capability to project vegetation responses to, and its feedbacks on, future climate and environmental change. If such a strong physiological response occurred at the continental scale, it would entail significant impacts on hydrological and biotic processes on the land surface, especially when considering the fact that 55–67% of annual land water loss in temperate and boreal forests consists of transpiration (Schlesinger & Jasechko, 2014), that is, water that enters the atmosphere through stomata. Though changes in the regional water cycle and energy budget are hard to directly link to the physiological CO2 effect experimentally, modeling studies using terrestrial biosphere models have demonstrated that land surface processes are sensitive to changes in $G_c$. Simulations showed that a CO2-induced reduction in $G_c$ triggers a reduction in ET, and consequently increases soil moisture, and continental runoff (Gedney et al., 2006; Betts et al., 2007; Cao et al., 2010), as well as sensible heat flux and land surface temperature (Boucher et al., 2009; Andrews et al., 2011). Owing to the tight coupling of $G_c$ and canopy photosynthesis, substantial large-scale changes in $G_c$ are also likely to affect GPP and net biome productivity (NBP) at the regional to global scale, ecological processes which affect the concentration of atmospheric CO2 and its seasonal amplitude (Randerson et al., 1997; Forkel et al., 2016).
Here we tested the plausibility of the strong increase in ecosystem IWUE from 1992 to 2010 as found by K13. We incorporated the assumed physiological driver of the trend, stomatal closure in response to rising atmospheric CO2 concentrations, into the process-based terrestrial biosphere model JSBACH (Reick et al., 2013), thereby forcing the observed trend in the model. The implications of the increased IWUE trend to carbon and water cycling at the continental scale were subsequently investigated by comparing JSBACH simulations of ET, continental runoff, and the seasonal amplitude of atmospheric CO2 across the extratropical northern hemisphere with observation-based ET products (Mueller et al., 2013), runoff measurements at major rivers, and observed atmospheric CO2 concentrations across ground-based monitoring sites.

**Material and Methods**

**JSBACH model description**

The JSBACH model (Reick et al., 2013; Knauer et al., 2015; version 3.10, revision 687) is the land component of the MPI Earth System Model (Giorgetta et al., 2013). Moisture, energy, and momentum fluxes between the land surface and the lower atmosphere are simulated using classical bulk transfer relations, in which aerodynamic land–atmosphere coupling is based on the Monin–Obukhov similarity theory (Roeckner et al., 2003). Simulated evapotranspiration (ET) comprises transpiration by vegetation, soil evaporation, and evaporation of intercepted water, all of which are affected by seasonally varying vegetation cover and leaf area. Soil hydrological processes are represented in a five-layer scheme (Hagemann & Stacke, 2014). Surface runoff and drainage enter a river routing scheme which simulates lateral water fluxes on the land surface (HD model) (Hagemann & Dümenil, 1998). Vegetation in the model is represented as plant functional types (PFTs), which differ in their biochemical and biophysical attributes. Radiative transfer in the canopy is based on the two-stream approximation (Sellers, 1985). C3 photosynthesis is simulated according to the model by Farquhar et al. (1980) and stomatal conductance ($g_s$) is calculated with the Ball–Berry equation (Ball et al., 1987):

$$g_s = g_0 + g_1 \frac{A_n \cdot rH}{c_a} \quad \text{(Eqn 1)}$$

where $A_n$ is net assimilation (mol m$^{-2}$ s$^{-1}$), $rH$ is relative humidity ($-$), and $c_a$ is atmospheric CO2 concentration (mol mol$^{-1}$). $g_0$ (0.005 mol m$^{-2}$ s$^{-1}$) and $g_1$ (9.3) are fitted parameters, which are kept constant across all C3 vegetation types and which represent the minimum stomatal conductance in darkness, and the sensitivity of $g_s$ to $A_n$, respectively. Leaf-level values of $A_n$, $g_s$, and $c_i$ are iteratively solved for three canopy layers, and scaled to their bulk canopy equivalents ($\text{GPP}, \ G_c, \ C_i$) with LAI.

**Sensitivity of WUE to atmospheric CO2 concentration**

According to the Ball–Berry model (Eqn 1), $iWUE (A_n/g_s)$ changes in proportion to $c_a$ if $rH$ and $g_1$ are assumed to remain unchanged with increasing $c_a$ and $g_0 = 0$. In this case, a fractional change in $c_a$ is expected to lead to the same fractional change in $iWUE$. This proportionality diminishes with increasing $\eta = g_0/g_s$, the fraction of $g_s$ functionally not under guard cell control of the stomata and therefore not responding to an increase in $c_a$ in the Ball–Berry model:

$$\frac{\text{d}WUE}{iWUE} = (1 - \eta) \frac{dc_a}{c_a} \quad \text{(Eqn 2)}$$
At the ecosystem level, the sensitivity of WUE to $c_a$ diminishes further as a result of two main factors: partial decoupling of the canopy from the atmosphere; and water fluxes other than transpiration (i.e. soil evaporation and interception). The strength of canopy–atmosphere decoupling depends on the ratio of aerodynamic conductance ($G_a$) to $G_c$, and was quantified as the dimensionless decoupling coefficient $\Omega$ (Jarvis & McNaughton, 1986), which ranges from 0 (perfectly coupled) to 1 (completely decoupled):

$$\Omega = \frac{\varepsilon + 1}{\varepsilon + 1 + G_a/G_c} \quad \text{(Eqn 3)}$$

where $\varepsilon$ is the change of latent heat content relative to the change of sensible heat content of saturated air. An important implication of this concept is that with increasing $\Omega$, the physiological control of transpiration by stomata is reduced:

$$\frac{dT}{T} = (1 - \Omega) \frac{dG_c}{G_c} \quad \text{(Eqn 4)}$$

That means a given fractional change in $G_c$ leads to a weaker fractional change in $T$, with the attenuation being determined by the value of $\Omega$. In addition, soil evaporation and interception are not directly affected by changes in $G_c$. Consequently, the sensitivity of WUE to $c_a$ decreases with increasing fraction of soil evaporation and interception on the total ecosystem water loss ($\phi$).

Accounting for these factors, and assuming that $\Omega$ does not affect plant carbon uptake, the relation between ecosystem WUE (GPP/ET) and $c_a$ can be written as:

$$\frac{dWUE}{WUE} = (1 - \eta)(1 - \Omega)(1 - \phi) \frac{dc_a}{c_a} \quad \text{(Eqn 5)}$$

It can be seen from Eqns 2 and 5 that WUE is not exactly proportional to an increase in $c_a$ and that the responsiveness further decreases with increasing scale from leaf to ecosystem. Inserting typical values of $\eta$, $\Omega$, and $\phi$ (see Supporting Information Table S1; Fig. S1) in Eqn 5 suggests that the sensitivity of WUE at ecosystem level is reduced compared with that at leaf level by c. 30% (Fig. S1).

Simulating increased stomatal sensitivity to atmospheric CO2 concentration

To incorporate a stronger WUE response to $c_a$ into the JSBACH model, we modified the Ball–Berry equation (Eqn 1) such that $g_s$ shows an increased sensitivity to $c_a$:

$$g_s = g_0 + g_1 \frac{A_n H}{c_a} \frac{1}{\max(1, 1 + \xi((c_a - c_{a,\text{base}})/c_{a,\text{base}}))} \quad \text{(Eqn 6)}$$

where $\xi$ is a constant stomatal sensitivity factor to $c_a$, and $c_{a,\text{base}}$ is the baseline atmospheric CO2 concentration, set to the value observed in 1992 (355.37 ppm), the beginning of the eddy covariance observations analyzed by K13. This formulation translates into a stronger stomatal response to CO2 if $c_a$ exceeds $c_{a,\text{base}}$, with the strength of the response determined by $\xi$. In this case, the following relation can be established at the ecosystem level:
The sensitivity factor $\xi$ was estimated for each site by numerically solving Eqn 7 using simulated site values of $\eta$, $\Omega$, and $\dot{\phi}$ (see Table S1), such that $dWUE/WUE$ corresponded to the median annual trend observed by K13 (2.3% yr$^{-1}$). Note that Eqn 6 has no purpose other than increasing the stomatal sensitivity in the model, thereby causing IWUE to rise at a similar rate as reported by K13.

Model setup and analysis

We conducted two main simulations: a standard run (ST) with the original Ball–Berry stomatal model (Eqn 1) and a CO$_2$-sensitive run (SE) with an increased stomatal sensitivity to $c_a$ from 1992 onwards (Eqn 6). Both model versions were run at ecosystem level for eddy covariance sites within the FLUXNET network, and also globally at T63 spatial resolution ($c. 1.875^\circ \times 1.875^\circ$). The focus of the analysis was on forested regions in the extratropical northern hemisphere during the period 1992–2010, consistent with the analysis conducted by K13.

Two different meteorological reanalysis datasets were used to force the JSBACH model – CRUNCEP v.6 (http://dods.extra.cea.fr/data/p529yiov/cruncep/readme.htm) and WFDEI (Weedon et al., 2014) – which provide air temperature, precipitation, specific humidity, longwave and shortwave radiation, and surface wind speed at subdaily resolution. All forcing variables were brought to half-hourly resolution. Atmospheric CO$_2$ concentration was provided globally at annual resolution as specified in Le Quéré et al. (2015). Land cover was prescribed from the HYDE 3.1 historical land-cover inventory (Klein Goldewijk et al., 2011), combined with the SYNMAP vegetation map (Jung et al., 2006).

Site-level simulations

We performed site-level simulations at 21 FLUXNET sites to test the effects of the modified physiology on simulated IWUE. The sites correspond to those investigated by K13 and comprise deciduous broadleaf and evergreen needle-leaf forest ecosystems in the temperate and boreal zones. Site characteristics relevant for this study are listed in Table S1. We used reanalysis climate forcing rather than meteorological forcing from the towers to have continuous simulations for all sites over the entire 1992–2010 period, which was not available from the FLUXNET database. For overlapping years, the meteorology measured at the flux towers is in relatively good agreement with the one from the reanalyses (Fig. S2), but shows stronger trends in $rH$ (Fig. S3). All climate variables were extracted from the pixel of the climate forcing fields (at original 0.5$^\circ$ resolution) where the respective site was located. For each meteorological data set, two runs were conducted, which served to attribute changes in IWUE to either $c_a$ or other climate variables: all climate variables held constant (i.e. an average site year with respect to precipitation, temperature, and air humidity was repeated throughout the entire simulation period) but $c_a$ allowed to vary; and all climate variables, including $c_a$, allowed to vary. Basic plant physiological (e.g. maximum carboxylation rate) and structural (LAI, vegetation height) attributes, as well as basic soil parameters (e.g. soil depth, particle size distribution) were adjusted to observed or estimated values for each site, if available. Mean annual summertime IWUE at site level was calculated as follows:

$$\frac{dWUE}{WUE} = (1 - \eta)(1 - \Omega)(1 - \dot{\phi}) \frac{d \left( c_a + \xi \frac{c_a^2 - c_{a,\text{base}} c_a}{c_{a,\text{base}}} \right)}{c_a + \xi \frac{c_a^2 - c_{a,\text{base}} c_a}{c_{a,\text{base}}}}$$

(Eqn 7)
IWUE = Median \left( \frac{GPP \cdot VPD}{ET} \right) \quad \text{(Eqn 8)}

where GPP (gC m$^{-2}$ s$^{-1}$), ET (kg H$_2$O m$^{-2}$ s$^{-1}$), and VPD (hPa) represent filtered half-hourly values in the summer months June, July, and August. Modeled data were filtered as described in K13 to exclude photosynthetically inactive time periods to avoid phenological effects as a result of possible shifts in the growing season. Days with precipitation and the following day were excluded to reduce the fraction of nontranspirational (i.e. not physiologically controlled) water fluxes on ET. Annual summertime IWUE trends were estimated with the Theil–Sen single median method.

To investigate whether the simulated IWUE trends are sensitive to the representation of canopy photosynthesis in the model, we tested two alternative model versions at site level, one in which photosynthesis is calculated separately for sunlit and shaded canopy fractions (Spitters, 1986; denoted as ‘sunlit_shaded’ run), and one in which photosynthesis and $g_s$ were explicitly coupled to the energy balance (‘leaf_EB’ run), in contrast to the version used in this study, which assumed equal canopy surface and air temperatures.

Continental simulations and evaluation datasets

For the global runs, the model was brought into equilibrium with respect to its water and carbon cycle using preindustrial climate forcing, atmospheric CO$_2$ concentration, and land use. We then ran the model with a transient forcing from 1860 to 2010 and with annually updated land cover. The sensitivity factor $\xi$ for the continental runs was set to the mean value of all sites ($\xi = 7.6$). Simulated monthly ET was compared with the diagnostic datasets and reanalyses of the LandFlux-EVAL multi-dataset synthesis (Mueller et al., 2013), which were aggregated to the resolution of the model via conservative remapping. The analysis was restricted to regions north of 35°N and where forest cover (based on SYNMAP) exceeds 30%. Daily river discharge time series were downloaded from the Global Runoff Data Centre (GRDC; Koblenz, Germany: http://www.bafg.de/GRDC/EN/02_srvcs/21_tmsrs/riverdischarge_node.html) and aggregated to mean annual discharges. Missing years were filled with the mean of the respective time series. Rivers with more than 3 years missing from 1992 to 2010 were discarded. Data from 42 river-gauging stations in America (21) and Eurasia (21), whose river catchments cover c. 19.8 Mio km$^2$, were used for the analysis (Table S2; Fig. S4).

The seasonal amplitude of atmospheric CO$_2$ from 1985 to 2010 was simulated using the atmospheric transport model TM3 (Rödenbeck et al., 2003) in Jacobian representation (Kaminski et al., 1999). Input to the TM3 model comprises global net biome productivity (NBP) from the JSBACH simulations, fossil fuel emissions (CDIAC, Boden et al., 2013), and net ocean carbon fluxes from the Global Carbon Project (Le Quéré et al., 2015). Simulated CO$_2$ amplitudes were compared with estimates from flask and continuous measurements collected by various institutions (see Rödenbeck, 2005). We selected six remote measurement stations (Table S3) whose seasonal cycle is predominantly influenced by the terrestrial biosphere north of 35°N (Randerson et al., 1997). Both observed and simulated seasonal CO$_2$ amplitudes were calculated based on monthly averaged CO$_2$ time series as the difference between the maximum and the minimum atmospheric CO$_2$ concentrations in each calendar year, and normalized to the 1985–1991 reference period. Normalized amplitude trends and their uncertainties were calculated using linear mixed-effects models with station as random effect.
Results

Site-level simulations

The effects of the modified model formulation on simulated vegetation physiology, GPP, ET and WUE at site level are shown in Fig. 1 (for WFDEI forcing; see Fig. S5 for CRUNCEP forcing). Results from the CO2-sensitive (SE) model formulation start to differ from those of the standard (ST) version after 1992, when $c_a$ exceeds $c_{a,base}$ (Eqn 6). Between 1992 and 2010, the higher CO2 sensitivity in the SE run induces strong stomatal closure, which is apparent in the c. 53% reduction in $g_s$ by the end of the simulation period (Fig. 1b). ET is reduced in parallel, but at an attenuated rate as a result of the contribution of nontranspirational water fluxes and canopy–atmosphere decoupling. The same holds true for IWUE when compared with the GPP/$G_c$ response. In addition, $C_i$ and GPP respond clearly to the partial stomatal closure and show a c. 20% reduction in 2010 compared with the reference period. The stronger decrease in ET compared with GPP leads to a strong increase in IWUE between 1992 and 2010 at all sites. Mean IWUE in 2010 exceeded that of the reference period by 54% and 60% for WFDEI and CRUNCEP forcing, respectively. The simulated increases in IWUE over all sites (median of 2.0% yr$^{-1}$ for WFDEI and 2.2% yr$^{-1}$ for CRUNCEP forcing, respectively) closely approach the annual IWUE increase of 2.3% yr$^{-1}$ as observed by K13 (Fig. 2).

Figure 1.
Mean daytime summer (JJA) values (± SD) of canopy conductance ($G_c$), gross primary production (GPP), intercellular CO2 concentration ($C_i$), evapotranspiration (ET), GPP/$G_c$, and
inherent water-use efficiency (IWUE = (GPP × VPD)/ET) for: (a) the standard (ST) run; and (b) the CO₂-sensitive (SE) run. All variables are normalized to the mean of the 1979–1991 period (gray shaded area). Shown are results for WFDEI climate forcing (see Supporting Information Fig. S5 for CRUNCEP climate forcing). Values are averaged across the 21 eddy covariance sites.

Figure 2.

Distribution of simulated inherent water-use efficiency (IWUE) trends (1992–2010) across all 21 flux tower sites for the standard (ST) and CO₂-sensitive (SE) runs with constant (Const.) climate, where all climate variables except atmospheric CO₂ concentrations were kept constant for an average site year, and variable (Var.) climate, where all climate variables, including atmospheric CO₂ concentrations, were allowed to vary. The boxes, bold horizontal lines, and circles indicate the interquartile ranges, medians, and data points outside 1.5 times the interquartile range, respectively. The right box depicts the corresponding observed trends reported by Keenan et al. (2013).

To attribute the changes in modeled IWUE to cₐ or other climate variables, the simulated IWUE trends were compared between model runs forced with constant climate (CO₂ effect) and variable climate (both CO₂ and climate effects) in the ST model version. cₐ caused a relatively constant contribution of c. 0.45% yr⁻¹ to the IWUE trend across sites (Fig. 2), which agrees with the expected theoretical behavior and the formulation implemented in the model. All other climate variables reduced IWUE at some sites and enhanced it at others and thus introduced a large intersite variability to the IWUE trend (Fig. S6). However, the median across all sites remained almost constant for both CRUNCEP and WFDEI forcing (Fig. 2). Compared with the ST scenario, significantly higher IWUE trends were simulated in the SE scenario for all sites. SE runs with constant climate showed a similar IWUE response to the SE runs with variable climate (Fig. 2). These results suggest that the simulated IWUE trend in the SE version can be primarily attributed to CO₂ effects, and not to those of other climate variables (Fig. S7).

Simulated IWUE trends at site level in both alternative model versions (‘sunlit_shaded’ and ‘leaf_EB’) were in good agreement with the ones presented here (see Figs S8 and S9). An
explicit coupling of photosynthesis and \( g_s \) to the energy balance as in the ‘leaf_EB’ run led to an increase in temperature and humidity at the canopy surface. However, these emerging meteorological gradients between the surface and the free air were constrained by the prescribed meteorological forcing and had little effect on the simulated IWUE trends.

**WUE responses to atmospheric CO\( _2 \) concentration at leaf and ecosystem levels**

Ecosystem WUE is less sensitive to rising \( c_a \) than its leaf-level equivalent, because factors such as nonstomatal water fluxes and aerodynamic resistance emerge at the ecosystem level that are negligible at the leaf level (Eqn 5). This scale dependency of the CO\( _2 \) sensitivity of WUE implies that an observed IWUE trend at ecosystem level is associated with a stronger iWUE trend at leaf level. To evaluate whether this affects the physiological interpretation of trends in ecosystem WUE, we performed idealized JSBACH simulations at the leaf and ecosystem levels using constant climate forcing to isolate the effects of increasing \( c_a \) (Fig. 3). The simulations at leaf and ecosystem levels were identical with respect to the calculation of photosynthesis and \( g_s \) (see Material and Methods), but the ecosystem-level simulations included scale-dependent feedbacks with the physical environment that are attenuated or nonexistent in the leaf-level simulations. We evaluated two common physiological scenarios with respect to stomatal responses to a rise in \( c_a \) (Saurer et al., 2004): one in which stomatal closure leads to a constant \( c_i/c_a \) (as assumed by the Ball–Berry model), and one in which \( c_i \) remains constant over time (as proposed by K13, implying a somewhat stronger stomatal closure). Run 1 served as a reference and employed the Ball–Berry model (Eqn 1) with \( c_a \) as measured in 1992. According to the constant \( c_i/c_a \) scenario, the increase in \( c_a \) between 1992 and 2010 causes a slight decrease in \( g_s \), and consequently a rise in iWUE, which is proportional to the change in \( c_a \) (run 2). Keeping \( c_i \) constant at the level of 1992 (run 3) requires an increased stomatal response to \( c_a \) which causes a larger iWUE trend between 1992 and 2010. In run 3, iWUE increases more than IWUE, which can be explained by the stronger impact of the attenuating factors (Eqn 5) at ecosystem level compared with leaf level. Importantly, the response associated with the constant \( c_i \) scenario is not sufficient to cause an IWUE trend in the magnitude as reported by K13 (median of 2.3% yr\(^{-1} \); Fig. 2). To obtain an IWUE response similar to the one observed at the ecosystem level (run 4), the required physiological response at leaf level would need to involve a decrease in \( c_i \) over time.
Figure 3.
(a) Simulated ecosystem inherent water-use efficiencies (IWUEs) and their trends for four runs differing in their stomatal response to atmospheric CO$_2$ concentration: (1) reference run: constant ratio of intercellular to atmospheric CO$_2$ concentrations ($c_i/c_a$) for $c_a$ of 1992 (Ball–Berry); (2) constant $c_i/c_a$ for $c_a$ of 2010 (Ball–Berry); (3) constant $c_i$; and (4) stomatal closure inducing an IWUE increase of c. 2% yr$^{-1}$. Numbers on the left indicate simulated IWUEs (gC kg$^{-1}$ H$_2$O hPa) in 2010, and their mean annual relative trends from 1992 to 2010 (in brackets). Each point represents one site and the slopes of the lines are across-site estimates of IWUE. IWUE was simulated by the JSBACH model, forced with WFDEI reanalysis, for the 21 FLUXNET sites characterized in Table S1. Non-CO$_2$ climate forcing was held constant in all runs. The following model settings were used for the respective simulations: (1) standard (ST) model version with $c_a$ of 1992; (2) ST model version with $c_a$ of 2010; (3) CO$_2$-sensitive (SE) model version with a mean sensitivity factor ($\xi$ in Eqn 7) of 2.85 and $c_a$ of 2010; (4) SE model version with a mean $\xi$ of 7.6 and $c_a$ of 2010. (b) The corresponding behavior at leaf level, simulated as in (a) but with a stand-alone version of the coupled photosynthesis-$g_s$ model in JSBACH (Farquhar et al., 1980; Ball et al., 1987). The slope of the line originating at the abscissa is $-1/g_s$. 
and its intersection with the $A_n/C_i$ curve (‘operating point’) gives the corresponding $A_n$ and $c_i$ values (Long & Bernacchi, 2003). Simulations were run with mean climate forcing from all sites (air temperature = 20.7°C, relative humidity = 52.7%, photosynthetically active photon flux density = 942 μmol m$^{-2}$ s$^{-1}$) and with $V_{cmax} = 40$ μmol m$^{-2}$ s$^{-1}$, $J_{max} = 76$ μmol m$^{-2}$ s$^{-1}$, $g_1 = 9.3$, $g_0 = 0.005$ mol m$^{-2}$ s$^{-1}$ and with Rubisco kinetic parameters taken from Bernacchi et al. (2001).

Continental-scale implications of the observed IWUE trend

At the continental scale, the different physiological responses to $c_a$ embedded in the ST and SE model versions are clearly reflected in ET, particularly in the summer months (Fig. 4a). The ST runs show a slight increase in ET across forested regions of the extratropical northern hemisphere from 1992 to 2005, which is in line with the reanalyses and the diagnostic ET products presented in Mueller et al. (2013). By contrast, the strong CO$_2$-induced decline in $G_c$ in the SE scenario causes a significant decrease in ET, totaling c. 1% yr$^{-1}$, which is not in accordance with the observation-based ET products (Fig. 4b). The choice of the climate forcing dataset had only minor effects on these results. The absolute mean summer values (Fig. S10a) demonstrate that simulated ET in the ST model version is underestimated compared with the data products and that their temporal dynamics are in moderate agreement (correlation coefficients ($r$) between 0.45 and 0.56). Although the ST and SE scenarios differ strongly, the difference between continental simulations was significantly lower than at site level as a result of the lower $T$/ET fraction in the absence of any data filtering, and the averaging across different vegetation types holding different aerodynamic properties.
(a) Normalized time series (gray shaded area: reference period 1989–1991) of observation-based (i.e. diagnostic and reanalysis products; see Mueller et al., 2013) and simulated mean summer (JJA) evapotranspiration (ET). Error bars denote standard errors of the mean. (b) Confidence intervals for the trend in normalized ET from 1992 to 2005 based on ordinary least-squares (OLS) regression. (c) Normalized time series (reference period 1979–1991) of observed and simulated continental discharge, calculated as the sum of 42 individual river discharges. The location of the individual gauging stations and characteristics of the rivers are shown in Fig. S4 and Table S2, respectively. (d) Confidence intervals for the trend in normalized continental discharge from 1992 to 2010 based on OLS regression.

A consequence of the modeled reduction in ET is an increase in simulated continental runoff (Fig. 4c,d). Across 42 river gauges (Table S2), normalized observed discharges show a slight, but not significant upward trend from 1992 to 2010. This behavior differs among rivers (Fig. S11). Simulated continental discharges in the ST versions are in agreement with the observations, but show stronger upward trends. The two SE model simulations show significantly higher discharge trends than both the ST runs and the observations (Fig. 4c,d). Both forcing products resulted in a good agreement of the modeled interannual variability with the observations ($r_{WFDEI} = 0.88$ and $r_{CRUNCEP} = 0.68$ for the 1992–2010 period). However, the use of WFDEI forcing yields more realistic absolute discharges (Fig. S10b) and weaker trends for the 1992–2010 time period than the CRUNCEP dataset. The strong underestimation of discharge (c. 40%) in simulations forced by the CRUNCEP dataset is indicative of a negative precipitation
bias in this product, probably to some extent caused by the nonapplication of a precipitation undercatch correction (e.g. Biemans et al., 2009). The altered physiology in the SE model version had considerable implications for carbon cycling in the model. The strong stomatal closure affected vegetation carbon uptake (GPP) and NBP at large scales, which led to changes in the simulated seasonality of atmospheric CO₂ concentrations. Observations show an increase in the seasonal amplitude of atmospheric CO₂ concentrations in the northern hemisphere, corresponding to an intensified net carbon exchange across temperate and boreal terrestrial ecosystems (Graven et al., 2013; Forkel et al., 2016). The ST model runs simulated no changes to weak increases in the seasonal CO₂ amplitude at six ground-based measurement stations (Fig. 5). The SE runs, by contrast, showed significant decreasing trends, which are clearly unrealistic given the observations (Fig. 5). The progressive decrease in the CO₂ amplitude in the SE model version indicates a weakening of the seasonal carbon exchange in these ecosystems, which is caused by the marked decrease in GPP (Fig. S12) in response to the successively increasing stomatal limitations to photosynthesis.

Figure 5.
(a) Individual (faint) and mean (bold) time series of normalized seasonal amplitudes of atmospheric CO₂ (gray shaded area: reference period), calculated as the difference between maximum and minimum CO₂ concentrations within a calendar year, based on six ground-based measurement stations (Table S3; Fig. S4). (b) Confidence intervals for the linear trends. Trends and confidence intervals were calculated using linear mixed-effects models assuming station as random effect.

To assess whether observed large-scale carbon and water fluxes are consistent with a constant $C_1$ over time, we repeated the continental simulations using a model parameterization that yields a constant $C_1$ at ecosystem level across FLUXNET sites (Eqn 6 with $\zeta$ set to 2.85). As
expected, the resulting trends in ET, discharge, and atmospheric CO2 amplitude showed an intermediate behavior between the ST and SE runs (Fig. S13). Nonetheless, this scenario is less consistent with the observations than the ST simulations, for all three observational datasets.

**Discussion**

**WUE responses to atmospheric CO2 concentration and other factors**

Rising atmospheric CO2 concentration is expected to increase plant WUE as a result of stomatal closure, but the exact magnitude of this effect is still under debate (e.g. Saurer et al., 2004). Studies at the leaf to stand scale suggest stomatal closure commensurate with a constant $c_i/c_a$ and $iWUE$ at leaf level to rise in proportion to $c_a$ (‘constant $c_i/c_a$’ scenario) (e.g. Ainsworth & Long, 2005; Frank et al., 2015). The strong $iWUE$ trend found by K13 has been attributed to the same physiological mechanism, but their results imply a much stronger stomatal response to $c_a$, which, as has been argued by K13, is consistent with an invariant $C_i$ over time. Increasing the stomatal sensitivity to $c_a$ in the JSBACH model resulted in increases in $iWUE$ at site level that are similar to those observed by K13 from 1992 to 2010. However, the degree of stomatal closure necessary to cause this trend led to decreasing levels of $C_i$, GPP, and ET, which are inconsistent with observations from the eddy covariance sites. This implies that it is unlikely that CO2-induced stomatal closure would have been the primary driving force behind the observed $iWUE$ trend. Our simulations support previous empirical findings of a physiological regulation towards a constant $c_i/c_a$ as $c_a$ increases rather than a constant $c_i$ (Fig. S13), and suggest a constant yet moderate contribution of $c_a$ to the increase in $iWUE$, accounting for approximately one-quarter of the trend found by K13.

Besides atmospheric CO2 concentration, other abiotic and biotic factors may have contributed to the trend. Climate change, for instance, has been found to influence WUE of grasslands and forests (De Boeck et al., 2006; Yu et al., 2008; Niu et al., 2011), with the sign and magnitude of the response depending on the type of ecosystem and the prevailing climatic conditions (Tian et al., 2010; Zhu et al., 2011; Zhang et al., 2014). Our model simulations at site level emphasize the strong climatic control on WUE. Climate factors other than $c_a$ (e.g. VPD) enhanced, reduced, or, for some sites, reversed the positive effects of $c_a$ on WUE in the ST scenario (Figs 2, S7). Additionally, changing biotic factors such as LAI can involve changes in WUE (Hu et al., 2008; Zhang et al., 2014). This and other biotic (e.g. canopy height) and abiotic (e.g. surface roughness) factors show no systematic changes over the study period and thus have been excluded as drivers for the WUE trend across sites by K13. Nevertheless, variables other than $c_a$ may still have contributed to the IWUE trend nonuniformly across sites. The eddy covariance data used for the analysis by K13 might be subject to a sampling bias in space and, particularly, in time, considering that analyzed time series were as short as 7 yr for some sites. The magnitude of the trend found by K13 remains unexplained but might not be robust enough to draw conclusions on a ‘mean’ WUE response, representative across extratropical forest ecosystems, over the last two decades.

**WUE definitions and their implications**

Many different ways of calculating WUE have been proposed, depending on the scale and purpose of the investigation (see Kuglitsch et al. (2008) for an overview). For entire ecosystems,
WUE is commonly defined as GPP/ET (e.g. Law et al., 2002; Ponton et al., 2006; Yu et al., 2008; Huang et al., 2015) and in some studies additional data screening is applied to ensure that ET represents mostly \( T \) (e.g. Ponton et al., 2006). However, WUE calculated in this way is strongly influenced by the effects of VPD on ET (e.g. Law et al., 2002; Ponton et al., 2006; Tang et al., 2014) with the consequence that observed dynamics in GPP/ET cannot be attributed to plant physiological function. To remove the confounding effects of VPD on WUE, an ‘inherent’ WUE (IWUE = (GPP × VPD)/ET) has been proposed as a proxy of iWUE at the ecosystem level (Beer et al., 2009). This formulation was adopted by subsequent studies. Recent considerations, however, have pointed out that the IWUE formulation neglects VPD effects on \( c_i/c_a \) (Zhou et al., 2014), which decreases as a result of stomatal closure in response to rising VPD (e.g. Leuning, 1995). Based on the optimality theory (Cowan & Farquhar, 1977; Lloyd & Farquhar, 1994), Zhou et al. (2014) derived a new WUE metric termed ‘underlying’ WUE (uWUE = (GPP × √VPD)/ET), which they found to better capture the GPP–ET relationship. Importantly, uWUE and IWUE predict different WUE trends depending on the concomitant change in VPD (Fig. 6). As most sites investigated by K13 showed an increase in VPD over time (mean over all sites ≈ 1.25% yr\(^{-1}\)), the magnitude of the WUE trend would probably be smaller if calculated as uWUE, the physiologically more appropriate WUE metric. Considering the large effect of the WUE metric on the calculation of WUE trends as well as the central role ascribed to VPD in future climate change (Cook et al., 2014), the choice of the WUE formulation is key when relating changes in WUE to plant physiological behavior.

![Graph showing FLUXNET, WFDEI, and CRUNCEP data](image)
Figure 6.
Difference in water-use efficiency (WUE) calculated with different metrics (inherent WUE (IWUE) – underlying WUE (uWUE)) in dependence of a vapor pressure deficit (VPD) trend for observations from 10 FLUXNET sites and simulations for 21 FLUXNET sites forced with WFDEI and CRUNCEP reanalysis.

WUE response to atmospheric CO₂ concentration at leaf and ecosystem levels
Our considerations (Eqns 2-7) suggest that the sensitivity of WUE to $c_a$ decreases with increasing scale from leaf to ecosystem, with the consequence that an observed CO₂ response of WUE at the ecosystem level corresponds to an even stronger physiological response within the leaves (Fig. 3). Thus, the required stomatal response at leaf level would have to involve a decline in $c_i$ (Fig. 3), which is physiologically unlikely to happen (Saurer et al., 2004). One reason for the difference across scales is aerodynamic conductance ($G_a$), which, depending on vegetation type and surface roughness, can exert strong control on canopy water use. The effect of $G_a$ was discussed extensively by Jarvis & McNaughton (1986) in their ‘omega’ theory, which effectively describes the sensitivity of $T$ to changes in $G_c$ as a consequence of canopy–atmosphere decoupling. $\Omega$ calculated from micrometeorological measurements of $G_a$ and derived $G_c$ in temperate forests is usually in the range of 0.2–0.3 (e.g. Magnani et al., 1998; Wullschleger et al., 2000, 2002; Martin et al., 2001). Modeled $\Omega$ by JSBACH (Table S1) was in accordance with field studies with a daytime mean of 0.21, indicating that the strength of the canopy–atmosphere decoupling is adequately represented in the model.

Not only does $T$ tend to get less sensitive to $c_a$ with increasing scale, but also $G_c$ itself has been ascribed a lower responsiveness to $c_a$ than its leaf-level equivalent $g_s$. Gunderson et al. (2002) and Wullschleger et al. (2002), for instance, found that stomata at lower canopy levels responded less to elevated $c_a$ than those in the upper canopy. In the Ball–Berry model (Eqn 1), as in most other state-of-the-art stomatal models (e.g. Leuning, 1995; Medlyn et al., 2011), the constant $g_0$ term reduces the sensitivity of $g_s$ to $c_i$ (Eqn 2) and further leads to a diminished response of $G_c$ compared with $g_s$ as a result of a larger $g_0/g_s$ ($\eta$) fraction in lower canopy layers with lower photosynthetic rates. Given the firm physiological basis of $g_0$ and its importance for canopy transpiration (Barnard & Bauerle, 2013), its role in modeling $G_c$ and WUE in ecosystem and land surface models deserves further investigation.

The analysis of IWUE usually relies on the assumption that ET consists almost entirely of $T$ if an appropriate data filter is employed (see the Material and Methods section). This a critical assumption because nontranspirational water fluxes are not directly responsive to $c_a$ and thus reduce the sensitivity of ecosystem water loss to rising atmospheric CO₂ concentrations, regardless of the physiological state of the vegetation. Our model simulations showed a low average residual contribution of evaporation of 4% across sites, indicating that the data screening applied here is sufficient to exclude water fluxes other than transpiration. It is worth mentioning that, in the absence of any data filter, evaporation and interception comprise a much larger fraction of ET (see Schlesinger & Jasechko, 2014), which leads to a considerably lower CO₂ effect on WUE over longer timescales (e.g. annually) (e.g. Wullschleger et al., 2002; Leuzinger & Körner, 2007), which is also apparent in our continental-scale analyses.
Role of stomata in the hydrological response of the land surface to rising CO₂

At the continental scale, simulated ET showed a marked reduction in response to the strong stomatal closure in the SE scenario, which is in line with previous studies that have emphasized the high sensitivity of ET to $G_c$ even at large spatial scales (Friend & Kiang, 2005; Gedney et al., 2006). The implications of CO₂-induced stomatal closure on ET and the land surface energy budget, known as ‘physiological forcing’ (Betts et al., 2007) is simulated in an exaggerated manner in the SE run, but shows qualitatively the same response as previous studies (Betts et al., 2007; Boucher et al., 2009; Cao et al., 2010), including increases in continental runoff and land surface temperatures (but note Piao et al., 2007).

One consequence of the reduced ET in the SE scenario was an increase in soil water content, a major indirect ecological effect of rising $c_a$ (e.g. Morgan et al., 2004). This effect plays only a minor role in this study as the focus was on regions where water limitation is of minor ecological importance. In water-limited regions, the simulated IWUE increase in the SE scenario is expected to be much weaker as a result of a positive feedback of increased water availability on vegetation productivity and ET.

In addition to its physiological effect through stomatal closure, rising $c_a$ can affect vegetation structure through increases in biomass production and LAI (Cowling & Field, 2003). Experimental studies have reported increases in foliage cover in response to elevated $c_a$ except for sites where the maximum leaf area carrying capacity has already been reached (Norby & Zak, 2011). This structural CO₂ effect through increased LAI is assumed to enhance transpiration and thus counteract the physiological CO₂ effect. However, its strength is poorly constrained and so are its implications for continental runoff (Gerten et al., 2014). In simulation studies, the structural CO₂ effect was small in Betts et al. (2007), but considerable in other studies (Kergoat et al., 2002; Bounoua et al., 2010), and Piao et al. (2007) even identified an increase in runoff caused by $c_a$. The JSBACH model lacks a productivity–LAI feedback, which leads to an unchanged foliage cover throughout the simulation period despite clear changes in GPP. A more realistic representation of vegetation growth in the model would probably, to some extent, offset the simulated CO₂ response of both ET and GPP, leading to lower responses in continental runoff as well. In the ST runs, the simulated increase in discharge (Fig. 4c,d) may be partly attributed to the missing vegetation structure feedback in the model. Notwithstanding this, the trends in the SE run are strongly dominated by the pronounced simulated physiological effect (Fig. 2), which makes a strong compensatory effect of LAI unlikely in this model version.

Stomatal responses to atmospheric factors, including $c_a$ and VPD, as well as the resulting ET are subject to multiple feedbacks at different scales (Field et al., 1995; Wilson et al., 1999; Vilà-Guerau de Arellano et al., 2012), involving changes in the surface energy budget, temperature, convective boundary layer height, and cloud formation. The JSBACH model gives only a simplified representation of the mechanisms involved. In particular, the model was not coupled to the atmosphere, and thus any boundary layer feedbacks were precluded in the simulations. Although these additional feedbacks are assumed to stabilize the ET response at larger scales (Field et al., 1995), a coupled model run would be necessary to test this assumption and to obtain a more complete representation of land–atmosphere interactions.
Does the observed ecosystem IWUE trend occur throughout the northern hemisphere?

The response of the terrestrial hydrological and carbon cycles to rising atmospheric CO$_2$ concentrations and their feedbacks on the climate system are key issues in climate change research (Gerten et al., 2014). This work supports the majority of previous studies reporting moderate physiological responses of $g_s$ and WUE to $c_a$ at the plant scale compared with the recent suggestions by K13. The sensitivity of the total land–atmosphere water flux to the rise in $c_a$ is further attenuated with increasing scale as a result of feedbacks with the physical environment. The combined implications of these two aspects are reflected in our results, which indicate that the magnitude of the ecosystem IWUE trend as reported by K13 is not in accordance with observed large-scale trends in continental discharge, ET, and the seasonal CO$_2$ exchange in temperate and boreal regions of the northern hemisphere over the 1992–2010 time period (Figs 4, 5). The simulations demonstrate that changes in ecosystem IWUE in the magnitude as found by K13 would result, if they occurred at the continental scale, in altered carbon and water fluxes at the land surface that would be clearly detectable in signals responding to biogeochemical changes in the terrestrial biosphere. We thus conclude that the magnitude of the IWUE trend observed at temperate and boreal forest ecosystems is not a large-scale phenomenon.

Acknowledgements

This work used eddy covariance data acquired by the FLUXNET community (see Table S1; available at www.fluxdata.org) and, in particular, by the following networks: AmeriFlux (US Department of Energy, Biological and Environmental Research, Terrestrial Carbon Program (DE-FG02-04ER63917 and DE-FG02-04ER63911)), CarboEuropeIP, and Fluxnet-Canada (supported by CFCAS, NSERC, BIOCAP, Environment Canada, and NRCan). We acknowledge the financial support to the eddy covariance data harmonization provided by CarboEuropeIP, FAO-GTOS-TCO, iLEAPS, Max Planck Institute for Biogeochemistry, National Science Foundation, University of Tuscia, Université Laval and Environment Canada and US Department of Energy and the database development and technical support from Berkeley Water Center, Lawrence Berkeley National Laboratory, Microsoft Research eScience, Oak Ridge National Laboratory, University of California – Berkeley, University of Virginia. This study further uses the LandFlux-EVAL merged benchmark synthesis products of ETH Zurich produced under the aegis of the GEWEX and ILEAPS projects (http://www.iac.ethz.ch/url/research/LandFlux-EVAL/). S.Z. was supported by the European Research Council (ERC) under the European Union's H2020 programme (grant no. 647304; QUINCY). We are grateful to Steffen Richter, Kerstin Sickel and Christian Rödenbeck for technical assistance.

Author contributions

S.Z. and J.K. designed the study. J.K. performed the simulations and the analysis. S.Z., M.R., M.F., B.E.M., S.H. and C.W. contributed ideas to the analysis. J.K. wrote the manuscript, with contributions from all authors.
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**Supporting Information**

Additional Supporting Information may be found online in the Supporting Information tab for this article:

Fig. S1 Mean summer (JJA) values across all sites for g, O, and / (Eqn 5) for WFDEI and CRUNCEP forcing.

Fig. S2 Mean summer (JJA) air temperature, precipitation, VPD, and relative humidity as measured at the eddy flux towers and in the reanalysis products.

Fig. S3 Relative trends of summer (JJA) air temperature and relative humidity at the eddy flux towers and in the reanalysis products.

Fig. S4 Location of FLUXNET sites, ground-based CO2 measurement stations, and discharge gauging stations analyzed in this study.

Fig. S5 As Fig. 1, but with CRUNCEP climate forcing.

Fig. S6 IWUE trends (1992–2010) for all sites simulated with constant and variable climate in the standard (ST) model formulation, and for variable climate in the CO2-sensitive (SE) model formulation.

Fig. S7 Contribution of climate variables other than atmospheric CO2 concentration to the IWUE trend in the SE scenario.

Fig. S8 Results from an alternative model version, in which photosynthesis was calculated separately for sunlit and shaded fractions of the canopy.

Fig. S9 Results from an alternative model version, in which photosynthesis and stomatal conductance were explicitly coupled to the energy balance (EB).

Fig. S10 Mean summer ET of diagnostic and reanalysis products and mean annual discharges.

Fig. S11 Relative trends in measured and simulated discharge (with WFDEI climate forcing) for all rivers analyzed in this study.

Fig. S12 Time series of simulated GPP for the standard (ST) and CO2-sensitive (SE) runs and WFDEI and CRUNCEP climate forcing, normalized to the 1985–1991 reference period.

Fig. S13 Confidence intervals for the trend in ET (as in Fig. 4b), continental discharge (as in Fig. 4d), and the seasonal CO2 amplitude (as in Fig. 5b), including the ‘constant Ci’ scenario.

Table S1 Characteristics of flux tower sites used in this study

Table S2 Characteristics of rivers and associated discharge gauging stations used in this study
Table S3 List of CO2 monitoring stations used in this study

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