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# **Forest water use and water use efficiency at elevated CO<sub>2</sub>: a model-data intercomparison at two contrasting temperate forest FACE sites**

*Running head:* model water use at elevated CO<sub>2</sub>.

Keywords: climate change, water, models, stomatal conductance, plant physiology,  
elevated CO<sub>2</sub>, CO<sub>2</sub> fertilisation, FACE.

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## Abstract

Predicted responses of transpiration to elevated atmospheric CO<sub>2</sub> concentration (eCO<sub>2</sub>) are highly variable among process-based models. To better understand and constrain this variability among models, we conducted an intercomparison of 11 ecosystem models applied to data from two forest free-air CO<sub>2</sub> enrichment (FACE) experiments at Duke University and Oak Ridge National Laboratory. We analysed model structures in order to identify the key underlying assumptions causing differences in model predictions of transpiration and canopy water-use efficiency. We then compared the models against data to identify model assumptions that are incorrect or are large sources of uncertainty. We found that model-to-model and model-to-observations differences resulted from four key sets of assumptions, namely: (i) the nature of the stomatal response to elevated CO<sub>2</sub> (coupling between photosynthesis and stomata was supported by the data); (ii) the roles of the leaf and atmospheric boundary layer (models which assumed multiple conductance terms in series predicted more decoupled fluxes than observed at the broadleaf site); (iii) the treatment of canopy interception (large inter-model variability, 2-15 %) ; and (iv) the impact of soil moisture stress (process uncertainty in how models limit carbon and water fluxes during moisture stress). Overall, model predictions of the CO<sub>2</sub> effect on WUE were reasonable (inter-model  $\mu = \sim 28 \pm 10 \%$ ) compared to the observations ( $\mu = \sim 30 \pm 13 \%$ ) at the well-coupled coniferous site (Duke), but poor (inter-model  $\mu = \sim 24 \pm 6 \%$ ; observations  $\mu = \sim 38 \pm 7 \%$ ) at the broadleaf site (Oak Ridge). The study yields a framework for analysing and interpreting model predictions of transpiration responses to eCO<sub>2</sub>, and highlights key improvements to these types of models.

## Introduction

Forest biomes play a key role in land-atmosphere exchanges of mass and energy, covering ~30 % of the land surface and recycling up to 56 % of precipitation (Eltahir and Bras, 1996; Bonan, 2008). The potential effects of increasing atmospheric carbon dioxide concentration ( $[\text{CO}_2]$ ) on forest biomes remain a key uncertainty in global change research (Denman, 2007). At the leaf scale, elevated  $[\text{CO}_2]$  ( $\text{eCO}_2$ ) increases carbon uptake via increasing photosynthetic rates (Kimball, 1993; Curtis and Wang, 1998; Mooney *et al.*, 1999) and reduces water loss via lower stomatal conductance ( $g_s$ ) (Morison, 1985; Saxe *et al.*, 1998; Medlyn *et al.*, 2001; Ainsworth and Rogers 2007). Although these direct impacts on physiological processes are well understood and have been well-quantified at the leaf scale, it remains unclear how these impacts will translate into changes at the ecosystem scale.

The reduction in  $g_s$  under  $\text{eCO}_2$ , when implemented in models, commonly results in a strong physiological forcing that affects transpiration, run-off and surface temperatures (Idso and Brazel 1984; Henderson-Sellers *et al.*, 1995; Pollard and Thompson, 1995; Sellers *et al.*, 1996; Gedney *et al.*, 2006; Betts *et al.*, 2007; Cao *et al.*, 2010). In model simulations by Gedney *et al.*, (2006), reduced  $g_s$  under  $\text{eCO}_2$  resulted in global reductions in transpiration and increases in runoff, results that they argued were supported by increases in observed continental runoff records over the 20<sup>th</sup> century. Betts *et al.*, (2007) modified the Land Surface Model (LSM) used by Gedney *et al.*, (2006), to account for atmospheric boundary layer feedbacks, and found similar results, predicting an increase in global runoff of ~6 % for a doubling in  $[\text{CO}_2]$ . In a similar vein, Cao *et al.*, (2010) showed with a coupled simulation that a

doubling of [CO<sub>2</sub>] resulted in an increase in global runoff (~8 %) due to physiological forcing controls.

However, a number of authors have argued that the effect of eCO<sub>2</sub> on transpiration (*E*) in such studies is overstated, due to atmospheric boundary layer feedbacks (Field *et al.*, 1995; Körner *et al.*, 2007), increasing leaf area index (LAI) (Woodward, 1990; Schäfer *et al.*, 2002; Gerten *et al.*, 2008), CO<sub>2</sub>-driven structural changes in vegetation and human-induced disturbance. Field *et al.*, (1995) suggested that the sensitivity of *E* to changes in *g<sub>s</sub>* is dependent on atmospheric feedback driven by the humidity of the boundary layer, wind speed and the canopy temperature. In agreement with this argument, Wullschleger *et al.*, (2002) found that canopy-atmosphere decoupling at the Oak Ridge Free-Air CO<sub>2</sub> Enrichment (FACE) site was high during the summer, which suggests that CO<sub>2</sub> driven changes in *g<sub>s</sub>* may have a relatively small effect on canopy transpiration fluxes. Wullschleger *et al.*, (2002) estimated that for a 24 % change in *g<sub>s</sub>*, there would only be a 12 % reduction in transpiration (peak of summer). A number of potential feedbacks via LAI are also possible. It has been argued that increased carbohydrate availability at eCO<sub>2</sub> will result in increased LAI, which would act to increase transpiration, offsetting “water savings” (Woodward, 1990; but see Warren *et al.*, 2011). Experimental results from FACE experiments suggest that eCO<sub>2</sub> can increase LAI in forest stands with relatively low LAI but not in stands with high LAI (Gielen *et al.*, 2001; Schäfer *et al.*, 2002; McCarthy *et al.*, 2007; Uddling *et al.*, 2008; Norby and Zak, 2011). As a result of such an eCO<sub>2</sub>-induced increase of LAI at Duke FACE, annual transpiration was unaffected over three years of measurements (Schäfer *et al.*, 2002). A series of modelling studies that allowed for increases in LAI with rising [CO<sub>2</sub>] highlighted an increase in transpiration, which, at the global scale,

was found to decrease global runoff amounts, in direct contrast to Gedney *et al.*, (2006; see above) (Piao *et al.*, 2007; Gerten *et al.*, 2008; Bounoua *et al.*, 2010).

The differing results among studies highlight the current uncertainty about plant water use in response to rising [CO<sub>2</sub>] and the incomplete nature of ecosystem water budgets in experiments. As changes in [CO<sub>2</sub>] are projected to extend beyond our observation record (Petit *et al.*, 1999), we are reliant on relatively short-term elevated [CO<sub>2</sub>] manipulation experiments to evaluate our models. The task, therefore, is to synthesise what we have learned from [CO<sub>2</sub>] manipulation experiments to improve our projections of plant water fluxes in response to eCO<sub>2</sub>. Although there is a long history of [CO<sub>2</sub>] manipulation experiments (glasshouse and open top chambers) for forest species, it is often difficult to scale observed results to the stand or ecosystem. Confounding factors such as limited rooting depth, short duration of experiments and age of plants, can complicate interpretation of results. For these reasons, FACE experiments are arguably the state of the art in this field and provide us with a unique series of long-term, stand-scale data sets against which to test models (Ainsworth and Rogers, 2007).

The goal of this study is to compare simulations of water fluxes by 11 state-of-the-art ecosystem models, evaluating simulations against forest carbon and water fluxes in response to eCO<sub>2</sub> at two forest FACE sites in the United States of America. Our aim is to contrast and analyse the responses of the models in order to identify the key model assumptions that lead to different predicted effects of CO<sub>2</sub> on transpiration. We also aimed to evaluate the simulations against data from the two forest FACE experiments, in order to identify which model assumptions are plausible, implausible

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or in need of further refinement. Additionally, the results of this intercomparison will help inform future experimental work, identifying existing gaps in our understanding, particularly as to which measurements we need to obtain in order to constrain uncertainty in model simulations.

The approach taken was to focus on water use efficiency (WUE), or carbon uptake per unit water transpired. Almost all of the models considered here (as well as many other ecosystem models) simulate transpiration based on the observed leaf-level coupling between photosynthesis and stomatal conductance (Wong *et al.*, 1979; Ball *et al.*, 1987). This coupling implies that assimilation is an important driver of transpiration, and consequently that the CO<sub>2</sub> effect on transpiration can be predicted from the CO<sub>2</sub> effect on assimilation. Models based on this coupling may thus differ in their predictions of transpiration either because they differ in their prediction of productivity or because they differ in their prediction of WUE. Model simulations of the CO<sub>2</sub> effect on productivity will be considered in a companion paper (Zaehle *et al.*, in prep). This paper considers how and why models differ in their predictions of the CO<sub>2</sub> effect on WUE, using a simple version of the coupled photosynthesis-stomatal conductance model as a baseline for comparing the behaviour of the different models. Having identified the key assumptions underlying model differences, we then evaluated the models against actual measurements. Together with the impacts on productivity, this information allows us to identify the uncertainties that lead to models differing in their predictions of CO<sub>2</sub> effects on transpiration.



## Materials and Methods

### *Experimental data*

The Duke FACE site is located in a loblolly pine (*Pinus taeda*) plantation (35.97 °N, 79.08 °W) established in 1983 in open woodland partially covered with grass harvested as fodder. The site experiences a mean annual temperature of 15.8 °C. Mean annual rainfall is 1145 mm, which is evenly distributed throughout the year, but the site regularly experiences drought during the growing season (Ellsworth *et al.*, 2012; McCarthy *et al.*, 2007). The majority of fine roots are restricted by a hard pan to the upper 0.35 m of the soil, making the forest highly sensitive to even short periods of drought (Oren *et al.*, 1998). The soil is relatively nutrient poor, showing a substantial response to nitrogen (N) fertilization (Crous *et al.*, 2008; Maier *et al.*, 2008; Oren *et al.*, 2001). Furthermore, natural variation in N availability controls net primary productivity (NPP), LAI, carbon allocation above *versus* belowground, and the proportion of LAI of the dominant pine *versus* the broadleaved species naturally established among the pines, as well as the responses of these variables to elevated CO<sub>2</sub> (Finzi *et al.*, 2002; Palmroth *et al.*, 2006; McCarthy *et al.*, 2007). At the start of the experiment trees were 15-years-old and approximately 14 m tall, with a mean summer LAI of 3–4 m<sup>2</sup> m<sup>-2</sup> (for the dominant pine species). In this study we examined the experimental period that covered the years between 1996 and 2008. The CO<sub>2</sub> treatment began in August 1996, with the three elevated rings (25–30 m in diameter) receiving continuous enhanced CO<sub>2</sub> concentrations tracking ambient conditions +200 µmol mol<sup>-1</sup> (mean ~ 542 µmol mol<sup>-1</sup>).

The Oak Ridge FACE site was similarly a former grassland area until a sweetgum (*Liquidambar styraciflua*) plantation was established in 1988. The site is located in Tennessee at the Oak Ridge National Laboratory (35.9 °N, 84.33 °W). The soil at the site, which is classified as an Aquic Hapludult, developed in alluvium washed from upland soils derived from a variety of rocks including dolomite, sandstone and shale. It has a silty clay loam texture and is moderately well drained. The soil is slightly acid (water pH approximately 5.5–6.0) with high base saturation largely dominated by exchangeable Ca (Norby *et al.* 2001). The site experiences a mean annual temperature of 13.9 °C with average annual rainfall of 1371 mm, falling evenly throughout the year (Warren *et al.*, 2011b).

The Oak Ridge FACE experiment lasted from 1998 to 2009 (data through to 2008 were used in this exercise). Five plots 25 m in diameter were laid out in 1996, and FACE apparatus was assembled in four of them. The stand can be characterised as a closed canopy deciduous sweetgum (*Liquidambar styraciflua*) forest. At the start of the experiment, the trees (~90 per plot) were 12 m tall with average diameter at breast height of 0.11 m and stand basal area of 0.28 m<sup>2</sup> m<sup>-2</sup>. The trees were in a linear growth phase, leaf area index was 5.5 m<sup>2</sup> m<sup>-2</sup>, and the canopy was no longer expanding (Norby *et al.* 2003). Exposure to elevated [CO<sub>2</sub>] commenced in two plots in April 1998, and continued during daylight hours of each growing season (April–November). The average daytime [CO<sub>2</sub>] from 1998 to 2008 growing seasons was 547 μmol mol<sup>-1</sup> in the two CO<sub>2</sub>-enriched plots and 395 μmol mol<sup>-1</sup> in ambient plots.

Data measured at the leaf and stand scale were used to test modelled responses. Measurements of leaf gas exchange, including assimilation and stomatal conductance,

were made on *in situ* foliage throughout the Duke FACE experiment (Ellsworth *et al.*, 2012). At ORNL, leaf gas exchange was measured *in situ* during several campaigns in 1998 – 2000 (Gunderson *et al.*, 2002; Sholtis *et al.*, 2004) and on cut branches in 2008–2009 (Warren *et al.*, in prep). At the stand scale, annual net primary production (NPP) was estimated at both sites from annual increments of foliage, wood, and fine-root production (see McCarthy *et al.*, 2009 for Duke and Norby *et al.*, 2002 for Oak Ridge). Stand-scale transpiration was derived from sap flow measurements for the years 1999, 2004, 2007 and 2008 at Oak Ridge (see Wullschleger *et al.*, 2002; Warren *et al.*, 2011a, b) and for 1998–2007 at the Duke site (see Drake *et al.*, 2010). Annual stand water use efficiency was estimated from these measurements as annual NPP / annual transpiration. Note that this measure is not identical to the modelled WUE considered in this paper, which is calculated as the ratio of gross primary production (GPP) to transpiration. The difference between the two measures is the ratio of NPP:GPP. Comparisons of modelled values against data therefore need to take into account the possibility that the ratio NPP:GPP changes under elevated  $C_a$ . In the majority of models, the effect of  $CO_2$  treatment on the NPP:GPP ratio is generally in the range of 0–5%. This issue is explored in more detail in a companion paper (De Kauwe *et al. in prep.*) and so to simplify, we do not examine modelled NPP/E, but rather GPP/E. For completeness, Figs. 7 and 8 are reproduced in the supplementary material, S1 and S2 calculating WUE as NPP/E. A summary of the observed site responses is provided in the supporting information.

### *The Models*

The 11 process based models considered in this study, encompassing stand, (GDAY, CENTURY, TECO), age/size-gap (ED2), land surface (CABLE, CASA, CLM4,

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EALCO, ISAM, O-CN), and dynamic vegetation models (LPJ-GUESS, SDGVM), vary widely in terms of their structure, emphasis and complexity. A detailed overview of the models is provided in Walker *et al.* (*in prep*). Here, we give some basic information about each of the models and summarise the key assumptions in each model that affect the simulated water fluxes (see Table 1).

### *Model simulations*

Model participants submitted simulations that covered the time periods representative of the FACE experiments. Modellers were provided with forcing meteorological and CO<sub>2</sub> concentration data, general site history information and stand characteristics with the intention that simulations be representative without being “tuned” to the observations. These data sets are available at: <http://public.ornl.gov/face/index.shtml>. Model outputs were provided at the two time steps hourly and daily, if appropriate. These outputs contained estimates of the various carbon, N and water fluxes and pools.

### *Model analysis*

The approach taken to analyse the model simulations was to make predictions based on a simple model, then to investigate reasons for the departure of each model from this simple model. By taking this process-oriented approach, our results can also be applied to other models not participating in this study. The simple model is based on the coupling between stomatal conductance and assimilation, which is widely observed experimentally (Wong *et al.*, 1979). Ball *et al.* (1987) found that this correlation was modified by humidity and atmospheric CO<sub>2</sub> concentration, and synthesised their observations into a simple empirical model. Several alternative

forms of this stomatal conductance model exist (Table 1). We use the form derived by Medlyn *et al.* (2011a) from the optimal stomatal theory of Cowan and Farquhar (1977). They obtained the following expression for stomatal conductance:

$$g_s = g_0 + 1.6 \left(1 + \frac{g_1}{\sqrt{D}}\right) \frac{A}{C_a} \quad (1)$$

where  $A$  is the gross assimilation rate ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ ),  $g_0$  ( $\text{mol m}^{-2} \text{s}^{-1}$ ),  $g_0$  and  $g_1$  (dimensionless) are fitted terms representing the minimum stomatal conductance and the sensitivity of the conductance to the assimilation rate, respectively,  $C_a$  is the atmospheric  $\text{CO}_2$  concentration, and  $D$  is the vapour pressure deficit (kPa) at the leaf surface. The minimum conductance,  $g_0$ , is small and in the simple model is assumed to be zero. In well-coupled atmospheric conditions (i.e. transpiration rate is largely determined by stomatal conductance), transpiration ( $E$ ) ( $\text{mol H}_2\text{O m}^{-2} \text{s}^{-1}$ ) can be approximated as:

$$E = g_s \frac{D}{P} \quad (2)$$

where  $P$  is the atmospheric pressure (kPa).

We can then combine equations 1 and 2 and re-arrange to show that if  $g_1$  and  $D$  are assumed to be unchanged by  $\text{CO}_2$  treatment then the instantaneous leaf WUE is directly proportional to the  $\text{CO}_2$  concentration:

$$\text{WUE} = \frac{A}{E} \propto C_a \quad (3)$$

Thus, for a given increase in  $[\text{CO}_2]$ , this simple model would predict a directly proportional increase in WUE. This model is clearly overly simple, but provides a

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baseline expectation that we can use to understand responses of more realistic models and to explore the root cause of model-to-model and model-to-observation differences.

We can analyse model behaviour by comparing the predicted change in WUE with  $eCO_2$  against the proportionality arising in the simple model. We examined each model's predictions to see how far that model deviated from proportionality, and then analysed the models to identify the assumptions causing this deviation. In the results, we first discuss the differences in assumptions among the models, and the impacts of these assumptions on model predictions; we then compare the models against data from the FACE experiments.

## Results

### Analysis of model behaviour

#### *Proportionality of modelled WUE response to $CO_2$ treatment*

Model results were examined by plotting the  $CO_2$  effect (elevated/ambient) on WUE (GPP per unit transpiration) for each day against the proportional increase in  $CO_2$  for that day. These plots are shown for the year 2002 for the Duke and ORNL sites in Figs. 1 and 2, respectively (for all years see S3-20). Most models show a relationship between the  $CO_2$  effect on WUE and the  $CO_2$  enhancement. However, in most cases there is a departure from direct proportionality; the slope of the relationship between the  $CO_2$  effect on WUE and the  $CO_2$  enhancement is less than 1. Also, at Duke (Fig. 1) there are noticeable drops in the WUE response to  $[CO_2]$  at high levels of enhancement in several models (CABLE, ED2 and O-CN). These drops occur under simulated soil moisture stress and tend to occur during the middle of the year when the  $CO_2$  enhancement is at its highest. We investigated the reasons for the departures from proportionality for each model, using the simple model as a basis for our investigation. The major reasons for the departures from proportionality as suggested

by the simple model can be classified as follows: (1) the model does not couple  $A$  and  $g_s$ , or uses only partial coupling; (2)  $A/g_s$  is not directly proportional to the change in  $[CO_2]$ ; (3)  $E$  is not proportional to  $g_s$ ; and (4) soil moisture stress modifies the coupling between  $A$  and  $g_s$ . Finally, we want to reiterate that these departures from the simple model do not necessarily represent model failures, but rather are a means of classifying and understanding model behaviour.

*Lack of coupling, or partial coupling, between  $A$  and  $g_s$ ,*

The DAYCENT model does not couple the assimilation and transpiration calculations. Instead, transpiration is calculated as a function of the potential evapotranspiration, soil water stress and LAI. The effect of  $eCO_2$  on transpiration is explicitly specified, based on average measured responses of  $g_s$  to  $eCO_2$  at the two FACE sites. The hypothesised response of WUE to  $eCO_2$  is thus not applicable to simulations by this model. Figs. 1 and 2 therefore show no relationship between the  $CO_2$  effect on WUE and the  $CO_2$  enhancement in this model.

The CLM4 model shows a subset of points with WUE response below proportionality for the Duke site (Fig. 1), and noticeable scatter with a WUE response below proportionality for the Oak Ridge site (Fig. 2). The CLM4 model does use a coupled stomatal model to calculate transpiration, but  $A$  and  $g_s$  become progressively decoupled as the limitation to new growth from the availability of mineral N increases. Under N-limitation,  $A$  is reduced below its potential value, but in the calculation of  $g_s$  the potential  $A$  rate is used, rather than the N-limited  $A$  rate. This decoupling of the two processes results in a low  $CO_2$  effect on WUE, because the  $CO_2$  effect on  $A$  is reduced under N-limitation but the transpiration losses are unchanged.

The model predicts higher N-limitation at both sites during the summer and under eCO<sub>2</sub>.

#### *Proportionality of A/g<sub>s</sub> to atmospheric CO<sub>2</sub>*

In the original Ball *et al.* (1987) model (Equation 1), A/g<sub>s</sub> is proportional to atmospheric CO<sub>2</sub> concentration. Some models replaced the C<sub>a</sub> term in Equation (1) with a different CO<sub>2</sub> dependence.

In the O-CN model, the C<sub>a</sub> term in Equation (1) is replaced with a non-linear response function ( $f_{CO_2}$ ) to model the effect of rising CO<sub>2</sub> by using a relationship based on C<sub>i</sub> rather than C<sub>a</sub> (Friend and Kiang, 2005):

$$f_{CO_2} = \frac{C_i + 0.004}{K_i C_i} \quad (4)$$

where  $K_i$  is a fitted parameter which equals 5. The parameters for this CO<sub>2</sub> dependence were obtained by fitting this model to data from a mini-ecosystem elevated CO<sub>2</sub> experiment on European Beech (Friend *et al.*, 2005). With this CO<sub>2</sub> dependence,  $g_s$  is reduced as [CO<sub>2</sub>] increases; however, unlike the classical Ball-Berry model, the C<sub>i</sub>:C<sub>a</sub> is not constant with C<sub>a</sub>, and the relationship between A and  $g_s$  is therefore no longer proportional to C<sub>a</sub>. As a result, there is a less-than-proportional CO<sub>2</sub> effect on WUE, the magnitude of which is sensitive to the fitted parameter ( $K_i$ ).

Simulations by the EALCO model impose a less than proportional change in the ratio of A to  $g_s$  as the [CO<sub>2</sub>] increases, by modifying the slope parameter as a function of [CO<sub>2</sub>], ( $f_{CO_2}$ ):



$$f_{CO_2} = \frac{1}{C_a(1.0 + 0.5(C_a - aCO_2)/aCO_2)} \quad (5)$$

where  $aCO_2$  is the  $CO_2$  is the baseline ambient  $[CO_2]$ . This equation translates to an increase in  $A/g_s$  that is half the increase in  $CO_2$  concentration above the baseline ambient value. Consequently, the WUE increases at half the rate of increase in  $CO_2$  concentration.

#### *Proportionality of transpiration with stomatal conductance*

In the simple model, transpiration is assumed to be proportional to stomatal conductance (Equation 2). This assumption only holds when stomata strongly control transpiration rates, i.e. when the canopy is well-coupled to the atmosphere. In reality, the boundary layer between the forest and atmosphere reduces the effect of stomatal conductance on transpiration rate. Jarvis and McNaughton (1985) showed that:

$$\frac{dE}{E} = (1 - \Omega) \frac{dg_s}{g_s} \quad (6)$$

where  $\Omega$  is the decoupling factor and ranges from 0 for a canopy fully coupled to the atmosphere to 1 for a completely decoupled canopy. The decoupling factor increases as the ratio of boundary layer conductance to stomatal conductance decreases; the canopy becomes decoupled when boundary layer conductance is low or when stomatal conductance is high. In a canopy that is decoupled from its local atmosphere, the  $CO_2$  effect on WUE is reduced, because transpiration is not reduced in proportion to stomatal conductance. In the case of a completely decoupled canopy, transpiration

will be unaffected by the CO<sub>2</sub> effect on  $g_s$ , and the CO<sub>2</sub> effect on WUE will reduce to the CO<sub>2</sub> effect on A.

The boundary layer conductance is determined differently amongst the models: some models calculate a canopy boundary layer conductance, others a leaf boundary layer conductance, and others use both conductances in their calculations. For example GDAY, O-CN and SDGVM, determine atmospheric coupling through the ratio of  $g_s$  to canopy boundary layer conductance,  $g_a$ , which accounts for the influence of turbulence. Canopy conductance (and hence coupling) increases with canopy roughness and wind speed. Fig. 3a shows how changes in  $g_a$ , shown here by varying canopy roughness, change the CO<sub>2</sub> effect on WUE. The CO<sub>2</sub> effect on WUE is proportional to CO<sub>2</sub> for rough canopies with high  $g_a$ . SDGVM effectively assumes  $g_a$  only varies with LAI, fixing the wind speed to 5 m s<sup>-1</sup>. This results in the model predicting a WUE response to eCO<sub>2</sub> along the saturating portion of the line shown in Fig. 3a, i.e. proportionality between  $g_s$  and  $E$ . However, as the model predicts higher LAI at Oak Ridge, the model also predicts a reduction in boundary layer conductance and thus a reduced WUE response to CO<sub>2</sub>. In contrast to SDGVM, GDAY accounts for the influences of day-to-day wind speed variations, which tend to reduce  $g_a$ . GDAY thus predicts a reduced CO<sub>2</sub> effect on WUE during stable atmospheric conditions.

Instead of canopy conductance, ISAM and TECO simulate leaf boundary layer conductance,  $g_b$ , which is determined by wind speed, the difference between the canopy and air temperature, and leaf size. Fig. 3b shows the influence of modelled leaf size on the response of WUE to CO<sub>2</sub> enhancement for a model using  $g_b$ . As leaf

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size increases, the conductance of the boundary layer decreases, transpiration is reduced and the proportionality of the WUE response to CO<sub>2</sub> is reduced. Leaf size is quite different between the two sites: at Duke the canopy is composed of thin needles, whereas leaf widths are ~0.12 m at Oak Ridge. Therefore, we would expect models using this approach to simulate different effects of CO<sub>2</sub> on WUE at the two sites, with a lower effect at ORNL. However, in some models, such as ISAM and TECO, the leaf width was fixed rather than being a parameter, so this difference does not appear.

The more complex LSMs, including CABLE, CLM4, EALCO and ED2 combine all three conductances (stomatal, leaf and canopy boundary layer). The overall decoupling factor thus depends on both leaf and canopy boundary layer conductances. We observed that models using all three conductances tended to have a higher decoupling factor than the simpler models using just two conductances, and thus predicted a lower CO<sub>2</sub> effect on WUE. For example, the CO<sub>2</sub> effect on WUE in CABLE is low (50–57 % of CO<sub>2</sub> enhancement, Figs. 1 and 2) compared to that in GDAY (77–88 % of CO<sub>2</sub> enhancement) although both models simulate a similar effect on  $A/g_s$  (Fig. 4, see below).

In LPJ-GUESS (and with it the entire LPJ family of models), the atmospheric demand for transpiration is simulated with an empirically calibrated hyperbolic function of canopy conductance (Huntingford and Monteith, 1998) rather than the Penman-Monteith equation used by the other models. This empirical function is parameterised with a scaling conductance ( $g_{h-m}$ ), which is the conductance at which transpiration reaches half its maximum value. When canopy conductance  $g_s$  exceeds  $g_{h-m}$ , as occurs

for both sites simulated here, the canopy becomes decoupled and the transpiration rate is thus relatively insensitive to CO<sub>2</sub>- driven changes in  $g_s$ .

We compare four models with different levels of coupling (GDAY, CABLE, LPJ-GUESS and O-CN) in Fig. 4. GDAY and O-CN only consider  $g_a$  and both have tight coupling. For both these models the WUE response is therefore similar to the  $A/g_s$  response. However for O-CN, the WUE response is lower than for GDAY; this is because the response of  $A/g_s$  to CO<sub>2</sub> is less than proportional, due to the different stomatal conductance model (see above). In both CABLE and LPJ-GUESS, the response of  $A/g_s$  to CO<sub>2</sub> is proportional, but coupling is low, reducing the WUE response. In CABLE,  $g_a$  and  $g_b$  operate in series (see above), reducing the coupling, such that the WUE response is about 64 % of the response of  $A/g_s$ . In LPJ-GUESS, stomatal conductance exceeds the scaling conductance, resulting in a very low WUE response that approaches the CO<sub>2</sub> effect on  $A$ .

The effect of the boundary layer is non-linear (Figure 3b), and consequently the time step of the model matters when estimating the CO<sub>2</sub> effect on WUE. We used a stand scale model, MAESTRA (Medlyn *et al.*, 2007), in conjunction with GDAY to quantify the likely impact of temporal (30 minute vs. day) resolution on the CO<sub>2</sub> effect on WUE, when other factors were fixed. Our sensitivity analyses suggested that models which operate on daily time steps are likely to predict higher WUE responses to CO<sub>2</sub> enhancement (mean ( $\mu$ ) =  $2.2 \pm 1.8$  %; range =  $-1.6$ – $7.3$  %). This bias is more pronounced during summer than winter because of the larger diurnal variability in the decoupling factor. This existence of this bias strongly suggests that sub-daily time step models are desirable to predict impacts of elevated CO<sub>2</sub> on WUE.

Finally, in some models such as CABLE, ED2, and OC-N, which consider  $g_b$ , differences in leaf-to-canopy temperatures drive differences in VPD, i.e. breaking from the assumption in the simple model that VPD does not change with CO<sub>2</sub> treatment. We tested the effect of these temperature driven differences by again running the MAESTRA model and found that at Duke leaf temperatures did not depart from the air temperature so did not affect the WUE response. At Oak Ridge, larger sized leaves resulted in some differences in the VPD due to higher leaf temperatures and led to a small increase in the WUE response to CO<sub>2</sub> (~4 %).

#### *Role of interception*

A disconnect between transpiration and stomatal conductance can also occur when the canopy is wet. Some of the models assume that intercepted water is lost from the system prior to any water balance and physiology calculations. However, several models, including CABLE, CLM4, EALCO, LPJ-GUESS, ISAM and O-CN, assume that if the canopy, or a fraction of it, is wet and there is an atmospheric deficit, canopy evaporation meets the atmospheric water demand for the wet fraction. As a consequence, during these periods,  $E$  is not related to  $g_s$ , but rather depends only on LAI and on the antecedent rainfall conditions, which determine the amount of interception. The corresponding transpiration is reduced, resulting in a high apparent water use efficiency during the period when the canopy is wet. Changes in LAI with CO<sub>2</sub> treatment influence the amount of intercepted water and therefore affect the CO<sub>2</sub> response of WUE, resulting in a non-proportional response. For example, LPJ-GUESS simulates increases in LAI at eCO<sub>2</sub> of between 3 and 30 % at Duke and up to 10 % at Oak Ridge. This effect is stronger at Duke, as the model assumes a higher interception in evergreen canopies (Gerten *et al.*, 2004), ~8 % of incoming rainfall.

Models differed strongly in how they simulated interception, indicating a high level of process uncertainty (Table 1). Rates of interception varied from 2 to 19 % of total rainfall and models disagreed whether, and how, interception impacts on leaf gas exchange.

#### *Effect of soil moisture stress on the WUE response to $eCO_2$*

Day-to-day variability in the  $CO_2$  effect on WUE may be additionally controlled by soil moisture stress, depending on how the soil moisture stress is assumed to affect gas exchange. In some models (CLM4, EALCO and ED2), soil moisture stress is assumed to directly affect photosynthetic rates. Stomatal conductance is consequently indirectly reduced by drought, but the ratio of  $A/g_s$  is unaffected. In these models, soil moisture stress does not affect the  $CO_2$  response of WUE. In other models (e.g. CABLE, GDAY, ISAM, O-CN and TECO), soil moisture stress is assumed to reduce the slope of the relationship between stomatal conductance and assimilation. In these models, the  $CO_2$  response of WUE typically decreases during soil moisture stress. This effect is demonstrated for the GDAY model in Fig. 5, which shows the impact of  $CO_2$  enrichment on modelled soil moisture availability and the corresponding  $g_1$  parameter (sensitivity of stomatal conductance to assimilation), which is reduced during water stressed periods. Under  $eCO_2$ , transpiration is reduced, resulting in slower soil moisture depletion than at  $aCO_2$ . Soil moisture stress results in an increase in WUE; accordingly the WUE at  $aCO_2$  is increased relative to the less stressed  $eCO_2$  simulation (assuming the effects of  $D$  to be equal) and this reduces the response of WUE to  $CO_2$ . The impact of soil moisture stress upon WUE can clearly be seen in Fig. 5, where there are distinct and prolonged reductions in the WUE effect size highlighted by grey shading. Fig. 5 also shows a pronounced drop in the response

of WUE to eCO<sub>2</sub> during the end and beginning of a given year, which is a consequence of variability in the CO<sub>2</sub> enrichment signal at the Duke site. In the model SDGVM, it is assumed that water stress affect both stomatal conductance and V<sub>cmax</sub> (and hence J<sub>max</sub>). During water stressed periods this will result in a similar response to those models that reduce the slope linking g<sub>s</sub> and A.

The reduction in the WUE response to enriched CO<sub>2</sub> is seen clearly in Fig. 1 in the GDAY and CABLE simulations for example. In other models the effect is not apparent; this is either because soil moisture stress attenuates the assimilation rate, or because the model does not simulate soil moisture stress in the years shown.

The model LPJ-GUESS simulates water stress somewhat differently to the other models. In this model, transpiration is given by the minimum of the atmospheric demand and the supply of water, the latter depending on root distribution-weighted soil moisture and a maximum transpiration rate (Gerten *et al.*, 2004). However, in the simulations presented here, low soil moisture availability rarely occurred. Instead, water supply was mainly limiting during periods of high atmospheric demand, when demand exceeded the maximum capacity of the plants to extract water. These periods when demand exceeds supply occurred frequently throughout the summer. During these periods, there is no stomatal influence on transpiration. Consequently, the CO<sub>2</sub> effect on WUE becomes the CO<sub>2</sub> effect on GPP.

Finally there are a number of other minor factors that change the CO<sub>2</sub> effect upon WUE. These include the residual stomatal conductance term, leaf sheltering, use of the atmospheric CO<sub>2</sub> concentration rather than the concentration at the leaf surface,

and the gross rather than net assimilation rate. These factors are addressed in the supporting information.

## Model comparison against data

### *Leaf-scale instantaneous transpiration efficiency*

Stomatal conductance data from both sites were used to test modelled leaf-level responses. The simple stomatal conductance model (Eq. 1) fitted the data well (Fig. 6), supporting the assumption of coupling between assimilation and stomatal conductance. Importantly, at the ORNL site, N content of the foliage declined strongly over the course of the experiment (Norby *et al.* 2010), but neither the slope of the stomatal model, nor the response of  $A/g_s$  to  $\text{CO}_2$ , was altered by this decline (Fig. 6b). These data indicate that the coupling between stomatal conductance and assimilation is not affected by N limitation (Fig 6b). The data therefore tend to support coupled models over uncoupled, or partially coupled, models such as DAYCENT and CLM4.

The data also tend to support a dependence on  $C_a$  as originally proposed by Ball *et al.* (1987), i.e. a proportionality between  $A/g_s$  and  $C_a$ . We tested the dependence on  $C_a$  by fitting the expression (cf Eq 1.) to each data set, and obtaining confidence intervals for the  $C_a$  dependence ( $b$ ).

$$g_s = 1.6 \left( 1 + \frac{g_s}{A} \right) A C_a^{-b} \quad (7)$$

Estimates for  $b$  were 0.969 (ORNL, 1999), 0.999 (ORNL, 2009) and 1.138 (Duke, 1998-2006). Confidence intervals from each data set were combined using meta-analysis, to obtain an overall confidence interval for  $b$  of (0.9, 1.07), strongly



supporting an inverse proportional dependence on  $C_a$ . Alternatives to this  $CO_2$  dependence, such as those used in O-CN (Equation 4) and EALCO (Equation 5), were tested against the data using dummy variable regression and were found not to be supported by the data.

#### *Annual stand WUE*

At the stand-scale, the observed mean annual WUE response to  $CO_2$  was lower at Duke:  $\mu = 29.7 \pm 13.8 \%$  ( $1\sigma$  = inter-annual variability; years = 10) than Oak Ridge:  $\mu = 37.6 \pm 7.1 \%$  (years = 4), though between sites, responses are consistent when accounting for inter-annual variability (Figs. 7 and 8). However, the enhancement in WUE was notably lower than (i.e. not directly proportional to) the mean  $[CO_2]$  increase, which was  $\mu = 45.4 \pm 13.8 \%$  and  $\mu = 40.3 \pm 11.5 \%$ , at Duke and Oak Ridge respectively. The mean increase in WUE was thus ~65 % (Duke) or ~93 % (ORNL) of the mean increase in  $[CO_2]$ .

The simulated annual mean WUE response to  $eCO_2$  is compared with observed values in Figs. 7 and 8. At Duke the model responses can clearly be seen to fall into three broad categories: higher than the observed inter-quartile range (GDAY, ISAM, SDGVM and TECO); within the observed inter-quartile range (CABLE, CLM4, ED2 and O-CN); and lower than the observed inter-quartile range (DAYCENT, EALCO, LPJ-GUESS). However, there is considerable year-to-year variability in the observed inter-quartile WUE response and the mean of all of the models ( $\mu = 27.8 \pm 9.7 \%$ ) falls within the inter-annual variability bounds of the observed response. In contrast, at Oak Ridge, the modelled WUE response ( $\mu = 24.1 \pm 6.4 \%$ ) is broadly below the observed. At Oak Ridge, ISAM, O-CN, SDGVM and TECO predict the highest

modelled responses to CO<sub>2</sub> treatment, similar to that found for Duke. Overall, most modelled simulations, with the exception of DAYCENT, EALCO and LPJ-GUESS, predict a lower WUE response to CO<sub>2</sub> than at Duke; LPJ-GUESS and CLM4 predict the smallest responses.

The overall model responses can be understood from our analysis, whereby various assumptions combine to alter the CO<sub>2</sub> effect on WUE from strict proportionality. As described above, the assumed leaf-level responses to CO<sub>2</sub> were not consistent with experimental data in the DAYCENT, CLM4 and EALCO models, explaining why these models generally predicted lower than observed mean CO<sub>2</sub> responses of WUE. Leaf-level responses in O-CN were not consistent with data either, but this model nonetheless captured the mean CO<sub>2</sub> response of WUE.

The assumptions regarding soil moisture stress and interception vary strongly among the other models, indicating significant process uncertainty. However, these assumptions have a smaller influence at an annual time scale than the boundary layer, because drought and rainfall events are typically shorter-lived incidents. The most important difference among models lies in the degree of atmospheric coupling. In general, the “simplest” models tended to predict the highest WUE responses (over-prediction at Duke), while the more “complex” models tended to predict WUE response to CO<sub>2</sub> similar to the observations at the well coupled site (Duke), but  $\sim 7 \pm 5$  % lower than observed at the more decoupled site (Oak Ridge). Thus, the comparison against data indicates three sets of assumptions (interception, soil moisture stress, and atmospheric coupling) give rise to considerable variability among models and therefore require further investigation.

### *Annual stand transpiration*

The modelled WUE responses, when considered with the modelled GPP responses, help to explain why the models differ in the predictions of the CO<sub>2</sub> effect on *E*. Model predictions of the CO<sub>2</sub> effect on *E* were poor for both sites, but for different reasons. At Duke, modelled WUE responses are broadly consistent with the observed, but the modelled *E* responses to CO<sub>2</sub> are not, and the inter-model variability is considerable,  $\mu = -6.1 \pm 7.7 \%$  (min = -25.9 %, max = 9.4 %) (Fig. 7c). Following our simple model, the GPP response to CO<sub>2</sub> must on the whole be poorly simulated (Fig. 7b). At Duke the variable GPP responses relate to the availability of canopy N, discussed in more detail by Zaehle, 2012 (*in prep*). At Oak Ridge, on the other hand, the models generally predicted the GPP response well, but poorly predicted the WUE response to eCO<sub>2</sub>. Consequently, as at Duke, model predictions for the CO<sub>2</sub> response of *E* were also poor and again varied between models (inter-model  $\mu = -6.4 \pm 7.8 \%$ , min = -31.2 %, max = 10.6 %).

## **Discussion**

We evaluated 11 models against leaf-scale and stand-scale water use efficiency data from two long-term forest FACE experiments. Simply comparing models against data would not be insightful, since the outcomes would apply to these versions of these models only. Instead, as advocated by Medlyn *et al.* (2011b), we first analysed the models in order to identify the key mechanisms driving model behaviour. This allowed us to compile a checklist of model assumptions that could be used to analyse predictions by any model of the effect of rising CO<sub>2</sub> on stand transpiration. Comparison of the models against the experimental data then allowed us to

discriminate among these model assumptions and to clearly identify areas of uncertainty that need to be resolved.

Following experimental evidence (Cowan and Farquhar, 1977; Wong *et al.*, 1979), most models assume that transpiration is coupled to carbon assimilation (Ball *et al.*, 1987; Collatz *et al.*, 1992; Leuning 1995; Katul *et al.*, 2010; Medlyn *et al.*, 2011a). We therefore analysed model outcomes in terms of water use efficiency, or the ratio of assimilation to transpiration. The simplest coupled model predicts that WUE should scale in direct proportion to changes in  $C_a$  in well-watered conditions (Equation 3). In this study, models predicted  $C_a$  effects on WUE that differed among models, but were generally less than direct proportionality (Figs. 1 and 2). We identified a number of principal causes that currently lead to differences among models, in particular: (i) assumptions about the stomatal response to elevated  $CO_2$ ; (ii) the roles of the leaf and atmospheric boundary layer (Figs. 3 and 4); (iii) treatment of canopy interception; and (iv) the impact of soil moisture stress (Fig. 5). In each of these areas, there are real discrepancies among models in the way the process is represented; but we believe that data are available to resolve these discrepancies in each case.

#### *The stomatal response to elevated $CO_2$*

The empirical stomatal model of Ball *et al.* (1987) and related theoretical models (Leuning 1995; Medlyn *et al.*, 2011a) proposed that for well-watered conditions, at a given relative humidity or  $D$ , stomatal conductance should be proportional to assimilation divided by  $C_a$ . This response is equivalent to stating that the  $C_i:C_a$  ratio is

independent of  $C_a$  (see also Katul *et al.*, 2000). This stomatal response to elevated  $C_a$  was recently shown to be consistent with optimal stomatal theory (Medlyn *et al.*, 2011a; but see also Katul *et al.*, 2010). Data from the two forest FACE sites support this elevated  $C_a$  response of stomata (Fig. 6). The response is generally supported wherever empirical data has been fitted to this stomatal model (Medlyn *et al.*, 2001, Leavitt *et al.* 2003; Leakey *et al.* 2006; Ainsworth and Rogers 2007; Barton *et al.*, 2012). The hypothesis that the  $C_i:C_a$  ratio is independent of  $C_a$  also has widespread experimental support (Drake *et al.*, 1997; Ainsworth and Long, 2005). Models sometimes employ alternative  $C_a$  dependences parameterised from individual experiments (e.g. Equations 4, 5) but the bulk of experimental data and our analyses of the Duke and Oak Ridge data would appear to be consistent with the original response hypothesised by Ball *et al.* (1987).

#### *Leaf and canopy boundary layer conductance*

We have shown that the magnitude of WUE response to  $C_a$  predicted at the stand-scale depends on the assumed coupling between the foliage and the atmosphere. For strongly-coupled, well-watered trees, the relationship between WUE and  $C_a$  should be independent of scale. This prediction is supported by experimental data (Barton *et al.*, 2012); in a well-coupled *Eucalyptus saligna* canopy, instantaneous transpiration efficiency increased in proportion to  $C_a$  at both leaf and whole-canopy scale. However, as canopy decoupling increases, the  $CO_2$  response of whole-canopy WUE is predicted to decline from proportionality.

From our model comparison, it is apparent that models that adopt simpler boundary layer treatments tend to have the highest canopy-atmosphere coupling and therefore

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predict the highest WUE responses. In contrast, models with more complex representations of canopy-atmosphere coupling often add leaf and canopy boundary layer conductances in series, resulting in a low overall boundary layer conductance, high decoupling and therefore a low WUE response. To understand a given model's prediction of CO<sub>2</sub> effects on transpiration, therefore, it is important to understand the level of decoupling assumed by the model. For this purpose, modelling studies should be very explicit about what boundary layer conductances that have been assumed, and what values have been used for the key parameters, namely roughness length, leaf width and wind speed, decoupling factors (*sensu* Jarvis and McNaughton, 1986) could also be derived from model output and reported explicitly. Importantly, there is clearly scope to reduce the large model-to-model differences relating to assumed coupling (Fig. 4) by using eddy covariance data to determine appropriate decoupling factors for use in models. We suggest that such data analyses are a priority for reducing model uncertainty.

### *Interception*

Another key difference among models was in how interception was treated. Changes in leaf area are often speculated to impact upon any potential water savings under eCO<sub>2</sub> (Woodward *et al.*, 1990; Field *et al.*, 1995). We have deliberately not discussed simulated changes in LAI in response to CO<sub>2</sub> here because the coupled A-g<sub>s</sub> relationships assumed by the various models implicitly consider these changes. Any increase in LAI due to additional photosynthate at eCO<sub>2</sub>, will be accounted for by an increase in GPP (due to increased light interception) and water loss, due to increased stomatal conductance. The WUE response (equation 3) to CO<sub>2</sub> accounts for these leaf area changes.

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However, effects on LAI play an important role in determining effects when canopies are wet. If LAI increases under eCO<sub>2</sub>, as simulated by most models, canopy interception will increase. Several models use intercepted water to meet a proportion of atmospheric demand. In these models, the increase in interception will result in a smaller CO<sub>2</sub> effect on WUE. Models differed in how they treated interception, and in the estimated proportion of intercepted canopy water (~2 to 14 %). Interception rates estimated from measurements as the difference between precipitation and throughfall are considerably higher than these modelled values. Values given by Schäfer et al., (2003) for the Duke site are approximately 27 % of precipitation. Data were not available for the ORNL site but interception rates for other hardwood forests in the vicinity are of the order of 16 % (Oishi et al., 2008). This model process uncertainty is another key area where discrepancies among models could be significantly reduced through data synthesis.

#### *Soil moisture stress*

There was a great deal of variability between the models as to when drought stress begins, duration of droughts and its impact on WUE (Egea *et al.*, 2011). These differences arise through different approaches to parameterisation. However, more fundamentally, we also identified considerable process uncertainty: models disagreed on the mechanisms by which moisture stress affects photosynthesis and transpiration fluxes. Some models assumed moisture stress affects photosynthetic capacity, others assumed it reduces the slope of A-g<sub>s</sub> relationship. Recent research suggests that neither of these processes alone is sufficient to capture the full drought effect (Keenan *et al.*, 2010; Egea *et al.*, 2011). There remains a need to find more mechanistic models to

explain coupled carbon and water responses, particularly at ecosystem scales (e.g. Katul *et al.*, 2010; Medlyn *et al.*, 2011a; Buckley *et al.*, 2012), which would allow us to make predictions under drought conditions that did not rely on simple empirical modifiers. Given the data available on plant responses to moisture stress, this is another important avenue of research that would allow us to close the gap between the models, and the model and observations.

#### *Comparison with FACE data*

Stand-level WUE, evaluated as  $\text{NPP}/E$ , often does not increase in proportion to  $C_a$ . For example, over the 20<sup>th</sup> century there has been a continuous rise in the  $[\text{CO}_2]$  (~23 %), whereas the change in plant WUE inferred from stable carbon isotope measurements has been considerably more variable (Saurer *et al.*, 2004; Waterhouse *et al.*, 2004; Gagen *et al.*, 2011; Peñuelas *et al.*, 2011). This suggests additional site-specific constraints when extrapolating our experimental understanding to the landscape scale (Peñuelas *et al.*, 2008; Linares *et al.*, 2009; Andreu-Hayles *et al.*, 2011).

At our two experimental FACE sites, the observed WUE increase was 66 % (Duke) or 93 % (ORNL) of the treatment enhancement of  $C_a$ . There is a possibility that this discrepancy is due to the necessity of calculating stand-level WUE from the observations of net primary productivity, rather than gross primary productivity, divided by transpiration. If the  $\text{NPP}:\text{GPP}$  ratio decreases under  $e\text{CO}_2$ , the  $C_a$  effect on observed WUE will be reduced. However, we have not addressed the  $\text{NPP}:\text{GPP}$  ratio in this paper (see De Kauwe *et al.*, in prep.).



Leaving aside the possibility of changes in the NPP:GPP ratio, our model comparison suggests that boundary layer and soil moisture feedbacks are the main factors attenuating the WUE response to CO<sub>2</sub>. Decoupling between the foliage and atmosphere due to the existence of a boundary layer can reduce the effect of CO<sub>2</sub> on WUE. Whilst decoupling might be an explanation for the lower-than-proportional CO<sub>2</sub> response of WUE at Oak Ridge, this is less likely to be the explanation for Duke, where the thin needle canopy should be well coupled to the atmosphere. More specific to the Duke site, effects of needle age and inter-annual variability in meteorological forcing (precipitation, storm damage and droughts), may have affected the magnitude of the WUE response to eCO<sub>2</sub> (see Ellsworth *et al.*, 2012). Domec *et al.* (2009) showed that  $g_s$  was reduced under eCO<sub>2</sub>, but only during well-watered conditions. At Duke the rooting depth (0.75 m), imposed by a hard clay pan in the soil, is shallow for a forest (Oren *et al.*, 1998). Consequently, water stress is common and may have been a key factor in reducing the CO<sub>2</sub> effect on WUE.

Experimental data on NPP and transpiration include many sources of uncertainty. Both terms comprise multiple primary measurements (e.g. litter mass, stem circumference, tree height, fine root length in mini-rhizotron tubes, and sap flux) with different degrees of precision, and critical scaling assumptions that may introduce biases. Heterogeneity across the tree plantation also contributes to substantial plot-to-plot variation, with coefficients of variation for NPP at ORNL of 20-24 %.

It can also be questioned whether the turbulence regime in the FACE rings is different from natural conditions. Wullschleger *et al.*, (2002) argued that the canopy decoupling in FACE rings might be lower than in natural canopies. However a

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detailed study using arrays of 3D sonic anemometers found no effect on turbulence regime (He *et al.* 1996 cited with additional information in Hendrey *et al.* 1999). Therefore, at Duke, the 26 m diameter region inside the 30 m total plot is considered uninfluenced by gas ports in terms of CO<sub>2</sub> concentration or turbulence.

#### *Implications for other model studies*

A number of models have previously been applied to predict eCO<sub>2</sub> effects on transpiration fluxes. For example, Cramer *et al.*, (2001) showed that the physiological CO<sub>2</sub> effect on runoff estimated by five DGVMs for the period 1990-2100 resulted in a change of anywhere from -3 to +47 %. Our study has developed a “checklist” approach (cf. Medlyn *et al.* 2011b) that can be used to assess and compare such model studies. The key questions to ask of any model study are as follows. First, is stomatal conductance coupled to assimilation rate? If so, assessments should focus on CO<sub>2</sub> effects on GPP and WUE, since these processes determine CO<sub>2</sub> effects on *E*. Secondly, is the ratio  $A/g_s$  proportional to  $C_a$ ? Increasing experimental evidence supports this assumption. Thirdly, how well coupled is the canopy to the atmosphere? Predicted effects on transpiration will be highest in model simulations that assume strong coupling. Fourthly, how is drought stress assumed to affect fluxes? Finally, what percentage of rainfall is intercepted, and does interception reduce transpiration fluxes? This checklist provides a relatively straightforward means to assess model simulations of transpiration responses to elevated CO<sub>2</sub>. In addition, it highlights key areas where data synthesis could significantly reduce discrepancies among models.

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## Figure Captions

Figure 1: Comparison of the ratio of WUE at eCO<sub>2</sub> to WUE at aCO<sub>2</sub>, plotted against  
the enhancement in CO<sub>2</sub> for 2002 at the Duke FACE site. The dashed black line is the  
1:1 line, whilst the solid grey line is the fit to the points, forced through the origin.

Model names are given on each panel, as are the slopes of the fitted lines.

Figure 2. Comparison of the ratio of WUE at eCO<sub>2</sub> to WUE at aCO<sub>2</sub>, plotted against  
the enhancement in CO<sub>2</sub> for 2002 at the ORNL FACE site. The dashed black line is  
the 1:1 line, whilst the solid grey line is the fit to the points, forced through the origin.

Model names are given on each panel, as are the slopes of the fitted lines.

Figure 3: Sensitivity of the WUE response to CO<sub>2</sub> enhancement for varying (a)  
canopy boundary layer conductance and (b) leaf boundary layer conductance.

Sensitivities were estimate using the MAESTRA model (Medlyn et al. 2007) as a  
function of (a) roughness length and (b) leaf width, carried out using the MAESTRA  
model. In panel (b) the grey shading indicates 1 standard deviation in the annual  
WUE response to CO<sub>2</sub>.

Figure 4: Modelled effects of CO<sub>2</sub> on the mean annual ratio of GPP to canopy conductance ( $A/g_s$ ), the ratio of GPP to transpiration (WUE), and GPP ( $A$ ) for GDAY, CABLE, LPJ-GUESS and O-CN for the year 2003.

Figure 5: The impact of soil moisture stress on the modelled WUE response to eCO<sub>2</sub> for the GDAY model for 2007 at the Duke site. Panel (a) shows how the soil moisture availability ( $\beta$ ) changes as a function of day of year, panel (b) shows how the  $g_1$  parameter is adjusted as  $\beta$  changes, and panel (c) shows the CO<sub>2</sub> effect on WUE and how it is impacted by these drought episodes. The light gray shading indicates periods of strong drought.

Figure 6: Measured leaf level stomatal conductance as a function of stomatal index  $A/(C_a\sqrt{D})$  at the (a) Duke (b) Oak Ridge sites. Fitted linear regression lines are shown. The stomatal model (Equation 1) was fitted to both data sets. There was no significant difference in slope between ambient and elevated CO<sub>2</sub> treatments at either site. Duke:  $g_1 = 2.56$  (Amb) and  $2.64$  (Elev). Test of different slopes:  $p = 0.58$ , overall model  $r^2 = 0.51$ . Oak Ridge:  $g_1 = 4.20$  (Amb) and  $4.11$  (Elev). Test of different slopes:  $p = 0.71$ , overall model  $r^2 = 0.83$ .

Figure 7: Box and Whisker plots showing the mean annual response of (a) WUE, (b) GPP and (c) transpiration ( $E$ ) to CO<sub>2</sub> enhancement at Duke, between 1996-2007, for observations and 11 models. Models (boxes) are shown in order of WUE response to CO<sub>2</sub>. Note: NPP is used in place of GPP in the observations. The ends of the boxes show the lower (25<sup>th</sup>) and upper (75<sup>th</sup>) quartiles. The horizontal whiskers show the full range of the data. The lines in the boxes are the medians and stars are the means.

Figure 8: Box and Whisker plots showing the mean annual response of (a) WUE, (b) GPP and (c) transpiration ( $E$ ) to CO<sub>2</sub> enhancement at Oak Ridge, for the years 1999, 2004, 2007 and 2008, for observations and 11 models. Models (boxes) are shown in order of WUE response to CO<sub>2</sub>. Note: NPP is used in place of GPP in the observations. The ends of the boxes show the lower (25<sup>th</sup>) and upper (75<sup>th</sup>) quartiles.

The horizontal whiskers show the full range of the data. The lines in the boxes are the medians and stars are the means.

**Table 1. Summary of model assumptions important for predicting transpiration and water use efficiency.**

	CABLE	CLM4	DAYCENT	EALCO
Model Name	CSIRO Atmosphere Biosphere Land Exchange	The Community Land Model version 4	Daily version of CENTURY	Ecological Assimilation of Land and Climate Observations
Reference	Kowalczyk <i>et al.</i> , 2006; Wang <i>et al.</i> , 2010, 2011	Oleson <i>et al.</i> , 2011	Parton <i>et al.</i> , 1983	Wang <i>et al.</i> , 2008, Wang <i>et al.</i> , 2007
Timestep	30-min	30-min	Daily	30-min
Assimilation	Farquhar <i>et al.</i> (1980)	Collatz <i>et al.</i> (1991) (no co-limitation)	$f(\text{nitrogen, temperature, soil water, PAR})$	Farquhar <i>et al.</i> (1980)
Stomatal Conductance	$g_s = g_0 + \frac{g_1}{1 + \frac{g_1}{g_0}}$	$g_s = g_0 + g_1 A$	$g_s = f(\text{LAI, PET})$	$g_s = g_0 + g_1 A$
CO <sub>2</sub> function	$f_{\text{CO}_2} = \frac{1}{(C_s - P)}$	$f_{\text{CO}_2} = \frac{1}{C_s}$	NA	$f_{\text{CO}_2} = \frac{1}{(1 + 0.2(C_s - P))}$
Transpiration	Iterative Penman-Monteith calculation at the leaf scale accounting for both $g_b$ and $g_a$ and limitation of soil water supply	Calculation at the canopy scale determined by atmospheric demand and accounting for both $g_b$ and $g_a$	$f(\text{PET, soil water stress and LAI})$ When LAI > 4.0, transpiration will equal PET	Iterative solution to the energy balance at sunlit vs. shaded canopy scale using $g_a$ only.
$g_0$ (mol (H <sub>2</sub> O) m <sup>-2</sup> s <sup>-1</sup> )	0.006	0.002	NA	0.0008
$g_a$	$f(\text{wind speed, canopy stability})$	$f(\text{wind speed, height})$	NA	$f(\text{wind speed, height, canopy stability})$
$g_b$	$f(\text{wind speed, leaf width})$	$f(\text{wind speed, leaf width})$	NA	NA
Interception effect on WUE; average fraction of intercepted rainfall at Duke / ORNL	Interception does not reduce transpiration; 2.4 – 2.2%	Atmospheric demand can be satisfied by evaporation of intercepted water; 5.1 – 3.5%	Interception does not reduce transpiration; 5.6 – 5.7%	Intercepted water used to meet atmospheric demand, which reduces transpiration fluxes but does not affect GPP calculations; 2.1 – 2.8 %
Soil Moisture stress	Modifier attenuates $g_1$	Modifier attenuates $V_{\text{cmax}}$	Directly affects transpiration	Modifier attenuates $J_{\text{max}}$

	parameter			and $V_{\text{cmax}}$
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**Table 1. Continued**

	ED2	GDAY	ISAM	LPJ-GUESS
Model Name	Ecosystem Demography version 2	Generic Decomposition and Yield	Integrated Science Assessment Model	General Ecosystem Simulator (GUESS) version of the combined Lund-Potsdam-Jena (LPJ)-GUESS modelling framework
Reference	Medvigy <i>et al.</i> , 2009	Comins and McMurtrie, 1993	Jain and Yang, 2005	Smith <i>et al.</i> , 2001, with unpublished implementation of nitrogen cycle (Smith <i>et al.</i> in prep.)
Time step	15-min	Daily	30-min	Daily
Assimilation	Farquhar <i>et al.</i> (1980)	Farquhar <i>et al.</i> (1980); Sands <i>et al.</i> 1996; Sands <i>et al.</i> 1995	Farquhar <i>et al.</i> (1980)	Collatz <i>et al.</i> (1991)
Stomatal conductance in well-watered conditions	$g_s = g_0 + \frac{g_1 A_n}{1 + D}$	$g_s = g_0 + 1.6 \left(1 + \frac{A_n}{g_0}\right)$	$g_s = g_0 + g_1 A_n$	$g_s = g_0 + 1.6 \frac{A_n}{1 + D}$
Stomatal conductance $\text{CO}_2$ function	$f_{\text{CO}_2} = \frac{1}{(C_s - \Gamma)}$	$f_{\text{CO}_2} = \frac{1}{C_s}$	$f_{\text{CO}_2} = \frac{1}{C_s}$	$f_{\text{CO}_2} = \frac{1}{C_s}$
Transpiration	Dynamic flux calculation from $g_s$ , $g_b$ , and leaf and canopy air vapour pressures	Penman-Monteith calculated at the canopy scale using $g_a$	Iterative solution to the energy balance at sunlit vs. shaded canopy scale, using both $g_a$ and $g_b$	Lesser of water supply, determined by plant-root-weighted soil moisture, and atmospheric demand, calculated as a semi-empirical hyperbolic function of canopy conductance (Gerten <i>et al.</i> 2004)
$g_0$ (mol $\text{H}_2\text{O}$ $\text{m}^{-2} \text{s}^{-1}$ )	0.0	0.0	0.016	0.012 – 0.02
$g_a$	$f$ (wind speed, vegetation profile)	$f$ (wind speed, vegetation profile)	$f$ (wind speed, height)	NA
$g_b$	$f$ (leaf temperature, leaf width, wind)	NA	$f$ (leaf temperature, leaf	NA

	<i>speed)</i>		<i>width, wind speed)</i>	
Interception effect on WUE; average fraction of intercepted rainfall at Duke / ORNL	Does not affect WUE calculations; 11.8 - 2.8%	Does not affect WUE calculations; 19.1 – 5.3%	Intercepted water used to meet atmospheric demand, which reduces transpiration fluxes but does not affect GPP calculations; 4.9 – 4.2%	Intercepted water used to meet atmospheric demand, which reduces transpiration fluxes but does not affect GPP calculations; 11.4 – 4.8%
Soil Moisture stress	Modifier attenuates assimilation and transpiration fluxes	Modifier attenuates $g_1$ parameter	Modifier attenuates $g_1$ parameter	During periods of stress, conductance is reduced until transpiration matches the supply rate. Photosynthesis rates are reduced accordingly

**Table 1. Continued**

	<b>O-CN</b>	<b>SDGVM</b>	<b>TECO</b>
Model Name	Orchidee CN	Sheffield Dynamic Vegetation Model.	Terrestrial Ecosystem Model
Reference	Zaehle et al, 2010	Woodward et al., 1995	Weng <i>et al</i> , 2008
Timestep	30-min	Daily	30-min
Assimilation	Kull and Knijt, 1998	Farquhar et al. (1980) as formulated by Harley et al. (1992)	Farquhar et al. (1980)
Stomatal Conductance	$g_s = \alpha \beta_D f_{CO_2} f_h A f(T)$	$g_s = g_0 + \frac{g_1(T)A}{(1 + 0.66D)} f_c$	$g_s = g_0 + \frac{g_1 A NSC}{1 + D/D_0} f_c$
CO <sub>2</sub> function	$f_{CO_2} = \frac{C_i + 0.004}{K_i C_i}$	$f_{CO_2} = \frac{1}{(C_s - 154T)}$	$f_{CO_2} = \frac{1}{(C_s - T)}$
Transpiration	Iterative Penman-Monteith calculation at the leaf canopy scale accounting, $g_a$	Penman-Monteith calculated at the canopy scale using $g_a$	Iterative Penman-Monteith calculated at the leaf scale using $g_b$
$g_0$ (mol (H <sub>2</sub> O) m <sup>-2</sup> s <sup>-1</sup> )	0.001-0.002	0.005	0.01
$g_a$	$f$ (wind speed, friction velocity)	$f$ (wind speed, height, LAI)	NA



$g_b$	NA	NA	$f$ (leaf temperature, leaf width, wind speed)
Interception effect on WUE; average fraction of intercepted rainfall at Duke / ORNL	Does not affect WUE calculations; 2.6 – 2.5%	Does not affect WUE calculations; 14.1 – 11.8%	Not calculated
Soil Moisture stress	Modifier attenuates $g_1$ parameter	Modifier attenuates $V_{\text{cmax}}$ and the $g_1$ parameter	Modifier attenuates $g_1$ parameter

Notes:  $A$  is the assimilation rate;  $g_s$  is stomatal conductance;  $g_0$  is the residual stomatal conductance as the assimilation rate reaches zero;  $g_1$  represents the slope of the sensitivity of stomatal conductance to assimilation,  $\text{CO}_2$  concentration and environmental controls (e.g. VPD); residual conductance to water vapour  $Rh$  is relative humidity at the leaf surface;  $D$  is the vapour pressure deficit;  $D_0$  is an empirical constant;  $C_s$  is the  $\text{CO}_2$  concentration at the leaf surface;  $\Gamma$  is the  $\text{CO}_2$  concentration point;  $P$  is the atmospheric pressure;  $g_a$  is the canopy scale boundary layer conductance;  $g_b$  is the leaf level boundary layer conductance;  $NSC$  is the non-structural carbon;  $PAR$  is the photosynthetically active radiation;  $LAI$  is the leaf area index;  $PET$  is the potential evapotranspiration;  $SMC$  is the soil moisture content;  $a\text{CO}_2$  is the ambient  $\text{CO}_2$  concentration;  $e\text{CO}_2$  is the elevated  $\text{CO}_2$  concentration;  $\beta$  is an empirical constant;  $V_{\text{cmax}}$  is the maximum rate of carboxylation;  $J_{\text{max}}$  is the maximum rate of electron transport;  $fh$  is a function describing the effect of canopy height on stomatal conductance;  $f(D)$  is a function describing the effect of atmospheric humidity upon stomatal conductance;  $\alpha$  and  $K_i$  are empirical constants;  $\beta_2$  is a soil moisture availability factor

















