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# Use of a crop model ensemble to quantify $CO_2$ stimulation of water–stressed and well-watered crops

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**Abstract.**

Increased atmospheric concentrations of carbon dioxide ($CO_2$) will benefit the yield of most crops. Two free Air $CO_2$ Enrichment (FACE) meta–analyses have shown increases in yield of between 0 and 73% for C3 crops. Despite this large range, few crop modelling studies quantify the uncertainty inherent in the parameterisation of crop growth and development. We present a novel perturbed–parameter method of crop model simulation, which uses some constraints from observations, that does this. The model used is the groundnut (i.e. peanut; *Arachis hypogaea* L.) version of the General Large–Area Model for annual crops (GLAM). The conclusions are of relevance to C3 crops in general.

The increases in yield simulated by GLAM for doubled $CO_2$ were between 16 and 62%. The difference in mean percentage increase between well–watered and water–stressed simulations was 6.8. These results were compared to FACE and controlled environment studies, and to sensitivity tests on two other crop models of differing levels of complexity: CROPGRO, and the groundnut model of Hammer et al. (1995). The relationship between $CO_2$ and water stress in the experiments and in the models was examined. From a physiological perspective, water–stressed crops are expected to show greater $CO_2$ stimulation than well–watered crops. This expectation has been cited in literature. However, this result is not seen consistently in either the FACE studies or in the crop models. In contrast, leaf–level models of assimilation do consistently show this result. An analysis of the evidence from these models and from the data suggests that scale (canopy versus leaf), model calibration, and model complexity are factors in determining the sign and magnitude of the interaction between $CO_2$ and water stress.

We conclude from our study that the statement that 'water–stressed crops show greater $CO_2$ stimulation than well–watered crops' cannot be held to be universally true. We also conclude, preliminarily, that the relationship between water stress and assimilation varies with scale. Accordingly, we provide some suggestions on how studies of a similar nature, using crop models of a range of complexity, could contribute further to understanding the roles of model calibration, model complexity and scale.

**Keywords:** Crop model, climate change, carbon dioxide, water stress, spatial scale

## 1. Introduction

Atmospheric concentrations of carbon dioxide are now substantially higher than they have been for hundreds of thousands of years (Siegenthaler et al., 2005) and they will continue to rise over the coming decades. Efforts to understand the impact of elevated $CO_2$ on annual crops are crucial to quantifying likely future food production. Studies of climate change routinely use single– or multi– model ensembles in order to quantify uncertainty in simulations (e.g. Murphy et al., 2004). These studies vary the equations and/or parameters that are used to predict climate, in order to produce an ensemble of output values rather than a single set. The current study applies these methods to the prediction of the impact of elevated $CO_2$ on crops, by varying the crop model parameters and hence producing an ensemble of simulations that sample uncertainty. This is not something that is commonly done in crop modelling studies (Challinor et al., 2005a).

Elevated $CO_2$ increases the rate of photosynthesis, decreases water use and can change leaf area index (LAI), above– and below– ground biomass, specific leaf area (SLA), radiation use efficiency (RUE) and harvest index (see e.g. Tubiello and Ewert, 2002). Table I illustrates some of these changes. In C4 crops, the principle mechanism for increased yield under elevated $CO_2$ is reduced water use. In C3 crops, both assimilation and water use are beneficially modified and increases in water use efficiency and yield can be mediated principally through the former (e.g. Clifford et al., 1993), the latter (e.g. Hartwell Allen. et al., 1996), or both.

Tubiello and Ewert (2002) and Ewert et al. (2002) present comparative reviews of the modelling methods used to simulate the impacts of elevated $CO_2$ on the growth and development of a C3 crop (wheat). One interesting issue that emerges is the difference in $CO_2$ stimulation between well–watered and water–stressed crops. From a physiological perspective, one would expect greater stimulation for stressed crops (see e.g. IPCC, 2001) and this effect can be seen in the measurement of daily integrated carbon assimilation (Bernacchi et al., 2006). Tubiello and Ewert (2002) show that many crop models capture this differential response. However, whilst some measurements of more integrated quantities such as biomass and yield show the same response (Kimball et al., 2002), some show greater $CO_2$–stimulation for non–stressed crops (Ainsworth and Long, 2005).

Consensus on the likely magnitude of the impact of elevated $CO_2$ on crops will only be achieved through ongoing dialogue between simulation and experimentation. Recent meta–analyses of free air $CO_2$ enrichment (FACE) experiments have indicated that the magnitude of $CO_2$–stimulation may be lower than previously thought (Long et al., 2005). It has been suggested that crop models are more likely to reproduce chamber–derived levels of $CO_2$ stimulation than the rather lower levels suggested by these more recent FACE studies (Long et al., 2006). However, Tubiello et al. (2007a) present evidence that crop simulation results are consistent with FACE studies.

The methods used in the current study provide a way of using observational constraints within a modelling framework, in order to make maximum use of the available information and so increase confidence in the results. The implications of this are discussed further in section 5. The study builds on the work of Challinor et al. (2005a), where it was shown that transpiration efficiency is a key source of uncertainty in predicting yields under future climates. That study also showed that uncertainty in climate simulation is an important component of uncertainty in yield variability. For the simulation of mean yields, however, climate model uncertainty did not act systematically across space, whilst uncertainty in the crop model did. Hence crop model uncertainty is particularly important in assessing mean yields. The current study focusses on this issue: the impact of crop model uncertainty on mean yields.

This study has three principal objectives: (i) to produce a validated ensemble of parameter sets for the General Large–Area Model for annual crops (GLAM) for exploring uncertainty in doubled $CO_2$ environments; (ii) to use these parameter sets to produce an ensemble of crop yields with which to assess the uncertainty associated with the response of a crop to elevated $CO_2$; (iii) to use these yield ensembles, together with sensitivity studies performed on two other crop models (CROPGRO: Boote and Jones, 1998; and the groundnut model of Hammer et al., 1995) and published crop measurements to assess the relationship between water stress and $CO_2$ stimulation. In particular we ask with what level of generality and conviction we should believe that "Relative enhancement of growth owing to $CO_2$ enrichment might be greater under drought conditions than in wet soil because photosynthesis would be operating in a more $CO_2$– sensitive region of the $CO_2$ response curve" (IPCC, 2001).

## 2. Methods

### 2.1. CROP MODEL DESCRIPTION

GLAM is a process–based model designed for use with daily time series of regional–scale (≈10–300 km) weather data, which is usually taken from climate models. Three soil hydrological parameters are required: the drained upper limit, saturated limit (i.e. field capacity) and lower limit. Data on the planting window are also required, since the simulated planting date is the first day within the planting window when soil moisture exceeds a specified fraction (50%) of the available soil water at the drained upper limit.

A schematic of the model is presented in figure 1. The model is of intermediate complexity — less complex than point–based models such as CROPGRO and more complex than, for example, the crop coefficient method of Doorenbos and Kassam (1979). It is based on the finding that, at least for groundnut in India, there is a relationship between crop yield and climate at the regional scale (Challinor et al., 2003). The model therefore assumes that sub–grid variability in weather, soils and management practices do not play a major role in determining yield at the grid scale. Hence sub–grid heterogeneity is not parameterised in the model. Further assumptions made by the model are also based on observed processes and quantities. These are described in sections 2.1.1–2.1.3, with a particular emphasis on the parameterisations that are affected by elevated $CO_2$.

The present study focusses on the groundnut (i.e. peanut; *Arachis hypogaea* L.) crop in India, for which extensive evaluation of GLAM has been carried out (Challinor et al., 2006, 2007, 2005b, 2005c, 2004). The processes included in the simulations under doubled $CO_2$ are: changes in assimilation rates, water use and SLA. No changes to the harvest index are simulated, since no consistent response emerged from the data (table I). Fertilisers may be needed in order to take full advantage of $CO_2$ stimulation (e.g. Kimball et al., Reilly and Schimmelpfennig, 2002, 1999). Since GLAM does not simulate nutrients directly — but rather through a yield gap parameter — the simulations in the study do not explicitly include this interaction. However, in order to capture uncertainty, high and low estimates of the increase in transpiration efficiency are used, and variation in nutrients contributes to this uncertainty.

For the current study, three changes were made to the original GLAM formulation (Challinor et al., 2004). The first of these is that the impact of water stress during flowering was simulated, after Challinor et al. (2006). The second change to the model relates to the parameterisation of assimilation, which is described in section 2.1.2. The third change, which is described in section 2.1.3, improves the consistency between biomass and LAI. The resulting improvements to the model skill are evaluated in section 3.1.

### 2.1.1. *Water use*

GLAM has a full soil water balance, with daily simulation of runoff, drainage, infiltration and uptake through growing roots. The model is therefore capable of simulating the impact of the timing of rainfall on yield. For example, in Challinor et al. (2004) two simulations with very similar rainfall totals (394 and 389 mm), but different distributions within the season, produced different yields (1059 and 854 kg ha$^{-1}$); this was reflected in observations (1360 and 901 kg ha$^{-1}$).

LAI growth in GLAM is limited by a parameterisation of soil water stress based on the availability of water relative to potential (energy–limited) transpiration. LAI is in turn used to determine the physiologically–limited transpiration. Actual transpiration is then the smaller of three values: energy–limited, water–limited and physiologically–limited. Of these, only the latter is affected directly by elevated CO$_2$. The physiologically–limited transpiration, $T^p_{Tpot}$, is affected by LAI ($L$) only when LAI is below a critical value ($L_{CR}$):

$$T^p_{Tpot} = \begin{cases} T_{Tmax}\left(\frac{L}{L_{CR}}\right) & L < L_{CR} \\ T_{Tmax} & L \geq L_{CR} \end{cases} \tag{1}$$

This equation is based on the data of (Azam-Ali, 1984). The physiologically–limited maximum transpiration, $T_{Tmax}$, will fall with rising CO$_2$, as stomata partially shut. Whilst $T_{Tmax}$ is not usually measured directly, it is strongly related to water use. Reducing water use in this way, rather than altering the Priestley–Taylor coefficient, means that the reduction in water use is physiologically, rather than energetically, constrained. It also means that only transpiration, and not evaporation, is altered (see discussion in Tubiello and Ewert, 2002). The reduction in $T_{Tmax}$ for the current study was determined by tuning $T_{Tmax}$ to give plausible changes in transpiration (section 2.3.2).

### 2.1.2. *Assimilation*

Biomass is determined as the product of a normalised transpiration efficiency ($E_{TN}$), with units of g kg$^{-1}$, and transpiration. $E_{TN}$ is given by

$$E_{TN} = \min(\frac{E_T}{V}, E_{TN,max}) \tag{2}$$

where $V$ is the vapour pressure deficit (VPD, measured in kPa) and $E_T$ is the transpiration efficiency in Pa (i.e. kPa × g $\mathrm{kg}^{-1}$). $E_T$ is often found to vary little across a range of environments, for a given crop variety at constant nutrient and $CO_2$ levels (Chapman et al., 1993). Since field estimates of $E_T$ are rarely made at very low VPD, GLAM employs a maximum normalised transpiration efficiency, $E_{TN,max}$, to avoid very high value of transpiration efficiency at low VPD.

The use of a transpiration efficiency to determine biomass makes GLAM primarily a water–driven model. However, since solar radiation is used to calculate potential transpiration rates, it is possible to assess the response of the model to radiation. Such an internal consistency check was performed by Challinor et al. (2004), who found observed and simulated values of radiation use efficiency to be in broad agreement.

In the original GLAM formulation (Challinor et al., 2004), $E_T$ and $E_{TN,max}$ were independent parameters that took unique calibrated values. In the current study, more than one set of parameter values is used (see section 2.3). It is therefore important that these variables are co–varied, in order to ensure consistency. With one exception (see section 2.3.1), this was achieved for simulations under baseline (1966–1989) concentrations of $CO_2$ by applying

$$E_{TN,max} = E_T \, \frac{E^c_{TN,max}}{E^c_T} \tag{3}$$

where superscript $c$ indicates the calibrated values of Challinor et al. (2004): $E^c_{TN,max}$=3 g $\mathrm{kg}^{-1}$ and $E^c_T$=1.4 Pa. Under elevated $CO_2$, $E_T$ increases and $E_{TN,max}$ may also change. Consistency between $E_T$ and $E_{TN,max}$ under elevated $CO_2$ was achieved by applying

$$E_{TN,max} = (1 - T_{fac}) \, E^c_{TN,max} + T_{fac} \, E_T \, \frac{E^c_{TN,max}}{E^c_T} \tag{4}$$

where $T_{fac}$ is a new variable introduced for this study. It is used for elevated $CO_2$ only and takes values between 0 and 1. For $T_{fac}$=0, $E_{TN,max}$ is unchanged from its baseline value, so that at low VPD there is no $CO_2$ stimulation. For $T_{fac}$=1, $E_{TN,max}$ increases by the same fraction as $E_T$. $T_{fac}$ exerts no control on assimilation at high VPD: for VPD> $E_T/E_{TN,max}$ (see equation 2), the increase in $E_T$ (between baseline and elevated $CO_2$ values) is the sole determinant of changes in assimilation. Hence $T_{fac}$ controls the differential response of assimilation to elevated $CO_2$ across low and high humidity environments. It is the value of $T_{fac}$, together with the increase in $E_T$, that determines the impact of elevated $CO_2$ on normalised transpiration efficiency, $E_{TN}$. Figure 2 illustrates this relationship. $E_{TN}$, together with transpiration, determines biomass and, though a harvest index equation, yield.

### 2.1.3. *Specific leaf area*

The original GLAM formulation simulates biomass and LAI independently, as described above. Specific leaf area (SLA = LAI divided by above–ground biomass) is then calculated as an output variable. The resulting end–of–season values of SLA for simulations in recent climates are usually realistic (Challinor et al., 2004), although in water–stressed environments very high values can sometimes occur. Because of this, and given the number of changed parameters in the current study, and the introduction of parameters to represent the crop response to elevated $CO_2$, an internal control of SLA was added for this study. This also presented an opportunity to reduce the unrealistically high values of SLA that occurred in the first few days of most simulations.

This control on SLA was implemented by imposing a maximum SLA, $S_{max}$. This maximum value is used to modify the calculated values of either biomass or LAI. For the first $N_D$ days after emergence biomass is increased if necessary, to ensure that SLA$\leq S_{max}$. From day $N_D + 1$ until the growth stage when LAI stops increasing, $S_{max}$ is imposed by limiting increases to LAI. Once the LAI has levelled off, both biomass and LAI are allowed to evolve freely. Since biomass generally increases over this period, SLA tends to fall, as is seen in observations (Hunt, 1990)

Sensitivity analysis revealed that the model is relatively insensitive to the choice of $N_D$, within the range 5–10 days. The lowest of these values was chosen, in order to ensure the least possible interference with the model calculation of biomass, which is calculated using a more independently–measurable crop–specific parameterisation than LAI. Under current–climate (baseline) conditions, $S_{max}$ was given the value of 300 $cm^2g^{-1}$, a typical value for groundnut (Banterng et al., 2003). In a doubled–$CO_2$ environment SLA is expected to fall (White and Montes-R., 2005; Kimball et al., 2002; Ainsworth and Long, 2005), and $S_{max}$ can be reduced accordingly.

### 2.2. Crop model inputs

The input weather data for the crop model came from the PRECIS regional climate model (http://precis.metoffice.com/) simulation of baseline (1961–1990) climate, on a 0.44° grid, carried out by IITM (2004). This simulation was also used by Challinor et al. (2007, 2006). The simulation of climate shows good representation of maximum temperature during the monsoon, and some over-estimation of the monsoon rainfall over central India (IITM, 2004). Similarly, Bhaskaran et al. (1996) found that precipitation over land during the Indian summer monsoon was 20% greater in the Hadley Centre RCM of the time, than in the corresponding GCM, due to the stronger vertical motions arising from finer horizontal resolution. Further discussion of the impact of increased horizontal resolution on the simulation of the Asian summer monsoon can be found in Martin (1999) and Stephenson et al. (1998). Rainfall in southeast India, and in some parts of northeast India, is underestimated in the PRECIS simulations. Further details on the performance of the baseline climate simulation, together with a more detailed description of the simulations themselves, can be found in IITM (2004). Two further sets of input data are required to run the model (see section 2.1). The soils data used here is that of (FAO/Unesco, 1974) and the data on planting windows is from (Reddy, 1988)

The groundnut yield data for calibration of the crop model are from the district–level database of agricultural returns compiled by the International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), Patancheru, India. The time series of pod yield, for the period 1966 to 1989, for each individual district was linearly detrended to 1966 levels in order to remove the influence of improved varieties and management methods. Each grid cell was assigned uniquely to a district according to the location of its centre. The yield data combine both the monsoon (rainfed) season and winter (irrigated) season. Figure 3 presents the mean and coefficient of variation of the yield data. Challinor et al. (2003, 2004) have more discussion on these data.

### 2.3. An ensemble of crop yields

The input data described above was used together with GLAM to produce an ensemble of crop yields. Each ensemble member was driven with the same weather, soils and planting data, but had one or more parameter values which differed from those of the other ensemble members. The parameters varied are described in the following sections, and summarised in table II. In the baseline simulations, key parameters determining the response of the crop to $CO_2$ were varied. In the simulations under elevated $CO_2$, every parameter that is influenced by $CO_2$ was either varied, or else tested to see if variation was required in order for observed $CO_2$ responses to be seen.

### 2.3.1. *Baseline simulations*

Four baseline simulations were performed. These differed in the values of those parameters that are important sources of uncertainty in estimating the response of yield to doubled $CO_2$. Specifically, the transpiration and transpiration efficiency of the crop were both varied. In naming the simulations, and referring to transpiration efficiency in general, the abbreviation TE will be used to denote either form of transpiration efficiency: the conserved quantity $E_T$, or the VPD–dependent quantity $E_{TN}$ (see equation 2). The context (i.e. reference, or not, to a dependence on VPD) and/or the use of the original mathematical symbols, will ensure clarity.

The Control simulation used the parameter set of Challinor et al. (2004), which corresponds broadly to the TMV2 variety. The High Baseline TE simulation used a higher value of $E_T$. This choice was made because the Control value of $E_T$ is at the lower end of the observed range, and baseline TE has been identified as an important contributor to uncertainty in yield under future climates (Challinor et al., 2005a). The Reduced Physiological Transpiration Limitation simulation used an increased value of the physiologically–limited maximum transpiration, $T_{Tmax}$ in equation 1. Since this parameter is not well-constrained under baseline $CO_2$ concentration, and since it is also used to reduce transpiration in the doubled $CO_2$ simulations, it is an important source of uncertainty. The final baseline simulation, the Reduced VPD–TE Interaction simulation, used a relationship between TE and vapour pressure deficit that is less sensitive to differences in VPD. Specifically, this simulation maintained, for baseline $CO_2$ concentration, a constant $E_{TN}$ over a larger range of VPD (0–1.1 kPa) than is the case for the other simulations (0–0.5 kPa see figure 2). This was achieved by altering $E_{TN,max}$ in equation 2, instead of applying equation 3 (which was used for all other simulations). This change alters assimilation rates, and in particular the difference in assimilation between well–watered and water–stressed environments. It is therefore a potentially important source of uncertainty.

Each of these baseline simulations was individually calibrated, using a spatially–variable yield gap parameter (YGP). This parameter was varied across the range 0.05–1 in steps of 0.05. YGP multiplies the potential maximum rate of change of leaf area index in order to give a value that is limited by non-climatic factors such as pests, diseases and nutrients. The calibrated value of YGP is that value which minimises the difference between observed and simulated yields. A calibrated value of YGP was obtained for each unique input weather time series, so that in practise YGP can also act to correct bias in the input weather data. The calibration process is described in more detail in Challinor et al. (2007).

### 2.3.2. *Simulations under elevated $CO_2$*

The impact of doubled $CO_2$ was simulated by increasing $E_T$ and reducing the physiologically–limited maximum transpiration, $T_{Tmax}$. Since these quantities are measurable, this has the advantage of constraining the model with observations. The reduction in $T_{Tmax}$ was derived by examining the changes in transpiration as $T_{Tmax}$ was varied. A reduction of 17% in $T_{Tmax}$ gave a decrease in transpiration of up to 10% in the Reduced Physiological Transpiration Limitation simulation, and 15% in the Control simulation. This is in broad agreement with measured values (table I). In order to capture uncertainty, two values of the percentage increase in $E_T$ under elevated $CO_2$ (TE_FRAC) were used (24% and 40%). These values are based on the measurements of Stronach et al. (1994) and Clifford et al. (2000). They follow Challinor et al. (2005a), except that the upper value was reduced in order to reflect the recent result that $CO_2$ stimulation in the field may be lower than that observed in controlled environments (Long et al., 2005).

The relationship between VPD and TE under doubled $CO_2$ was also altered in some of the simulations, by using the new variable $T_{fac}$ (equation 4). Low values result in low $CO_2$ stimulation at low VPD. A value in the range 0.3–0.5 was suggested by examining low–VPD response of assimilation and net primary productivity in the land surface scheme of a general circulation model (MOSES; Cox et al., 1999). Thus 0.4 was chosen as one of the values of $T_{fac}$. The other value chosen was zero, as this encourages a differential response to $CO_2$ between well–watered (low VPD) and water–stressed (high VPD) environments (see section 2.1.2). It follows from equations 2 and 4that under elevated $CO_2$, $E_{TN}$ remains constant for VPD greater than 0.5 ($T_{fac} = 0$), 0.55 ($T_{fac} = 0.4$, TE_FRAC=24%), or 0.58 ($T_{fac} = 0.4$, TE_FRAC=40%) kPa. For the Reduced VPD–TE Interaction simulations, a value of 0.1 was chosen for $T_{fac}$, since when 0 or 0.4 were used, unrealistic changes in TE resulted. Under elevated $CO_2$ in the Reduced VPD–TE Interaction simulations, $E_{TN}$ remains constant for VPD greater than 0.89 (TE_FRAC=24%) or 0.99 (TE_FRAC=40%) kPa.

The final parameter change for doubled $CO_2$ adjusts the relationship between biomass and LAI. Since a reduction in SLA may be expected under elevated $CO_2$, the maximum SLA ($S_{max}$; see section 2.1.3) was reduced, by a percentage S_FRAC, in some simulations. Note, however, that it is not only these simulations that result in a reduction in SLA. S_FRAC was chosen to be 10%, which is in the centre of the range suggested by table I.

Whether or not $S_{max}$ is reduced, it can exert a control over LAI for the period from $N_D + 1$ until LAI stops increasing (see section 2.1.3). The maximum LAI increases linearly with biomass, with a constant of proportionality $S_{max}$. Hence transpiration efficiency drives biomass and $S_{max}$ regulates the response of LAI to that change. Since transpiration efficiency increases under elevated $CO_2$, this mechanism allows LAI to increase in response $CO_2$. The second effect of $CO_2$ on LAI is mediated through the potential for reduced water stress (i.e. the reduction in $T_{Tmax}$), which also tends to increase LAI.

The baseline and doubled $CO_2$ simulations are summarised in table III. Every possible combination of simulations was performed. For each baseline simulation, there is a maximum of $2^3 = 8$ elevated $CO_2$ simulations (two values each of TE_FRAC, $T_{fac}$ and S_FRAC). Since the Reduced VPD–TE Interaction parameter set had its own value of $T_{fac}$, that parameter was not varied, leaving that baseline simulation with 4 associated doubled $CO_2$ simulations. This resulted in a total of $(3 * 8) + (1 * 4) = 28$ doubled $CO_2$ simulations. Since all simulations used the same input climate, any differences in yield are due to the crop model parameters representing doubled $CO_2$.

### 2.4. Selection of ensemble members

Observed ranges of yield, SLA and LAI were used as criteria to select simulations for further analysis. The observations used were the full ranges from table I, with one modification: the range of yield values, which is relatively large, was reduced by replacing the five–fold yield increase observed by Clifford et al. (1993) with the maximum associated dry matter increase (128%). This upper limit, which was not approached by the GLAM output, is still quite high, especially considering the lower changes in yield seen in FACE studies. Values of yield change from FACE studies were not used directly. Instead, the use of FACE yield data (which does not include groundnut) for C3 crops was reserved as an independent test of simulated crop yield (section 3.3). The crop model outputs used for the comparison were the thirty–year mean values of yield, SLA and LAI. The criterion applied in each case was that at least 90% of the simulated values from all (787) grid cells lie within the ranges from observations.

### 2.5. Sensitivity analysis

Sensitivity analyses were performed with two further crop simulation models, in order to compare the response of these models under doubled $CO_2$ to that of GLAM. The two models used were CROPGRO (Boote and Jones, 1998) and the groundnut model of Hammer et al. (1995). This second model, referred to from here onwards as QNUT, formed the base for the development of the legume model template in APSIM (Wang et al., 2002). CROPGRO and QNUT were not calibrated to reproduce observed yields. Instead, standard parameter values were used where possible in order to ensure that the model was being used within operational limits. This avoids over–tuning of the model (obtaining the correct yield for potentially the wrong reason), which would be an area of particular concern since neither QNUT not CROPGRO were designed to operate at the spatial scale of the observed yields. The parameter set used for the QNUT model was that of Virginia Bunch, with one modification: the thermal requirement was reduced in order to give the crop a duration of around 140–150 days, closer to the observed and simulated values for India (Challinor et al., 2003, 2004). The parameter set used for the CROPGRO simulations was the TMV2 parameter set calibrated for use in India by Kakani (2001). Weather inputs for the two crop models came from the PRECIS simulations (section 2.2) of the regions shown in figure 4, each of which has between 23 and 25 grid cells. The crop was sown on the same day as in the GLAM simulations. The final yield from all simulations within each region were averaged in order to produce a value for each region under the baseline and doubled $CO_2$ environments.

It is possible that calibrated results would produce a different response to that presented here. However, all results are normalised by baseline yields, in order to minimise calibration bias. For the CROPGRO model, some attempt to examine a range of calibrations was made: two values (High and Low: 0.82 and 0.22) of the soil fertility factor (SLPF) were used. Within CROPGRO a further variation was introduced: simulations were performed using both the canopy– and leaf– level photosynthesis modules. All four combinations of these two options were carried out. Comparison with FACE yields from the literature adds further data to this assessment, as well as indicating the general level of agreement between the GLAM simulations and observations. Since FACE studies have not been conducted with groundnut, C3 crops were used for this comparison.

## 3. Results

### 3.1. Crop yield ensemble in the baseline climate

Calibrated values of YGP were in the range 0.05–1 for the Control and the Reduced Physiological Transpiration Limitation simulations. For the other two baseline simulations, YGP was in the range 0.10–1.0. Figure 5 shows the level of agreement between the simulated and observed mean yields for two of the simulations: the Control simulation, and the least accurate, overall, of the other three 1*$CO_2$ simulations (High Baseline TE). The Control simulation is an improvement on the simulations using the earlier version of GLAM (v1.0) with the same parameter set (Challinor et al., 2007): root mean square error assuming perfect correlation (see Challinor et al., 2007) in the new simulations is lower in 576 out of 787 grid cells. In a number of grid cells across central India there are improvements in the simulation of mean yield. The errors in mean yield in the southern part of India are common to all four baseline simulations and may in part be due to errors in the input rainfall (Challinor et al., 2007, 2005c). In southern and north–western parts, the standard deviation of yield is lower, and closer to observations, in the new simulations than in those GLAM v1.0 (not shown). In many parts of central and eastern India, the standard deviation increases, again bringing closer agreement with observations (not shown).

Four regions were analysed in more detail. These were chosen for both geographical and climatic variation, in particular variation in water stress. Figure 4 is a map of the mean simulated levels of crop water stress across India for the Control simulation, showing also the location of the four chosen regions: north–west (NW), the north–western part of Gujarat (GJ), a region in central India (CE) and part of the southern peninsula (SP). Simulated water stress is particularly high in SP (which has a mean transpiration deficit, relative to the potential, of 66% in the Control simulation), leading to the errors in simulated yields cited above. There is also water stress in NW (mean transpiration deficit in the Control simulation of 44%), where the model is more accurate (figure 5). The other two regions show very little water stress. However, note that the simulated rainfall in GJ is higher than that observed: over 50cm during the simulated crop season, which is approximately the observed June–Dec seasonal total (Challinor et al., 2003). Whilst the pattern of water stress remains the same across the simulations (not shown) there is some variability in the magnitude. However, this variability is less than the inter-annual standard deviation.

The four baseline simulations are compared in figure 6. Comparisons with observations are of limited used, since the observed yields are on a district scale, and there are only four (GJ) or six (CE) districts in each region. However, in both cases the range of within–region variability is represented well. In GJ, three of the four baseline simulations are very similar. The High TE simulation extends the range of mean yields in both directions. In contrast, in CE only one of the simulations (Reduced Physiological Transpiration Limitation) is similar — in this case very similar — to the control. This may be because compared to CE, yield in GJ is more constrained by climate, particularly via VPD (not shown).

### 3.2. CROP YIELD ENSEMBLE UNDER DOUBLED $CO_2$

Of the 28 crop simulations under doubled $CO_2$, 18 passed the criteria described in section 2.4. Most of these (12) had the decreased maximum SLA parameter value. All except for one of the High Baseline TE simulations without the SLA decrease failed to pass the criteria, due to high LAI. This section analyses the the 18 ensemble members in terms of their differential response to $CO_2$ between well–watered and water–stressed environments. Absolute measures of the impact of $CO_2$ stimulation on yield for the two environments are presented, together with those from the other two crop models and results from FACE experiments, in section 3.3.

A different response to $CO_2$ between well–watered and water–stressed environments was seen in both the simulations with no TE increase at low–VPD ($T_{fac}$=0) and those with ($T_{fac}$=0.4). This can be shown using the yields averaged over all ensemble members, all years and all grid cells within two pairs of regions: well–watered (GJ plus CE) and water–stressed (NW plus SP). To quantify the differential response, we define $Y_{dif}$ as the percentage change in average yield in the well–watered environment minus the percentage change in average yield in the water–stressed environment. The simulations with no TE increase at low–VPD have $Y_{dif}$=4.3. The same figure for the simulations with a TE increase at low–VPD is, as expected, higher (9.1). These simulations especially favoured well–watered conditions when parameters conducive to higher LAI were used: the simulations with no decrease in SLA had $Y_{dif} = 13\%$. Using individual ensemble members, rather than averages, $Y_{dif}$ is positive in all 18 cases. If ensemble averages over single regions are used to calculate $Y_{dif}$, so that there are four results (GJ minus NW, GJ minus SP, etc) then, again, all of these numbers are positive. Hence using this metric, the GLAM simulations show greater stimulation in well–watered than in stressed environments. Note, however, that if individual ensemble members from single regions are used to calculate $Y_{dif}$ then the result is slightly less clear: 0, 2, 4 or 8 of the eighteen ensemble members favour the water–stressed regions SP or NW.

Table IV illustrates the reason for the well–watered regions having greater $CO_2$ stimulation than NW and SP: LAI increases under doubled $CO_2$ in all of the simulations, hence increasing light capture and, potentially, transpiration. Since only the well–watered regions have enough water to substantially increase transpiration, these show greater increases in yield under doubled $CO_2$. The SP region showed the lowest increases in LAI. Most of the simulations in SP show decreased water use under elevated $CO_2$, and all simulations showed a decrease in water stress: the change in the fraction of potential transpiration realised, averaged across time and space, ranged across ensemble members from 2.9 to 10%. Of the 7 simulations that showed increased water use, 6 used Reduced Physiological Transpiration Limitation parameters — i.e. the simulations where the absolute reduction in transpiration due to stomatal closure is smallest. In NW, the increase in water use in these 6 simulations resulted in increases in LAI that in turn resulted in an increase in average water stress.

### 3.3. Sensitivity analysis and synthesis of results

The differential response to $CO_2$ between well–watered and water–stressed environments is shown for the GLAM results and for the sensitivity analysis results from the two other crop models (section 2.5) in figure 7. Also shown are the yield changes for C3 crops from two FACE meta–analyses. Whilst the ranges are large, it is worth noting that, using the average response, the two FACE results do not agree on whether droughted or non–stressed crops will benefit most from elevated $CO_2$. However, FACE2 (Ainsworth and Long, 2005) does show reduced benefit under 'wet conditions'. This highlights an important issue in making this kind of comparison: meta–analyses necessarily simplify the data so that information, in this case regarding exact levels of water stress, is lost.

The well–watered GLAM simulations are within the range suggested by the FACE studies, as are most, but not all, of the water–stressed simulations. When all the GLAM simulations are taken together, the difference between the well–watered and water–stressed regions is positive and very small. The QNUT model showed a similar response to GLAM, with the water–stressed regions having larger increases in yield than the well–watered regions. Three of the four CROPGRO configurations show the opposite response.

In all cases the CROPGRO simulations with canopy–level photosynthesis calculations resulted in higher stimulation than the leaf–level simulations, and the difference between well–watered (GJ plus CE) and water–stressed simulations (NW plus SP) was less. Similarly, in all cases increased soil fertility (High–SLPF) was associated with smaller differences between well–watered and water–stressed simulations. The same effect can be seen, for example, in the yield results presented by Kimball et al. (2002). Given these results, it is not surprising that the one CROPGRO configuration that did not result in greater stimulation under water–stress is the the High–SLPF simulation with canopy–level photosynthesis. This highlights the importance of model calibration, since different conclusions would be reached in this case for the two different values of SLPF.

## 4. Discussion

### 4.1. Yield, LAI and water use

The GLAM results, which were selected for SLA and LAI from FACE and chamber studies, and yields from chamber studies, show broad agreement with the yields of C3 crops from FACE studies. This can be seen in figure 7, which shows that the increases in yield simulated by GLAM for doubled $CO_2$ were between 16 and 62%, and those of the FACE studies were between 0 and 73%.

For all GLAM simulations, LAI increased under doubled $CO_2$, by a similar range to that found in FACE studies (cf tables I and IV). As a result, water use mostly remained the same or increased. Similar results, where increases in LAI cause transpiration increases that compensate for partial stomatal closure, have been suggested (Field et al., 1995) and reported (Goudriaan and Unsworth, 1990) in the literature. For some of the simulations in water–stressed regions, transpiration decreased, by up to 4.6%. This is a similar amount to that seen in FACE studies, (table I) but less than the decrease of 14% reported by Clifford et al. (1995) (see table I). This may be because typical values of LAI in the field, and those of the GLAM simulations, are considerably lower than those of Clifford et al. (1995). At lower LAI, transpiration is more sensitive to increases in LAI (equation 1). This means that in the GLAM simulations presented here, water storage in the soil may not be prolonged under elevated $CO_2$ in the same way as it is for crops with higher LAI.

In contrast to the GLAM results, FACE studies of wheat under well–watered conditions have shown that water use falls under elevated $CO_2$ (e.g. by 3.3 to 6.7% in the meta–analysis of Kimball et al., 2002). Hence increases in LAI do not compensate for stomatal closure under these conditions. This may again be due to higher LAI. In contrast, under stressed conditions, Kimball et al. (2002) reported that water use may increase or decrease (−2.2 to +4.5%). Differences in the sign of this change across experiments may be due to differences in the timing of application of water during the growing season. The timing in the model simulations is not the same as the timing in the FACE experiments.

### 4.2. Interaction between water stress and assimilation

The interaction between water stress and assimilation in this study differed between models (sections 3.2 and 3.3). In the GLAM results, no greater stimulation of stressed crops was seen, despite the mechanism for such a result being included in the model. QNUT behaved in a similar fashion. This is a particularly noteworthy result since the difference in absolute yield increases between well–watered crops and stressed crops is even larger than their percentage counterparts. CROPGRO, however, which simulates leaf–level processes, showed the converse result. Furthermore, when the canopy–level photosynthesis module within CROPGRO was used, the magnitude of this response was reduced.

In order to understand the reason for these differences, a little more analysis is required. Figure 8 shows the relationship between yield and incident radiation in simulations of irrigated crops using canopy– and leaf– level photosynthesis in the CROPGRO model. Both $CO_2$ concentration and the choice of photosynthesis module have an effect on this relationship. However, the choice of photosynthesis module did not result in a larger percentage difference, between baseline and elevated $CO_2$, in either the slope or the value of yield at high (20.7 MJ day$^{-1}$) radiation. The lack of a difference between photosynthesis modules when water is not limiting suggests that it is the response to elevated $CO_2$ under water stress that is responsible for the contrasting behaviour of these modules.

To examine this possibility, we need only examine the absolute yields from the simulations under water stress under baseline $CO_2$ concentrations: the mean yields from NW and SP are smaller with the leaf–level photosynthesis (783 and 694 kg ha$^{-1}$, respectively) than with the canopy–level photosynthesis (862 and 752 kg ha$^{-1}$, respectively). Smaller yields are more likely to produce larger percentage differences, especially since both photosynthesis modules produce absolute differences in yield (elevated minus baseline $CO_2$) that are greater for well–watered crops than for water–stressed crops. This again highlights the importance of calibration: simulations of future changes in yield are reliable only if the crop model reproduces accurately yields in the baseline environment. In the current study, this has only been attempted with GLAM.

Does the issue of calibration alone explain the differences between GLAM and CROPGRO? Model formulation is likely to play a role, especially since the water–stressed baseline yields in GLAM are lower than those in DSSAT, making GLAM prone to larger percentage changes under elevated $CO_2$. GLAM uses normalised transpiration efficiency to convert water to biomass. The relationship between transpiration and biomass * VPD is linear (equation 2). The only interactions between water stress and assimilation are those that are determined by enforced changes in model parameters between baseline and elevated $CO_2$. These have either been empirically fitted (physiologically–limited maximum transpiration) or else a range of plausible values has been used (relationship between VPD and TE; changes in SLA). This is substantially different from simulating assimilation at the leaf or canopy levels. QNUT also uses a linear relationship to determine biomass — in this case a radiation use efficiency. Hence differences between the models in the level of organisation at which biomass accumulation is simulated, and subsequently scaled up to produce field–scale biomass and yield, may be one of the reasons for the differences in model behaviour between CROPGRO and the other two models. Similarly, the differences between the two sets of CROPGRO simulations may be due to differences between the simulation of photosynthesis directly at the canopy–level and simulation at the leaf–level with subsequent upscaling being done elsewhere in the model. Ultimately, the reasons for the differences between these models can only be determined using fully–calibrated CROPGRO and QNUT simulations, based on yield data at the appropriate spatial scale, and with adequate sampling of uncertainty.

### 4.3. Levels of complexity in crop modelling

The above analysis suggests that differences between model output may be due to differences in the calibration of the model and/or in the level of complexity of the model itself. Since models of differing complexity have produced different results, it seems logical to ask whether or not this is due simply to insufficient complexity in some of the models. In other words, is complexity a prerequisite for quantifying the impact of elevated $CO_2$ and its interaction with water stress? Tubiello and Ewert (2002), in their review of available models, find that it is not. Given that a range of approaches is feasible, what are the advantages and disadvantages of complexity in modelling?

Quantities such as yield integrate a number of non–linear processes. In the current study, observations of yield, SLA and LAI were used to constrain the GLAM model. The model also contains other parameters that have been previously constrained with, or tested against, observations (e.g. water use, harvest index and transpiration efficiency; Challinor et al., 2004, 2005a). Thus a model of intermediate complexity such as GLAM has the advantage of having a large fraction of its parameters that can be linked directly to observations. Models that simulate crop growth at a more fundamental level have more parameters. These cannot always be linked directly to observations. This results in a greater likelihood that there are a number parameter sets that lead to the same baseline yields (c.f. Beven, 2006). These different parameter sets may not respond in the same way to elevated $CO_2$. For this reason, crop models should be evaluated not only in terms of yield, but in terms of their skill in simulating other quantities and processes. The evaluation of skill in yield simulation then becomes a test of the interactions between these processes. These interactions are often complex and non–linear, leading some authors to conclude that the appropriate level of complexity for a model is one level — and no more — below the quantity of interest (Sinclair and Seligman, 2000).

More complex models, then, are more difficult to constrain with observations than less complex models. This would suggest a preference for lower complexity (e.g. Brooks et al., 2001), particularly when estimates over large areas are required (see Challinor et al., 2003). However, it is important to remember that more complex models may include processes and interactions that are, or become, a significant determinant of yield. Hence the difficulty in constraining complex models with observations should not be seen as a reason for avoidance. Rather, it is a reason to exercise caution in using crop model parameter sets outside the model domain in which they have been tested. Where parameters are uncertain, the impact of this uncertainty on yield should be estimated.

### 4.4. Complexity and spatial scale

Section 4.2 suggests that insufficient model complexity, and differences in model calibration, are likely contributers to differences in model output. However, section 4.3 suggests that model complexity and accuracy are not necessarily directly related. Hence we consider now a third possible reason for model differences: since the complexity of a plant model is in general related to its spatial scale (Raupach and Finnigan, 1988), it is possible that the range of responses across some models reflects a real–world scaling issue.

Certainly real scaling issues exist in biological and physical systems. Indeed, the question of how the impacts of elevated $CO_2$ scale across leaf, canopy and regional scales is crucial for our predictions of the impacts of climate change on crops (Ewert, 2004), natural vegetation (El Maayar et al., 2006), and the hydrological cycle (Field et al., 1995). Of particular relevance to the current study, Medlyn et al. (2003) and Rosati and Dejong (2003) find that leaf–level photosynthesis may not scale up linearly to the regional or canopy scale. Long et al. (2004) provide a description of the response of assimilation at the leaf level. Using the Farquhar–von-Caemmerer–Berry photosynthesis model, the authors show how stomatal limitation on assimilation is reduced at high $CO_2$. At the canopy level, Ewert (2004) found that simulated $CO_2$ stimulation (ratio of canopy assimilation rate in doubled and ambient conditions) fell with increasing LAI. Since low LAI is associated with water stress, this suggests higher $CO_2$ stimulation for stressed crops. However, the effect reported by Ewert (2004) is not large ($\approx$27% stimulation at LAI=1, and $\approx$21% at LAI=10). The authors also found that measurements of $CO_2$ stimulation (under 1.5*ambient conditions) of wheat biomass showed a small (statistically insignificant) difference between water–stressed and well-watered crops. Hence LAI (and water stress) exerted greater control over biomass than $CO_2$ levels.

The character of the above results is summarised in figure 9, by using data from a range of studies. The figure shows measurements and simulations from the literature of assimilation at different values of water stress, measured through stomatal conductance, Palmer crop moisture index and LAI. All of these show a negative value of $Y_{dif}$ (the percentage change in yield in well–watered environments minus the percentage change in yield in the water–stressed environments). Crop model results for yield, from the current study and one other study, are also presented. Models with detailed simulation of photosynthesis tend to show negative $Y_{dif}$ and models with less detailed approaches show positive $Y_{dif}$. Hence using both observations and simulations (predominantly the latter), a pattern has emerged: $Y_{dif}$ increases with increasing levels of biological organisation.

Some of the differences in figure 9 are likely to be due to differences in model complexity (section 4.2). However, since some of the models examined in the current study operate on different spatial scales, these differences may be justified, rather than simply being the result of model error. Hence for at least some of the data in figure 9, the pattern of increasing $Y_{dif}$ with increasing levels of biological organisation could potentially be explained by differences between measures of assimilation at the leaf, field and large–area levels.

To determine the likelihood of this, modelling and field work need to be carefully combined. In this study we have not compared field experiments to simulations on a one–to–one basis. We are therefore unable to discern whether it is model error, model calibration, or model spatial scale that is primarily responsible for the different behaviours seen in figure 9. Since the effect is small relative to the uncertainties (figure 7) such discernment may not be easy. Furthermore, difficulties are likely to be compounded by non–linear interactions between the level of soil nutrients, water stress and $CO_2$ levels (section 3.3; Kimball et al., 2002, Ainsworth and Long, 2005). This effect is one of at least three which has not been simulated in detail in the current study. The second of these is downregulation or acclimation to elevated $CO_2$, which are sometimes used interchangeably (El Maayar et al., 2006) and sometimes not (Long et al., 2004). This refers to a reduction in assimilation with increasing exposure to elevated $CO_2$ conditions. For a discussion of short–term versus long–term impacts of $CO_2$, see Morison (1998). Such effects could mean that the long–term increase in TE under elevated $CO_2$ is lower than that used in this study. Increases in surface ozone (Long et al., 2005) are another mechanism by which TE could be reduced. However, ozone and $CO_2$ do not interact linearly and under elevated $CO_2$ the reduction in assimilation due to high ozone can be small (Bernacchi et al., 2006).

Notwithstanding the limitations above, could a carefully designed combination of modelling and field work determine the roles of model error, model calibration and model spatial scale? Since greater complexity leads to greater difficulty in applying observational constraints (section 4.3), and since complexity itself is likely to be a cause of model differences (section 4.2), it follows that such a task would not be trivial. Perhaps only by also examining theory can a complete picture emerge. For example, under well–watered conditions the response of plants to light differs with spatial scale: at the canopy level assimilation tends to respond linearly to radiation (e.g. Chen and Coughenour, 2004), whilst at the leaf scale the linear response can reach saturation (e.g. Rosati and Dejong, 2003). This is a measurable effect, and models can be used to develop mechanistic explanations for it (Dewar et al., 1998). Canopy architecture is the obvious difference across these two spatial scales, and is likely to play a role in the different behaviour observed. Any crop has leaves with a distribution of ages and a distribution of light levels, and this is likely to smooth out the cutoff point where increases in incident radiation no longer produce increases in assimilation. The fact that linearity in the response of the crop to $CO_2$ emerges more fully as time progresses (Medlyn et al., 2003) supports the hypothesis that different levels of organisation may produce different responses to elevated $CO_2$ (since the crop has more time to integrate across a range of incident light levels).

## 5. Conclusions

This study has confirmed previous findings that complexity in modelling is not a prerequisite for capturing the impact of elevated $CO_2$ on crops. However, as with any modelling approach, observations are needed to constrain model parameters. Additionally, in this study, the ensemble output was itself constrained with FACE data of SLA and LAI (although yields from FACE studies were not used as a constraint). Hence the model output presented here is partially tuned, rather than being an entirely independent result. Whilst there are valid reasons for wanting to avoid such partial tuning, it has the advantage of assimilating knowledge from experimental crop science into the modelling study. This pragmatic approach is routinely used by meteorologists when creating (e.g. Kalnay et al., 1996) and using (e.g. Betts et al., 2003) reanalyses of atmospheric and oceanic fields.

Results from the crop yield ensemble produced in this study estimate the uncertainty in yield associated with a doubling of $CO_2$ to be similar to the magnitude of the effect (approximately 40%), in broad agreement with FACE studies (figure 7). Despite these uncertainties, some conclusions may be drawn regarding the relationship between water stress and $CO_2$ stimulation. Firstly we find, in both models and observations, a low level of conviction and generality associated with the statement "Relative enhancement of growth owing to $CO_2$ enrichment might be greater under drought conditions than in wet soil because photosynthesis would be operating in a more $CO_2$– sensitive region of the $CO_2$ response curve" (IPCC, 2001). This is an important conclusion, since the nature of the relationship between water stress and $CO_2$ stimulation has implications for rainfed and irrigated agriculture (rainfed crops are more likely to experience water stress). If the relative $CO_2$ enhancement of growth is less under drought conditions than in wet soils, this may place demands on irrigation water resources that are additional to those already identified (Tubiello et al., 2007b). For the potential benefits of elevated $CO_2$ to be maximised, agronomic practice needs to adapt as $CO_2$ rises — something that is not reflected in recent releases of at least some cultivars Ziska et al., 2004.

The second conclusion is a preliminary one, drawn using results from a number of modelling and experimental studies of the mean response of crops to elevated $CO_2$. These results suggest a relationship that is not preserved across spatial scale: on small spatial scales, and correspondingly low levels of organisation, water–stressed crops benefit more from elevated $CO_2$, in terms of percentage changes in assimilation and yield, than well–watered crops. On larger spatial scales, yields suggest this relationship is weakened and even reversed. However, this study has shown that variations in spatial scale may not be the only reason for differences in the response of simulated crops to elevated $CO_2$. Inappropriate level of model complexity and insufficient model calibration may also play a role. Further studies using a range of models, with results interpreted in terms of fundamental theory and processes, would help to determine the relative contributions of these causes. Hence the methods used in the current study could be profitably applied to crop models of varying levels of complexity and spatial scale. Such studies would tell us how differences across models in their scaling–up of assimilation and water use to yield (section 4.2) relate to real–world scaling issues (section 4.4).

This work would present a number of challenges, some of which have been at least partially addressed in the literature. Only one–to–one comparisons between field data and simulations can determine whether or not a model is sufficiently complex to capture observations. Also, the models would need to be fully calibrated, preferably under both baseline and elevated $CO_2$ concentrations. Calibration should be on yield and, if possible, other quantities. Hence a significant amount of data for calibrating, and possibly constraining, the models would need to be available. For comparisons at large spatial scales, heterogeneity in weather and soils would need to be accounted for in one–to–one comparisons between data and models. If constraining data is used then techniques for its integration with the model (e.g. Chen and Coughenour, 2004) will also be needed. There are also challenges associated with fully representing parameter uncertainty. Sensitivity analyses can be used to identify key parameters (e.g. Makowski et al., 2006) and associated uncertainty. To ensure a minimum number of unconstrained parameters, some authors have systematically simplified complex models, in order to eliminate redundant parameters (e.g. Brooks et al., 2001).

In conclusion, the ensemble approach to crop modelling, with or without constraints from observations, could be profitably applied to a range of crop models. By providing objectively–determined uncertainty ranges, and by sampling across different modelling approaches, such studies would increase confidence in our estimates of the impacts of elevated $CO_2$ on crop yield.

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Table I. Summary of observations of changes in crop growth under elevated $CO_2$ relevant to the current study. Specific Leaf Area (SLA), Leaf Area Index (LAI), water use (usually calculated as quantity of water applied minus the increase in soil water content over the season), Harvest Index (HI) and yield are presented. All groundnut studies were conducted under 100% elevated $CO_2$, whilst the Free air $CO_2$ enrichment (FACE) studies used a range of $CO_2$ concentrations, resulting in elevations of approximately 60 to 70%. Brackets give ranges. The Kadiri-3 experiments were conducted in glasshouses and the Georgia Red experiments were conducted in a growth chamber. Notes: [1] Dry matter increases were more modest: 115% (101 to 128).

| **Crop or species** | **SLA** | **LAI** | **Water use** | **HI** | **Yield** | **Ref.** |
|---|---|---|---|---|---|---|
| | | | ***FACE meta–analyses*** | | | |
| C3 crops | −8(−5 to −9)% | +10 (−8 to +32) | — | — | — | Ainsworth and Long (2005) |
| C3 crops | −20 to 0 | ≈11% (−6 to 24%) | −3 to +5% | — | — | Kimball et al. (2002) |
| C3 crops | −6(−4 to −8)% | +7 (−1 to +16) | — | — | — | Long et al. (2004) |
| | | | ***Groundnut in controlled environment*** | | | |
| Kadiri-3 (irrig.) | — | ≈6% | — | 0.20→0.20 | 25% (14 to 38) | Clifford et al. (1993) |
| Kadiri-3 (irrig. to 22 or 35 DAS) | — | ≈40% | -14% | 0.05→0.15 | 510% (365 to 720)[1] | Clifford et al., Clifford et al. (1993, 1995) |
| Georgia Red | −15% | Area/leaf:+18% | — | 24.5→29.1 | ≈50% | Stanciel et al. (2000) |

Table II. Crop model parameters varied in order to create the ensemble of yield simulations. The first of these relates to water use, the next four control assimilation and the last controls the limitation on specific leaf area (SLA).

| **Parameter** | **Units** | **Reference** | **Description** |
|---|---|---|---|
| $T_{Tmax}$ | cm day$^{-1}$ | Eqn. 1 | Physiologically–limited maximum transpiration |
| $E_T$ | Pa | Eqn. 2 | Transpiration efficiency in Pa |
| $E_{TN,max}$ | g kg$^{-1}$ | Eqns. 2 and 3 | Max. normalised transpiration efficiency |
| TE_FRAC | — | Eqn. 2 | Increase in $E_T$ under elevated $CO_2$ |
| $T_{fac}$ | — | Eqn. 4 | Controls increase in $E_{TN,max}$ under elevated $CO_2$ |
| S_FRAC | — | Sec. 2.1.3 | Decrease in maximum SLA, $S_{max}$, under elevated $CO_2$ |

Table III. The simulations carried out. Four of the crop model parameter sets act on both the baseline and doubled $CO_2$ simulations. A further three parameter variations, each consisting of two options, affect only the simulations under doubled $CO_2$. Percentages increases under doubled $CO_2$ are measured with respect to the control parameter value. All doubled–$CO_2$ simulations used a value of $T_{Tmax}$ that was 17% lower than the corresponding baseline value. Equation 3 was turned off for the Reduced VPD–TE Interaction simulation in order to permit the lower value of $E_{TN,max}$. Notes: [1] $T_{fac}$ only affects crop simulation at elevated $CO_2$. [2] This simulation also used the higher baseline value of $E_T$ (2.2 Pa).

**Baseline and doubled $CO_2$**

| Name | Parameter changed | Value | | Description |
|---|---|---|---|---|
| | | Standard | Actual | |
| Control | — | — | — | Standard parameter set |
| High Baseline TE | $E_T$ | 1.4 | 2.2 | Baseline transpiration efficiency increased by 57%. |
| Reduced Physiological Transpiration Limitation | $T_{Tmax}$ | 0.30 | 0.55 | Physiologically–limited maximum transpiration increased by 83% |
| Reduced VPD–TE Interaction | $T_{fac}$ & $E_{TN,max}$ | —[1] & 3 | 0.1 & 2 | $E_{TN}$ is constant over a larger range of VPD [2] |

**Doubled $CO_2$ only**

| Name | Parameter changed | Value 1 | Value 2 | Description |
|---|---|---|---|---|
| Small/Large TE Increase | TE_FRAC | 24% | 40% | Increase in $E_T$ under 2*$CO_2$ |
| Reduced/Same SLA Limit | S_FRAC | 10% | 0% | Do, or do not, reduce maximum SLA under 2*$CO_2$ |
| (No) TE Increase at Low–VPD | $T_{fac}$ | 0 | 0.4 | At low VPD, $E_{TN}$ does (not) increase under 2*$CO_2$ |

Table IV. Percentage changes between doubled $CO_2$ and baseline values of two crop characteristics. Means and ranges are across all 18 ensemble members. SP and NW are water–stressed regions. GJ and CE are well–watered regions.

| . | **LAI** | | | **Transpiration** | | |
|---|---|---|---|---|---|---|
| Region | Mean | Median | Range | Mean | Median | Range |
| SP | 14.0 | 15.1 | 6.9 – 21.9 | 1.9 | -0.9 | −4.6 – 6.1 |
| NW | 18.4 | 20.5 | 8.6 – 25.7 | 6.9 | 6.8 | 0.8 – 11.7 |
| GJ | 24.4 | 28.2 | 9.0 – 33.6 | 12.0 | 12.1 | 1.1 – 20.6 |
| CE | 19.5 | 19.6 | 6.0 – 32.3 | 11.6 | 12.3 | 3.7 – 19.9 |

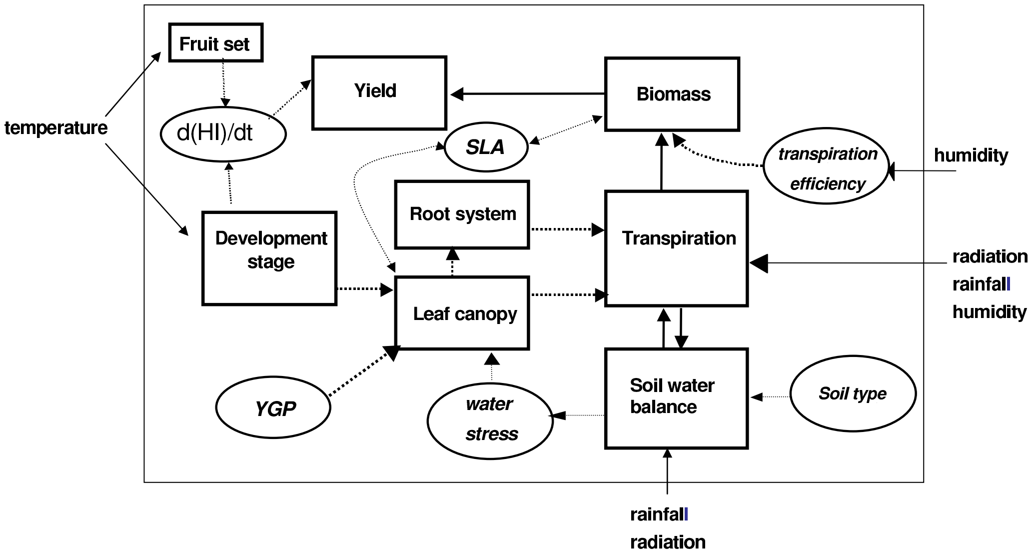


*Figure 1.* Schematic representation of the GLAM model. d(HI)/dt denotes the rate of change of leaf area index. YGP is the yield gap parameter. Prognostic variables, or groups of variables, are shown in rectangles. Intermediate variables and constants are shown in ovals. The daily driving variables are shown outside the model box.

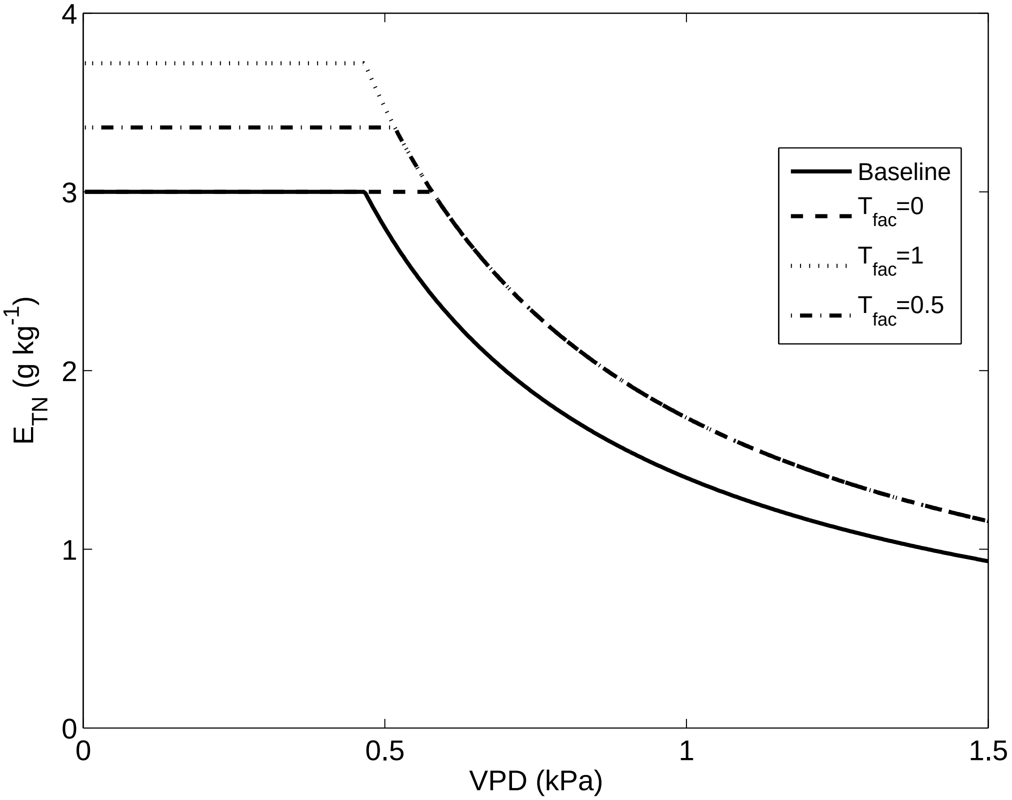
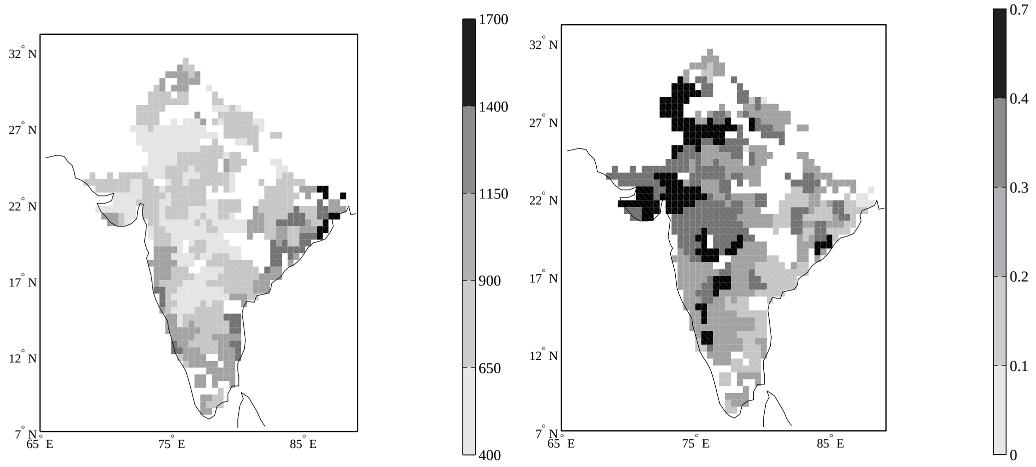


*Figure 2.* Relationship between normalised transpiration efficiency ($E_{TN}$) and vapour pressure deficit (VPD) in the baseline environment (solid line) and in the elevated $CO_2$ environment with an increase of 24% in $E_T$ (dotted, dashed and dot–dashed lines). $T_{fac}$ controls the response of $E_{TN}$ to VPD at low VPD (see equation 4).



(a) Mean

(b) CV/100

*Figure 3.* Mean (kg ha$^{-1}$) and coefficient of variation (CV) of observed groundnut yield in India, over the period 1966–89, presented on the simulation grid.

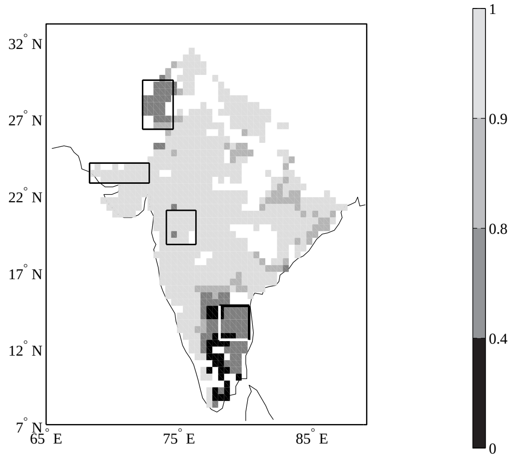
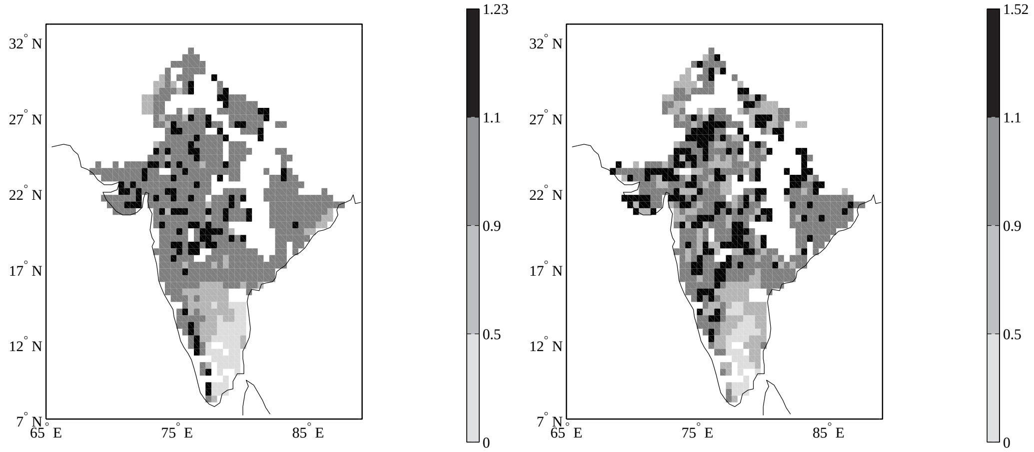
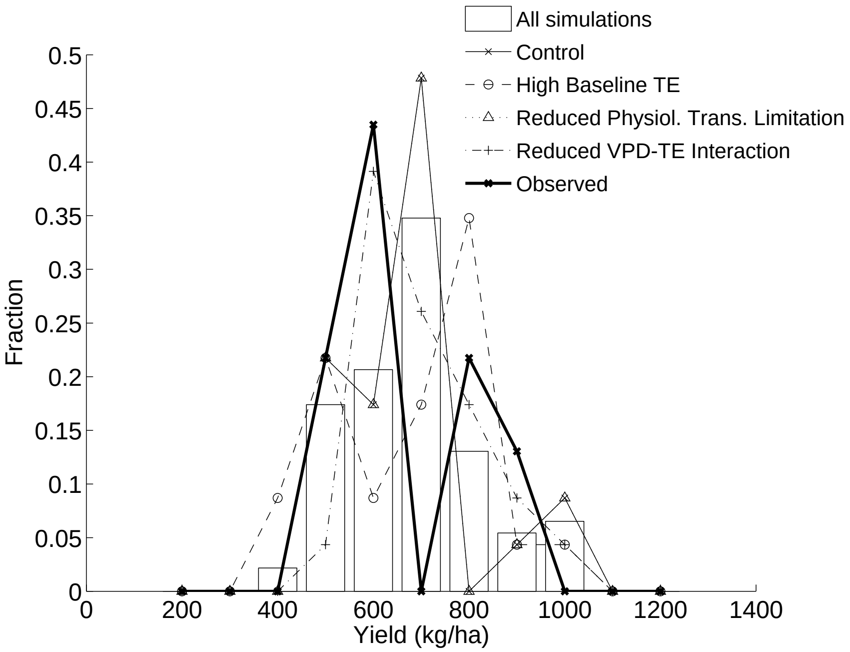


*Figure 4.* Actual transpiration divided by potential transpiration for the Control simulation. Also shown are the four regions, from north to south: NW, GJ, CE and SP (bounded by two white and two black lines).

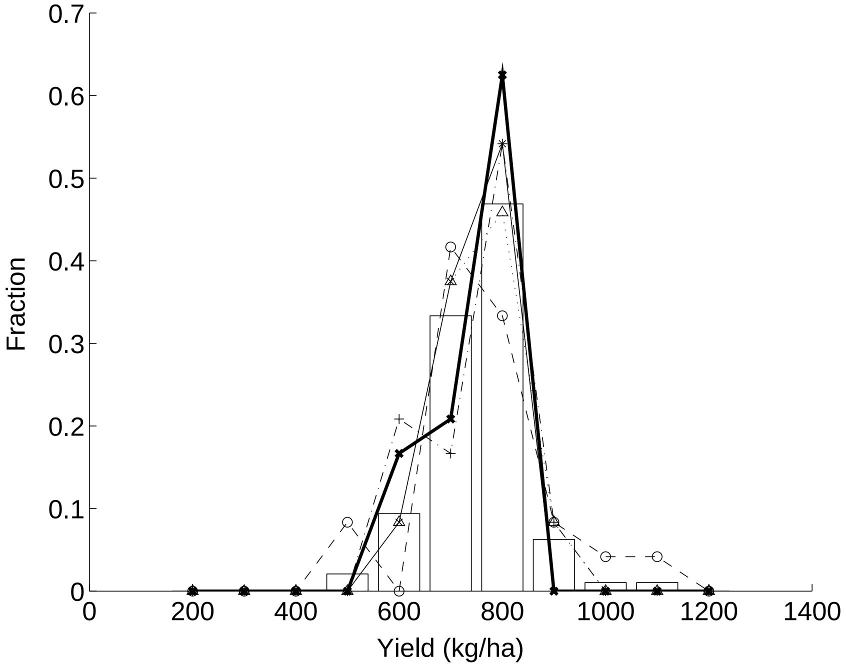


(a) Control (b) High Baseline TE

*Figure 5.* Thirty–year mean simulated baseline yields normalised by observed mean 1966-89 yields. The two sets of simulations shown are described in more detail in table III and section 3.1.



(a) CE



(b) GJ

*Figure 6.* Histograms of thirty–year mean simulated baseline yields for two regions in the four baseline simulations. All histogram counts are normalised by the total number of data points in the histogram. For CE this total number is 92 for the histogram of All Simulations and 23 for all other histograms. The GJ region contains one less data point per set of simulations. Although the observations contain 23 or 24 data points, they are not uniquely–valued since they come from district–level data, and the districts are larger than the grid cells (see section 2.5). Hence there are only four or six uniquely–determined yields in the histograms of observations.

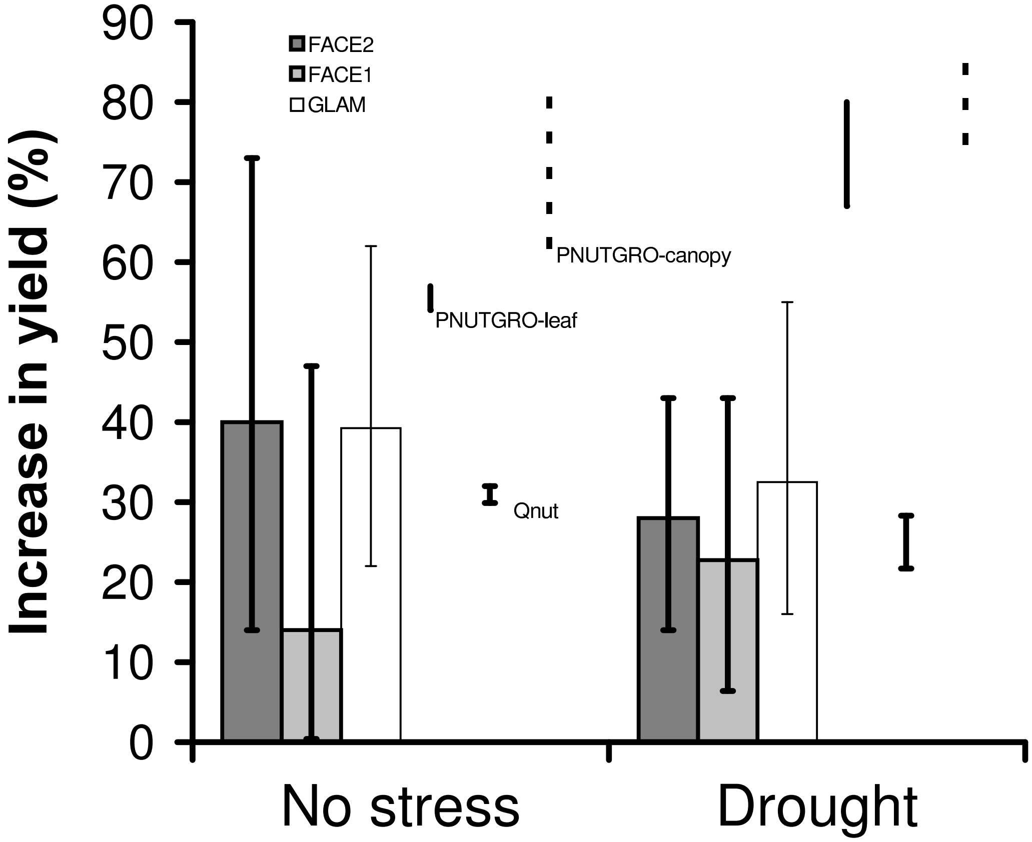


*Figure 7.* Effect of elevated $CO_2$ according to two FACE studies (FACE1: Kimball et al., 2002; FACE2: Ainsworth and Long, 2005) and the GLAM simulations. Bars show mean values. For the FACE studies, whiskers show the maximum and minimum values when standard error is taken into account. For GLAM, whiskers show the full range of model output. Also shown are the results of the sensitivity analyses on two further crop models: CROPGRO (i.e. PNUTGRO) and QNUT. For PNUTGRO, two sets of simulations, both with the high value of SLPF (0.82), are shown: simulations using leaf–level photosynthesis, and simulations using canopy–level photosynthesis. All crop model values are based on average yields within two regions (CE and GJ for No stress, and NW and SP for Drought). Hence GLAM results are based on 36 ensemble members and PNUTGRO and QNUT are based on two points, one at each end of the bar.

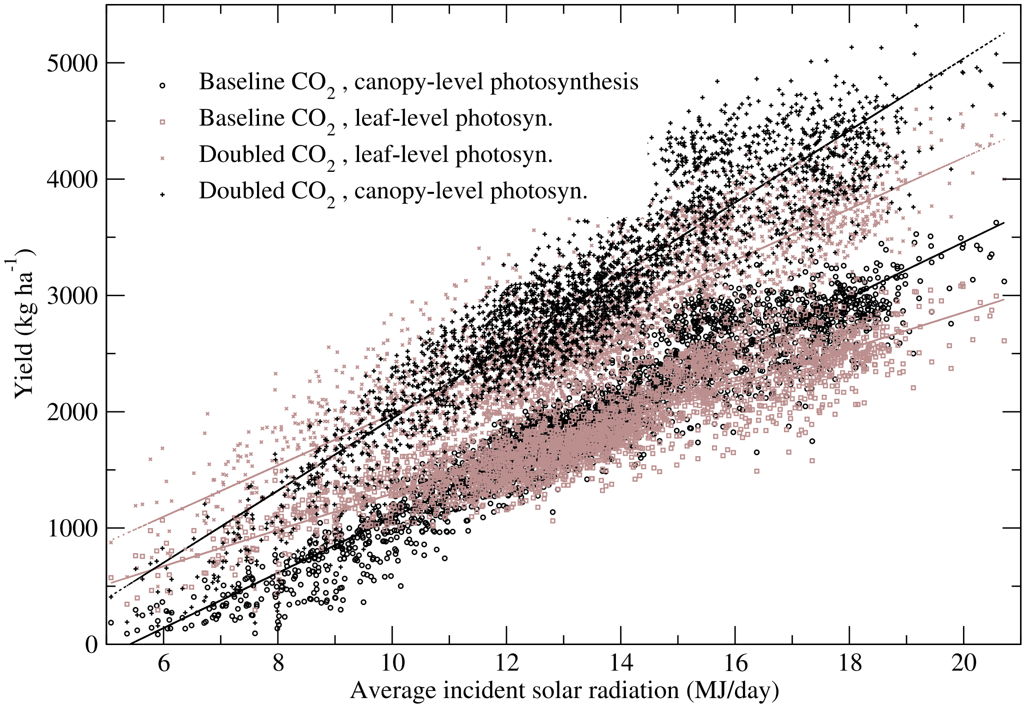


*Figure 8.* Impact of solar radiation on yield in simulations of irrigated crop cultivation using the CROPGRO model. Individual simulations, rather than average yields, were used. Hence there are approximately 30 (years) * 4 (study regions: CE, GJ, NW and SP) * 24 (grid cells per region) = 2880 data points. Two model configurations under two atmospheric CO$_2$ concentrations are shown. The linear regressions shown are all statistically significant, with $r \geq 0.88$ and $p < 0.0001$.

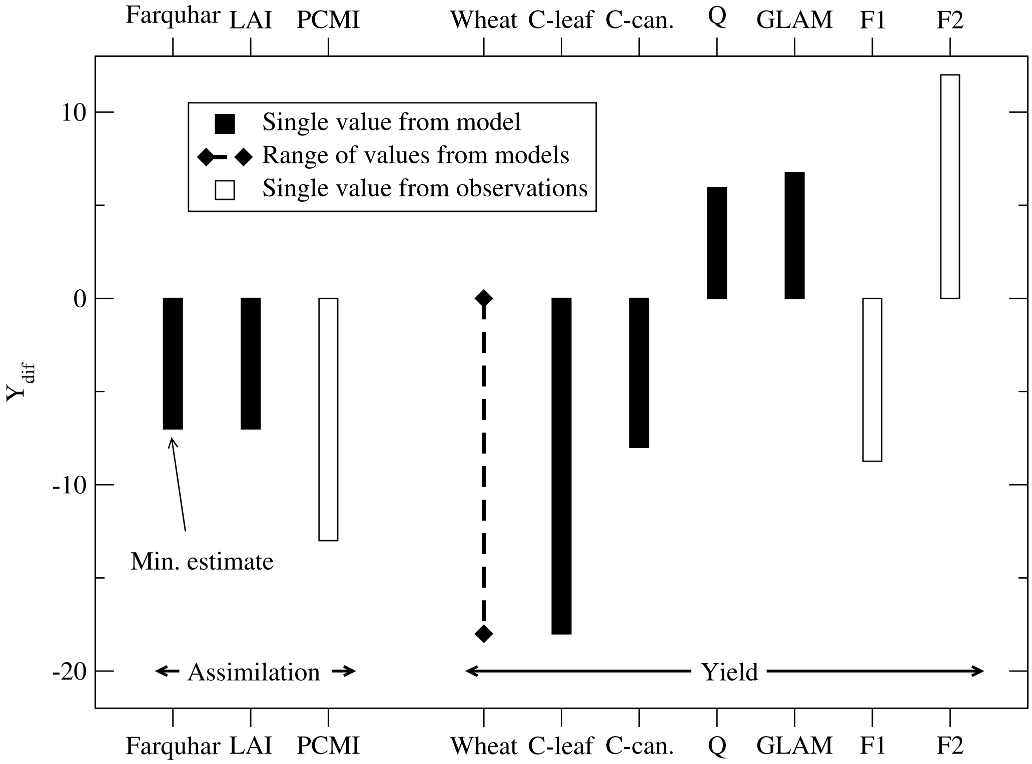


*Figure 9.* Mean percentage change in yield in well–watered environments minus the percentage change in yield in the water–stressed environments. Data for the six bars on the right is the mean response from the models and data in figure 7: CROPGRO (C) using the leaf– and canopy– level photosynthesis modules, QNUT (Q), GLAM and two FACE (F) studies. Also shown are the range of values from five wheat models run by Tubiello and Ewert (2002), and three differences in stimulation estimated from assimilation rates at different values of: Palmer crop moisture index (regression across PCMI=-1 to +1.5, Bernacchi et al., 2006); leaf area index (LAI=1 and 10, Ewert, 2004); stomatal conductance (using the Farquhar–von-Caemmerer–Berry model). The 'Farquhar' data point is calculated by using the supply=demand points, at baseline and elevated $CO_2$, in figure 1 of Long et al. (2004). The analysis is conducted at the leaf–level and assumes that the ratio of internal to external stomatal concentrations remains constant under elevated $CO_2$, and that there is no change in the demand function. The 'Farquhar' data point is for moderate stomatal closure, giving an assimilation of approximately 18 $\mu$mol m$^{-2}$ s$^{-1}$. Assuming a stomatal closure such that assimilation under baseline $CO_2$ is approximately half of this gives $Y_{dif} = -59\%$.

# List of abbreviations and symbols

| **Abbrev.** | **Symbol** | **Description** | **units** |
|---|---|---|---|
| FACE | | Free air $CO_2$ enrichment | — |
| GLAM | | General Large–Area Model for annual crops | — |
| LAI | $L$ | Leaf area index | Dimensionless |
| RUE | | Radiation use efficiency | g $MJ^{-1}$ |
| SLA | $S$ | Specific leaf area | $cm^2$ $g^{-1}$ |
| — | $T$ | Transpiration | cm |
| TE | $E_{TN}$ | Transpiration efficiency | g $kg^{-1}$ |
| TE | $E_T$ | Transpiration efficiency | Pa |
| VPD | $V$ | Vapour pressure deficit | kPa |
| YGP | | yield gap parameter | Dimensionless |

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