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# Uncertainty of wheat water use: Simulated patterns and sensitivity to temperature and CO<sub>2</sub>

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## 1. Introduction

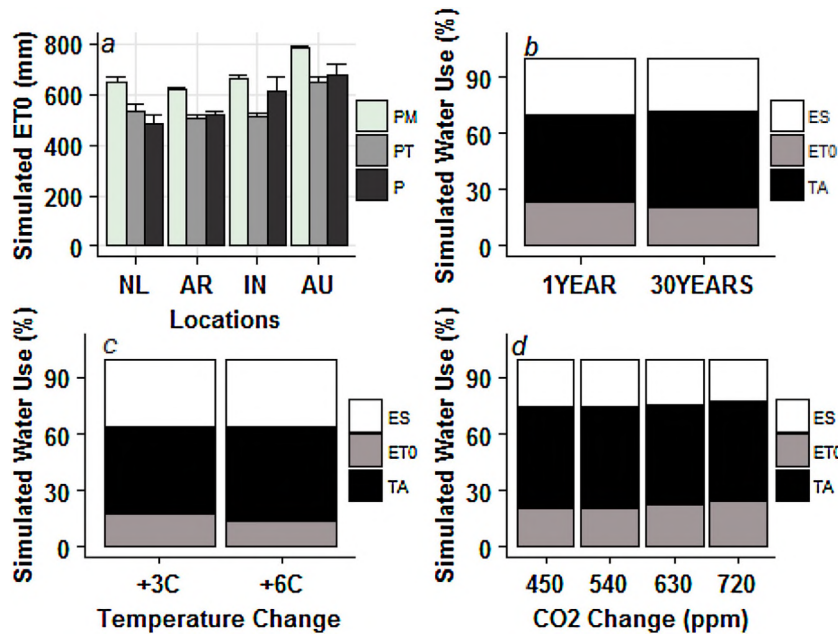
Globally, agriculture uses about 70% of all freshwater withdrawals for irrigation, although discrepancies exist in the quantified amount (Alcamo et al., 2007; Howell, 2001; Shen et al., 2008). About 70% of the world's wheat production comes from irrigated or high rainfall regions, with the majority of irrigation concentrated in developing countries with high population density, particularly large producers like China and India (Dixon et al., 2009; Reynolds and Braun, 2013). Projections that global food demand will double by 2050 highlight the challenges agriculture is facing with the need to produce more food with less land and less water (Foley et al., 2011; Godfray et al., 2010). Due to continued population growth, urbanization and industrialization, agriculture will increasingly compete with other sectors for freshwater (Godfray et al., 2010; Siebert and Doll, 2010; Tilman et al., 2011), and climate change may further limit water availability for irrigation in many cropping areas (Elliott et al., 2014). In rainfed agricultural environments, where crops rely on rainfall alone, future changes in rainfall patterns, temperature conditions, and increases in atmospheric carbon dioxide concentrations ( $[\text{CO}_2]$ ) will affect crop production (Challinor et al., 2014; Knox et al., 2012; Müller and Robertson, 2014; Rosenzweig and Parry, 1994; Rötter and Van de Geijn, 1999).

Passioura (2006) discussed how the term “water productivity”, in the context of agriculture, has different meanings to different people in terms of significance and timescale of interest. Similarly, different aspects of the water used in agriculture are of interest to different actors and stakeholders. These aspects are often characterized in terms of crop water use (WU, known also as actual evapotranspiration), water use efficiency (WUE, defined in Eq. (7)),

and transpiration efficiency ( $T_{\text{eff}}$ , defined in Eq. (8)). For example, breeders use the ratio of agronomic performance (e.g. grain yield) to cumulated WU (WUE) as a basis for identifying crop ideotypes with better productivity, agronomists use WUE as a benchmark for identifying management practices suitable for irrigated or rainfed cultivation, while farmers may be more interested in WUE from an economic point of view (e.g. the monetary outcome such as marketable yield, given a unit of input used to produce it) (Blum, 2005; Condon et al., 2002; Passioura, 2006; Passioura and Angus, 2010; Sadras and Angus, 2006; Semenov et al., 2014). The improvement of crop productivity through management and breeding for high WUE has been the subject of numerous studies (Condon et al., 2004; Condon et al., 2002; Sinclair and Muchow, 2001). Tools that extrapolate the effects of future temperature and  $[\text{CO}_2]$  changes on how WU, WUE, and  $T_{\text{eff}}$  are likely to respond can complement information from field/greenhouse-based experiments for developing guidance on suitable climate change adaptations.

Crop simulation models (CSMs) are increasingly used to explore and assess climate change impacts on agriculture (Angulo et al., 2013; Osborne et al., 2013; White et al., 2011a). CSMs can account for multiple interactions among climate, crop, soil and management. CSMs differ in the way they simulate soil-plant-atmosphere processes and in the number of parameters and inputs required (Rötter et al., 2012; White et al., 2011a). Some CSMs have been developed, evaluated and applied in specific agro-environments, and these models don't perform equally well across all environments.

Single CSMs have usually been used to assess biophysical impacts due to climate change, but it is not possible to evaluate various sources of uncertainty with a single CSM (White et al.,



**Fig. 1.** Simulated potential reference evapotranspiration ( $ET_0$ ) and percentage of simulated water use variance. (a) Simulated seasonal  $ET_0$  for the 30-year baseline calculated from the average of those models using Penman-Monteith (PM, 7 models), Priestley-Taylor (PT, 6 models), and Penman (P, 3 models) equations. Different letters indicate significant differences at  $\alpha = 0.05$ . (b–d) Simulated proportion of variance for water use explained by  $ET_0$  (light grey), crop transpiration ( $T_a$ ; black), and soil evaporation ( $E_s$ ; white) for (b) the experimental year and the 30-year baseline, (c) average daily air temperature increases, and (d) increasing atmospheric  $CO_2$  concentrations.

2011a). One method of studying uncertainties in climate models that has become common practice is to use ensembles of multiple global and regional climate models (Mearns et al., 1997; Tebaldi and Knutti, 2007). Until recently, model ensembles have seen limited use in modelling climate change impact on agriculture (Rötter et al., 2011). Mean or median simulations from multi-model ensembles are usually more accurate than any individual model (Asseng et al., 2013; Martre et al., 2015; Rötter et al., 2012). A further benefit of ensembles is that the variability among the simulations from an ensemble can be used to estimate the uncertainty range when using different CSMs.

In this paper we used simulations from a recent multi-model study (Asseng et al., 2013) that focused solely on wheat grain yield, to explore simulations of crop WU, WUE, and  $T_{eff}$  and their variability and sensitivity to temperature and  $[CO_2]$  changes.

The objectives of this study were to: i) quantify the contributions of sources of model uncertainty to calculations of crop transpiration, soil evaporation, and potential evapotranspiration; and to ii) estimate the relative changes, the patterns and the variability between models for the simulated WU, WUE,  $T_{eff}$ , yield, crop transpiration and soil evaporation at elevated temperatures and  $[CO_2]$ .

## 2. Materials and methods

### 2.1. Experimental sites

Experimental data from four locations with contrasting growing season rainfall and temperature were used which were described in details in Asseng et al. (2013). The locations were Wageningen – NL (Groot et al., 1991), Balcarce – AR (Travasso et al., 1995), New Delhi – IN (Naveen, 1986), and Wongan Hills – AU (Asseng et al., 1998). In particular, the experimental sites were defined in terms of yield and season length as high yielding and long season in the NL, high/medium yielding and medium season in AR, irrigated and short season in IN, and low yielding, rainfed, short season in AU (Asseng et al., 2013). These locations were chosen to represent

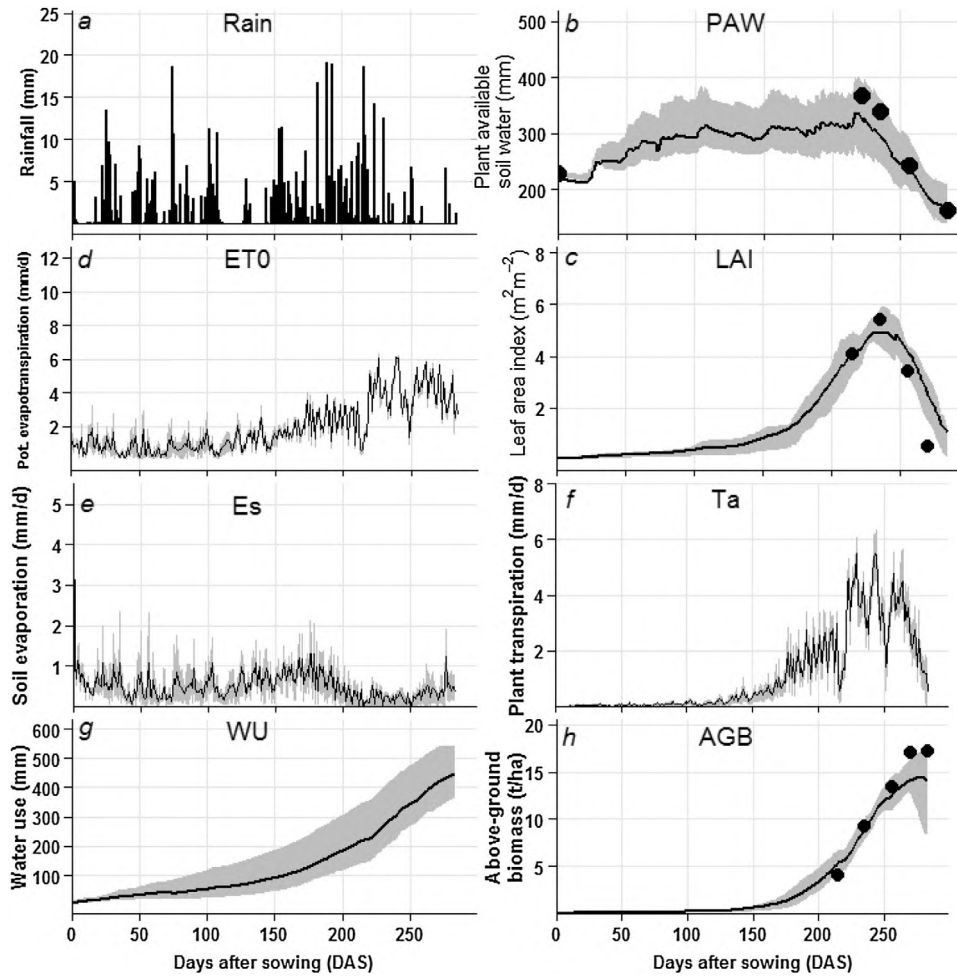
four different wheat mega-environments, a concept used by wheat breeders for testing cultivars (Monfreda et al., 2008) that accounts for about 80% of the wheat-growing area of the world (Additional details were provided in Tables S1 and S2).

The data were quality controlled and standardized using the AgMIP data protocols (Rosenzweig et al., 2011). The management information used at each site was obtained from the experimentalists. The crops were kept weed and disease-free. Daily weather data of solar radiation, maximum and minimum temperature and rainfall were recorded at weather stations on site, with the exception of IN, where solar radiation was obtained from the NASA POWER dataset (White et al., 2011b). At NL, the average daily wind speed at 2-m height was measured. At the three other locations daily wind speed was estimated using the NASA Modern Era Retrospective-Analysis for Research and Applications (MERRA) (Rienecker et al., 2011). At all locations dew-point temperature was estimated using MERRA. Atmospheric  $[CO_2]$  was assumed to be at 360 ppm for all the locations, in line with measured atmospheric  $[CO_2]$  for the mid-point (year 1995) of the baseline climate period 1980–2009.

Measured experimental field data used for this study were harvested grain dry matter yield ( $Y$ ,  $t\ ha^{-1}$ ), in-season measurements of total aboveground biomass (dry matter) (AGB;  $t\ ha^{-1}$ ), leaf area index (LAI,  $m^2\ m^{-2}$ ), water use (WU, mm), and soil water content to maximum rooting depth (SWC, Vol%). For each location soil the soil layers were supplied to all modelling groups (Table S2). For each soil layer ( $i$  for up to  $n$  layers) and from the layer-specific SWC, the plant available soil water content to maximum rooting depth (PAW, mm) was calculated using the lower limit of water extraction for each soil layer (LL, Vol%) which is similar to the soil moisture content at wilting point, and the thickness of each soil layer ( $st$ , m) as follows:

$$PAW = \sum_{i=1}^n st_i * (SWC_i - LL_i) \quad (1)$$

At NL, the SWC was measured down to 1 m, so the SWC and PAW were calculated assuming that the soil between 1 m and maximum rooting depth of 2 m was similar to the 0.6–1 m layers. At AR,



**Fig. 2.** Daily variability in plant water use and crop growth-related variables for an experimental site in the Netherlands (NL). (a) Daily growing season rainfall. (b–h) Average of 16 crop models (black line) with the interval between the 20th and 80th percentiles (shaded grey area) for plant available water (PAW), daily potential evapotranspiration (ET<sub>0</sub>), leaf area index (LAI), soil evaporation (Es), plant transpiration (Ta), water use (WU), and above-ground biomass (AGB). Observed values (closed symbols) are shown for plant available soil water, LAI, and above-ground biomass.

the SWC was measured down to 1.2 m and the maximum rooting depth was 1.3 m. While, in IN and AU the SWC was measured up to 1.5 m and 2.1 m, and the maximum rooting depth was 160 and 210, respectively.

Soil water balance (SWB) was calculated for each simulation run using the simulated drainage (mm), runoff (mm), crop transpiration (mm), soil evaporation (mm), and rainfall (mm) for NL, AR, AU, while for IN irrigation was also considered (mm). To calculate the  $\Delta$ Soil Water Change (SWB) the following equation was used:

$$\text{SWB} = \text{Rain} + \text{Irrigation} - \text{Drainage} - \text{Runoff} - \text{Transpiration} - \text{Evaporation} \quad (2)$$

## 2.2. Crop models

Based on a twenty-six member multi-model ensemble study conducted by Asseng et al. (2013), sixteen crop models which simulate crop transpiration ( $T_a$ ) and soil evaporation ( $E_s$ ) as separate fluxes were selected for detailed analysis of water use simulations (for more detailed information on the simulated processes see Table S3). The models, which varied in complexity and functionalities, have all been described and used in modelling wheat crops. Additional details on modelling procedures were described in Asseng

et al. (2013), for this study we used the models calibrated against phenology and yield. At the beginning of the study a questionnaire was sent to the modelers to provide information on which type of  $ET_0$  was used in the crop models. Information on different implementations of the  $ET_0$  calculation in the 16 wheat models using the Penman (P; Penman, 1948), Penman-Monteith (PM; Allen et al., 1998) or Priestley-Taylor (PT; Priestley and Taylor, 1972) equations (Table S3). Analysis of variance (ANOVA) for unbalanced designs was used to test the differences among the three  $ET_0$  formulas at each location.

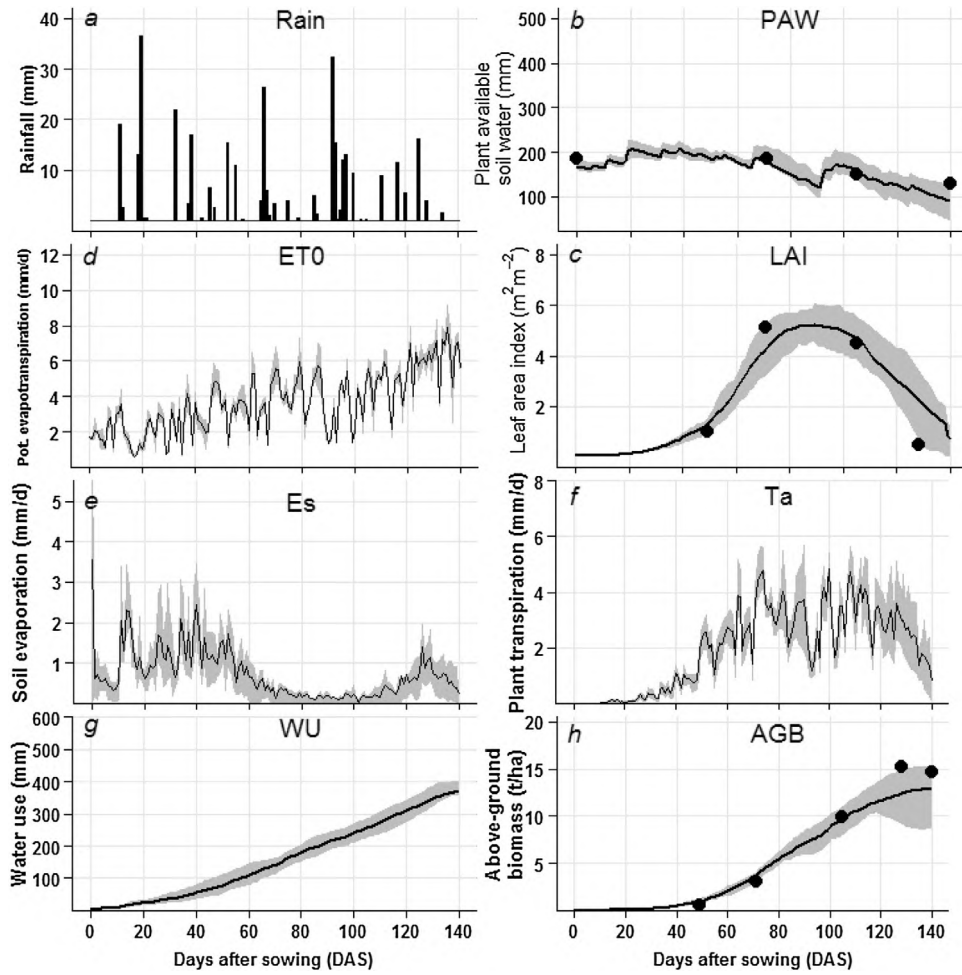
## 2.3. Data analysis

The partitioning of uncertainty of simulated WU was made to explore which component was responsible for most of the variability. WU can be expressed as follows, based on simulated cumulative  $\sum ET_0$ ,  $\sum Ta$  and  $\sum Es$ :

$$\text{WU} = \sum ET_0 * \left[ \frac{\sum Es}{\sum ET_0} + \frac{\sum Ta}{\sum ET_0} \right] \quad (3)$$

The variance is calculated as follows:

$$\text{Var}(\text{WU}) = \text{Var} \left( \frac{\sum Ta}{\sum ET_0} \right) * E \left( \sum ET_0 \right)^2 + \text{Var} \left( \frac{\sum Es}{\sum ET_0} \right)$$



**Fig. 3.** Daily variability in plant water use and crop growth-related variables for an experimental site in Argentina (AR). (a) Daily growing season rainfall. (b–h) Average of 16 crop models (black line) with the interval between the 20th and 80th percentiles (shaded grey area) for plant available water (PAW), daily potential evapotranspiration (ET0), leaf area index (LAI), soil evaporation (Es), plant transpiration (Ta), water use (WU), and above-ground biomass (AGB). Observed values (closed symbols) are shown for plant available soil water, LAI, and above-ground biomass.

$$*E\left(\sum ET_0\right)^2 + Var\left(\sum ET_0\right) * \left[E\left(\frac{\sum Es}{\sum ET_0} + \frac{\sum Ta}{\sum ET_0}\right)\right]^2 \quad (4)$$

where  $\sum Ta/\sum ET_0$  was transpiration as a fraction of evaporative demand and  $\sum Es/\sum ET_0$  was soil evaporation as a fraction of evaporative demand. A way of quantifying the contribution of  $\sum Ta/\sum ET_0$ ,  $\sum Es/\sum ET_0$ , and  $\sum ET_0$  to the overall uncertainty was through the first-order sensitivity coefficients (S1):

$$S1(Ta) = Var\left(\sum Ta/\sum ET_0\right) * E\left(\sum ET_0\right)^2 \quad (5)$$

$$S1(Es) = Var\left(\sum Es/\sum ET_0\right) * E\left(\sum ET_0\right)^2 \quad (6)$$

$$S1(ET_0) = Var\left(\sum ET_0\right) * \left[E\left(\sum Es/\sum ET_0 + \sum Ta/\sum ET_0\right)\right]^2 \quad (7)$$

If there are no interactions among terms,  $S1(x)$  is the fraction of overall variance contributed by factor  $x$  and the sum of the S1 can be somewhat larger or smaller than 1, depending on whether there were positive or negative correlations between terms. The larger the values of  $S1(x)$ , the greater the contribution of factor  $x$  to the overall variance. From the sum of the first-order sensitivity coefficients, we calculated the percentage contribution of each term.

Water use efficiency (WUE) was calculated as:

$$WUE = \frac{Y}{\sum WU} \quad (8)$$

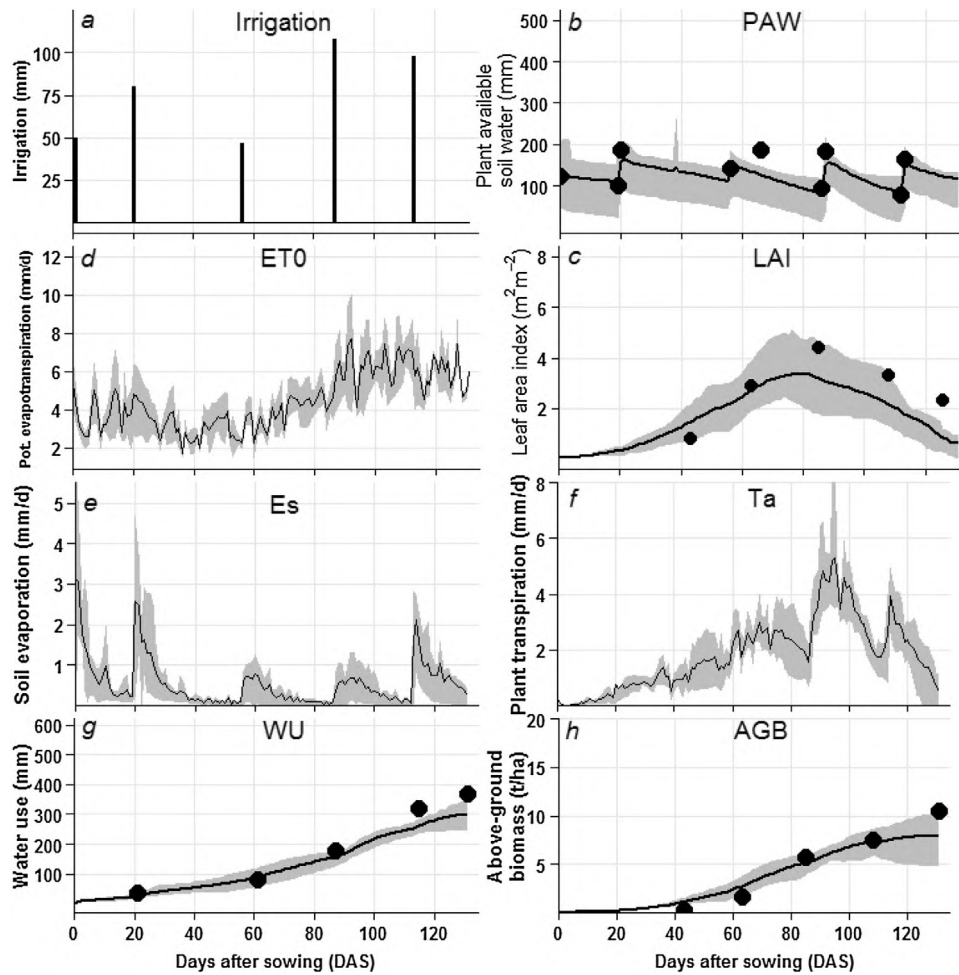
where  $Y$  is the simulated grain dry matter yield and  $\sum WU$  was the cumulative evapotranspiration calculated from sowing to harvest. Transpiration efficiency ( $T_{eff}$ ) on a grain yield basis was calculated following the definition of [Angus and van Herwaarden \(2001\)](#):

$$T_{eff} = \frac{Y}{\sum Ta} \quad (9)$$

where  $\sum Ta$  is the cumulative water transpired from sowing to harvest.

#### 2.4. Sensitivity analysis

In addition to the simulations based on the measured experimental conditions, simulations were conducted using daily weather data for the period 1980–2010 for all the locations to create a baseline. A sensitivity analysis of the sixteen models to temperature and  $[CO_2]$  was done using a partly-factorial design. Daily minimum and maximum temperature were increased by either 3 °C (+3C) or 6 °C (+6C) and  $[CO_2]$  was increased in 90 ppm increments from a baseline to a maximum of 720 ppm. Wind speed and relative humidity were kept unchanged with the increased temperatures, so vapor pressure was re-calculated using the modified



**Fig. 4.** Daily variability in plant water use and crop growth-related variables for an experimental site in India (IN). (a) Irrigation. (b–h) Average of 16 crop models (black line) with the interval between the 20th and 80th percentiles (shaded grey area) for plant available water (PAW), daily potential evapotranspiration ( $ET_0$ ), leaf area index (LAI), soil evaporation (Es), plant transpiration (Ta), water use (WU), and aboveground biomass (AGB). Observed values (closed symbols) are shown for plant available soil water, LAI, water use, and above-ground biomass.

temperatures. In order to understand the effects of climate factors alone on crop responses, soil and crop management were kept the same for all the simulations except that dates of irrigation and fertilization were adapted to the changed phenology.

The relative changes in  $Y$ , WU, Ta, Es, WUE, and  $T_{eff}$  were calculated as:

$$r_k = \frac{\bar{y}_{sensitivity,k} - \bar{y}_{baseline,k}}{\bar{y}_{baseline,k}} * 100 \quad (10)$$

where  $r_k$  is the predicted relative change with respect to the 30-year baseline according to model  $k$ ,  $\bar{y}_{sensitivity,k}$  is any of the above variables averaged over the 30 years of climate sensitivity according to model  $k$ , and  $\bar{y}_{baseline,k}$  are the variables averaged over the 30 years of baseline climate according to model  $k$ .

More detailed analysis of the multi-model intercomparison in terms of decomposition of the mean square error and other statistical indicators can be found in [Martre et al. \(2015\)](#).

### 3. Results

#### 3.1. Decomposition of the variability

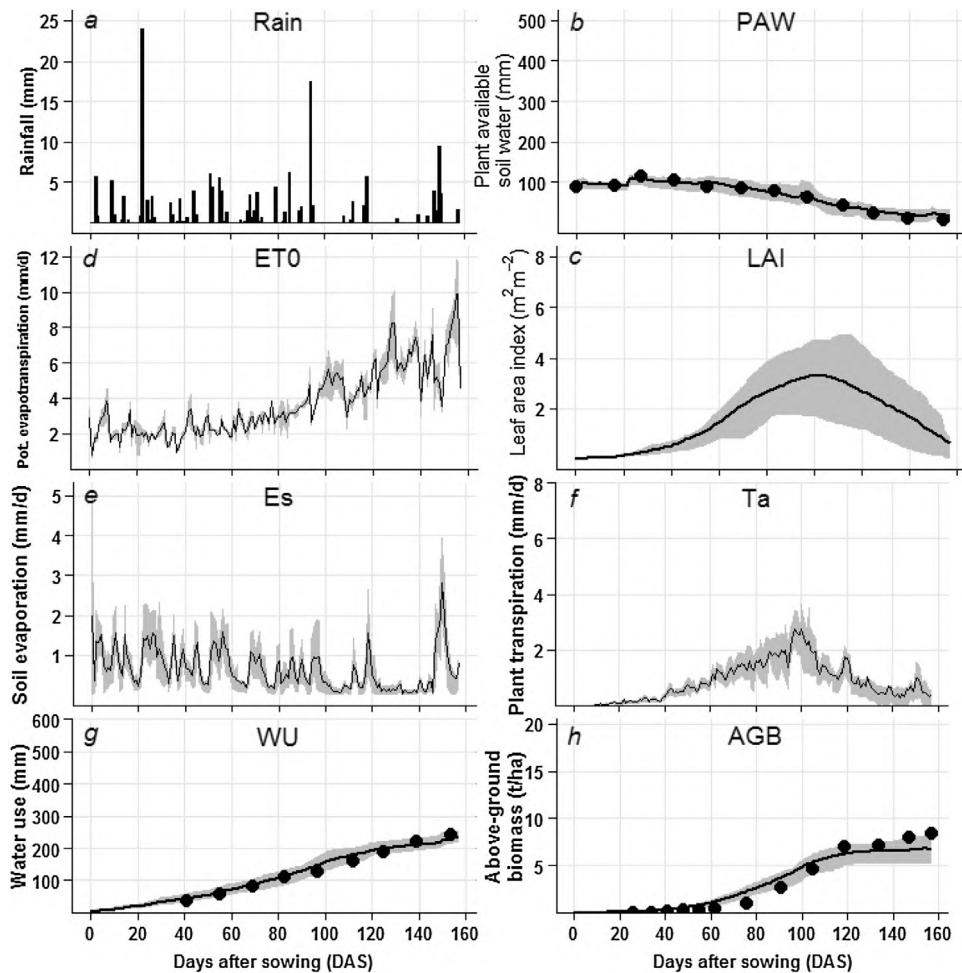
The simulated growing season  $ET_0$  using the three methods (PM, PT, and P) ranged from 786 mm for AU to 483 mm for the NL ([Fig. 1a](#)).

Total season  $ET_0$  values calculated by the three methods differed at each location ( $P < 0.05$ ; [Fig. 1a](#)).

When the uncertainty of simulated WU was partitioned between Ta, Es, and  $ET_0$ , and following equations [2] to [6], the first-order sensitivity coefficient  $S1(Ta)$  contributed the most to the variability in WU among models ([Fig. 1b–d](#)). For the single year dataset the term  $S1(Ta)$  was 46% of the variability,  $S1(Es)$  was 30%, and ( $ET_0$ ) was 24% ([Fig. 1b](#)). For the simulations averaged over the 30-year baseline,  $S1(Ta)$ ,  $S1(Es)$ , and  $S1(ET_0)$  were 51%, 28% and 21%, respectively ([Fig. 1b](#)). There was little change in the first order sensitivity coefficients as temperature increased. The  $S1(Ta)$ ,  $S1(Es)$ , and  $S1(ET_0)$  values were 46, 37, and 18% at +3C and 50, 36 and 14% at +6C ([Fig. 1c](#)). Simulations with four  $[CO_2]$  showed similar results with  $S1(Ta)$  ranging between 53 and 54% ([Fig. 1d](#)).

#### 3.2. Observed and simulated data

The daily patterns of growing season rainfall, observed and simulated PAW,  $ET_0$ , LAI, Es, Ta, WU, and AGB are shown for NL, AR, IN, and AU in [Figs. 2–5](#), respectively. The four wheat-growing locations differed in terms of the evaporative demand of the atmosphere, soil conditions, and the temporal variability of growing season rainfall and temperature ([Figs. 2–5](#)). For example, at AU rainfall occurred frequently throughout the season with occasional days of heavy rainfall in spring and summer ([Fig. 5a](#)). In contrast, there was no



**Fig. 5.** Daily variability in plant water use and crop growth-related variables for an experimental site in Australia (AU). (a) Daily growing season rainfall. (b-h) Average of 16 crop models (black line) with the interval between the 20th and 80th percentiles (shaded grey area) for plant available water (PAW), daily potential evapotranspiration (ET0), leaf area index (LAI), soil evaporation (Es), plant transpiration (Ta), water use (WU), and aboveground biomass (AGB). Observed values (closed symbols) are shown for plant available soil water, water use, and above-ground biomass.

rainfall at the IN site (Fig. 4a). NL and AR had frequent heavy rainfall during the growing season (Figs. 2a and 3a). The in-season observed values for the plant available soil water, aboveground biomass, water use, and LAI were within the range of the simulations in NL, AR, and AU (Figs. 2, 3 and 5). There were some discrepancies between observed and simulated values in IN for the LAI, PAW and WU (Fig. 4).

The end-of-season cumulative WU, WUE,  $T_{eff}$ , Es,  $T_{eff}$ , and Y for the single experimental year, and for the 30-year period from 1980 to 2009 are shown in Table 1. Simulated average values for WU was less variable than for WUE and  $T_{eff}$ . The coefficient of variation (CV) across locations for the single experimental year varied between 14 and 23% for WU, and between 16 and 37% for WUE. Average CV of simulated values varied between 20 and 33% for  $T_{eff}$ , between 34 and 73% for Es, and between 24 and 55% for  $T_{eff}$  (Table 1).

### 3.3. Crop simulation models sensitivity to average daily air temperature and atmospheric $CO_2$ concentration

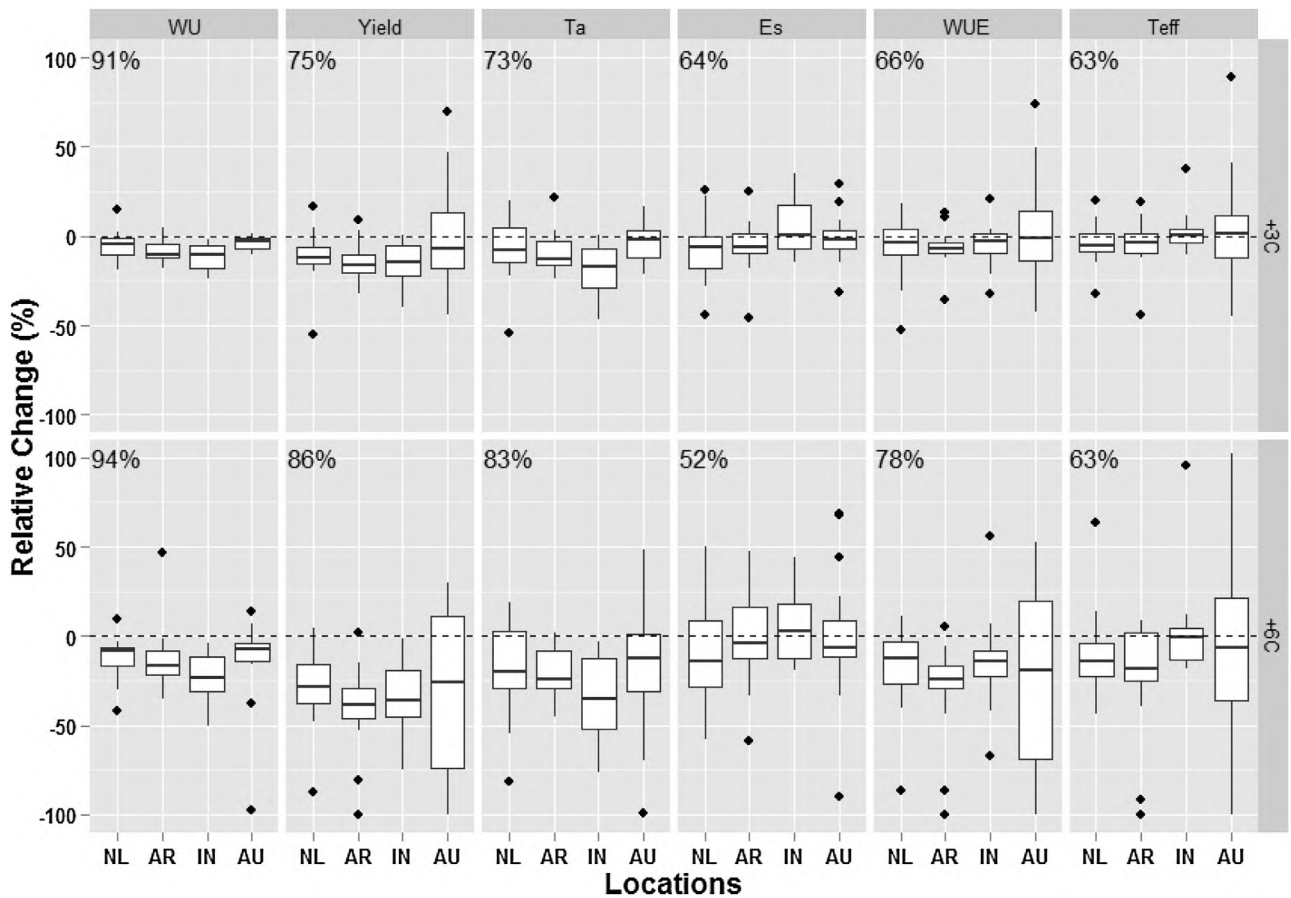
The average simulated WU, Y,  $T_a$ , Es, WUE, and  $T_{eff}$  decreased with increased temperature for all four locations (Fig. 6). However, the variability of the models increased as temperature increased for all the variables (Fig. 6). The models showed higher uncertainties for Australia, where except for the simulated WU which had little

variability. In Australia simulated  $T_{eff}$  varied between  $-100$  and  $+100\%$  when temperature was increased by  $+6C$  (Fig. 6).

Simulated average WU,  $T_a$ , and Es decreased with increasing  $[CO_2]$  while Y, WUE, and  $T_{eff}$  increased with increasing  $[CO_2]$  at all locations (Fig. 7). The simulated relative changes to  $[CO_2]$  showed less variability than temperature. This outcome seemed to be consistent across the models, with the exception of few outliers. At 720 compared to 360 ppm  $[CO_2]$  in the four locations, the overall simulated values changed by  $-4\%$  for WU,  $+31\%$  for Y,  $-2\%$  for  $T_a$ ,  $-9\%$  for Es,  $+38\%$  for WUE, and  $+34\%$  for  $T_{eff}$  (Fig. 7). Only the variability of WUE and  $T_{eff}$  was higher at 720 ppm than at 360 ppm, ranging between 0 and 100% changes at 720 ppm (Fig. 7).

The respective effects of changing temperature and  $[CO_2]$  interact in generating model outputs of the 16 crop models. For simulated WU, increasing  $[CO_2]$  to 720 ppm does not offset its reduction caused by temperature increase (Fig. 8). The effects of  $[CO_2]$  in compensating temperature-induced losses of WUE and  $T_{eff}$  were larger than for simulated WU (Fig. 8). For example, with a  $6^\circ C$  increase, WUE increased if  $[CO_2]$  was above 450 ppm in NL and IN, or above 550 ppm in AR and AU (Fig. 8).

Of particular interest is the variability in the direction of change in simulated responses to increased temperature or  $[CO_2]$ . It was studied by counting how many models showed similar trend; for example how many models simulated a decrease in WU at  $+6C$ , and how many simulated an increase in WU at  $+6C$ . Overall, with a



**Fig. 6.** Effects of higher temperatures, respect to the 30 years historical data, on simulated water use related variables and grain yield. Boxplot of the relative change of multi-model simulations with increases in average daily air temperature of 3 °C and 6 °C for water use (WU), grain yield (Y), cumulative crop transpiration ( $T_a$ ), cumulative soil evaporation ( $E_s$ ), water use efficiency (WUE), and transpiration efficiency ( $T_{eff}$ ), for experimental sites in the Netherlands (NL), Argentina (AR), India (IN), and Australia (AU). The percentage of individual models that predict the same trend is shown above each set of points.

**Table 1**

Average (AV), standard deviation (STD), and coefficient of variability (CV%) for the Netherlands (NL), Argentina (AR), India (IN), and Australia (AU) for seven parameters using the 16 crop simulation models.

Variable	Unit	AV	STD	CV%	AV	STD	CV%	AV	STD	CV%	AV	STD	CV%
1-Year		NL			AR			IN			AU		
ET0 <sup>a</sup>	(mm)	548.8	92.7	16.9	516.7	56.4	10.9	590.1	92.6	15.7	647.2	68.4	10.6
WU <sup>b</sup>	(mm)	445.4	100.3	22.5	371.3	51.7	13.9	301.9	49.9	16.5	234	38.4	16.4
$T_a$ <sup>c</sup>	(mm)	301.7	85.7	28.4	271.6	53.9	19.8	232.5	66.3	28.5	132.1	43.8	33.2
$E_s$ <sup>d</sup>	(mm)	143.7	60.6	42.2	99.6	33.4	33.5	69.4	50.7	73.1	101.9	39.8	39.1
Yield	(t ha <sup>-1</sup> )	7.7	0.4	5.7	6.1	0.5	9	4	0.4	10.4	2.2	0.5	21.9
WUE <sup>e</sup>	(kg ha <sup>-1</sup> mm <sup>-1</sup> )	18.1	4.1	22.6	16.6	2.6	15.6	13.8	2.6	19	9.9	3.7	37.3
$T_{eff}$ <sup>f</sup>	(kg ha <sup>-1</sup> mm <sup>-1</sup> )	29.2	16	55	23.3	5.6	24	19.3	7.4	38.4	18.9	8.2	43.2
Baseline (30-years)													
ET0	(mm)	556.7	88.3	15.9	539.6	55.4	10.3	564.6	68.7	12.2	692.7	68.8	9.9
WU	(mm)	449.9	99.3	22.1	365.9	58.9	16.1	329.4	52	15.8	258.6	49.7	19.2
$T_a$	(mm)	297.9	75.3	25.3	257	50.1	19.5	244.8	62.9	25.7	154.4	46.9	30.4
$E_s$	(mm)	152	56.9	37.5	109	35.9	33	84.7	46.7	55.1	104.2	44.2	42.4
Yield	(t ha <sup>-1</sup> )	7.4	0.9	12.3	5.5	0.4	8	5	0.6	12.2	2.8	0.6	21.4
WUE	(kg ha <sup>-1</sup> mm <sup>-1</sup> )	17.3	4.9	28.1	15.6	3.2	20.5	15.4	1.8	11.6	11.3	4.2	36.7
$T_{eff}$	(kg ha <sup>-1</sup> mm <sup>-1</sup> )	27.5	13.4	48.6	22.5	5.8	25.9	21.9	6.7	30.5	20.4	10.1	49.3

<sup>a</sup> Potential evapotranspiration.

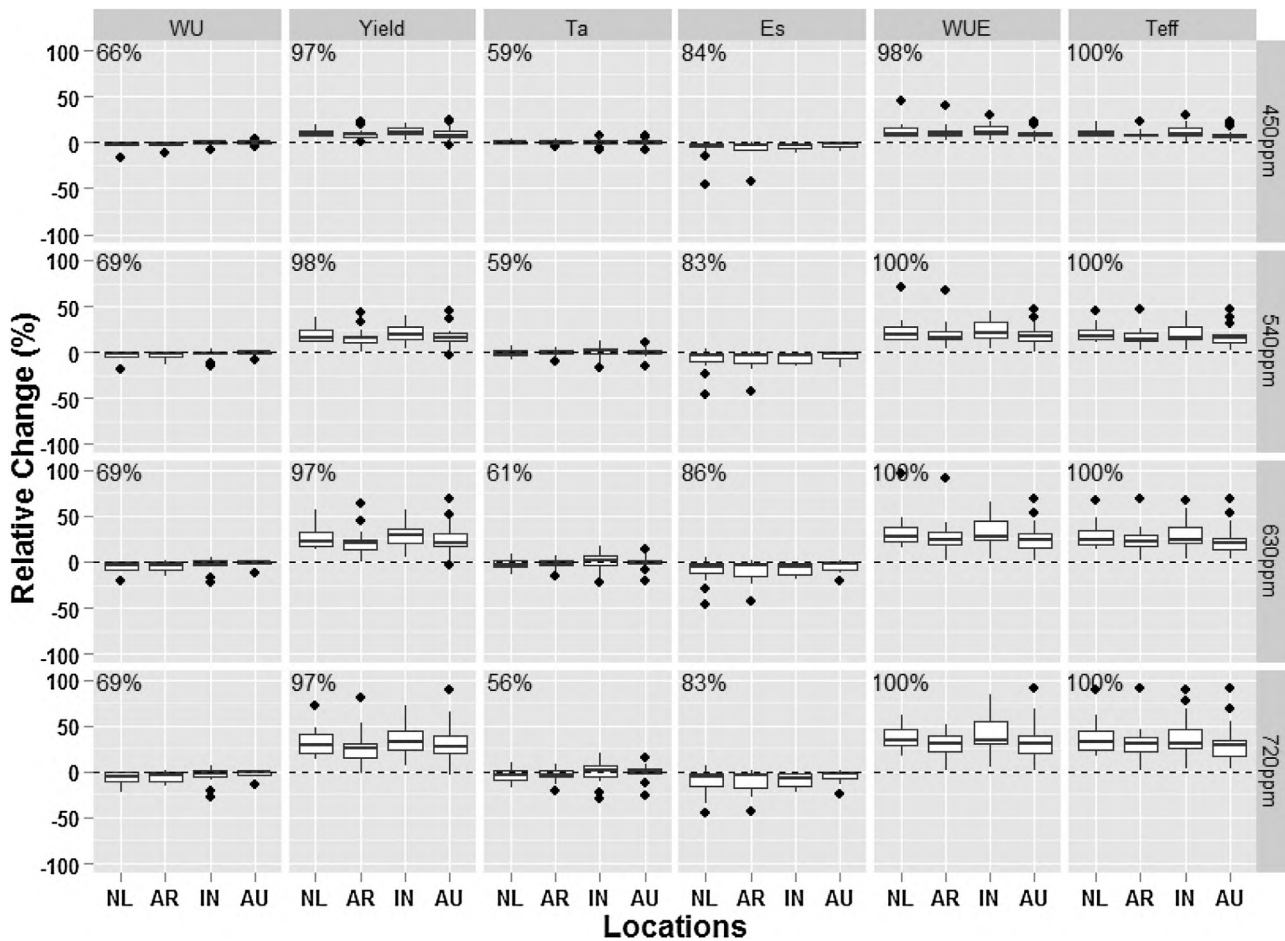
<sup>b</sup> Water use.

<sup>c</sup> Crop transpiration.

<sup>d</sup> Soil evaporation.

<sup>e</sup> Water use efficiency.

<sup>f</sup> Transpiration efficiency.



**Fig. 7.** Effects of increases in atmospheric CO<sub>2</sub> concentrations on simulated water use related variables and grain yield. Boxplot of the relative change of multi-model simulation with increased atmospheric CO<sub>2</sub> concentrations for water use (WU), grain yield (Y), cumulative crop transpiration (*T<sub>a</sub>*), cumulative soil evaporation (*E<sub>s</sub>*), water use efficiency (WUE), and transpiration efficiency (*T<sub>eff</sub>*), for experiment sites in the Netherlands (NL), Argentina (AR), India (IN), and Australia (AU). The percentage of individual models that predict the same trend as the multi-model mean is shown above each set of points.

6 °C increase across the four locations, 94% of the models computed that WU decreased, 83% that *T<sub>a</sub>* decreased, 52% that *E<sub>s</sub>* decreased, 78% that WUE decreased, and 63% that *T<sub>eff</sub>* decreased (Fig. 6). Modelling the effect of 720 ppm CO<sub>2</sub>, 69% of the models agreed that WU decreased, 97% that *Y* increased, 56% that *T<sub>a</sub>* decreased, and 83% that *E<sub>s</sub>* decreased. All models projected that WUE and *T<sub>eff</sub>* would increase (Fig. 7).

The calculated SWB using Eq. (2) showed that for both baseline and sensitivity to temperature and CO<sub>2</sub> the NL had a higher variability among the models with respect to the other locations (Fig. 9). The variability among the different components of Eq. (2) showed that transpiration (*T<sub>a</sub>*) was the component having the higher variability followed by the drainage (Fig. 10). For example, in the NL the simulated transpiration varied between 100 and 500 mm for the baseline runs (No temperature changes) and drainage between 0 and 400 mm, for the upper and lower hinge representing the 25th and 75th percentile, respectively. At +6C the variability of simulated crop transpiration among models ranged between 10 and 540 mm while simulated drainage ranged between 0 and 350 mm (Fig. 10a).

#### 4. Discussion

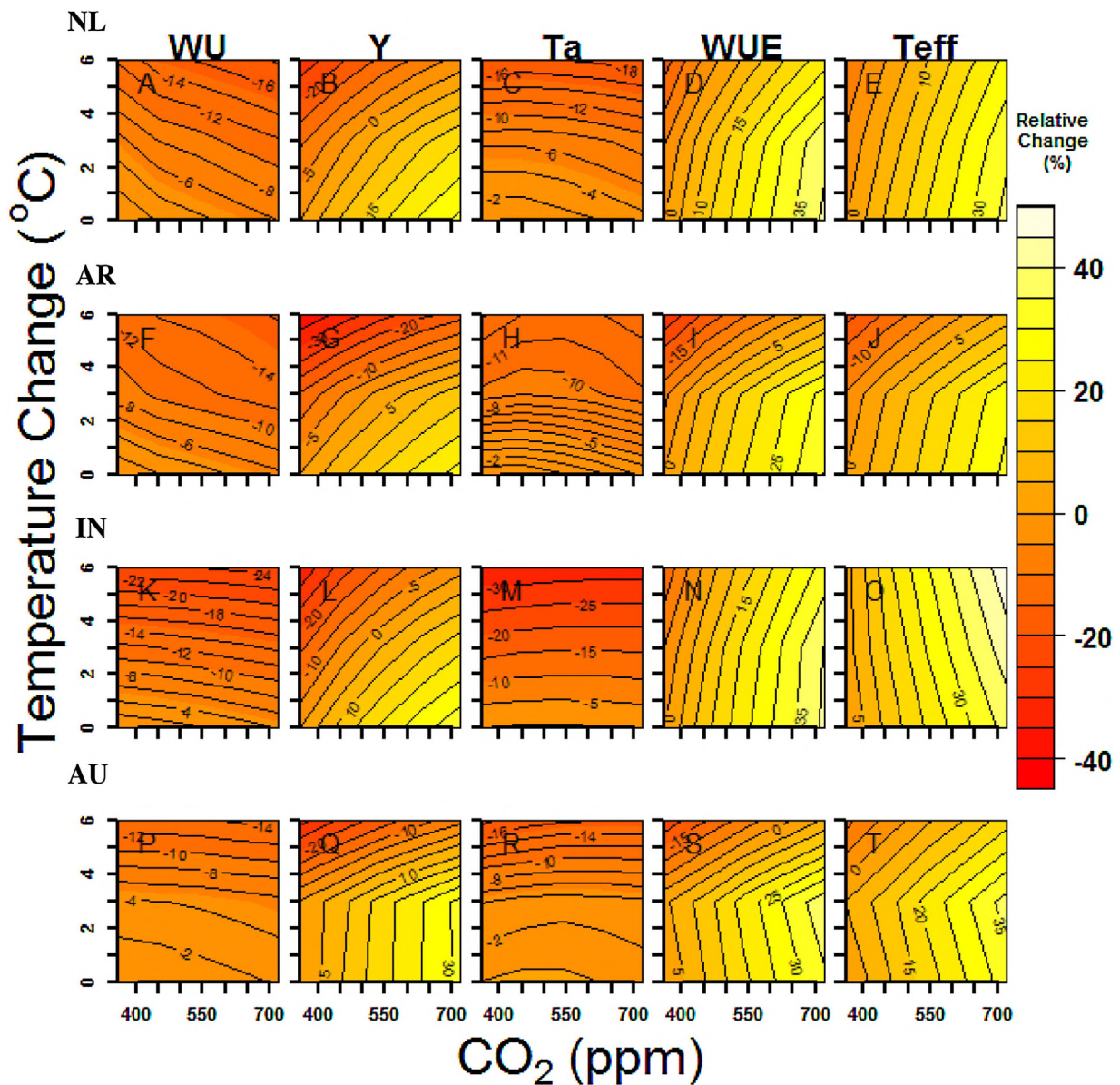
In this study, most of the variability in simulated WU was due to model differences in *T<sub>a</sub>/E<sub>to</sub>* and *E<sub>s</sub>/E<sub>to</sub>* rather than the choice of the *E<sub>T0</sub>* formula. This is true for the experimental years, the 30-year baseline and for the simulations with increased temperature

or CO<sub>2</sub>. While differences in the choice of the *E<sub>T0</sub>* formula have been shown to be important (Kingston et al., 2009; McAfee, 2013; McKenney and Rosenberg, 1993; Utset et al., 2004; Xu and Singh, 2002), studies focusing on the *E<sub>T0</sub>* formula have not analyzed how the partitioning of *E<sub>T0</sub>* between *E<sub>s</sub>* and *T<sub>a</sub>* would influence the simulations of crop WU. Other studies have focused on the partitioning within the growing season of the *E<sub>s</sub>* and *T<sub>a</sub>* only, showing that *E<sub>s</sub>* can account for 20% to 40% of WU (Kool et al., 2014; French and Schultz, 1984).

Although the overall first order effect of *T<sub>a</sub>/E<sub>to</sub>* accounted for 51% of the total of first order effects on WU for both different temperature and CO<sub>2</sub> changes across the four locations, no experimental data were available to validate these aspects of the simulation. Differences among models in simulating rooting depth/distribution and soil water extraction by roots could be an important reason for differences in *T<sub>a</sub>* estimation (Wu and Kersebaum, 2008).

Understanding the partitioning of WU between crop transpiration and soil evaporation is critical because of its implications for agricultural, ecological, and hydrological studies. In addition, considering the variability in the simulation of PAW, and particularly of simulated LAI, the differences in *T<sub>a</sub>/E<sub>to</sub>* are not surprising because the water is transpired by crops through stomata that are on leaves.

Given the variability of the simulated SWB, and of the other components like drainage, further research into the reasons of variation of different sub-routines among models is necessary. The



**Fig. 8.** Interaction patterns between temperature and atmospheric CO<sub>2</sub> concentration on simulated water use related variables and grain yield. Relative change in (a, f, k, and p) water use (WU), (b, g, l, and q) grain yield (Y), (c, h, m, and r) cumulative crop transpiration (*T<sub>a</sub>*), (d, i, n, and s) water use efficiency (WUE), and (e, j, o, and t) transpiration efficiency (*T<sub>eff</sub>*) simulations for experimental sites in (a–e) the Netherlands, (f–j) Argentina, (k–o) India, and Australia (p–t) with increases in average daily air temperature versus atmospheric CO<sub>2</sub> concentration.

hardest part is to get detailed and accurate measurements of each sub-component in a single experiment.

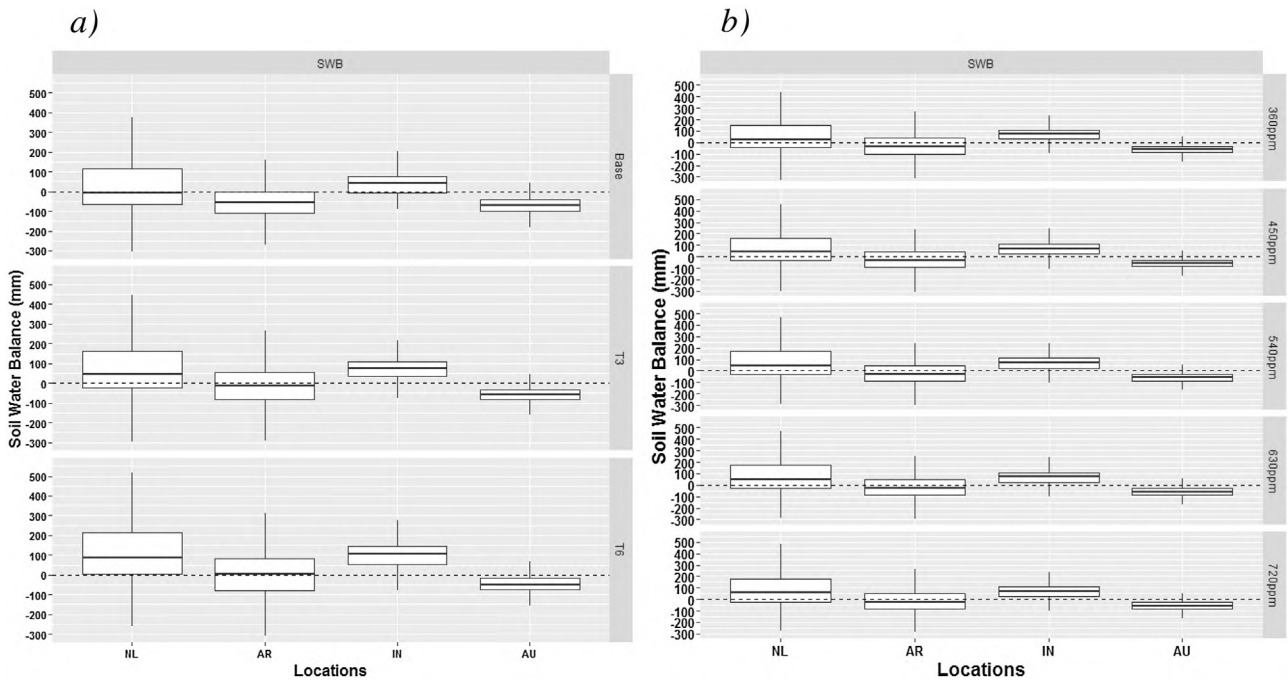
The large variability between models indicates that there are major differences in the way the processes that affect water use are modeled. Differences among models in simulating soil water extraction by roots could be an important reason for differences in *T<sub>a</sub>* estimation (Wu and Kersebaum, 2008). Variability in the simulation of PAW and LAI would have a direct effect on the differences in *T<sub>a</sub>/ET<sub>o</sub>*. Since PAW was among the given soil parameters, causes are primarily related to differences in the models' crop interfaces to soil (roots) and atmosphere (LAI).

Models have been tested against the same limited set of CO<sub>2</sub> response data, which are from open-top chamber or Free Air Carbon dioxide Enrichment Experiments (FACE) data. Models also typically include many processes that respond to temperature, while the response to CO<sub>2</sub> is often lumped at a higher level of integration as discussed in details by Kersebaum and Nendel (2014). Some

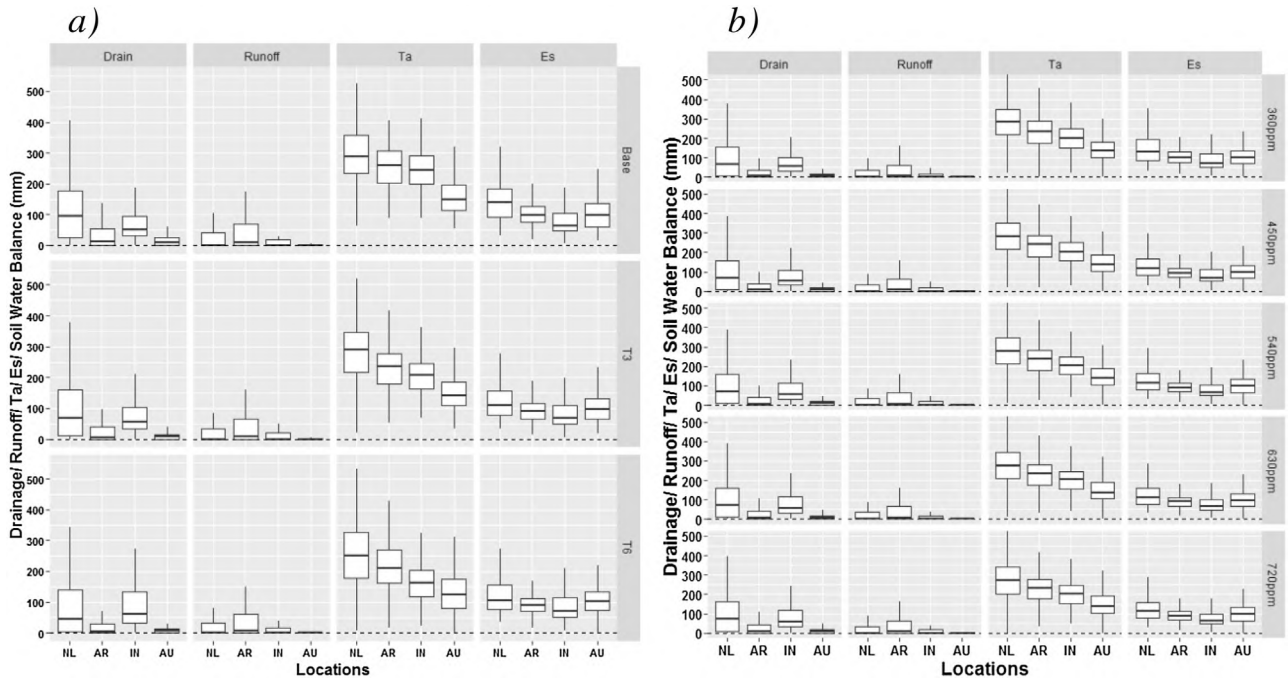
models used an empirical relationship between CO<sub>2</sub> and radiation use efficiency while other models used the CO<sub>2</sub> dependency of the photosynthesis light response curve (Tubiello and Ewert, 2002) or directly simulated stomatal conductance and rubisco-kinetics based photosynthesis.

However, there is no clear relationship between model results and model's structure because models are complex and many elements of structure interact with each other (Bassu et al., 2014; Li et al., 2015; Martre et al., 2015). Further research into the sources of variation of different sub-routines among models is necessary.

Increased [CO<sub>2</sub>] in field crops has led to decreases in WU of 3–8%, and an increase in Y of 8–31% (Hatfield et al., 2011; Kimball et al., 2002; Long et al., 2006; Manderscheid and Weigel, 2007; Tao and Zhang, 2013). The variability in the experimental results depends on crop management, CO<sub>2</sub> concentrations used in the experiments, the type of experiment (e.g. open-top chambers or field experiments), and the different scaling methods used to compare a crop



**Fig. 9.** Boxplots of the simulated Soil Water Balance (SWB) calculated using Eq. (2) for the Netherlands (NL), Argentina (AR), India (IN), and Australia (AU); (a) Effect of temperature on each of the model simulation of the baseline 30-years period (Base), the increases in average daily air temperature of 3 °C (T3) and 6 °C (T6); (b) for the increases in atmospheric CO<sub>2</sub> concentrations.



**Fig. 10.** Boxplots of the simulated components of the Soil Water Balance (SWB) calculated using Eq. (2). Simulated Drainage (*Drain*), Runoff (*Runoff*), crop transpiration (*Ta*), and soil evaporation (*Es*) are shown for the Netherlands (NL), Argentina (AR), India (IN), and Australia (AU); (a) Effect of temperature on each of the model simulation of the baseline 30-years period (Base), the increases in average daily air temperature of 3 °C (T3) and 6 °C (T6); (b) for the increases in atmospheric CO<sub>2</sub> concentrations.

response to CO<sub>2</sub> concentrations across different experiments (Long, 2012). A meta-analysis of wheat studies found that increasing [CO<sub>2</sub>] from 400 to 800 ppm increases WUE by between 5 and 38% (Hatfield et al., 2011; Kimball et al., 2002; Long et al., 2006; Manderscheid and Weigel, 2007; Tao and Zhang, 2013; Wang et al., 2013). The results of this study regarding the simulated response at the four locations for WU, Y, and WUE to [CO<sub>2</sub>] was in line with these studies. This concordance contrasts with claims that on average models

overestimate [CO<sub>2</sub>] effects (Ewert et al., 2007; Long et al., 2006; Tubiello et al., 2007).

Another important outcome of our study is to have traced the average pattern of WU, WUE, and  $T_{eff}$  change with temperature and [CO<sub>2</sub>] increases. Despite variability, the majority of models had the same direction of change in Y, WU, WUE, and  $T_{eff}$  in the sensitivity to temperature and [CO<sub>2</sub>]. This allowed us to draw conclusions about general crop responses when temperature and [CO<sub>2</sub>] both change.

The interaction between increase in temperature and increase in [CO<sub>2</sub>] showed that, depending on the location, Y, WUE, and  $T_{eff}$  reductions due to temperature can be largely offset by increasing [CO<sub>2</sub>]. The response of WUE to temperature is of particular interest since this response may be driving yield changes in many regions with limited rainfall and water for irrigation (Pirttioja et al., 2015).

The changes in temperature used in this study (+3 °C and +6 °C) caused more model output variability than the changes in atmospheric [CO<sub>2</sub>] (from 360 ppm to 720 ppm at 90 ppm intervals). But, the crop models' agreement related to the magnitude of changes is variable-specific. For example, crop models showed good agreement in terms of relative change of simulated Y under temperature and elevated [CO<sub>2</sub>] changes, WU showed good agreement under temperature changes and lower agreement under [CO<sub>2</sub>], while WUE, and  $T_{eff}$  showed less agreement under temperature changes and high agreement under elevated [CO<sub>2</sub>] (Figs. 6 and 7).

## 5. Conclusion

The largest uncertainty in simulated crop WU among CSMs is due to differences in how models simulate crop transpiration. The simulated response to increased temperature caused a decline in WU. The sixteen models showed greatest uncertainty of simulated WUE, and  $T_{eff}$  at increased temperatures and with interactions between temperature and [CO<sub>2</sub>]. To improve the simulated impacts of climate change on crop water dynamics, crop transpiration in CSMs needs to be improved with detailed experimental data.

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