How accurately do maize crop models simulate the interactions of atmospheric CO$_2$ concentration levels with limited water supply on water use and yield?

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ABSTRACT

This study assesses the ability of 21 crop models to capture the impact of elevated CO$_2$ concentration ([CO$_2$]) on maize yield and water use as measured in a 2-year Free Air Carbon dioxide Enrichment experiment conducted at the Thünen Institute in Braunschweig, Germany (Manderscheid et al., 2014). Data for ambient [CO$_2$] and irrigated treatments were provided to the 21 models for calibrating plant traits, including weather, soil and management data as well as yield, grain number, above ground biomass, leaf area index, nitrogen concentration in biomass and grain, water use and soil water content. Models differed in their representation of carbon assimilation and evapotranspiration processes.

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Stomatal conductance
Grain number
Water use

The models reproduced the absence of yield response to elevated [CO_2] under well-watered conditions, as well as the impact of water deficit at ambient [CO_2], with 50% of models within a range of +/−1 Mg ha^{-1} around the mean. The bias of the median of the 21 models was less than 1 Mg ha^{-1}. However under water deficit in one of the two years, the models captured only 30% of the exceptionally high [CO_2] enhancement on yield observed. Furthermore the ensemble of models was unable to simulate the very low soil water content at anthesis and the increase of soil water and grain number brought about by the elevated [CO_2] under dry conditions. Overall, we found models with explicit stomatal control on transpiration tended to perform better. Our results highlight the need for model improvement with respect to simulating transpirational water use and its impact on water status during the kernel-set phase.

1. Introduction

Given population growth and changes in dietary habits, global maize demands are expected to increase (Pingali, 2001). Water deficits, air temperature and atmospheric CO_2 concentrations ([CO_2]) are expected to rise significantly by 2050 and beyond (IPCC 2013). For instance, [CO_2] of approximately 540 parts per million (ppm) is projected for 2050–2100 under the radiative concentration pathways (RCP) 8.5 or 4.5 scenarios, respectively (Van Vuuren et al., 2011). Projections of maize production remain unclear partly due to the large uncertainty in the response of C_4 crops to elevated [CO_2] and interaction with water and temperature stresses (Markelz et al., 2011; Deryng et al., 2016,); a better mechanistic understanding of the underlying processes as they are affected by climate change can reduce that uncertainty. Mechanistic crop models are valuable tools to both integrate the complex interactions of climate variables and to make reliable estimates of projected impacts of rising [CO_2] on crop yields and resource use. During the last few decades, the models have evolved from cropping system models to agricultural production system models and are used in a large variety of domains or sectors like food security (Matthews et al., 2013), agricultural policy assessment (Bryan et al., 2011; Van Ittersum and Cassman, 2013; Gutzler et al., 2015), plant breeding (Banterng et al., 2004; Boote et al., 2011; Heinemann et al., 2015), climate change impacts assessment (Kapetanaki and Rosenzweig, 1997; Kassie et al., 2015; Tao et al., 2009; Sultan et al., 2013; Deryng et al., 2016; Rosenzweig et al., 2014) and adaptation design (Tao and Zhang, 2010).

The various crop models use different coding and parameterizations in their simulation of [CO_2] effects on key crop processes and yield under climate scenarios (White et al., 2011; Kersebaum and Nendel, 2014; Deryng et al., 2016). These approaches may provide useful insights on the direction and magnitude of the impacts of expected climate change effects and scenarios on important crops, such as maize.

Nevertheless, the uncertainty due to the way models simulate maize growth responses to increasing [CO_2] concentrations precludes more precise projections of maize production and related food security scenarios (Leakey et al., 2012; Deryng et al., 2016). Crop plants respond to [CO_2] *via* its impact on stomatal conductance. For wheat, Yin (2013) suggested that many crop models, for which parameters were identified with growth chamber experiments, tend to overestimate the beneficial effects of elevated [CO_2] on productivity. The knowledge and testing of [CO_2] effects to simulate the reduced transpiration rate using maize models is even more rudimentary.

A previous intercomparison study of multiple maize models, based on experimental data at four sites in France, Brazil, USA, and Tanzania, showed large variability in simulated yield responses to different levels of [CO_2] and under non-limiting water conditions (Bassu et al., 2014). In that study, models that explicitly considered effects of doubled [CO_2] between 360 and 720 ppm on carbon

assimilation and transpiration *via* stomatal conductance resulted in yield increase of 0–19%. The study also revealed that the simulated crop water use through evapotranspiration exhibited even higher variability among models. These modeling uncertainties can partly be explained by the different formalisms used in the models to represent the CO_2 fertilization effect, often based on empirical functions (Yin, 2013) or developed and/or calibrated using data from experiments that failed to represent open-field responses (Long et al., 2006; Ainsworth and Long 2005). Furthermore, the development of these models' parameters were made using a very limited number of data, thus reducing their reliability. For that reason, complex interactions between water, temperature, radiation and [CO_2] have not been investigated fully. We believe that gathering the experience of many years of improvement of models and their embedded formalisms and parameters may provide insight into these complex interactions and may advance our capacities for a more certain projection of climate change on maize yield. This approach may be implemented by cross-comparing model results with open-field Free Air CO_2 Enrichment (FACE) data, as FACE experiments provide more realistic production conditions (O'Leary et al., 2015; Boote et al., 1996; Tubiello and Ewert, 2002). In this way, possible sources of model discrepancies can be examined, hints on specific weaknesses extracted, and overall model ability to simulate response to varying [CO_2] conditions enhanced.

While the response of C_3 crops to CO_2 fertilization is comparatively better documented and analyzed in the scientific community, the response of C_4 crops to elevated [CO_2] is much smaller and is also less documented in chamber and FACE experiments. The effect is expected to be small due to the C_4 photosynthesis pathway in which CO_2 is pre-fixed by PEP-Carboxylase and substrate saturation of that carboxylase occurs at about 400 ppm *i.e.* the current ambient [CO_2]. Two papers on FACE-experiments on C_4 crops report very little yield sensitivity under good water supply, but show greater response, near 20% yield increase under dry conditions. This effect of CO_2 on C_4 crops is illustrated by the results of Manderscheid et al. (2014) and Manderscheid et al. (2015), who conducted a maize-FACE experiment in Braunschweig, Germany, in 2007 and 2008. The experiment evaluated two [CO_2] levels at two water regimes. Under dry conditions only, significant effects on maize yields were observed in 1 of 2 years with a very large [CO_2]-induced increase in yields of 40% and with the same total crop water use as the ambient [CO_2] levels. That experiment provided results of an unusually positive CO_2 fertilization effect of 550 ppm [CO_2] on maize yields under water limited conditions. The data of that experiment are therefore valuable for evaluating the variability of maize models to simulate such considerable impacts.

The objectives of this study were:

(i) to test the ability of multiple maize models to simulate the yield response to the different [CO_2] levels and water regimes of the two year FACE experiment (Manderscheid et al., 2014), notably the strong response to [CO_2] under water limitation,

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(ii) to test the degree to which the models could correctly simulate the measured low soil water contents, and the complex relationships between CO_2 and crop water relations,

(iii) to compare simulated responses of relevant variables among groups of models, using as grouping criteria, contrasting approaches to compute such variables, to gain insight into the possible reasons for model variability,

(iv) to highlight potential model improvements for enhancing their abilities to simulate the response of maize plant growth to the increasing $[CO_2]$.

This study is the second phase of the Maize pilot of the Agricultural Model Intercomparison and Improvement Project (AgMIP), which is a major international research effort that brings together climate, crop and economic modelling communities with cutting-edge information technology to conduct model intercomparisons and improvements, and to coordinate multi-assessments of future climate impacts and adaptation on the agri-food sector (Bassu et al., 2014; Rosenzweig et al., 2014).

2. Materials and methods

Here we: 1) briefly describe the conditions and design of the field experiment, 2) present the data supplied to the 21 individual modelling groups to perform this work, and 3) provide a short overview of the CO_2 response mechanisms used in the participating models.

2.1. Field experimentation background

The underlying data of the presented simulations originate from a FACE-experiment performed on a 10-ha research field site at the Thünen Institute, Braunschweig, Germany (N 52°18′, E 10°26′, 79 m a.s.l.) in two consecutive growing seasons 2007 and 2008. The FACE-experiment is described in detail by Manderscheid et al. (2014). Additional details on sap flow in plants and crop microclimate are given in Manderscheid et al. (2015). To test the interactions of $[CO_2]$ levels and water availability on *Zea mays* L. cv. 'Romario' growth, a modified 2×2 factorial experiment with three replications was set up in a fully randomized design. Sarlangue et al. (2007) measured approximately 1595 growing degree days for the cultivar 'Romario' from emergence to physiological maturity. The texture of the Luvisol soil is characterized by 6–7% clay, 24–32% silt and 61–70% sand (0–40 cm soil depth) with an increasing sand fraction with soil depth (40–60 cm). The maximum rooting depth (*i.e.* depth of root water uptake) is limited to 60 cm.

The FACE system used a modified set up with 6 circular rings (diameters: 20 m) installed following Weigel et al. (2005). The factors controlled included (a) two levels of $[CO_2]$ concentrations: AMBIENT (387 ppm) and (b) FACE (550 ppm) and two levels of water supply: IRR and DRY giving four treatments in total: IRR_AMBIENT, IRR_FACE, DRY_AMBIENT, DRY_FACE. IRR comprised non-limiting water conditions by rainfall and drip irrigation as required. DRY comprised operation of rain shelter from mid July to exclude most of heavy daily rainfalls (>10 mm). Atmospheric CO_2 enrichment started in early June of both years, when leaf area index (LAI) exceeded 0.5 $m^2 m^{-2}$. Pest control and fertilisation were performed based on best farmers practice. The applied total irrigation amounts and total fertilizer applications are presented in Table 1.

Daily air temperature, relative humidity, global radiation and precipitation were measured in a nearby weather station. Soil water content was measured 20 (2007) and 25 (2008) times per growth period using TDR probes down to 60 cm depth. Total aboveground dry matter, grain yield, LAI, and grain number were measured four and five times during the season in 2007 and 2008, respectively.

2.2. Simulation protocol

The 21 modellers involved in this work were provided with basic information on the experimental field conditions (physical and chemical soil properties and initial conditions, weather data, maximum rooting depth), management of the different treatments (tillage, fertilizer application, nitrogen fertilization, CO_2 enrichment; Table 1), and essential information on measurements (development stages and dates: sowing, anthesis and physiological maturity, harvest) and limited cultivar information from the seed company (approx. degree days from emergence to maturity). Modellers were asked to calibrate and run their models based on the provided information for the treatments IRR_AMBIENT for 2007 and 2008. Subsequently they applied their models to simulate all treatments of both years (see Table 1).

2.3. Evaluation of simulation results

The simulation results of the individual models and multi-model ensemble were compared to the respective measured values and evaluated by means of absolute and relative (response ratios) graphical representations using boxplots and time series analysis. Additionally, a number of statistical tools were used to evaluate the ability of the models to simulate the measured plant growth and soil water dynamics of the FACE experiment.

2.3.1. Nash-Sutcliffe-Efficiency

The Nash-Sutcliffe efficiency (NSE) is related to the RMSE and defined by Nash and Sutcliffe (1970) (Eq. (1)).

$$NSE = 1 - \frac{\sum_{i=1}^{n}(m_i - s_i)^2}{\sum_{i=1}^{n}(m_i - \bar{m})^2} \tag{1}$$

Where m_i and s_i are the measured and simulated values, and $\bar{m}$ is the measured mean. The NSE values are dimensionless and can take values from $-\infty$ to 1.0. A NSE value of 1.0 is given for a perfect match of simulation and measurement, if $NSE \geq 0$, the model is better than when the observed mean is used as a predictor, while negative values indicate that the observed means is a better estimate.

2.3.2. Root mean square error

Deviations from the measurements are estimated by the root mean square error (RMSE, Eq. (2)) in total values and units with respect to the observed variable:

$$RMSE = \sqrt{1/n \sum_{i=1}^{n}(m_i - s_i)^2} \tag{2}$$

2.4. Key characteristics of the participating models

The main characteristics of the participating maize and agroecosystem models can be found in Bassu et al. (2014) and in the individual model documentations. Eleven models consider the $[CO_2]$ effects on maize growth through the primary modification of daily biomass accumulation using either coefficients for the radiation use efficiency (RUE) or transpiration efficiency (TE) or both simultaneously. Ten more mechanistic maize models used algorithms based on biochemical photosynthesis processes (Table 2). Six models specifically used routines to compute the grain number, all based on the growth rate of the above ground biomass during a short period from anthesis to beginning grain growth. Finally, 15 models included an explicit impact of $[CO_2]$ on leaf (or canopy) stomatal resistance and hence transpiration rate, although 6 did not (Table 2).

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Table 1
Total irrigation and fertilization amounts for the individual treatments, as well as averaged [CO_2] concentrations. Dates of anthesis and observed total water use (estimated from soil water content measurements). Underlined and bold figures were provided to modellers. After Manderscheid et al. (2014). The last column shows the median of models'simulations. Figure in brackets are one standard deviation, n = 3 for measurements and n = 21 for simulations.

		Irrigation [mm]	Atm. CO_2 [ppm]	Nitrogen fertilization [kg N/ha]	Date of anthesis	Water use measured (mm)	Water use simulations (mm)
2007	AMBIENT/IRRIGATED	**34**	**387**	**173**	**18 July**	**320 (6)**	391 (69)
	AMBIENT/DRY	0	387	173	18 July	277 (5)	376 (72)
	FACE/IRRIGATED	34	550	173	18 July	327 (1)	364 (70)
	FACE/DRY	0	550	173	18 July	277 (7)	364 (74)
2008	AMBIENT/IRRIGATED	**119**	**387**	**198**	**25 July**	**300 (1)**	392 (63)
	AMBIENT/DRY	20	387	198	25 July	198 (5)	284 (68)
	FACE/IRRIGATED	94	550	198	25 July	273 (0)	360(49)
	FACE/DRY	20	550	198	25 July	201 (5)	284 (51)

Table 2
Traits of the 21 models in terms of biomass production, stomatal conductance and grain number simulation. More information on models can be found in Bassu et al. (2014) and in individual model's papers.

	RUE or leaf photosynthesis (Lp)	Stomatal conductance[a]	Grain number
Agro-IBIS	Lp	Yes	No
APSIM	RUE	No	Yes
CERES-Maize	RUE	Yes	Yes
Daisy	Lp	No	No
EXPERT-N-Ceres	RUE	No	Yes
EXPERT-N-Spass	Lp	Yes	No
EXPERT-N-Sucros	Lp	No	No
GLAM	RUE	Yes	No
HERMES	Lp	Yes	No
IXIM	Lp	Yes	Yes
LP	Lp	Yes	No
MAIZSIM	Lp	Yes	No
MCWLA	Lp	Yes	No
Monica	Lp	Yes	No
PEGASUS	RUE	Yes	No
RZWQM2	RUE	Yes	Yes
SALUS	RUE	Yes	No
SARRA-H	RUE	No	No
SIMPLACE⟨1⟩	RUE	No	No
SIMPLACE⟨2⟩	RUE	Yes	No
STICS	RUE	Yes	Yes

[a] Only models identifying an independent stomatal conductance variable responding to CO_2 were considered.

3. Results

3.1. General agreement with experimental data

The median simulated date of anthesis was similar for all treatments and 3 days earlier than the measured values (Table 1), within a range of 4 and 6 days for 50% of models in 2007 and 2008, respectively.

For the 21 models used here, the median RMSEs of yield, AGB at anthesis, AGB at harvest and soil plant available water in the 60 cm soil layer (SPAW) were 1.8, 1.5 and 2.1 Mg ha^{-1} and 81 mm, respectively. As expected, the RMSEs of the model ensemble, computed with the median of the 21 model's results, and for the same variables were much smaller except for crop water use (Table 3).

Models exhibited an especially high variability for water use and that was also reflected in the variability of ET/ET° and SPAW. For the latter, the Nash-Suttclife coefficient varied between 0.74 and −35, with a median value of −0.39 for the 21 models. The main discrepancies between simulations of observations came from a very variable estimate of the initial soil water content in the 60 rooting depth, on sowing date, *i.e.* 30 days before the first data measured in the experiment.
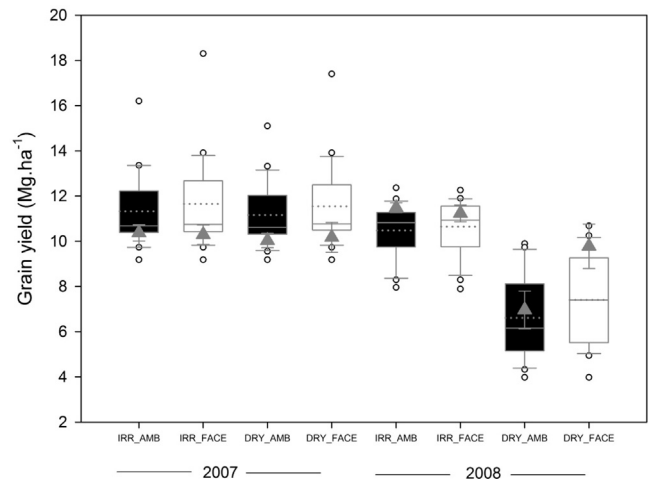

Fig. 1. Inter odel variability for yield in 2007 (4 boxes on the left) and 2008 (4 boxes on the right) under dry or wet conditions, at ambient or elevated [CO_2]. The box includes 50% of models, the error bars include 90% of models. The plain horizontal line in the boxes indicates the median and the dotted line indicates the mean. The triangles indicate the experimental means. Dots show outliers.

3.2. Interactions of water deficit and CO2 on crop yield and water use

The response of simulations to the various crop treatment conditions was analysed as followed. First we compared the models and the results at ambient CO2 and well-watered conditions. Secondly, we studied the impact of water deficit at AMBIENT CO2 and finally, we analysed the impact of [CO_2], first under well-watered conditions then during the drought of 2008.

3.2.1. At ambient [CO2] and optimal water conditions

The models were calibrated on the IRR AMBIENT treatments observations for 2007 and 2008. Not surprisingly, the median of model simulations were close to observations, showing a slight overestimation only of yields in 2007 and slight underestimate in 2008. 50% of models varied within a 1.8 and 1.4 Mg ha^{-1} interval around the median in 2007 and 2008, respectively (Fig. 1). The median of the 9 models having an explicit function for kernel number was also close to the observations (Fig. 2), *i.e.* approximately 4200 grains m^{-2}. 50% of models were within 600 grains m^{-2} in 2007 but that range nearly doubled in 2008 up to 1165 grains m^{-2}. The above ground biomass (AGB) was also rather well simulated in 2007 and 2008 although the median of models slightly underestimated the observed value (Fig. 3). The inter model range for 50% of models was similar both years and close to 1.6 Mg ha^{-1}, *i.e.* also similar to the range found for yields. Finally, the median of simulated ET/ET° ratio did not differ largely between two years at

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Table 3

Mean RMSEs for yield, above ground biomass at anthesis, above-ground biomass at harvest and crop water use simulations depending on (i) the way the biomass production is formalized (RUE: based on the simulation of radiation use efficiency of biomass production or based on a leaf photosynthesis response to light and [CO2]) and (ii) whether an explicit stomatal conductance function is used to simulate the response of crop transpiration to [CO2] or not and (iii) whether the grain number is computed or not. In each cell the left hand side figure is the median of individual model's RMSE and the right hand side figure is the RMSE for the model ensemble of each category. The superscript [HS] indicates a highly significant difference between the category of models.

|	Number of models in category	Yield RMSE ($Mg\,ha^{-1}$)	Above Ground Biomass at anthesis RMSE ($Mg\,ha^{-1}$)	Above Ground Biomass at harvest RMSE ($Mg\,ha^{-1}$)	Total water use RMSE (mm)
RUE	11	1.8/1.6	1.5/0.6	2.1/1.6	95/83
Leaf photosynthesis	10	1.8/1.2	1.2/0.9	1.8/1.0	57/66
Response of Stomatal conductance to [CO2]	15	1.4/0.7	1.3/0.4	2.0/1.2	78/72
No response of stomatal conductance to [CO2]	6	2.4^{HS}/2.3	1.9/1.0	2.3/1.6	121/123
With Grain simulation	6	1.5/0.8	1.2/0.4	1.5/1.6	86/87
No grain simulation	15	1.8/1.1	1.5/0.9	2.1/1.9	81/83
All models	21	1.8/1.0	1.5/0.6	2.1/1.2	81/82
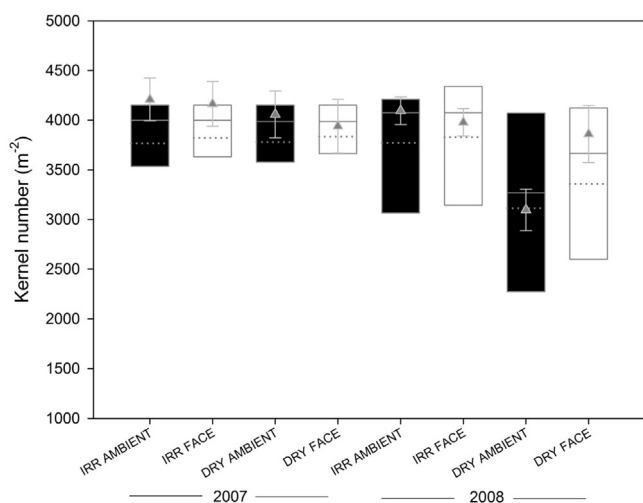
Fig. 2. Inter model variability for kernel number in 2007 (4 boxes on the left) and 2008 (4 boxes on the right) under dry or wet conditions, at ambient or elevated [CO2]. The box includes 50% of models, the error bars include 90% of models. The plain horizontal line in the boxes indicates the median and the dotted line indicates the means. The triangles indicate the experimental means. Dots show outliers.
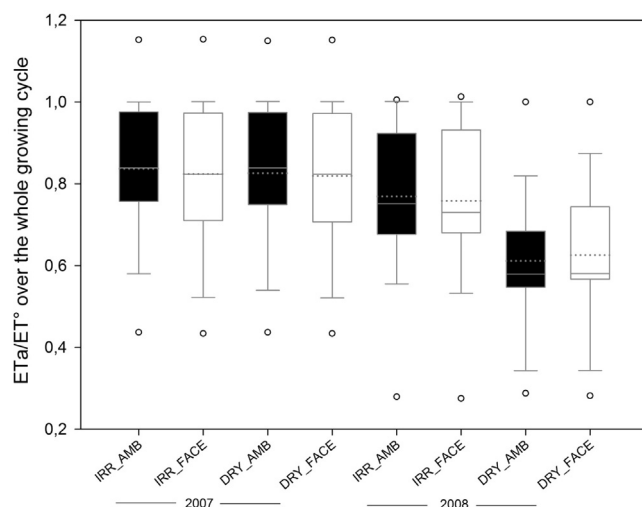

Fig. 4. Inter model variability for ratio of ET/ET° over the whole growing season in 2007 (4 boxes on the left) and 2008 (4 boxes on the right) under dry or wet conditions, at ambient or elevated [CO2]. The box includes 50% of models, the error bars include 90% of models. The plain horizontal line in the boxes indicates the median and the dotted line indicates the mean. Dots show outliers.
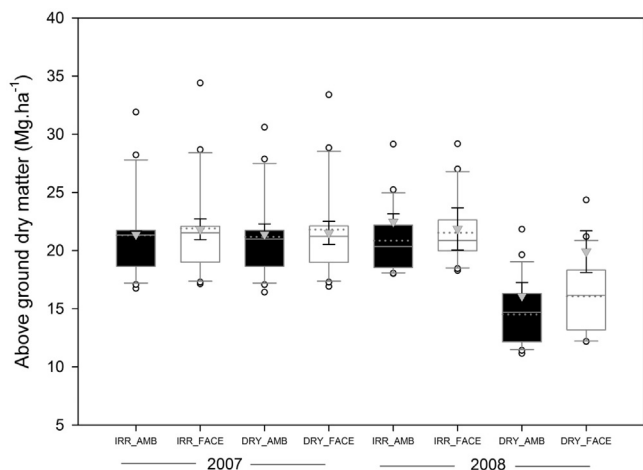

Fig. 3. Inter model variability for above ground biomass (AGB) in 2007 (4 boxes on the left) and 2008 (4 boxes on the right) under dry or wet conditions, at ambient or elevated [CO2]. The box includes 50% of models, the error bars include 90% of models. The plain horizontal line in the boxes indicates the median and the dotted line indicates the means. The triangles indicate the experimental means. Dots show outliers.

approximately 0.8 on average, with 50% of models ranging within an interval close to 0.2 around that median values (Fig. 4).

3.2.2. Impact of drought at AMBIENT [CO2]

In 2007 the water deficit treatment had no impact on simulated yields so that the AMBIENT DRY treatment could be considered as a replicate of the AMBIENT IRR treatment. This was fully consistent with the observations (Fig. 1). The same could be concluded for simulated kernel numbers (Fig. 2), AGB (Fig. 3) and ET/ET° (Fig. 4). The inter-model variability for the 2007 AMBIENT DRY treatments was also similar to IRR treatments for the same variables. In the following, the drought response will then only be considered for the year 2008, and the 2007 AMBIENT DRY will be considered a mere replicate of the AMBIENT IRR treatment.

In 2008 however, a significant impact of water limitation was simulated. Indeed drought reduced the median of 21 simulated values of ET/ET° from 0.75 to 0.58 (Fig. 4). Interestingly, the variability of that variable also diminished under DRY conditions in 2008. In that year, the simulated SPAW was close or higher than 53 mm (Fig. S1), half of the field capacity, in the AMBIENT IRR treatment whereas it remained lower than 40 mm for most of the growing season in the AMBIENT DRY plots, even declining down to 12 mm approximately at the date of anthesis. The 21 models' median simulated LAI (Fig. S2) in the second experimental year followed the
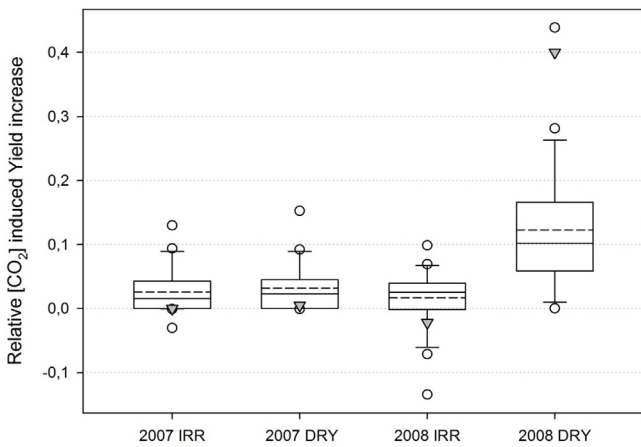
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Fig. 5. Simulated relative increase of maize yield at 550 ppm *versus* the ambient air [CO_2] in 2007 and 2008 for irrigated and dry plots: ((FACE – AMBIENT)/AMBIENT). Triangles are from average measured yields.
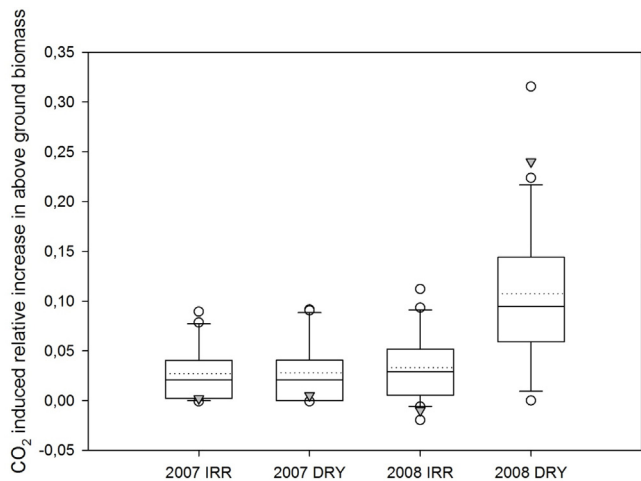

Fig. 6. Simulated relative increase of maize Above Ground Biomass at 550 ppm *versus* the ambient air [CO_2] in 2007 and 2008 for irrigated and dry plots: ((FACE-AMBIENT)/AMBIENT).

general trend of the data except at the end of the growth cycle where simulated results of the DRY treatment declined much less rapidly than in the experiment. In 2008 the simulated impact of drought on AGB at ambient [CO_2] in the DRY treatment was very clear (Fig. 3), the median of 21 models decreasing from 20.3 down to 14.5 Mg ha^{-1}. Simulations also exhibited an impact of water deficit on the grain number (Fig. 2), the median of the 6 relevant models decreasing to 3250 grains m^{-2} instead of 4100 in the IRR treatment. The inter-model variability also increased, models varying within a range of 1800 grains m^{-2}. These features were consistent with a simulated drought–induced decline in yield to approximately 6.1 Mg ha^{-1} instead of 10.8 Mg ha^{-1} in the control (Fig1). As for the IRR treatment, these simulated data generally were slightly lower than the measured yields. The variability between models increased in comparison to the range found in the three other IRR treatments (including the DRY AMBIENT in 2007). 50% of models simulated values within 2.86 Mg ha^{-1} instead of 1.6 Mg ha^{-1} in the IRR treatments on average.

3.2.3. Impact of CO2 in irrigated conditions

As in the experiment in the treatments receiving sufficient water (including the DRY treatments of 2007), there was no impact of [CO_2] level on yields (Fig. 5) or AGB (Fig. 6). There was no impact of [CO_2] on ET/ET$^\circ$ (Fig. 4) in the same situations and no signifi-

Table 4
Median values for 21 models of the impact of CO_2 on soil water content, biomass growth rate and ET/ET$^\circ$ in the DRY treatment in 2008.

	Median fraction of total plant available water in the 0–60 cm soil horizon during the growth cycle	Median rate of above ground dry matter increase around anthesis (20–30 July, Kg.ha^{-1}.day^{-1})	Median ratio ET/ET$^\circ$ at anthesis (25 July)
AMBIENT	0.39	156	0.63
FACE	0.40	176	0.88

cant impact on the simulated water consumptions exhibited either (Table 1). However, the 21 models' medians of SPAW tended to be higher for the FACE treatment (Fig. S1 for 2008, 2007 not shown).

3.2.4. Impact of [CO2] in water restricted conditions

When water deficit had an impact (DRY treatments in 2008), models were able to simulate a compensating impact of [CO_2] but with less intensity than the one measured (Fig. 5).

At 550 ppm, the median simulated yield was 7.4 instead of 6.2 Mg ha^{-1} at ambient concentration, *i.e.* a 19% increase for the median of the model ensemble. However, because of the variability of the relative [CO_2] increase between models, the median increase of the 21 models was 10% only. This [CO_2] positive impact on yield under water deficit was less than half the measured increase, between 7 and 9.8 Mg ha^{-1} *i.e.*, 40% with 550 ppm compared to the ambient [CO_2] (Fig. 5).

The median simulated increase in grain number under high [CO_2] was negligible under well-watered conditions (Fig. 2), including the non-irrigated plots in 2007, and 13.0% for the dry treatment in 2008, again, less than the experimental result, where the grain number was increased by 25% with 550 ppm [CO_2]. The median decrease of SPAW in response to raising [CO_2] in the water limited treatment of 2008 was also less than the one measured (Fig. S1), with no impact on total water use (Table 1) or ET/ET$^\circ$ (Fig. 4) of the crop. However, the median simulated ET/ET$^\circ$ during the period of flowering, *i.e.* +/−5 days around anthesis, among all models rose from 0.63 up to 0.88 at 550 ppm [CO_2] (Table 4), indicating a more severe water deficit at ambient [CO_2] than at elevated [CO_2] during that particular phase, in line with the maximum soil water deficit as expressed by SPAW.

For the 6 models that simulated grain number, simulated growth rates of AGB between 5 days before and 5 days after flowering was computed. On average, models generally showed no [CO_2] effect on that variable. Even at low water availability in 2008, the difference between the two [CO_2] regimes *i.e.* at ambient and elevated [CO_2], respectively was not significant (156 and 176 kg ha^{-1} day^{-1}, respectively, Table 4).

Finally, the median of the ensemble model's simulation of AGB increased by 11% in the 2008 DRY FACE treatment, which was considerably less than the 24% observed in the experiment (Fig. 6).

4. Discussion

As previously reported in other work, the simulated maize yield was not increased by elevated CO_2 under well-watered conditions (Ghannoum et al., 2000; Leakey et al., 2006, Twine et al., 2013). For the 2008 season which exhibited significant water deficit; however, simulations were able to simulate a significant increase in yield with CO_2 enrichment, although less than observed in the same season. The measured impact of CO_2 was more than three times as large as the simulated one, considering the median of the 21 models. This is one of the highest experimental impacts of [CO_2] increase on maize recorded in the literature (Kimball et al., 2002; Leakey et al., 2006; Meng et al., 2014). Because no impact was found for

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the simulations of the 2008 experiment and in the 2007 wet treatments, and because the measured CO_2 impacts were not significant either, we concentrated the analysis of modeling of CO_2 impact on the dry treatment of 2008 only. It is under such conditions where model uncertainty (both precision and accuracy) may seriously challenge our capacity to understand climate change impacts and assess the effectiveness of long term adaptation options to climate change.

As analysed by Manderscheid et al. (2014), and further documented in their later paper (Manderscheid et al., 2015), the reasons for the dramatic increase of yield under 550 ppm [CO_2] as compared to the ambient concentration resulted from a reduction of transpiration rates at early stages of the crop cycle, enabling plants to conserve soil water when water was still non limiting. During the time period −5 and +5 days of anthesis, the actual difference in SPAW between the two [CO_2] levels in the dry and well-watered situation was approximately 18 mm. That was approximately five times more than the difference simulated by the models in general. Such higher SPAW under 550 ppm [CO_2] which brought about a much less stressful situation condition during kernel set and grain formation for the high [CO_2] treatment were, in general, not captured correctly by the models. This cumulative water-saving effect appears to occur primarily because the simulated CO_2 effect to reduce transpiration appears to be too weak in most of these maize models. Another causal factor is that the models on the whole also predicted ET to be too high compared to measured (Table 1 and Fig. S1), which would make this [CO_2] effect even more critical. Later, in August, the larger leaf area of the crop in the elevated [CO_2] treatment compensated the CO_2-induced decline in transpiration rate so that the water use from the beginning of June until harvest was similar in both treatments. Models were able to partially represent that complex kinetics, although missed the precise magnitude. This suggests that the response functions parameterized in some of the models may simulate interactions at the process level correctly. In the field, the decrease of the intensity of the transpiration rate induced by an increase in [CO_2] was almost exactly compensated by (i) the availability of more soil water at the time where ETo was highest and (ii) an increase in green leaf area. FACE treatments generally bring about a hotter and drier local microclimate (Twine et al., 2013; Manderscheid et al., 2015; Webber et al., 2016), resulting in very similar quantities of water use in both CO_2 treatments until the end of the growth cycle. Under ambient [CO_2] at the end of July, the observed fraction of SPAW reached levels lower than the 0.5 ratio of water holding capacity, which is often interpreted as a threshold for crop productivity (Allen et al., 2006). The saved water that was observed in the root zone provided a much higher SPAW and enabled the crop grown at 550 ppm [CO_2] to maintain a better water status, longer green leaf area duration and hence to harvest more energy and therefore produce more biomass. Again, all this could be followed in the kinetics of simulated variables, showing that the ensemble of models actually reproduced some of the impacts. What the models did not take into account was (i) the consequence of the altered water regime of plants on the microclimate (Twine et al., 2013; Manderscheid et al., 2015; Webber et al., 2016) and (ii) the absorption of light by the rainout shelters. But even if considered, these factors could not account for the full difference observed, all together. More important, was the impact of [CO2] level on the timing of the maximum water stress 3 days after the anthesis date, coincided with a very sensitive phase of kernel set in maize to plant water status (Turc et al., 2016).

The simulated timing of the maximum stress for the crop was fairly precise, with only 3 days difference. Therefore the drought relief effect of prior water conservation (partial stomatal closure induced by the elevated [CO_2]) would have impacted yield if the water conservation had been enough. Indeed, ensemble models simulated the ambient situation fairly well (Fig. S1) but largely

underestimated the impact of CO_2. Model algorithms to reflect the effect on stomata resistance are mainly based on findings for C3 crops (e.g. Nendel et al., 2009; but see Markelz et al., 2011). However, Akita and Moss (1973) showed that the response curve of the stomatal resistance to increasing CO_2 was much steeper for C4 than for C3 crops. This could be an indication that the main reason for a lesser impact of [CO_2] in the simulation was an insufficient reduction in plant transpiration in the early part of the season leading up to anthesis.

These data alone, based on one season of water use estimated by soil water balance, are not sufficient to verify the magnitude of reduction of transpiration under elevated [CO_2]. Additional testing of transpiration and evapotranspiration of maize models under elevated [CO_2] is needed, and present evidence indicates that the maize models are not sufficiently reducing transpiration with elevated [CO_2]. In the prior sensitivity evaluation of maize models to CO2 by Bassu et al. (2014), the median simulated reduction in transpiration was 8% for a doubling of [CO_2] from 360 to 720 ppm. By comparison, an 18% reduction in transpiration was reported for maize grown at 720 versus 360 ppm [CO_2] in two studies on maize conducted in sunlit, controlled-environment chambers (Allen et al., 2011; Kim et al., 2006; Chun et al., 2011,). We propose that if the maize models were updated to reflect this greater observed reduction in transpiration, that the model simulations of water conservation during the pre-anthesis phase would have been substantial, both improving the simulated soil water balance and giving a larger benefit of elevated [CO_2] for the water-stressed treatment in 2008.

Some consistency to that statement is given by the comparison of two groups of models: those which have an explicit impact of [CO_2] on the stomatal conductance and those which do not (Table 3.) For those models with explicit stomatal conductance, the seasonal water use was less and the mean RMSE for yield was significantly less, sustaining the hypothesis that a more mechanistical approach for the response of crop transpiration to [CO_2] is better. The RMSE for yield of the ensemble model made of the models with explicit stomatal conductance response was 0.7, i.e. even less than for the other ensemble, which did not differ from the median value of the models' RMSE of 2.3 for yield.

Although the main source of uncertainty in this study comes from the variability in water use, the grain number issue must be considered as well as shown by the experiment itself. It may be expected that once the water economy of the crop is improved, the setting of kernel number (sink strength) could be the next to be improved, because occurrence of water deficits at the critical timing of kernel number determination should have caused more [CO_2] effect on kernel number, but did not do so because the water conservation effect (transpiration reduction) was insufficient. Indeed, models with explicit grain number did not perform significantly better than those without simulating grain number (Table 3). Lack of significance might be due to the insufficient number of models in the first category (6), given the minimum number of maize crop models in an ensemble able to securely match the actual yields was found to be close to 10 in a previous study (Bassu et al., 2014). But above all, improved models also improve the ensemble of models (Maiorano et al., 2016). Also, the routines used to take this effect into account might not be relevant. In all 6 models able to compute a grain number, the process is based on the AGB growth rate around anthesis. But that variable averaged −/+5 days around anthesis for the DRY treatment in 2008 did not differ between both [CO_2] treatments (Table 4). Indeed recent findings by Turc et al. (2016) suggest that direct hydraulic influence on silk elongation set (i.e., affecting anthesis-silking-interval) might cause the decrease in grain number. The follow-on or feed-forward effect was that reduced kernel number on the ambient [CO_2] treatment actually caused sink limitation later during grain-filling when rains were received. Evidence

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for this sink limitation is provided by Manderscheid et al. (unpublished data) who observed less carbohydrate remobilization from the ambient treatment than observed for the elevated CO_2 treatment for the 2008 dry case. This interaction of water stress timing with kernel number set is what makes the CO2 impact larger for this experiment.

5. Conclusions

In this study, CO_2 affected maize yield primarily through crop water balance.

The coincidence of prior water conservation under elevated CO_2 and because most severe water stress occurred at anthesis can explain the particularly high impact of CO_2 in the data set and therefore, models missing this critical point in crop phenology cannot adequately simulate the high impact of CO_2 for this situation, regardless of the CO_2 impact algorithm implemented in the model. This poses a great challenge to regional applications of maize models in climate change impact assessments, since the accurate reproduction of sowing dates (which determines the subsequent simulation of phenology) at the regional scale is already very difficult. Probabilistic approaches to cover a satisfying representation of phenology could overcome this problem and prepare the way for making full use of improved CO_2 impact algorithms.

Crop transpiration/water balance and kernel number set (sink strength) are the modules that require special attention. More robust functions and good input data are required for making these model adjustments

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.eja.2017.01.002.

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