Physical robustness of canopy temperature models for crop heat stress simulation across environments and production conditions

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ABSTRACT

Despite widespread application in studying climate change impacts, most crop models ignore complex interactions among air temperature, crop and soil water status, CO₂ concentration and atmospheric conditions that influence crop canopy temperature. The current study extended previous studies by evaluating T_c simulations from nine crop models at six locations across environmental and production conditions. Each crop model implemented one of an empirical (EMP), an energy balance assuming neutral stability (EBN) or an energy balance correcting for atmospheric stability conditions (EBSC) approach to simulate T_c . Model performance in predicting T_c was evaluated for two experiments in continental North America with various water, nitrogen and CO₂ treatments. An empirical model fit to one dataset had the best performance, followed by the EBSC models. Stability conditions explained much of the differences between modeling approaches. More accurate simulation of heat stress will likely require use of energy balance approaches that consider atmospheric stability conditions.

Introduction

As temperatures warm with climate change, reductions in crop yields due to heat stress (Porter and Gawith, 1999; Wheeler et al., 2000) are expected to increase (Porter et al., 2014). Statistical models of crop yield response to weather have detected large yield declines across many regions as the number of days with extremely high temperature have increased (Lobell et al., 2011; Hawkins et al., 2013; Lobell et al., 2013; Hatfield, 2016). Heat stress depends on unique combinations of the timing and duration of high temperature events, crop phenological stage and varietal characteristics (Rezaei et al., 2015; Prasad et al., 2017), suggesting that process-based crop models may provide valuable insights into how high temperatures impact crop performance under climate change (White et al., 2011). It is only recently that process-based crop models have included heat stress effects on grain number, grain yield or crop senescence (Challinor et al., 2005; Asseng et al., 2011; Moriondo et al., 2011; Maiorano et al., 2017), with limited evaluation of their performance under heat stress conditions (Stratonovitch and Semenov, 2015; Gabaldón-Leal et al., 2016). Further, unlike their statistical counterparts, most process-based crop models do not account directly for the interaction of crop water status and high temperature events (Lobell and Asseng, 2017), although such interactions affect the magnitude of heat stress (Gourdji et al., 2013; Anderson et al., 2015; Troy et al., 2015). Recent efforts have estimated and evaluated canopy temperature (T_c) simulations in process-based crop models (Webber et al., 2016b; Webber et al., 2017), though with their evaluation limited to irrigated production in arid conditions. Canopy temperature has long been considered in irrigation scheduling (Jackson et al., 1977) and is used as a selection trait for drought and heat tolerance (Blum et al., 1982; Hatfield et al., 1987; Blum et al., 1989; Reynolds and Langridge, 2016). Typically, crops with cooler canopies maintain higher yields under water deficits or with heat stress under irrigated conditions (Blum et al., 1982; Blum et al., 1989; Olivares-Villegas et al., 2007; Lopes and Reynolds, 2010; Pinto and Reynolds, 2015), while Pinter et al. (1990) offer a slightly different interpretation.

The canopy temperature of crops generally follows ambient air temperature (T_{air}) but can drop below or rise above T_{air} due to the balance of radiative heating and transpirational cooling. The difference between T_c and T_{air} , termed canopy temperature depression ($\Delta T = T_c - T_{air}$) is larger and more negative with ample soil water supply and high vapor pressure deficit (VPD) (Idso et al., 1981; Jackson et al., 1981). Any factor which reduces the rate of transpiration, such as soil water deficit (Idso et al., 1981), low reference crop evapotranspiration (ET_o), typically driven by low VPD, or elevated atmospheric CO_2 concentrations (Kimball et al., 1999; Wall et al., 2000; Leakey et al., 2006; Wall et al., 2006; Gray et al., 2016) will reduce canopy cooling. When transpiration is restricted, T_c frequently exceeds T_{air} (Siebert et al., 2014).

Despite the importance of T_c for irrigation management and crop breeding, the complexity of calculations of T_c has likely discouraged wider application of T_c in crop models. Canopy temperature results from the energy balance at the crop surface, in which energy fluxes include net radiation, sensible and latent heat transfer as well as energy transfer with soils (Jackson et al., 1981). Beyond the complexity of stomatal regulation of gas exchange and its role in determining latent energy flux together with atmospheric evaporative demand (Jarvis and McNaughton, 1986), the stability of the air influences aerodynamic resistance, r_a , of the transfer of heat and vapor between the crop surface and the atmosphere (Monteith and Unsworth, 2007). For example, under stable atmospheric conditions, air near the canopy is heavier than the overlaying air such that buoyancy is inhibited and the aerodynamic resistance to heat and vapor transfer are relatively greater, whereas in unstable conditions, buoyancy of the air near the crop canopy reduces r_a (Monteith and Unsworth, 2007). The Monin-Obukhov Similarity Theory (MOST) is a common approach to determine r_a in which stability correction factors (Thom, 1975) are applied to logarithmic momentum, temperature and vapor fluxes (Monin and Obukhov, 1954), and constitutes the main approach to energy balance correcting for atmospheric stability conditions (EBSC). However, stability corrections depend on T_c among other factors (Webb, 1970), implying that a solution of T_c using an EBSC approach requires an iterative solution (Liu et al., 2007). Two main alternatives avoid the complexity of correcting for boundary layer stability. The first assumes neutral stability conditions and solves a

relatively straightforward energy balance (EBN) (Clawson et al., 1989), though the method implicitly assumes that T_c is close to T_{air} . The second option avoids an energy balance by using an empirical relationship (EMP) to relate T_c to main drivers, such as T_{air} , VPD and soil water status. The EMP methods have produced estimates of T_c similar to those of the EBSC methods for r_a (Liu et al., 2007) and T_c (Webber et al., 2017), but both studies noted that their results needed to be validated across a wider range of climates and growing conditions.

The main objective of this study was to assess the skill of different crop models in simulating T_c for a wide range of environmental conditions (locations, years, atmospheric CO₂ concentrations) and agronomic conditions (irrigated and rainfed, high and low nitrogen fertilization levels), extending a previous study which considered only potential production conditions under ambient CO₂ at one location. A second objective was to understand possible strengths of the different approaches for modeling T_c . The study is undertaken as part of the overall efforts of the Agricultural Model Intercomparison and Improvement Project (AgMIP; Rosenzweig et al., 2013) Wheat group (<http://www.agmip.org/wheat/>) to understand the impacts of high temperature on wheat yields.

Materials and Methods

Site and field experiment descriptions

Data from two series of experiments, here referred to as “FACE-Maricopa” and “China Wheat” were used to evaluate T_c simulations (Fig. 1). In the FACE-Maricopa dataset, a spring wheat (*Triticum aestivum* L.) cultivar was grown over four seasons with buried drip irrigation, ample optimal nitrogen and water regimes, and both ambient and elevated atmospheric CO₂ concentrations (Kimball et al., 1999; Kimball et al., 2017). In 1993 and 1994, an additional treatment was a limiting water supply (50% of the ample water treatment), and in 1996 and 1997, a limited nitrogen treatment was included. In total, 16 experimental treatments were available from the FACE-Maricopa experiments. The China Wheat dataset considered in

this study is a subset of the larger China Wheat dataset described in Reginato et al. (1988), which investigated winter wheat growth and development across a transect of five sites in North America (Fig. 1) over two growing seasons (harvest years 1985 and 1986). Our analyses focus on data for one cultivar, two water availability levels (rainfed and full irrigation) and one soil nitrogen level (near optimal for plant growth). In total, 18 experimental treatments were obtained from the China Wheat study.

Figure 1. Location of the FACE-Maricopa experiment and the five sites of the China Wheat experiment considered in this study

FACE-Maricopa experiment

The FACE-Maricopa experiment (Kimball et al., 1995; Hunsaker et al., 1996; Hunsaker et al., 2000) was conducted at Maricopa, AZ, U.S.A. (33.1° N, 112.0° W; 361 m a.s.l.) between 1993 and 1997. The soil is classified as a reclaimed, Trix clay loam, described in Kimball et al. (1999) as a fine-loamy, mixed (calcareous), hyperthermic Typic torrifluvents. The spring wheat cultivar Yecora Rojo was grown with a mid-December sowing date in each year in east-west rows, 0.25 m apart with an average plant density of 150 plants m⁻². Pest and weed controls were conducted to minimize damage. Plants were sampled weekly for crop height, phenology (Haun (1973) index and Zadoks (1974) stages of development), green leaf area index (LAI), green stem area index, and biomass of crown, stem, leaf, and grain components were

assessed at 7 to 10 day intervals. Final grain yield measurements were from 20 m² samples collected with machine harvesting from each plot in late May (Kimball et al., 2017).

To inject CO₂ into the plots, 25-m diameter rings of 0.305 m pipe were placed in the field shortly after planting. Vertical pipes of 2.5 m height were spaced around the rings at 2.4 m spacing, and blowers delivered CO₂-enriched air through the pipes to the plots out of tri-directional holes at approximately canopy height. Wind and CO₂ sensors near the center of the plots were used as inputs to control the flow rate of CO₂ such that near-target CO₂ levels were maintained throughout the growing season (Hendrey, 1993). The target CO₂ levels for the 1993 and 1994 harvest years were 550 ppm, whereas for the 1996 and 1997 harvest years, the CO₂ levels were maintained at approximately 200 ppm above ambient, which was approximately 360 ppm (Kimball et al., 1995). All FACE plots had blowers, whereas in 1993 and 1994, there were no blowers in the ambient-CO₂ plots. In 1996 and 1997, both FACE and ambient plots had blowers. Pinter et al. (2000) reported that at night the blowers increased T_{air} and T_c temperatures about 1.0°C compared to plots with no blowers, whereas during daytime, there was no effect of the blowers on T_c and a slight (-0.2°C) cooling of T_a . The increased temperatures associated with the blowers also apparently accelerated plant development such that anthesis was 4 days earlier, and senescence was similarly advanced compared to plots with no blowers.

Irrigation water was applied using a sub-surface drip system installed at 0.23 m depth (Hunsaker et al., 1996). The full-irrigation treatments received irrigation water to return the root zone soil water content to field capacity whenever the available soil water reached 30% depletion. For the experiment in 1993 harvest year, the semi-irrigated treatment received 50% of the water applied to the full irrigation treatment, whereas in the 1994 harvest year experiment, the semi-irrigated treatments received the same amount of water as the full irrigation treatment on every second application date. In the 1996 and 1997 harvest year experiments, all treatments received full irrigation (Hunsaker et al., 1996; Hunsaker et al., 2000).

Adequate nitrogen was applied to all plots in the 1993 and 1994 harvest year experiments at a rate of 271 and 261 kg N ha⁻¹, respectively (Hunsaker et al., 1996). In the 1996 and 1997 harvest year experiments, nitrogen was applied at a rate of 350 kg N ha⁻¹ to the high N plots and at a rate of 70 kg N ha⁻¹ (1996) and 15 kg N ha⁻¹ (1997) in the low N treatments, respectively. There was an addition of 30 and 33 kg N ha⁻¹ applied to the high and low N plots due to the N in the irrigation water (Kimball et al., 1999).

Hand-held infrared thermometers (IRTs; Model 110, 15° field-of-view, Everest Interscience, Tucson, Arizona, USA) were used to measure midday T_c . Almost all of the T_c data used for this model inter-comparison study were collected between 13:00 and 14:00 (mean solar time) from all plots generally two to five times per week from before emergence until harvest. Occasionally measurements were made at other time, though in this study only observations after 11:30 and before 15:00 were considered. The measurements were obtained from a walkway along the west side of the non-destructively sampled final harvest area in each plot. The IRTs were pointed toward the north at an angle of 20° below horizontal. At each plot, six measurements were obtained along the walkway. Plot averages were used in this study. Before and after each measurement run, the IRTs were pointed at a black-body source in the shade, and calibration measurements were obtained. Also, before and after each run, air dry and wet bulb temperatures were obtained with a psychrometer, and weather and data quality conditions were noted. Observations of T_c used in this study were based on selecting measurements when the IRT was sensing only crop canopy and not soil surface yet senescence had not started, based on results reported in Fig. 6 of Pinter et al. (2000) and Table 1 of Kimball et al. (1999).

Solar radiation, air dry and wet bulb temperatures, rainfall, and windspeed were measured at weather station located near the center of the field. No adjustments were made for night-time blower effects. Time series of the daily maximum air temperatures and canopy temperatures during the four growing seasons are shown in Fig. 2.

China Wheat experiment

The China Wheat experiment (named because originally there was a US collaboration with Chinese scientists in this experiment) was conducted along a transect at Lubbock, TX (33.63° N, 101.83° W, elev. 1830 m a.s.l.) on soils classified as a Olton Clay Loam, Manhattan, KS (39.09° N, -96.37° W, elev. 321 m a.s.l.) on a Muir silt loam, Tryon, NE (41.6° N, 100.8° W, 975 m a.s.l.) on a Valentine fine sand, Mandan, ND (46.8° N, 100.9° W, 549 m a.s.l.), a Williams loam and Lethbridge, AB (49.7° N, 112.8° W, 920 m a.s.l.) on Lethbridge silty clay loam. Details of the individual experiments were provided by Reginato et al. (1988) and accompanying papers. Time series of the daily maximum temperature at each site for the growing season in the two experimental harvest years are shown in Figs. 3 and 4. The winter wheat cultivar Colt was planted at each site with a row spacing of 0.15 to 0.30 m in north-south rows. Each plot measured at least 2 m long with variable width. Weeds and pests were controlled to minimize damage. Nitrogen fertilizer was applied as NO_3 at a rate to obtain a near optimal supply of nitrogen availability of 160 kg N ha^{-1} including soil available nitrogen determined from soil sampling prior to planting to a depth of 1.2 m. Other fertilizers were applied to avoid any nutrient deficiencies. At each site, rainfed and well-watered treatments were provided. The rainfed treatment relied on rainfall and necessary small irrigations at the time of planting or to prevent crop failure. The well-watered treatment received irrigations to maintain a high water content in the soil profile during the growing season. Irrigations were scheduled to allow for up to a 50% depletion of plant readily available water from the rooted profile, as determined with neutron probe soil moisture measurements.

Plant-development stages were recorded weekly using both the Haun and the Zadok scales. Crop height was measured on 10 plants per plot usually at a 7 to 14 day frequency. On the same dates, crop biomass was determined from samples of 12 plants per plot selected equally from four sections of the plot. Leaf green area and the area of dead leaves were determined on a subsample of these 12 plants. At maturity, grain yield and final total above ground biomass was determined in an area of at least 3 m^2 . The T_c

observations were the average of east and west oblique facing measurements (six in each direction) made with handheld infrared thermometers (Everest Interscience or Telatemp, depending on availability at each site) with a bandpass of 8-14 μm and a 4° field of view. Measurements used in this study were taken between 12:00 and 15:00. The frequency with which T_c values were available varied between sites and is indicated in Figs. 3 and 4. Values were restricted to T_c observations where the crop canopy was sufficiently developed, leaf area index (LAI) > 0.6 , to avoid bias from including soil surface in the instrument field of view. However, as not all sites had LAI time series, T_c values were additionally removed if rainfed T_c was much cooler than irrigated T_c or if irrigated plots were much hotter than air near the start of spring and no models came close to capturing the response.

Simulation experiment

Simulations were conducted for the 34 experimental treatments from the two experiments. The study considered nine crop models that differed in terms of their structure and parameterization of both crop growth and development, water, nitrogen and CO_2 responses, and their approach to simulate T_c (Table 1). Three models used an empirical (EMP) approach to simulate T_c (DN, FA and HU). Four models used an energy balance assuming neutral stability atmospheric conditions (HE, S2, SQ, and SS), while the remaining two models (L5 and SP) used an energy balance approach that corrected for atmospheric stability. All models used T_c to drive the heat stress responses (Webber et al., 2017), in some cases including feedback on T_c through impacts on crop LAI and height. Heat stress responses varied among the models based on the processes they consider, though all considered at least one of the following mechanisms: reduction in grain number, final grain size, or harvest index, accelerated senescence leading to shorter grain filling period. Further, the sensitive periods, high temperature thresholds and parameterization of heat stress responses differed among models (Table 1).

Simulations were conducted in two steps. In the first step, all available soil moisture and crop response data (LAI, biomass, and grain yield) and a limited amount of T_c data (T_c observations for two treatments

per experiment) were provided to the modelers to calibrate their models. To reduce effects of poor simulations of phenology, anthesis and physiological maturity dates were calibrated to within 5 days for each treatment, so phenology parameters for a given model may have differed among treatments. In the second step, modelers were given all available T_c observations to calibrate their T_c models. Only HU, SP, and L5 used T_c data for calibration, as the other models had no parameters to calibrate their T_c simulations (Table 1). The results presented in the main text are all based on the results of the calibrated models with additional results from the uncalibrated step in the SI materials. The HU model was treated as a reference for this study, and its results were considered separately from the other EMP models because the parametrization of the routine for maximum T_c (Neukam *et al.* 2016) was based on a subset of the available data of this study (Table 1) and all data are for continental North America. The underlying multiple linear regression model uses different parameter sets for pre- and post-heading phase to derive maximum T_c as a function of daily incoming global radiation, leaf area index, daily maximum air temperature ($T_{\max}$) and the ratio of actual and potential transpiration times the daily mean VPD. The T_c algorithms used in DN and FA were developed with independent datasets.

Table 1. Descriptions of model components related to canopy temperature (T_c) simulation and the sensitivity of T_c simulations to water and nitrogen, as well as atmospheric CO₂ concentration. The main approach to simulating T_c is indicated as an empirical (EMP), an energy balance assuming neutral stability (EBN) or an energy balance correcting for atmospheric stability conditions (EBSC). NA indicates non-applicable

Model (2-letter code; references)	T_c approach	Possible feedbacks of water stress on T_c	Possible feedbacks of N on T_c	Possible feedbacks of CO ₂ on T_c	Calibration to T_c observations
HUMEWheat (HU, Johnen et al., 2012; Ratjen and Kage, 2015)	<p>REF - EMP</p> <p>A statistical approach is used to determine regression models for daily minimum, mean and maximum T_c as described in Neukam <i>et al.</i> (2016). T_c observations in this study were considered to be the daily maximum.</p> <p>During pre- and post-heading phase different parameter sets for the covariates (p_1, p_2, p_3, p_4, and p_5) are used in the multiple linear regression model to predict daily maximum T_c ($T_{c,max}$):</p> $T_{c,max} = p_1 + p_2 R_{inc} + p_3 T_{a,max} +$	<p>The ratio of actual to potential transpiration quantifies drought stress and is considered in the multiple linear regression model to predict mean and maximum T_c (Neukam et al., 2016) as well as a reduced LAI development in presence of drought (Ratjen et al., 2016).</p>	<p>N deficit reduces LAI development (Ratjen and Kage, 2016) which is considered in the soil water balance calculation and multiple linear regression model to predict mean and maximum T_c.</p>	<p>Elevated CO₂ decreases transpiration rates. The decline in transpiration in comparison to ambient CO₂ (380 ppm) accounts for the change of minimum, mean</p>	<p>The ambient CO₂ concentration was set to 380 ppm for FACE-Maricopa data observations when the range of -5 to 5 ppm was used for calibration.</p>

	<p> $p_4 \log \text{LAI} + p_5 \left[\text{VPD} * \left(\frac{T_{\text{act}}}{T_{\text{pot}}} \right) \right]$, where R_{inc} is the amount of daily incident solar radiation, $T_{\text{a,max}}$ is the daily maximum air temperature, VPD is the mean daily vapour pressure deficit and T_{pot} is the potential transpiration which is the difference of potential evapotranspiration from the Penman-Monteith-equation (Thom and Oliver, 1977; Monteith and Unsworth, 2007) and the sum of interception evaporation and potential soil evaporation (Neukam et al., 2016). T_{act} is the actual transpiration determined as the sum of the soil water uptake by the plants calculated by a sink term approach (Feddes <i>et al.</i>, 1978). The partitioning of sinks over soil layers is controlled by the root length in each layer, modified by a root water uptake competition factor (Ehlers et al., 1991). </p>			and maximum T_c .	
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Nwheat (DN, Asseng <i>et al.</i> , 1998; Keating <i>et al.</i> , 2003; Asseng <i>et al.</i> , 2011)	EMP T_c is taken as 6 °C higher than T_{air} when the crop is fully stressed and 6 °C ^a cooler than T_{air} on average when the crop is fully transpiring (Ayeneh <i>et al.</i> , 2002; Maes and Steppe, 2012; Siebert <i>et al.</i> , 2014). Between these limits, the basis of the expression for T_c is the relationship between $T_c - T_{air}$ (ΔT) and the ratio of actual and potential evapotranspiration and vapor pressure deficit (Idso <i>et al.</i> , 1981; Jackson <i>et al.</i> , 1981)	ΔT is related to the actual and potential evapotranspiration and VPD of the atmosphere (Jackson <i>et al.</i> 1981). Water stress increases the canopy temperature and accelerates leaf senescence.	Low N which reduces crop growth also reduces water use and therefore T_c . Under low N, saved water later in the season can result in more transpiration later in season and lower T_c .	CO ₂ increases TE. Less transpiration from increased TE increases T_c . Water saved for later in the season can increase late- season transpiration and reduce T_c .	No calibration
FASSET (FA; Olesen <i>et al.</i> , 2002; Doltra <i>et al.</i> , 2014; Doltra <i>et al.</i> ,	EMP Based on an empirical relationship between midday crop temperature, evapotranspiration and net radiation (Seguin and Itier, 1983). Maximum and minimum T_c are calculated on a daily time	Water stress affects transpiration directly and indirectly through accelerated senescence, and the changed	N affects leaf area which influences transpiration and thus the radiative balance	Transpiration is reduced with higher CO ₂ affecting the radiative balance	No calibration

^a NWHEAT for this study was implement in a not yet released version of DSSAT

2015)	step	transpiration affects the radiative balance		(Doltra et al., 2014)	
Hermes (HE, Kersebaum, 2011; Kersebaum and Nendel, 2014)	<p>EBN</p> <p>T_c is calculated from a hourly energy balance by summing incident solar radiation, latent and sensible (H) heat fluxes and solving T_c from H.</p> <p>Hourly temperature and radiation values are determined following Hoogenboom & Huck (1986). The sensible heat flux is given by:</p> $H = \frac{\rho c_p (T_c - T_a)}{r_a}$ <p>where ρ is air density, c_p the specific heat of air, T_a is air temperature and r_a is the aerodynamic resistance which is calculated according to Thom and Oliver (1977) as $r_a = [4.72 [\ln((z - d + z_0)/z_0)]^2] / (1 + 0.54u)$ where u is wind speed at reference height z, d the zero-displacement height equal $1.04h^{0.88}$ and z_0 the roughness length for momentum and heat transfer each equal to $z_0 = 0.062h^{1.08}$, where h is</p>	<p>Cooling effect of evapotranspiration is considered in the energy balance. Consequently limited water reduces cooling and resulting higher T_c accelerates phenological development.</p>	<p>Limited N may reduce LAI for light interception of the canopy, but also transpiration. N stress accelerates phenological development</p>	<p>Stomatal resistance is modified by CO₂. (Kersebaum and Nendel, 2014). Therefore, elevated CO₂ slightly increase T_c through reduced transpiration and higher LAI</p>	No calibration

	the crop height. In the hourly energy balance, with the Penman-Monteith ET_0 equation and crop coefficient (Allen et al., 1998) where the stomatal resistance term is adjusted to consider ambient CO_2 levels (Kersebaum and Nendel, 2014).				
<i>SiriusQuality</i> (SQ; Martre et al., 2006; http://www1.clermont.inra.fr/siriusquality/ ; Maiorano et al., 2017)	EBN T_c is calculated from a daily energy balance by summing incident solar radiation, soil, latent and sensible (H) heat fluxes and solving T_c from H (Jamieson et al., 1995). The sensible heat flux is given by: $H = \frac{\rho c_p (T_c - T_a)}{r_a}$, where ρ is air density, c_p the specific heat of air, T_a is air temperature and r_a is the aerodynamic resistance which is calculated assuming neutral stability conditions according to Monteith (1973) as: $r_a = k^2 u / [\ln((z - d) / z_o)]^2$ with k the von Karman constant equal to 0.40, u the wind speed at reference height z , d the	Indirectly through reduced transpiration and accelerated canopy senescence.	Indirectly through reduced LAI under low N conditions.	No direct feedbacks of CO_2 .	No calibration

	<p>zero-displacement height equal to $0.13 \times h$ and z_o the roughness length for momentum and heat transfer each equal to $0.63 \times h$, where h is the crop height.</p>				
SSM-Wheat (SS, Soltani et al., 2013)	<p>EBN</p> <p>T_c is calculated from a daily energy balance by summing incident solar radiation, soil, latent and sensible (H) heat fluxes and solving T_c from H.</p> <p>The sensible heat flux is given by: $H = \frac{\rho c_p (T_c - T_a)}{r_a}$, where ρ is air density, c_p the specific heat of air, T_a is air temperature and r_a is the aerodynamic resistance which is calculated assuming neutral stability conditions according to Monteith (1973) as: $r_a = k^2 u / [\ln((z - d) / z_o)]^2$ with k the von Karmin constant equal to 0.40, u the wind speed at reference height z, d the zero-displacement height equal to $0.13 \times h$ and z_o the roughness length for momentum and heat</p>	<p>Indirect. Water stress affects (reduces) the daily accumulation of biomass and LAI, thus modifying the evaporation from soil and the transpiration. These, in turn, affect the energy balance.</p>	<p>Indirect. Daily LAI formation, and in turn biomass accumulation, is regulated by nitrogen availability, thus affecting daily evapotranspiration and, in turn, the energy balance.</p>	<p>Indirect. CO₂ affects daily biomass accumulation through modifying the radiation use efficiency and the transpiration efficiency. Evapotranspiration may vary accordingly, thus affecting the</p>	No calibration

	transfer each equal to $0.63 \times h$, where h is the crop height (Jamieson et al., 1995).			energy balance.	
Sirius2014 (S2; Jamieson et al., 1998; Jamieson and Semenov, 2000; Lawless et al., 2005)	EBN T_c is calculated from a daily energy balance by summing incident solar radiation, soil, latent and sensible (H) heat fluxes and solving T_c from H (Jamieson et al., 1995). The sensible heat flux is given by: $H = \frac{\rho c_p (T_c - T_a)}{r_a}$, where ρ is air density, c_p the specific heat of air, T_a is air temperature and r_a is the aerodynamic resistance which is calculated assuming neutral stability conditions according to Monteith (1973) as: $r_a = k^2 u / [\ln((z - d) / z_o)]^2$ with k the von Karman constant equal to 0.40, u the wind speed at reference height z , d the zero-displacement height equal to $0.13 \times h$ and z_o the roughness length for momentum and heat transfer each equal to $0.63 \times h$, where h is the crop height.	T_c is affected by increased water stress which causes transpiration to decrease altering the energy balance (Jamieson et al., 1995)	No direct feedbacks of N. However, N affects canopy growth and, potentially, dynamics of T_c (Lawless et al., 2005)	No direct feedbacks of CO_2 . However, CO_2 affects canopy growth and, potentially, dynamics of T_c (Lawless et al., 2005)	No calibration

SIMPLACE< Lintul2 >* (SP; Gaiser et al., 2013)	EBSC T_c is calculated from an hourly energy balance by summing incident solar radiation, soil, latent and sensible (H) heat fluxes and solving T_c from H . Atmospheric stability is considered by using Monin-Obukhov Similarity Theory (MOST) and empirical stability correction factors to solve for r_a . T_c is calculated for two bounding extremes: upper (no transpiration) and lower (full transpiration) limits of T_c , avoiding the need to specify canopy resistance terms at intermediate transpiration rates. With these two extreme potential values of T_c , actual $T_c = T_{c,L} + (1 - K_{ws})(T_{c,U} - T_{c,L})$ where K_{ws} is soil water stress index. A full description is given in Webber et al. (2016b).	Soil water stress index is used to determine T_c between the upper (no transpiration) and lower (full transpiration) limit of T_c . The rate of transpiration also influences the energy balance of each limit as well as the stability correction terms.	No-feedback	No effect of CO ₂ on hourly transpiration or T_c . However, daily transpiration is reduced using an empirical reduction function in response to elevated CO ₂ and this affects soil water content which has an effect on T_c .	Varietal canopy resistance term and terms that control wind speed due to assumptions of height of surrounding vegetation
SIMPLACE< Lintul5>**	EBSC T_c is calculated from an hourly energy balance	Soil water stress index used to determine T_c	Indirect. Daily LAI formation, and in turn	Direct. Linear function	Varietal canopy resistance term

(L5; Gaiser et al., 2013)	by summing incident solar radiation, soil, latent and sensible (H) heat fluxes and solving T_c from H . Atmospheric stability is considered by using Monin-Obukhov Similarity Theory (MOST) and empirical stability correction factors to solve for r_a . T_c is calculated for two bounding extremes: upper (no transpiration) and lower (full transpiration) limits of T_c , avoiding the need to specify canopy resistance terms at intermediate transpiration rates. With these two extreme potential values of T_c , actual $T_c = T_{c,L} + (1 - K_{ws})(T_{c,U} - T_{c,L})$ where K_{ws} is soil water stress index. A full description is given in Webber et al. (2016b).	between the upper (no transpiration) and lower (full transpiration) limit of T_c . The rate of transpiration also influences the energy balance of each limit as well as the stability correction terms.	biomass accumulation, is regulated by nitrogen availability, thus affecting daily evapotranspiration and, in turn, the energy balance.	decreases canopy resistance (r_c) term, such that canopy resistance increased by 20% as atmospheric CO ₂ increased from 370 to 550 ppm.	
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* SIMPLACE<Lintul2> is the shortened name for SIMPLACE<Lintul2,CC,DailyHeat,CanopyT>.

** SIMPLACE<Lintul5> is the shortened name for SIMPLACE<Lintul5,FAO-56,HourlyHeat,CanopyT>.

Model evaluation

Three measures of model performance were considered. The square root (RMSE) of the mean squared error and the coefficient of determination (R^2) were determined for ΔT , grouped across similar nitrogen and CO₂ levels, across years in the FACE-Maricopa experiment and grouped across water treatments, years and sites (five China Wheat experiments plus FACE-Maricopa). The RMSE was calculated as:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (\Delta T_{s,i} - \Delta T_{o,i})^2} \quad (1)$$

where $\Delta T_{o,i}$ is the i th observation of ΔT , $\Delta T_{s,i}$ is the i th simulated ΔT value, and N is the total number of observation and simulation pairs. Observations and simulations for a particular treatment were pooled across dates and years for the FACE-Maricopa experiment, and across dates, years and sites for the China Wheat experiment.

Analyses of variance for multivariate linear regressions were conducted using PROC GLM in the SAS statistical software (version 9.4, SAS Institute; Cary, NC). Sequential sums of squares (Type I) were used to quantify the variation described by a factor, given any variation attributable to variables previously included in the linear model. Given the importance of how the variables were ordered, various sequences were explored. Typically, variables were introduced sequentially based on their explaining progressively less variation or based on their relevance for testing specific hypotheses relating to comparisons of observed vs. simulated data.

For the FACE data, four basic linear models were considered. The first used year, treatment and finally weather to characterize variation in observed ΔT . In the second group of tests, daily weather variables were tested first, followed by treatment effects to explain variation in observed ΔT . These analyses helped characterize how treatments and environmental variables drove variability in observed ΔT . In the third model, simulated ΔT , followed by year and treatment effects were considered to determine how well the

simulated ΔT explained variation in the observations, as well as assess how much variation remained due to years and the treatments not explained by a given crop model. In the final group of tests, VPD at T_{max} (VPD_{Tmax}), followed by the simulated ΔT and then the treatment factors were used to assess how much variation in observed ΔT a model could explain beyond that of the expected, large VPD effect. The linear models tested for the China Wheat data were similar but differed in that site was the highest level of the hierarchy. Given evidence that ensembles of crop models often out-perform any individual model (Martre et al., 2015), two multi-model ensembles were created from the mean (e.mean) and the median (e.median). The reference HU model was excluded from the ensemble analyses.

To explicitly evaluate if the performance of the EBSC models was infact related to stability conditons and not another confounding factor, we estimated the stability conditions of the boundary layer for each observation of T_c using the formulation of Richards' number (Ri) as reported in Mahrt and Ek (1983) as:

$$Ri = \frac{g(T_a - T_c)z}{T_a u^2}$$

Where g is the acceleration due to gravity in ms^{-2} , z is the height that atmospheric measurement observed at in m, and u is the wind speed in ms^{-1} .

Results

Canopy temperature and canopy temperature depression observations and simulations

There was considerable intra- and inter-annual variation in daily maximum air temperature (T_{max}) for the FACE-Maricopa experiment (Fig. 2a to 2d) and additionally, among sites for the China Wheat experiment (Figs. 3a to 3d and 4a to 4d), with observed T_c largely following T_{max} . In the FACE-Maricopa experiment, observed ΔT in the fully irrigated conditions tended to be negative, whereas under semi-irrigated conditions observed ΔT was less negative and frequently positive in 1993 (Fig. 2a and 2b). Similarly, in

the China Wheat experiment, ΔT tended to be negative indicating canopy cooling in the irrigated treatments (Fig. 3f to 3j, and Fig. 4e to 4h) except at Tryon, NE (site NESAs) which had sandy soil and the measured ΔT values suggest frequent water deficits even under irrigation. The effect of elevated CO_2 and nitrogen status were more subtle (Fig. 2e to 2h) though ΔT tended to be less negative under elevated CO_2 , and with low nitrogen levels. As reported in Kimball et al. (1999), elevated CO_2 raised T_c by 0.6°C and 1.1°C compared to ambient CO_2 concentrations at high and low nitrogen levels, respectively. These results are consistent with decreases in stomatal conductance and similar increases in T_c observed on leaves in cuvettes obtained with portable photosynthesis systems (Wall et al., 2000; Wall et al., 2006).

With few exceptions, observed variation in ΔT in the FACE-Maricopa experiment was captured by at least one model in the ensemble, as indicated by the grey banding of Figure 2e to 2h, though individual models differed widely (Fig. S2 and Tables 2 and 3). The multi-model ensemble median (e.median) correlations across the various nitrogen and CO_2 treatments are presented in Table 2. The EBSC models consistently had the highest R^2 and lowest RMSE values while the reference model HU in most cases had better performance in these well-watered treatments. The e.median estimator failed to capture the differences between 1993 and 1994 in which 1993 had positive ΔT values for the semi-irrigated treatment, whereas observations in 1994 had large negative ΔT in both the full- and semi-irrigated treatments. Likewise, the reference model HU calibrated to the ambient CO_2 data for these treatments had a R^2 of only 0.22. In the China Wheat experiment, there were relatively more instances where observed ΔT was outside of the range of simulated ΔT (Figs. 3 and 4, Fig. S3). When data were pooled across all sites of the China Wheat experiment, e.median had R^2 values of 0.41 and 0.26 ($P < 0.05$) for the irrigated and rainfed treatments, respectively, except from the HU model which was independently parametrized from this data. The EBSC models had the best agreement with observations. The EMP models generally performed better than the EBN models. However, it is hard to generalize across the EBN models, as the performance of individual models varied with treatment and R^2 values sometimes had insignificant or near zero correlations with observations.

Figure 2. Time course of observed daily maximum air temperature (T_{max} , blue line), mid-day canopy temperature (T_c) observations (symbols) and the range (shaded areas) and median (red and black lines) values of simulated daily maximum T_c across models for the FACE-Maricopa experiment in (a) 1993, (b) 1994, (c) 1996, and (d) 1997. The differences between T_c and T_{max} ($\Delta T = T_c - T_{max}$) are presented for the (e) 1993, (f) 1994, (g) 1996, and (h) 1997 harvest years. In all panels, star symbols are ambient CO_2 and triangles are elevated CO_2 . In (a), (b), (e), and (f) the black symbols are full irrigation, red symbols are semi irrigated, the dark grey banding is full irrigation, light grey is semi irrigated, their

intersection is medium grey, and black and red lines are median values of model simulations for full irrigation and semi irrigated, respectively. In (c), (d), (g), and (h) the black symbols are high nitrogen fertilizer rates, red symbols are low nitrogen fertilizer rates, the dark grey banding is high nitrogen, light grey is low nitrogen, their intersection is medium grey and black and red lines are median values of model simulations for high and low nitrogen, respectively. Observations of T_c and ΔT are only shown when the canopy was near fully closed.

Figure 3. Time course of observed daily maximum air temperature (T_{max} , blue lines), mid-day canopy temperature (T_c) observations (symbols) and the range (shaded areas) and median (red and black lines) values of simulated daily maximum T_c across models for the China Wheat experiment in 1985 at (a) Lubbock, TX, (b) Manhattan, KS, (c) Tryon, NE, (d) Mandan, ND and (e) Lethbridge, AB. The differences between T_c and T_{air} ($\Delta T =$

$T_c - T_{\max}$) are presented for (f) Lubbock, TX, (g) Manhattan, KS, (h) Tryon, NE, (i) Mandan, ND and (j) Lethbridge, AB. The black symbols are full irrigation, red symbols are semi irrigated, the dark grey banding is full irrigation, light grey is semi irrigated, their intersection is medium grey, and black and red lines are median values of model simulations for full irrigation and semi irrigated, respectively. Observations of T_c and ΔT are only shown when the canopy was near fully closed.

Figure 4. Time course of observed daily maximum air temperature (T_{air} , blue line), mid-day canopy temperature (T_c) observations (symbols) and the range (shaded areas and median (red and black lines) values of simulated daily maximum T_c values across models for China Wheat experiment

in 1986 at (a) Lubbock, TX, (b) Tryon, NE, (c) Mandan, ND and (d) Lethbridge, AB. The difference between T_c and T_{air} ($\Delta T = T_c - T_{air}$) are presented in (e) Lubbock, TX, (f) Tryon, NE, (g) Mandan, ND and (h) Lethbridge, AB. The black symbols are full irrigation, red symbols are semi irrigated, the dark grey banding is full irrigation, light grey is semi irrigated, their intersection is medium grey, and black and red lines are median values of model simulations for full irrigation and semi irrigated, respectively. Observations of T_c and ΔT are only shown when the canopy was near fully closed.

Table 2. Coefficient of determination (R^2) of observed vs. simulated ΔT ($\Delta T = T_c - T_{air}$) across production conditions and water, nitrogen, and CO₂ factors by experiment. The values for water supply treatments (Irr - irrigated and Rain - rainfed) for the China Wheat (CW) experiment consider data pooled across sites and years. Data from the FACE-Maricopa experiment are pooled across years for all treatments. Only R^2 values that were statistically significant at $P = 0.05$ are reported.

T_c		FACE Water		FACE Nitrogen		FACE CO2		CW Water	
model		Semi							
type	Model	Full Irr	Irr	High	Low	Amb	Elev	Irr	Rain
REF	e.mean	0.54	0.16	0.52	0.47	0.5	0.47	0.41	0.25
REF	e.median	0.50	0.13	0.48	0.47	0.47	0.43	0.41	0.26
REF-									
EMP	HU	0.52	0.22	0.51	0.45	0.51	0.53	0.40	0.48
EMP	DN	0.31	-	0.23	0.28	0.24	0.24	0.27	0.14
EMP	FA	0.12	0.15	0.25	-	0.19	0.17	0.20	0.12
EBN	HE	0.25	0.04	0.27	0.25	0.20	0.22	0.14	-
EBN	SQ	0.32	0.08	0.27	0.21	0.24	0.27	0.16	-
EBN	SS	0.28	0.13	0.29	0.22	0.28	0.26	-	0.10
EBN	S2	0.03	-	0.07	-	0.08	0.04	0.13	-
EBSC	L5	0.49	0.03	0.34	0.51	0.34	0.32	0.27	0.27
EBSC	SP	0.36	0.13	0.37	0.31	0.37	0.34	0.41	0.30
obs		357	122	368	110	239	240	53	52

Table 3. Root mean square error (RMSE) of ΔT ($\Delta T = T_c - T_{air}$) across production conditions and water, nitrogen, and CO₂ factors by experiment. The values for water supply treatments (Irr-irrigated and Rain-

rainfed) for the China Wheat (CW) experiment considered data pooled across sites and years. Data from the FACE-Maricopa experiment were pooled across years for all treatments.

T_c		FACE Water		FACE Nitrogen		FACE CO2		CW Water	
model		Full	Semi						
type	Model	Irr	Irr	High	Low	Amb	Elev	Irr	Rain
REF	e.mean	1.59	1.65	1.65	1.46	1.75	1.45	2.86	3.37
REF	e.median	1.55	1.66	1.63	1.39	1.68	1.48	2.83	3.36
REF-									
EMP	HU	1.36	1.55	1.42	1.39	1.42	1.4	2.89	3.1
EMP	DN	2.07	2.76	2.37	1.87	2.09	2.42	2.91	3.66
EMP	FA	1.87	1.85	1.77	2.17	1.76	1.97	3.33	4.3
EBN	HE	2.09	3.21	2.57	1.89	2.56	2.29	3.88	5.21
EBN	SQ	2.94	2.04	2.69	2.93	3.08	2.36	3.42	5.84
EBN	SS	2.35	1.9	2.24	2.28	2.44	2.04	5.25	3.64
EBN	S2	2.92	3.1	3.11	2.45	3.21	2.71	3.94	3.97
EBSC	L5	1.49	2.11	1.76	1.32	1.71	1.63	3.01	3.23
EBSC	SP	1.59	2.05	1.75	1.6	1.83	1.61	2.67	3.39

Decomposing sources of variation in ΔT

Four types of analysis were used to assess which factors explained the most variation in observed ΔT , including multiple regression models in which various treatments factors (water, CO₂, and nitrogen), year effects or weather effects (VPD_{Tmax}, ET_o, solar radiation) were examined. For the FACE-Maricopa dataset, VPD_{Tmax} explained the greatest amount of variation in observed ΔT , explaining 33% of the variation, with solar radiation explaining an additional 10% (Fig. 5a). After the weather variables were

controlled for, treatment effects of CO₂, nitrogen and water, tested in that order, explained an additional 5, 2 and 5%, respectively. The remaining residual variation in the observations was 38%. For the China Wheat experiment, VPD_{Tmax} explained only 1% of variation in observed ΔT (Fig. 5b), with little additional variation explained by the weather variables assessed next. The greatest amount of variation (28%) was due to experimental site after weather variables were controlled for. Year effects explained a further 10% of variation with water treatment explaining 27% of variation. Readers should be reminded that unlike the FACE-Maricopa experiment in which observations spanned the season over a wide temperature range (Fig. 2), in the China Wheat experiment there were a limited and variable number of observations per year and site (Figs. 3 and 4). For this reason, caution must be taken in interpretation of Fig. 5b, as it represents the drivers of variation in the available observations, not the expected drivers of ΔT over the entire growing season.

Figure 5. Type I sums of squares in an ANOVA of the sources of variation explaining observed ΔT (°C), where $\Delta T = T_c - T_{air}$, expressed as a percentage of the total sums of squares for (a) the FACE-Maricopa and (b) China Wheat experiments. Sources of variation were controlled for in the following order for FACE-Maricopa: VPD_{Tmax}, ETo, daily cumulative solar radiation, windspeed, year, CO₂ (year), nitrogen

(year) and water (year); and for China Wheat: VPD_{Tmax} , ET_o , daily cumulative solar radiation, windspeed, site, year (site) and water (site x year), as indicated from bottom to top in both panels.

From the analyses of variance for FACE-Maricopa, ΔT simulations from all crop models explained a significant portion of variation in observed ΔT , but this portion ranged from 5% to 35% (Fig. 6a). The reference EMP model (HU) explained 50%, while the e.median explained 45%. Of the three T_c model approaches, simulations of ΔT by the EBSC models explained 34% of the variation in observed ΔT , more than either of EBN (19%) or EMP (20%) types. The models differed in how much variation remained across years and the various treatment factors. For CO_2 treatment effects, in the EBSC models, only 1% variation remained unexplained by L5 whereas 5% remained unexplained by SP. The within group differences were less pronounced for the other two modelling approaches. The three modelling approaches were similar with regards to explaining variation due to nitrogen with the EMP models explaining the greatest variation. Wider variation within modelling approaches was observed for the amount of unexplained variation related to water supply level. For the China Wheat experiment, all models except SQ explained a significant portion of variation in observed ΔT , though the amount of variation explained was generally lower than the variation explained in the FACE-Maricopa experiment (Fig. 6b). On average the EMP (excluding HU), EBN and EBSC models explained 24, 7 and 40% of variation in observed ΔT , respectively while the reference model HU explained 51% of variation. All models left a large amount of variation due to site unexplained, at 17, 28 and 17% for the EMP, EBN and EBSC model averages, respectively. There was no strong pattern within modelling approach as to how much variation remained after controlling for year. On average, EBSC models had only 5% variation due to water treatment remaining, whereas EMP and EBN models had 16% and 20% unexplained variation due to water treatment respectively, and the reference HU 8% remaining.

Figure 6. Type I sums of squares in an ANOVA of the sources of variation explaining observed ΔT ($^{\circ}\text{C}$), where $\Delta T = T_c - T_{air}$, expressed as a percentage of the total sums of squares for (a) the FACE-Maricopa and (b) the China Wheat experiments. Sources of variation for FACE-Maricopa (a) were controlled for in the following order: simulated ΔT (green), year (yellow), CO_2 (year) (blue), nitrogen (year) (orange) and water (year) (light green), with the residual error in red, as indicated from bottom to top. Sources of variation for China Wheat (b) were controlled for in the following order: simulated ΔT (green), site (dark blue), year (site) (yellow), water (site $\times$ year) (light green), with the residual error in red, as indicated from bottom to top in the figure. In both panels, the percentage sums of square terms are shown from left for the reference EMP model HU, the mean across models (e.MN), the model median (e.MD), the two EMP models (DN and FA), four EBN models (HE, S2, SQ and SS) and two ENSC models (L5 and SP).

Considering the drivers of variability in observed ΔT as well as the remaining residuals, we explored what variability the simulated ΔT accounted for and what remained unexplained. As the analyses used Type I Sums of Squares, caution is needed in directly comparing the terms between the ANOVAs with and without the simulations. As a first step, we noted that the simulations explained at most 50% (HU reference) and 34% (EBSC approach) of the variation in observed ΔT in the FACE-Maricopa experiment. Likewise, VPD_{Tmax} explained 38% of the variation in the observations when considering only

environmental or treatment factors. Therefore, we endeavored to test the hypothesis that the models explained more variation than the $VPD_{T_{max}}$ did by performing an ANOVA in which $VPD_{T_{max}}$ was controlled for first, followed by simulated ΔT . For the FACE experiment, all models explained more variation than $VPD_{T_{max}}$, whereas in the China Wheat experiment two of the EBN models were unable to explain more variation in observations after $VPD_{T_{max}}$ was controlled for (Table 4). In both experiments, the HU reference explained the highest level of variation followed by the EBSC, EMP and EBN models.

Variation between observed and simulated ΔT also might result from differences in how well the models simulated crop growth, including effects of nitrogen or water regimes. For example, if a given model simulated values of LAI that were unrealistically low, this might lead to underestimation of transpiration. We tested for an effect of simulated LAI on the residual of observed vs. simulated ΔT (SI Fig. S3). Allowing for a site effect, LAI and its interaction with site explained from 2.6% to 12.6% of the variation ($P < 0.01$, data not shown), suggesting that skill in simulating crop growth also contributed a relatively small proportion of the error in simulating ΔT .

Table 4. Type I sums of squares variation (%) explained by simulated values of ΔT after variation due to $VPD_{T_{max}}$ was controlled for expressed as a percentage of total variation across years, production conditions and CO_2 factors in the FACE-Maricopa experiment and across years, locations and water supply treatment in the China Wheat experiment. Only values that were statistically significant at $P = 0.05$ are reported. e.mean and e.median are the mean and median across models, respectively.

T_c model type	Model	FACE	China Wheat
REF	e.mean	15.9	42.9
REF	e.median	13.0	42.9
REF-EMP	HU	17.0	51.0

EMP	DN	5.7	36.0
EMP	FA	2.7	17.7
EBN	HE	1.5	19.3
EBN	SQ	5.5	-
EBN	SS	5.9	-
EBN	S2	3.2	5.6
EBSC	L5	7.3	36.4
EBSC	SP	8.3	42.2

Response to CO₂

Modeled response of T_c to CO₂ was assessed for all observational pairs of the difference in T_c at elevated and ambient CO₂ for each water supply and nitrogen fertilizer treatments (Fig. 7). The observed CO₂ response exhibited variation that the models would not necessarily be expected to reproduce. Two of the models, the EBN model HE and the EBSC model L5, reproduced the median response in the observations, while the EMP model DN captures some response in the water supply treatments, though not in the nitrogen supply treatments. The ability of the various models to capture the response of T_c to water and nitrogen treatments is presented in the SI (Fig. S5), though the variation is high due to the variation in water and nitrogen stress levels over the course of the season.

Figure 7. Absolute T_c response (°C) to elevated atmospheric CO_2 concentration relative to ambient CO_2 in the FACE-Maricopa experiment in (a) 1993 and 1994 for across water supply treatment levels and (b) 1996 and 1997 across nitrogen fertilizer treatment levels. The boxes show the 25th and 75th percentile of the paired data points, the top whisker indicates either the maximum value or the 75th percentile value plus 1.5 times the difference between the 75th and 25th percentile, the circles above the top whisker indicate any values larger than the value of the top whisker, the bottom whisker indicates either the minimum value or the 25th percentile value minus 1.5 times the difference between the 75th and 25th percentile and the circles beneath the bottom whisker indicate any values smaller than the bottom whisker. In both panels, the response is presented from left for the reference EMP model HU, the mean (e.mean) and the median (e.median) across models, the two EMP models (DN, FA), four EBN models (HE, S2, SQ, SS) and two ENSC models (L5, SP).

Discussion

Extension of and limitations of the study

To our knowledge, this is the first study to compare approaches for simulation of T_c over a wide range of locations and management conditions, extending previous T_c and r_a model comparisons by Webber et al. (2017) and Liu et al. (2007), respectively. Despite the wide range of production conditions and latitudes considered, all study locations were continental, and a high humidity site with low VPD was not included. Many tropical African, Asian and South American regions fall into the latter category, and T_c may be expected to rise above T_{air} in periods of soil water stress. Given that daily maximum temperatures are already close to high temperature thresholds in these regions (Schlenker and Lobell, 2010; Lobell et al., 2011) and is expected to increase with climate change, further study is warranted. Further, the EMP T_c models evaluated in this study were originally developed using data from Maricopa either directly in this study or based on relationships reported by Pinter, Zipoli et al (1990). It should be noted that the HU model was originally developed from two sites in Germany, but before parameterization with the FACE-Maricopa data, it had performance similar to the other EMP models (Table S3).

Our study also did not consider genotypic variability in the degree of canopy cooling, although stomatal conductance and the degree of canopy temperature depression typically varies among genotypes under heat (Amani et al., 1996) and also varies between spikes and leaves, with the reproductive spike being warmer than leaves at least partially due to lower stomatal density (Pinter et al., 1990; Ayeneh et al., 2002). However, there is also evidence that floral structures may show differential ability to cool at key reproductive stages (Steinmeyer et al., 2013). We know of no studies evaluating models for their ability to distinguish canopy temperature depression across varieties. This is an obvious next step for crop models to aid in investigating genotype by environment by management (G×E×M) interactions for heat stress risk assessments. The fact that aerial instrument platforms can now assess T_c at high throughput -and with greater precision than using ground based approaches- (Tattaris et al., 2016) provides an opportunity to calibrate and validate models for this trait on a large scale.

Related to assisting (G×E×M), the current study did not evaluate whether consideration of simulated T_c can improve heat stress simulations of production, as the focus was on the skill of T_c routines across production conditions and locations. Some authors (Hatfield et al., 1984) have argued that canopy temperature in cereal crops is a poor indicator of heat stress, as the spikes will generally be at the same temperature as the air rather than that of the bulk canopy. In fact, a canopy temperature gradient within the crop, varying between canopy and spike in wheat (Amani et al., 1996; Ayeneh et al., 2002), or the ear in maize (Edreira and Otegui, 2012), has been reported. In the case of wheat, although the spike was 0.5 to 1° C warmer than the canopy in Obregon, Mexico, under irrigated conditions, it still obtained a temperature depression relative to T_{air} of 3 to 4.3° C (Ayeneh et al., 2002). That the spike temperature will differ from T_{air} and be close to T_c is also supported by Amani et al. (1996). In any case, if T_c is to replace T_{air} in simulation of heat stress effects, models will need re-calibration or parameterization.

A further issue is that our analysis of the drivers of observed ΔT were limited in that we used mainly the summary weather data as used by the crop models as input (i.e., daily radiation sum, average wind speed, daily maximum temperature and corresponding VPD) whereas actual ΔT is driven by instantaneous values of VPD, air temperature, and water stress. Further study of this issue is possible with our FACE-Maricopa dataset, making use of sub-hourly data (Kimball et al., 1999). However, temperature and vapor profiles with the crop's boundary layer vary rapidly as the distance from the crop surface increases (Monteith and Unsworth, 2007), such that conducting an energy balance of a cropped surface is sensitive to where atmospheric conditions are measured (Jarvis and McNaughton, 1986). As the objective of this study was to investigate T_c in the context of simple approaches to model heat stress, we believe a daily analysis, considering daily T_{max} and $VPD_{T_{max}}$ was appropriate. A future challenge will be to extend the use of T_c to growth and development processes that respond to temperatures other than T_{max} .

Potential for model improvement

In our current study, many of the comparisons were based on comparing individual model performance against the observations and testing model performance for simulating crop response to nitrogen stress, water deficits or atmospheric CO₂ concentration. This contrasts with our previous model intercomparison (Webber et al., 2017), which placed more emphasis on the approach to simulating T_c (i.e., EMP, EBN, ENSC). There was sometimes considerable variation within a modelling approach that may be related to how sensitive the crop models were to nitrogen or water availability, which will affect stomatal conductance and LAI, both of which feedback to T_c simulations as discussed further below. Nevertheless, comparing across the R^2 (Table 2 and S1), RMSE (Tables 3 and S2) and level of variation explained (Fig. 6), as a group, the EBSC models performed better than the EMP or EBN models, as in Webber et al. (2017). This is particularly evident when the performance of the models for the China Wheat experiment where the EBSC models could explain 30 to 40% of the variability in the observed ΔT and had R^2 values of 0.27 – 0.30 for the rainfed treatments across sites, whereas three of the four EBN models had no significant correlations, and the EMP models had an average R^2 value of 0.13. However, in the FACE water stress treatments as well as the high N and all CO₂ treatments, the empirical HU model performed markedly better than even the EBCS models, though the difference was reduced or reversed in the irrigated and nitrogen limited treatments. Collectively, this suggests the hypothesis that simulation of T_c across diverse environments and conditions is improved with stability correction to account for the differences in r_a or that empirical models must be fit on sufficient data for a particular environment. Our study does not allow us to definitely conclude whether the superior performance of the EBSC models compared to other models in the ensemble is due to stability correction or rather due to other factors (e.g. improved simulation of evapotranspiration), as discussed in more detail below. However, there was a clear relationship between how much variation in observed ΔT could be explained by simulated ΔT , and the remaining variation variability explained by stability conditions, as indicated by the bulk Richardson number (Ri ; Fig 8). This indicates that the reference empirical model HU and the EBSC models were able to capture more variability associated with boundary layer stability conditions than the other models. To more directly test this, it would be better to compare our modelled estimates of r_a to measurements of

turbulence obtained using a 3D sonic anemometer, but such measurements were not made in the FACE experiment. Despite the smaller total error for the EBSC models, in some cases the error, $T_{c,obs} - T_{c,sim}$, was still correlated with Ri and exhibited a positive slope demonstrating that the stability conditions were not completely corrected for, although the Ri relation with error for EBSC models was generally less than that for the EBN or EMP models (Figs S6 and S7, Tables S3 and S4). Surprisingly, the error associated with one of the EBN models (HE) generally exhibited less correlation (and lower slope) with Ri, though the simulations explained less variation in observed ΔT than did the EBSC models. The question of whether stability correction or an empirical approach is needed may simply depend on the application, the extent of the study and the data available to construct or calibrate an empirical model.

Figure 8. Type I sums of squares in an ANOVA of variation in observed $\Delta T = T_c - T_{air}$ ($^{\circ}\text{C}$) explained by simulations of ΔT , expressed as a percentage of the total sums of squares, for each of the FACE-Maricopa and the China Wheat experiments plotted against the remaining Type I sums of squares variation explained by the Richardson number (Ri). Different colors indicate the model approach to simulate T_c , with EBN models in red, EBSC models in green and EMP models in blue. The letter indicates the model

name and the two occurrences of each model are to indicate the values for each of the FACE-Maricopa and China Wheat experiments which are not distinguished in this figure.

Beyond corrections for stability, ability to correctly simulate T_c depended on the respective models' response to water, nitrogen and CO₂ levels. This presumably explains why unlike Webber et al. (2017), this study did not reveal as decisively that the EBN models were consistently worse than EMP models at the Maricopa site. It was surprising to us that the EMP models performed better for the China Wheat dataset than the EBN models, as they were developed based on relationships derived in Maricopa. This is particularly the case for the HU model, which although treated as a reference model for FACE-Maricopa, was not trained on the data for the China Wheat experiment. However, as already discussed all study locations were continental and do not include high humidity conditions. Interestingly, no models were able to perform well under the semi-irrigated conditions in the FACE Maricopa experiment, including HU, and further study is needed to understand the drivers of variation in these observations. It should be noted that in the first step of this study in which limited T_c observations were available for calibration, the HU model performed similar to the other EMP models (SI material, Table S3). However, we place limited emphasis on the first set of simulations as some models had prior access to the observations and other than HU, there was limited ability to calibrate the T_c simulations to observations.

After VPD_{Tmax} was accounted for, the simulations were able to explain 4.2, 4.0 and 7.8 % of the variation for the EMP, EBN and EBSC approaches for FACE-Maricopa, respectively. The agreement among these values contrasted with the wide variation in skill in capturing the variation in observed ΔT across modelling approaches suggests that the difference among the simulation approaches relates to how well models capture the effects of VPD driving transpirational cooling or lack thereof. In general, the EBSC models also explained the greatest amount of variation across the well-watered treatments for both FACE and China Wheat experiments, in which cooling is largely driven by VPD_{Tmax} and air is typically stable (SI Material, Tables S2 and S3). The superior performance of the EBSC models compared to other

models in the ensemble was less pronounced when observations over all water stressed treatments from both experiments were combined. Furthermore, within the EBN approaches, there was wide variation in terms of the variation explained across water stress treatments. Correct simulation of the response of T_c to water stress requires that a model must correctly simulate root depth, soil water dynamics, water demand and uptake as well as the crop response to water stress. Therefore, poor performance of a T_c approach here may reflect either the ability of a given crop model to correctly simulate water use and water stress or the T_c model's sensitivity to water stress. A further caveat to the interpretation of the results under water-limited conditions is that the HU reference model trained on the FACE-Maricopa data could only explain 22% of variation in the water stressed observations from that experiment, but when observations were pooled with the China Wheat experiment, its correlation with observed ΔT increased to 43%. More work is needed to understand the source of variation in this treatment.

Regarding the effect of different simulations of evaporative demand and water use on simulated T_c , consider the two EBSC models, L5 and SP, which share the same T_c model, but differ in other respects. Considering the FACE irrigated treatments, where soil water deficit would have been minimal, the differences between their simulations are probably related to the degree of evaporative cooling and resulting stability conditions, as L5, with higher correlation for these treatments, generally simulates higher ET_0 (Webber et al., 2016a) with the FAO-56 methodology (Allen et al., 1998) than SP with a Penman based approach (Penman, 1948). However, the SP model had better performance considering the water limited conditions and the China Wheat experiment, in which correct simulation of the water balance and various feedbacks on LAI would have been more important, as both feedback onto r_a and T_c . Clearly a prerequisite of improving T_c simulations is to have good estimates of ET_0 and simulation of soil water dynamics. For the nitrogen treatments, there was no large pattern across model groups, although the EMP models were able to explain more variation than the other types (data not shown). Likewise, there was little differentiation between the model groups with respect to explaining variation due to CO_2 levels with one model in each of the EBN and EBSC capturing the median response (Fig. 7). This suggests that

regardless of the approach, it should be possible to include this response in T_c models and this study identified this as a relatively straightforward model improvement. As previously stated, while the two EBSC models used the same T_c model, L5 accounted for CO₂ effects on canopy resistance (r_c) term, such that canopy resistance increased by 20% as atmospheric CO₂ increased from 370 to 550 ppm. The T_c model of L5 did not feedback onto the calculation of transpiration. Instead, it used the crop coefficient and ET_o concept (Allen et al., 1998), so its daily potential transpiration rate was adjusted to limit water use under elevated CO₂ (Zhao et al., 2015). However, this strategy was insufficient to describe the reduced stomatal conductance on an hourly basis to determine T_c in our previous study (Webber et al., 2016b), suggesting that further model development is needed. Collectively, beyond accounting for stability conditions or having a strong empirical model built on adequate data, correct simulation of T_c across a range of conditions also requires that crop models account for water demand, soil water dynamics and response to CO₂.

Use of T_c in climate change impact assessments

As the frequency of crop heat stress increases with climate change (Field, 2012), it will become increasingly important for crop models to improve their consideration of the impacts of heat stress damage on crop yields (White et al., 2011). Observational evidence demonstrates that transpirational cooling in irrigated systems (Lobell et al., 2008; Puma and Cook, 2010) has mitigated damages during periods of high temperatures in past episodes of high temperature in maize production in the US (Carter et al., 2016). Likewise, Lobell et al (2011) detected more severe yield losses due to the number of hot days in drought as compared to well-watered conditions. Despite this widely documented and physically well understood phenomenon, few crop models consider the interaction of high temperature and water availability, suggesting heat stress assessments will likely overestimate damages under irrigated conditions, and this bias will increase as climates become warmer (Siebert et al., 2017). Consideration of T_c explicitly accounts for this interaction and should improve the accuracy of climate change impact assessments, particularly for irrigated systems (Rezaei et al., 2015). However, consideration of heat and

drought stress is also expected to be important for tropical regions where daily maximum temperatures are already close to limits for crop heat stress and short episodes of high temperature and drought are likely to coincide. Correct simulation of this will depend on a good approach to simulating T_c as well as adequate depiction of crop water demand and use dynamics and possible interactions with CO₂ concentrations.

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