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Canopy temperature for simulation of heat stress in irrigated wheat in a semi-arid environment: A multi-model comparison

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ABSTRACT

Even brief periods of high temperatures occurring around flowering and during grain filling can severely reduce grain yield in cereals. Recently, ecophysiological and crop models have begun to represent such phenomena. Most models use air temperature (T_{air}) in their heat stress responses despite evidence that crop canopy temperature (T_c) better explains grain yield losses. T_c can deviate significantly from T_{air} based on climatic factors and the crop water status. The broad objective of this study was to evaluate whether simulation of T_c improves the ability of crop models to simulate heat stress impacts on wheat under irrigated conditions. Nine process-based models, each using one of three broad approaches (empirical, EMP; energy balance assuming neutral atmospheric stability, EBN; and energy balance correcting for the atmospheric stability conditions, EBSC) to simulate T_c , simulated grain yield under a range of temperature conditions. The models varied widely in their ability to reproduce the measured T_c with the commonly used EBN models performing much worse than either EMP or EBSC. Use of T_c to account for heat stress effects did improve simulations compared to using only T_{air} to a relatively minor extent, but the models that additionally use T_c on various other processes as well did not have better yield simulations. Models that simulated yield well under heat stress had varying skill in simulating T_c . For example, the EBN models had very poor simulations of T_c but performed very well in simulating grain yield. These results highlight the need to more systematically understand and model heat stress events in wheat.

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1. Introduction

The rising temperatures expected with climate change are likely to reduce wheat yields (Asseng et al., 2015), although the impact may be moderated by positive CO₂ fertilization effects. Without

consideration of adaptations in crop variety, the dominant effect of warming is to accelerate crop development. Evidence suggests that heat stress consisting of even brief periods of high temperatures above crop specific critical thresholds (Ferris et al., 1998; Porter and Gawith, 1999; Wheeler et al., 2000; Jagadish et al., 2007; Vignjevic et al., 2015) are already causing large reductions in cereal yield (Schlenker and Roberts, 2009; Hawkins et al., 2013; Lobell et al., 2013; Fontana et al., 2015). It is expected that negative impacts of high temperature on crop yields will become more frequent with increased climate variability and higher mean temperatures (Field

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et al., 2012). To date, few climate change impact studies using crop models have considered such heat stress effects (Teixeira et al., 2013; Deryng et al., 2014).

High temperatures affect a number of crop growth and development processes that together result in the heat stress impacts observed in the field (Rezaei et al., 2015). Photosynthesis rates in wheat decrease when temperature exceeds optimum values (Sage and Kubien, 2007) due to reduction in the efficacy of photosystem II (Nash et al., 1985), thylakoid membrane instability (Bukhov et al., 1999) and reduced RUBISCO activity (Crafts-Brandner and Law, 2000). Reduced photosynthesis rates, together with increased respiration at high temperature (Brooks and Farquhar, 1985), result in reduced net assimilation. The reduction in net assimilation is reversible, though if coinciding with anthesis may result in large reductions in grain number and yield (Porter and Gawith, 1999). However, as compensation for the negative effects of heat stress on net assimilation, remobilization of non-structural carbohydrates (NSC) to grains during grain filling increases and is considered vital to ensuring yield during high temperatures (Tahir and Nakata, 2005). The tradeoff is that high temperature accelerates leaf senescence due to oxidative damage (Harding et al., 1990). Development rates are accelerated with temperature (Roberts and Summerfield, 1987) resulting in lower yields due to the shorter grain filling period. Finally, reproductive failure, including pollen infertility, flowering and fertilization failure and grain abortion are significant and irreversible sources of yield loss under high temperatures associated primarily with a reduction in grain number (Porter and Gawith, 1999; Barnabás et al., 2008).

While many crop models account for the temperature effects on net assimilation and development rate, it is only recently that crop models have attempted to explicitly simulate heat stress effects such as accelerated senescence or the reduction of grain number due to the failure of reproductive processes (Asseng et al., 2011; Moriondo et al., 2011; Eitzinger et al., 2013). The later heat stress responses can be considered, and are represented in crop models, as discontinuities in the regular temperature responses driving grain yield formation. Further, much evidence supports that genotypes that maintain relatively higher yield levels under heat or drought stress have cooler canopies than genotypes with the greatest yield reductions (Pinto et al., 2010; Pinto and Reynolds, 2015). These authors hypothesize that the genotypic differences conferring cooler canopies are related to the ability of the roots to extract more water from the soil profile. As such, it is important to accurately estimate the absolute temperature of the affected plant tissue. As an example, consider that yield loss due to irreversible grain sterility begins at 31 °C (Wheeler et al., 1996a,b; Porter and Gawith, 1999), but no grain abortion occurs at 30 °C. In this case, being off by 1 °C could result in large errors of either under or overestimation of heat stress effects. This may not be true for the temperature dependence of net assimilation and radiation use efficiency (RUE) functions, for example, as both types of functions are continuous and being a few degrees off with the crop temperature implies a relative error proportional to the ratio of the error in temperature to the range of temperatures over which the function is defined. In spite of the need to correctly specify the crop temperature, most crop modelling attempts to account for heat stress have used air temperature (T_{air}), which can differ by several degrees from actual crop canopy temperature (T_c). Siebert et al. (2014) found that stress thermal time, an index of heat stress that sums temperatures greater than a high temperature threshold during a period in which crops are sensitive to heat stress (Blumenthal et al., 1991), computed with T_c and not T_{air} , is a more appropriate predictor of heat stress impacts on grain yield. Herein we hypothesize that T_c and not T_{air} must be used to simulate yield reductions under high temperature (Siebert et al., 2014) and the related progression of crop senescence (Kimball et al., 2012).

Critically, T_c can deviate significantly from T_{air} (Siebert et al., 2014; Rezaei et al., 2015). For example, when soils are wet, as after a rainfall or irrigation, T_c may be several degrees cooler than the air. In contrast, with a dry soil profile, canopies can be several degrees warmer than the air due to reduced transpiration rates associated with stomatal closure under water deficit (Clawson et al., 1989; Wall et al., 2006). However, low transpiration rates can also occur when soils are wet, for example when the air-canopy vapor pressure deficit (VPD) is low as is common in humid cool environments. Further, weather variables such as the amount of incident solar radiation and wind speed (which drives advection) have a large direct effect on T_c via the heat balance of the cropped surface (Monteith and Unsworth, 1990), and also indirectly through their influence on crop water use.

There are various way in which T_c for crop canopies can be simulated, ranging from very simple empirical relationships (e.g. Choudhury et al., 1986; Shuttleworth and Gurney, 1990) to solutions of the energy balance at a cropped surface. Within the energy balance approaches, there are two very different methods: complex energy balance approaches considering the stability conditions of the atmosphere (EBSC) (e.g. Thom, 1975) and greatly simplified methods which assume neutral atmospheric conditions (EBN). In any energy balance approach, net incident radiation, energy fluxes to the soil, latent energy to evaporate water from the cropped surface and sensible heat flux (energy to warm or cool the cropped surface) are summed to equal zero. Therefore, T_c can be solved from the sensible heat term. Both the latent and sensible energy terms depend on the resistance of the surface to transfer water vapour and heat to the air, respectively. The differences between the energy balance methods that assume neutral stability versus those that correct for atmospheric stability are related to how they calculate these aerodynamic resistance terms (Liu et al., 2007). To understand this difference, one must consider the concept of the dry adiabatic lapse rate (DALR). As imaginary small air pockets immediately next to the surface rise, they cool at the DALR, which is the equal to the temperature change needed to supply just enough energy to allow the expansion of the air such that its pressure decreases to that of the surrounding air (Monteith and Unsworth, 2008). The process is adiabatic as there is no net transfer of energy in or out of the air pocket. When air over hot and dry surfaces rises, it also cools at the DALR with the result that it is warmer than the surrounding air as it rises. As a result, the continued rise of the warmer (lighter) air is enhanced due to buoyant forces. The end result of this is that the resistance to heat and vapour transfer (via the rising air) is lower than it would be if the surface were not warm. The opposite occurs, i.e. resistance is greater, when a surface is relatively cool as occurs on clear nights with high radiative heat transfer from the surface, or under conditions with high evaporative cooling such as with wet soils in high and high evapotranspiration environments (Monteith and Unsworth, 2008). To account for this in energy balance methods requires iteration, as the solution and even the appropriate methods to determine the resistance terms are a function of the canopy (surface) temperature, which is unknown (Monteith and Unsworth, 2008). An alternative is to assume that the resistance is not affected by atmospheric stability, or that the actual lapse rate of the air is equal to the DALR, as assumed in the EBN methods. In this case, calculation of the resistance to heat and vapour transfer is just a function of the crop height and wind speed (Liu et al., 2007). However, the error made in this method may be significant depending on a number of factors.

To date, crop models typically employ more empirical (EMP) approaches (e.g. STICS) or the simplified EBN approach (e.g. Sirius2014). The more mechanistic EBSC approaches are found in other types of models for describing the plant environment (Mihailovic and Eitzinger, 2007) or ecosystem processes (Grant et al., 2012) or for controlling experimental heating for agronomic trials (Kimball

et al., 2008, 2015). In general, the data requirements for mechanistic approaches are similar to those required to estimate evapotranspiration using the American Society of Civil Engineers (Allen et al., 2005) or FAO-56 (Allen et al., 1998) Penman–Monteith method, but correction for atmospheric stability requires iteration as exact solutions are not possible (Liu et al., 2007). This is due to the interdependence of heat transfer to and from the cropped surface and T_c (Monteith and Unsworth, 1990). The EBN models neglect this interdependence. As a result, the main disadvantages of mechanistic approaches are the computational time and that they may also require more detailed meteorological data for their estimation. Empirical approaches are much simpler computationally, and in specific environments produce similar estimates of aerodynamic resistance compared to Thom (1975), as evaluated in Liu et al. (2007) and Shahrokhnia and Sepaskhah (2011). However, these methods are likely unreliable in other environments, especially in semi-arid regions.

The broad aim of this study is to evaluate whether simulation of T_c improves the ability of crop models to capture heat stress impacts on wheat under irrigated conditions in a semi-arid environment. The specific objectives are: (1) to assess the skill of different T_c models, representing three approaches (EMP, EBN and EBSC), to simulate T_c ; (2) to assess if crop models designed for and using T_c on a number of processes are better able to simulate grain yields under heat stress than crop models that only use T_c on processes related to heat stress. The research question behind this second objective is whether T_c should be used to model many crop processes or whether it is sufficient to use T_c only for processes sensitive to an absolute threshold of high temperature; (3) to determine if the use of simulated T_c , compared to T_{aai} , on processes sensitive to heat stress improves simulation of grain yield under heat stress; and (4) to assess which approach of simulating T_c results in the best simulation of grain yield under heat stress.

2. Materials and methods

2.1. Experimental description

The Hot Serial Cereal (HSC) experiment (Wall et al., 2011; White et al., 2011; Kimball et al., 2012, 2015; Ottman et al., 2012) in Maricopa, Arizona, U.S.A. (33°4'12" N, 111°58'12" W; 361 m above sea level) in which the spring wheat cultivar Yecora Rojo was grown between 2007 and 2009 provided the data to test the models. Maricopa is a hot and semi-arid environment and wheat was grown with full irrigation. To capture a range of temperature regimes, the crop was planted approximately every six weeks. For each sowing date and replication combination, the cumulative stress thermal time was calculated by summing daily maximum air temperatures greater than 31 °C between emergence and physiological maturity (Table 1). This information was used as the basis to determine the degree of heat stress in different sowing dates. For the purposes of the current canopy temperature study, data is presented by replication as individual plots within the same treatment had slightly different phenological development and were observed to senesce at different times, having a large impact on T_c . Seeds were sown (288 seeds m⁻²) in north-south rows, 0.19 m apart. Individual seeded blocks (sowing date) were 11 by 11 m in size and the plots were circular (3 m diameter) and centered within each block (Wall et al., 2011). Data are not available for the wheat planted in the summer as those crops did not survive due to heat and to intense competition with C₄ weeds. Final grain yield measurements were taken from 0.95 m² samples near the centre of each plot which were harvested between physiological maturity and harvest ripe stage (Ottman et al., 2012). Grain yield measurements were corrected to 0% moisture content.

Table 1

Cumulative stress degree days (°C days, threshold temperature 31 °C) in the Hot Serial Cereals (HSC) experiment based on daily maximum air temperatures during the period from emergence to physiological maturity for each sowing date by replication combination.

Emergence Date	Replication	Cumulative °days over 31 °C
27/03/2007	1	199.3
27/03/2007	2	175.3
27/03/2007	3	175.3
28/04/2007	1	396.3
10/11/2007	2	9.4
13/01/2008	1	43.1
13/01/2008	2	43.1
13/01/2008	3	41.5
20/02/2008	1	82.3
20/03/2008	1	160.3
20/03/2008	2	169.1
20/03/2008	3	154
06/05/2008	1	299.4
12/10/2008	1	36.5
05/11/2008	1	6.3
21/12/2008	1	54.5
21/12/2008	2	63.1
21/12/2008	3	40.2
23/01/2009	1	100.5

T_c was measured with infrared thermometers (IRTs; Model IRR-PN, Agogee Instruments Inc., Logan, UT, USA). Before January 2008, the IRTs were 1.0 m above the crop and pointing downward at an angle of 45° (Wall et al., 2011). However, at this height and angle, the sensor detected a large soil signal when the ground cover was still low and this created problems for controlling infrared heaters in adjacent plots (not considered in this study). As a result, the thermometers position was changed to 0.3 m height and at an angle of 30° below the horizontal (Wall et al., 2011). The T_c measurements used in this study are limited to those when the crop had full ground cover and maximum normalized difference vegetation index (NDVI) value (Kimball et al., 2012). Before this period of maximum NDVI, the soil temperature (Wall et al., 2013) had a dominating effect on the infrared temperature measurements and after this period, reduced stomatal conductance increased canopy temperatures as the crop senesced. Further, measured T_c were only available for every second sowing date (Table 1). A weather station on the site provided minimum and maximum temperature, solar radiation and wind speed. To cover times in which the weather station was not in operation, data from regressions between the Arizona meteorological station (AZMET) (<http://ag.arizona.edu/AZMET/06.htm>) weather station (1 km from site) and the site were used. Dew point temperature and precipitation were always from the AZMET station.

2.2. Model descriptions

The models used in this study are described in detail in other publications (see Asseng et al., 2015). The information presented in Table 2 summarizes key elements of how each model simulates canopy temperature, how heat stress is treated, and how T_c is applied in the current simulations to simulate heat stress effects.

2.3. Simulation setup

The models simulated 19 sowing date/replicate combinations of the HSC experiment, excluding treatments with frost damage. Modelers were supplied with daily weather data for simulations, but also provided with hourly weather and T_c data for their reference. Modelers were asked to set phenology dates to within ±1 day for each treatment according to observations of anthesis and maturity to exclude effects of incorrect phenology in this exercise. Soil

Table 2
Overview of the approaches to simulating canopy temperature (T_c). NA indicates non-applicable.

Model (2-letter code; references)	T_c approach	Approach to simulate heat stress (uses T_c step 1)	Other processes using T_c
APSIM Nwheat (AN, Asseng et al., 1998; Keating et al., 2003; Asseng et al., 2011)	EMP T_c is taken as 6 °C higher than air temperature (T_{air}) when the crop is fully stressed and 6 °C cooler than T_{air} on average when the crop is fully transpiring (Ayeneh et al., 2002; Maes and Steppe, 2012; Siebert et al., 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 et al., 1981; Jackson et al., 1981)	Heat stress effects only for leaf senescence with no effects on grain number or grain filling. Between maximum daily temperatures (T_{max}) of 32 and 34 °C, there is a linear transition between no acceleration of leaf senescence at $T_{max} < 32$ °C to a 50% increase at 34 °C. Leaf senescence is accelerated 3-fold at 40 °C (modified after Porter and Gawith, 1999)	None
Ecosys (EC, Grant et al., 2011)	EBSC T_c is that at which closure of the canopy energy balance [net radiation (R_{nc}) + sensible heat flux (H_c) + latent heat flux (LE_c) + change in heat storage ($G_c = 0$)] is achieved. Boundary layer resistance (r_a) is affected $T_c - T_a$ through the Richardson number. Canopy resistance, (r_c) is affected by canopy water status through canopy water and turgor potentials solved from soil-root-canopy-atmosphere hydraulic scheme	Seed set reduced by 0.01 during each hour that T_c rises above 33 °C (for wheat) or below 0 °C during anthesis and post-anthesis growth stages	All canopy CO ₂ fixation, growth, respiration and phenology processes
FASSET (FA, Olesen et al., 2002; Doltra et al., 2015)	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 step	9.5% increase in the rate of senescence when $T_{max} > 30$ °. No heat stress effects on grain number, grain filling or final yield	Phenology
SIMPLACE<Lintul2>* (SP, Gaiser et al., 2013; Zhao et al., 2015)	EBSC MOST used to solve for aerodynamic resistance (r_a). Calculate upper (no transpiration) and lower (full transpiration) limit of T_c and use soil water stress index to interpolate between the two limits	Grain yield reduced during period around flowering, with maximum reductions occurring above 40 °C and no reductions occurring when the temperature is cooler than 31 °C. The reduction factor varies linearly between these two extremes. Based on Challinor et al. (2005) as described in Eyshi Rezaei et al. (2013)	None
SIMPLACE<Lintul5>** (L5, Gaiser et al., 2013; Zhao et al., 2015)	EBSC Monin-Obukhov Similarity Theory MOST used to solve for r_a . Calculate upper (no transpiration) and lower (full transpiration) limit of T_c and use soil water stress index to interpolate between the two limits	Grain yield reduced when hourly temperature over 30 °C in the period 50 °C days before to 150 °C days after anthesis. Yield reduction factor used with $T_c - 0.03$ (°C hr) ⁻¹ whereas the yield reduction factor used with $T_{air} - 0.005$ (°C h) ⁻¹ . No heat stress effects on senescence	None
SiriusQuality (SQ, Martre et al., 2006; http://www1.clermont.inra.fr/siriusquality/)	EBN Described in Jamieson et al. (1995a,b)	Leaf senescence rate is accelerated by 45% per °C increase of T_c above 35 °C and 4-fold when T_c exceeds 34 °C. The acceleration factor is applied to 3-h T_c . No heat stress effects on grain number, grain filling or final yield	Grain dry matter and nitrogen (N) accumulation Leaf and stem N turn-over and remobilization Leaf (surface area) and internode (length) expansion*** Leaf emergence rate*** (for Haun index >4.) Leaf senescence RUE temperature response
Sirius2014 (S2, Jamieson et al., 1998; Jamieson and Semenov, 2000; Lawless et al., 2005)	EBN	Leaf senescence rate is accelerated by 10.8% per °C of 3-h T_c above 28.9 °C. In a period from 10 days before to anthesis, grain number is reduced by 2% per °C of $T_{c,max}$ above 32.5 °C. In a period of from 5 to 12 days after anthesis, the potential single grain dry mass is reduced by 0.1% per °C of $T_{c,max}$ above 38.6 °C Grain filling stops when $T_{c,max}$ is above 38 °C	After Haun stage 4 canopy temperature is used for all processes of wheat growth and development
STICS EMP (T1, Brisson et al., 2003; Brisson et al., 2008)	EMP T_c based on a relationship between midday surface temperature and daily evapotranspiration, also taking into account the net daily radiation and the canopy height (De Sanctis et al., 2013). $T_{c,max}$ cannot be lower than $T_{air,max}$ and $T_{c,min}$ is always equal to $T_{air,min}$	Grain filling stops when $T_{c,max}$ is above 38 °C	Phenological stages Leaf growth (LAI and biomass by radiation use efficiency) Root growth and senescence Grain water content Grain filling Senescence
STICS EBN (T2, Brisson et al., 2003; Brisson et al., 2008)	EBN Two instantaneous energy balances are calculated by an iterative convergence procedure to estimate $T_{c,max}$ and $T_{c,min}$, assumed to occur at midday and at the end of the night, respectively. Minimum and maximum values of net radiation, soil heat, evapotranspiration and r_a are taken into account. This method needs wind speed and humidity data	Grain filling stops when $T_{c,max}$ is above 38 °C	Phenological stages Leaf growth leaf area index (LAI) and biomass by RUE) Root growth and senescence Grain water content Grain filling Senescence

* SIMPLACE <Lintul2> is the shortened name for SIMPLACE<Lintul2,CC,DailyHeat,CanopyT>.

** SIMPLACE <Lintul5> is the shortened name for SIMPLACE<Lintul5,DRUNIR,HourlyHeat,CanopyT>.

*** Use near-surface soil temperature (Jamieson et al., 1995a) for Haun index <4.

properties, initial conditions, and crop management were provided as inputs. As modelers had already simulated these experiments in another study (Grant et al., 2011; Asseng et al., 2015), all observed crop growth data (grain yield and its components, aboveground biomass and nitrogen for grain, leaves and stems, leaf area index) were provided for calibration. Atmospheric CO₂ concentration was set at 385 ppm.

To accommodate the wide range of ways T_c is already used in some crop models, and for its use to simulate heat stress in models not previously using T_c , a simulation exercise was designed with two steps summarized in Fig. 1. In Step 1, all models used their simulated values of T_c as an input to processes judged to drive heat stress effects (acceleration of senescence reducing final grain weight, reduction in grain number or final yield resulting from failure of flowering, failure of fertilization and/or grain abortion), not already captured in the temperature responses of net assimilation related processes. This varied widely across the models (Table 2). Models normally using only T_a (AN, FA, L5 and SP) had to apply T_c to at least one heat stress related process. Models that were already using T_c continued to use T_c as per usual on other processes and in some cases did not need to make any changes for this step (EC, SQ, S2, T1 and T2). This step allowed a first comparison, as stated in the second objective of the study, of whether or not models normally using T_c do better at simulating grain yield under heat stress than models that normally use only T_{air} . In Step 2 (Fig. 1) referring to the third objective, models simulations were conducted using T_{air} on processes sensitive to heat stress. This implies that AN, FA, L5 and SP used T_{air} for all processes whereas the models that normally use T_c (SQ and S2) were run using T_{air} on processes sensitive to heat stress (i.e. grain number, harvest index, final grain yield and/or leaf senescence), but used T_c as per normal with other processes affecting crop growth or development. Three models did not perform Step 2 because of technical difficulties re-coding the models (T1 and T2) or because the modellers felt it was inappropriate to use T_{air} on the heat stress response in their model (EC). Results from Step 1 and Step 2 were compared for the six models that completed both steps to investigate if use of T_c compared to the use of T_{air} for heat stress effects improved simulations of grain yield. Modelers were able to calibrate their models for steps 1 and 2, but re-calibration between steps was to be limited to parameters controlling processes to which T_c versus T_{air} were switched and only for parameters related to the temperature response for that process.

2.4. Analysis of results

While a number of metrics may be used to evaluate model performance relative to the observations (Wallach et al., 2013), we used four main measures. The square root (RMSE) of the mean squared error (MSE) gives information in the same units as the variable of interest, whereas the root mean squared relative error (RMSRE) enables more meaningful comparison of errors across treatments, though being too sensitive for very low observed values. Further, the coefficient of determination (R^2), calculated as the square of the Pearson correlation coefficient. MSE and RMSE were calculated as:

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_{s,i} - y_{o,i})^2 \quad (1)$$

and

$$RMSE = \sqrt{MSE} \quad (2)$$

where $y_{o,i}$ is the i th observation of grain yield, $y_{s,i}$ is the i th simulated grain yield value, and N is the total number of observation and simulation pairs.

RMSRE was calculated as:

$$RMSRE = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{y_{s,i} - y_{o,i}}{y_{o,i}} \right)^2} \quad (3)$$

Additionally, MSE for grain yield was decomposed into three components: the squared bias (SB), a term related to the slope of the regression (b) between $y_{s,i}$ and $y_{o,i}$ (NU; non-unity slope), and a term related to the correlation (R^2) between $y_{s,i}$ and $y_{o,i}$ (LC; lack of correlation) using the method developed in Gauch et al. (2003). The three components sum to MSE, such that:

$$MSE = SB + NU + LC$$

where,

$$SB = (\bar{y}_{s,i} - \bar{y}_{o,i})^2; \quad NU = (1 - b)^2 \times \left(\frac{\sum_{i=1}^N y_{s,i}^2}{N} \right); \quad \text{and}$$

$$LC = (1 - R^2) \times \left(\frac{\sum_{i=1}^N y_{o,i}^2}{N} \right) \quad (5)$$

with b the slope of the least squared regression of $y_{o,i}$ on $y_{s,i}$. All calculations and plotting were done using the statistical software R (R Core Team, 2013) with the RStudio software package (version 0.98.953).

3. Results

3.1. Canopy temperature simulations

The time course of daily maximum temperature over the period of the experiment is plotted in Fig. 2a. The figure also shows daily maximum observed T_c values and the spread of simulated T_c values. The ability of the models to reproduce the observed difference between daily maximum values of T_c and T_{air} , ($\Delta T = T_c - T_{air}$) is shown in Fig. 2b and in Figs. 3 and 4. Observations were only available for approximately one half of the sowing dates, and also only when the crop had a full ground cover and had not yet started senescence, constituting the key phase when crops are sensitive to heat stress (Barlow et al., 2015; Rezaei et al., 2015). Of the approaches to simulate T_c , the EBSC models had the highest degree of correlation with observations, and also the lowest RMSE (2.9 °C) while the EBN exhibited the highest RMSE at 6.7 °C. The performance of the EMP models was similar to the EBN in terms of correlation with observations, with R^2 values of 0.10 and 0.02, respectively. On the other hand, the RMSE of the EMP models (3.9 °C) was close to that of the EBSC models, much lower than that of the EBN models. All three groups exhibit some degree of bias towards over-estimation of T_c , but this is greatest for the EBN models. The EBN models' simulated ΔT_{sim} was better when ΔT_{obs} was close to zero, as is expected with EBN approaches. The error in their simulations increased as ΔT_{obs} became more negative, indicating that T_c was cooler than T_{air} . No simple single variable regression relationships were found between the studentized residuals of the regressed ΔT_{obs} and ΔT_{sim} values and either of T_{air} , daily air vapour pressure deficit (VPD) or daily incident solar radiation (Fig. 5).

Within the three groupings, additional error was introduced by the specific implementation of T_c and/or its interactions with other processes in the individual crop models (Fig. 4). The R^2 values of the three EMP models ranged between 0.00 (STICS-EMP) and 0.37 (FAS-SET), and their RMSE values ranged from 2.3 °C (APSIM Nwheat) to 5.9 °C (STICS-EMP). The high RMSE indicated a tendency to overestimate T_c as the observed T_c was less than T_a . All three EBN models had a positive bias with similar values of RMSE of 5.7 °C (SiriusQuality) to 8.0 °C (STICS-EBN). In all cases the error increased as observed T_c became increasingly lower than T_a whereas there was more variation in terms of correlation, with R^2 values ranging between

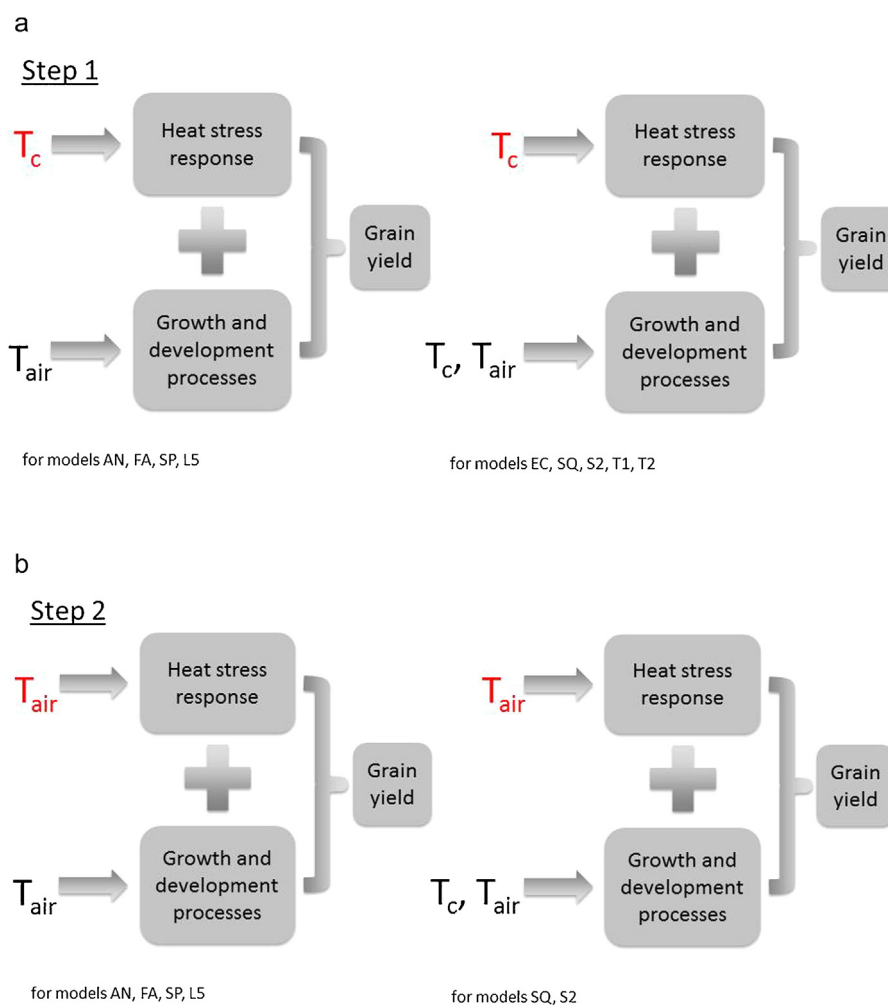


Fig. 1. Overview of the two steps in the simulation exercise and list of models that participated in each step. In Step 1, T_c was applied in all models to simulate heat stress effects. T_c was additionally used in EC, SQ, S2, T1 and T2 in other processes, whereas T_{air} was used for all other processes in AN, FA, SP and L5. All models were required to participate in Step 1. In Step 2, T_{air} was applied in all models to simulate heat stress effects. T_c was additionally used in SQ and S2 in other processes. Step 2 was designed for a subset of models to enable a comparison of grain yield simulations when T_c versus T_{air} was used to simulate heat stress responses. Not all models in Step 1 were able to complete Step 2.

0.24 (SiriusWheat) and 0.00 (STICS-EBN). In the final group, the EBSC models, two of the models had little bias with RMSE values of 1.4 °C (SIMPLACE <Lintul5>) and 2.0 °C (SIMPLACE <Lintul2>), whereas a third model in this group had a positive bias and RMSE of 4.4 °C (ecosys). However, all three models had a better correlation with observations than models in other groups, with R^2 values ranging between 0.4 (ecosys) and 0.75 (SIMPLACE <Lintul5>). Two of the crop models in this group (SIMPLACE <Lintul2> and SIMPLACE <Lintul5>) used the same T_c implementation but embedded in different crop models. Their T_c simulations are not identical (Fig. 4g and 4h) due to interactions in the models between LAI, crop height, water stress, and T_c .

3.2. Grain yield simulations using canopy temperature

All models were run using their simulated values of T_c to account for heat stress effects as defined by the modelers. Some models were modified for this exercise to have these processes responsive to T_c instead of T_{air} (discussed in the next section), whereas other models did not require modification as they already used T_c (Table 2). Taken across all treatments, the models that use T_c on a number of processes in addition to heat stress responses (i.e. ecosys, SiriusQuality, Sirius2014, STICS EMP, STICS EBN) had a RMSE of 2.2 t ha⁻¹, (RMSRE of 0.42) and an R^2 of 0.42 (Fig. 6a), whereas

those which used T_c only for heat stress responses (i.e. APSIM Nwheat, FASSET, SIMPLACE <Lintul2>, SIMPLACE <Lintul5>) had a RMSE of 1.5 t ha⁻¹, (RMSRE of 0.36) and a R^2 of 0.66 (Fig. 6b). To see if improvement in models performance using T_c depended on the magnitude of heat stress, we considered sowing date/repetition combinations having more than 150 °C days (threshold temperature 31 °C calculated with daily maximum air temperature) (Porter and Gawith, 1999) between sowing and maturity (Table 1). While much evidence suggests that the most critical period for heat stress is around anthesis and grain filling (Wheeler et al., 2000), we considered the whole growing period as the models employ different critical periods and we wanted to avoid biasing the comparison among models. The group of models that considered T_c only for heat stress processes (i.e. APSIM Nwheat, FASSET, SIMPLACE <Lintul2> and SIMPLACE <Lintul5>) simulated final grain yield with a RMSE of 1.1 t ha⁻¹, (RMSRE of 0.42) and a R^2 value of 0.78 in the heat stress treatments (Fig. 6b), as compared to a RMSE of 2.0 t ha⁻¹, (RMSRE of 0.42) and a R^2 value of 0.47 for the models that used T_c on many processes (Fig. 6a). The models using T_c on many processes exhibit higher bias or SB, as well as NU, than the models using T_c only for their heat stress response (Fig. 7). However, for both types of models, the NU error, associated with a deviation between the 1:1 line in the linear relationship between observed and simulated values decreases when only the heat stress treat-

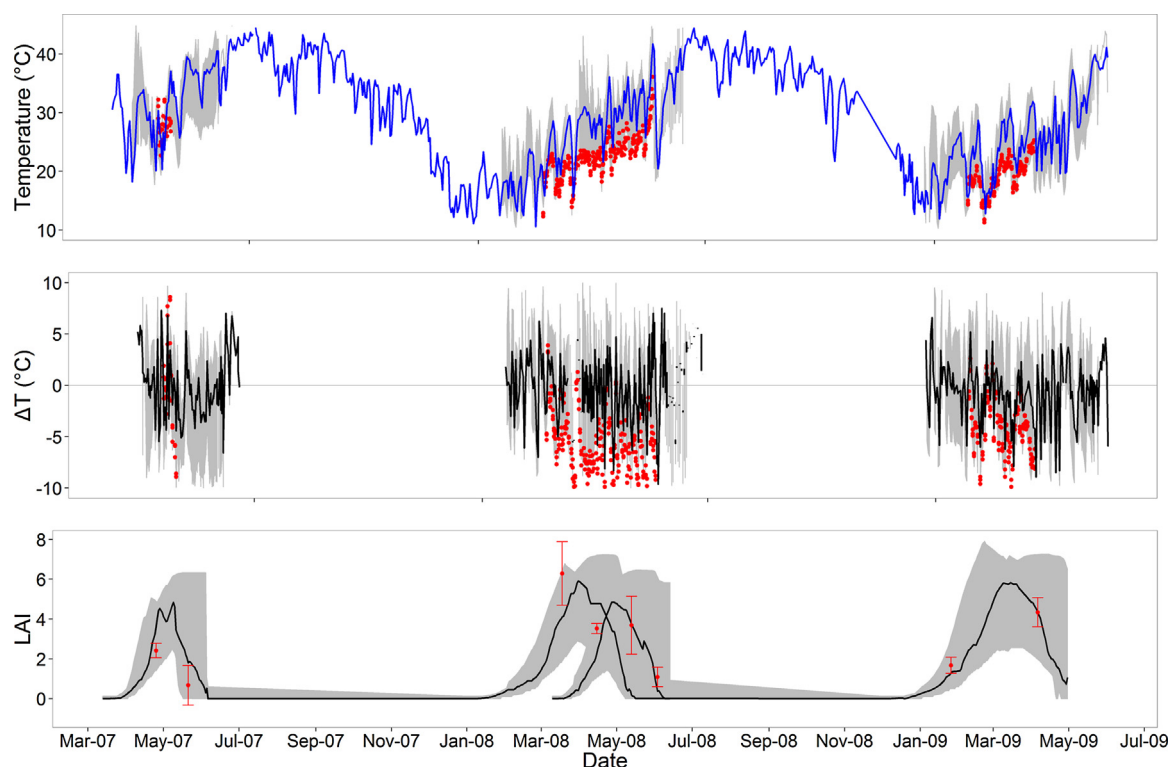


Fig. 2. Measurements of daily maximum air temperature (T_{air} , blue line) at the experimental site and canopy temperature (T_c , red circles) compared to the range (grey shading) of simulated T_c values across models are shown in panel (a). Panel (b) shows observed ΔT ($\Delta T = T_c - T_{\text{air}}$, red circles) for daily maximum values compared to the median (black line) and the range (grey shading) of simulated ΔT values across models. Simulations are only shown for the periods in which simulations were conducted. Observations of T_c and ΔT are only shown when the canopy was fully closed and the crop was not yet senescent and which were further only available for one half of the sowing dates. Panel (c) contains the median (black line) and range across models (grey shading) of LAI simulations. LAI observations are shown as red circles and the standard deviation of the observations are shown with red error bars. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

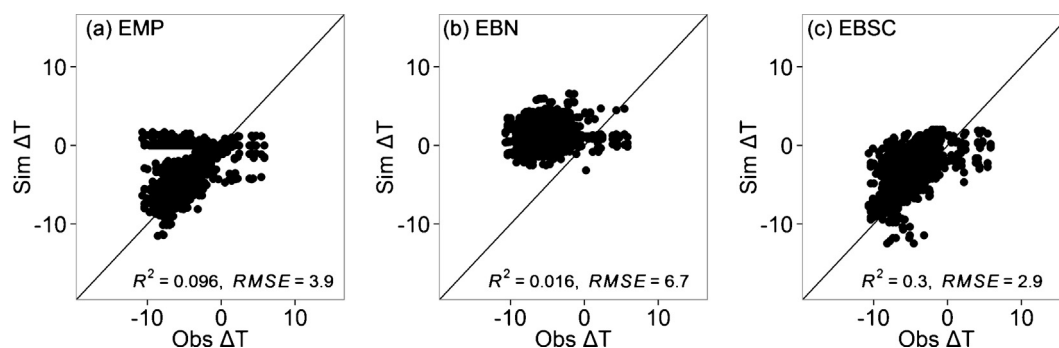


Fig. 3. Simulated vs. observed ΔT (°C), where $\Delta T = T_c - T_{\text{air}}$, for daily maximum values of T_c and T_{air} , over all sowing date/repetition combinations for (a) empirical (EMP), (b) energy balance assuming neutral stability (EBN) and (c) energy balance correcting for atmospheric stability (EBSC) approaches. Solid lines represent the 1:1 line.

ments are considered. Likewise, the LC error, associated with the degree of correlation between simulated and observed differences, decreases for both model groups when only the heat stress treatments are considered and was smaller for the models that used T_c only for heat stress responses.

Regardless of whether T_c was used on many processes or only to simulate the heat stress response, the models which used EBN simulated grain yields with a RMSE value of 1.7 t ha^{-1} (RMSRE of 0.39), slightly better than EMP or EBSC models, which had RMSE values of 1.8 (RMSRE of 0.42) and 2.3 t ha^{-1} (RMSRE of 0.45), respectively (Fig. 8). Likewise, the correlation between observations and simulations of the EBN approach ($R^2 = 0.60$) was slightly higher than those of the EMP ($R^2 = 0.55$) or EBSC ($R^2 = 0.44$) approaches, despite the fact that the latter two approaches were superior in simulat-

ing T_c (Fig. 3). Examination of the error components of each model type did not reveal a consistent relationship between the lack of agreement with the slope, lack of correlation or systematic error in explaining the different model types' ability to simulate grain yield (Fig. 9). In all cases, there was more bias (SB) when only the heat stress treatments were considered, though the EBSC models had the least bias for the heat stress treatments.

There appears to be no definite relationship between the quality of the T_c and grain yield simulations for the models across all treatments (Fig. 10a) based on the ranking of the models for skill in simulating the two variables. The ranking is intended to visually demonstrate possible patterns in the relationship between T_c and grain yield simulations, though the use of only nine models is insufficient to allow much confidence in the ranking results. The models

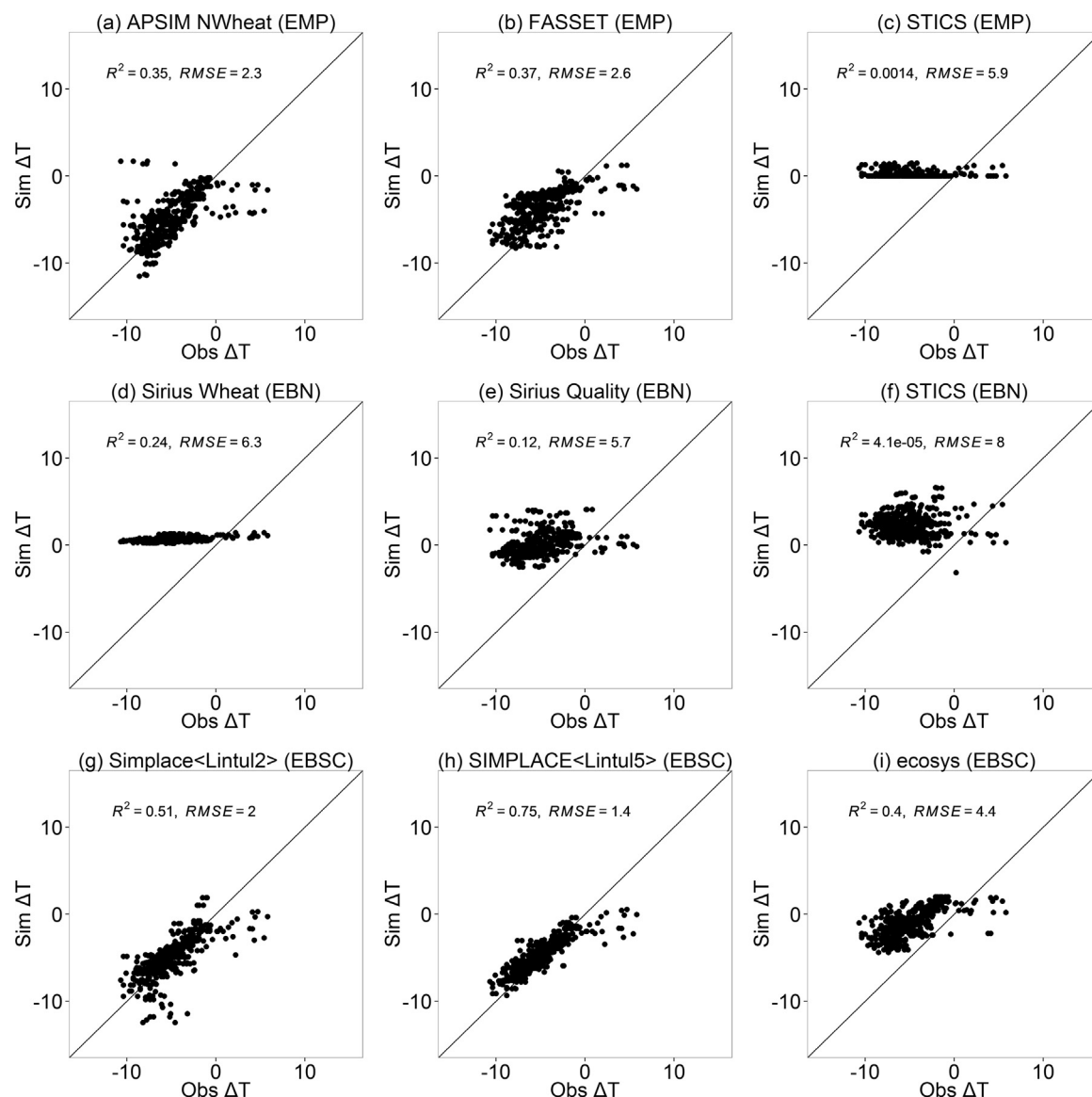


Fig. 4. 1-to-1 plots of simulated vs. observed ΔT ($^{\circ}\text{C}$), where $\Delta T = T_c - T_{\text{air}}$, for daily maximum values of T_c and T_{air} , for the eight crop models over all sowing date/repetition combinations. Model simulations in panel (a)–(c) use empirical (EMP) expressions to simulate T_c , (d)–(f) use approaches based on an energy balance but assume neutral stability atmospheric conditions (EBN), while (g)–(i) use energy balance approaches with corrections for atmospheric stability conditions (EBSC).

ranked in the top positions for grain yield simulations included both models ranked at the top for T_c simulation, as well as those ranked poorly or moderately for simulating T_c . However, the models with the lowest rankings for skill in simulating grain yield also had the lowest ranking for simulating T_c . All three approaches to simulating T_c were among the highest ranked models for simulating yield, regardless of their skill in simulating T_c . Likewise, considering only the treatments with heat stress shows that there was not a strong relationship between the skill of the model in simulating T_c and grain yield, as the second highest ranked model for simulating grain yield was ranked 8th for simulating T_c (Fig. 10b). As in the case of all treatments, the models with the lowest rank for simulating grain yield under heat stress also had low ranks for simulating T_c .

For the six models that were run using both T_c and T_{air} on processes driving heat stress responses, across all treatments, the use of T_c lead to lower values of RMSE for grain yield for five of the models, and no change for one model (Fig. 11 and Table 3). When only the treatments with heat stress are considered, defined as having greater than 150°days over 31 $^{\circ}\text{C}$ (Table 1), five of the models show a decrease in RMSE with the use of T_c and only the Sirius2014

Table 3

Change in RMSE ($\Delta\text{RMSE} = \text{RMSE}_{T_{\text{air}}} - \text{RMSE}_{T_c}$) of grain yield model simulations over all treatments and treatments with heat stress when T_c is used in place of T_{air} to simulate heat stress effects. Only the SIMPLACE < Lintul5> model was re-calibrated between steps.

Model	ΔRMSE	
	All treatments	Treatments with heat stress
APSIM NWheat (EMP)	0.09	0.09
FASSET (EMP)	0.09	0.30
SIMPLACE < Lintul2> (EBSC)	0.01	0.06
SIMPLACE < Lintul5> (EBSC)	1.29	2.45
SiriusQuality (EBN)	0.73	1.15
Sirius2014 (EBN)	0.00	0.00

model shows no change (Fig. 12). In the treatments with heat stress, grain yields tended to be smaller when T_{air} was used. This is due to irrigation in semi-arid conditions, which frequently resulted in the T_c being several degrees lower than T_{air} with the result of less heat stress. Four of the models, FASSET, SIMPLACE<Lintul2>, SIMPLACE<Lintul5> and SiriusQuality showed a greater improvement in

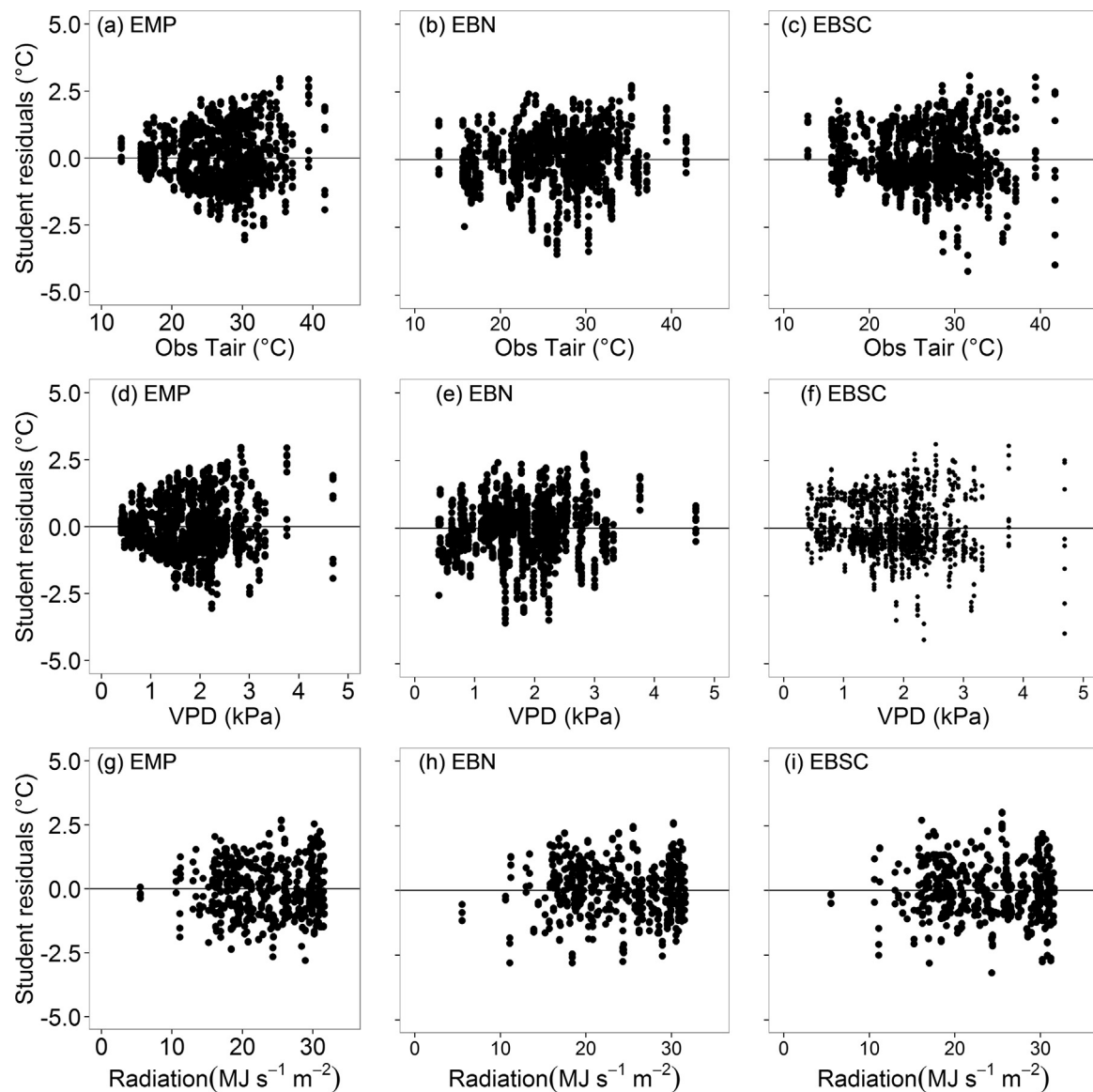


Fig. 5. Studentized residual errors of ΔT ($\Delta T = T_c - T_{air}$) for the three model types EMP (a, d, g), EBN (b, e, h) and EBSC (c, f, i) regressed against T_{air} (a)–(c), vapour pressure deficit (VPD) (d)–(f), and daily incident solar radiation (g)–(i). In each figure, the black line is $y = 0$.

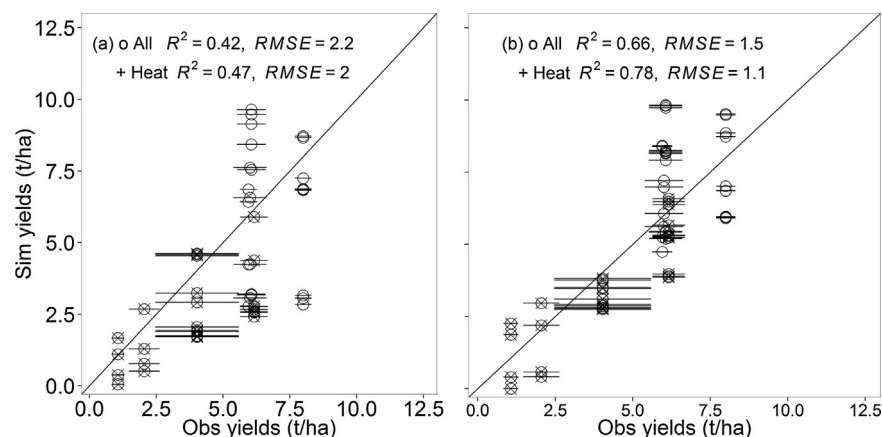


Fig. 6. 1-to-1 plot of simulated (Sim) vs. observed (Obs) final grain yield over all sowing dates/replications combinations (o symbol) and the sowing dates/replications combinations (x symbol) with heat stress for models (a) using T_c with many processes and (b) using T_c only for their heat stress responses with T_{air} with all other processes. Solid horizontal lines show the SD of the observations. The 1:1 runs diagonally in the figures.

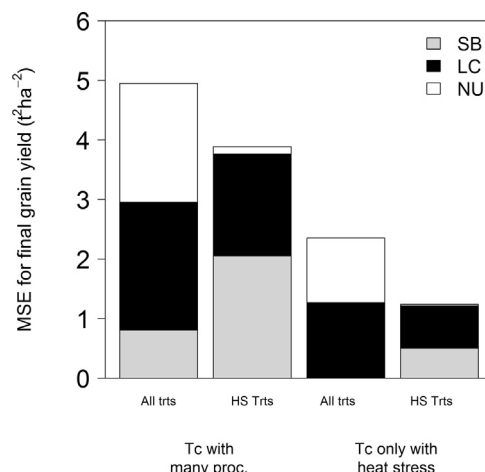


Fig. 7. MSE and its components, squared bias (SB), non-unity slope (NU), and lack of correlation (LC), calculated with simulated and observed final grain yield for models using T_c with many processes and using T_c only for their heat stress responses with T_{air} with all other processes. MSE is shown over all sowing dates/replications combinations (All trts) and the sowing dates/replications combinations with heat stress (HS Trts).

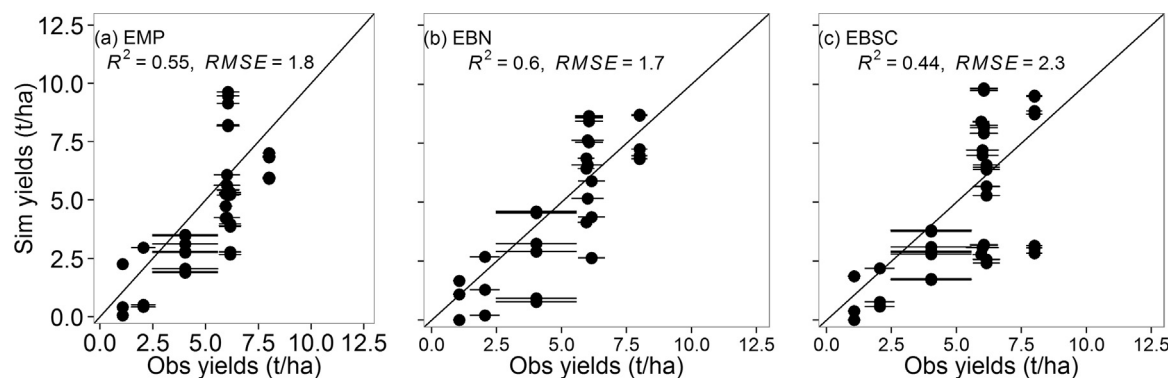


Fig. 8. 1-to-1 plot of simulated (Sim) vs. observed (Obs) final grain yield over all treatments separated according to the approach to simulate T_c : (a) empirical (EMP), (b) energy balance assuming neutral stability (EBN) and (c) energy balance correcting for atmospheric stability (EBSC). Solid horizontal lines show the SD of the observations. The 1:1 runs diagonally in the figures.

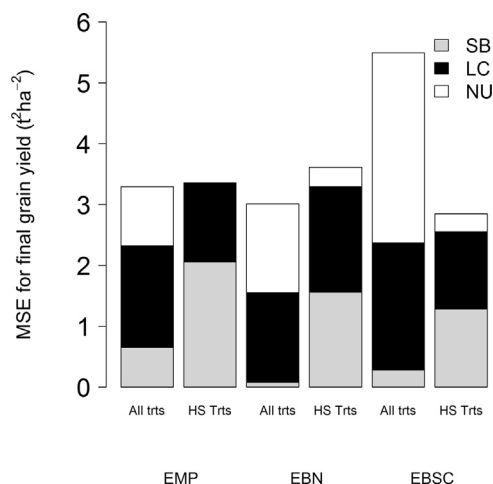


Fig. 9. MSE and its components, squared bias (SB), non-unity slope (NU), and lack of correlation (LC), calculated with simulated and observed final grain yield for models using the EMP, EBN and EBSC approaches to simulate T_c . MSE is shown for all sowing dates/replications combinations (All trts) and the sowing dates/replications combinations with heat stress (HS Trts).

4. Discussion

To the best of our knowledge, this is the first study to evaluate the use of T_c to simulate heat stress effects in cereals. We tested nine different methods embedded in widely applied crop models, representing three approaches to simulate T_c . While the analysis is not fully orthogonal for reasons discussed later, they are likely to be overcome in future studies. Nevertheless, our results point to some key findings which can guide future model inter-comparison and improvement work related to heat stress.

In our model comparison, we found a wide variation in the skill of the three approaches to simulate T_c of irrigated wheat in a semi-arid environment. The EMP approaches performed almost as well as the EBSC approaches, and much better than the EBN models. However, caution is needed if one is to extend the EMP approach to other environments or possibly even to the same location in climate change impact studies. Due to the nature of empirical approaches, it cannot be assumed that the relationships among the main variables controlling T_c (T_{air} , radiation, windspeed, vapor pressure deficit) will be the same in other environments or climates. Therefore, future studies should evaluate the potential of empirical approaches across environments.

The poor performance of the EBN methods in simulating T_c was not surprising, given that the assumption of neutral stability implies that there is little heat transfer between the cropped surface and ambient air, and that T_{air} and T_c should therefore be largely

grain yield simulation with the use of T_c in the treatments with heat stress than they did when all treatments were considered (Table 3).

similar. While assumptions of neutral stability are frequently made for calculations of reference crop ET, such calculations assume a well-watered crop and estimate water use over a day (Allen et al., 1998). However, while most of the models evaluated here also use a daily time step, they are estimating a daily maximum T_c which occurs for a relatively short period of the day and is often associated with large heat fluxes, thereby invalidating the neutral stability assumptions (Allen et al., 1998). However, for the irrigated conditions of the HSC experiment investigated in this study, T_c was infrequently higher than T_{air} and the error in ΔT is expected to be larger under other production/environment conditions where transpiration is less and/or water stress is frequent. Further, the STICS models both limit $T_{c,max}$ to be no cooler than $T_{a,max}$ which occurred infrequently with the measurements in this experiment.

This study revealed that the EBN models simulated grain yield well despite their relatively poor simulation of T_c , compared to the other models. By coincidence, the EBN models sampled in this study, also use T_c for processes other than heat stress effects and have been calibrated over many other experiments with their simulations of T_c . It may be that the bias in T_c estimates with the EBN approach are compensated by the parameterization of the threshold temperature for their heat stress response, as we hypothesized to happen when T_{air} is used. For example, in STICS grain filling stops when temperature are greater than 38 °C, SiriusQuality uses a threshold temperature of 35 °C to accelerate senescence, and Sirius2014 uses 32.5 °C to reduce grain number and 38.6 °C to limit grain filling. All of these thresholds are higher than 31 °C which is the threshold widely held to explain yield reductions under heat stress (Wheeler et al., 1996a,b; Porter and Gawith, 1999).

In trying to answer whether consideration of T_c can improve grain yield simulations under heat stress, we compared various aspects of the problem. First, we considered whether models that explicitly model effects of T_c on a number of processes simulate grain yield better than models that use only T_{air} and have been modified for this study to use T_c only for processes driving their heat stress response. We found that across all models, the group of models normally using only T_{air} and modified to use T_c on processes sensitive to heat stress performed better than models normally using T_c . This trend held for simulations across all sowing date/replicate combinations as well as simulations in combinations with heat stress (Fig. 6). When individual models were considered, models of each type ranked best and worst in simulating grain yield (Fig. 10). From this, we loosely conclude that simulation of heat stress does not require crop models to be completely reworked to use T_c on all processes. However, the models using T_c on many processes (STICS EMP, STICS EBN, SiriusQuality, Sirius2014 and ecosys) all had positive bias on their T_c simulations, so it is not possible to know if their yield simulations would improve with better T_c simulations.

Secondly, we evaluated whether models improved their skill in grain yield simulation when T_c replaced T_{air} in heat stress responses, and if the magnitude of the improvement depended on whether there was heat stress. In general, the use of T_c reduced RMSE values and increased the R^2 value, though the improvement was modest in all but three of the models (SiriusQuality, FASSET and SIMPLACE <Lintul5>) (Figs. 11 and 12). There are many reasons that may explain why the use of T_c did not improve simulations to a greater extent. The first is in how the individual models represent heat stress. In SIMPLACE <Lintul5>, which showed the greatest improvement when T_c replaced T_{air} , each °C hour above 30 °C results in a grain yield reduction 2.5%. If only T_{air} is used, even with a much smaller value of the reduction factor (e.g. 0.5%) after calibration (taken as the lower limit of the parameter), the result was that too much heat stress was simulated, as T_c was generally a few degrees cooler than T_a . If models do not have such functions

that operate with a threshold and discontinuity, they are unlikely to pick up large improvements by using T_c .

Secondly, this dataset was used in a previous model comparison (Martre et al., 2003; Asseng et al., 2015), in which modellers calibrated their grain yield simulations but had no information on the T_c . Only the SIMPLACE <Lintul5> did not participate in the earlier studies, and it is this model which, perhaps coincidentally, shows the greatest improvement in grain yield simulations when T_c is used rather than T_{air} . Also, though each modeller had the opportunity to re-calibrate between steps 1 and 2, only SIMPLACE <Lintul5> did. This is very likely due to the fact that during calibration in the earlier simulation exercise, the other models set threshold temperatures for heat stress higher than 31 °C (Wheeler et al., 1996a,b; Porter and Gawith, 1999), with the exception of FASSET and SIMPLACE <Lintul2>. It should be noted that FASSET simulations also showed improvement when T_c replaced T_{air} in its heat stress response.

Finally, we examined if there was a relationship between the skill in grain yield simulation and skill in T_c simulation. Considered over all treatments, generally the models that did well in simulating T_c also did well in simulating final grain yield and conversely (Fig. 10). However, some models that performed only moderately well with T_c simulations, such as SiriusQuality and Sirius2014, estimated final grain yield better. Both of these models use the EBN approach to simulate T_c and had considerable positive bias though relatively good correlation with observed T_c (Fig. 4). Perhaps this is explained in these models by either (1) little sensitivity of the models to heat stress, and/or (2) their use of higher temperature thresholds than encountered in reality (Wheeler et al., 2000; Porter and Semenov, 2005) as discussed above. Much like the challenge of using EMP models, this approach of adjusting the threshold temperature cannot be assumed to be robust across climatic conditions or production systems. For example, in rainfed systems with frequent drought conditions or very little atmospheric evaporative demand, it is not unusual for T_c to be several degrees warmer than T_{air} , and such conditions would require heat stress temperature thresholds to be lower than reality (Siebert et al., 2014). Furthermore, such systems can also have T_c below T_a after a rainfall event when the crop is well watered and atmospheric evaporative demand is high, with the result that too much heat stress would be simulated. More generally, this raises the question of the relative importance of heat stress responses in many of the models tested here, and in particular their importance as compared to other processes (e.g., phenology, dry matter production, crop nitrogen response), which determine grain yield. It is beyond the scope of our study to investigate the sensitivity to the models to heat stress as the approaches and thresholds differed greatly between models. By coincidence, the EBN models all include functions to reduce grain yield or seed set with high temperature, whereas the EBN and EMP models contain variations of accelerating senescence, reducing yield or seed set, reducing grain weight, or stopping grain filling with no consistency between EBN and EMP approaches. As many of the models did not show a significant improvement in grain yield simulation with the use of T_c , it is not possible to relate an acceptable error in T_c simulations to enable simulation of grain yield with a given confidence interval. For a model such as SIMPLACE <Lintul5> which reduces grain yield for cumulative degree hours above a high temperature threshold, one could do a sensitivity analysis to determine what error in T_c is acceptable to still simulate yield with a given error range. However, this is not reasonable for the SiriusQuality and Sirius2014 models which had large error (bias) in their T_c estimates, but simulated final grain yield well, as discussed above.

Canopy temperature depression is a key trait used by breeders to select wheat lines with tolerance to heat and drought stress (Pinto et al., 2010; Pinto and Reynolds, 2015). The mechanism responsible for canopy cooling seems to be deeper roots in dry soils and

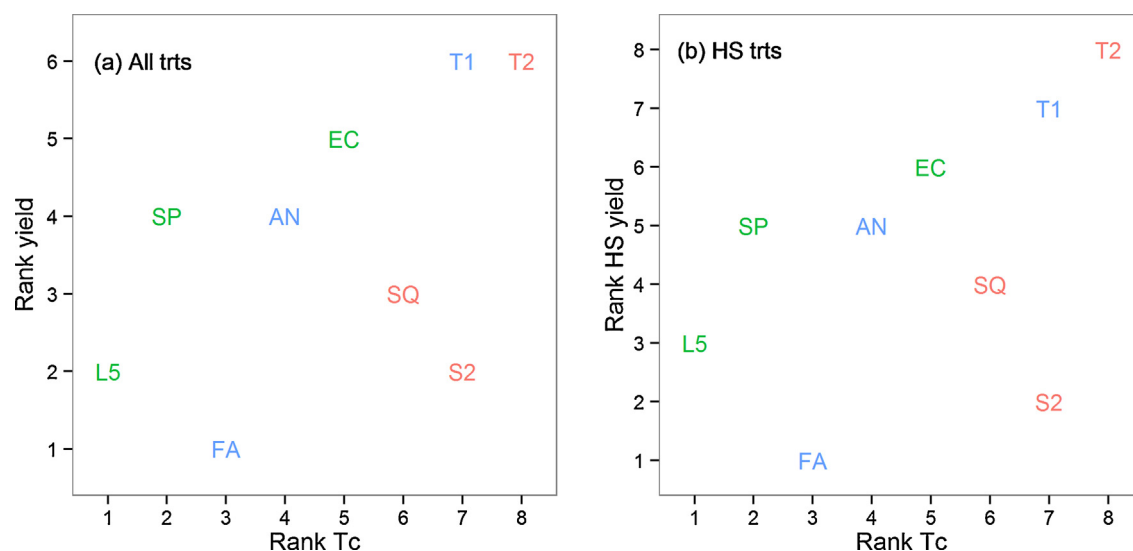


Fig. 10. Models are ranked by their ability to simulate canopy temperature (T_c) on the horizontal axis and final grain yield on the vertical axis over (a) all treatments and (b) HS treatments defined as having greater than 150 °C days (base temperature 31 °C) between sowing and maturity. In both cases, the ranking was based on taking the average of the rank for RMSE (lowest values rank highest) and the rank for the correlation coefficients (highest values rank highest) and further ranking the average ranking. Models in blue are EMP, models in pink were EBN and model names that are green are EBSC. Two letter codes for each model are given in Table 2.

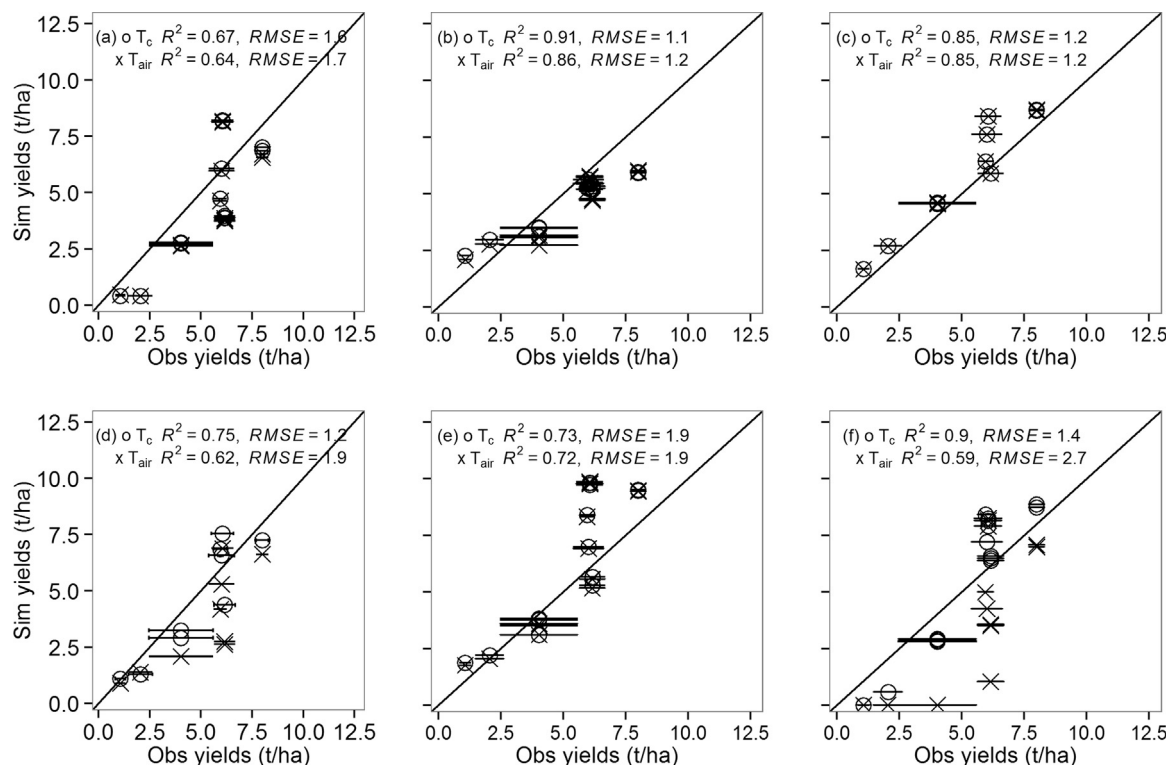


Fig. 11. Simulated vs. observed final grain yield for the six crop models that were able to simulate both steps 1 and 2, over all sowing date repetition combinations. Model simulations in panel (a) APSIM Nwheat and (b) FASSET have EMP expressions for T_c , (c) Sirius2014 and (d) SiriusQuality use EBN expressions, while (e) SIMPLACE <Lintul2> and (f) SIMPLACE <Lintul5> use EBSC approaches. Open circles are for simulations with canopy temperature and crosses are for simulations with air temperature. Solid lines represent 1:1 lines.

greater root biomass when high temperatures occur under irrigated conditions (Pinto et al., 2010; Pinto and Reynolds, 2015). Though this study did not consider the ability of models to distinguish between genotypes, many of the modelling approaches presented should be able to do so, as their canopy temperature simulations are a function of soil water status. Testing canopy temperature model performance across genotypes should be the focus of further investigation.

Our study focused on the effects of simulating heat stress, i.e. effects of maximum canopy temperature. Similar considerations may be applied to the simulation of effects of minimum temperature on cold damage in plants. However, even though the same physical principles are applied for the heat balance during night, it is principally different since low canopy and surface temperatures typically occur under clear sky conditions with little longwave incoming radiation and with low wind speed resulting in mete-

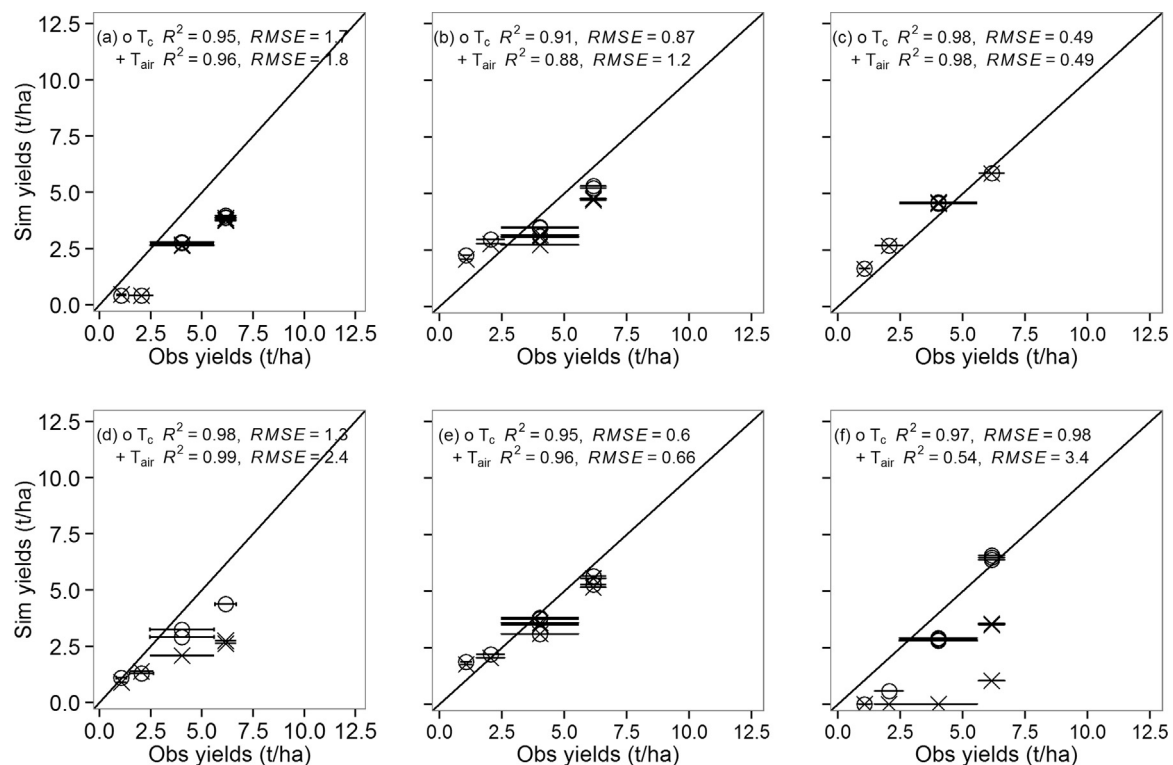


Fig. 12. Simulated vs. observed final grain yield for the six crop models that were able to simulate both steps 1 and 2, for the treatments with heat stress. Model simulations in panel (a) and (b) have EMP expressions for T_c , (c) and (d) use EBN expressions, while (e) and (f) use EBSC approaches. Open circles are for simulations with canopy temperature and crosses are for simulations with air temperature. Solid lines represent 1:1 lines.

orological inversion conditions. Therefore, simulating minimum canopy temperatures may be principally different from the effects of maximum temperatures presented here.

5. Conclusions

This study evaluated whether simulation and use of T_c improve the ability of crop models to simulate heat stress impacts on wheat grain yields under irrigated conditions. Nine process-based crop models, each using one of three broad approaches (EMP, EBN and EBSC) to simulate T_c , were compared under a range of temperature conditions. The models varied widely in their ability to reproduce the observed T_c with the commonly used energy balance approaches assuming neutral stability conditions performing much worse than either empirical or energy balance approaches correcting for atmospheric stability. While we generally saw an improvement in the simulation of grain yields under heat stress with T_c compared to T_{air} , this effect was not as pronounced as we expected. However, the improvement was substantial for two models, and for all six models, the reduction in RMSE was larger when only the heat stress conditions were considered. The use of T_c on more processes than just the heat stress response did not result in better grain yield simulations. Models that did well in simulating grain yield under heat stress had varying skill in simulating T_c , highlighting the need to more systematically understand and quantitatively model heat stress events in wheat.

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