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

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A B S T R A C T
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 a) in their heat stress responses despite evidence that canopy temperature (T c) better explains grain yield losses. T c can deviate significantly from T a 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 a 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 (Tair), which can differ by several degrees from actual crop canopy temperature (Tc). 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 Tc and not Tair, is a more appropriate predictor of heat stress impacts on grain yield. Herein we hypothesize that Tc and not Tair 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, Tc can deviate significantly from Tair (Siebert et al., 2014; Rezaei et al., 2015). For example, when soils are wet, as after a rainfall or irrigation, Tc 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 Tc 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 ways in which Tc 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, Tc 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 vapor 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. Siritus 2014). 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., 2012).
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 Shahrokhiinia 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 $T_a$ 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 $T_a$, 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.

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

$T_c$ was measured with infrared thermometers (IRTs; Model IR-SPN, 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.

<table>
<thead>
<tr>
<th>Model (2-letter code; references)</th>
<th>$T_c$ approach</th>
<th>Approach to simulate heat stress (uses $T_c$ step 1)</th>
<th>Other processes using $T_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>APSIM Wnheat (AN, Asseng et al., 1998; Keating et al., 2003; Asseng et al., 2011)</td>
<td>EMP $T_c$ is taken as 6°C higher than air temperature ($T_a$) when the crop is fully stressed and 6°C cooler than $T_a$ 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, 1981)</td>
<td>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 $T_{max}$ &lt; 32°C to a 50% increase at 34°C. Leaf senescence is accelerated 3-fold at 40°C (modified after Porter and Gawith, 1999)</td>
<td>None</td>
</tr>
<tr>
<td>Ecosys (EC, Grant et al., 2011)</td>
<td>$T_c$ is at which closure of the canopy energy balance (net radiation ($R_{net}$) + sensible heat flux ($H_s$) + latent heat flux ($L_E$) + change in heat storage ($G_c = 0$)) is achieved. Boundary layer resistance ($r_b$) 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 hydrodynamic scheme</td>
<td>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</td>
<td>All canopy CO₂ fixation, growth, respiration and phenology processes</td>
</tr>
<tr>
<td>FASSET (FA, Olesen et al., 2002; Doltra et al., 2015)</td>
<td>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</td>
<td>9.5% increase in the rate of senescence when $T_{max} = 30°C$. No heat stress effects on grain number, grain filling or final yield</td>
<td>Phenology</td>
</tr>
<tr>
<td>SIMPLACE&lt;Lintul2&gt; (SP, Gaiser et al., 2013; Zhao et al., 2015)</td>
<td>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</td>
<td>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 Chällinor et al. (2005) as described in Eyshi Rezaei et al. (2013)</td>
<td>None</td>
</tr>
<tr>
<td>SIMPLACE&lt;Lintul5&gt; (LS, Gaiser et al., 2013; Zhao et al., 2015)</td>
<td>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</td>
<td>Grain yield reduced when hourly temperature over 30°C in the period 50-100°C days before to 150°C days after anthesis. Yield reduction factor used with $T_c = 0.03 (°C h)^{-1}$ whereas the yield reduction factor used with $T_{max} = 0.005 (°C h)^{-1}$. No heat stress effects on senescence. Leaf senescence rate is accelerated by 455% per °C increase of $T_c$ above 35°C and 4-fold when $T_c$ exceeds 34°C. The acceleration factor is applied to 3-4°C $T_c$. No heat stress effects on grain number, grain filling or final yield</td>
<td>None</td>
</tr>
<tr>
<td>SiriusQuality (SQ, Martre et al., 2006; <a href="http://www1.clermont.inra.fr/siriusquality/">http://www1.clermont.inra.fr/siriusquality/</a>)</td>
<td>EBN Described in Jamieson et al. (1995a,b)</td>
<td>Granin dry matter and nitrogen (N) accumulation</td>
<td>Leaf and stem N turn-over and remobilization</td>
</tr>
<tr>
<td>Sirius2014 (S2, Jamieson et al., 1998; Jamieson and Semenov, 2000; Lawless et al., 2005)</td>
<td>EBN</td>
<td>Leaf senescence rate is accelerated by 10.8% per °C of 3-4°C $T_c$ above 28.9°C. In a period from 10 days before to anthesis, grain number is reduced by 2% per °C of $T_{max}$ above 32.5°C. In a period of 5 to 12 days after anthesis, the potential single grain dry mass is reduced by 0.1% per °C of $T_{max}$ above 38.6°C. Grain filling stops when $T_{max}$ is above 38°C</td>
<td>Phenological stages (Leaf growth (LAI and biomass by radiation use efficiency), Root growth and senescence, Grain water content, Grain filling, Senescence, Phenological stages)</td>
</tr>
<tr>
<td>STICS EMP (T1, Brisson et al., 2003; Brisson et al., 2008)</td>
<td>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). $T_{max}$ cannot be lower than $T_{min}$ and $T_{min}$ is always equal to $r_{max}$</td>
<td>Grain filling stops when $T_{max}$ is above 38°C</td>
<td>Leaf growth (LAI and biomass by radiation use efficiency), Root growth and senescence, Grain water content, Grain filling, Senescence, Phenological stages</td>
</tr>
<tr>
<td>STICS EBN (T2, Brisson et al., 2003; Brisson et al., 2008)</td>
<td>EBN Two instantaneous energy balances are calculated by an iterative convergence procedure to estimate $T_{max}$ and $T_{min}$, 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</td>
<td>Grain filling stops when $T_{max}$ is above 38°C</td>
<td>Leaf growth leaf area index (LAI) and biomass by RUE, Root growth and senescence, Grain water content, Grain filling, Senescence</td>
</tr>
</tbody>
</table>

* 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 TC is already used in some crop models, and for its use to simulate heat stress in models not previously using TC, a simulation exercise was designed with two steps summarized in Fig. 1. In Step 1, all models used their simulated values of Tc 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 TA (AN, FA, L5 and SP) had to apply TC to at least one heat stress related process. Models that were already using TC continued to use TC 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 TC do better at simulating grain yield under heat stress than models that normally use only Tair. In Step 2 (Fig. 1) referring to the third objective, models simulations were conducted using Tair on processes sensitive to heat stress. This implies that AN, FA, L5 and SP used Tair for all processes whereas the models that normally use TC (SQ and S2) were run using Tair on processes sensitive to heat stress (i.e. grain number, harvest index, final grain yield and/or leaf senescence), but used TC 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 Tair 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 TC compared to the use of Tair 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 TC versus Tair 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 (R2), calculated as the square of the Pearson correlation coefficient. MSE and RMSE were calculated as:

\[
\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (y_{si} - y_{o,i})^2 \quad (1)
\]

and

\[
\text{RMSE} = \sqrt{\text{MSE}} \quad (2)
\]

where \( y_{si} \) is the \( i \)th observation of grain yield, \( y_{o,i} \) is the \( i \)th simulated grain yield value, and \( N \) is the total number of observation and simulation pairs.

RMSRE was calculated as:

\[
\text{RMSRE} = \left( \frac{1}{N} \sum_{i=1}^{N} \left( \frac{y_{si} - y_{o,i}}{y_{o,i}} \right)^2 \right)^{1/2} \quad (3)
\]

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 \( y_{si} \) and \( y_{o,i} \) (NU; non-unity slope), and a term related to the correlation \( (R^2) \) between \( y_{si} \) 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:

\[
\text{MSE} = \text{SB} + \text{NU} + \text{LC}
\]

where,

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

\[
\text{LC} = (1 - R^2) \times \left( \frac{\sum_{i=1}^{N} y_{si}^2}{N} - \bar{y}_{si} \bar{y}_{si} \right) \quad (5)
\]

with \( b \) the slope of the least squared regression of \( y_{o,i} \) on \( y_{si} \). 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 \( T_{air} \) (\( \Delta T_c = T_c - T_{air} \)) 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 \( \Delta T_{obs} \) 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 \( \Delta T_{obs} \) and \( \Delta T_{sim} \) 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 (FASSET), 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 \( T_{air} \). All three EBSC 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 \( T_{air} \) whereas there was more variation in terms of correlation, with \( R^2 \) values ranging between
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 ($T_{\text{air}}$, 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 $\Delta T$ ($\Delta T = T_{c} - T_{\text{air}}$, red circles) for daily maximum values compared to the median (black line) and the range (grey shading) of simulated $\Delta T$ values across models. Simulations are only shown for the periods in which simulations were conducted. Observations of $T_{c}$ and $\Delta T$ 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 $\Delta T$ (°C), where $\Delta T = T_{c} - T_{\text{air}}$, for daily maximum values of $T_{c}$ and $T_{\text{air}}$, 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-
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°C (Table 1), five of the models show a decrease in RMSE with the use of $T_c$ and only the Sirius2014 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. 4. 1-to-1 plots of simulated vs. observed ∆T (°C) where ∆T = $T_c - T_{air}$, 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).](image-url)

Table 3

<table>
<thead>
<tr>
<th>Model</th>
<th>∆RMSE All treatments</th>
<th>∆RMSE Treatments with heat stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>APSIM NWheat (EMP)</td>
<td>0.09</td>
<td>0.09</td>
</tr>
<tr>
<td>FASSET (EMP)</td>
<td>0.09</td>
<td>0.30</td>
</tr>
<tr>
<td>SIMPLACE&lt;Lintul2&gt; (EBSC)</td>
<td>0.01</td>
<td>0.06</td>
</tr>
<tr>
<td>SIMPLACE&lt;Lintul5&gt; (EBSC)</td>
<td>1.29</td>
<td>2.45</td>
</tr>
<tr>
<td>SiriusQuality (EBN)</td>
<td>0.73</td>
<td>1.15</td>
</tr>
<tr>
<td>Sirius2014 (EBN)</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

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Fig. 5. Studentized residual errors of $\Delta T (\Delta T = T_c - T_{air})$ 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.
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).

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 $T_c$ ($T_{aw}$, 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 $T_{aw}$ and $T_c$ should therefore be largely
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 $\Delta T$ is expected to be larger under other production/environment conditions were transpiration is less and/or water stress is frequent. Further, the STICS models both limit $T_{c,max}$ to be no cooler than $T_{air,max}$ 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 $^\circ$C, SiriusQuality uses a threshold temperature of 35 $^\circ$C to accelerate senescence, and Sirius2014 uses 32.5 $^\circ$C to reduce grain number and 38.6 $^\circ$C to limit grain filling. All of these thresholds are higher than 31 $^\circ$C which is the threshold widely held to explain yield reductions under heat stress (Wheeler et al., 1996a,b; Porter and Gwavth, 1995).

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 effect 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 $T_{air}$. 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 < Lintu5>) (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 < Lintu5>, which showed the greatest improvement when $T_c$ replaced $T_{air}$, each $^\circ$C hour above 30 $^\circ$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 $T_{air}$. 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 < Lintu5> 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 < Lintu5> 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 $^\circ$C (Wheeler et al., 1996a,b; Porter and Gwavth, 1999), with the exception of FASSET and SIMPLACE < Lintu2>. 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 rainfall 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 $T_0$ 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 determines 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 EBSC 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 < Lintu5> 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
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-
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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