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2 **Performance of DSSAT-Nwheat across a wide range of current and future growing**

3 **conditions**

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6

7 **Abstract**

8 Crop models are widely used in agricultural impact studies. However, many studies have reported large
9 uncertainties from single-model-based simulation analyses, suggesting the need for multi-model
10 simulation capabilities. In this study, the APSIM-Nwheat model was integrated into the Decision Support
11 System for Agro-technology (DSSAT), which already includes two wheat models, to create multi-model
12 simulation capabilities for wheat cropping systems analysis. The new model in DSSAT (DSSAT-Nwheat)
13 was evaluated using more than 1,000 observations from field experiments of 65 treatments, which
14 included a wide range of nitrogen fertilizer applications, water supply (irrigation and rainout shelter),
15 planting dates, elevated atmospheric CO₂ concentrations, temperature variations, cultivars, and soil types
16 in diverse climatic regions that represented the main wheat growing areas of the world.

17 DSSAT-Nwheat reproduced the observed grain yields well with an overall root mean square deviation
18 (RMSD) of 0.89 t/ha (13%). Nitrogen applications, water supply, and planting dates had large effects on
19 observed biomass and grain yields, and the model reproduced these crop responses well. Crop total
20 biomass and nitrogen uptake were reproduced well despite relatively poor simulations of observed leaf
21 area measurements during the growing season. The low sensitivity of biomass simulations to poor
22 simulations of leaf area index (LAI) were due to little changes in intercepted solar radiation at LAI >3 and
23 water and nitrogen stress often limiting photosynthesis and growth rather than light interception at low
24 LAI.

25 The responses of DSSAT-Nwheat to temperature variations and elevated atmospheric CO₂
26 concentrations were close to observed responses. When compared with the two other DSSAT-wheat
27 models (CERES and CROPSIM), these responses were similar, except for the responses to hot
28 environments, due to different approaches in modeling heat stress effects.

1 The comprehensive evaluation of the DSSAT-Nwheat model with field measurements, including a
2 comparison with two other DSSAT-wheat models, created a multi-model simulation platform that allows
3 the quantification of model uncertainties in wheat impact assessments.

4
5 Key words: DSSAT-Nwheat, crop growth model, model evaluation, multi-model simulations, model test
6 data sets

7 8 **1. Introduction**

9 Dynamic crop simulation models are widely used for decision support when analyzing cropping
10 systems, assessing climate impacts, and evaluating crop management options. Crop models can
11 integrate the complex interactions of soil properties, climatic conditions, crop management
12 practices, and crop genetic characteristics. This enables a better understanding of complex
13 interactions across a range of factors that affect crop growth processes. One of the main aspects
14 of crop simulation models is the possibility to use them across various environmental and
15 management conditions, provided that they have been evaluated under a wide range of growing
16 conditions. Thus, many crop models have been developed in the past decades (see e.g. Asseng *et al.*,
17 2015; White *et al.*, 2011), and these models are increasingly being applied in agricultural and
18 environmental studies as complimentary tools to field experiments (Matthews *et al.*, 2013). The
19 Decision Support System for Agro-technology Transfer (DSSAT) modeling platform (Jones *et al.*,
20 2003) and the Agricultural Production Systems Simulator (APSIM) (Keating *et al.*, 2003;
21 Holzworth *et al.*, 2014) are leading crop modeling systems that are widely applied in various
22 environments. Both DSSAT and APSIM are modelling platforms that consist of modules for
23 crop growth and development, soil water, nutrient and organic matter dynamics, data
24 management, and a central engine that controls simulation processes.

25 Nwheat is a crop system simulation model for wheat in APSIM (Holzworth *et al.*, 2014;
26 Asseng *et al.*, 1998; Keating *et al.*, 2003). It is a derivative of the Crop Environment Resource

Synthesis model (CERES) (Ritchie *et al.*, 1998) with various modifications. The most important modifications in Nwheat are the replacement of the crop water uptake routine of CERES with an approach based on a critical fraction of available soil water, a linkage of crop water demand to biomass via transpiration efficiency instead of being a function of potential evapotranspiration and LAI as in the original CERES-Wheat, the inclusion of a high temperature stress factor to accelerate senescence of leaf area (CERES-Wheat has no heat stress factor for leaf senescence) and a modification of the functions controlling the frost damage, the specific leaf area, the light extinction coefficient and the simulation of aeration stress on crop growth (Keating *et al.*, 2001). These modeling differences result in simulation differences between the Nwheat and CERES-Wheat models.

The APSIM-Nwheat model has been tested and applied in many studies of wheat cropping systems in diverse environments, showing that it is a robust crop model (Asseng *et al.*, 2008; Heng *et al.*, 2007; Milroy *et al.*, 2008; Wessolek and Asseng, 2006; Bassu *et al.*, 2011; van Ittersum *et al.*, 2003; Yunusa *et al.*, 2004; Ludwig and Asseng, 2006; Asseng *et al.*, 1998; Asseng *et al.*, 2013; Asseng *et al.*, 2015; O'Leary *et al.*, 2015).

The first objective of this study was to integrate Nwheat (the crop component only) into the DSSAT modeling platform and to share common soil water and nutrient modules with other plant growth routines in DSSAT. The goal of integrating Nwheat into DSSAT was to provide a suite of alternative crop models for a multi-modeling approach to quantify and reduce uncertainties in wheat cropping system studies. Recent research had indicated that outputs from a single crop model simulation showed large uncertainties, potentially leading to biased conclusions and decisions (Rotter *et al.*, 2011). For instance, Asseng *et al.* (2013) used 27 different wheat models in a multi-model inter-comparison to study the uncertainty in wheat yield

estimates under climate change conditions and found large uncertainty associated with individual crop models. Similar crop model uncertainties were confirmed with maize (Bassu *et al.*, 2014) and rice (Li *et al.*, 2015). Asseng *et al.* (2013) suggested that three or more crop models are required to reduce model uncertainty of model-ensemble medians to be comparable to field experiment errors. Multi-model ensemble medians have been shown to be better predictors of yields and many other cropping system variables across a wide range of environments (Martre *et al.*, 2015).

The second objective of this study was to evaluate the performance of the new model (DSSAT-Nwheat) under diverse environmental and management conditions with detailed field measurements. Performance of crop models need to be evaluated for their response to major environmental variables, however, rigorous model evaluation is limited (White *et al.*, 2011). The performance of the Nwheat model within the DSAT framework was evaluated with varying factors and environmental variables including atmospheric CO₂ concentrations, temperature, water and nitrogen supply, and sowing dates. The third objective was to benchmark the new model against the two existing wheat models in DSSAT under contrasting management and environmental conditions, and to evaluate the new multi-model capability of DSSAT.

2. Materials and Methods

2.1 Study sites

Model performance was evaluated based on experimental data from diverse environmental conditions that represented agricultural regions of low to high potential for wheat production.

Study sites included USA (Arizona), Netherlands (Bowling, EEST, and PAGV), Australia (Cunderdin), New Zealand (Lincoln), and Mexico (Obregon) (Fig. 1). In terms of agro-climate,

the study sites represented a dryland Mediterranean climate, an irrigated area in an arid climate, humid continental, and humid sub-tropics.

<Fig 1>

Experimental data sets for evaluating model performance

This study used large data sets representing main wheat growing regions and environments around the world. Data used were quality checked and had been published in earlier studies (Asseng *et al.*, 1998; Asseng *et al.*, 2000; Kimball *et al.*, 1995; Kimball *et al.*, 1999; Groot and Verberne, 1991; Sayre *et al.*, 1997). A total of 65 experimental treatments with more than 1,000 observed data of wheat growth variables were used to test model performance. The data set includes 16 treatments from four years of a Free-Air Carbon Dioxide Enrichment (FACE) experiment conducted in Arizona, USA; 18 treatments from two years and three sites of nitrogen fertilizer application trials of high-quality detailed experiments from the Netherlands; 25 treatments with various water deficit levels at Cunderdin, Australia and Lincoln, New Zealand; and 6 years of experiments with air temperature variability at Obregon, Mexico (Table 1).

The FACE experiment at Arizona consisted of ambient (360 ppm) and elevated (550 ppm) atmospheric CO₂ concentrations during the experiment years. In addition, the FACE experiment included dry and wet treatments as well as low and high nitrogen fertilizer treatments to study the interactive effects of elevated atmospheric CO₂ concentration with water and nitrogen supply. Details of the FACE experiment are given in Kimball *et al.* (1995), Kimball (2006), and Wall *et al.* (2006). Nitrogen fertilizer experiments conducted in the Netherlands ranged from zero (no nitrogen fertilizer application) to 240 kg N/ha. Details for these experiments can be

found in Asseng et al. (2000) and Groot and Verberne (1991). Water deficit treatments at Cunderdin, Western Australia, consisted of three sowing dates ranging from 6 June (sowing 1) to 20 July (sowing 3) and irrigation treatments during the 1997 growing season. Experiments at Lincoln, New Zealand consisted of treatments with different levels of irrigation water applied, varying from no irrigation to a high irrigation rate (550 mm) under a rainout shelter. The growing season temperature at Obregon, Mexico varied by up to 1.7°C during the growing season across six years in a well-watered and well-fertilized experiment.

Different cultivars were used in each of the experiments, including Arminda, Gamenya, Rongotea, Spear, Wilgoyne, and Yecora. Planting time varied from the first week of June (in Australia) to the first week of December (in USA), depending on the planting window for each experimental site. Measured crop growth data used for model evaluation included in-season development of total crop biomass, leaf area index (LAI), crop nitrogen uptake, grain nitrogen, and grain yield. Data for initial soil water content, initial soil nitrogen, and crop residue measured during each experimental year were available.

<Table 1>

2.2. Description of the Nwheat model

Nwheat model

Nwheat was developed based on the CERES-Wheat model (Ritchie *et al.*, 1998). The model simulates crop development and growth, water and nitrogen dynamics, as well as different stress

factors and stress responses of wheat in daily time steps (Keating *et al.*, 2001; Asseng *et al.*, 2004). Crop phenology in Nwheat is a function of accumulated degree-days, photoperiod, and vernalization requirements. Potential dry matter production is driven by radiation use efficiency, solar radiation, temperature, and leaf area index (LAI). Sub-optimal water and nitrogen supply can reduce the potential dry matter production. Potential crop water demand is a function of transpiration efficiency and vapor pressure deficit. Actual water uptake depends on uptake demand, root density, and available soil water within the soil profile. Grain yield depends on grain number, grain filling, and carbohydrate remobilization. Carbohydrates available for remobilization to grain are defined in the model as 75% of biomass growth from before anthesis to the beginning of the linear grain-filling stage.

The simulation of plant nitrogen dynamics is similar to that of the CERES-Wheat model, which is driven by nitrogen content of the various plant components, potential nitrogen uptake capacity of the root system, crop nitrogen demand, and nitrogen remobilization (Ritchie *et al.*, 1995). Nitrogen concentration of each plant organ is calculated as a function of plant growth stage. Actual crop nitrogen demand is the difference between potential and actual nitrogen concentrations, including the nitrogen amount required for new growth and excluding the nitrogen remobilization to the grain. Nitrogen remobilization to the grain is driven by temperature. The process stops at the end of grain filling, although nitrogen can be remobilized from leaves and stems to the grain until a minimum concentration is reached. Grain nitrogen content is constrained at very low ($<1.2\%$) and very high ($>4\%$) grain N-concentrations. Potential nitrogen uptake capacity is a function of root density, soil nitrate and ammonium concentrations, and soil water content. A nitrogen stress factor is calculated as a quotient of actual nitrogen content in the crop and a critical nitrogen concentration. The nitrogen stress

factor affects LAI, photosynthesis, and leaf senescence. Only the crop component of Nwheat is integrated into the DSSAT and it shares common soil nitrogen and soil water modules with the other wheat models. Water balance dynamics in the DSSAT wheat models is determined by soil characteristics provided as model inputs for lower limits (LL), drained upper limit (DUL), and saturated volumetric water content (SAT). Water balance is modeled using a cascading approach, meaning that water moves vertically from top to bottom when the water content of a soil layer exceeds the field capacity. The model considers the effect of crop cover and surface residue on runoff and soil evaporation.

Nwheat captures the effect of elevated atmospheric CO₂ concentration on crop growth, radiation use (RUE), and transpiration efficiency (TE) based on an independent RUE-CO₂-temperature function and an independent CO₂-TE functions (Reyenga *et al.*, 1999). Scaling of radiation use efficiency was calculated as the ratio of light-limited photosynthetic response at enhanced CO₂ concentration relative to a current CO₂ concentration (Asseng *et al.*, 2004). Elevated atmospheric CO₂ concentration affects transpiration efficiency by multiplying the transpiration efficiency with a factor that increases linearly from 1.0 to 1.37 when the CO₂ concentration increases from 350 to 700 ppm (Asseng *et al.*, 2004).

Model inputs

Similar to most other dynamic crop models, DSSAT-Nwheat requires inputs that describe daily weather, cultivar growth and development characteristics, management events, and soil characteristics. The minimum weather data requirements are daily temperature (e.g., minimum and maximum), solar radiation, rainfall, and station information (e.g., latitude). The model uses seven main genetic coefficients for a cultivar: vernalization requirement, photoperiod sensitivity,

thermal time requirement, kernel number per biomass, kernel growth rate, maximum stem dry weight, and phyllochron interval (Table 2). Vernalization and photoperiod affect phenology between emergence and floral initiation. Grain yield potential is controlled by a coefficient of kernel number per ear (Grno) and maximum kernel growth rate (Fillrate). Tillering depends on potential final dry weight of a single stem (stmwt). Leaf appearance is associated with degree day accumulation by the phyllochron parameter. Main soil inputs include initial soil water content, lower and drained upper limits, saturated water content, water drainage and runoff coefficients, rooting growth factors, first stage evaporation, and soil albedo. Crop management information includes planting date and depth, plant population, fertilizer and irrigation application rates and dates, as well as measured or estimated initial soil water and nitrogen content.

<Table 2>

2.3 Evaluation of model performance

Statistical evaluation

Statistical indices such as coefficient of determination (r^2) of a 1:1 regression line, slope of regression (forced through the origin), and root mean square deviation (RMSD) were used to evaluate model performance. The coefficient of determination (r^2) for a 1:1 line ($y=x$) provides the degree of association between model simulations and measured values. Values of r^2 higher than 0.5 were considered as acceptable or satisfactory and values closer to 1 indicate strong association between model simulation and measured values (Santhi *et al.*, 2001). Absolute magnitude of error (deviation of simulations from expected 1:1 line) is provided by the root

mean squared deviation. Model performance was evaluated as excellent when normalized RMSD is <10%, satisfactory when RMSD is 10-30% and poor when RMSD >30% (Bannayan and Hoogenboom, 2009; Jamieson *et al.*, 1991). Direction of a possible under- or overestimation was evaluated by the slope (m) of a best fit regression line forced through the origin. The slope of a regression line that passes through the origin provides better estimate for the relationship between the model simulated and observed values (Bellocchi *et al.*, 2010). If not forced through the origin, the slope would not be useful to quantify a possible under-or over estimation.

Sensitivity analysis

A sensitivity analysis was conducted using data from the multi-model inter-comparison from Asseng *et al.* (2013). This study used 30 years of observed weather data from Australia and the Netherlands to evaluate how the model responds to changes in input data and to benchmark the new model against the two existing wheat models in the DSSAT. For the sensitivity analysis scenario, temperature was increased by 3, 6, and 9°C, and atmospheric CO₂ concentration levels were set at 360, 450, 540, 630, and 720 ppm. The DSSAT-Nwheat sensitivity to changes in temperature and atmospheric CO₂ concentration was compared to the sensitivity of the two existing wheat models in the DSSAT (CERES and CROPSIM) (Asseng *et al.*, 2013; Asseng, 2015).

3. Results

The DSSAT-Nwheat model reproduced observed grain yields well with an overall root mean square deviation (RMSD) of 0.89 t/ha (13%) (Table 3). Observed grain yields varied from 10 t/ha at Lincoln, New Zealand to 0.9 t/ha at Cunderdin, Australia. The model was able to

reproduce this large difference with the highest yield simulation for Lincoln (10.7 t/ha) and lowest for Cunderdin (0.7 t/ha) (Fig. 2).

< Table 3>

< Fig. 2>

Total crop biomass was simulated well (Fig. 3a). The coefficient of determination (r^2) for biomass simulations was high ($r^2=0.95$), and the RMSD was low (RMSD= 1.35 t/ha (15%)) (Table 3). The strong correlation between simulated and observed crop biomass was also shown by a slope (forced through the origin) of nearly one ($m= 0.98$). The effect of nutrient and water supply on total crop biomass production was well simulated by the model, but the simulations for leaf area index (LAI) showed poor agreement with measured values (RMSD = 1.15 (46%)) (Fig. 3b). The model tended to overestimate LAI, particularly for the maximum leaf development under low nitrogen supply and underestimated some of the high irrigation treatments. Despite the poor simulations of leaf area index, the simulations for grain yields (Fig. 2), aboveground biomass (Fig. 3a), grain number, grain size, crop nitrogen uptake, and grain protein were reasonably good (Fig. 3c, d, e, & f).

< Fig 3>

Water supply, nitrogen applications, atmospheric CO₂ concentration, and planting dates had large effects on observed biomass and grain yields, and the model reproduced these crop responses well (Fig. 4). For instance, water deficit at Lincoln reduced the observed biomass from

24 t/ha to 16 t/ha and observed grain yield from 10 t/ha to 4.5 t/ha. The model simulation showed a biomass reduction from 24 t/ha to 13 t/ha and grain yield from 10.7 t/ha to 5.5 t/ha due to water deficit at Lincoln (Fig 4a). However, the model tended to slightly overestimate the grain yield for water deficit conditions. Differences between simulated and observed grain yields for water deficit conditions might be attributed to an overestimation of soil water content by the model simulation, however, there was no measured soil water data to validate this.

Observed biomass and grain yield variations for several nitrogen application rates were also captured by the model. Low nitrogen application at PAGV, Netherlands, for instance, reduced the observed biomass from 18 to 14 t/ha and grain yield from 8 to 6 t/ha. A corresponding simulation showed biomass reduction from 17 to 15 t/ha and yield reduction from 8 to 7 t/ha (Fig 4b). At EEST, increasing the nitrogen application from 0 to 160 Kg N/ha showed an increase in observed crop biomass from 10 to 18 t/ha and grain yield from 4.5 to 7.6 t/ha. The corresponding model simulation showed an increase in crop biomass from 12.5 to 16.6 t/ha and grain yield from 5.8 to 7.2 t/ha (not shown). In general, the model captures the effects of nitrogen application rates. For low nitrogen treatments, there is a tendency of slight overestimation, for instance, at PAGV the observed yield at low nitrogen is 6.3 t/ha while the model simulates 6.8 t/ha i.e. model simulates 8% grain yield higher than the observed (Fig. 4b).

An increase in atmospheric CO₂ concentration from 360 to 550 ppm under well-irrigated conditions at Arizona, USA, showed an increase in crop biomass from 18 to 20 t/ha (11%) and grain yield from 8 to 9 t/ha (12.5%). The response of the DSSAT-Nwheat model to elevated atmospheric CO₂ concentration was very similar to observed responses with an increase in crop

1 biomass from 17 to 19 t/ha (11.8%) and an increase in grain yields from 8 to 9 t/ha (12.5%) (Fig
2 4c). The relative increase in crop biomass and grain yield due to increased atmospheric CO₂
3 concentration was higher for water deficit conditions. Delaying planting dates reduced observed
4 crop biomass from 7.6 to 3.5 t/ha and grain yield from 2.7 to 1 t/ha at Cunderdin, Australia,
5 under terminal drought and heat stress conditions. The model simulation showed similar
6 responses to a delayed planting date with a decrease in crop biomass from 8.1 to 3.3 t/ha and
7 grain yield from 2.7 to 0.6 t/ha (Fig 4d).

8
9 <Fig 4>

10
11 The performance of the model was further evaluated with consideration of interactions among
12 environmental factors and crop management such as elevated atmospheric CO₂ concentration
13 with water and nitrogen availability. The model response to such interactions was found to be
14 generally in agreement with field observations (Fig. 5). A combination of irrigation and elevated
15 atmospheric CO₂ concentration increased observed yield from 8.5 to 9.4 t/ha (10.6%) during the
16 1993-94 growing season at Arizona, and the model simulation showed similar yield changes. For
17 low nitrogen treatments, both observed and model-simulated yields did not change with elevated
18 atmospheric CO₂ concentration. High nitrogen in combination with elevated atmospheric CO₂
19 concentration showed observed yield changes from 8 to 9 t/ha (13%), and the model simulation
20 indicated similar relative yield changes during the 1995-96 growing season.

21
22 < Fig 5>

Compared with the two other DSSAT wheat models (CERES and CROPSIM), the response of Nwheat DSSAT for increased temperature and elevated atmospheric CO₂ concentrations was similar, except for extreme heat environments, e.g., Australia (Fig. 6). For instance, an increase in temperature by 6°C (from the baseline) resulted in a decrease in grain yield by 1 t/ha as predicted by the CERES model for the Netherlands, and a prediction with DSSAT-Nwheat showed a similar yield reduction (Fig. 6a). For an extreme environment in Australia, DSSAT-Nwheat and CROPSIM showed similar response to temperature changes, whereas the CERES response deviated (Fig. 6b). The CERES model was more sensitive to increased temperature effects than the DSSAT-Nwheat and CROPSIM models at extreme environments. An increase in atmospheric CO₂ concentration from 360 to 720 ppm, according to a prediction by CERES and CROPSIM models, resulted in a grain yield increase by 2 t/ha in the Netherlands, and a similar response to elevated CO₂ concentration was predicted by DSSAT-Nwheat (Fig. 6c). The simulated response of yield to an increase in CO₂ as predicted by CERES and CROPSIM was small (<1 t/ha) for Australia, and DSSAT-Nwheat simulation showed a similar response (Fig. 6d). The DSSAT-Nwheat model also captured the effect of growing season rainfall on yield similar to the other models (Fig. 6e)

< Fig 6>

4. Discussion

Crop simulation modeling is a complex process involving interaction of various environmental and crop factors (soil, climate and crop variables), but simulation results contain uncertainty. When using a single crop model, this uncertainty cannot be quantified. Ensemble model simulations, using multiple models for the same task, has been suggested to quantify crop model

1 uncertainty (Martre *et al.*, 2015), for example by expanding existing modeling platforms (Feng *et*
2 *al.*, 2014). Hence, an additional wheat model was added to the existing wheat models of the
3 DSSAT platform.

4
5 A comprehensive evaluation of crop simulation models with adequate data sets from different
6 environments, management, cultivars, and soil types is critical in order to use a crop model with
7 confidence in agricultural systems analysis (White *et al.*, 2011). The Nwheat model has been
8 evaluated and widely applied within APSIM. In this study, the Nwheat model (crop module
9 only) was evaluated within the DSSAT modeling platform. Crop model evaluation is a common
10 procedure in adopting and using a crop model in a new environment or in a new modeling
11 framework (Matthew *et al.*, 2015; Matthews *et al.*, 2013; Zacharias *et al.*, 2015; Jones *et al.*,
12 2001; Angulo *et al.*, 2013); however, most crop models are not yet well tested across a wide
13 range of current and future growing conditions in combination with atmospheric CO₂ and
14 temperature interactions (White *et al.*, 2011). Interactions of atmospheric CO₂ concentration,
15 temperature, nutrient and water supply are the main drivers of crop response to climate change
16 (Asseng *et al.*, 2013). This study demonstrated the wider implications of considering main
17 environmental interactions to assess model performance for crop growth simulation and impact
18 studies.

19
20 The comprehensive test of model performance confirmed reliability of the Nwheat model
21 simulations in the DSSAT platforms across a wide range of management and environmental
22 conditions. The overall performance of DSSAT-Nwheat across the various environmental and
23 growing conditions was good. The model predicted grain yield responses to environmental and

management factors well. Although model evaluation studies are environmental and cultivar-specific and not directly comparable, the root mean square deviation (RMSD) between observed and simulated yield reported in this study (0.89 t/ha) is comparable to that of findings in other model evaluation studies (e.g. Ko *et al.*, 2010; Asseng *et al.*, 2004; Singh *et al.*, 2008) .. The DSSAT-Nwheat model has also very close simulations with APSIM-Nwheat reported in earlier studies (Asseng *et al.*, 1998; Asseng *et al.*, 2000).

The prediction for crop biomass dynamics was generally accurate. Simulations for crop nitrogen, grain protein, grain number, and grain size were also acceptable. However, there was a bias in LAI simulations with LAI in general being poorly simulated. The slope of a regression line (forced through the origin) for the LAI indicated a value of 1.2, which implies a tendency of overestimation of LAI with the Nwheat model. Interestingly, the poor simulations for LAI did not affect crop biomass and crop nitrogen uptake simulations. Crop biomass accumulation in Nwheat is a function of intercepted radiation, which in turn is a function of LAI. Simulated crop nitrogen uptake is a function of crop biomass growth. The low sensitivity of biomass simulations to poor simulations of leaf area index (LAI) were due to little changes in intercepted solar radiation at LAI >3. Asseng *et al.* (2004) found that crop growth and yield simulations were less sensitive to LAI >3 as higher LAI contributed only marginally to intercepted radiation in wheat. Poor simulation of LAI before the canopy closure could be because of water and nitrogen stress effects often limiting photosynthesis and growth rather than light interception at low LAI. While potential radiation interception is closely linked to LAI of up to 3, water or nitrogen stress can reduce photosynthesis and growth, therefore overwriting any bias of LAI simulations at low LAI at any growth stage. Meinke *et al.* (1997) also showed that a LAI simulation bias did not reduce

the accuracy of crop biomass simulation. Accurate simulation of LAI remains difficult due to complex interactions of assimilate allocation controlling leaf development (Ewert, 2004). Some studies indicated that crop nitrogen uptake is proportional to LAI expansion during the vegetative growing period and suggested that the simulation of crop nitrogen demand be linked with leaf area growth (Lemaire *et al.*, 2007). However, such functionality would require a better simulation of LAI dynamics. Therefore, linking N uptake demand to biomass growth in Nwheat appears to be a reasonable and robust alternative.

DSSAT-Nwheat was able to reproduce the response of wheat growth and grain yields to the various crop management practices, environments, and their interactions. The model was able to capture important feedbacks, such as increased grain yields and crop biomass accumulations, when water and nitrogen supply were not limiting growth. Treatments with adequate soil water and nitrogen resulted in higher observed yields than those with water or nitrogen stress, and the model simulations captured these yield changes among the treatments. The dynamics of CO₂-water-nitrogen interactions were reproduced with the Nwheat model simulations. Relative increases of grain yield and crop biomass due to elevated atmospheric CO₂ concentration were higher under water stress conditions. For example, elevated atmospheric CO₂ concentration increased yields by 34% under water stress conditions in the 1992-93 growing season at Arizona compared to 14% in the high-irrigated treatments. While a reduction in stomatal conductance is not directly simulated in Nwheat, the model captures this effect through an increase in transpiration use efficiency under elevated atmospheric CO₂ concentrations (Asseng *et al.*, 2004). Various FACE experiments (e.g. Ko *et al.*, 2010; Kimball *et al.*, 1995; Wall *et al.*, 2006; Grant *et al.*, 1995; Kimball *et al.*, 2002; Mitchell *et al.*, 1993) showed that the relative increase in

1 crop biomass and grain yield due to elevated atmospheric CO₂ are higher for water stress than
2 well-watered conditions, which the model reproduced well in this study.

3 The DSSAT-Nwheat response (directional changes) to increased temperature and elevated
4 atmospheric CO₂ was in general comparable with the responses of the two existing other wheat
5 models in the DSSAT (CERES and CROPSIM). However, the models differ in the degree of
6 sensitivity. An increase in temperature by 6°C showed a very similar yield response for DSSAT-
7 Nwheat and CERES (15% and 17% yield reduction, respectively), while CROPSIM showed no
8 response in the Netherlands. For a hot environment (Australia), DSSAT-Nwheat and CROPSIM
9 simulated yield reduction by 42% and 33%, respectively, and CERES showed complete crop
10 failure when temperature increased by 9°C beyond the baseline. Increase in atmospheric CO₂
11 concentration from 360 to 720 ppm increased wheat yield by 21% according to DSSAT-Nwheat,
12 while it increased by 28% and 37%, according to CERES and CROPSIM, respectively, in the
13 Netherlands. For a hot environment in Australia, DSSAT-Nwheat showed lower response (10%)
14 compared to CERES (32%) and CROPSIM (24%) for an increase in atmospheric CO₂ from 360
15 to 720 ppm. The sensitivity to elevated atmospheric CO₂ response is slightly higher for CERES
16 than the other models in hot environments. The simulated yield gain due to increased elevated
17 atmospheric CO₂ for all three models is comparable to other FACE experiments reported; for
18 instance, 6-35% was reported in USA (Kimball, 2006; Kimball *et al.*, 1995; Wall *et al.*, 2006),
19 Germany (Ewert *et al.*, 2002), and China (Li *et al.*, 2007; Ynag *et al.*, 2007).

20
21 The difference in the degree of sensitivity and responsiveness among the models may be due to
22 differences in model structure and parameterization and the way they captured extreme
23 temperature and elevated atmospheric CO₂ concentration effects. Temperature and atmospheric

CO₂ affects the various growth and development processes of a crop through their influence on stomatal conductance and rate of physiological processes. The relationship between crop development and temperature responses varies among the crop models. For instance, the DSSAT-Nwheat model has a factor to accelerate leaf senescence in response to extreme temperature, and this relationship reduces the leaf area index incrementally for each day over 32°C. However, in CROPSIM, crop growth versus temperature response is driven by mean air temperature (Hunt and Pararajasingham, 1995) and does not consider effects of extreme temperatures. For computing the effects of elevated CO₂, the evapotranspiration routine of CERES and CROPSIM includes a ratio of transpiration under elevated atmospheric CO₂ concentrations to that of under ambient concentrations (Hoogenboom, 2012). DSSAT-Nwheat uses functions to describe the RUE-CO₂-temperature effects and CO₂-TE effects (Reyenga *et al.*, 1999; Asseng *et al.*, 2004).

The integration of the Nwheat model into DSSAT created a multi-model platform allowing simulations using three wheat models and quantification of model uncertainties in impact assessments. Crop models describe crop-climate interactions differently (White *et al.*, 2011), which can result in diverging model outcomes. Accordingly, uncertainty in crop growth simulations and impact assessments has been an increasing concern among the modeling community. Simulation studies using a single crop model cannot identify model uncertainties in impact assessments (Rotter *et al.*, 2011; Asseng *et al.*, 2013; Bassu *et al.*, 2014; Li *et al.*, 2015), but a multi-models simulation approach can (Martre *et al.*, 2015; Rosenzweig *et al.*, 2014; Asseng *et al.*, 2015). This new method of putting three crop models in a single platform with shared soil and water process modules narrows the uncertainty calculations to the crop growth and development portions of the model. While the three models share the same soil nitrogen and

soil water balance sub-routines, simulation results differ due to different crop growth functions, including crop water uptake, leaf area development, light interception and heat stress sensitivity.

Conclusions

A comprehensive testing of the DSSAT-Nwheat model with field measurements including a comparison with two other DSSAT models revealed that the new DSSAT-Nwheat model has reliably good performance under diverse environmental and growing season conditions. The model can now be used in the DSSAT modeling platforms for assessing impacts of various agronomic management strategies and decisions in wheat cropping systems under current and anticipated climate change. It can be employed to explore the integrated effects of temperature, atmospheric CO₂ concentrations, water, nutrients, and agronomic management practices in a range of wheat growing environments. Furthermore, integrating Nwheat in DSSAT created a multi-model platform that allowed the quantification of model uncertainties in impact assessments.

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FIGURE CAPTIONS

Fig. 1 Map of study sites for DSSAT-Nwheat model evaluation. Wheat producing regions are based on Monfreda *et al.*, (2008).

Fig. 2. Observed versus simulated grain yields with the DSSAT-Nwheat model for FACE experiments (Arizona, USA), nitrogen fertilizer experiments (BOUW, EEST, and PAGV, the Netherlands), increased levels of water deficit (Lincoln, New Zealand and Cunderdin, Australia) and variable air temperature (Obregon, Mexico).

Fig. 3. Observed versus DSSAT-Nwheat model simulated (a) total biomass, (b) leaf area index (LAI), (c) grain number, (d) grain size, (e) crop nitrogen, and (f) grain protein. The symbols used here represent the same as the legend in Fig. 2.

Fig. 4. Observed (symbols) and DSSAT-Nwheat model simulated (lines) total biomass and grain yield for treatments (a) water supply at Lincoln, New Zealand; (b) nitrogen supply at PAGV, the Netherlands, in the 1982-83 growing season; (c) normal and elevated atmospheric CO₂ concentrations at Arizona, USA, in the 1992-93 growing season; and (d) normal and late planting dates at Cunderdin, Australia, in the 1997 growing season.

Fig. 5. Observed (dark filled bars) and DSSAT-Nwheat model simulated (gray filled bars) grain yields for interactions of CO₂, water, and nitrogen treatments. Labels of the x-axis indicate sowing year followed by D-dry, W-wet, N-low nitrogen, NN-high nitrogen and C-elevated atmospheric CO₂ concentration (550 ppm). Dry and wet treatments are from FACE 1993-94 and low and high nitrogen treatments are from FACE 1995-96 experiments.

Fig. 6. Sensitivity of the DSSAT-Nwheat model to levels of temperature and CO₂ concentrations in comparison to the existing DSSAT-wheat models (CERES and CROPSIM). Simulations for CERES and CROPSIM are based on Asseng *et al.* (2013). Trend lines in Fig. 6e & 6f are for DSSAT-Nwheat simulations.

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Table 1: Experimental data sets used for testing DSSAT-Nwheat. Normal and elevated atmospheric CO₂ concentration refers to 360 and 550 ppm respectively. N1, N2 and N3 are nitrogen fertilizer application levels (kg N/ha).

Experiments	Years	Treatments
1. FACE experiment (Arizona, USA)		
FACE dry	1992	Normal and elevated CO ₂ ; dry
	1993	Normal and elevated CO ₂ ; dry
FACE wet	1992	Normal and elevated CO ₂ ; wet
	1993	Normal and elevated CO ₂ ; wet
FACE low N	1995	Normal and elevated CO ₂ ; low N
	1996	Normal and elevated CO ₂ ; low N
FACE high N	1995	Normal and elevated CO ₂ ; high N
	1996	Normal and elevated CO ₂ ; high N
2. Nitrogen application experiments (Netherlands)		
EEST	1983	N1= 0 N2= 60 N3= 180
	1984	N1=110 N2= 150 N3= 150
PAGV	1983	N1= 80 N2= 140 N3= 240
	1984	N1= 80 N2= 180 N3= 240
BOUWING	1983	N1= 0 N2= 60 N3= 160
	1984	N1= 70 N2= 170 N3= 230
3. Increased level of water deficit (Lincoln, New Zealand)	1991	Treatments with water deficit (rainout shelter with irrigation treatments)
4. Temperature sensitivity experiment (Obregon, Mexico)	1989-1994	Years with variable growing season temperature
5. Increased levels of water deficit (Cunderdin, Australia)	1997	Treatments with planting dates resulting in increased terminal water stress

Table 2. Main genetic coefficients used in DSSAT-Nwheat model

Genetic coefficients	Coefficient code	Minimum and maximum values (Range)
Sensitivity to vernalization	P1v	1-5
Sensitivity to photoperiod	P1d	1-5
Thermal time (start of grain filling to maturity)	P5	600-800°C
Kernel number per stem weight (at the beginning of grain filling)	Grno	20-30 kernel/g-stem
Maximum kernel growth rate	Fillrate	2-2.5 mg/kernel/day
Potential final dry weight of a single stem	Stmwt	1-4 g/stem
Phyllochron interval	Phint	70-120°C-days/leaf appearance

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2 Table 3. Summary of DSSAT-Nwheat model performance under various environmental
 3 conditions (r^2 is the coefficient of determination for $y=x$ regression line; m is slope of a
 4 regression line forced through the origin; and RMSD is the root mean square deviation).

Sites and model attributes	Number of paired data points	$r^2(1:1)$	M	RMSD
Maricopa, USA				
Grain yield	47	0.64	1.05	0.87
Biomass	354	0.91	1.01	1.92
LAI	328	0.72	0.91	0.95
BOUW, Netherlands				
Grain yield	6	na	0.91	0.72
Biomass	43	0.97	0.98	1.04
LAI	43	0.69	1.3	1.07
Crop Nitrogen	43	0.89	1	23.21
EEST, Netherlands				
Grain yield	6	na	0.63	1.01
Biomass	43	0.97	0.97	0.94
LAI	40	0.68	1.2	0.97
Crop Nitrogen	43	0.84	1.15	27.84
PAGV, Netherlands				
Grain yield	6	na	0.98	0.44
Biomass	43	0.97	0.95	1.06
LAI	40	0.63	1.3	1.26
Crop Nitrogen	43	0.74	1.19	35.18
New Zealand				
Grain yield	7	na	1.16	1.45
Biomass	84	0.92	1.01	1.8
LAI	94	0.43	0.98	1.51
Mexico				
Grain yield	6	na	0.89	1.17
Australia				
Grain yield	15	0.83	0.89	1.14

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