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Assessing crop model improvements through comparison of sorghum (sorghum bicolor L. moench) simulation models: A case study of West African varieties

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Field Crops Research Volume 201, 1 February 2017, Pages 19–31

DOI: <u>http://dx.doi.org/10.1016/j.fcr.2016.10.015</u>

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Article type: Review

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Key words *Sorghum bicolor* L. moench; Photoperiod sensitivity; APSIM; DSSAT; Samara

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 cultivars

4 Abstract

5 Better defining niches for the photoperiod sensitive sorghum (sorghum bicolor L. Moench) cultivars of West Africa into the local cropping system might help to improve the resilience of 6 7 food production in the region. In particular, crop models are key tools to assess the growth and development of such cultivars against climate and soil variability. In this study, we 8 compared the performance of three proceed-based crop models (APSIM, DSSAT and 9 10 Samara) for prediction of diverse sorghum (Sorghum bicolor L. Moench) germplasm having 11 widely varying photoperiod sensitivity using detailed growth and development observations from field trials conducted in West Africa semi-arid region. Our results confirmed the models 12 13 capability to reproduce diverse PPSen for the selected cultivars. Simulated phenology and 14 morphology organs during calibration and validation were within the closet ranged of 15 measured values with the evaluation of model error statistics (RMSE and R²). With the 16 exception of high PPSen cultivar (IS15401), APSIM and Samara estimates indicate the lowest value of RMSE (< 7days) against the observed values for phenology compared to 17 DSSAT model. Across the cultivars, there was over-estimation for simulated leaf area index 18 19 (LAI) while total leaf number (TLN) fitted perfectly into the observed values. Samara estimates were found to be the closet with the lowest value for RMSE (< 3leaves for TLN 20 and $< 1.0m^2/m^2$ for LAI) followed by DSSAT and APSIM respectively. Contrary to the good 21 performance of Samara model for simulating phenology and morphology, there was a 22 significant variability and large error estimates between model-simulated and field-observed 23 values for total grain yield and biomass. For both calibration and validation, the estimates by 24 APSIM were found to be closer to the observed with the lowest RMSE, NRMSE (%) and R² 25 26 followed by DSSAT and Samara models. The uncertainty and large error against the

observed values were traced to the models ability to better simulate final biomass and grain
yield rather than early vegetative phase of the crop growth (above-ground biomass).

Keywords: Model calibration and validation, comparison and improvement, sorghum bicolor
L. moench, photoperiod sensitivity.

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1. INTRODUCTON

7 Sorghum (sorghum bicolor L. MOENCH) is the fifth most important cereal crop in the world 8 and is a dietary staple food of more than 500 million people in more than 30 countries 9 (ICRISAT 2009). Besides, its primary staple food for humans, it serves as an important source of feed and fodder for animals particularly in semi-arid regions. It makes 10 comparatively quick growth and gives not only good yield of grain but also enormous 11 12 quantities of fodder. In West Africa, sorghum production is primarily grown under rainfed 13 conditions and length of the growing period (LGP) is mainly a function of the date of the first 14 rains (Sivakumar, 1988), which is delayed with latitude and varies widely from year-to-year. Sorghum is a short day photoperiod sensitive crop. Progress towards flowering is 15 16 accelerated when daylength decreases (Folliard et al., 2004). In West Africa, favourable 17 conditions for sorghum cultivation usually extend from May to November. Most of the plant growth thus takes place under decreasing daylength, explaining why cycle duration shortens 18 when sowing is delayed. Farmers use the photoperiod (PP) sensitive varieties, that allows 19 for grouped flowering at the end of the rainy season for a wide range of planting dates 20 21 (Traore' et al., 2000). This feature is useful to minimize grain mold and insect and bird damage, which typically affect early maturing varieties. Furthermore it, avoids incomplete 22 grain filling, a problem for late maturing varieties faced with soil water shortage at end of 23 season (Vaksmann et al., 1996). The extensive genetic and phenotypic diversity of sorghum 24 (Clerget et al., 2008; Murray et al. 2008) and its adaptation to harsh climatic and cropping 25 conditions (Nasidi et al., 2010) offers the opportunity to develop Food-Fodder-Fuel(FFF) 26

plants for a multitude of environmental conditions, including the semi-arid environments
 found in West Africa.

Traditionally, conducting field trials are used to evaluate the performance of the different 3 planting material under a range of climate conditions. However, field trials are time 4 5 consuming and financially demanding and are difficult to extrapolate to other sites and 6 seasons. Hence, crop-climate models can help with the interpretation of experimental data 7 and, after careful calibration and validation, can be used in a prospective way in conjunction 8 with field data to draw recommendations for improved climate-induced risk adaptation 9 strategies. For sorghum, there are crop models implemented in simulation frameworks such 10 as DSSAT - Decision supportfor Agro-Technology Transfer (Jones et al., 2003), APSIM -11 Agricultural Productions Systems slMulator (Holzwoth et al., 2014) or Samara (Dingkuhn et 12 al. 2011). These models differ in the description of the processes and consequently in their 13 outputs. Thus, comparison of different modelling approaches can help reveal the uncertainties relating to crop growth and yield predictions (Palosuo et al., 2011). These 14 15 include the uncertainty related to the model structure, which is the most difficult source of 16 uncertainty to quantify (Chafield, 1995). Also, comparison can help to identify those parts in 17 the model that produce systematic errors and require improvements (Adam et al., 2012). Recently, there is a growing body of studies comparing models and outputs (Asseng et al., 18 2013, Bassu et al. 2014, Li et al. 2015). Though, the selected models are widely used in 19 Africa and elsewhere, our findings show that the models are not very well calibrated and 20 validated for the diverse photoperiod sensitivity sorghum cultivars found in West Africa. 21 Considering the growing importance of crop simulation models in assessing the impacts of 22 current and future climatic conditions, improving the ability of the models to simulate more 23 accurately the response of crops to environmental conditions is an important step in making 24 realistic assessment of impacts of climate and other management practices on crop 25 performance Therefore, the objectives of this study are to; (i) calibrate and validate sorghum 26 modules implemented in the model framework of APSIM, DSSAT and Samara for the 27 photoperiod sensitivity cultivars given the detailed crop growth data obtained from the field 28

trials (ii) and finally identify major strengths and weaknesses among the models to give
recommendations for improvements.

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2. Materials and Methods

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2.1 Calibration and validation data

6 The experimental data used for model calibration were collected from on-station field trial 7 during 2013 growing season at the International Crops Research Institute for the Semi-Arid Tropics (ICRISAT), Bamako, Mali Republic (12.52°N and -8.07°W). The experimental 8 protocol was designed to observed crop phenology, morphology and above ground dry 9 10 matter dynamics, yield and yield components under non-limited water and nutrient supply. The experiment had cultivar (ten) and sowing date (3) as treatments in a randomized 11 12 complete block design (RCBD) with four (4) replications. The cultivars were sown on June 14 represents early planting date (PD_1), July 9 represent medium planting date (PD_2) and 13 August 5 represents late planting date (PD_3) respectively. These sowing dates covered the 14 15 widest range of farmer's sowing window for sorghum in the Sudano-sahelian zone. Plant 16 population was 67,000 hills/ha (0.75m between rows and 0.20m between hills), and was 17 thinned to 1plant/ hill15 days after planting (DAP). The crop was fertilized using 100kg/ha of Di-ammonium phosphate at sowing and 50kg/ha of Urea (46%N) at 40 days after planting. 18 19 Insecticides were used according to local recommendations and weeding was done manually. Each plot was 8 m long by 5.25 m wide and consists of seven (7) rows. The outer 20 two rows were excluded from sampling in order to prevent border effect on the 21 measurements. Leaf area index (LAI) and above-ground biomass (separated into leaf, stem 22 and panicle) were sampled within the three rows at 1m² per sampling time at every 15days 23 interval beginning from 25DAP for PD_1, 27 DAP for PD_2 and 30 DAP for PD_3 until 24 grain filling stage. The samples were oven dried at 72 °C for 72 h. At maturity, harvest was 25 done on 4 m² area within each plot (4-replication per cultivar) for the determination of final 26 biomass and grain yield. The fresh weights of these samples were taken and thereafter sub-27 28 sample of 20 % of the total harvested leaves and stems together with the total harvested

panicles grain were oven-dried at 72 °C for 72 h. Phenology and leaf development were recorded as emergence, 50% flag leaf date, 50% flowering and maturity dates, total leaf number (TLN) and leaf area index (LAI). Also, the soil of the experimental plot was sampled at a depth of 0- 30cm prior to sowing and application of fertilizers. The soil is a well-drained, sandy loam(55% sand, 35% silt, and 20% clay)Soil organic carbon content was low at 0.24%.Nutrient analyses provided 224.5mg/kg total N, available phosphorus (Bray- P1) 94.94mg /kg, 2.47cmol/kg CEC and pH of water 5.3.

8 Four (4) out of ten (10) genotypic plant materials experimented were selected and directly calibrated in three contrasted process-based models (as described in section 2.2)from 9 10 observed data collected over three planting dates in 2013 growing season. The cultivars were CSM63E, CSM335, Fadda and IS15401 respectively. These four cultivars were 11 12 selected for their sharply contrasting phenology and morphology as well as their responses to photoperiod. The duration of their crop growing cycle varies from early to late maturity and 13 characterized as Guinea landrace plant group (Harlan and de Wet, 1972). Their 14 geographical origin emerged from both Mali and Burkina Faso. CSM63E, locally named 15 16 "Jakumbe", is an early (85-100days) maturity, an intermediate height type, low biomass, 17 enough grain and low photoperiod sensitivity (PPSen). CSM335 otherwise called "Tieble", is a traditional local variety with medium physiological maturity ranging from 105 to 135 days, 18 19 an intermediate plant height, high biomass, low grain and moderate PPSen. Fadda is an improved hybrid, medium maturity days (100 – 135), high-yielding dual purposes (biomass 20 and grain), intermediate plant height and also moderate PPSen. IS15401 also called 21 Soumalemba is a late maturity cultivar varied from 100 to 155 days, improved traditional tall 22 variety, high-yielding dual purposes (biomass and grain), and high PPSen. 23

In addition to these data, we gathered a large data set for validation of the models by using results from field experiments carried out between 2000 and 2008. These experiments were part of research study on sorghum physiology project developed by CIRAD and ICRISAT for two locations (Bamako and Cinzana, Mali) and during different cropping seasons. Details of

these experiments have been reported by Clerget et al., (2005; 2007). The agronomic
 practises and relevant observations used for this study are presented in Table 1.

3

4 [Insert Table 1 near here]

5

6 2.1.1 Environmental conditions

7 Daily climatic condition was monitored during 2013 growing season using automatic weather 8 station (AWS) installed within the station (less than 500m to the experimental site). The data observed include rainfall, solar radiation, maximum and minimum temperature relative 9 10 humidity wind speed and direction. Also, the long-term (1970- 2010) daily climatic data was 11 obtained to establish comparison with the cropping year at the station. The record shows 12 that 2013 total rainfall (1190mm) was above long-term average (1970-2010) and classified 13 as a wet year. Also, the analysis of monthly rainfall at the station indicates a distinct mono-14 modal pattern with the peak amount in August and varied between May and October (Figure 15 1). It was found that over 50% of the total rainfallwas received in the month of July and August, while both minimum and maximum temperatures decrease uniformly throughout the 16 growing season. 17

18

19 [Insert Figure 1 near here]

20

To further define the climatology of the station (Table 2), the onset date of growing season was computed after Omotosho et al., (2000), while cessation of rainy season was computed after Traoré et al., (2000).Average monthly air temperature varies from 26.2 °C to 32.3 °C; average solar radiation observed was 18.7MJ/m²/day. Also, growing season astronomical day length varies from 11 h 15 min to 12 h 45 min and civil daylength from 12 h 10 min to 13 h 38 min.

- 1 [Insert Table 2 near here]
- 2
- 3

2.1.2 Calculation of derived parameters

- 4 Additional parameters for calibration data calculated as follows:
- 5 Daily growing degree-days (GDD, ⁰C day) were calculated as (Streck, 2002):

 $6 \quad \text{GDD} = (T_{\text{mean}} - T_{\text{b}}) / \text{day} \qquad (1)$

where Tb is the base temperature, assumed 11°C as found in most literatures for sorghum (Folliard et al., 2004; Clerget et al., 2004) and T_{mean} is the daily mean temperature. The accumulated growing degree-days from planting (AGDD) was calculated by adding up the GDD values, i.e. AGDD = Σ GDD.

Phyllochron was calculated for each planting date and cultivar by the linear regression between the number of leaves produced and the thermal time in each sampled period. The thermal time (°C) necessary for the appearance of a leaf is equal to 1/b, where b is the slope t of the regression.

The coefficient of light extinction was computed from LAI-2000 plant canopy analyzer (LI-COR 15 Inc., Lincoln, NB, United States). The LAI2000 estimates light transmitted by the ratio of 16 17 radiative measurements below and above the canopy. The fraction of radiation intercepted was calculated by multiplying the instrument output DIFN (Diffuse Not Intercepted) by a 18 value of 0.94 assuming only 6% of visible light reflected by green canopy (Dingkun et al., 19 1999). The reliability of this assumption was confirmed by the analysis of spectral reflectance 20 data obtained by field spectroradiometer, data not showed, (Stroppiana et al., 2005). Light 21 extinction coefficient k is then calculated inverting Lambert-Beer's law as: 22

23

 $K_{df} = -\ln (0.94 \text{PAR}_{\text{transmitted}})^* \text{ LAI}^{-1} \qquad (2)$

Representative values of k for the two cultivars at different development stages were in both cases derived by regressing of In (PAR_{transmitted}) vs LAI (Casanova *et al.*, 1998; Dingkuhn *et al.*, 1999). Also, Radiation Use Efficiency (RUE) was calculated as the slope of the linear regression between values of above ground biomass and cumulated APAR - Absorbed photosynthetically active radiation (calculated using Eq. 3) (Sinclaire and Muchow, 1 1999). The Photosynthetic Active Radiation (PAR) was calculated from daily solar radiation 2 (SR; obtained from weather station records during growing period), assuming that PAR 3 comprised 45 % of SR (Howell et al., 1983). Meanwhile, daily fAPAR time series was estimated by Lambert-Beer formula using the k values in Lambert- Beer's law 4 $APAR_d = PAR_d \times fAPAR_d$ (3) 5 In the equation the subscript letter d refers to the daily value and $fAPAR_d = 1 - exp^{-k^*LAI}$. 6 7 8 2.2 Model Descriptions 9

The three process-based models were examined for comparison and recommendation for improvement in this study; they are DSSAT, APSIM and Samara. Table 3 provides an overview of the modelling approaches applied regarding the major processes that determine crop growth and development relative to their similarities and differences. All the models used were designed for sorghum crop, and also capable of simulating crop phenology, total above-ground, LAI, leaf number, grain yield, and field water balance components in daily time steps.

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2.2.1 Model calibration and analysis of differences

Models were calibrated by matching directly both the observed and derived parameters from 19 2013 field experiment. The calibration procedure followed four phases which include 20 21 phenology, morphology, above-ground biomass and grain yield. All the models considered thermal time after planting and it was computed using an algorithm by Jones and Kiniry 22 (1986), considering that growth speed increases as a linear function of temperature between 23 a base and an optimal temperature, and then decreases linearly between an optimal and 24 maximal temperature. Thus, the cardinal temperatures used across the models were 11°C 25 for base temperature below which no development takes place (Lafarge et al., 2002; Clerget 26

et al., 2004); and 44°C for maximum temperature, above which development is also nil 1 2 (Ritchie and Alagarswamy, 1989). Instead of a single value for the optimum temperature 3 (34°C according to Ritchie and Alagarswamy, 1989; confirmed by Clerget et al., 2004), resulting in a sharp maximum for development rate, we used an optimal range of 4 temperatures between 28 and 36°C (Dingkuhn et al., 2008). These cardinal temperatures 5 form a doubly broken stick model with a plateau between the two optimal temperatures 6 7 (Kouressy et al., 2008). The daily civil day length (sun 6^o below the horizon at beginning and end of the day) was calculated according to Keisling (1982) based on latitude and Julian 8 calendar date. Plant available water capacity was derived from field measurements. 9 Parameter in APSIM related to water dynamics such as runoff curve number and 10 evaporation terms were defined as Hoffmann et al. (accepted). In DSSAT and APSIM, the 11 12 nitrogen related parameters in the soil modules were according to soil analysis data obtained 13 from experiment which include organic carbon and initial nitrogen. The Samara model used model default does not need this input as it does not account for nitrogen. Calibration of leaf 14 15 number in the model followed the leaf appearance rate (phyllochron) calculated from the 16 field-observed data. Also, derived light extinction coefficient (k), and radiation use efficiency 17 (RUE) served as input for the calibration of above-ground biomass and grain yield. The simulated output for each cultivar for different parameters of crop growth and development 18 19 were analyzed compared to the observed data and relate to the modelling approaches used. 20 While the main differences and similarities in model predictions led to the recommendations for model improvements as provided below. 21

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23 [Insert Table 3 near here]

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25

2.3 Evaluation of the models

We first calibrated the models using the information from the detailed field trial during 2013.
Thereafter, we used the additional data set to independently validate the models (Clerget et

al. 2005, Table 1). In the calibration process we aimed to achieve a good agreement with the
observed. For calibration and validation we assessed the goodness-of-fit between model
simulated and observed values of yield and above-ground biomass as well as phenological
events Model-estimated (simulated) were compared with observed using the following listed
statistics;

6

1. Root mean square error (RMSE):

7 RMSE = $[n^{-1}\Sigma$ (simulated – observed) ²]^{0.5}Eqn. (4) 8 2. The normalized root mean square error (NRMSE) express in percent, calculated 9 according to Loague and Green (1991) with eqn.(4)

10 NRMSE = $[n^{-1}\Sigma$ (simulated – observed) $^{2}]^{0.5}X = \frac{100}{M}$ Eqn. (5)

11 M is the mean of the observed variable. NRMSE gives a measure (%) of the relative 12 difference of simulated versus observed data. The simulation is considered excellent 13 with a NRMSE less than 10%, good if the NRMSE is greater than 10% and less than 14 20%, fair if the NRMSE is greater than 20% and less than 30% and poor if the 15 NRMSE is greater than 30% (Jamieson*et al.*, 1991).

- Linear regression (1:1) plot was taken as an indicator to inform whether the models
 under- or overestimated measured yields, i.e. the direction and magnitude of bias.
- Additionally, for comparison, the traditional R² regression statistic (least-squares
 coefficient of determination) was calculated though it does not take into account
 model bias, which is central when assessing the performance of simulation models.
- 21

22 [Insert Table 4 near here]

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- 24
- 25
- 26

1 **3. Results**

2 **3.1 Calibration**

3.1.1

3

Photoperiod sensitivity

After careful calibration, all models reproduced the diverse photoperiod sensitivity (PPSen) 4 5 of the cultivars satisfactorily. Furthermore, estimated model-fitted for crop developmental phases (Figure 2a) showed how the cultivars response to PPSen between the emergency 6 7 and flag leaf initiation (E-FI) stage. These ranged from low PPSen for CSM63E to high PPsen for IS15401. The results show a decrease in thermal time (E-FL) with the late PD 3 8 observed reducing day length hour, which signified the level of PPSen of across cultivar. 9 CSM63E indicated as low PPSen cultivar with the lowest thermal time E-FI across the 10 sowing dates ranging from 103 to 57°Cdays. Also, CSM335 and Fadda indicate as the 11 12 moderately PPSen cultivars with the observed thermal time E-FI at a medium ranged between 330 and 117ºCdays while the high PPSen cultivar (IS15401) observed the longest 13 thermal time E-FI ranging from 464 to 196°Cdays. 14

15

16 [Insert Figure 2a near here]

17

Also, Table 4 presents the final calibrated genetics coefficients for cultivar's PPSen. In 18 19 APSIM, the critical photoperiod hours 1&2 were the same for all cultivars; the values were adjusted to 12.8h for photoperiod crit 1 and 13.2h for photoperiod crit 2. The calibrated 20 photoperiod slope varied between 150°C/H (CSM63E) and 900°C/H (IS15401). Also, DSSAT 21 presents the photoperiod hour ranging from 12.6H (CSM335 and IS15401) to 13.2H for 22 Fadda with lowest PPSen coefficient (P2) for CSM63E (50 °Cday) and highest value for 23 24 IS15401 (450°Cdays). The PPSen calibration in Samara followed a different modelling approach by using a dimensionless value ranging from 0.3 for highly sensitive cultivars to 25 0.95 for insensitive cultivars (Dingkuhn et al., 2008). The low PPSen cultivar (CSM63E) was 26 calibrated with coefficient value of 0.85 while high PPSen cultivar (IS15401) obtained a 27

coefficient value of 0.5. As shown on the Table 4, APSIM and DSSAT followed similar 1 2 pattern in the photoperiod slope values while Samara indicates opposite for the same 3 purpose. For instance, the low coefficient value (0.5) in Samara indicates high PPSen cultivar which contrasts to APSIM and DSSAT models. Also, the calibrated photoperiod 4 5 critical hours (lower and upper limits) expressed similar pattern for APSIM and Samara. The same values were calibrated for all the cultivars, while DSSAT was calibrated by the 6 7 photoperiod critical hours (P2O) as a single value for each cultivar, varied from 12.6 hrs 8 (CSM335 and IS15401) to 13.2 hrs (Fadda).

9

10 [Insert Table 4 near here]

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12 3.1.2 Development phases

Table 5 presents calibrated cultivars genetics coefficients for the crop development phases, 13 although the models were very similar but name identification was different. The genetics 14 15 coefficients were obtained by matching the observed phenology with the model-simulated. 16 The models were calibrated for about six or seven coefficients that defined their growth stages between emergence and maturity. In APSIM, CSM63E obtained the lowest value 17 (190°Cday) from emergence to end of the juvenile phase followed by medium cultivars 18 19 (Fadda and IS15401) while CSM335, the late maturity obtained the highest value of 220°Cday. End of juvenile varied across the cultivars, the least value (50°Cday) was 20 obtained by CSM63E while the highest value (180°Cday) was obtained from late maturity 21 cultivar (IS15401). All the cultivars observed similar characteristics from flag leaf to 22 flowering and also from flowering to start of grain, the calibrated values are 170 and 23 24 80ºCday. DSSAT-CERES-sorghum model coefficients parameter also varied among the cultivars, the early maturity cultivar CSM63E had the lowest value (190°Cday) indicates as 25 P1 (thermal time from seedling emergence to the end of the juvenile phase) while the late 26 27 maturity cultivar IS15401 had the highest value of 550°Cday. P2 indicates as end of the

1 juvenile phase to panicle initiation, the obtained values ranged between 50°Cday (CSM63E) 2 and450°Cday (IS15401). P2O (critical photoperiod or the longest daylength hour at which 3 development to occurs at maximum rate) ranged from 12.6h (for CSM335 and IS15401) to 13.2h for Fadda. Also, cultivars expressed similar characteristics, thermal time from end of 4 5 tassel initiation to anthesis (PANTH) except for late variety (IS15401) that differs with 6 calibrated value of 640.5°Cday The values of P3 (thermal time from the end of flag leaf 7 expansion to anthesis) and P5 (thermal time from beginning of the grain-filling to physiological maturity) varied between cultivars. The calibrated values ranged from 170.5 to 8 300.5°Cday for P3 and 400 to 480°Cday for P5. 9

10

11 [Insert Table 5 near here]

12

For Samara model, only the basic vegetative phase (BVP) differed among the cultivars, the 13 calibrated values ranged from 260°Cday for CSM63E to 450°Cday for IS15401. Maturation 14 15 phase #1 (SdjMatu1) and maturation phase #2 (SdjMatu2) did not varied much among the 16 cultivars. SdjMatu1 ranged from 350°Cday to 400°Cday andSdjMatu2 obtained a fixed value of 40°Cday across cultivars. Thus, Figure 2b indicates DSSAT total thermal time estimates 17 to be the closest to the field-calculated thermal time for all the cultivars (with exception of 18 19 IS15401). The differences between the model-simulated and field-calculated could be linked 20 to the modelling approaches described earlier in Table 3.

21

22 [Insert Figures 2b near here]

23

Furthermore, the simulated phenology (flowering and maturity) were observed to be in good agreement with the field-observed values (Table 6). The models captured the strong effect of planting date on growth development to a wide extent. Across the cultivars, APSIM and Samara simulations showed the lowest value of RMSE against the observed values for

flowering and maturity compared to DSSAT. Also, there were no significant differences of
 mean between the model-simulated and observed for most of the cultivars except for
 CSM335 (P<0.02 for flowering) and also Fadda and IS15401 (P<0.03 for maturity).

4

5 [Insert Table 6 near here]

6 **3.1.3 Leaf appearance rate and light interception**

7 As displayed in Table 7, APSIM cultivar's genetics coefficients for leaf appearance rate 8 followed two steps i.e. leaf appearance to develop most leaf liqule (leaf app rate 1) and last 9 leaf ligule (leaf_app_rate_2). The calibrated values (53°Cd/leaf and 26.5°Cd/leaf) were the same for all the cultivars. The values justified the increase in the observed leaf number (>20) 10 11 per plant most of the cultivars; it also prevented over-simulation of TLN against the observed values. DSSAT and Samara followed a similar pattern for all the cultivars; both models 12 expressed the leaf appearance rate as PHINT and Phyllochron interval. DSSAT calibrated 13 values varied from 55 to 60°Cd/leaf while Samara varied from 38 to 40°Cd/leaf. The 14 15 calibrated value was the same for CSM63E, CSM335 and Fadda in both model, 60ºCd/leaf 16 in DSSAT and 40°Cd/leaf in Samara. IS15401 indicates slightly lower value of 55°Cd/leaf for DSSAT and 38°Cd/leaf for Samara. This value justified the longer thermal time of vegetative 17 phase resulting to more leaf produced by the cultivar. Although, none of the models 18 19 reproduced the estimated phyllochron values for PD_3 that had no effect of PPsen but the simulated leaf number showed a close match with observed values for all the cultivars with 20 lowest error statistics estimated (Figure 3). The RMSE and R² ranging from 1.3 to 2.2 leaves 21 and 0.66 to 0.97 for the simulated leaf number of all the cultivars and models. Samara and 22 23 DSSAT simulations showed to be the most accurate for most cultivars while, APSIM performance was the best for IS15401 as indicated by the estimates of RMSE and R^2 24 (Figure 3). Furthermore, the models captured the differences in observed leaf number 25 relative to the sowing dates (Figure 4). There was no significant difference of means (P< 26 27 0.05) between the mode-simulated and observed values. Across planting date, the highest

1 TLN was obtained at early (PD_1) which was significantly higher than medium (PD_2) and 2 both were significantly higher than TLN at late (PD_3). Due to shortening of the vegetative 3 phase, late (PD_3) observed a reduction of about seven (7) leaves compared to early 4 (PD_1) resulting from cultivar's response to variation of sowing date. This result implicated 5 that the end of vegetative phase could be largely dependent on temperature and variation in 6 planting date.

7

8 [Insert Table 7 near here]

9

10 The simulated LAI for the cultivars show over-estimation against the observed LAI with the high values of estimated error statistics. The RMSE and R² ranging from 0.56 to 1.46m²/m² 11 12 and 0.3 to 0.83 for the LAI simulated by all the models (Figure 5). For most cultivars, Samara 13 estimates were closer to the observed values compared to APSIM and DSSAT. The overestimation could be linked to early senescent rate observed from the field trial for all the 14 15 cultivars with exception of CSM63E (Figure 6). Leaf senescence might not be properly 16 simulated by the models. Samara simulation was different from APSIM and DSSAT due to 17 its ability to simulate based on organo-genesis of plant growth which including the senescent rate of the leaf production. 18

19

20 [Insert Figure 3 near here]

21

The light extinction coefficients, k values showed that there was no significant difference between cultivars but it slightly differed across the planting dates (result not shown). Pooling the sowing dates together for each cultivar, the estimated mean value of k was 0.8. In addition, observed the analysis of covariance at different growth stages (Akinseye, 2015) indicate no significant difference in k-value among the four cultivars but slightly differed across sowing dates despite the large differences in plant height between the early and late

1 maturity cultivars. The result suggests that aspects of canopy architecture likely to affect k, 2 such as leaf angle distribution, did not differ among these diverse cultivars. As shown on 3 Table 7, the k value of 0.85 was used in DSSAT for all cultivars and Samara (except for Fadda). The high k-value used by the models prevents against under-estimation of above-4 5 ground biomass and grain yield outputs. The model-calibrated was closed to the field-6 estimated which was in agreement to previous studied by Porter et al., (1993) who found 7 that the higher the crop will intercept the value of k, the more of the incident PAR particularly 8 at low LAI, and thus dry matter production could be over-estimated.

9

10 [Insert Figure 4 near here]

11

12 **3.1.4** Radiation use efficiency, and partitioning for yield formation

There was a strong effect of variation of sowing date on estimated RUE between PD_1 and 13 14 PD_3 from field trial with the high values obtained from early PD_1 and decreased with late PD 3. On the average, the highest value was observed for Fadda (6.9g/MJ), followed by 15 IS15401 and CSM335 (5.8g/MJ and5.0/MJ) while CSM63E gave the lowest value of 3.3g/MJ 16 respectively. The model-calibrated values confirmed the genotypic differences as estimated 17 from field experiment (Table 7). This estimated RUE was significantly higher than those 18 found in the literatures for sorghum (Kiniry et al., 1989; Muchow, 1989). The high RUE 19 values (>3.0 g/MJ) obtained could be linked to the cultivar-specific traits especially for the 20 21 PPSen sorghums found in West Africa. For APSIM, RUE was determined as individual value between emergency and maturity during the crop growth period while DSSAT and Samara 22 determined as a single value between emergency and maturity. The APSIM calibrated 23 coefficients ranged from 1.25 g/MJ (CSM63E) to 1.85 g/MJ (Fadda - improved hybrid). In 24 25 DSSAT, the calibrated RUE value was 3.8 g/MJ for CSM63E, CSM335 and IS15401 while Fadda obtained higher value of 5.2g/MJ, which justified for the high biomass production as 26 hybrid. Also, the T-conversion signifies RUE in the Samara, the values ranged from 4.5g/MJ 27

forCSM63E to 6.9g/MJ for Fadda. Across the models, only Samara calibrated RUE were closer to the field-estimated (except for CSM63E). The model-calibrated was found to be higher than the commonly used range found in the literatures e.g. Sinclair and Muchow, (1999) used 1.2–1.4 g/MJ as calibrated value for sorghum.

5 [Insert Figure 5 near here]

6

Interestingly, there was a relatively good agreement between the model-simulated and
observed for total above-ground biomass (Figure 7a). APSIM estimated the lowest RMSE
(1536 kg/ha), NRMSE (11.5%) and very strong coefficient of determination (R²- 0.9) followed
by DSSAT with RMSE (1708 kg/ha), NRMSE (12.8 %) and very strong R² (0.9) and Samara
gave RMSE of 1849 kg/ha, NRMSE (13.8 %) and strong R² (0.8).

12

13 [Insert Figure 6 near here]

14

15 [Insert Figure 7a near here]

16

The simulated grain yield was a product of grain number and grain size. Maximum grain 17 yield number is a function of the change in plant biomass between panicle initiation and the 18 start of grain filling, while grain size is determined by grain growth rate, the effective grain-19 filling period, and the re-distribution of assimilates post-anthesis. For DSSAT, the G2 (scale 20 for partitioning of assimilates to the panicle ranged from 0.5 mg/day for CSM63E to 21 2.5mg/day for improved hybrid Fadda and IS15401. Samara estimated as function of 22 Coeff_Pan_Sink_Pop*Pan_Struct_Mass_Max/1000-grain weight. Panicle structure mass 23 maximum (Pan Struct Mass Max) was calibrated between 3.0g (CSM63E and CSM335) 24 and 3.5g (Fadda and IS15401. The simulation outputs showed that APSIM and Samara 25 26 estimates for grain yield were closer to the observed values compared to DSSAT (Figure

7b). Across the cultivar, APSIM indicated a better agreement relative to the observed values
 with estimated lowest RMSE (397 kg/ha), NRMSE of 20.3% and R² of 0.8. Samara and
 DSSAT slightly over-estimated with the RMSE (538 and 771 kg/ha), NRMSE (27.6 and 39.5
 %) and R² (0.6 and 0.5) respectively.

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6 [Insert Figure 7b near here]

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3.2 Validation

3.2.1 Phenology, total leaf number, total biomass and grain yield

The valuation results for the simulated phenology and total leaf number (TLN) against 10 observed values over the different growing seasons for all the cultivars showed a good 11 matched with a minimum statistical error (Figure 8). For the duration to flowering (Figure 8a), 12 Samara estimated observed the lowest RMSE of 6.6 days and R² of 0.8 while APSIM and 13 DSSAT estimates were close with RMSE of 8.3 and 8.7 days. In the case of duration to 14 15 physiological maturity (Figure 8b), APSIM showed the lowest RMSE value of 7.6days and followed by DSSAT with RMSE of 8.9 days, both had correlation (R²) of 0.9 while Samara 16 17 estimates was the highest with the RMSE of 9.2 days and correction (R²) of 0.8. In general, the model-simulated for phenology shows a slight overestimation against the observed with 18 a reasonable bias error. Samara estimates was the most accurate compared to APSIM and 19 DSSAT for flowering while APSIM estimates indicate the best accurate compared to DSSAT 20 21 and Samara for physiological maturity. For TLN, Samara estimates indicate the lowest RMSE (0.7 leaf) followed by APSIM and DSSAT (Figure 8c). 22

23

24 [Insert Figure 8 near here]

The model-simulated for both grain yield and total biomass showed significant variations against the observed data (Figure 9). None of the models could closely reproduce

1 observations across the cultivars. The simulated grain yield was slightly under-estimated by APSIM and DSSAT while Samara slightly over- estimated it. The results showed no 2 3 significant difference of mean at 5% level of probability (P<0.05) between the models and observed values for grain yield. Similarly, average total biomass showed over-estimation for 4 5 all the models against observed values and well as significantly difference of mean between the models and observed. As displayed in Figure 10, the statistical errors found APSIM 6 7 estimates to be well corresponds to the observed values with the lowest RMSE, NRMSE (%) and R² compared to DSSAT and Samara. For both grain yield and total biomass, APSIM 8 results showed the RMSE (472 and 2452 kg/ha), NRMSE (22.6 and 23.3%) and R² (0.7 and 9 0.8). Meanwhile, Samara indicates the highest RMSE (762 and 4058 kg/ha), NRMSE (35.7 10 and 38.8 %) and weak R² (0.4 and 0.5) respectively. 11

12

13 [Insert Figure 9 near here]

14

15 **4 Discussion**

A comparison of crop simulation models served two purposes in this study which include: (i) 16 17 the modelling assessment for their ability to predict crop growth and development with detail 18 information linked to photoperiodism during calibration and (ii) possible identification of the 19 parts that produce systematic errors for further improvements. When an error has been 20 identified, steps can be taken to improve model performance on the basis of better analysis 21 of the processes involved. Then, complementary processes of the model development and experimentation become cyclic and mutually supportive (Palosuo et al., 2011). Some 22 aspects of the performance of the models were very satisfactory (e.g. Phenology and leaf 23 number) but there was also a clear indication for model improvements should be sought for 24 the parts that present high significant error (e.g. LAI and grain yield). 25

26

- 1 [Insert Figure 10 near here]
- 2
- 3

4.1 Improvements to simulated phenology

The calibration process over the three planting dates showed that model-simulated for the 4 5 phenological phases (duration to flowering and physiological maturity) were well 6 corresponds to the observed values (Table 6). This result underlined the capability of the 7 models to predict crop duration for the agronomic relevant range of sowing dates under 8 varying daylength period. However, the results confounded the models adaptability to predict 9 West African diverse photoperiod sensitivity varieties. Large error (>7days) estimated for the high PPSen cultivar (IS15401) by all models, which suggests further improvement on 10 cultivar's photoperiodism for phenological growth stages. 11

In addition, the validation presented over different growing seasons (non-limiting water and 12 13 nutrients supply) and locations (Bamako and Cinzana) corroborates the strength of models for simulating phenology growth of sorghums for semi-arid cultivars (Figure 8a&b). The 14 results showed a near perfect fit of for the model-simulated phenology (flowering and 15 maturity) against the corresponding observed values. The large error estimated by APSIM 16 and DSSAT for flowering, DSSAT and Samara for maturity could be linked to the high 17 PPSen cultivar among them. The imperfect model fit can be expected to have significant 18 19 effect on other parts of the simulation results for example LAI. The result found suggests that crop models be used to determine the crop duration for the widest range of sorghum 20 21 varieties in West African semi-arid region, reinforcing the studied by Traoré et al., (2007).

22

4.2 Improvements to leaf area development, biomass partitioning and yield formation

Model-estimated for TLN agreed jointly with the observed values both for the calibration and
 validation. Samara ranked as the best estimates with the lowest RMSE, NRMSE (%) and R²
 seen for most cultivars except IS15401, followed by APSIM and DSSAT respectively. Also,

1 the model-simulated errors across the cultivars for LAI were seen to be very large with the estimated RMSE and NRMSE (%).In general, the model over-estimated against the 2 3 observed that could be as a result of early senescent leaves observed. But Samara gave the lowest RMSE and NRMSE (%) and strong R² for all the cultivars (with exception CSM63E) 4 compared to APSIM and DSSAT. As observed from the calibration, APSIM and DSSAT 5 6 simulation for LAI show more response to biomass accumulation development but Samara 7 response to the detail organogenesis procedure for the plant growth beginning from crop 8 emergency. Also, the performance of Samara could be linked to limited crop platform (only sorghum and rice) parameterized in model. In addition, Samara addressed the drawback 9 10 already mentioned in the literatures by Ewert et al., (2002), Traoré et al., (2007) and Adam et 11 al., (2011) in order to better represent the leaf area development in crop model. The 12 approach chosen was derived from the plant level model ECOMERISTEM (Dingkuhn et al., 13 2006) which included the capability to simulate competition for assimilates (supply) among growing organs (demand) and to adjust accordingly the growth rate and final size of different 14 organs in the plant. 15

16 Furthermore, simulation for above-ground biomass and grain yield suggest a need for 17 significant improvement. The model performances were contrary to the results obtained for the phenology and TLN. APSIM was more accurate in terms of both calibration and 18 19 validation of grain yield and total biomass compared to DSSAT and Samara. For calibration (Figure 7), the model errors estimated by APSIM were seen to be the lowest values with the 20 RMSE (397 and 1536 kg/ha), NRMSE (20.3 and 11.5 %) and strong R² (0.8 and 0.9) 21 respectively. The validation demonstrated a significant variation between the model-22 simulated and observed values. The results confirmed further that the model uncertainty lied 23 in the prediction of above-ground biomass and grain yield relative to the measured-observed 24 values (Figure 9). Samara estimates for grain yield resulted a slight over-estimation (with 25 high variability against the measured values) while APSIM and DSSAT predicted slight 26 underestimation and less variability. In the case of total biomass, model-simulated showed 27 28 overestimation with less variability against the observed values. The model error estimated

1 by APSIM was found to be better and accurate in the prediction of grain yield and total 2 biomass compared to DSSAT and Samara models. As observed during the calibration 3 process, the time-course results (figures not shown) across the cultivars indicated only Samara model exhibited ability to reproduce close to the measured-observed values of 4 5 above-ground biomass at early vegetative stage of the crop sampled at different times 6 during growing season. Due to the large errors estimated for both grain yield and biomass 7 across models, it is therefore suggested that more efforts are still required on model 8 partitioning for simulating aboveground biomass and grain yield formation especially PPSen sorghums. 9

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11

4.3 Sources of uncertainties

12 As observed from this study, the model uncertainty lied majorly on partitioning for simulating 13 above ground biomass at the early growing phase (vegetative) and grain yield formation particular for the PPSen cultivars. Although, the models captured final biomass and yield 14 15 values, but the estimated error was too larger compared to phenology and morphology simulation. This uncertainty could be attributed to three possible sources; (i) model structure 16 (ii) bad parameterization or (iii) quality of field trial data. On model structure, all the models 17 18 simulated above-ground biomass based on light interception/absorbed coefficient (k) and 19 radiation use efficiency (RUE) and water demand but Samara was built on model ECOMERISTEM (Dingkuhn et al., 2006). This platform shows better capability to simulate 20 competition for assimilates (supply) among growing organs (demand) and to adjust 21 22 accordingly the growth rate, this approach led to reproduction of early growing phase. 23 However, APSIM and DSSAT respond to soil parameterization (e.g. SLPF in DSSAT and 24 initial nitrogen in APSIM) as well nutrients supply. As observed during calibration, there was a carryover effect of soil parameterization and nutrients applied to APSIM and DSSAT 25 resulting to model over-estimation of LAI against the field observed values. The measure 26 27 was used to prevent model underestimating the final biomass and grain yield. On model

1 parameterization, we pointed out the difficulties to assess critical parameters such as GDD 2 from emergence to end of the juvenile stage. Another factor that observed to be responsible 3 for significant variations between the simulated and observed results was plant population. For instance, the calibrations were performed on a specific planting density 4 5 (67000plants/hills), thereafter validated with different planting densities. This approach was 6 observed to introduced large error between the models for the simulated grain yield and total 7 biomass e.g. Samara. We thereby suggest that validation of the models could be better for 8 total biomass and grain yield, if the same level of plant populations is considered, the way 9 model response to different level of nutrient supply. Finally, the quality of field trial data, we 10 can discuss the importance of sowing dates trials to assess the phyllochron (Clerget et al., 11 2007) properly while in our case though the late PD_3 sowing was a late sowing, it might not 12 late enough to assess the phyllochron properly. The field trials used for evaluation were 13 considered to be non-limited by nutrients, however, the strong contrast to the simulated yield 14 led to the suspension that there were potentially hidden nutrient deficiencies.

15

16

17 **5.** Conclusion

18 A novel and apparent merit of this study is that commonly used crop growth models for 19 sorghum were tested for diverse PPSen cultivars for calibration and validation. The results established the capability of the process-based models to predict crop duration for the 20 agronomical relevant range of farmer's planting window and photoperiod sensitivity for 21 sorghums cultivars in the region. All the models showed minimum error estimates for 22 23 phenology and morphology parameter against observed ones obtained over different 24 growing seasons. However, differences in the simulating yield and biomass with the lowest possible error estimates like what we observed for phenology could be trace to the 25 contrasting ways in model partitioning for this parameters. In conclusion, the level of 26 27 uncertainty in simulating final grain yield and biomass were found to be lower in APSIM and

1 DSSAT compared to Samara. This further confirmed their reliability to predict climate 2 impacts on yield and yield variability. Longer yield series for clearly defined growth and 3 management conditions for calibration that used in this study would greatly enhance the 4 outcome of model comparison studies for subsequent model on the level of uncertainty.

5 Acknowledgement

6 This work constitutes part of doctoral research studies funded by WASCAL Graduate 7 research programme and also supported by ICRISAT, Mali for the experimentation. The 8 authors thank Dr. Neil Huith for his assistance during calibration of the cultivars in APSIM 9 and also Dr. Clerget Benoit permission to used part of his data reported on physiology of 10 sorghum project experiments in West Africa for the validation of the models.

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Figure 1: Comparison of the long-term (1970-2010) monthly rainfall, minimum air temperature and maximum air temperature and cropping year 2013



Figure 2a: Estimated model-fitted crop growth stages between emergency and flag leaf initiation (E-FI) indicating cultivar's response to photoperiod sensitivity (PPSen).











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Figure 4: Comparison between the model-simulated and observed for leaf number over the three sowing dates. The significance difference of mean between the models and observed at 5% level of probability (P<0.05) are as follows; 0.24(CSM63E); 0.37(CSM335); 0.77(Fadda) and 0.32 (IS15401) respectively.



Figure 5: Model-simulated leaf area index (LAI) against the observed LAI over the three planting dates. (a) CSM63E: APSIM – RMSE = 0.56 m²/m², R² = 0.62; DSSAT- RMSE= 0.81 m²/m², R²= 0.64; Samara - RMSE= 0.68, R²= 0.87. (b) CSM335: APSIM – RMSE = 1.4 m²/m², R² = 0.45; DSSAT- RMSE= 1.1 m²/m², R²= 0.62; Samara - RMSE= 0.8 m²/m², R²= 0.83. (c) Fadda: APSIM – RMSE = 0.92 m²/m², R² = 0.73; DSSAT- RMSE= 0.92 m²/m², R² = 0.89; Samara - RMSE= 0.87 m²/m², R² = 0.91. (d) IS15401: APSIM – RMSE = 1.46 m²/m², R² = 0.31; DSSAT- RMSE= 1.4 m²/m², R² = 0.68; Samara - RMSE= 0.9 m²/m², R² = 0.78.



rigure o. Observed average senescent leaves over rour replications for each cultivar in trifee sowing dates



Figure 7a: Simulated total biomass against observed total biomass for all cultivars over the three planting dates. APSIM: RMSE=1536kg/ha, NRMSE (%) =11.5, R²= 0.87; DSSAT: RMSE=1708kg/ha, NRMSE (%) =12.8, R²= 0.85; Samara: RMSE= 1840kg/ha, NRMSE (%) =13.8, R²= 0.82



Figure 7b: Simulated grain yield against observed grain yield for all cultivars over the three planting dates. APSIM: RMSE=397kg/ha, NRMSE (%) =20.3, R²= 0.8; DSSAT: RMSE=771kg/ha, NRMSE (%) = 39.5, R²= 0.5; Samara: RMSE= 538kg/ha, NRMSE (%) =27.6, R²= 0.6.



Figure 8: Model comparison for simulated phenology and total leaf number (TLN) against observed values for all the cultivars over different growing seasons, planting density and planting dates. (a) **Flowering:** APSIM - RMSE= 8.3 days; R^2 = 0.9; DSSAT- RMSE= 8.7 days; R^2 = 0.8; Samara - RMSE= 6.6 days; R^2 = 0.8. (b) Maturity: APSIM - RMSE=7.6 days; R^2 = 0.9; DSSAT- RMSE= 9 days; R^2 = 0.9; Samara - RMSE= 9.2 days; R^2 = 0.8. (c) TLN: APSIM - RMSE=1.2 leaves; R^2 = 0.96; DSSAT- RMSE= 1.3 leaves; R^2 = 0.97; Samara - RMSE= 0.7 leaves; R^2 = 0.99.



values for the all cultivars over different growing seasons, planting density and dates. Boxes indicate the inter-quartile range (25-75 percentiles) and whiskers show the high and low extreme values. The significance difference of mean between the models and observed at 5% level of probability (P<0.05) are as follows; 0.25 for grain yield and 0.00008 for Total biomass.



Figure 10: (a) Model comparison for simulated grain yield and total biomass against the observed values for all the cultivars over different growing seasons, planting density and planting dates. (a) Grain yield: APSIM - RMSE= 472 kg/ha; NRMSE (%) =22.6; R²= 0.68; DSSAT- RMSE= 719 kg/ha; NRMSE (%) = 34.8; R²= 0.4; Samara - RMSE= 762 kg/ha; NRMSE (%) =35.7; R²= 0.4.(b) Total biomass: APSIM - RMSE= 2452kg/ha; NRMSE (%) =23.3; R²= 0.75; DSSAT- RMSE= 3138kg/ha; NRMSE (%) =36.8; R²= 0.66; Samara - RMSE= 4058 kg/ha; NRMSE (%) =38.8 %; R²= 0.45.

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