



# Novel methodology to evaluate and compare evapotranspiration algorithms in an agroecosystem model

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## ABSTRACT

Efforts to improve agroecosystem models require methods for unbiased comparisons among simulation algorithms. With focus on evapotranspiration (ET) in Cotton2K, the objectives were to develop a novel methodology for evaluating model parameterization options and to compare model performance using three ET algorithms. The Cotton2K model was updated to include a standardized ET method, and two Penman approaches were also tested. Sobol global sensitivity analysis and multiobjective optimization were used to identify influential parameters and select feasible parameterization options. The three ET methods led to differences in simulation accuracy for ET, soil water contents, and several plant growth metrics ( $p < 0.05$ ). However, no ET method could consistently outperform the other two methods, and ET simulation errors were up to 60%. The simulation methodology permitted unbiased comparison of three ET methods in Cotton2K and highlighted areas for model improvement, including the surface evaporation simulation and the linkage between simulated ET and crop growth.

## 1. Introduction

Evapotranspiration (ET) is commonly the greatest pathway of water loss from crop production systems. As a result, the accuracy of water balance simulations in agroecosystem models is highly dependent on how well the model simulates ET. Moreover, the calculations of other model components, including soil nutrient and crop growth and development algorithms, depend on the accuracy of ET and water balance simulations. These concerns have driven recent efforts to evaluate and improve ET calculations in many agroecosystem models, including the Decision Support System for Agrotechnology Transfer (DSSAT) Cropping System Model (CSM) (Attia et al., 2016; DeJonge et al., 2012b; Marek et al., 2017; Sau et al., 2004; Thorp et al., 2014b), the Root Zone Water Quality Model (RZWQM) (Anapalli et al., 2016), and the Soil and Water Assessment Tool (SWAT) (Marek et al., 2016). Several of these model evaluation efforts have incorporated high-quality daily ET data sets, such as those provided by the large weighing lysimeters at Bushland, Texas (Anapalli et al., 2016; Marek et al., 2016, 2017). Among various methods for ET measurement, weighing lysimeters that are properly designed, installed, and managed can provide accurate ET data for agroecosystem model evaluation (Farahani et al.,

2007).

A variety of methods exist for ET simulation in agroecosystem models, each having unique limiting assumptions, algorithm complexity, and input data requirements. Naturally, comparisons of different ET approaches both within and among models have aimed to identify the better performers. Farahani and Bausch (1995) found better ET estimates from the Shuttleworth and Wallace (1985) method as compared to a Penman-Monteith approach. Ma et al. (1999) demonstrated improved ET simulations with energy combination methods as compared to pan evaporation approaches, particularly when transpiration occurred. Lascano and Van Bavel (2007) compared explicit and recursive combination methods for computing Penman-based ET, finding the former to calculate as much as 25% less ET than the latter on hot summer days in Lubbock, Texas. Anothai et al. (2013) compared Priestley-Taylor and Penman-Monteith ET approaches in the DSSAT CSM, finding the latter method to better agree with measured ET data from Bowen ratio instrumentation. Kang et al. (2009) performed a comprehensive comparison of ET simulations from three wheat (*Triticum aestivum* L.) models (CROPWAT, MODWht, and DSSAT CSM-CERES-Wheat) using measured ET from the Bushland weighing lysimeters and from gravimetric water content measurements at a site in

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China. They noted overall poor simulation performance among the models and suggested considerable revisions were necessary to improve ET calculations. They also discussed the effects of interacting model components on ET simulation performance, highlighting for example the contribution of leaf area index (LAI) simulation error to ET error and vice versa. Further demonstrating the divergent nature of ET methods in agroecosystem models, Kimball et al. (2019) reported large variability in ET simulation results from an intercomparison of 29 maize (*Zea mays* L.) models parameterized for Iowa conditions.

The barriers to unbiased comparison of ET methods in agroecosystem models are substantial. Most agroecosystem models are manually calibrated, meaning input parameters are adjusted until performance is deemed acceptable through simple statistical calculations (Jacovides and Kontoyiannis, 1995) and human assessment of measured versus simulated data plots. Computational approaches can eliminate the potential for modeler bias to influence the calibration effort. For example, Soldevilla-Martinez et al. (2014) developed a simulated annealing global optimization method to calibrate and compare the DSSAT CSM and the Water and Agrochemicals in soil, crop, and Vadose Environment (WAVE) model using measured drainage and ET data from a weighing lysimeter and soil water measurements from capacitance sensors. While the approach highlighted differences in the drainage simulations among the two models, a primary disadvantage of simulated annealing and similar iterative optimization approaches is that only one solution is recommended by the algorithm despite substantial computational expense. One alternative seeks to first develop a comprehensive database of model input and output relationships, and any assessment of simulation output in comparison with measurements occurs subsequently (Irmak et al., 2000; Welch et al., 2001). In addition to the benefit of fully representing model responses to input parameterization, the database approach can also improve computational efficiency, because simulations can be easily parallelized on high-performance computers (Lamsal et al., 2018).

As recognized by Kang et al. (2009), another barrier to objective evaluation of ET methods in agroecosystem models involves the shared feedback between the ET algorithm and other model components. For example, parameter adjustments that improve ET simulations might also worsen crop yield simulations and vice versa (DeJonge et al., 2012a). Better ET algorithms should demonstrate better performance in multiple aspects of the model simulation, not just in the ET simulation itself. This means that the model parameterization effort requires the optimization of multiple, often conflicting objectives, as embodied in the comparison of measurements and simulation output for multiple types of agronomic data (e.g., LAI, plant dry matter, crop height, yield, ET, soil water content, etc.). Many approaches for multiobjective optimization have been developed for solving engineering design problems (Chianducci et al., 2012; Zio and Bazzo, 2012); however, application of these methods to agroecosystem model evaluation and comparison is relatively uncommon. As one example, Charoenhirunyingyos et al. (2011) combined measured and simulated data for LAI, ET, and soil water content into a single objective function and used a genetic algorithm to optimize the Soil Water Atmosphere Plant (SWAP) model. Similarly, Thorp et al. (2015) used an objective function that combined measured and simulated data for LAI, ET, crop height, and seed cotton yield to parameterize CSM-CROPGRO-Cotton using simulated annealing optimization. Neither of these studies incorporated the database approach of Welch et al. (2001) and therefore suffered the disadvantage of computationally intensive iterative optimization techniques resulting in only one solution. Furthermore, Welch et al. (2001) described an additional drawback of efforts to combine multiple variables into a single objective function; it permits the optimizer to differentially gain accuracy in one variable by sacrificing accuracy in another. An improved strategy for multiobjective optimization problems involves the computation and assessment of solutions among the Pareto optimal set (Cheikh et al., 2010; Mishra and Harit, 2010; Taboada et al., 2007; Welch et al., 2001), which is the subset of

possible solutions that are not dominated by any other solution (mathematical definition to follow). Unfortunately, a single solution rarely optimizes all objective functions in multiobjective problems; however, the set of plausible solutions can be objectively narrowed by computing the Pareto optimal solutions.

A final barrier to unbiased evaluation of ET methods in agroecosystem models involves the statistical approaches used to make comparisons. Evaluations of models rarely entail more than calculations of simple statistical metrics, such as root mean squared error (RMSE) or mean bias error (MBE). Jacovides and Kontoyiannis (1995) demonstrated how RMSE and MBE can be combined to calculate the *t*-statistic, which when compared to a critical *t* value from standard statistical tables can assess the statistical significance of the model's calculations at a given confidence level. In their comparison of four ET simulation methods, the best performer was sometimes improperly selected if statistical hypothesis tests were not incorporated in the analysis. Based on hierarchical linear regression modeling, Thorp et al. (2014b) showed that CSM-CROPGRO-Cotton simulations of yield and ET could explain variability in the measured data, independent of the growing season. Their methodology provided statistical support that the model was responding appropriately to the agronomic treatments imposed in a given year. By using assessments of statistical inference to compare ET methods in agroecosystem models, the conclusions regarding the relative performance of each method can be strengthened.

The overall goal of this study was to develop a novel methodology for unbiased evaluation and comparison of three ET algorithms in the Cotton2K agroecosystem model (<http://departments.agri.huji.ac.il/fieldcrops/cotton/>). Field data for the analysis included ET measurements from weighing lysimeters at Bushland, Texas and other agronomic measurements from surrounding field experiments that compared fully irrigated, deficit irrigated, and dryland cotton (*Gossypium hirsutum* L.) production. Specific objectives were to 1) incorporate global sensitivity analysis, multiobjective optimization, and high-performance computing to fully evaluate Cotton2K parameterization options, 2) compare the effects of three ET algorithms on the accuracy of simulated ET, cotton fiber and seed yield, soil water content, and plant growth metrics using statistical inference, and 3) evaluate ET simulation behavior in Cotton2K using crop coefficient methods.

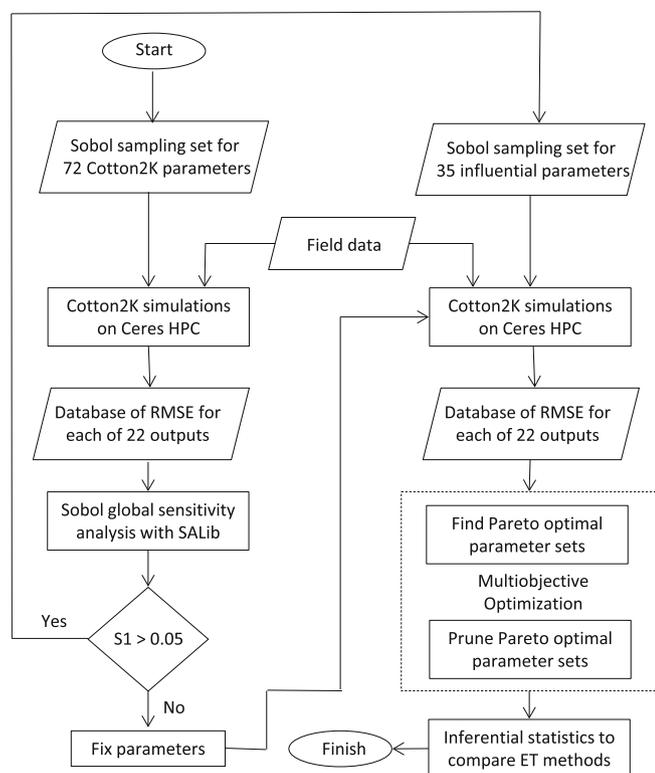
## 2. Materials and methods

### 2.1. Simulation workflow

A novel simulation approach was developed for unbiased analysis and comparison of simulation results for three ET algorithms in Cotton2K (Fig. 1). Aspects of the workflow included 1) a Sobol sampling scheme to choose large numbers of input parameterization options from a high-dimensional parameter space, 2) high-performance computing to efficiently conduct large numbers of Cotton2K simulations, 3) a database approach to link input parameter sets with error statistics from comparisons of measured and simulated data, 4) a global sensitivity analysis (GSA) to identify influential Cotton2K input parameters, 5) a multiobjective optimization (MOO) method to calculate Pareto optimal solution sets by evaluating model error statistics among multiple agroecosystem metrics, 6) a pruning algorithm to cull Pareto optimal solutions based on a user-specified order for objective function priority, and 7) classical inferential statistics to assess differences in model performance among the pruned Pareto optimal sets for each ET algorithm. Further details on the field measurements, the Cotton2K model, and the workflow implementation are described in the following sections.

### 2.2. Field measurements

Cotton field experiments to quantify ET of fully irrigated, deficit irrigated, and dryland cotton production were conducted in four



**Fig. 1.** Workflow to incorporate 1) a Sobol global sensitivity analysis using Python's Sensitivity Analysis (SALib) module, 2) Cotton2K simulations on the Ceres high performance computer (HPC), 3) a database approach for linking Sobol parameter sets with root mean squared error (RMSE) between measured and simulated data, 4) multiobjective optimization to identify Pareto optimal parameter sets, and 5) inferential statistics on RMSE from pruned Pareto optimal parameter sets for unbiased comparison of three evapotranspiration (ET) methods.

weighing lysimetry fields at the USDA-ARS Conservation and Production Research Laboratory (CPRL) near Bushland, Texas (35.187°N; 102.097°W; 1170 m above mean sea level) during the 2000 and 2001 growing seasons (Howell et al., 2004). Also, the Bushland Evapotranspiration and Agricultural Remote sensing EXperiment (BEAREX08) quantified ET for fully irrigated and dryland cotton production at the same site during 2008 (Evetts et al., 2012). The soil texture at the site was predominantly clay loam and silty clay loam, as determined from textural analysis of soil samples (Tolk et al., 1998). Growing season precipitation (short crop reference ET) from April through September amounted to 155 (1707), 160 (1579), and 230 (1624) mm in 2000, 2001, and 2008, respectively. Strong regional advection from the south and southwest typically led to high reference ET values at the site, and low precipitation levels led to water limitation and need for irrigation. In all three seasons, irrigation was applied using a 10-span lateral-move overhead sprinkler irrigation system (Lindsay Manufacturing, Omaha, Nebraska) equipped with mid-elevation spray application (MESA) nozzles at a height of approximately 1.5 m above the ground surface. The machine was oriented from north to south, traveled in an east or west direction, and irrigated two lysimeter fields simultaneously.

Four large weighing lysimeters were installed at the Bushland field site in the 1980's (Marek et al., 1988) and have been used to monitor ET for a variety of crops for nearly three decades (Evetts et al., 2012, 2016; Howell et al., 1995, 2004). During the 2000 and 2001 cotton studies, the southeast and northeast lysimeter fields were managed using full and limited irrigation, respectively. Full irrigation was defined as weekly irrigation to replenish root zone soil water content to field capacity, and limited irrigation was half of the full rate. In 2008 season,

both the northeast and southeast lysimeter fields were fully irrigated. The northwest and southwest lysimeter fields were not irrigated (dry-land production) in 2001 or 2002, and less than 130 mm was applied in the 2008 early season to encourage germination and emergence. Soil water content was periodically measured at two access tube locations in each lysimeter using a calibrated neutron scattering probe (model 503DR Hydroprobe, CPN International, Inc., Martinez, California), which provided data from 0.1 to 1.9 m in 0.2 m incremental depths. Specific protocols for weighing lysimeter measurements during the three cotton growing seasons were given by Howell et al. (2004) and Evetts et al. (2012). Howell et al. (1995) discussed the calibration technique for mass measurement within the lysimeter, which can provide ET estimates at time scales less than 1 h. More recently, Marek et al. (2014) presented techniques for quality assurance and quality control of data collected from the lysimeters. Based on this post-processing protocol, lysimeter ET data for the present study was aggregated on a daily basis from 1 January through 31 December in 2000, 2001, and 2008.

Cotton planting dates ranged from mid-May to early June in the three growing seasons. After establishment, cotton plants were destructively sampled on a two-week basis from small areas (1.0–2.0 m<sup>2</sup>) more than 10 m away from the lysimeter. The samples were processed in the laboratory to estimate leaf area index (LAI), leaf dry matter (LDM), stem dry matter (SDM), boll dry matter (BDM), canopy height (CHT), mainstem node count (NOD), green boll count (GBL), and mature boll count (MBL). Cotton harvest dates ranged from late October to early December in the three growing seasons. Yield measurements were obtained by sampling mature bolls from five 10.0 m<sup>2</sup> areas in each lysimeter field. Turnout percentages were measured using a small research gin, which provided data for fiber yield (FBY), cottonseed yield (SDY), and seed cotton yield (SCY).

### 2.3. Cotton2K

The Cotton2K agroecosystem model is described online at the website provided previously and was recently reviewed by Thorp et al. (2014a). Model development descended from several early and notable efforts in cotton growth modeling, including GOSSYM (Baker et al., 1972, 1983), SIMCOTI (Baker et al., 1972), SIMCOTII (Jones et al., 1974), and CALGOS (Marani et al., 1992a, b, c). Primarily, Cotton2K made these models more relevant for cotton production in arid, irrigated environments, such as the western U.S. and Israel. Whereas GOSSYM calculates water balance processes on a daily time step, Cotton2K uses hourly weather information to calculate hourly water and energy balances, which is thought to improve the accuracy of the model's ET calculations.

Cotton2K simulates a two-dimensional soil profile with a depth of 2 m and width equal to the cotton row spacing (Lambert et al., 1976; Bar-Yosef et al., 1982). The soil profile is divided into a fixed number of small compartments, both horizontally and vertically. Water and nitrogen contents and root growth are calculated in each compartment. Additionally, the compartments are grouped vertically into a set of nine soil horizons, each with a thickness of 15 cm. Van Genuchten (1980) parameters are used to define the soil water holding and hydraulic conductivity characteristics in each soil horizon. These were determined by fitting the model to soil water measurements and other data, as discussed later. Due to lacking experimental data, initial conditions for nitrate and ammonium were assumed to be 5.0 kg ha<sup>-1</sup> for all soil horizons and all simulations. Initial organic matter was specified uniquely for each experimental year based on limited pre-season measurements of surface organic matter at the field site and estimates of vertical organic matter distribution from a USDA soil survey of the study area. Initial soil water content was estimated as the average of neutron scattering probe readings during the subsequent growing season and were specified uniquely for each lysimeter field. Management information required by the model, including irrigation and

fertilization schedules and dates of planting and harvest, was specified as recorded for each lysimeter field.

Highly detailed and comprehensive simulations of cotton development and growth and are possible with Cotton2K. The model simulates development of mainstem nodes in response to air temperature using heat unit concepts, and the development of vegetative or fruiting branches from each mainstem node is also simulated. Development of leaves and reproductive structures, including squares, green bolls, and mature bolls, is simulated at individual sites along the vegetative and fruiting branches. This permits simulation of cotton plant maps, where the position of each reproductive structure on the simulated plant is explicitly considered. Growth rates of unique plant organs, including roots, stems, leaf blades, petioles, squares, green bolls, and mature bolls, are based on carbon supply and demand relationships. Effects of water stress on simulated plant growth are calculated as a function of leaf water potential, and nitrogen stress effects depend on supply and demand relationships for nitrogen in vegetative material, fruits, and roots (Jones et al., 1974). Stress alters simulated plant growth via reductions in organ growth potential and shedding of squares and bolls (i.e., abscissions). A set of 51 variety parameters are used to simulate the effects of genetics on cotton growth and development responses.

A number of source code edits were required to facilitate efficient model input/output (I/O) for high-performance computing and to correct any encountered coding errors. For example, the model code was altered to directly output soil water contents corresponding to the positions of neutron scattering probe measurements. Also, some parameter sets caused underflow or overflow errors at run time, which required coding edits to restrict ranges for certain state variables. A Fortran version of Cotton2K was obtained from the developers of the PALMScot landscape-scale cotton modeling tool (Booker et al., 2014, 2015). Although a newer C++ version of Cotton2K exists, the code for cotton growth simulations is interwoven with code for its Microsoft Windows-based graphical user interface (GUI), which precluded its use on a Linux high-performance computing system. After incorporating coding edits, the model was compiled using “gfortran” within the open-source “GNU's Not Unix!” (GNU) compiler collection ([www.gnu.org](http://www.gnu.org)).

#### 2.4. Evapotranspiration methods

The ET methodology in Cotton2K is based on the California Irrigation Management Information System (CIMIS) algorithm using the modified Penman equation (Snyder and Pruitt, 1985). Two options are possible for obtaining the required hourly weather information: either input hourly data directly as measured (CIMIS-HR) or use the methodology of Ephrath et al. (1996) to estimate hourly data from daily measurements (CIMIS-DY). Both of these options were tested in this study (Table 1). Required hourly meteorological information, including solar irradiance ( $\text{MJ m}^{-2}$ ), air temperature ( $^{\circ}\text{C}$ ), dew point temperature ( $^{\circ}\text{C}$ ), and wind speed ( $\text{km d}^{-1}$ ), was obtained from a Texas High Plains ET Network weather station, which was positioned over a well-watered, clipped grass surface adjacent to the field site. Hourly precipitation data (mm) were obtained from a tipping bucket rain gauge managed by the experimentalists at the field site. Daily weather inputs included maximum and minimum daily air temperature along with the daily aggregations of the other weather measurements.

Since the initial development of the Cotton2K model, efforts in the

ET community have aimed to standardize ET computations (Allen et al., 1998; Walter et al., 2005). Therefore, a third ET option (ASCEK-HR, Table 1) was added to Cotton2K based on the findings of DeJonge and Thorp (2017), who demonstrated the use of more modern and standardized ET methodologies to identify problematic ET responses in another agroecosystem model. Computations of short crop reference ET ( $\text{ET}_{\text{os}}$ ) or tall crop reference ET ( $\text{ET}_{\text{rs}}$ ) from meteorological data form the basis of standardized ET ( $\text{ET}_{\text{cz}}$ ) calculations (Walter et al., 2005). The standard algorithm for hourly  $\text{ET}_{\text{os}}$  was added to Cotton2K, which required the same hourly weather data as discussed previously. Similar to DeJonge and Thorp (2017), a dual crop coefficient methodology (Allen et al., 1998) was used in the ASCEK-HR ET method to calculate basal crop coefficients ( $K_{\text{cb}}$ ) from simulated LAI:

$$K_{\text{cb}} = K_{\text{cbmin}} + (K_{\text{cbmax}} - K_{\text{cbmin}})(1 - \exp[-S_{\text{Kc}}(\text{LAI})]) \quad (1)$$

Maximum  $K_{\text{cb}}$  ( $K_{\text{cbmax}}$ ) was specified as 1.25, based on the FAO-56 tabulated value for cotton with appropriate adjustment for the Bushland environment. The  $K_{\text{cbmin}}$  and  $S_{\text{Kc}}$  factors were fixed at 0.0 and 0.6, respectively, as discussed in DeJonge and Thorp (2017). Evaporation coefficients ( $K_{\text{e}}$ ) were calculated using the methods described in FAO-56 (Allen et al., 1998). Daily  $\text{ET}_{\text{os}}$  was summed from hourly  $\text{ET}_{\text{os}}$  and used to calculate daily potential transpiration ( $\text{EP}_{\text{o}} = K_{\text{cb}}\text{ET}_{\text{os}}$ ) and potential soil water evaporation ( $\text{ES}_{\text{o}} = K_{\text{e}}\text{ET}_{\text{os}}$ ). Although a standardized  $\text{ET}_{\text{os}}$  algorithm for daily weather data also exists (Walter et al., 2005), it was deemed nonsensical for the current study, because the Cotton2K water balance fundamentally operates with an hourly time-step. Even with the CIMIS-DY ET method (Table 1), daily weather data was immediately converted to hourly data upon input to the model (Ephrath et al., 1996).

#### 2.5. Simulations

Cotton2K was setup to run 12 simulation scenarios based on the three cotton growing seasons and four uniquely managed lysimeter fields (Table 2). Simulations were initiated on 1 January of each year and concluded on the recorded harvest date for each lysimeter field. Within the southwest lysimeter field in 2001, twin rows spaced 25 cm apart were planted on 76 cm centers. Because Cotton2K did not consider this planting configuration, a row spacing of 38 cm (i.e., half of 76 cm) was simulated.

Simulations were conducted using USDA's new high performance computing resource called Ceres, which consists of 64 compute nodes each having 40 logical cores on Intel Xeon processors with hyper-threading and a shared 2PB storage system with Lustre design. The operating system on Ceres was a Linux CentOS distribution (ver. 6.7). Located in Ames, Iowa, access to Ceres occurred via the dedicated high-speed networking resource called SCINet. About 60 Cotton2K simulations  $\text{s}^{-1}$  were possible on Ceres, as compared to no more than 3 simulations  $\text{s}^{-1}$  on a modern desktop machine. Thus, high performance computing increased simulation capability by a factor of 20.

A Python script ([www.python.org](http://www.python.org)) that incorporated Python's “multiprocessing” package was developed to manage the simulation tasks on Ceres. The Python script loaded a list of parameter sets into a processing queue, created 40 working directories for conducting simulations in parallel, and copied pertinent Cotton2K files to each directory. It then established 40 independent worker processes, one for

**Table 1**  
Summary of Cotton2K evapotranspiration (ET) algorithms tested in this study.

Method	Description
CIMIS-DY	California Irrigation Management Information System (CIMIS) algorithm using the modified Penman equation (Snyder and Pruitt, 1985). Required hourly weather data is computed from daily data based on Ephrath et al. (1996).
CIMIS-HR	CIMIS algorithm using the modified Penman equation (Snyder and Pruitt, 1985). Required hourly weather data is input directly as measured.
ASCEK-HR	American Society of Civil Engineers (ASCE) standardized short crop reference ET ( $\text{ET}_{\text{os}}$ ) algorithm (Walter et al., 2005) adjusted for cotton based on a dual crop coefficient methodology (Allen et al., 1998; DeJonge and Thorp, 2017). Required hourly weather data is input directly as measured.

**Table 2**

Summary of the 12 cotton management scenarios evaluated with Cotton2K. Field experiments were conducted within the four weighing lysimeter fields at Bushland, Texas, USA in 2000, 2001, and 2008.<sup>a</sup>

Year	Lysimeter	Planting	Row	Plant	Irrigation	Rainfall <sup>b</sup>	Harvest
	Field	Date (DOY)	Spacing	Spacing	Depth	Depth	Date (DOY)
			(cm)	(p m <sup>-1</sup> )	(mm)	(mm)	
2000	NE	16 May (137)	76	17.6	292	203	6 Dec (341)
2000	NW	15 May (136)	76	23.0	0	203	6 Dec (341)
2000	SE	16 May (137)	76	18.6	534	203	6 Dec (341)
2000	SW	15 May (136)	25	18.8	0	203	6 Dec (341)
2001	NE	16 May (136)	76	14.9	213	277	3 Nov (307)
2001	NW	16 May (136)	76	12.3	0	277	20 Oct (293)
2001	SE	16 May (136)	76	15.3	403	277	16 Nov (320)
2001	SW	16 May (136)	38	7.1	0	277	20 Oct (293)
2008	NE	21 May (142)	76	12.6	409	334	24 Nov (329)
2008	NW	5 Jun (157)	76	10.1	129	334	29 Nov (334)
2008	SE	21 May (142)	76	11.5	410	334	25 Nov (330)
2008	SW	5 Jun (157)	76	13.5	129	334	24 Nov (329)

<sup>a</sup> Day of year, DOY; northeast, NE; northwest, NW; southeast, SE; southwest, SW.

<sup>b</sup> 1 January to 30 September.

**Table 3**

Agroecosystem metrics evaluated for 12 cotton management scenarios within the lysimeter fields at Bushland, Texas, USA. The 22 metrics are listed in priority order for evaluation of the Cotton2K agroecosystem model using multiobjective optimization techniques.

Metric	Description	Unit	<i>n</i>
ET	Evapotranspiration	mm d <sup>-1</sup>	3761
FBY	Fiber yield	kg ha <sup>-1</sup>	12
LAI	Leaf area index	m <sup>2</sup> m <sup>-2</sup>	72
SCY	Seed cotton yield	kg ha <sup>-1</sup>	12
CHT	Canopy height	m	72
SDY	Cottonseed yield	kg ha <sup>-1</sup>	12
NOD	Mainstem node number	nodes	42
LDM	Leaf dry matter	kg ha <sup>-1</sup>	72
SDM	Stem dry matter	kg ha <sup>-1</sup>	44
GBL	Green boll number	bolts	24
MBL	Mature boll number	bolts	32
BDM	Boll dry matter	kg ha <sup>-1</sup>	44
SWC010	Soil water content at 10 cm	cm <sup>3</sup> cm <sup>-3</sup>	106
SWC030	Soil water content at 30 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC050	Soil water content at 50 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC070	Soil water content at 70 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC090	Soil water content at 90 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC110	Soil water content at 110 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC130	Soil water content at 130 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC150	Soil water content at 150 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC170	Soil water content at 170 cm	cm <sup>3</sup> cm <sup>-3</sup>	107
SWC190	Soil water content at 190 cm	cm <sup>3</sup> cm <sup>-3</sup>	98

each requested processing core. Each worker process iteratively selected an item from the processing queue, adjusted Cotton2K input files to incorporate the current parameter set, conducted the 12 simulation scenarios, and extracted simulated data from Cotton2K output files for pairing with associated measurements. Measured and simulated data for 22 agroecosystem metrics (Table 3) were aggregated among the 12 simulation scenarios (Table 2) for each tested parameter set by calculating the percent root mean squared error (%RMSE) uniquely for each metric:

$$\%RMSE_i = f_i(\mathbf{m}_i, \mathbf{s}_i) = \frac{100}{\mathbf{m}_i} \sqrt{\frac{1}{n_i} \sum_{j=1}^{n_i} (m_{ij} - s_{ij})^2} \quad (2)$$

where  $\mathbf{m}_i$ ,  $\mathbf{s}_i$ , and  $n_i$  are the measured and simulated data vectors and vector length, respectively, among the 12 scenarios for the  $i$ th metric (Table 3). The Python script and simulation job concluded by outputting a model response database that included the Cotton2K input parameter sets with associated %RMSE statistics for each of the 22

agroecosystem metrics.

## 2.6. First sobol sampling

The simulation workflow entailed two main phases: one leading to a Sobol global sensitivity analysis and another leading to a multiobjective optimization approach for model calibration (Fig. 1). Both phases began by using a Sobol sampling procedure to choose high-dimensional parameter sets for input to Cotton2K. A Python script that incorporated the Sensitivity Analysis Library (SALib) was developed to conduct the Sobol sampling and later to compute the Sobol sensitivity indices (Saltelli, 2002; Saltelli et al., 2010; Sobol, 2001). Sobol sampling techniques were previously shown to be advantageous and more efficient to develop databases that describe high-dimensional model input and output relationships (Lamsal et al., 2018), because the Sobol algorithm can select parameter sets that are more evenly dispersed across the multidimensional parameter space.

Initially, 72 model input parameters were sampled for inclusion in the Sobol GSA (Table 4): 1) 18 parameters that defined the sand and clay contents for each of the nine soil horizons, 2) two parameters that define the soil matric potential at field capacity (SMPFC) and at which free drainage occurs (SMPFD), 3) the 51 cotton variety parameters (VARPAR01 through VARPAR51), and 4) the  $S_{Kc}$  parameter for ET simulations with the ASCEK-HR method (Eq. (1)). The sand and clay contents chosen by the Sobol algorithm were input to the Rosetta pedotransfer function (Zhang and Schaap, 2017) to calculate the associated Van Genuchten (1980) parameters for each soil horizon. Appropriate parameter ranges (Table 4) for sand and clay were based on texture measurements of soil samples collected at the field site (Tolk et al., 1998). Based on recommendations in the model documentation, SMPFC ranged from  $-0.38$  to  $-0.28$  bars, and SMPFD ranged from  $-0.15$  to  $-0.05$  bars (1 bar = 100 kPa). Appropriate ranges for variety parameters were chosen by using spreadsheet software (Excel, 2013; Microsoft Corporation, Redmond, Washington) to test outcomes of the model equations that incorporated each parameter (Table 4). The appropriate equations were taken from the model code and programmed into the spreadsheet to facilitate tests of equation outcomes with different input parameter values, which permitted specification of reasonable parameter ranges. The  $S_{Kc}$  parameter was varied from 0.5 to 0.9 based on the recommendation of DeJonge and Thorp (2017). Many of the Cotton2K variety parameters are unitless variables used in empirical equations that drive specific plant growth or development characteristics.

The  $N$  parameter of the Sobol sampling algorithm was set to 34,723

**Table 4**

Cotton2K parameters included in the Sobol global sensitivity analysis (GSA) and their ranges. Influential parameters are denoted (\*). Optimized parameter values for three Cotton2K evapotranspiration methods (CIMIS-DY, CIMIS-HR, and ASCEK-HR) are provided for influential parameters, and the remaining parameters were specified with default values.<sup>a</sup>

Parameter	Function	LB	UB	GSA	CIMIS-DY	CIMIS-HR	ASCEK-HR
CLAY015	Clay at 15 cm (%)	25.0	45.0	*	26.3	30.5	30.5
CLAY030	Clay at 30 cm (%)	25.0	45.0	*	30.9	29.0	29.0
CLAY045	Clay at 45 cm (%)	25.0	45.0	*	32.3	35.1	35.1
CLAY060	Clay at 60 cm (%)	25.0	45.0	*	26.1	39.8	39.8
CLAY090	Clay at 90 cm (%)	25.0	45.0	*	39.5	31.9	31.9
CLAY120	Clay at 120 cm (%)	25.0	45.0	*	26.7	28.7	28.7
CLAY150	Clay at 150 cm (%)	25.0	45.0	*	34.8	26.9	26.9
CLAY180	Clay at 180 cm (%)	25.0	45.0	*	26.5	37.8	37.8
CLAY210	Clay at 210 cm (%)	25.0	45.0	*	43.3	36.0	36.0
SAND015	Sand at 15 cm (%)	15.0	25.0	*	24.9	17.8	17.8
SAND030	Sand at 30 cm (%)	15.0	25.0	*	16.5	20.5	20.5
SAND045	Sand at 45 cm (%)	15.0	25.0	*	16.3	20.9	20.9
SAND060	Sand at 60 cm (%)	15.0	25.0	*	22.1	21.8	21.8
SAND090	Sand at 90 cm (%)	15.0	25.0	*	22.8	19.9	19.9
SAND120	Sand at 120 cm (%)	15.0	25.0	*	24.5	17.1	17.1
SAND150	Sand at 150 cm (%)	15.0	25.0	*	17.1	21.5	21.5
SAND180	Sand at 180 cm (%)	15.0	25.0	*	24.3	15.7	15.7
SAND210	Sand at 210 cm (%)	15.0	25.0	*	21.2	22.7	22.7
SMPFC	SMP at field capacity (bars)	-0.38	-0.28	*	-0.379	-0.355	-0.355
SMPFD	SMP for free drainage (bars)	-0.15	-0.05	*	-0.126	-0.139	-0.139
VARPAR01	Plant density effect on growth	0.00	0.08	*	0.03012	0.03964	0.03964
VARPAR02	Leaf growth at prefruiting nodes	0.00	0.60		0.30	0.30	0.30
VARPAR03	Leaf growth at prefruiting nodes	0.00	0.10		0.014	0.014	0.014
VARPAR04	Leaf growth at prefruiting nodes	0.00	1.00	*	0.12897	0.32599	0.32599
VARPAR05	Leaf growth on mainstem nodes	0.50	3.00		1.60	1.60	1.60
VARPAR06	Leaf growth on mainstem nodes	0.00	0.02		0.010	0.010	0.010
VARPAR07	Leaf growth on mainstem nodes	18.0	28.0		24.0	24.0	24.0
VARPAR08	Leaf growth on fruiting branches	0.00	0.20		0.10	0.10	0.10
VARPAR09	Boll growth period (PD)	18.0	38.0		28.0	28.0	28.0
VARPAR10	Boll growth rate (g PD <sup>-1</sup> )	0.10	0.45		0.3293	0.3293	0.3293
VARPAR11	Maximum dry boll mass (g)	3.00	15.0		8.800	8.800	8.800
VARPAR12	Pre-squaring stem growth	0.00	2.00	*	0.21521	0.02576	0.02576
VARPAR13	Pre-squaring stem growth	0.00	2.00		0.040	0.040	0.040
VARPAR14	Pre-squaring stem growth	0.00	0.08		0.014	0.014	0.014
VARPAR15	Post-squaring stem growth	1.00	4.00		2.4	2.4	2.4
VARPAR16	Post-squaring stem growth	0.50	2.00		1.50	1.50	1.50
VARPAR17	Post-squaring stem growth	0.00	1.00		0.40	0.40	0.40
VARPAR18	Post-squaring stem growth	0.00	0.20		0.140	0.140	0.140
VARPAR19	Vertical mainstem growth	0.00	0.50		0.20	0.20	0.20
VARPAR20	Vertical mainstem growth	0.00	0.10		0.02	0.02	0.02
VARPAR21	Vertical mainstem growth	10.00	18.0	*	14.34033	12.94189	12.94189
VARPAR22	Vertical mainstem growth	-4.00	-2.00	*	-2.07385	-2.00330	-2.00330
VARPAR23	Vertical mainstem growth	0.09	0.12		0.10	0.10	0.10
VARPAR24	Vertical mainstem growth	0.00	0.50		0.175	0.175	0.175
VARPAR25	Vertical mainstem growth	1.00	4.00		2.20	2.20	2.20
VARPAR26	Vertical mainstem growth	0.70	1.30	*	1.18629	1.03512	1.03512
VARPAR27	Mainstem node delay, C stress	0.50	1.00		0.82	0.82	0.82
VARPAR28	Fruiting site delay, C stress	1.00	3.00		2.15	2.15	2.15
VARPAR29	Fruiting site delay, C stress	1.00	3.00		1.36	1.36	1.36
VARPAR30	Temperature effect on squaring	0.70	1.30	*	1.15787	1.00377	1.00377
VARPAR31	Prefruit node development (PD)	1.00	5.00	*	2.70044	2.50366	2.50366
VARPAR32	Prefruit node development (PD)	1.00	3.00	*	2.43665	1.21277	1.21277
VARPAR33	Prefruit node development (PD)	0.50	1.00		0.80	0.80	0.80
VARPAR34	Initial leaf area (dm <sup>2</sup> )	0.01	0.10	*	0.06023	0.01491	0.01491
VARPAR35	Fruiting branch development	-32.0	-26.0	*	-27.34802	-26.05164	-26.05164
VARPAR36	Fruiting site development	-57.0	-49.0		-54.00	-54.00	-54.00
VARPAR37	Fruiting site development	0.00	2.00		0.80	0.80	0.80
VARPAR38	Defoliant effect on leaf age	0.00	5.00		3.20	3.20	3.20
VARPAR39	Temperature effect, dehiscence	-306.0	-240.0		-292.0	-292.0	-292.0
VARPAR40	Temperature effect, dehiscence	0.70	1.30		1.08	1.08	1.08
VARPAR41	Temperature effect, turnout	45.0	60.0		56.80	56.80	56.80
VARPAR42	Temperature effect, turnout	0.30	0.90		0.5500	0.5500	0.5500
VARPAR43	Shedding intensity, C stress	0.30	0.70		0.53	0.53	0.53
VARPAR44	Shedding intensity, water stress	0.30	0.70		0.48	0.48	0.48
VARPAR45	Probability of square abscission	0.10	0.50		0.24	0.24	0.24
VARPAR46	Probability of square abscission	0.00	0.15		0.08	0.08	0.08
VARPAR47	Probability of boll abscission	1.00	10.0	*	2.75616	3.04620	3.04620
VARPAR48	Probability of boll abscission	0.30	1.50	*	0.58030	0.32908	0.32908
VARPAR49	Probability of boll abscission	5.00	15.0	*	11.67297	11.25305	11.25305
VARPAR50	Probability of boll abscission	0.20	1.20	*	0.90380	0.68602	0.68602
VARPAR51	Seed cotton mass per boll (g)	2.00	8.00		5.00	5.00	5.00

(continued on next page)

Table 4 (continued)

Parameter	Function	LB	UB	GSA	CIMIS-DY	CIMIS-HR	ASCEK-HR
ETSKC	ASCEK-HR ET method parameter	0.50	0.90		0.60	0.60	0.60

<sup>a</sup> Carbon, C; lower bound, LB; physiological day, PD; soil matric potential, SMP; upper bound, UB.

Table 5

Details of the Sobol sampling and Cotton2K simulations for two phases in the simulation workflow: Sobol global sensitivity analysis (GSA) and multiobjective optimization (MOO).

	GSA	MOO
<i>N</i> for Sobol sampling	34,723	34,723
No. of parameters ( <i>n</i> )	72	35
No. of Sobol sets ( $N(2n + 2)$ )	5,069,558	2,500,056
No. of scenarios per set	12	12
No. of tested ET methods	1	3
No. of simulations	60,834,696	90,002,016
Simulation duration (CPU hr)	60,217	89,889
Simulation duration (hr)	301	449

with specification to prepare for calculation of second-order sensitivity effects. Thus, the number of *n*-dimensional parameter sets ( $n = 72$ ) chosen by Sobol for the Sobol GSA was  $N(2n + 2) = 5,069,558$ , as defined within the Sobol algorithm (Table 5). The value of *N* was selected based on preliminary estimates of the rate of simulations on Ceres, with plans to contain the simulation timeframe to within a couple weeks. Most importantly, as revealed by later tests, the number of simulations was more than satisfactory to ensure stability of Sobol sensitivity indices. With 12 simulations per parameter set, the Sobol GSA needed a total of 60,834,696 simulations, which required 60,217 CPU hr on Ceres and approximately 301 h of wall-clock time. To minimize computational expense, simulations for the GSA were conducted only for the ASCE-HR ET method (Table 1).

## 2.7. Global sensitivity analysis

To gain insights on Cotton2K responses to adjustment of model input parameters, a Sobol GSA (Cariboni et al., 2007; Pianosi et al., 2016; Saltelli et al., 2000) was conducted using algorithms from the SALib package in Python (Saltelli, 2002; Saltelli et al., 2010; Sobol, 2001). An astute reader will note that less computationally intensive sensitivity analyses are normally conducted first, followed by more intensive methods like Sobol GSA. Here, only Sobol GSA was used, because 1) the availability of high-performance computing resources ensured efficiency of simulations and 2) subsequent portions of the workflow also incorporated the Sobol sampling aspect of the Sobol GSA (Fig. 1).

Using algorithms from the SALib package, first-order, second-order, and total sensitivity indices were calculated for each combination of the 72 input parameters and 22 agroecosystem metrics. The %RMSE statistic for each agroecosystem metric was used as the objective function for sensitivity index calculations. Based on the recommendation of Zhang et al. (2015), any parameter having a first-order sensitivity index greater than 0.05 for any of the 22 agroecosystem metrics was considered an influential parameter and remained flexible in the subsequent analysis (Fig. 1; Table 4). Other parameters were considered non-influential and were fixed to default values for the remainder of the analysis. The overall purpose of the Sobol GSA was to eliminate non-influential parameters prior to using multiple objective optimization for model calibration.

## 2.8. Second sobol sampling

The GSA results suggested that only 35 of the 72 Cotton2K

parameters influenced the simulation outcomes (Table 4). Subsequently, the Sobol sampling algorithm in SALib was again used to choose Cotton2K parameter sets but only among the influential parameters as identified by the Sobol GSA. A second GSA based on the reduced parameter set was not conducted. Instead, simulation results based on the second Sobol sampling was used for multiobjective optimization to identify the parameter sets that provided optimal agreement between measured and simulated results. It was assumed that the best solutions to the multiobjective optimization problem were among the parameter sets chosen by the second iteration of Sobol sampling (Fig. 1).

Each Sobol parameter set was used for simulations of the 12 Cotton2K scenarios (Table 2) using three different ET methods in the model (Table 1), resulting in three model response databases that linked parameter sets to %RMSE outcomes for each agroecosystem metric (Table 3). Using the same Sobol *N* parameter for these runs ( $N = 34,723$ ), the number of *n*-dimensional parameter sets ( $n = 35$ ) chosen by Sobol was  $N(2n + 2) = 2,500,056$ . With 12 simulations per parameter set for three ET approaches, this analysis needed 90,002,016 simulations, which required 89,889 CPU hr on Ceres and approximately 449 h of wall-clock time (Table 5).

## 2.9. Multiobjective optimization

Because there were 22 agroecosystem metrics to consider (Table 3), optimizing the Cotton2K parameterization required multiobjective optimization (MOO) techniques (Taboada et al., 2007). The objective function to be optimized incorporated *k* unique %RMSE calculations, one for each agroecosystem metric ( $k = 22$ ), expressed as

$$f_{\text{MOO}}(\mathbf{m}, \mathbf{s}) = (f_1(\mathbf{m}_1, \mathbf{s}_1), f_2(\mathbf{m}_2, \mathbf{s}_2), \dots, f_k(\mathbf{m}_k, \mathbf{s}_k)) \quad (3)$$

where the terms are as described for Equation (2). Equation (3) represents the set of %RMSE calculations (Eq. (2)) for each of *k* agroecosystem metrics, based on the results of simulations for a given parameter set among more than 2.5 million sets tested (Table 5). The first step toward reduction of plausible parameter sets was to calculate the subset of Pareto optimal solutions (Cheikh et al., 2010), which were the solutions that were not dominated (or non-dominated) by any other solution. In mathematical terms, a solution  $x_1$  dominates another solution  $x_2$  if the following two conditions are met:

- $f_i(x_1) \leq f_i(x_2)$  for all  $i \in \{1, 2, \dots, k\}$
- $f_j(x_1) < f_j(x_2)$  for at least one  $j \in \{1, 2, \dots, k\}$

In words, a solution dominates another if the %RMSE calculations for *k* agroecosystem metrics are all less than or equal to that for the other, and at least one %RMSE calculation is less than that for the other. The goal was to find the parameter sets with %RMSE calculations that were not dominated by the %RMSE calculations for any other parameter set. A Python script was developed to calculate the Pareto optimal solution set for each Cotton2K ET method. Efficiencies in computation were gained by sorting the data set such that non-dominated solutions were more likely evaluated first (Mishra and Harit, 2010), ceasing evaluation of a solution immediately after determining it was dominated, and using Python's "multiprocessing" package to divide computational load among processors on Ceres.

A known problem with Pareto optimal sets is that they often remain large and cumbersome, and they do not adequately ease the burden of selecting one or several practical solutions. Taboada et al. (2007) tested

two approaches to aid selection of practical solutions by “pruning” the Pareto optimal set: one based on a clustering technique and another based on a user-defined priority ranking among the set of objective functions (Eq. (3)). Borrowing from the latter strategy, a Python script was created to reevaluate each Pareto optimal solution and combine the  $k$  objective function outcomes to a single evaluation criterion by assigning random weightings approximately in order of objective function priority. Specifically,  $k$  random weightings ( $\mathbf{w}$ :  $\sum_{i=1}^k w_i = 1.0$ ) were computed by using Python’s “numpy” package to 1) generate  $k$  random numbers from a uniform distribution ( $\mathbf{r}$ :  $0 \leq r_i \leq 1 \forall i \in \{1,2,\dots,k\}$ ), 2) sort  $\mathbf{r}$  from highest to lowest, and 3) calculate  $w_i = \left( r_i / \sum_{j=1}^k r_j \right) \forall i \in \{1,2,\dots,k\}$ . Given the objectives of this study and that crop yield and water use are commonly the most important of agroecosystem metrics, the priority of objective functions were specified in the following order: ET, FBY, LAI, SCY, CHT, SDY, NOD, LDM, SDM, GBL, MBL, and BDM, followed by the ten soil water content measurements from top to bottom in the profile (Table 3). Weightings were iteratively assigned to objective function in order of priority, but to relax strictness of the subjectively chosen order, weightings were assigned randomly from the highest three remaining weightings. (This allowed the algorithm to vary the objective function priority at each iteration while generally preserving the priority overall.) The evaluation criterion,  $c$ , was then computed for each solution in the Pareto optimal set

$$c = \sum_{i=1}^k w_i f_i(\mathbf{m}_i, \mathbf{s}_i) \quad (4)$$

and the solution having the minimum  $c$  was identified as a “pruned” Pareto optimal solution. To ensure equal treatment among objective functions, the values  $f_i(\mathbf{m}_i, \mathbf{s}_i)$  for each objective function (i.e., see Equation (2)) were normalized from 0.0 to 1.0 prior to computing  $c$ . The process of random weighting computation and  $c$  computation was iterated until 100,000 iterations passed without identification of a new pruned solution. The set of pruned Pareto optimal solutions determined from this process was used for all further analysis.

The Pareto optimal sets for each of the three Cotton2K ET methods were pruned using identical random weightings. Multiple trials of the pruning algorithm produced very similar results, which highlighted the consistency of the approach. Because the algorithm also counted the number of times a particular pruned solution was selected, a single, “most popular” solution could be identified. However, according to the definition of multiobjective optimization, all solutions in the Pareto optimal set have equal feasibility as a solution to the optimization problem.

### 2.10. ET method comparison

The performance of the three Cotton2K ET methods (Table 1) was compared by conducting an analysis of variance (ANOVA) on %RMSE results for each of the 22 agroecosystem metrics (Table 3) among the pruned Pareto optimal solutions. Tukey’s multiple comparisons tests were also conducted to identify which Cotton2K ET method resulted in statistically different %RMSE values for each agroecosystem metric ( $p \leq 0.05$ ), and the lowest of these identified the better ET method for a given metric. Statistical analysis was conducted using the R Project for Statistical Computing software ([www.r-project.org](http://www.r-project.org)).

Further efforts involving measured and simulated crop coefficient plots were used to evaluate and compare ET time series for the “most popular” Pareto optimal solution for each ET method. DeJonge and Thorp (2017) demonstrated how crop coefficient methods can be used to assess the ET outputs of agroecosystem models relative to either measured or theoretically expected crop coefficient time series (Allen et al., 1998). The approach required daily calculation of the evaporation coefficient ( $K_c = E/ET_{os}$ ), the basal crop coefficient adjusted for

water stress ( $K_{cb}K_s = T/ET_{os}$ ), and the single crop coefficient ( $K_c = ET/ET_{os}$ ), where  $E$ ,  $T$ , and  $ET$  are the daily Cotton2K-simulated outputs for soil water evaporation, plant transpiration, and evapotranspiration, respectively. Furthermore, measured  $K_c$  values were computed from the weighing lysimeter data.

## 3. Results

### 3.1. Global sensitivity analysis

The GSA identified 35 influential parameters of the 72 included in the analysis (Table 4). These parameters contributed most substantially to sensitivity in the model outputs. As expected, sand and clay parameters at each soil depth had the greatest influence on the simulated soil water contents near that depth. The SMPFC parameter (soil matric potential at field capacity) was most influential on simulated soil water content in the deeper soil layers from 120 to 200 cm, while the SMPFD (soil matric potential at which free drainage occurred) parameter was influential on soil water content throughout the entire soil profile.

Six variety parameters were influential for four or more of the agroecosystem metrics: VARPAR01, VARPAR04, VARPAR31, VARPAR32, VARPAR47, and VARPAR49. Four of the 22 agroecosystem metrics, including LAI, LDM, CHT, and NOD, were sensitive to the VARPAR01 parameter, which adjusts plant growth simulations in response to plant density. The VARPAR04 parameter, which controls growth potential of leaves at prefruiting nodes, mainly influenced ET and soil water contents at 10, 70, and 90 cm, likely through its effects on LAI. The VARPAR31 parameter had greatest effects on ET, CHT, and soil water contents at all the soil depths. The parameter defines the physiological days required for developing the fourth through the ninth prefruiting nodes and thus has great effect on late stage vegetative growth prior to fruiting. Similarly, VARPAR32 defines the physiological days for development of the first and second prefruiting nodes and was influential on ET and soil water contents at 3 of the 10 depths. VARPAR47 through VARPAR50 are used to calculate the probability of fruit abscission as a function of fruit age, and these were the most influential parameters on GBL, FBY, SDY, and SCY.

Other influential parameters had more specific effects on Cotton2K outputs. VARPAR12, which controls stem growth potential, primarily influenced SDM. VARPAR21 and VARPAR22 both influenced CHT through their effects on calculations of mainstem growth as a function of prefruit node age after second square. Likewise, VARPAR26 has a multiplicative effect on daily vertical stem growth and was therefore influential on CHT simulations. Booker et al. (2014) also identified VARPAR26 as a highly influential parameter. VARPAR30 acts as a multiplier on the temperature function used to calculate squaring date, and it was influential on GBL. As expected, both LAI and LDM were sensitive to VARPAR34, which sets the initial leaf area of prefruiting leaves. VARPAR35, which was influential on CHT, affects the calculation of physiological days between successive fruiting branches. Results of the GSA were often intuitive and helped to identify influential model parameters for subsequent model parameterization efforts (Table 4; Fig. 1).

### 3.2. Multiobjective optimization

Recalling that the second Sobol sampling resulted in 2,500,056 Cotton2K parameter sets that were evaluated using multiobjective optimization (Table 5), calculation of the Pareto optimal solutions for the CIMIS-DY, CIMIS-HR, and ASCEK-HR ET methods reduced the number of plausible solutions to 461,448, 369,347, and 419,784, respectively. Thus, the Pareto optimal solution set eliminated up to 85% of the total evaluated solutions, although the remaining number was still very large. Pruning the Pareto optimal solutions using the objective function weighting approach further reduced the number of solutions to 19, 12, and 22 for the CIMIS-DY, CIMIS-HR, and ASCEK-HR ET methods,

**Table 6**

Analysis of variance results ( $F$  statistics and  $p$  values) and Tukey's multiple comparisons tests among the pruned Pareto optimal solutions from Cotton2K simulations using three evapotranspiration methodologies (CIMIS-DY, CIMIS-HR, and ASCEK-HR). The group means for percent root mean squared errors (%RMSE) are given for each evapotranspiration method and agroecosystem metric, and statistically better performing methods for each metric are highlighted in bold. <sup>a</sup>

Metric	$F$	$p$ value	CIMIS-DY	CIMIS-HR	ASCEK-HR
			%RMSE	%RMSE	%RMSE
ET	5.84	0.0053**	60.5 a	60.9 a	<b>59.6 b</b>
FBY	0.26	0.7700	47.6 a	45.5 a	46.4 a
LAI	4.67	0.0138*	<b>62.6 ab</b>	64.6 a	<b>60.7 b</b>
SCY	6.20	0.0039**	<b>40.7 a</b>	<b>43.9 ab</b>	44.6 b
CHT	7.10	0.0019**	30.9 a	31.7 a	<b>27.1 b</b>
SDY	17.97	0.0000***	<b>41.8 a</b>	47.7 b	48.3 b
NOD	7.85	0.0011**	<b>17.0 a</b>	21.9 b	<b>16.1 a</b>
LDM	3.54	0.0366*	<b>56.9 a</b>	<b>61.1 ab</b>	61.1 b
SDM	2.18	0.1240	88.4 a	87.1 a	83.5 a
GBL	30.38	0.0000***	96.8 a	113.5 b	<b>81.2 c</b>
MBL	5.67	0.0060**	<b>94.6 ab</b>	106.9 b	<b>80.3 a</b>
BDM	2.57	0.0863	58.8 a	64.5 a	59.8 a
SWC010	10.22	0.0002***	<b>36.6 a</b>	<b>36.7 a</b>	40.0 b
SWC030	29.87	0.0000***	<b>21.3 a</b>	<b>20.2 a</b>	23.7 b
SWC050	3.31	0.0449*	<b>22.6 a</b>	<b>23.5 ab</b>	23.9 b
SWC070	0.19	0.8240	28.8 a	29.1 a	28.6 a
SWC090	2.19	0.1230	32.6 a	33.1 a	31.5 a
SWC110	0.74	0.4830	30.6 a	30.8 a	29.9 a
SWC130	4.84	0.0120*	35.8 a	36.4 a	<b>33.8 b</b>
SWC150	4.25	0.0197*	<b>34.0 ab</b>	35.7 b	<b>33.6 a</b>
SWC170	1.37	0.2630	37.8 a	39.6 a	37.2 a
SWC190	4.97	0.0108*	<b>31.7 a</b>	35.3 b	<b>32.2 a</b>

<sup>a</sup> Boll dry matter, BDM; canopy height, CHT; evapotranspiration, ET; fiber yield, FBY; green boll number, GBL; leaf area index, LAI; leaf dry matter, LDM; mature boll number, MBL; mainstem node number, NOD; cottonseed yield, SDY; seed cotton yield, SCY; stem dry matter, SDM; soil water content; SWC.

respectively. This means the multiobjective optimization technique could reduce the solution set to better than 0.0009% of the total evaluated solutions. The result highlighted the difficulty of practical decision making from the Pareto optimal set, while pruning the set based on limited user input (i.e., the order of objective function importance) substantially reduced the number of solutions and improved the practicality of determining a feasible model parameterization.

### 3.3. Statistical analysis

Simulation results among the three ET methods in Cotton2K (Table 1) were different ( $p \leq 0.05$ ) for 15 of the 22 agroecosystem metrics: ET, LAI, SCY, CHT, SDY, NOD, LDM, GBL, MBL, and soil water content at 10, 30, 50, 130, 150, and 190 cm (Table 6). With the ASCEK-HR method, ET was simulated significantly better than with the other two ET methods, although the mean %RMSE improvement was less than 1%. Because the %RMSE calculation for ET involved more than 3700 data values (Table 3), %RMSE variation among the pruned Pareto optimal sets was low, which contributed to the significant difference among ET methods. The ASCEK-HR method also performed significantly better than the other two ET methods for CHT, GBL, and soil water content at 130 cm. However, the CIMIS-DY method performed significantly better than both the other two methods for SDY. The CIMIS-HR method did not perform significantly better than both the other methods for any of the agroecosystem metrics. Collectively, CIMIS-DY and CIMIS-HR both performed better than ASCEK-HR for SCY, LDM, and soil water contents at 10, 30, and 50 cm. Thus, the statistical results demonstrated no clear winner among the three ET methods. Generally, each ET method statistically outperformed the other methods for one or more metric but not without significantly underperforming on a different metric. An exception was in the

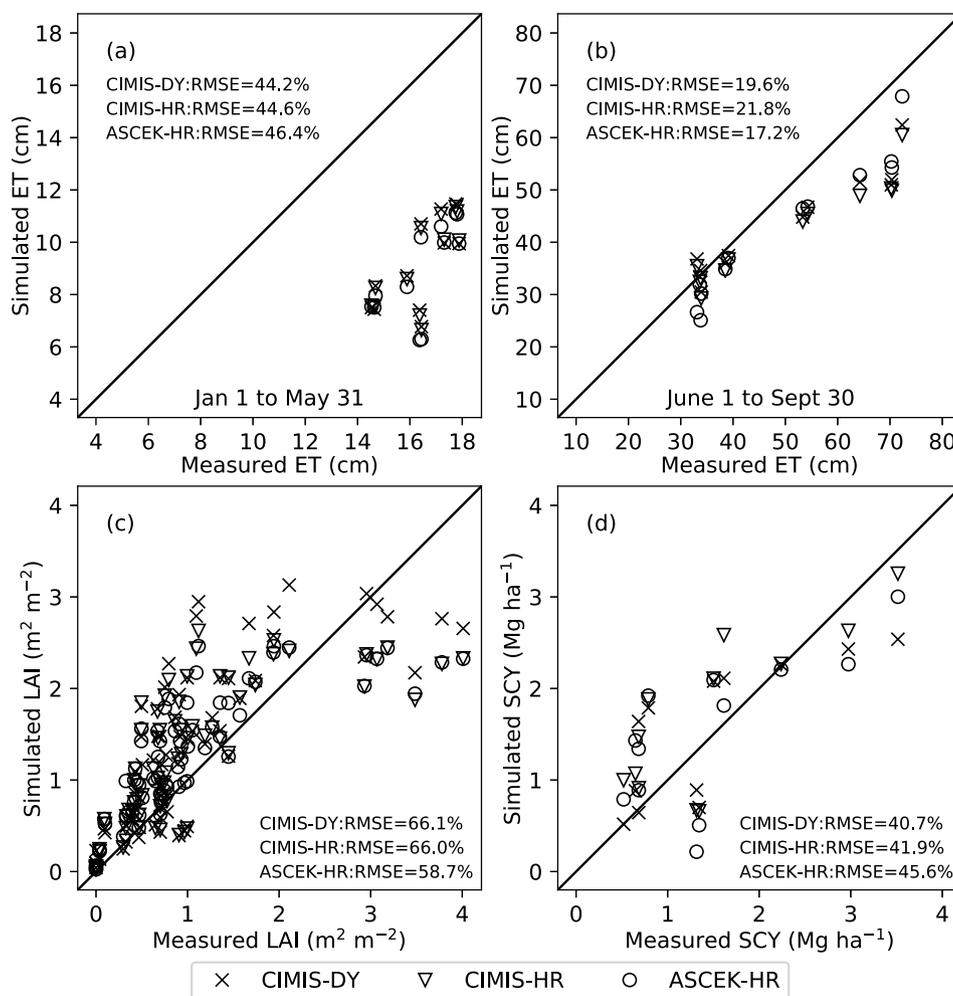
comparison of CIMIS-DY and CIMIS-HR, where the results showed no advantage to using directly measured hourly weather data (CIMIS-HR) as compared to estimating hourly weather from daily measurements based on Ephraïm et al. (1996) (CIMIS-DY). That is, CIMIS-DY performed as well as or better than CIMIS-HR for all 22 agroecosystem metrics, an unexpected result but nonetheless demonstrated statistically. Importantly, based on comparisons to daily measurements from weighing lysimeters at Bushland, the ASCEK-HR standardized ET method statistically outperformed the CIMIS-DY and CIMIS-HR methods for simulating ET in Cotton2K.

### 3.4. Model evaluation

The pruning algorithm iterated 465,213 times to identify 22 or less pruned Pareto optimal solutions for each ET simulation method. Among the results at each iteration, the most popular solutions for the CIMIS-DY, CIMIS-HR, and ASCEK-HR methods were selected 63%, 86%, and 61% of the time. The most popular solutions for CIMIS-HR and ASCEK-HR were identical (Table 4), perhaps because these two ET approaches used the same weather input data. For CIMIS-DY, a different solution was most popular. The solution identified as the most popular for each method (i.e., most commonly selected by the pruning algorithm) was used to parameterize Cotton2K for all further evaluations of the model. Of the 2,500,056 evaluated parameter sets, only one parameter set was commonly present in the pruned Pareto optimal solutions for all three ET methods, but it was not a most popular solution for any method.

To more fully evaluate the ET simulations in Cotton2K, the simulation timeframe was divided into sections dominated by soil water evaporation (1 January through 31 May) and transpiration (1 June through 30 September). (Because Cotton2K simulations terminated on the specified harvest date (Table 2), availability of information for November and December was inconsistent, so it was not included here.) Cotton2K consistently underestimated cumulative ET during the soil water evaporation-dominated portion with %RMSE > 44% for all three ET methods (Fig. 2a). Because soil water evaporation is simulated based only on the water content of the top soil layer, the underestimation may be due to inadequate simulation of upward water flux from deeper soil layers. For example, if the simulated soil water evaporation demand is larger than the upward water flux into the top soil layer, soil water evaporation will decline even though the next deepest soil layer may have plenty of water to meet the demand. Cumulative ET during the transpiration-dominated period was also consistently underestimated by the model (Fig. 2b) for all ET methods. The %RMSE for the ASCEK-HR method (17.2%) was lowest among the ET methods with better performance apparent at the extreme levels of ET, corresponding to fully irrigated treatments. Overall, after thorough evaluation of Cotton2K parameterization options with three ET simulation strategies, Cotton2K consistently underestimated ET as compared to ET measurements from the Bushland weighing lysimeters (Fig. 2).

The Cotton2K simulations of LAI were mostly overestimated for LAI < 2.5 m<sup>2</sup> m<sup>-2</sup> and underestimated for LAI > 2.5 m<sup>2</sup> m<sup>-2</sup> (Fig. 2c). Only the fully irrigated treatments in 2001 and 2008 achieved a maximum LAI of 3.0 m<sup>2</sup> m<sup>-2</sup> or more. Thus, the model was generally unable to fully respond to plant growth conditions under full irrigation, while also often drastically overestimating LAI for water-limited conditions. Simulation results for SCY were moderately accurate (Fig. 2d), although the SCY results for the ASCEK-HR ET method were worse than for the other two methods. Overall, Cotton2K simulations of LAI and SCY were poorer than that obtained with a different agroecosystem model at a nearby research station in west Texas (Modala et al., 2015) and in central Arizona (Thorp et al., 2017). Note that the %RMSE statistics for LAI and SCY are different in Fig. 2 as compared to Table 6, because the latter provides mean %RMSE among solutions in the pruned Pareto optimal set while the former reports %RMSE for the most popular pruned Pareto optimal solution.



**Fig. 2.** Cotton2K simulated versus measured data for a) evaporation-dominated cumulative evapotranspiration prior to the cotton growing season (January 1 through May 31), b) transpiration-dominated cumulative evapotranspiration during the cotton growing season (June 1 through September 30), c) cotton leaf area index (LAI), and d) seed cotton yield (SCY). Results are shown for three ET simulation methods: CIMIS-DY, CIMIS-HR, and ASCEK-HR.

### 3.5. Evapotranspiration behavior

As suggested by DeJonge and Thorp (2017), analysis of the crop coefficients (i.e.,  $K_c$ ,  $K_{cb}K_s$ , and  $K_e$ ) as computed from simulated ET variables and  $ET_{os}$  can reveal insights about model behavior and functionality, as well as the reasonableness of simulated transpiration and soil water evaporation time series. The approach is also useful for further comparisons among ET simulation methods. Crop coefficient plots for simulations of the fully irrigated 2008 NELYS field generally showed similar behavior between the three ET methods (Fig. 3). For example, all three methods demonstrated similar pre-season (DOY 100–160) and post-season (DOY 275–300) spikes in  $K_e$ , indicating increased soil water evaporation (and  $K_e$ ) due to precipitation events. However, the pre-season peaks in simulated  $K_e$  were not as high as measured  $K_e$  from the lysimeter, indicating underestimated soil water evaporation no matter which ET algorithm was used. Mid-season  $K_e$  from DOY 190 to 240 was better simulated with the ASCEK-HR method than with the CIMIS methods, as compared to  $K_e$  from lysimetry. Gross underestimation of  $K_e$  at the end of the season from DOY 260 to 275 contributed to the general trend of underestimated ET during the transpiration-dominated portion of the season (Fig. 2b) and indicates need for improvements to the late-season transpiration calculations.

Other aspects of the crop coefficient curves highlighted localized differences among the simulated ET time series. Although the %RMSE between measured and simulated ET were not different for CIMIS-HR and CIMIS-DY (Table 6), visual differences in mid-season  $K_e$  (DOY

220–240) indicated different simulated ET time series for the two CIMIS methods (Fig. 3). During this time, the field received 106 mm of precipitation over a five day period (DOY 226–230). Despite simulation of full canopy during these days ( $LAI > 2.6$ ; not shown), the CIMIS-DY method simulated higher evaporation with  $K_e$  ranging from 0.37 to 0.50. This resulted in high  $K_e$  values reaching 1.74 for CIMIS-DY on DOY 230 (Fig. 3a). The  $K_e$  results for CIMIS-HR and ASCEK-HR were smaller during this time: 0.29–0.34 (Figs. 3b) and 0.19–0.31 (Fig. 3c), respectively. This reduced  $K_e$  to 1.22 or less for CIMIS-HR and ASCEK-HR, which is closer to a more typical mid-season value. The result was likely due to providing precipitation data in hourly versus daily amounts. Specifying rain events hourly allowed infiltration processes to be simulated over several timesteps, while specifying daily rainfall amounts filled the top soil layer in a single timestep and increased opportunity for soil water evaporation thereafter.

Because the ASCEK-HR method generally had high LAI (Fig. 2c) and thus  $K_{cb}$  (Eq. (1)), the  $K_e$  peaks generally decreased as the season progressed from DOY 180 to 280 (Fig. 3c). This was a sensible response because increases in plant growth should further limit soil water evaporation, and similar behavior was recently found with another agroecosystem model (DeJonge and Thorp, 2017). However, neither  $K_e$  time series for CIMIS-DY (Fig. 3a) nor CIMIS-HR (Fig. 3b) demonstrated this declining trend over the season. The results indicated that the soil water evaporation routine for the CIMIS methods in Cotton2K should be further investigated and potentially improved.

Another interesting finding was the drastic changes in transpiration

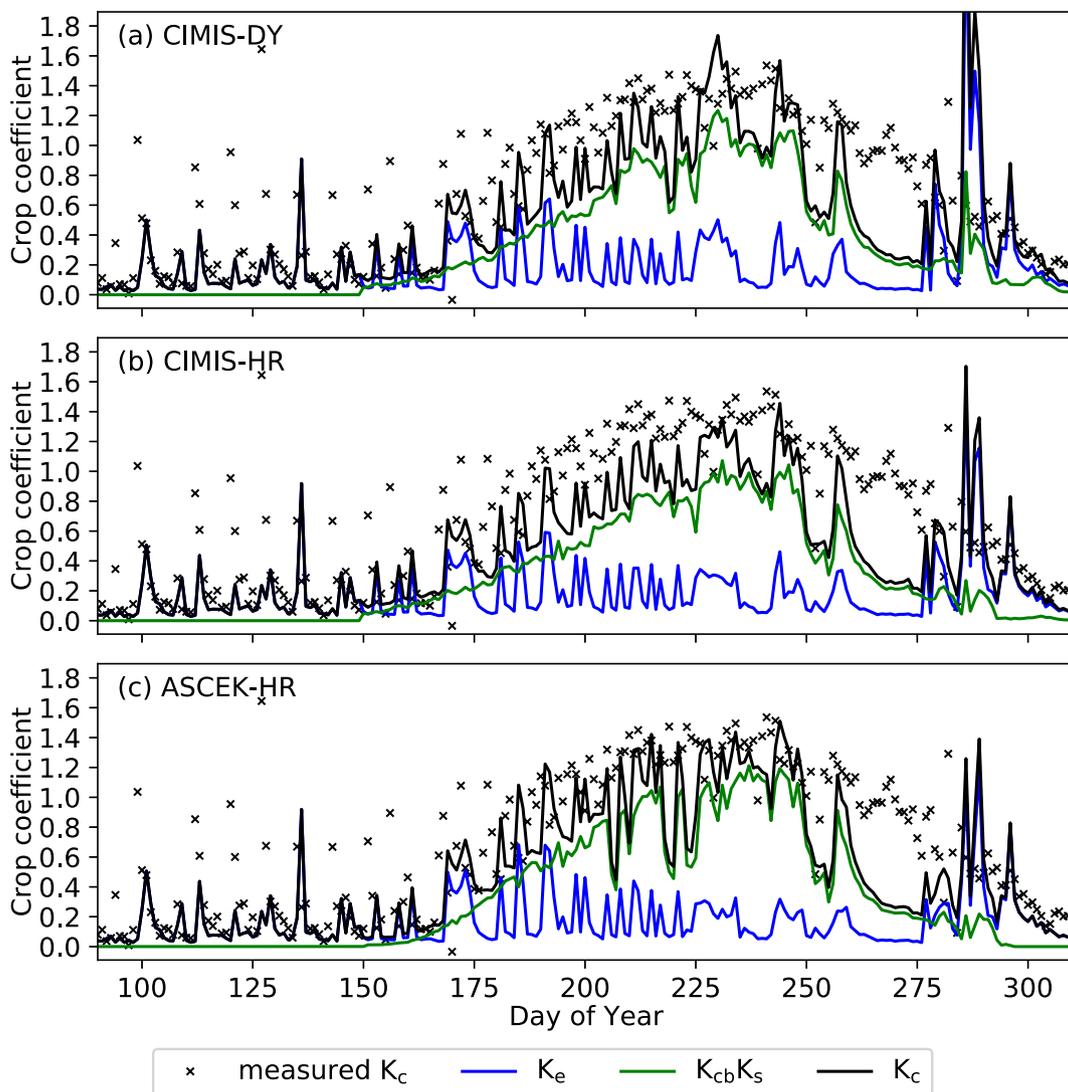


Fig. 3. FAO-56 crop coefficients simulated by Cotton2K using three evapotranspiration methods (CIMIS-DY, CIMIS-HR, and ASCEK-HR) and measured with the northeast lysimeter under fully irrigated cotton production at Bushland, Texas in 2008.

(i.e.,  $K_{cb}K_s$ ) as simulated for the 2000 SWLYS field with dryland cotton production, particularly for the CIMIS ET methods (Fig. 4). Crop coefficients from the CIMIS ET methods exhibited tremendous and seemingly unrealistic transpiration variability, whereas the ASCEK-HR method resulted in a more steady increase in transpiration. For example, over a sixteen day period from DOY 178–193,  $K_{cb}K_s$  for CIMIS-HR varied from 0.15 to 1.11 and back to 0.28 (Fig. 4b). Because LAI was simulated as a steadily increasing curve over this time period (not shown), it seems unlikely that the crop's transpiration potential shifted from near zero to full potential and back to near zero in just a few days. The CIMIS-DY method also exhibited a similar large swing in  $K_{cb}K_s$  values at this time (Fig. 4a). However, the ASCEK-HR method demonstrated a more typical  $K_{cb}K_s$  curve that generally followed the pattern of biomass growth, because the method intrinsically linked simulated LAI with transpiration via Equation (1) (Fig. 4c). Because simulated  $K_{cb}K_s$  often appeared incongruent with simulated LAI time series (not shown), the interaction between vegetation production and transpiration needs further investigation to achieve more reasonable crop coefficient time series, particularly under water-limited conditions with the CIMIS methods in Cotton2K.

#### 4. Discussion

Verifying the accuracy of simulation results from agroecosystem models is a fundamental research question that has generated numerous studies on techniques for model evaluation, sensitivity analysis, and model intercomparison. Herein, a novel approach was developed to compare and highlight deficiencies in Cotton2K simulations based on three ET algorithms. The main advantage of the approach was its inherent objectivity; there was very little effect of subjectivity in the model comparisons. When subjectivity was required, for example in specifying the parameter ranges (Table 4), the threshold for sensitivity indices, or the priority order of agroecosystem metrics (Table 3), the decision could be applied uniformly among all ET methods. Thus, the comparisons were more scientifically robust and repeatable, as compared to model intercomparison techniques that involve more subjective model parameterization decisions. Through the use of high-performance computing, the approach also permitted evaluation of many more parameter sets than could be practical using manual model parameterization techniques. Thus, the comparisons could be conducted with a more thorough assessment of model responses to variability in parameterization.

The results also reinforced an important lesson about agroecosystem model evaluation when multiple types of measured data are available;

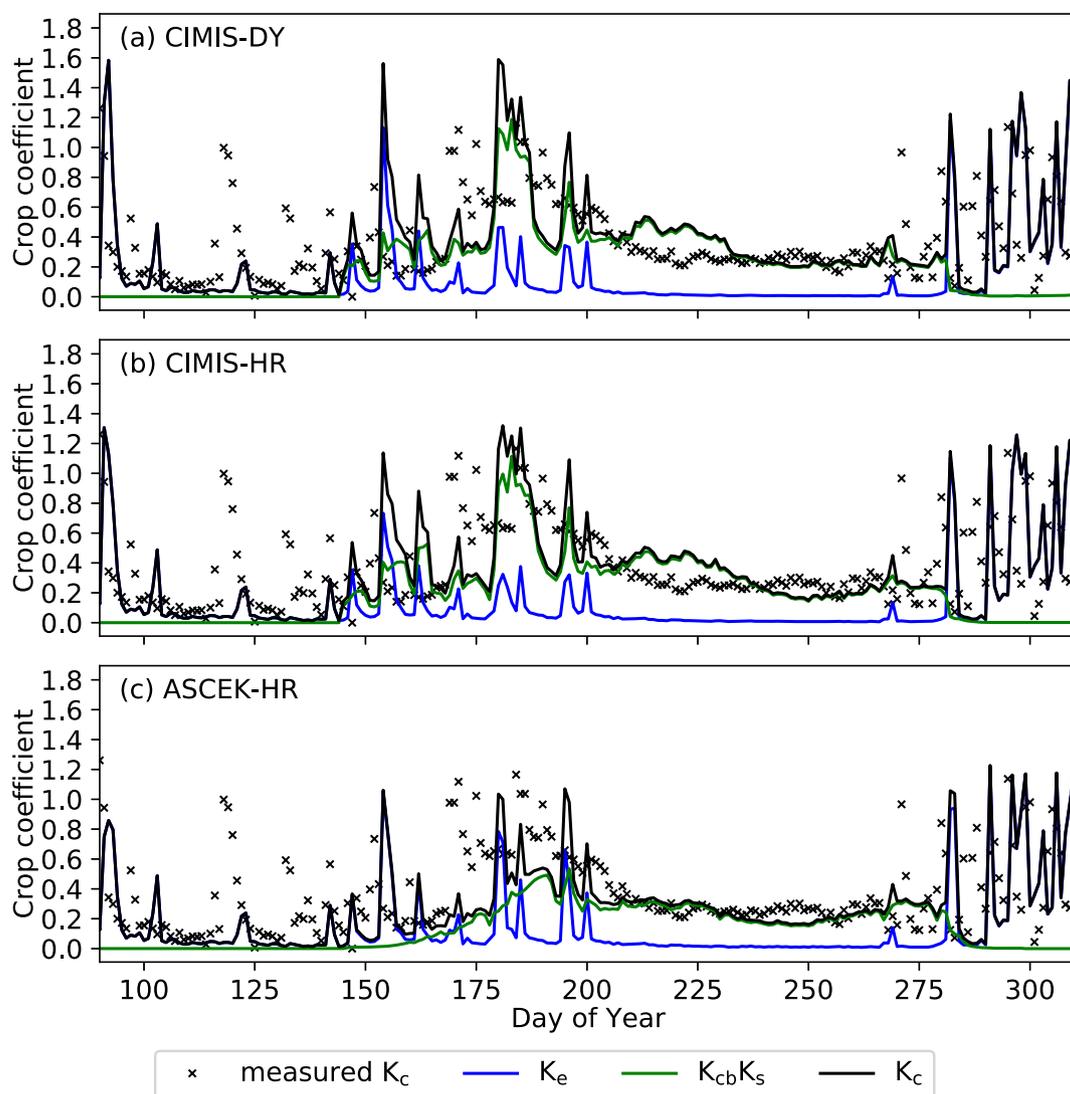


Fig. 4. FAO-56 crop coefficients simulated by Cotton2K using three evapotranspiration methods (CIMIS-DY, CIMIS-HR, and ASCEK-HR) and measured with the southwest lysimeter under dryland cotton production at Bushland, Texas in 2000.

it can be difficult to find solutions that improve simulations of all metrics simultaneously. Given any two model parameterizations considered in this study, there was a 15%–18% chance that one parameterization was no better than the other when considering all 22 agroecosystem metrics. The implications for manual calibration are potentially freeing for perfectionist modelers who are frustrated when they can no longer improve simulations of one metric without worsening simulations of another. That is, the calibration effort may have approached a solution within the Pareto optimal set, and further efforts to reduce simulation error among all metrics may be futile. Furthermore, the number of solutions among the Pareto optimal set is likely too large to be assessed adequately using manual calibration methods, but more advanced computational techniques could be used for further assessment.

The GSA highlighted opportunities to condense and simplify the crop variety parameters in Cotton2K. Only 15 of 51 variety parameters were identified by the GSA to substantially influence the simulation results. Many of the parameters work together in empirical equations to control a particular aspect of the simulation. For example, three parameters are involved in leaf growth on the mainstem nodes, four parameters affect post-squaring stem growth, and four other parameters control the probability of boll abscission (Table 4). Efforts to merge the effects of such parameters could possibly increase their sensitivity,

while also reducing the complexity of the model parameterization. However, realistic simulation detail should not be lost in the effort to reduce parameters. Conducting the GSA for each of the 12 scenarios separately may also reveal differences in model sensitivity that are caused by environment.

Using three ET algorithms, Cotton2K simulated ET, LAI, and SCY with %RMSE between measured and simulated data ranging from 59.6% to 60.9%, 60.7%–64.6%, and 40.7%–44.6%, respectively (Table 6). However, as reported by Modala et al. (2015) and Thorp et al. (2017), the %RMSE results for these important agroecosystem metrics were lower for a different cotton simulation model based on data from different sites in the western U.S. This result is surprising, because Cotton2K simulates cotton growth and development and soil water balance processes in more detail than other cotton simulation models. For example, Cotton2K simulates a two-dimensional soil profile and considers development and growth of individual cotton bolls; whereas, other models simulate these processes with greater simplicity. Future efforts will focus on evaluation of other cotton models using the data sets from Bushland, Texas. This will allow a more direct comparison of Cotton2K performance to other models with reduced complexity.

No matter which ET method was used, Cotton2K generally underestimated ET as compared to data from the Bushland weighing

lysimeters (Fig. 2). Borrowing the terminology of Lamsal et al. (2018), Cotton2K likely suffered from a lack of “expressibility”, which means there were possibly no parameterization options that would prevent the model from underestimating ET, particularly for the CIMIS approaches. Adjustments of  $K_{cbmax}$  (Eq. (1)) higher than the value recommended by FAO-56 could possibly increase the transpiration component of ET, but only for the ASCEK-HR ET method. Alternatively, transpiration might be increased by expanding the simulated root profile, which is also two-dimensional in Cotton2K. Because soil water evaporation is supplied only by the water content of the top soil layer in Cotton2K, underestimation of evaporation is likely related to a water limitation in that layer. Increasing the thickness of the top layer in Cotton2K is a potential solution to increase the water supply available for evaporation (Lascano and Van Bavel, 1986). Future work should further investigate and possibly improve the Cotton2K soil water balance simulation, particularly focusing on how the simulated soil and root profile supplies water for ET and on the simulated relationships between plant growth and ET. Also, due to the importance of ET partitioning in models of soil-plant-atmosphere systems (Kool et al., 2014), data sets that better describe the soil water evaporation and plant transpiration components of ET are needed for more thorough model evaluation and improvement.

## 5. Conclusions

With the development of a novel methodology for making unbiased Cotton2K parameterization decisions, the study demonstrated how three ET simulation methodologies could be intercompared while reducing modeler bias and subjectivity. The methodology was useful for determining statistically whether one ET method performed better than another. While the present study provided a specific example related to comparison of ET methods, the approach is likely also useful for comparisons of other agroecosystem model components.

The study demonstrated differences ( $p < 0.05$ ) in Cotton2K simulations of ET and other agroecosystem metrics among three ET simulation methods. However, none of the tested ET methods could perform as well as or better than both of the other methods when considering all metrics collectively. Considering ET alone, the ASCEK-HR method led to minimal but significant improvements in simulated ET, and crop coefficient curves were often more realistic. While the three ET methods had many qualitative and programmatic differences that led to localized differences in simulated ET time series, the overall contribution of these differences toward comprehensive improvement of the simulation results was negligible. To improve ET simulations with Cotton2K, future research should investigate the simulation methodologies used for soil water flux near the soil surface and for linking water use with crop growth.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.envsoft.2019.06.007>.

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