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Assessing fiber quality variability among modern upland cotton cultivars and incorporating it into the GOSSYM-based fiber quality simulation model

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Abstract

Background GOSSYM is a mechanistic, process-based cotton model that can simulate cotton crop growth and development, yield, and fiber quality. Its fiber quality module was developed based on controlled experiments explicitly conducted on the Texas Marker-1 (TM1) variety, potentially making its functional equations more aligned with this cultivar. To assess the model's broader applicability, this study analyzed fiber quality data from 40 upland cotton cultivars, including TM1. The measured fiber quality from all cultivars was then compared with the model-simulated fiber quality.

Results Among the 40 upland cultivars, fiber strength varied from 28.4 $cN \cdot tex^{-1}$ to 34.6 $cN \cdot tex^{-1}$, fiber length ranged from 27.1 mm to 33.3 mm, micronaire value ranged from 2.7 to 4.6, and length uniformity index varied from 82.3% to 85.5%. The model simulated fiber quality closely matched the measured values for TM1, with the absolute percentage error (APE) being less than 0.92% for fiber strength, fiber length, and length uniformity index and 4.7% for micronaire. However, significant differences were observed for the other cultivars. The Pearson correlation coefficient (*r*) between the measured and simulated values was negative for all fiber quality traits, and Wilmotts's index of agreement (WIA) was below 0.45, indicating a strong model bias toward TM1 without incorporating cultivar-specific parameters. After incorporating cultivar-specific parameters, the model's performance improved significantly, with an average *r*-value of 0.84 and WIA of 0.88.

Conclusions The adopted methodology and estimated cultivar-specific parameters improved the model's simulation accuracy. This approach can be applied to newer cotton cultivars, enhancing the GOSSYM model's utility and its applicability for agricultural management and policy decisions.

Keywords Cotton, GOSSYM, Crop modeling, Fiber quality, Cultivar-specific parameter

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Background

Cotton fiber quality is pivotal in market profitability for both cotton growers and the textile industry (Liu et al. 2023). Cotton fiber quality, including fiber length, also known as upper half mean length (UHML), fiber strength, micronaire, length uniformity index, color grade, etc., affects yarn (hairiness, evenness, strength, and spinning efficiency) and fabric performance (appearance, strength, and pilling). Fiber length refers to the average length of the 50% longest fibers by weight (Krifa 2006). The length uniformity index represents the fiber length distribution and is obtained as a ratio between the mean length of the fibers and the UHML of the fibers (Ramey et al. 1989). Fiber strength expressed in centinewtons per tex ($cN \cdot tex^{-1}$) is the force required to break a bundle of fibers that is one tex unit in size, where a tex unit is equal to the weight in grams of 1 000 m of fiber. Fiber strength is vital for advanced spinning technologies and affects the hairiness and strength of both the yarn and fabric (Bradow et al. 2010). Micronaire (an indirect measure of fiber fineness and maturity) influences fiber processing and dyeing consistency (Rodgers et al. 2017). Color grade measures fiber's reflectance, brightness, and yellowness, which influence dyeing properties (Xu et al. 1998). Growers always aim to produce the best quality cotton to gain market profitability (Liu et al. 2023). In the USA, each bale of cotton produced is graded based on the quality attributes as per the quality standards/charts regulated by the United States Department of Agriculture-Agricultural Marketing Service (USDA-AMS) (Pinnamaneni et al. 2021). High-quality cotton, which meets the USDA's grading standards, is eligible for premium pricing in the markets. Conversely, low-quality fiber, often resulting from adverse weather conditions, pest damage, improper harvesting and ginning practices, etc., may receive discounted prices.

Cotton fiber quality is influenced by cultivars, environmental conditions, and management practices (Lokhande et al. 2014; Mehran et al. 2023; Baghyalakshmi et al. 2024). For instance, a reduction of 12% in the micronaire was observed when shifting from rainfed treatment to irrigated treatment (Pinnamaneni et al. 2021). A study on the contribution of environment and genotype to cotton yield and quality, using seven cotton cultivars across 33 environments, showed that both factors influence fiber quality, with the environment playing a more significant role (contribution ranging from 47% to 80%) in governing it (Snider et al. 2013).

Crop simulation models that can simulate the interactive effect of cultivar, environmental, and management conditions have an important role in agricultural management (Thorp et al. 2014). Since the 1980s, numerous cotton simulation models have been developed, such as GOSSYM (Baker et al. 1983), OZCOT (Hearn et al. 1985; Hearn 1994), CSM-CROPGRO-Cotton (Hoogenboom et al. 1992), COTCO2 (Wall et al. 1994), and Cotton2K (Marani 2004). Among the existing cotton simulation models, GOSSYM stands out as one of the most widely validated and applied in on-farm decision-making and management practices (Lemmon 1986; Reddy et al. 1995b, 2002, 2003, 2008). It is a mechanistic, process-level simulation model that estimates crop growth, development, and yield based on the environmental conditions (solar radiation, temperature, humidity, rain, wind, CO_2, etc.), soil physical and hydraulic properties, and management practices (irrigation, fertilizer application, tillage) (Baker et al. 1972, 1983; Whisler et al. 1986). It has also been applied in policy areas across the cotton-growing areas (Doherty et al. 2003; Liang et al. 2012a, 2012b). Over time, GOSSYM has been refined and improved through insights gained from laboratory experiments, field trials, and controlled-environment studies (Landivar et al. 1983; Boone et al. 1993; Reddy et al. 1995a, 1997, 2003; Staggenborg et al. 1996; Baker et al. 2015). Recent enhancements to GOSSYM include improved estimations of photosynthesis and transpiration by integrating the Farquhar biochemical model and Ball-Berry leaf energy balance model (Beegum et al. 2023b). A notable addition to the GOSSYM model is a fiber quality simulation module, which is the first of its kind among process-based cotton models (Beegum et al. 2023a, 2024b).

The GOSSYM model can simulate four major fiber quality traits: fiber strength, length, micronaire, and length uniformity index. The mathematical functional relationships between these four fiber quality metrics and the major factors influencing fiber quality (temperature, water, and nutrient status) used in the developed model were established based on several sets of control chamber experiments (Beegum et al. 2023a). One of the main highlights of all the experiments was that they were all performed on the same cotton cultivar, Texas Marker-1 (TM1), a common cultivar used as a reference genome in cotton research (Kohel et al. 1970; Beegum et al. 2023a; Sreedasyam et al. 2024). Therefore, the fiber quality module integrated into GOSSYM may be biased towards or more predictive of the TM1 variety. Thus, the model needs testing for its performance with other cultivars. If the model doesn't simulate well for other cultivars, cultivar-specific parameters in the fiber quality module in GOSSYM will need to be developed.

The study aims to assess fiber quality variability among different cotton cultivars and to evaluate and improve the GOSSYM model's fiber quality simulations. The specific objectives are (a) to analyze the variability in fiber strength, fiber length, micronaire, and length uniformity index among different cotton cultivars, including the TM1 variety used for model development; (b) to evaluate the fiber quality module in GOSSYM for its accuracy in simulating fiber quality across cultivars; and (c) to estimate cultivar-specific parameters based on observed variability in fiber quality.

Materials and methods

Cotton fiber quality module in GOSSYM

Fiber quality estimation in the GOSSYM model follows a two-step algorithm. First, the model estimates the potential fiber quality, which is a function of temperature and represents fiber quality under optimal conditions without other stresses. Next, it calculates the actual fiber quality by modifying the potential fiber quality based on stress factors (water and nutrient stresses). Water and nutrient stresses are represented as functions of leaf water potential and leaf nitrogen concentration, respectively (Lokhande et al. 2014; Beegum et al. 2023a). In the model, the fiber quality traits (fiber strength, length, micronaire, and length uniformity index) are estimated for each of the cotton bolls, and the plant-level quality is estimated as a mass-weighted average of the fiber quality of individual bolls (Beegum et al. 2023a).

Obtaining data for analyzing fiber quality variability among cotton cultivars

Data for analyzing fiber quality variability among cotton cultivars (a total of 40), including the TM1 variety, was obtained as part of another experimental study that was focused on quantifying the growth and development of different cotton cultivars (Beegum et al. 2024a, 2024c). All cultivars were grown under the same environmental and management conditions to isolate variability in the fiber quality as a genetic characteristic of the cultivar and exclude the influence of other factors. All cultivars were grown under non-limiting water and nutrient conditions.

This study was conducted in 2022 at the Environmental Plant Physiology Laboratory at the Mississippi Agricultural and Forestry Experimentation Station, Mississippi State University, Mississippi, USA (33°28′ N, 88°47′ W). The details of the experiment's design can be found in studies by Beegum et al. (2024a; 2024c). The data set on fiber quality was from a total of 40 different upland cotton cultivars with three replications and five plants per replication. The 8–10 cotton bolls per plant were hand-picked from the first and second positions (closest to the mainstem). This was done to eliminate age-related factors and any variations in the duration from flowering to boll opening that could impact the fiber quality. The cotton bolls were ginned at the Crop Science Research Laboratory, United States Department of Agriculture-Agricultural Research Service (USDA-ARS), which has a Continental/Moss Gordin 10-saw, 10-inch diameter gin stand (Continental Eagle Corporation, USA), powered by 3-phase 240-V electricity. Four major fiber quality traits (fiber strength, length, micronaire, and length uniformity index) were assessed using high-volume instrumentation (HVI) (Uster HVI 1000, Uster Technologies AG, Switzerland) at the Fiber and Biopolymer Research Institute, Texas Tech University. Fiber quality measurements included four readings for micronaire and ten each for fiber length and fiber strength in each replication. The mean of these values within each replication was used for analysis.

Evaluating fiber quality variability and cultivar-specific parameters

The cultivar-specific fiber quality parameters were estimated using the methodology developed by Beegum et al. (2024c). The first step was to run the GOSSYM model using the same environmental and management conditions that prevailed during the experiments. Then, we compared the measured and simulated fiber quality values. Since the model was initially developed using the TM1 cultivar, the first step was to compare the model-simulated quality for TM1 with the measured value to determine whether the model exhibited a bias toward this cultivar.

Based on the variation percentage observed between the measured and simulated fiber quality across all cotton cultivars, they were grouped into categories. Since the parameters in the fiber quality functional equations act as multipliers, the cultivar-specific parameters were determined by scaling the variation in the measured and simulated values from the base parameter value of 1.0. A similar scaling procedure had previously been used in GOSSYM to estimate cultivar-specific parameters for several functions in GOSSYM, such as the time to square, time from square to open boll, time to flower, fruit loss, and plant height functions (Reddy et al. 1988).

To categorize cultivars, a bandwidth of ± 2.5% around the simulated values was first estimated. This facilitates setting a cultivar-specific parameter value of 1.0 for all cultivars that have their measured fiber quality values within this band (–2.5% to +2.5%). A band of ± 5%, ± 10%, ± 15%, etc., from the simulated values was not adopted because this would result in a larger band (–5% to +5%) close to the simulated values compared with subsequent bands. Starting from the ±2.5% band, an additional 5% is added on either side (–7.5%, +7.5%) of the simulated values for fiber quality traits. The calibrated values for the cultivars within +2.5% to +7.5% were set to 1.05, and within –2.5% to –7.5% were set to 0.95, which was based on the relative variation from a value of 1.0 for parameters for cultivars within –2.5% to +2.5%. Similarly, the calibrated values for the cultivars within +7.5% to +12.5% and within –7.5% to –12.5% were set to 1.10 and

0.90, respectively. This approach determined cultivar-specific parameters based on the variation in the measured fiber strength, fiber length, micronaire, and length uniformity index from the GOSSYM simulated values.

Performance evaluation for GOSSYM model

The comparison of the measured and simulated fiber quality, as well as the performance of the methodology used for cultivar-specific parameter estimation, are evaluated based on the absolute percentage error (APE), root mean square error (RMSE), Willmott's index of agreement (WIA), and Pearson correlation coefficient (*r*) (Willmott 1982). Lower APE values indicate higher accuracy in the simulation, as the simulated values are closer to the actual measured values. Lower RMSE values indicate the closeness of the measured values to the simulated ones. WIA reflects the degree to which the simulated variable accurately estimates the measured variable, with a value of 1.0 indicating perfect agreement and 0.0 indicating no agreement (Willmott 1981). The *r* is a statistical measure that describes the extent to which the simulated and measured variables are linearly related. The values of *r* range from −1 to 1. An *r* value of 1 indicates a perfect positive linear relationship, –1 indicates a perfect negative linear relationship, and 0 signifies no linear relationship. All the performance evaluations are performed in RStudio software. APE, RMSE, WIA, and *r* are estimated using Eqs. 1, 2, 3, and 4, respectively. The terms *simulated* and *measured* in the equations refer to simulated and measured data. The $simulated_{\text{mean}}$ and $measured_{\text{mean}}$ indicate the average of all the simulated and measured values in the dataset, respectively. The number of observed data points is represented by *n*, and *i* is the index representing each individual data point in the dataset.

$$APE = \left|\frac{measured - simulated}{measured}\right| \times 100 \tag{1}$$

$$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}(simulated_i - measured_i)^2\right]^{1/2} \tag{2}$$

$$WIA = 1 - \left[\frac{\sum_{i=1}^{n}(simulated_i - measured_i)^2}{\sum_{i=i}^{n}\left(\left|simulated_i - measured_{\text{mean}}\right| + \left|measured_i - measured_{\text{mean}}\right|\right)^2}\right] \tag{3}$$

$$r = \left[\frac{\sum_{i=1}^{n}(simulated_i - simulated_{\text{mean}})(measured_i - measured_{\text{mean}})}{\sqrt{\sum_{i=1}^{n}(simulated_i - simulated_{\text{mean}})^2}\sqrt{\sum_{i=1}^{n}(measured_i - measured_{\text{mean}})^2}}\right] \tag{4}$$

Genetic algorithm-based optimization for cultivar parameter estimation

To evaluate the cultivar-specific parameter estimation method adopted in this study (Beegum et al. 2024c) against other approaches, genetic algorithm (GA)-based optimization was used for a comparative analysis (Forrest 1996). The GA optimization began with an initialization step, where a population of cultivar-specific parameter values was randomly generated within the 0.5 to 1.5 range. This range was selected because the multiplier parameters in the GOSSYM typically fall within these bounds (Beegum et al. 2024c). Each solution was evaluated using the fitness function defined as the RMSE between the measured and simulated fiber quality indices. Selection, crossover, and mutation operations were performed over 10 generations or until an early stopping criterion was met. The early stopping criterion was triggered if the APE between the simulated and measured values fell below 2.5%, which aligned with the accepted variability threshold used when grouping cultivars based on relative variability. The GA continued iterating until the maximum number of generations was reached or the early stopping condition was satisfied. The best solution from the final population was selected as the optimal parameter set for each cultivar. Parameter estimation using GA was conducted individually for each cultivar. The GA-based optimization was implemented in RStudio software using the GA package.

Results

Fiber quality of the 40 cotton cultivars

The mean of the fiber strength, length, micronaire, and length uniformity index for 40 upland cotton cultivars was 30.98 cN·tex^{-1}, 31.2 mm, 3.7, and 84.0%, respectively (Fig. 1a-d). Fiber strength varied from 28.4 cN·tex^{-1} to 34.6 cN·tex^{-1}, fiber length ranged from 27.1 mm to 33.3 mm, micronaire ranged from 2.7 to 4.6, and length uniformity index varied from 82.3% to 85.5%. The coefficient of variation was 4.5%, 4.17%, 13.3%, and 0.81% for fiber strength, length, micronaire, and length uniformity index, respectively. A significantly negative correlation was observed between micronaire and fiber length (*r*= –0.51), as well as

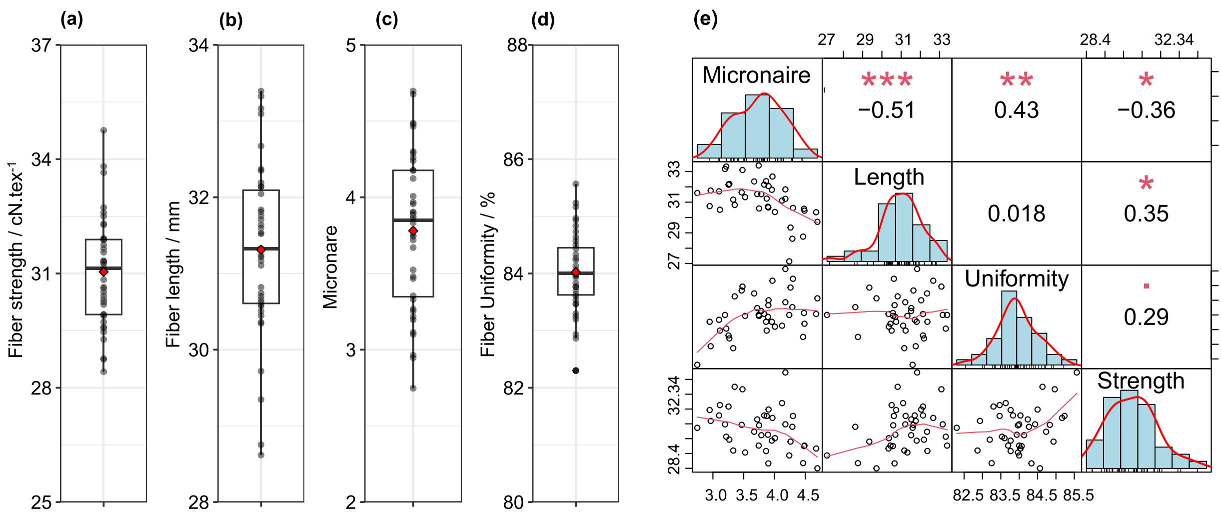

Fig. 1 Variation in fiber strength (**a**), length (**b**), micronaire (**c**), length uniformity index (**d**) among all the cultivars, and (**e**) the distribution and Pearson correlation among the fiber quality traits. The horizontal line inside the box plot gives the median, and the red point represents the mean value. ***, **, *, and ·, represent the significance at $P < 0.001$, $P < 0.01$, $P < 0.05$, $P < 0.1$, respectively

between micronaire and fiber strength ($r=-0.36$) (Fig. 1e). A positive correlation was observed between fiber strength and length ($r=0.35$) as well as between length uniformity index and micronaire ($r=0.43$). A mild positive correlation was observed between the length uniformity index and fiber length ($r=0.018$) (Fig. 1e).

Simulated and measured fiber quality without cultivar-specific parameters

The GOSSYM model-simulated and the measured fiber quality are shown in Fig. 2. First, the model-simulated value was compared with the measured fiber quality from the TM1 variety. The model accurately predicted the TM1 variety for all fiber quality traits. The simulated values for fiber strength, fiber length, micronaire, and length uniformity index for TM1 were 29.69 $cN \cdot tex^{-1}$, 30.42 mm, 4.27, and 83.1%, while the measured values were 29.42 $cN \cdot tex^{-1}$, 30.44 mm, 4.48, and 83.7%, respectively. The APE was less than 0.92% for fiber strength, fiber length, and length uniformity index and 4.7% for micronaire.

When comparing the absolute percentage difference between the measured and simulated values of fiber quality traits for all the cultivars, the maximum difference observed was 55.6%, which occurred in micronaire for the cultivar PHY332 W3 FE. The r values between the simulated and measured data were negative, and WIA was less than 0.45 for all the fiber quality traits. The average absolute percentage difference between the measured and simulated values for fiber strength, fiber length, micronaire, and length uniformity index was 5.4%, 3.8%, 16.7%, and 1.15%, respectively (Fig. 2). These results demonstrate that the GOSSYM model effectively simulates the fiber quality of the TM1 variety as anticipated. However, there is a considerable disparity between the simulated and measured fiber quality for other cultivars, emphasizing the necessity for specific parameters tailored to each cultivar in order to simulate fiber quality accurately.

The classification of the cultivars based on the variability between measured and GOSSYM-simulated quality values is illustrated in Fig. 2a-d. Cultivars are organized into groups, represented by horizontal dashed lines, with each band forming a distinct category based on their variability. Once grouped, their corresponding cultivar-specific parameters are determined (Fig. 2). The cultivar-specific parameter values estimated using this approach are given in Table 1.

Simulated and measured fiber quality after incorporating the cultivar-specific parameters

Once the cultivar-specific parameters were estimated based on the simulated and measured fiber quality (Table 1), the GOSSYM model was rerun by including the cultivar-specific parameters. The simulated and measured fiber quality values after incorporating the cultivar-specific parameters in the fiber quality functions of the GOSSYM model are presented in Fig. 3. The model simulated the fiber quality for all the cultivars with better accuracy, as shown by higher values of r (−0.06 versus 0.84) and WIA (0.42 versus 0.88) and reduced RMSE compared with simulations without cultivar-specific

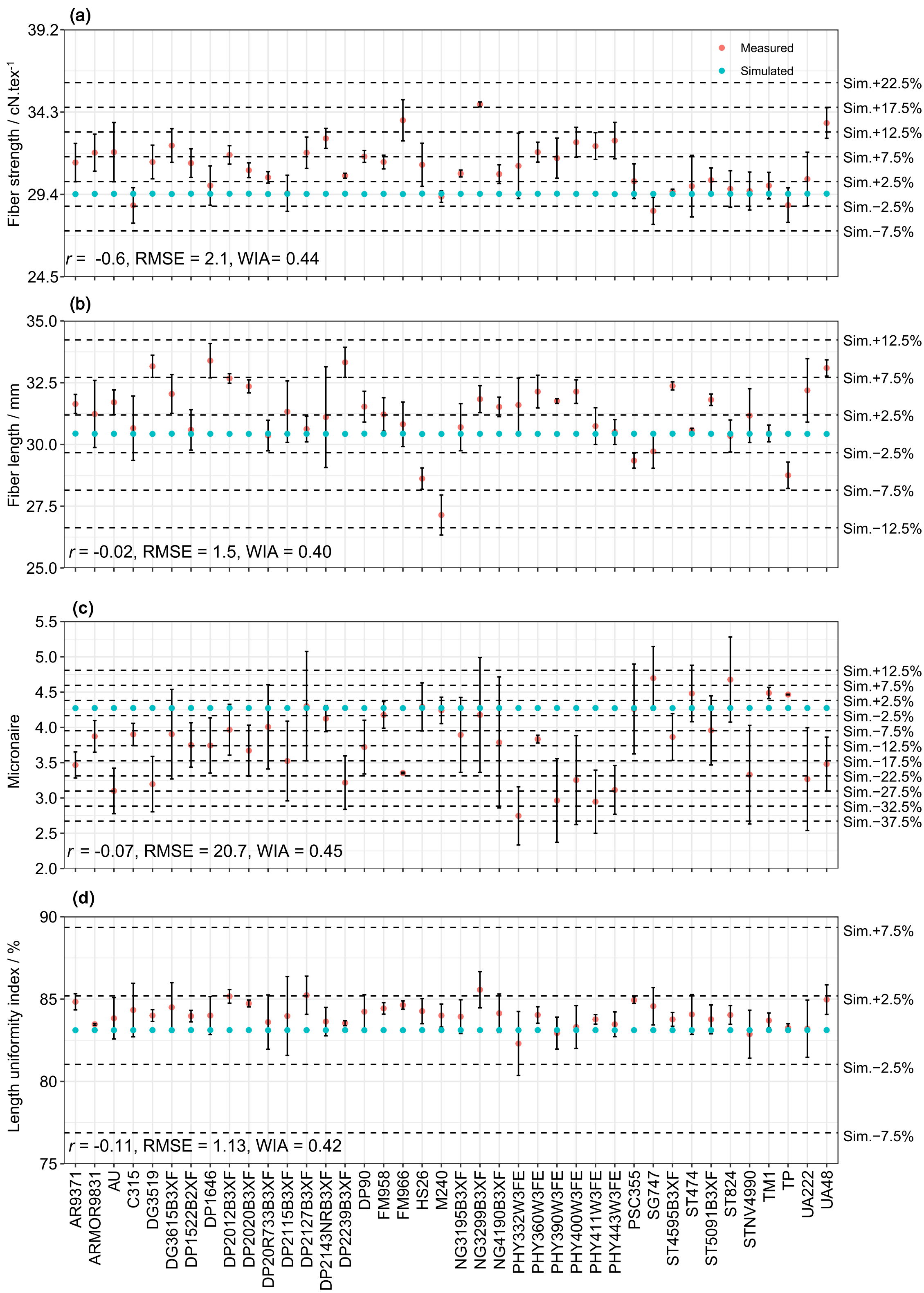

Fig. 2 Simulated and measured values for fiber strength (**a**), fiber length (**b**), micronaire (**c**), and length uniformity index (**d**). Horizontal dashed lines represent the simulated values ± 2.5% (Sim. +2.5%, Sim. −2.5%), ± 7.5% (Sim. +7.5%, Sim. −7.5%), ± 12.5% (Sim. +12.5%, Sim. −12.5%), ± 17.5% (Sim. +17.5%, Sim. −17.5%), and ± 22.5% (Sim. +22.5%, Sim. −22.5%). *RMSE* root mean square error, *r* Pearson correlation coefficient, *WIA* Willmott's index of agreement

Table 1 Cultivar-specific parameter values for fiber strength, fiber length, micronaire, and length uniformity index for the 40 cotton cultivars were estimated

Cultivar name	Fiber strength	Fiber length	Micronaire	Length uniformity index
AR9371	1.05	1.05	0.80	1.00
ARMOR9831	1.10	1.05	0.90	1.00
AU	1.10	1.05	0.75	1.00
C315	1.00	1.00	0.90	1.00
DG3519	1.05	1.10	0.75	1.00
DG3615B3XF	1.10	1.05	0.90	1.00
DP1522B2XF	1.05	1.00	0.90	1.00
DP1646	1.00	1.10	0.90	1.00
DP2012B3XF	1.10	1.05	0.95	1.00
DP2020B3XF	1.05	1.05	0.85	1.00
DP20R733B3XF	1.05	1.00	0.95	1.00
DP2115B3XF	1.00	1.05	0.8	1.00
DP2127B3XF	1.10	1.00	1.00	1.05
DP2143 NRB3XF	1.10	1.00	0.95	1.00
DP2239B3XF	1.05	1.10	0.75	1.00
DP90	1.10	1.05	0.85	1.00
FM958	1.05	1.05	1.00	1.00
FM966	1.15	1.00	0.80	1.00
HS26	1.05	0.95	1.00	1.00
M240	1.00	0.90	1.00	1.00
NG3195B3XF	1.05	1.00	0.90	1.00
NG3299B3XF	1.20	1.05	1.00	1.05
NG4190B3XF	1.05	1.05	0.90	1.00
PHY332 W3 FE	1.05	1.05	0.65	1.00
PHY360 W3 FE	1.10	1.05	0.90	1.00
PHY390 W3 FE	1.05	1.05	0.70	1.00
PHY400 W3 FE	1.10	1.05	0.75	1.00
PHY411 W3 FE	1.10	1.00	0.70	1.00
PHY443 W3 FE	1.10	1.00	0.75	1.00
PSC355	1.05	0.95	1.00	1.00
SG747	1.00	1.00	1.10	1.00
ST4595B3XF	1.00	1.05	0.90	1.00
ST474	1.00	1.00	1.05	1.00
ST5091B3XF	1.05	1.05	0.95	1.00
ST825	1.00	1.00	1.10	1.00
STNV4990	1.00	1.00	0.80	1.00
TM1	1.00	1.00	1.05	1.00
TP	1.00	0.95	1.05	1.00
UA222	1.05	1.05	0.75	1.00
UA48	1.15	1.10	0.80	1.00

parameters (Figs. 2 and 3). This highlights that the parameter estimation methodology efficiently improved fiber quality simulations.

Genetic algorithm-based cultivar parameter estimation

Cultivar-specific parameters were estimated using a GA-based optimization technique. The measured and simulated fiber quality values after incorporating the parameters estimated using the GA optimization technique into the GOSSYM model are shown in Fig. 4. A comparison of the parameters estimated using the method adopted in this study and the GA-based method is presented in Fig. 5. After incorporating parameters estimated using both methods into GOSSYM, the model equally improved the estimation ability. There were only very minor variations in the performance indices when comparing the efficiency of the methods, with the difference in the average of r and WIA between the methods being 0.025 and 0.015.

Discussion

Process-based crop models are essential for simulating crop growth and development under varying management and climatic conditions, analyzing the effectiveness of different cropping systems, optimizing agricultural productivity, etc. (Boote et al. 1996). These models help assess interactions between cultivars, environmental factors, and management practices, aiding resource management and evaluating environmental impacts. Cultivar-specific parameters are employed in these models to represent different cultivars and reflect their phenological and physiological differences, thereby accurately simulating crop growth and development (Jones et al. 2011). Identifying these parameters typically requires extensive experimental data across multiple environmental and management conditions, which is time-consuming and resource-intensive. With the rapid development of new cultivars, it becomes increasingly challenging to develop cultivar-specific parameters for each new cultivar (Mongiano et al. 2019). Despite these challenges, identifying these parameters is crucial for effectively utilizing crop models.

In crop models, cultivar-specific parameters can function as multipliers, modifiers of functional relationships, limits of variables, or arguments in equations. For example, in the GOSSYM model, parameters for potential

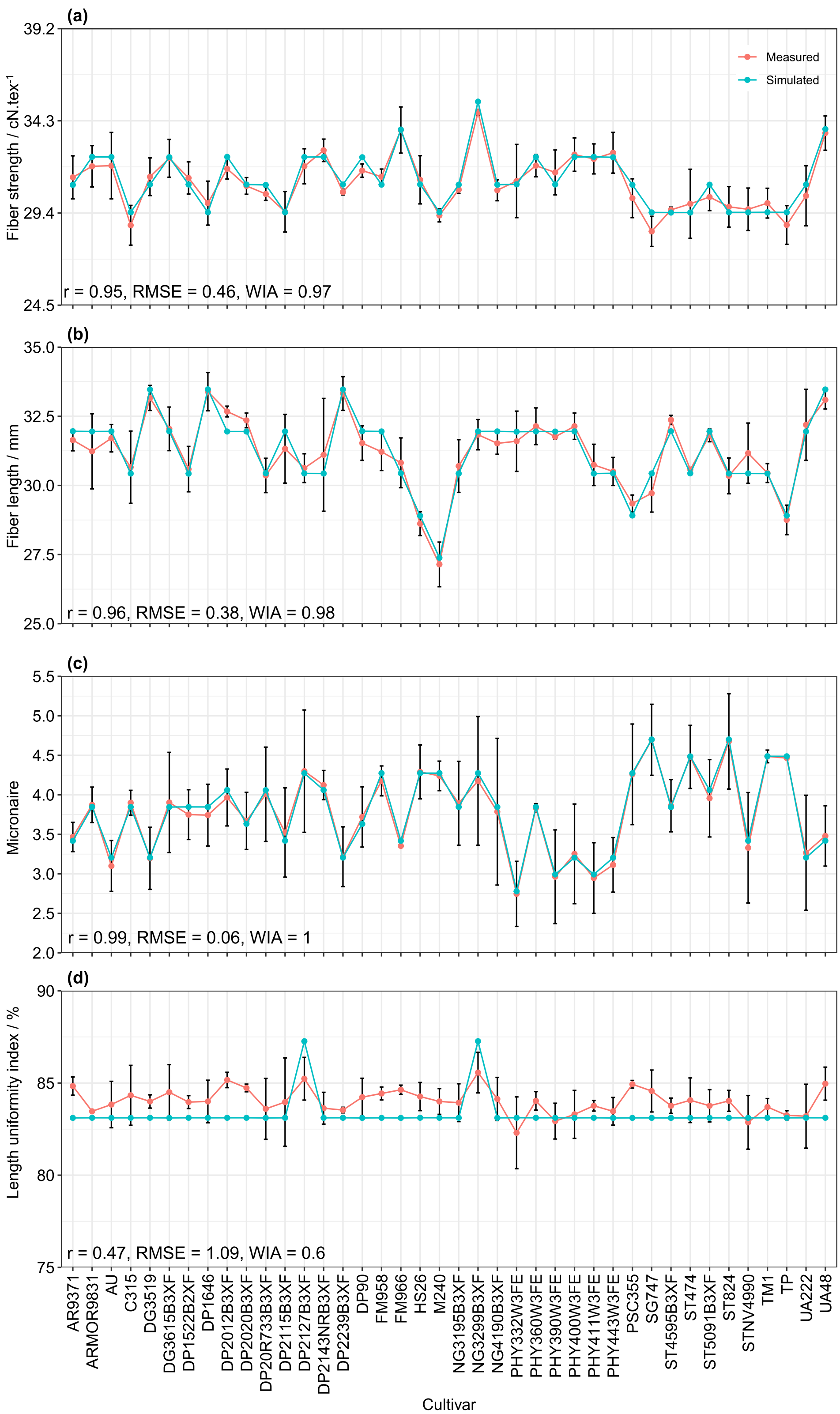

Fig. 3 Simulated and measured fiber strength (**a**), fiber length (**b**), micronaire (**c**), and length uniformity index (**d**) after incorporating cultivar-specific parameters in the fiber quality simulation module in the GOSSYM. *RMSE* root mean square error, *r* Pearson correlation coefficient, *WIA* Willmott's index of agreement

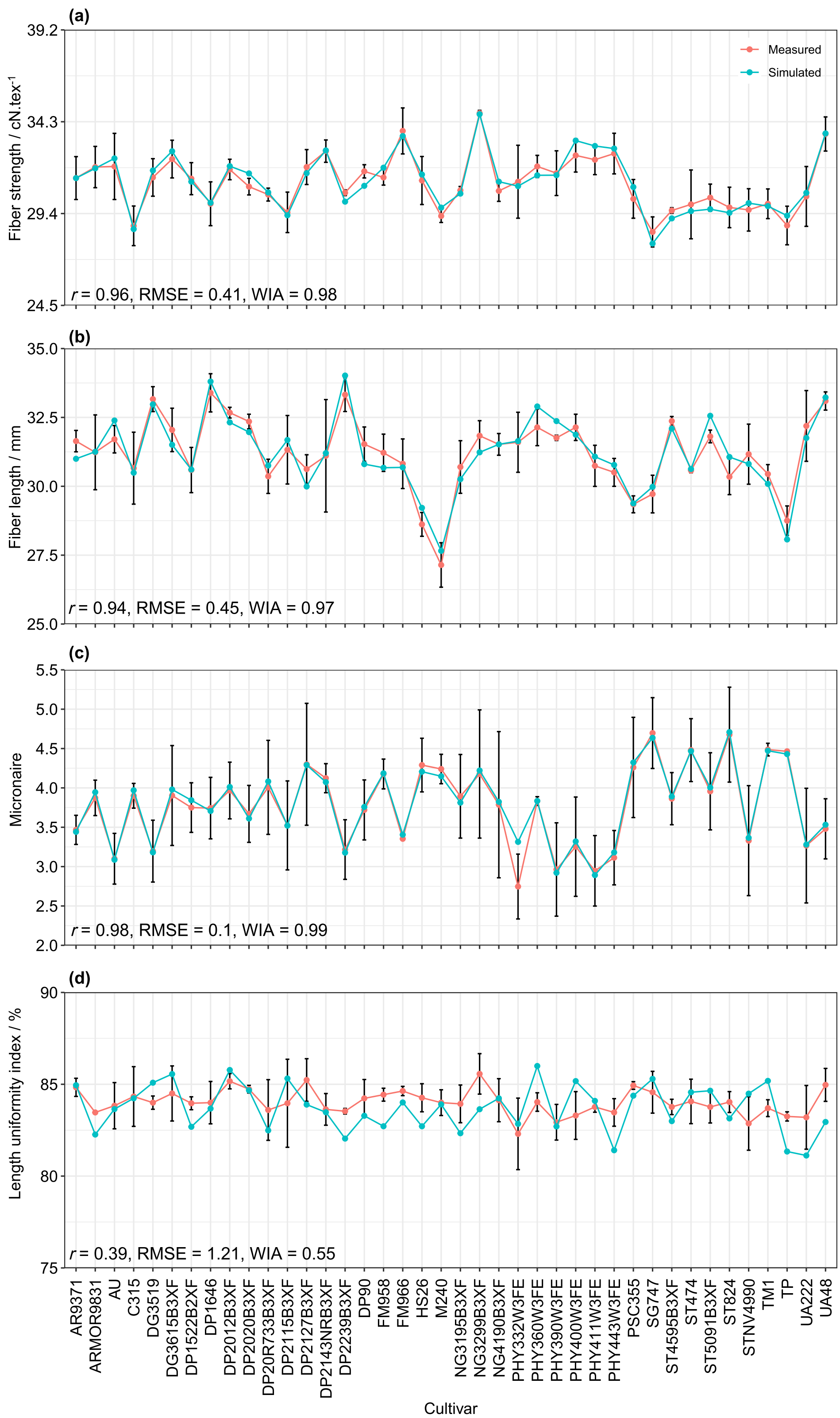

Fig. 4 Simulated and measured fiber strength (**a**), fiber length (**b**), micronaire (**c**), and length uniformity index (**d**) after incorporating cultivar-specific parameters identified using genetic algorithm-based optimization into GOSSYM. *RMSE* root mean square error, *r* Pearson correlation coefficient, *WIA* Willmott's index of agreement

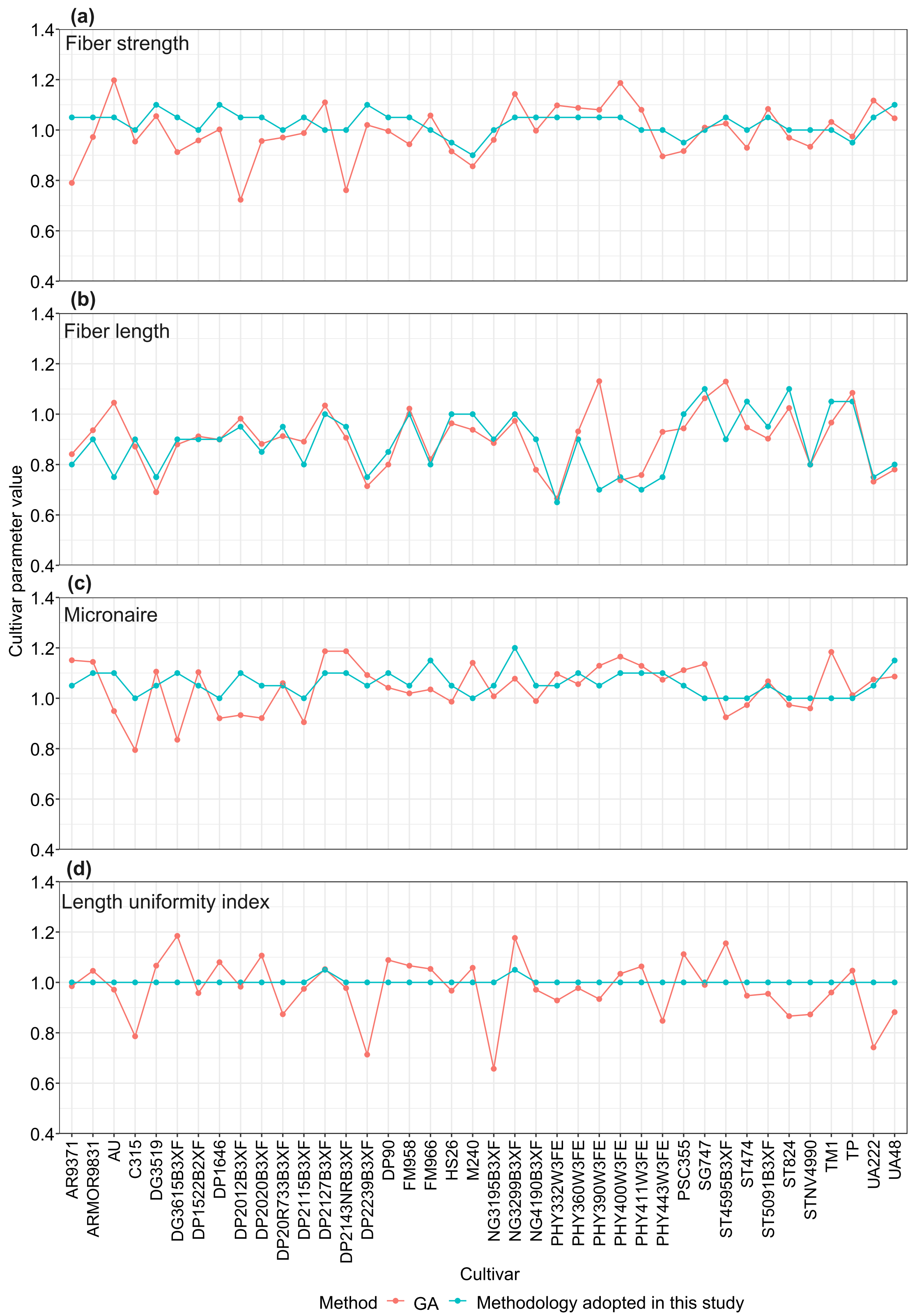

Fig. 5 Cultivar-specific parameters for each of the 40 cultivars for fiber strength (**a**), fiber length (**b**), micronaire (**c**), and length uniformity index (**d**) estimated using parameter estimation methodology adopted in this study and genetic algorithm (GA)-based parameter estimation method

cotton boll growth and stem growth act as limits, while parameters for the delay in fruiting node formation and cotton boll abscission act as arguments.

Cultivar-specific parameters in GOSSYM related to plant growth and development have already been determined and incorporated into GOSSYM for different cotton cultivars, including the 40 examined in this study (Beegum et al. 2024c). However, the cultivar-specific parameters related to fiber quality were not explored before. The cultivar-specific parameters in the fiber quality module act as multipliers, with the variety TM1 serving as a baseline for functional equations. By carrying out experiments using 40 upland cotton cultivars alongside TM1 under the same environmental and management conditions, the present study was able to isolate the impact of cultivars on fiber quality variability and understand the relative variation in fiber quality with TM1.

The results revealed significant variability in fiber quality among different cultivars, with micronaire showing the highest variability, followed by fiber strength and fiber length, and length uniformity index exhibiting the least variability (Fig. 1). Significant variability in fiber quality among cultivars has also been reported by Teodoro et al. (2019). Consistent with this study, other studies have also observed that micronaire and fiber strength display the greatest genetic variability when comparing fiber quality across cotton cultivars (Meredith et al. 1973; Snider et al. 2013). The observed negative correlation between micronaire and fiber strength can be attributed to fiber fineness and the effect of the bundle testing method used in HVI testing. Lower micronaire values indicate finer fibers, which result in a higher number of fibers within the bundle test (LaFave et al. 2023). During the fiber strength test, the increased fiber count allows for better force distribution, leading to higher measured fiber strength. Alternatively, fibers with higher micronaire values have thicker cell walls, reducing their flexibility and capability to withstand stress, thereby reducing their ability to bear loads without breaking (Bradow et al. 2000). The positive correlation between fiber strength and length observed in this study aligns with findings from other studies (Hussain et al. 2022). Understanding the impact of ginning on this relationship is essential, as stronger fibers resist breakage during ginning and retain their original length, while weaker fibers are more prone to breakage, reducing their length (Armijo et al. 2013). This difference in response to ginning amplifies the correlation between strength and length after the ginning, making it more pronounced compared with before ginning, when fibers retain their original length.

The study first analyzed the variability between simulated and measured cotton fiber quality without adding cultivar-specific parameters (Fig. 2). The model's predictions closely aligned with the TM1 variety, reflecting the specificity of the functional relationships developed from experiments on this cultivar. However, significant deviations were observed when applying the model to other cultivars, highlighting the need for cultivar-specific parameter estimation (Fig. 2). Given that cultivar-specific parameters for fiber quality act as multipliers and all governing functions in the fiber quality module of GOSSYM were developed based on the same cultivar (TM1), it was reasonable to group the cultivars based on their relative variability from the simulated values and identify the cultivar-specific parameters. Incorporating these parameters into the GOSSYM model significantly improved the accuracy of fiber quality predictions across all evaluated cultivars, as evidenced by increased *r* and WIA values and reduced RMSE (Figs. 2 and 3). The methodology focuses on reasonably estimating parameters by accounting for the crop model structure and functions rather than finding the most precise value to match observed fiber quality closely.

There are various existing calibration methods, such as GA (Pabico et al. 1999), sequential uncertainty fitting (Abbaspour et al. 2004), generalized likelihood uncertainty estimation (GLUE), parameter estimation and sensitivity testing (PEST), weighted least squares methods, optimization algorithms, evolutionary and bio-inspired algorithms (Zuniga et al. 2014), Bayesian approaches, and trial-and-error searches (Seidel et al. 2018). Studies have used these methods to estimate cultivar-specific parameters in crop models. Most of these methods often treat the model as a black box, transforming inputs into outputs without considering the model structure or the functional relevance of the parameters being calibrated (Zhao et al. 2014). These frequentist or Bayesian approaches can be used to estimate the cultivar-specific parameters for fiber quality. They could provide results similar to or better than the methodology adopted in this study, and the choice of method depends on user preference (Seidel et al. 2018). This study did not focus on comparing existing calibration methods, as that was not its primary aim. However, a GA-based parameter optimization was performed to compare the methodology used. GA was chosen randomly, as the study does not explicitly focus on comparing parameter estimation procedures. Analysis showed that both methods improved the fiber quality simulations.

In GA, the convergence criteria (population size and iterations) or early stopping criteria can be adjusted for more accuracy. For example, in the GA-based optimization carried out for this study, the early stopping criterion is triggered if the APE between the simulated and measured values falls below 2.5%, which can be varied by the user. The methodology adopted in this study facilitates simulating fiber quality within an error margin of ± 2.5%. Similar to GA, the methodology for determining cultivar-specific parameters based on grouping used in this study is also flexible, allowing users to adjust the error margin to suit their specific needs, ranging from broad agricultural assessments to more precise applications. The error margin is a choice of the model user, depending on the precision and accuracy required for the model's purpose (Boote et al. 1996).

Some general differences exist between the method adopted in this study and existing parameter calibration methods. Existing frequentist or Bayesian approaches do not inherently account for the model structure or functional equations where the parameters are used. Studies have shown that it is unwise to make adjustments without clearly understanding the parameters' relevance and the model structure, as it is essential to know how each cultivar-specific parameter is used in the mathematical functions within crop models because individual parameters can be connected to the model structure and there can be interactions between parameters (Wallach et al. 2001; Zhao et al. 2014). In contrast to existing calibration methods, the methodology adopted in this study grouped the cultivars based on the relative variation from simulated values and estimated cultivar-specific parameters for the groups. In this method, absolute variation is considered while grouping the cultivar, and cultivar-specific parameters are determined based on the relative differences in the group the cultivars belong to. This grouping approach allows for the assignment of the same cultivar-specific parameters to all cultivars within a group, enabling a structured crop database. For example, GOSSYM can identify a particular cultivar, determine its group, and assign the corresponding parameters for specific functions. Existing approaches do not perform this grouping during parameter estimation. Each cultivar has different values as opposed to the group approach (Table 1). Even if the parameter variation would have only resulted in minimal variation between the observed and simulated values, each cultivar will have one parameter value, which the user can decide if they would like to group based on the similarity or have independent parameter values for each cultivar. Most calibration methods calibrate the cultivar-specific parameters of a cultivar at a time; the methodology adopted in this study identified the cultivar-specific parameters of all the cultivars currently growing simultaneously. Only some studies have looked into estimating the cultivar-specific parameters collectively by accounting for the relative variability in the growth and development of the cultivars.

In the present study, the cultivar-specific parameters for 40 cultivars are estimated, evaluated, and incorporated into the GOSSYM model. From a practical standpoint, accurately predicting fiber quality for different cultivars using the GOSSYM model holds significant value for the cotton producers and industry. The model can be used to predict how fiber quality responds to varying environmental conditions and management practices (planting date, amount and timing of irrigation, fertilizer application, etc.), and can help optimize these factors to achieve superior fiber quality traits.

This study was the first detailed evaluation of the fiber quality module in the cotton simulation model, GOSSYM. It examined how well TM1 performed, considering that the model development was based on TM1. Additionally, the study assessed how well GOSSYM simulated fiber quality for cultivars other than TM1. Since this study involved comparisons across 40 different cultivars, an extensive experimental study was conducted to systematically evaluate cultivar-specific variation in fiber quality, followed by the estimation of cultivar-specific parameters for all cultivars together. This study helped establish that the parameter estimation method, based on the relative variation between simulated and observed fiber quality values, provided accurate estimates. Since the method proved promising, experiments such as those conducted in this study are not required if the GOSSYM model is to be used for fiber quality estimation of another cultivar that is not among the 40 cultivars. Instead, the cultivar-specific parameters for a new cultivar can be estimated through a straightforward process. The first step is to obtain the quality traits corresponding to any environment and management conditions for the new cultivar. The next step is to run GOSSYM simulations using the same environmental and management conditions but applying the cultivar-specific parameters corresponding to TM1. This can be quickly done by adding the name of the cultivar (in this case, TM1) from the cultivar list in the GOSSYM model. The simulated quality can then be compared with the measured quality of the new cultivar of interest. The absolute difference can be used to determine which band the cultivar falls in, followed by the determination of the cultivar-specific parameters as per the grouping method.

Not all cultivars included in this study are currently commercially grown in the USA, and the study is limited to upland cotton. However, as discussed above, cultivar-specific parameters can be developed for any cultivar of interest, including Pima cotton cultivars. In addition, the fiber quality data used in this study were obtained from hand-picked cotton samples. While hand-picking minimizes fiber damage and contamination, the results may still be influenced by ginning methods and HVI measurement procedures

(Delhom et al. 2020). The accuracy and consistency of HVI measurements can vary depending on instrument calibration and operational conditions. Therefore, the findings of this study may not fully represent fiber quality outcomes under different harvesting and ginning practices. While this study demonstrates the improved accuracy of the fiber quality simulation in the GOSSYM model with the developed cultivar-specific parameters, future studies should include additional validations by comparing the fiber quality of the cultivars in varying environmental and management conditions to further validate the cultivar-specific parameter estimation methodology presented in this study.

Conclusions

This study evaluated the capability of the GOSSYM model to simulate fiber quality by comparing the model-simulated and measured fiber quality values for different cotton cultivars. Cultivar-specific parameters were estimated to account for the cultivar-related variability in the model results. The parameter estimation methodology adopted, and the estimated cultivar-specific parameters improved the simulation capabilities of the model. The proposed methodology can be easily adapted to incorporate new cultivars, ensuring the model remains applicable, especially given the frequent development of new cultivars each year. Accurately simulating fiber quality is highly beneficial for agricultural management, as it helps simulate cultivar-environment-management interactions and their influence on fiber quality.

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Authors' contributions
Beegum S: Conceptualization, methodology, software, formal analysis, writing-original draft; Hassan MA: Software, formal analysis, writing- original draft; Reddy KN: Supervision, review, and editing; Reddy V: Supervision, review, and editing; Reddy KR: Conceptualization, methodology, software, experiments, data acquisition, writing-reviewing and editing preparation. All authors read and approved the final manuscript.

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Data availability
Data used in this study are available within the article. The latest version of the GOSSYM source code with the fiber quality module can be accessed from https://github.com/USDA-ARS-ACSL/GOSSYM-2DSOIL. There are no restrictions for accessing the source code.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Competing interests
The authors declare that they have no competing interests.

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