

Article

Evaluating the Performance of the STEMMUS-SCOPE Model to Simulate SIF and GPP Under Drought Stress Using Tower-Based Observations of Maize

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Highlights

What are the main findings?

- The STEMMUS-SCOPE model demonstrates higher accuracy than the SCOPE model in simulating SIF and GPP under drought stress.

What is the implication of the main finding?

- The simulation performance of STEMMUS-SCOPE under drought stress is validated;
- The potential of the STEMMUS-SCOPE model to investigate the SIF-GPP relationship under drought stress is demonstrated.



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Abstract

With advancements in solar-induced fluorescence (SIF) observation technology and the evolution of vegetation radiative transfer models, SIF signals can now be more effectively interpreted and leveraged from a mechanistic perspective. This, in turn, facilitates a deeper understanding of the mechanistic link between SIF and photosynthesis. Considering the impact of water stress on terrestrial ecosystems, this paper simulated SIF and gross primary productivity (GPP) values using the STEMMUS-SCOPE model at half-hour scales from 2017 to 2023 at the Daman site. The simulation results were compared and validated against flux tower observations and SCOPE model outputs. Taking advantage of irrigation events in the semi-arid irrigated farmland, we assessed the accuracy of STEMMUS-SCOPE in simulating SIF and GPP under drought stress, as well as its capability to quantitatively analyze the impacts of water stress on SIF and GPP. The results show that the accuracy of the SIF and GPP values simulated by the STEMMUS-SCOPE model is higher than that of the SCOPE model. The averaged R^2 and RMSE between the SIF simulated by STEMMUS-SCOPE model and the observed SIF values are 0.66 and $0.29 \text{ mW m}^{-2} \text{ nm}^{-1}$, and the averaged R^2 and RMSE between the GPP simulated by the STEMMUS-SCOPE model and the observed GPP values from 2017 to 2023 are 0.88 and $4.93 \text{ } \mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$, respectively. Especially under relatively drought conditions, the R^2 between the SIF simulated values and observed values is 0.84, and the R^2 between the GPP simulated values and observed values is 0.96. By further combining soil moisture content (SMC) and canopy conductance (G_s) analyses, we found that the response of the STEMMUS-SCOPE simulations under water stress was consistent with previous findings on the impacts of water deficits, thereby confirming the model's reliability for drought conditions. Under drought stress, the decline in fluorescence emission efficiency (Φ_F) with decreasing G_s and SMC was smaller than that of the light use

efficiency (LUE). Therefore, the STEMMUS-SCOPE model is promising for investigating the SIF–GPP relationship under drought stress.

Keywords: STEMMUS-SCOPE; drought stress; solar-induced chlorophyll fluorescence (SIF); gross primary productivity (GPP)

1. Introduction

In the photosynthesis of vegetation, chlorophyll molecules absorb photosynthetically active radiation (PAR) and release it through three energy dissipation pathways: photosynthetic carbon fixation, heat dissipation, and chlorophyll fluorescence, which is the most important biochemical process in terrestrial ecosystems [1]. Numerous studies have demonstrated that solar-induced chlorophyll fluorescence (SIF) and gross primary productivity (GPP) showed a good correlation at various spatial scales of leaves, individuals, canopies, and regions [2,3]. The light use efficiency (LUE) model proposed by Monteith (1972) simplifies the photosynthetic process by expressing GPP as the product of absorbed photosynthetically active radiation (APAR) and the LUE for CO₂ fixation [4]. Chlorophyll fluorescence originates from photochemical reactions and is simultaneously driven by APAR. Fluorescence emission efficiency (ΦF) is the fluorescence quantum efficiency at the photosystem level, and f_{esc} is the SIF escape probability from the photosystem to the canopy level (the ratio of canopy SIF in a certain direction to the total SIF emitted by the photosystem); the relationship between SIF and GPP can be linked through the ratio between LUE and ΦF .

In recent years, numerous studies have demonstrated that SIF is a novel approach for detecting vegetation photosynthesis and tracking photosynthetic dynamics owing to the physiological information it contains [5,6]. Especially under stress conditions or in evergreen ecosystems with little variation in vegetation structure, SIF can exhibit a stronger correlation between GPP and APAR [7–9].

In the observation and simulation of terrestrial ecosystems, substantial uncertainty still exists in the coupling relationship between SIF and photosynthesis. This uncertainty mainly arises from the influences of vegetation types and environmental factors, such as light stress, temperature stress, and drought stress, thereby posing challenges to the accurate estimation of photosynthesis [3,10–14]. The vertical heterogeneity of light distribution within plant canopies affects both the energy source for photosynthesis and spectral fluorescence responses. Previous studies have employed various modeling approaches to elucidate the effects of light conditions on leaf physiological processes [15,16]. Under temperature stress, low temperatures impair plant photosynthesis by altering key biochemical processes [17]. Numerous studies have demonstrated that the photosynthetic rate of high-latitude evergreen coniferous forests decreases significantly due to low winter temperatures [13,18]. By incorporating the maximum photochemical efficiency of photosystem II, Chen et al. developed a model based on the light-response mechanism (MLR) model that improves the accuracy of GPP estimation [19]. Numerous studies have demonstrated that drought exerts a significant influence on both ecosystem stability and productivity [20–22]. In response to drought stress, plant mechanisms are generally classified into stomatal regulation and non-stomatal regulation. When water stress occurs, plants reduce the rate of photosynthesis by adjusting the opening and closing of the stomata and maintain high leaf water potential or high relative water content of the leaves by controlling the opening and closing of the stomata to avoid tissue dehydration [23–25]. As drought stress intensifies, plant regulatory mechanisms shift from stomatal to non-stomatal regulation, leading to decreases in chlorophyll content, reductions in SIF, and leaf damage. It has been suggested that the decline in GPP-to-SIF ratios with reduced water availability may

be associated with stomatal responses [26]. Therefore, investigating the effects of drought stress on photosynthetic products and their interrelationships is of great importance.

Under drought stress, the observed relationship between SIF and GPP exhibited a nonlinear pattern, with increasing drought stress, the ratio of GPP to SIF declined. Compared with normalized difference vegetation index (NDVI) and enhanced vegetation index (EVI), SIF is more sensitive to drought and better captures vegetation dynamics driven by water and thermal variations. In addition, compared with LUE-based estimates, SIF-based GPP estimations exhibited a stronger correlation with observed GPP [27–30]. SIF exhibited more consistent declines with GPP losses induced by drought than APAR estimations during the drought period in space and time, where APAR had obvious lagged responses compared with SIF, especially in evergreen broadleaf forest land [31]. However, the emission mechanism of SIF is complex, and considerable uncertainties remain in its interpretation and analysis. Therefore, a mechanistic understanding of the interactions between SIF and vegetation structure, along with an examination of the main factors influencing SIF emission, will help to elucidate the relationships between SIF, photosynthesis, and biomass.

The SCOPE (Soil Canopy Observation of Photosynthesis and Energy) model is one of the most widely used models for the simulation of SIF [32]. Based on the energy balance, the model integrates the radiative transfer model and the photosynthesis model, which is a virtual laboratory for studies on surface energy balance, and SIF–photosynthesis. However, the SCOPE model does not track the moisture changes in soil and vegetation, nor does it parameterize the effects of soil moisture changes on photosynthesis or stomatal parameters, so the effects of soil moisture are only apparent when soil moisture affects the optical and thermal signals of vegetation [33]. Therefore, under drought and extreme heat conditions, the simulation performance of the SCOPE model is constrained. In 2019, Bayat et al. [33] incorporated the soil–plant–atmosphere continuum (SPAC) model into SCOPE, developing the SCOPE_SM model, which limited the maximum carboxylation rate by calculating the water stress coefficient of soil moisture, and its feasibility was evaluated through simulations at a grassland site. The results demonstrated that the model responds well to water stress; however, it neglects the dynamic distribution of vegetation roots. In 2021, Wang et al. developed STEMMUS-SCOPE by integrating the processes of photosynthesis, SIF, and soil water–heat transfer into the SPAC system [34]. This integration was achieved through the incorporation of a one-dimensional root growth model and an impedance scheme connecting the soil, roots, leaves, and atmosphere. Experimental results from maize and grassland sites demonstrated that, compared with the SCOPE and SCOPE_SM models, STEMMUS-SCOPE achieved higher simulation accuracy for water, heat, and carbon fluxes. These findings indicate that by coupling soil water–heat transport with dynamic root growth, the model can more accurately simulate ecosystem functions [34,35]. The advantage of the STEMMUS-SCOPE model lies in its coupling of a leaf-level photosynthesis model, a canopy radiative transfer model, and the soil–plant–atmosphere continuum (SPAC) model. This integration enables a quantitative analysis of the sensitivity of simulated SIF and GPP to different input parameters. By accounting for and separating the influences of physiological and non-physiological factors on SIF and GPP, the model provides a clearer understanding of the relationship between SIF and GPP, thereby filling the current research gap in quantitatively assessing how water stress affects this relationship. However, validation using long-term observational data is still lacking.

ChinaSpec is a continuous SIF ground observation network based on flux stations in the Chinese mainland [36]. Among them, the long-time flux and SIF observation data of the Daman site in recent years provide a good basis for the validation of the STEMMUS-SCOPE model in irrigated farmland within semi-arid areas. Based on this dataset, we employed flux, meteorological data, and vegetation parameters from the Daman site during 2017–2023, together with measured soil water content to evaluate the performance

of STEMMUS-SCOPE model in simulating SIF and GPP under drought stress and further evaluated the impact of crop drought stress on SIF, GPP at the Daman site. This study emphasizes the validation and evaluation of the STEMMUS-SCOPE model based on multi-year continuous observational data, along with mechanistic interpretations of its responses to SIF and GPP under drought stress, highlighting its important role in quantitatively assessing the effects of drought stress on SIF and GPP.

2. Materials and Methods

2.1. Study Area

The Daman site is located on flat terrain about 8 km southeast of Zhangye City, Gansu Province ($38^{\circ}51'20''\text{N}$, $100^{\circ}22'20''\text{E}$). It belongs to the temperate continental climate, with an average annual temperature of 8°C , an annual sunshine of 3000–3600 h, and an annual precipitation of about 300 mm. The observed feature type of this flux station belongs to crops, the type of which is maize, and there is no special irrigation and fertilization control [37]. The station is equipped with flux, meteorological, hydrological, and SIF observation systems, and the Daman site Vegetation Fluorescence Automatic Observation System has been observing and accumulating canopy spectral data for 7 consecutive years since 2017. In this article, the Daman site from June to September of each year from 2017 to 2023 was used for analysis. The CO_2 exchange between vegetation and the atmosphere was measured by a CO_2 flux observation system based on the eddy covariance (EC) technique [38]. The flux measurement system is located on a 5 m high platform on the flux tower in the crop area of the Daman site. The flux observation system consists of a high-frequency open-circuit infrared gas analyzer (IRGA) (Li-7500, Li-Cor, Lincoln, NE, USA) and a three dimensional sonic anemometer that measures the high-frequency instantaneous wind speed component and sound temperature. Turbulent flux data were sampled at a frequency of 10 Hz. The raw flux data collected by the flux measurement system (CR5000 at YK and GT, Campbell Scientific Inc., Logan, UT, USA; 27) is stored through a data logger and processed to obtain a net ecosystem exchange (NEE) of CO_2 . GPP is estimated from the NEE and ecological respiration (Re) measured by the equation $\text{GPP} = \text{Re} - \text{NEE}$.

The automatic weather station (AWS) system consists of a meteorological gradient observation device capable of observing environmental and meteorological variables, including PAR, air temperature (T_a), air pressure (Press), and air humidity (RH). The system is located on an EC flux observation tower [37]. All observations were processed to a 30 min resolution after removing outliers (more than 3 standard deviations) and then integrated into a daily mean [39].

An automatic fluorescence observation system of vegetation (Bergsun Inc., Beijing, China) is also erected on the flux tower, and the automatic fluorescence observation system adopts a QE65Pro spectrometer (QE65pro; Ocean Optics, Dunedin, FL, USA), with a spectral resolution of 0.31 nm, a sampling interval of 0.155 nm, and a spectral range of 650–815 nm. The upward and downward radiation observation uses a bifurcated optical fiber to connect to the spectrometer in a dual-field angle measurement method, a bare optical fiber observes the reflected radiation of ground objects at an inclination angle of 25° , and the other cosine probe measures the incident solar radiation vertically towards the zenith direction, and the “sandwich” sampling method is used to observe the downward solar radiation and upward canopy radiation through the electronic shutter and control software.

This study used the solar-induced chlorophyll fluorescence calculated by the fluorescence automatic observation system through the 3FLD algorithm. The 3FLD algorithm assumes a linear variation in fluorescence and reflectance within the absorption line, and this method has been shown to be more robust and accurate than the FLD and iFLD meth-

ods [15]. Therefore, in this study, the 3FLD algorithm was used to retrieve the SIF at the O₂-A band for the accuracy evaluation of the STEMMUS-SCOPE model.

In this study, half-hour-scale meteorological data observed at the tower base were used as inputs for the STEMMUS-SCOPE model to obtain half-hour-scale outputs of SIF and GPP. The half-hour-scale tower-based observations of SIF and GPP were used to compare with the corresponding outputs simulated by the STEMMUS-SCOPE model.

In this article, the fPAR was estimated based on the vegetation index. Several research results have shown that the NDVI is a good proxy for fPAR from a fixed perspective [40,41]. We use the wide dynamic range vegetation index (WDRVI), which has been shown to show a good linear correlation with fPAR [42]. WDRVI is defined as:

$$WDRVI = \frac{\alpha \cdot Ref_{800} - Ref_{680}}{\alpha \cdot Ref_{800} + Ref_{680}} \quad (1)$$

where Ref_{800} and Ref_{680} are the reflectance at 800 nm and 680 nm, respectively. α is the weight coefficient, which is set to a fixed value of 0.1, and the existing linear model is used to estimate the fPAR based on WDRVI:

$$fPAR = 0.516 \cdot WDRVI + 0.726 \quad (2)$$

2.2. STEMMUS-SCOPE Model

The STEMMUS-SCOPE model is an integrated soil–plant model that integrates the SCOPE model and STEMMUS model. The SCOPE model can predict leaf-to-canopy reflectance and SIF spectra, photosynthesis, and evapotranspiration, while the STEMMUS model can simulate root dynamic growth and root water uptake (RWU), addressing the limitation of the SCOPE model that does not account for root water uptake and the compensation mechanism among roots. By coupling the two, the model is able to link soil water and nutrient dynamics with photosynthetic and stomatal behaviors, allowing water stress to be considered before it manifests in vegetation optical or thermal signals [33]. This coupling enhances the model's capability to predict vegetation status under drought conditions without being hindered. The integrated model links below-ground ecophysiological and hydrological processes with leaf- and canopy-level photosynthesis and SIF. Consequently, it can serve as a forward simulator of SIF and VNIR–SWIR–TIR spectra while also constraining the coupled processes of water, energy, and carbon fluxes [43].

The STEMMUS-SCOPE model uses the STEMMUS module to simulate the initial soil moisture profile based on soil initial conditions. From this, a water stress factor is calculated, which is used in the Biochemical module of SCOPE to constrain the maximum carboxylation rate (V_{cmax}) and to compute the ΦF as well as the net photosynthetic rates (A_n) at the leaf and canopy levels. The GPP is subsequently derived from the net photosynthetic rate. Through the Fluspect (leaf fluorescence), RTMo (canopy optical radiative transfer), Ebal (energy balance), RTMt (canopy thermal radiative transfer), and RTMf (canopy fluorescence radiative transfer) modules of SCOPE, the model simulates various fluxes and variables, including energy fluxes (net radiation, R_n ; latent heat flux, LE ; sensible heat flux, H ; and soil heat flux, G), transpiration (T), soil surface temperature (T_s), and SIF. The STEMMUS module then uses the outputs and boundary conditions from SCOPE to compute RWU and other hydrological variables. Through iterative coupling, the STEMMUS-SCOPE model is able to calculate the leaf water potential (LWP), which reflects the plant's water status, based on soil moisture and soil hydraulic resistance. In this study, a time step of 30 min was adopted.

An example scatter plot of SIF and GPP simulated by the STEMMUS-SCOPE model is shown below (see Figure 1), which is during the DOY of 180–190 (no irrigation, no drought) in 2020 and with setting the cab to 50, the LAI to 3, and the V_{cmax} to 80. According to

the original average soil moisture content of each layer, the input measured soil moisture content is changed, and the lower the soil moisture content is, the lower the slope of the SIF-GPP linear regression line, which gradually presents a nonlinear state.

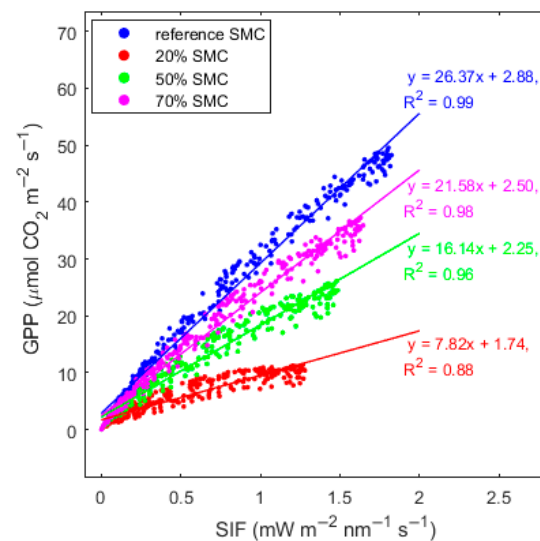


Figure 1. The relationship between SIF and GPP under different soil moisture contents.

In this study, the input parameters of the STEMMUS-SCOPE model were obtained through field measurement, reference to the literature, and inversion, and the key input parameters are listed in the Table 1. Among them, the meteorology parameters are obtained by actual measurement. The MERIS Terrestrial Chlorophyll Index (MTCI) was used to retrieve Cab. MTCI exhibits high accuracy in estimating Cab ($R^2 = 0.73$, RMSE = 11.16) and maintains good sensitivity even during the high-chlorophyll-concentration stage in maize [44,45]. The multi-angular NDVI (MAVI) was used to retrieve LAI, with the aim of reducing the effects of soil background and saturation on LAI estimation. The MAVI achieves high accuracy in LAI retrieval ($R^2 = 0.945$, RMSE = 0.345) [46]. The leaf inclination was spherical, which has been shown to be a good approximation in crops such as maize [47,48].

Table 1. List of parameters and values used in this study.

Parameter	Description	Symbol	Unit	Value/Source
Leaf	Leaf chlorophyll content	Cab	$\mu\text{g cm}^{-2}$	Inversion
	Leaf carotenoid content	Cca	$\mu\text{g cm}^{-2}$	0.25 Cab
	Leaf dry matter content	Cdm	g cm^{-1}	0.012
	Senescent material content	Cs	/	0
	Ball–Berry stomatal conductance parameter	m	/	6.8, 10
Canopy	Leaf area index	LAI	$\text{m}^2 \text{m}^{-2}$	Inversion
	Leaf inclination distribution function	LIDF _a	/	−0.35
	Leaf inclination distribution function	LIDF _b	/	−0.15
	Maximum carboxylation rate	Vcmax		60–80
Meteorology	Incoming shortwave radiation	Rin	W m^{-2}	Measurement
	Air temperature	Ta	$^{\circ}\text{C}$	Measurement
	Wind speed	u	m s^{-1}	Measurement
	Air vapor pressure	ea	hPa	Measurement
	CO ₂ concentration	Ca	$\mu\text{mol m}^{-3}$	Measurement
	Incoming longwave radiation	Rli	W m^{-2}	Measurement
	Relative humidity	RH	%	Measurement
	Relative humidity	VPD	hPa	Measurement
	Air pressure	P	hPa	Measurement
	Soil moisture content	SMC	%	Measurement
	precipitation	Rain	mm	Measurement

2.3. Calculation of Canopy Conductance

Canopy conductance is the degree of stomatal opening at the canopy scale, is the main factor affecting the photosynthesis and respiration of plants, and can also be used as a comprehensive basis for determining the overall impact of drought; we use the daily mean canopy conductance (G_s) as a comprehensive parameter reflecting the drought stress experienced by plants. G_s can be calculated using the vorticity flux data to extrapolate the Penman–Monteith equation [4,49]:

$$G_s = \frac{\gamma \cdot g_a \cdot LE}{\Delta \cdot (R_n - G) + \rho \cdot c_p \cdot g_a \cdot VPD_a - (\Delta + \gamma) \cdot LE} \quad (3)$$

Among them, γ is the humidity constant (kPa K^{-1}), which is related to atmospheric pressure; g_a is the aerodynamic conductivity (ms^{-1}); Δ is the slope of the saturated water vapor pressure difference curve (kPa K^{-1}); LE is the latent heat flux (W m^{-2}); R_n is the net radiation (W m^{-2}); and G is the soil heat flux below the canopy (W m^{-2}). In addition, ρ is the density of the air (kg m^{-3}), which depends on temperature, pressure, and humidity; c_p is the specific heat capacity of air ($\text{kJ kg}^{-1} \text{K}^{-1}$); and VPD_a is the atmospheric vapor pressure difference, defined as the difference between the atmospheric vapor pressure at ambient temperature and the actual vapor pressure [50]. In this equation, the unit of G_s is m s^{-1} , and these units can be converted to $\text{mol m}^{-2} \text{s}^{-1}$ using ideal gas quantification [51]. g_a can be calculated by the following formula:

$$g_a = \frac{k^2 \cdot u}{\left[\ln\left(\frac{z-d+zH}{zH}\right) + \psi_H \right] \cdot \left[\ln\left(\frac{z-d+zM}{zM}\right) + \psi_M \right]} \quad (4)$$

where z is the anemometer wind speed (m); d is the zero plane displacement (m); and zH and zM represent the roughness length (m) of the sensible thermal momentum, respectively. ψ_H and ψ_M represent the stability correction factors for heat and momentum, respectively. k is the von Karman constant; and u is the wind speed at altitude z . Both d and zM can be estimated as a function of canopy height, with h and zH as a function of zM (usually $d = 0.67 h$, $zM = 0.67 h$, $zH = 0.2 zM$).

2.4. Irrigation and Changes in Soil Moisture in 2023

The irrigation management at the Daman site provides an opportunity to quantify the performance of the STEMMUS-SCOPE model in SIF and GPP under drought stress. According to the irrigation and precipitation data at the Daman site, we can select the period of drastic change in soil water content, compare the differences between the SCOPE model and the STEMMUS-SCOPE model before and after the drastic change in soil water content, and evaluate the simulated value caused by the STEMMUS-SCOPE model for tracking the change in soil water content. Due to the obvious irrigation events in 2023, the period between the second and third irrigation, which is the mid-growth stage of maize, was chosen as the representative period for evaluating the performance of the STEMMUS-SCOPE model in different soil moisture conditions. According to the half-hour-scale changes in soil water content and precipitation in 2023 (see Figure 2), it can be inferred that the irrigation events in 2023 occurred at the time points of 156, 205, and 240 DOY.

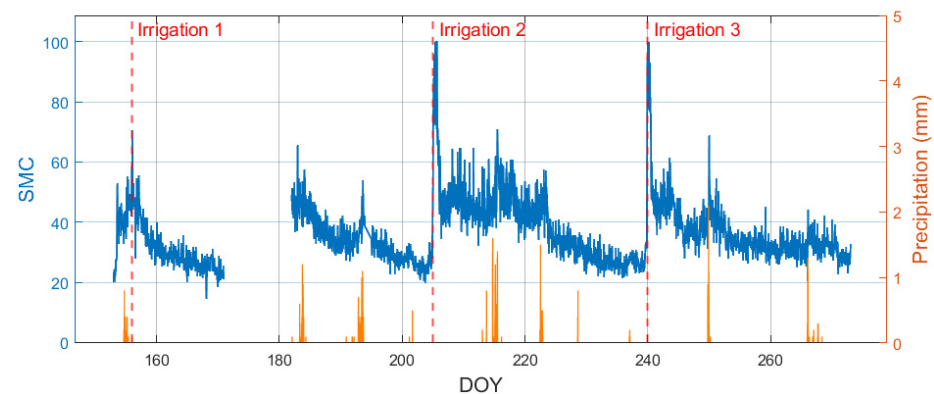


Figure 2. Soil volume moisture content and rainfall during the growth period of maize in 2023.

Previous studies have shown that crops in the study area experience significant drought stress when soil moisture falls below 20% [52,53]. However, the study area is located in a typical irrigated farmland in a semi-arid region of China, where a well-developed irrigation infrastructure and advanced agricultural management practices ensure that soil moisture is carefully regulated within an optimal range for crop growth. As a result, soil moisture rarely drops below 20%. When soil moisture approaches the stress threshold, irrigation is usually applied promptly to prevent severe water deficits. Therefore, soil moisture exhibits pronounced fluctuations before and after irrigation. Based on this pattern, we selected the soil moisture conditions during the three days before irrigation as the standard for defining drought. Periods with soil moisture below 30% or canopy conductance below 0.3 were classified as relatively dry conditions, whereas periods after irrigation characterized by a rapid increase in soil moisture were defined as relatively non-drought conditions.

3. Results

3.1. Comparison of the Accuracy of the STEMMUS-SCOPE and SCOPE Models for GPP and SIF Simulation

Based on the half-hour-scale SIF and GPP data of simulations and observations, we analyzed the accuracy of the simulated SIF and GPP values of the STEMMUS-SCOPE model from 2017 to 2023 (see Table 2). Across all years, both models showed reasonable agreement with tower-based observations, but the STEMMUS-SCOPE model consistently achieved slightly higher accuracy. For SIF, the R^2 of the STEMMUS-SCOPE model ranged from 0.46 to 0.83, and the RMSE ranged from 0.21 to 0.35 $\text{mW} \cdot \text{m}^{-2} \cdot \text{nm}^{-1}$, comparable to or slightly better than those of the SCOPE model. For GPP, the STEMMUS-SCOPE model exhibited clear improvements, with R^2 values ranging from 0.80 to 0.93 and RMSE values from 3.14 to 5.93 $\mu\text{mol CO}_2 \cdot \text{m}^{-2} \cdot \text{s}^{-1}$, outperforming the SCOPE model ($R^2 = 0.71\text{--}0.88$, $\text{RMSE} = 4.62\text{--}7.64 \mu\text{mol CO}_2 \cdot \text{m}^{-2} \cdot \text{s}^{-1}$). The results indicate that the STEMMUS-SCOPE model provides more accurate and stable simulations of both SIF and GPP, particularly for GPP, reflecting the benefit of incorporating soil moisture dynamics and root water uptake processes. Take 2023 as an example, for the STEMMUS-SCOPE model, the R^2 between the observed SIF and the simulated SIF was 0.79, with an RMSE of 0.19 $\text{mW} \cdot \text{m}^{-2} \cdot \text{nm}^{-1}$, and the R^2 between the observed GPP and the simulated GPP was 0.93, with an RMSE of 3.14 $\mu\text{mol CO}_2 \cdot \text{m}^{-2} \cdot \text{s}^{-1}$. For the SCOPE model, the R^2 between the observed SIF and simulated SIF was 0.77, with an RMSE of 0.20 $\text{mW} \cdot \text{m}^{-2} \cdot \text{nm}^{-1}$, and the R^2 between the observed GPP and simulated GPP was 0.88, with an RMSE of 4.62 $\mu\text{mol CO}_2 \cdot \text{m}^{-2} \cdot \text{s}^{-1}$ (see Figures 3 and 4). The results show that, throughout the entire growth period of summer maize at the Daman site in 2023, the STEMMUS-SCOPE model achieved a higher accuracy of SIF and GPP than the SCOPE model, and the

simulation results in the middle of the crop growth period were better than those in the early and late stages of crop growth period in 2023. During DOY 215–240, the SCOPE model significantly overestimated GPP, whereas the STEMMUS-SCOPE model did not exhibit such overestimation. On DOY 241, the simulated GPP from the STEMMUS-SCOPE model showed a sudden increase, which was likely caused by an irrigation event that led to a rise in simulated values.

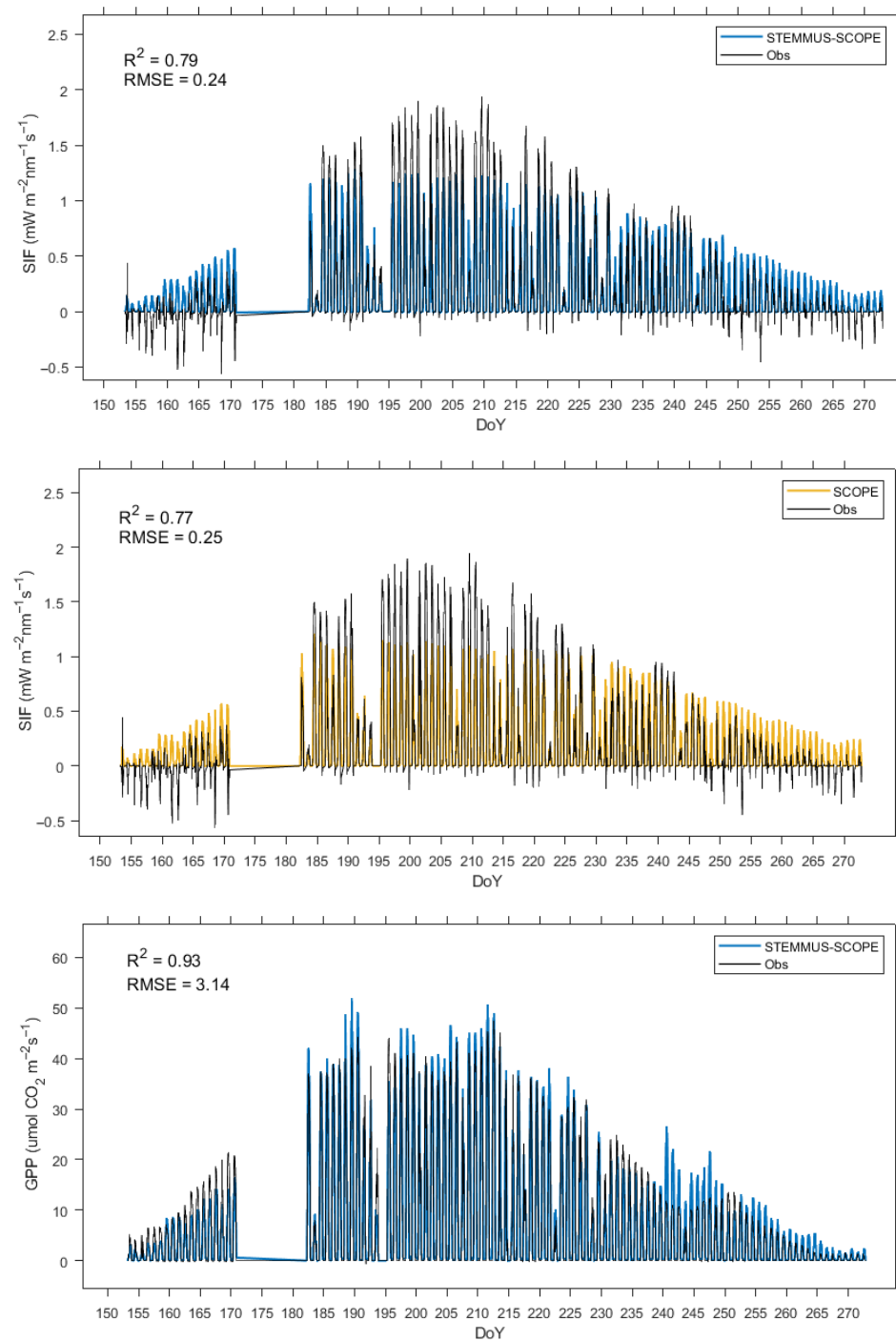


Figure 3. Cont.

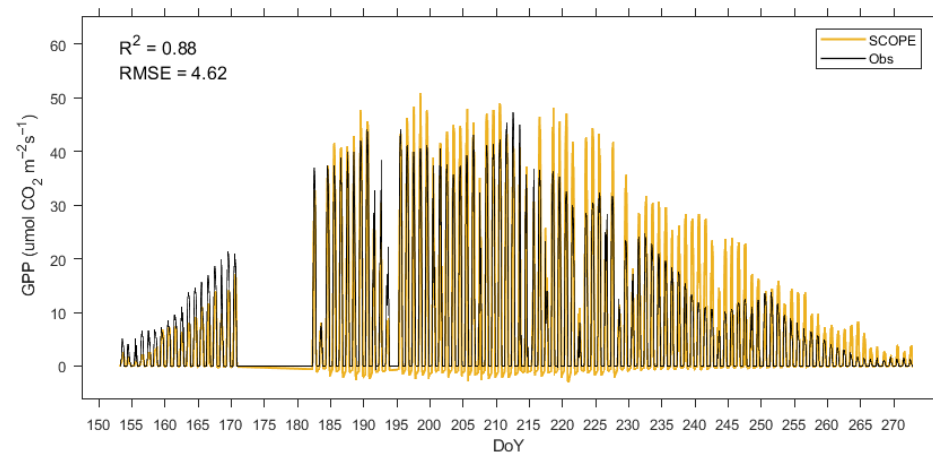


Figure 3. Comparison of simulated and observed values of the STEMMUS-SCOPE model and the SCOPE model in 2023.

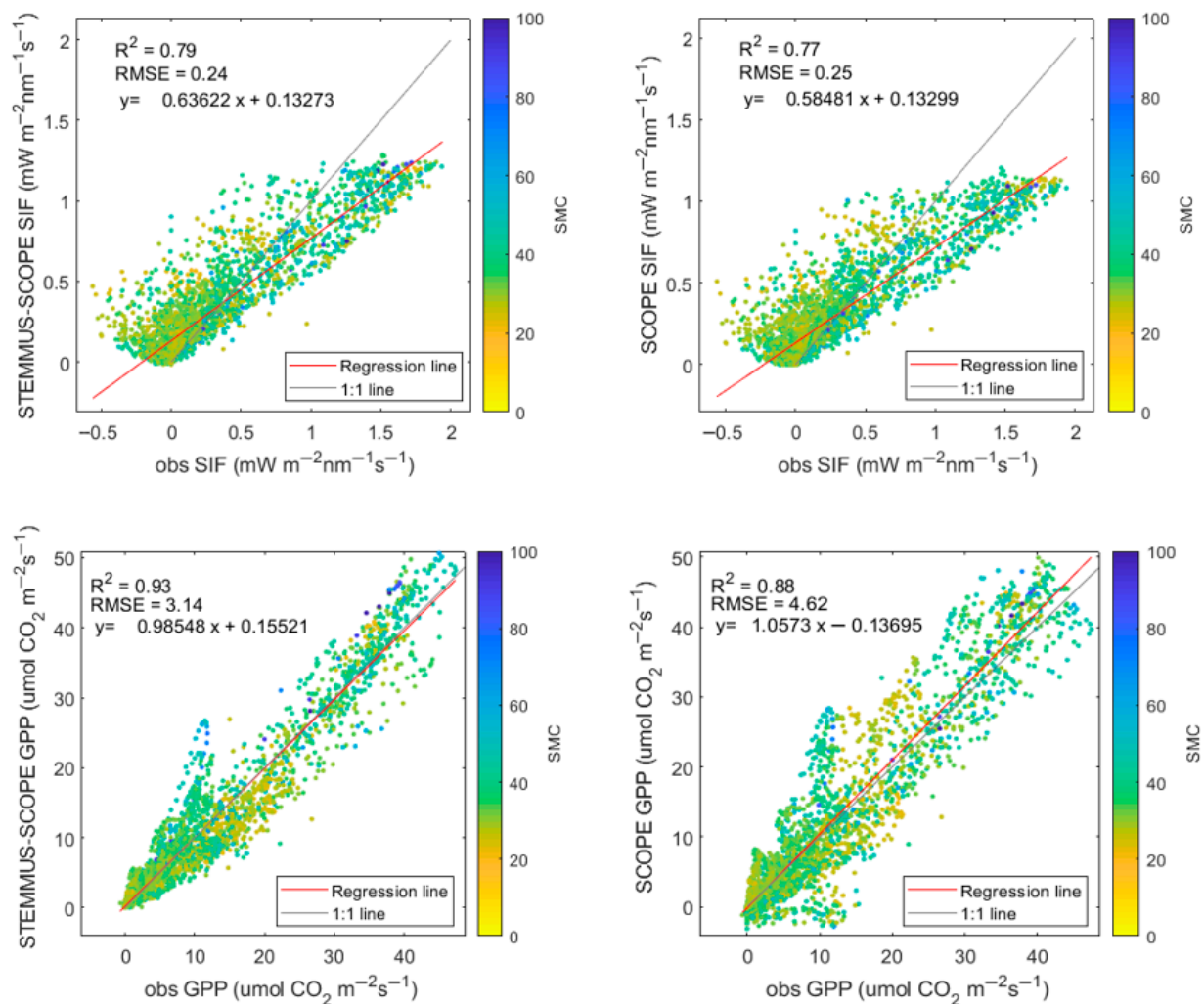


Figure 4. Scatter plots of the 2023 STEMMUS-SCOPE model and SCOPE model simulations and observations.

Table 2. Half-hour-scale simulation accuracy of the STEMMUS-SCOPE model and SCOPE model from 2017 to 2023.

Year	SIF				GPP			
	STEMMUS-SCOPE		SCOPE		STEMMUS-SCOPE		SCOPE	
	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
2017	0.46	0.33	0.46	0.30	0.80	5.93	0.71	7.64
2018	0.62	0.35	0.61	0.27	0.90	5.75	0.88	6.82
2019	0.61	0.33	0.62	0.29	0.89	4.96	0.86	6.85
2020	0.56	0.33	0.55	0.30	0.86	5.18	0.83	5.77
2021	0.83	0.24	0.83	0.32	0.90	4.77	0.86	5.60
2022	0.74	0.21	0.73	0.20	0.89	4.78	0.86	6.17
2023	0.79	0.24	0.77	0.25	0.93	3.14	0.88	4.62

3.2. Performance of the STEMMUS-SCOPE Model in Tracking the Effects of Drought Stress

The performance of the STEMMUS-SCOPE model in simulating SIF and GPP under changing soil water conditions was evaluated based on the variations in soil water content between the second and third irrigation events at the Daman site.

As shown in Figure 5, during the period between the second and third irrigation, the R² between the observed SIF and the SIF simulated by the STEMMUS-SCOPE model was 0.83, and the RMSE was 0.22 mW m^{−2} nm^{−1}. For SCOPE model, the R² between the observed SIF and simulated SIF was 0.79, and the RMSE was 0.25 mW m^{−2} nm^{−1}. During DOY 206–221, when soil moisture was relatively high after the second irrigation, the SIF simulated by the STEMMUS-SCOPE model was higher than that simulated by the SCOPE model. In contrast, during DOY 231–239, when soil moisture was relatively low before the third irrigation, the SIF simulated by the STEMMUS-SCOPE model was slightly lower than that of the SCOPE model. During the period between the second and third irrigation, the R² between the observed GPP and the GPP simulated by the STEMMUS-SCOPE model was 0.96, and the RMSE was 2.88 μmol CO₂ m^{−2} s^{−1}. For the SCOPE model, the R² between the observed SIF and simulated SIF was 0.79, and the RMSE was 5.35 μmol CO₂ m^{−2} s^{−1}. During this period, the SCOPE model tended to overestimate GPP, with the overestimation particularly pronounced before the third irrigation. In contrast, the STEMMUS-SCOPE model effectively addressed this issue, showing improved simulation performance not only before the third irrigation but also during other periods when the SCOPE model exhibited overestimation. Specifically, the linear regression slope of the GPP simulated by the STEMMUS-SCOPE model between the second and third irrigation events was 1.0023, indicating that the STEMMUS-SCOPE model achieved better GPP simulation performance than the SCOPE model under varying soil moisture conditions, especially when soil moisture was relatively low.

As shown in Figure 6, in periods before all irrigations in 2023, the accuracy of SIF simulated by the STEMMUS-SCOPE model was slightly better than the simulations by the SCOPE model, with an R² of 0.84 and an RMSE of 0.26 mW m^{−2} nm^{−1}, and its regression line was closer to the 1:1 line. The accuracy of GPP simulated by the STEMMUS-SCOPE model was significantly higher than that of the SCOPE model, with an R² of 0.96, an RMSE of 2.69 μmol CO₂ m^{−2} s^{−1}, and a regression slope of 1.0237. The observation-to-simulation ratios under different soil moisture conditions indicated that, under lower soil moisture, the variability in these ratios for the STEMMUS-SCOPE model was smaller than that for the SCOPE model, demonstrating its superior simulation accuracy during drought periods (see Figure 7).

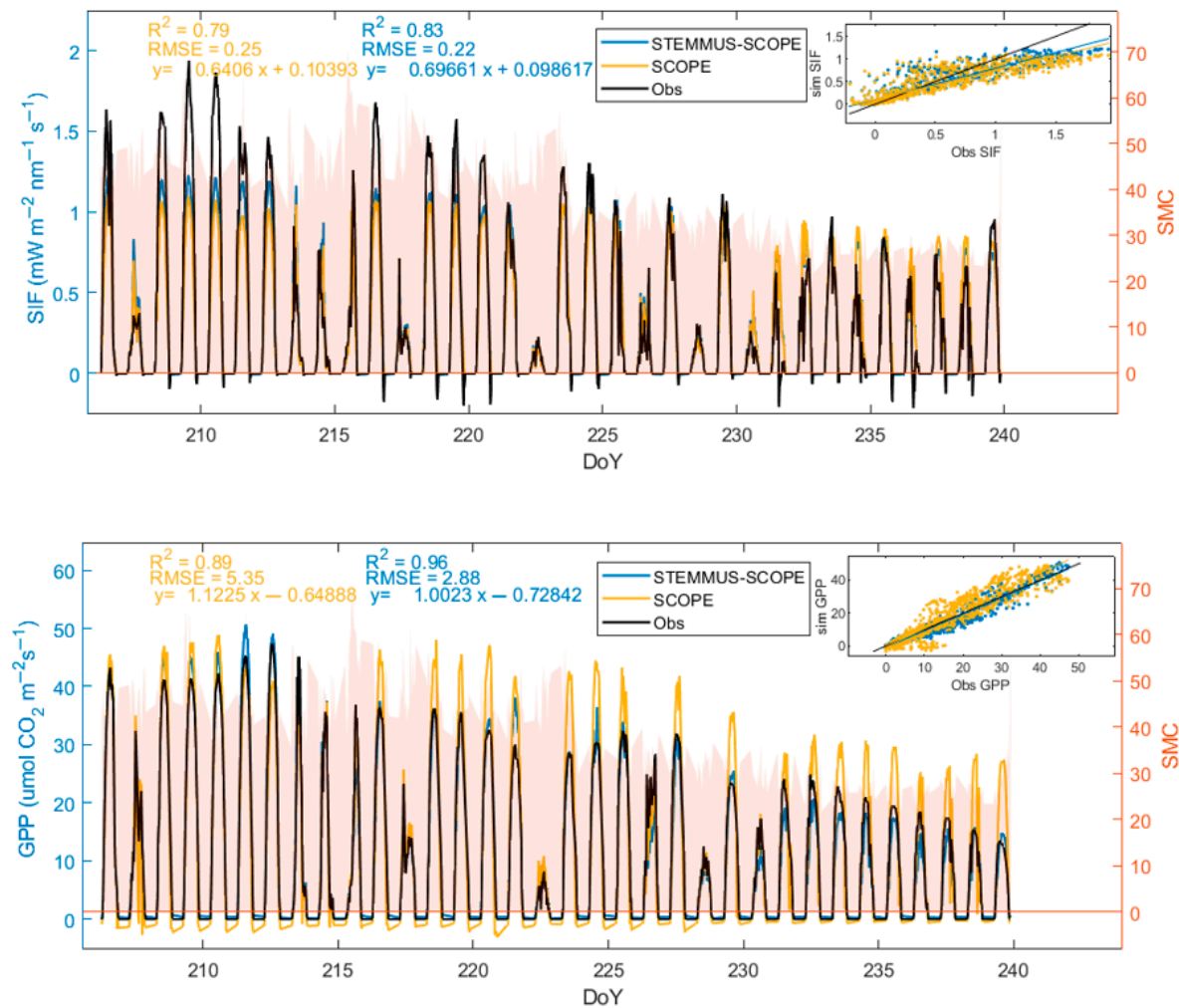


Figure 5. Comparison of half-hour-scale simulation performance of SCOPE and STEMMUS-SCOPE models during the period between the second and third irrigation events.

3.3. Responses of STEMMUS-SCOPE-Simulated ΦF and LUE to Varying SMC

Based on the daily-scale ΦF and LUE values obtained from tower observations as well as those simulated by the STEMMUS-SCOPE model, we discuss their relationships with varying soil moisture content and canopy conductance in 2022 (see Figures 8 and 9).

Under relatively non-drought conditions, the model simulations showed that the correlation between ΦF and SMC ($R^2 = 0.0699$) was slightly stronger than that between ΦF and G_s ($R^2 = 0.0208$), while the correlation between LUE and SMC ($R^2 = 0.4046$) was significantly stronger than that between LUE and G_s ($R^2 = 0.0627$). Under relatively drought conditions, the correlation between ΦF and G_s ($R^2 = 0.1806$) was stronger than that between ΦF and SMC ($R^2 = 0.0193$), and the correlation between LUE and G_s ($R^2 = 0.4857$) was significantly stronger than that between LUE and SMC ($R^2 = 0.1645$). These results indicate that under relatively drought conditions, G_s carries more physiological information about the crop, whereas under relatively non-drought conditions, SMC performs better. This pattern is consistent with the results observed from the flux tower measurements. It is noteworthy that the correlation between LUE and SMC simulated by the STEMMUS-SCOPE model under non-drought conditions was significantly higher than that between LUE and SMC observed from the tower measurements ($R^2 = 0.0732$).

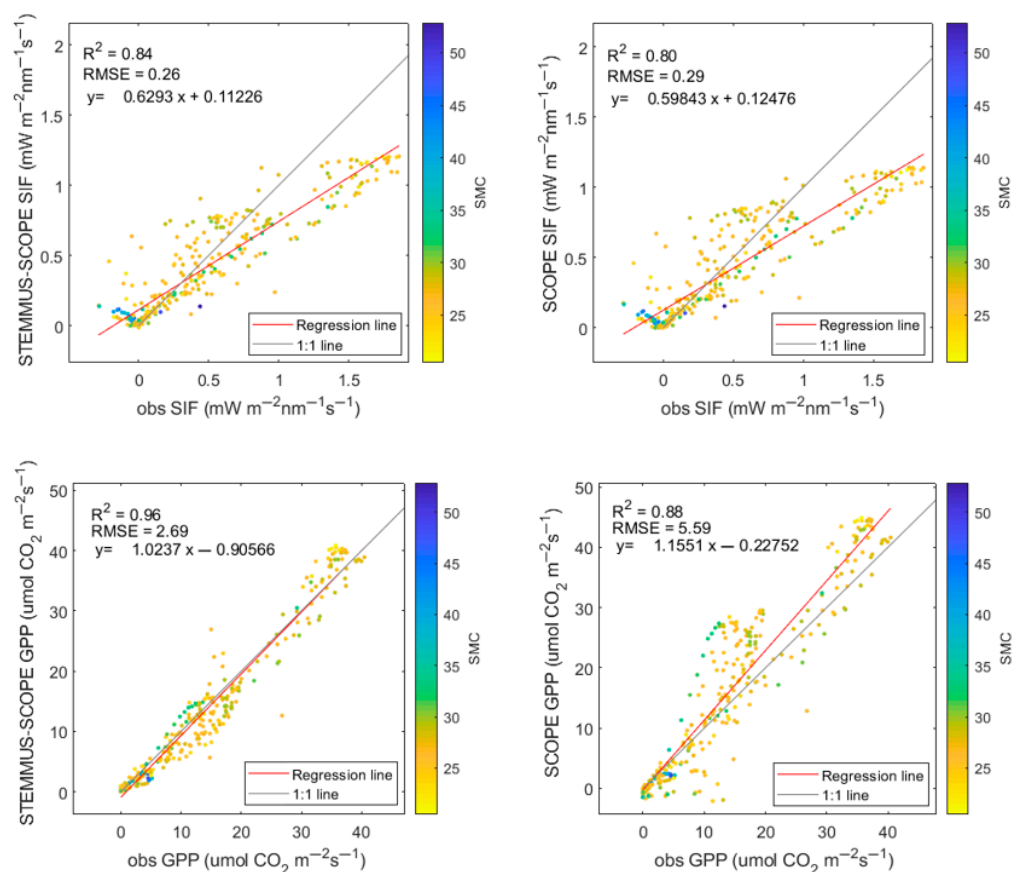


Figure 6. Comparison of half-hour-scale GPP and SIF simulated by the STEMMUS-SCOPE model and the SCOPE model during the 2023 drought.

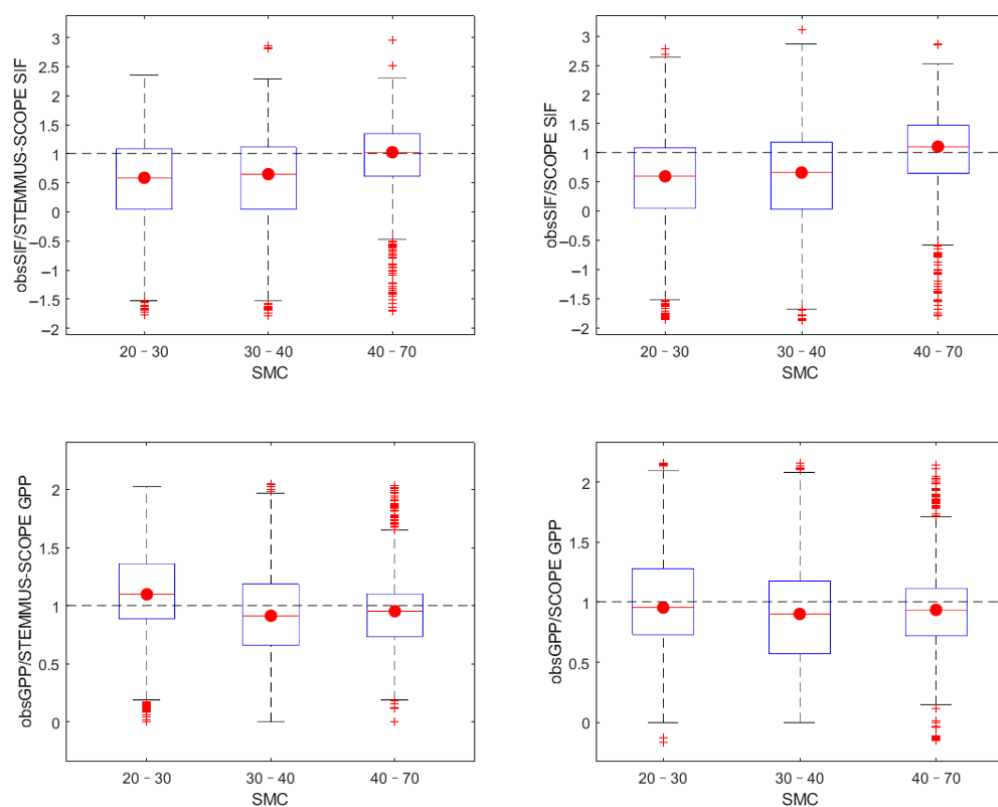


Figure 7. Half-hour-scale SIF and GPP box plots simulated by the STEMMUS-SCOPE model and the SCOPE model for different soil moisture contents in 2023.

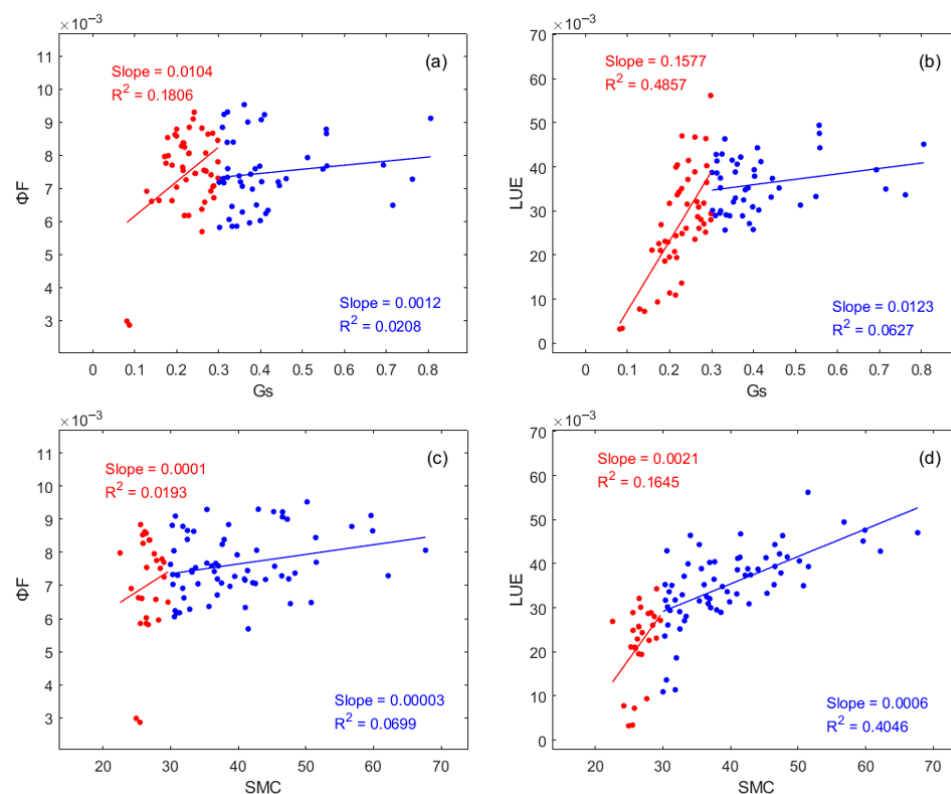


Figure 8. The relationship between (a) ΦF and (b) LUE simulated by the STEMMUS-SCOPE model and Gs; the relationship between (c) ΦF and (d) LUE simulated by the STEMMUS-SCOPE model and SMC. The red areas represent relatively drought conditions, while the blue areas represent relatively non-drought conditions.

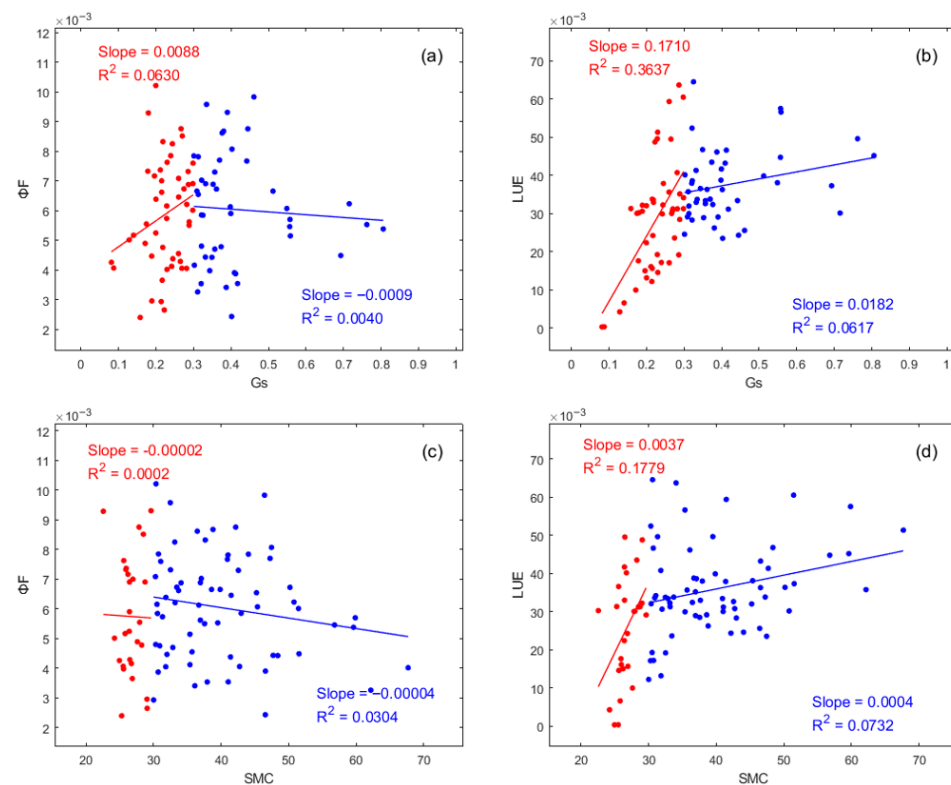


Figure 9. The relationship between (a) ΦF and (b) LUE observed at the tower base and Gs; the relationship between (c) ΦF and (d) LUE observed at the tower base and SMC. The red areas represent relatively drought conditions, while the blue areas represent relatively non-drought conditions.

Moreover, both the tower observations and STEMMUS-SCOPE simulations show that ΦF and LUE decreased with a declining water availability index; however, their response patterns differ. As drought severity increases, the observed decline in ΦF is smaller than that in LUE, whereas this asynchronous decline is partially constrained in the STEMMUS-SCOPE simulations.

4. Discussion

4.1. Performance of the STEMMUS-SCOPE Model for SIF and GPP Under Drought Stress

In this article, we evaluated the performance of the STEMMUS-SCOPE model at the Daman site, with a particular focus on drought periods and times of soil moisture variation. As shown in Table 2 and Figures 3 and 4, the simulation performance of the STEMMUS-SCOPE model has been validated, and its accuracy of SIF and GPP simulation can match or even exceed that of the SCOPE model. Wang et al. [34] compared and analyzed the simulation performance of the SCOPE, STEMMUS, and STEMMUS-SCOPE models in maize fields and grasslands by verifying the simulation capabilities of different terrestrial ecological types, indicating that the STEMMUS-SCOPE model has better simulation capabilities in different terrestrial ecological types, especially when the canopy experienced moderate water stress. Tang et al. [54] used the STEMMUS-SCOPE model in the desert grassland of northwest China to simulate the energy flux under shrub and grassland scenarios. Different from these studies, this study takes advantage of the pronounced soil moisture fluctuations in semi-arid irrigated farmland to focus on evaluating the STEMMUS-SCOPE model's performance in simulating SIF and GPP, particularly under relatively dry conditions and during periods of soil moisture variation. As shown in Figure 5, during the relatively dry period before the third irrigation, unlike the SCOPE model, the GPP simulated by the STEMMUS-SCOPE model was clearly constrained by water stress, resulting in a significant improvement in simulation accuracy. Figures 6 and 7 further demonstrate that STEMMUS-SCOPE outperforms SCOPE under drought conditions.

To evaluate the capability of STEMMUS-SCOPE to quantitatively assess the effects of drought stress on SIF and GPP, we also took into account the impact of stomatal response on SIF and GPP under relatively drought conditions. We calculated G_s on a daily scale based on Equations (3) and (4), and FPAR was calculated according to Equations (1) and (2). The determination of water stress is complex, involving multiple factors such as reduced soil moisture content as well as atmospheric and water demand. At present, vegetation indices and the CWSI are used as indicators for monitoring crop drought [55–57]. At the leaf scale, leaf water potential is a good parameter for determining water stress, but no measured leaf water potential data are available in this study area. Souza et al. [25] found that under drought stress, the declines in canopy conductance, respiration rate, and transpiration rate were consistent. Since stomatal responses directly affect plant photosynthesis, respiration, and transpiration, this may explain the change in the relationship between SIF and GPP. Previous studies have also suggested that G_s is associated with certain fluorescence parameters related to photosynthesis [58,59]. Therefore, in this article, G_s is also used as an index to determine drought status, and the simulation performance of the STEMMUS-SCOPE model for SIF and GPP is analyzed in combination with SMC. The variations in ΦF and LUE simulated by the STEMMUS-SCOPE model under different drought indicators were generally consistent with those observed at the tower. Chen et al. [27] pointed out that the decrease in ΦF under drought stress was less than the decrease in LUE, and this phenomenon was found in both observations at the tower base and model simulations. This may be because, although the light response of plant photosynthesis is weakened in relatively drought conditions, plants compensate for the decline in photochemical processes through stomatal reactions, thereby mitigating the effects of drought. In this article, the inconsistency between the declines in ΦF

and LUE with decreasing water availability was constrained (see Figure 8). This suggests that the SIF and GPP values simulated by STEMMUS-SCOPE exhibit strong correlations across different water conditions, which can be attributed to the model's consideration of the dynamic effects of water availability on the simulation. In addition, we found that the ΦF and LUE values simulated by the STEMMUS-SCOPE model are more strongly correlated with G_s , indicating that G_s can also serve as a comprehensive evaluation index, and it performs better than SMC as an indicator under drought conditions.

4.2. Advantages of STEMMUS-SCOPE in Quantifying Drought Effects on SIF and GPP

In this article, we demonstrated that the STEMMUS-SCOPE model can track the effect of water stress on the simulated values under drought conditions, whereas the SCOPE model lacks this capability. Although the input parameters of the SCOPE model also include a water stress factor, these parameters are not calculated based on measured soil moisture content or simulated soil moisture content, so they cannot accurately and specifically reflect the impact of drought stress on the simulation experiment. Especially under relatively drought conditions and the late growth stage of maize, the simulated GPP value of the SCOPE model tends to be higher, because water stress is one of the main factors restricting vegetation function [33,60]. Therefore, it is particularly important to combine hydraulic models. Bayat et al. [33] achieved better performance in estimating GPP and ET by integrating SPAC models into SCOPE. The STEMMUS-SCOPE model further incorporates the SPAC system and a root growth module to calculate the water stress factor. Compared with the SCOPE-SM model, the STEMMUS-SCOPE model introduces a one-dimensional root growth model, which can simulate the flux change under drought stress well [34]. By integrating a one-dimensional root growth model and an impedance scheme that links soil, roots, leaves, and the atmosphere, the STEMMUS-SCOPE model is able to simulate SIF and GPP under drought conditions or during rapid soil moisture changes more accurately than the SCOPE model.

One major reason for the uncertainty in the SIF–GPP relationship under drought conditions is that stomatal responses can occur more rapidly than changes in electron transport [61]. Under drought stress, rapid stomatal closure limits the entry of CO_2 into the leaf and chloroplasts, reducing the internal CO_2/O_2 ratio. This shift promotes higher rates of photorespiration and the Mehler reaction. Because these two processes consume only a small fraction of ATP compared with carbon fixation, the thylakoid proton gradient (ΔpH) increases substantially [62]. As ΔpH rises, the xanthophyll cycle is activated, enhancing non-photochemical quenching (NPQ). Consequently, thermal dissipation becomes increasingly important in the drought response, while SIF is reduced. In addition to stomatal limitation, severe drought can also trigger non-stomatal regulation, further suppressing photosynthesis. Intense water stress can impair the activity and activation state of Rubisco and chloroplasts, leading to declines in both photosynthesis and fluorescence. Helm et al. [63] noted that drought-induced reductions in CO_2 assimilation may result from restricted CO_2 diffusion due to stomatal closure or from downregulation of leaf biochemical processes caused by non-stomatal factors. However, the observed decrease in fluorescence was generally smaller than the reduction in CO_2 assimilation. This mismatch between the light reactions and carbon reactions may be a key contributor to the complex SIF–GPP relationship, as SIF is directly linked to the light reactions of photosynthesis.

The STEMMUS-SCOPE model calculates the water stress factor based on the soil moisture content and root length density of each soil layer. The obtained water stress factor is directly applied to the photosynthetic biochemical processes to constrain V_{cmax} . When soil moisture decreases, the stress factor significantly reduces V_{cmax} , leading to a decline in photochemical efficiency, an increase in thermal dissipation, enhanced NPQ, and reduced

fluorescence. As a result, SIF exhibits a decreasing trend that corresponds to the severity of drought (see Figures 5–9). The decline in $V_{\max}$ in the model directly limits carbon fixation capacity, leading to a reduction in simulated GPP. Especially under drought conditions, the water stress factor can effectively constrain the model outputs, thereby avoiding the overestimation commonly observed in the SCOPE model (see Figures 5 and 6).

For the uncertainty in the SIF–GPP relationship under drought conditions, a mechanistic explanation can be obtained through the different pathways by which the water stress factor in the STEMMUS-SCOPE model affects SIF and GPP. As soil moisture decreases, the slope between simulated SIF and GPP gradually declines (see Figure 1), highlighting the model's potential for assessing the influence of drought stress on the SIF–GPP relationship.

4.3. The Limitations of This Article

In this study, we conducted a long-term evaluation of the STEMMUS-SCOPE model using continuously monitored maize data, confirming that the model performs well in simulating processes within this agricultural ecosystem. However, several limitations remain that warrant improvement in future research. Maize is a typical C4 plant, and this study did not include long-term validation for other plant functional types. Since the photosynthetic processes of C3 and C4 plants differ, their responses to environmental stresses may involve distinct mechanisms [61,64]. Secondly, although the STEMMUS-SCOPE model provides a process-based description of the interactions among water, carbon, and energy, its performance still depends on the accuracy of key physiological parameterization such as Cab and LAI. Uncertainties in these parameters can introduce potential variability into the model outputs. Moreover, the soil profile in the study area is not vertically homogeneous, whereas this study assumes vertical uniformity, which may introduce certain biases when simulating the SPAC processes within the STEMMUS-SCOPE framework.

5. Conclusions

In this study, we used meteorological and flux data from the Daman site during 2017–2023, along with measured or retrieved vegetation parameters, to simulate half-hourly SIF and GPP using the STEMMUS-SCOPE model. Leveraging the irrigation events characteristic of semi-arid irrigated farmland, we evaluated and validated the model from two perspectives: accuracy in simulating SIF and GPP under drought stress and capability to quantitatively assess the impacts of water stress on SIF and GPP. The STEMMUS-SCOPE model exhibited strong simulation performance during the maize growing season. Taking 2023 as an example, the model achieved an R^2 of 0.79 for SIF and 0.93 for GPP. Compared with the SCOPE model, STEMMUS-SCOPE more effectively reduces the overestimation under water deficit conditions, indicating its improved ability to track the effects of soil moisture variability—an advantage particularly evident under low soil moisture. This article, thus, verified the simulation performance of the STEMMUS-SCOPE model and examined the model's ability to track the effects of soil moisture variability on simulated values under different water conditions.

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