Understanding Interactions between Terrestrial Water and Carbon Cycles Using Integrated SMAP Soil Moisture and OCO-2 SIF Observations and Land Surface Models

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Abstract

Recently, more advanced synchronous global-scale satellite observations, the Soil Moisture Active Passive enhanced Level 3 (SMAP L3) soil moisture product and the Orbiting Carbon Observatory 2 (OCO-2) solar-induced chlorophyll fluorescence (SIF) product, provide an opportunity to improve the simulations of both water and carbon cycles in land surface modeling. This study introduces a mechanistic representation of SIF to the Simplified Simple Biosphere Model version 4 (SSiB4) coupled with the Top-down Representation of Interactive Foliage and Flora Including Dynamics Model (TRIFFID). This newly developed model with the observed satellite data indicates that introducing dynamic processes can lead to substantial improvement in global carbon flux simulation. In the SSiB4/TRIFFID/SIF, four critical soil and vegetation parameters–B parameter, soil hydraulic conductivity at saturation (Ks), wilting point, and maximum Rubisco carboxylation rate (Vmax)–were identified through numerical sensitivity experiments. Among the four parameters, the B parameter has the most significant effects on both soil moisture and SIF simulations. With the optimized B parameter, both soil moisture and SIF simulations were improved substantially, with especially significant improvement for shrubs. The Ks and wilting point also affect both soil moisture and SIF but with reduced magnitude. The Vmax directly affects photosynthesis, and its modification can substantially improve the SIF simulation of needleleaf trees and C3 grasses. With all four calibrated parameters based on SMAP L3 and OCO-2 data, the root-mean-squared error (RMSE) of soil moisture and SIF simulations decreased from 0.076 to 0.063 m3/m3 and from 0.143 to 0.117 W/m2/µm/sr, respectively.

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Key Points:

- Dynamic vegetation processes substantially improve of terrestrial carbon flux simulation.
- Satellite products lead to advances in simulation and understanding of water and carbon cycles and their interactions.
- The B parameter, representing the slope of water retention curve, shows the most significant effects on both water and carbon cycles.

Abstract

Recently, more advanced synchronous global-scale satellite observations, the Soil Moisture Active Passive enhanced Level 3 (SMAP L3) soil moisture product and the Orbiting Carbon Observatory 2 (OCO-2) solar-induced chlorophyll fluorescence (SIF) product, provide an opportunity to improve the simulations of both water and carbon cycles in land surface modeling. This study introduces a mechanistic representation of SIF to the Simplified Simple Biosphere Model version 4 (SSiB4) coupled with the Top-down Representation of Interactive Foliage and Flora Including Dynamics Model (TRIFFID). This newly developed model with the observed satellite data indicates that introducing dynamic processes can lead to substantial improvement in global carbon flux simulation. In the SSiB4/TRIFFID/SIF, four critical soil and vegetation parameters--B parameter, soil hydraulic conductivity at saturation (K_s), wilting point, and maximum Rubisco carboxylation rate (V_{max})--were identified through numerical sensitivity experiments. Among the four parameters, the B parameter has the most significant effects on both soil moisture and SIF simulations. With the optimized B parameter, both soil moisture and SIF simulations were improved substantially, with especially significant improvement for shrubs. The K_s and wilting point also affect both soil moisture and SIF but with reduced magnitude. The V_{max} directly affects photosynthesis, and its modification can substantially improve the SIF simulation of needleleaf trees and C_3 grasses. With all four calibrated parameters based on SMAP L3 and OCO-2 data, the root-mean-squared error (RMSE) of soil moisture and SIF simulations decreased from 0.076 to 0.063 m^3/m^3 and from 0.143 to 0.117 $W/m^2/\mu m/sr$, respectively.

1 Introduction

The terrestrial carbon and water cycles are tightly coupled by biological plant processes (Niyogi and Xue, 2006; Scholze et al., 2016). The interactions between soil moisture and carbon flux have been confirmed by previous studies (Koster et al., 2016; Qiu et al., 2018). Surface soil moisture plays a crucial role in land-atmosphere interactions (Humphrey et al., 2021; McColl et al., 2017; Seneviratne et al., 2010). It directly affects the photosynthesis and transpiration processes (Cox et al., 2002; Zhan et al., 2003) and indirectly affects carbon assimilation through modulating phenological processes (Zhang et al., 2015). The amount of available soil moisture is a key limiting factor on photosynthesis and transpiration since it affects both the water use and carbon uptake of the plant through the leaf stomata gas exchange (Manzoni et al., 2013), which makes the interactions between vegetation and soil moisture dynamics contribute significantly to the structure and function in arid and semiarid ecosystems (Walker et al., 1981; Bhark and Small, 2003; D'Odorico et al., 2007). The terrestrial ecosystem provides feedback on the water cycle through transpiration and vegetation structure (Xue et al., 2004; Kang et al., 2007).

Surface soil moisture has large uncertainty in spatiotemporal distribution, and great efforts have been devoted to improving measurements using active or passive microwave instruments (Font et al., 2001; Njoku et al., 2003; Entekhabi et al., 2010; Kerr et al., 2012). The assimilation of the remotely sensed surface soil moisture has the potential to improve land surface processes modeling (Wander et al., 2014; Scholze et al., 2016). Wu et al. (2020) found that the Soil Moisture and Ocean Salinity (SMOS) soil moisture data can be used to constrain the simulations of the terrestrial biosphere carbon cycle to optimize soil hydrological and biophysical parameters simultaneously. The Soil Moisture Active Passive (SMAP) mission is the most recent space-borne mission at L-band and has been considered one of the most promising satellites for surface soil moisture monitoring (Wigneron et al., 2017). Recent studies suggest that SMAP outperforms other satellite products compared to in situ soil moisture measurements (Ma et al., 2019; Beck et al., 2021). Zhang et al. (2022) used the direct insertion of SMAP soil moisture observation to improve the simulated land-surface carbon fluxes across a variety of timescales. The SMAP product can provide a better representation of soil moisture, which suggests its potential for improvement in coupled carbon-water dynamics in terrestrial ecosystem models.

In recent years, remote sensing of solar-induced chlorophyll fluorescence (SIF) has been a rapidly advancing front in investigating carbon dynamics and other applications (Frankenberg et al., 2011; Sun et al., 2018; Doughty et al., 2022; Leng et al., 2022). The SIF retrieved from spaceborne spectrometers has been extensively used as a proxy for terrestrial photosynthesis to understand terrestrial ecosystem dynamics (Sun et al., 2017; Helm et al., 2020). As a signal emitted by the photochemically active centers of plants, SIF is directly linked to the actual process of photosynthesis (Porcar-Castell et al., 2014). Gonsamo et al. (2019) found that the Orbiting Carbon Observatory-2 (OCO-2) SIF can accurately capture the control of soil moisture on photosynthetic activity, especially for regions with distinct seasonality of rainfall. Lee et al. (2015) incorporated equations coupling SIF to photosynthesis in a land surface model and confirmed that SIF has the potential to improve photosynthesis simulation. Qiu et al. (2018) incorporated this mechanistic representation of SIF and the Greenhouse gases Observing SATellite (GOSAT) and the Global Ozone Monitoring Experiment-2 (GOME-2) SIF measurements into a global terrestrial biosphere model, the Simplified Simple Biosphere Model version 2 (SSiB2/SIF), to evaluate and investigate the model-simulated relationships between soil moisture and SIF. In this study, we incorporated this existing SIF module into SSiB version 4 (SSiB4) to enable the fluorescence simulation, which is directly linked to photosynthetic activity and gross primary production (GPP).

In most studies, the vegetation conditions are specified based on observed and satellite-derived data, which suppresses the interactions between soil moisture and carbon cycle dynamics and indicates an important deficiency in the representation of terrestrial carbon processes in coupled carbon balance-based dynamic vegetation models. Dynamic vegetation models (DVMs) can simulate vegetation establishment, growth, competition, and mortality (Sitch et al., 2008). Studies suggest that the DVMs can be used at seasonal/interannual/decadal scales to simulate the land/atmosphere feedback (Lu et al., 2001; Levis and Bonan, 2004; Kim and Wang, 2012; Zhang et al., 2021). The Top-down Representation of Interactive Foliage and Flora Including Dynamics model (TRIFFID) uses the CO_2 fluxes at the land-atmosphere interface to update plant distributions and soil carbon, which allows the changes in biophysical properties to provide feedback onto the atmosphere (Cox et al., 2001; Hawkins et al., 2019). TRIFFID has been validated across spatial scales and ecosystems (Cox et al., 2000; Cox et al., 2004; Piao et al., 2009; Zhang et al., 2015; Liu et al., 2019). It serves as the foundation of the Joint UK Land Environment Simulator (JULES) for global carbon budget assessment (Clark et al., 2011; Le Quéré et al., 2016) and was coupled to SSiB4 to study the connections between vegetation dynamics and climate variability (Zhang et al., 2015). Liu et al. (2019) validated the vegetation distribution and leaf area index (LAI) simulated by SSiB4/TRIFFID against satellite products. With the coupling of TRIFFID, the relevant land-surface characteristics of vegetation cover and structure are modeled directly, which suggests SSiB4/TRIFFID can be used to investigate the role and mechanisms of the interactions between soil moisture and carbon cycle dynamics.

This study used the SMAP L3 soil moisture data, in conjunction with the OCO-2 SIF measurements, to evaluate the soil moisture and SIF simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF as well as the relationships between the soil moisture and SIF simulation to investigate the effects of dynamic vegetation processes on soil moisture and carbon flux estimates. We integrated the two satellite measurements into SSiB4/TRIFFID/SIF to improve the model parameterization and to investigate the broad-scale relationships between soil moisture and carbon cycle dynamics, providing the opportunity to better understand the mechanistic processes in the global terrestrial biosphere model that bridges water and carbon cycles. This paper is organized as follows: Section 2 presents the model structure, experimental design, and the satellite datasets used for evaluation and calibration. The effects of the dynamic vegetation processes and key parameters on SM, SIF, and GPP simulations and the performance after calibration are illustrated in Section 3. Discussions and concluding remarks are presented in Section 4 and Section 5, respectively.

2 Model description, experimental design, and data

2.1 Model description

SSiB is a biosphere model that intends to simulate the biophysical exchange processes realistically (Xue et al., 1991 and 1996). Zhan et al. (2003) developed an analytical solution approach from a photosynthesis model (Collatz et al., 1991, 1992) and incorporated it into SSiB to generate SSiB2, which improved the land surface CO_2 fluxes simulation. The dynamic vegetation model, TRIFFID, which has been widely used in vegetation-climate interaction studies (Cox et al., 2000; Harper et al., 2016), was coupled to SSiB4 (Xue et al., 2006) to calculate vegetation dynamics. In SSiB4/TRIFFID, SSiB4 provides net plant photosynthesis assimilation rate, autotrophic respiration, and other surface conditions such as canopy temperature and soil moisture for TRIFFID. TRIFFID updates the vegetation dynamics, including the plant functional type (PFT) fractional coverage, vegetation height, and LAI, for SSiB4. Equations coupling SIF to photosynthesis, which were incorporated into the Community Land Model version 4 (CLM4, Lee et al., 2015), were incorporated into SSiB2 by Qiu et al.

(2018). In this study, the SIF module was incorporated into SSiB4/TRIFFID, forming SSiB4/TRIFFID/SIF, to enable the chlorophyll fluorescence simulation in photosynthesis.

2.2 Experimental design

In this study, SSiB2/SIF and SSiB4/TRIFFID/SIF were used to simulate the global soil moisture, SIF, and GPP and to assess the effects of the dynamic vegetation process on the simulations. The SSiB2/SIF model was driven by atmospheric forcing from 2010 to 2019 (Figure 1a). For the SSiB4/TRIFFID/SIF model, we first conducted spin-up simulations driven with climatological forcing and 1979 CO_2 concentration for 100 years to reach a quasi-equilibrium state as done by Liu et al. (2019) and Huang et al. (2020). Using the quasi-equilibrium simulation results as the initial vegetation conditions, such as each plant functional type's (PFT) fraction coverage, leaf area index (LAI), etc., we performed transient runs driven with historical meteorological forcing and yearly updated atmospheric CO_2 concentration from 1979 to 2019 (Liu et al., 2019) (Figure 1b). The time step of model integration is 3 h, and the spatial resolution of the model is 0.5°×0.5°. The experiments covered the period from 2010 to 2019 in SSiB2/SIF and 1979 to 2019 in SSiB4/TRIFFID/SIF, and the results from April 2015 to

December 2019, when the soil moisture and SIF satellite data were both available, were analyzed.

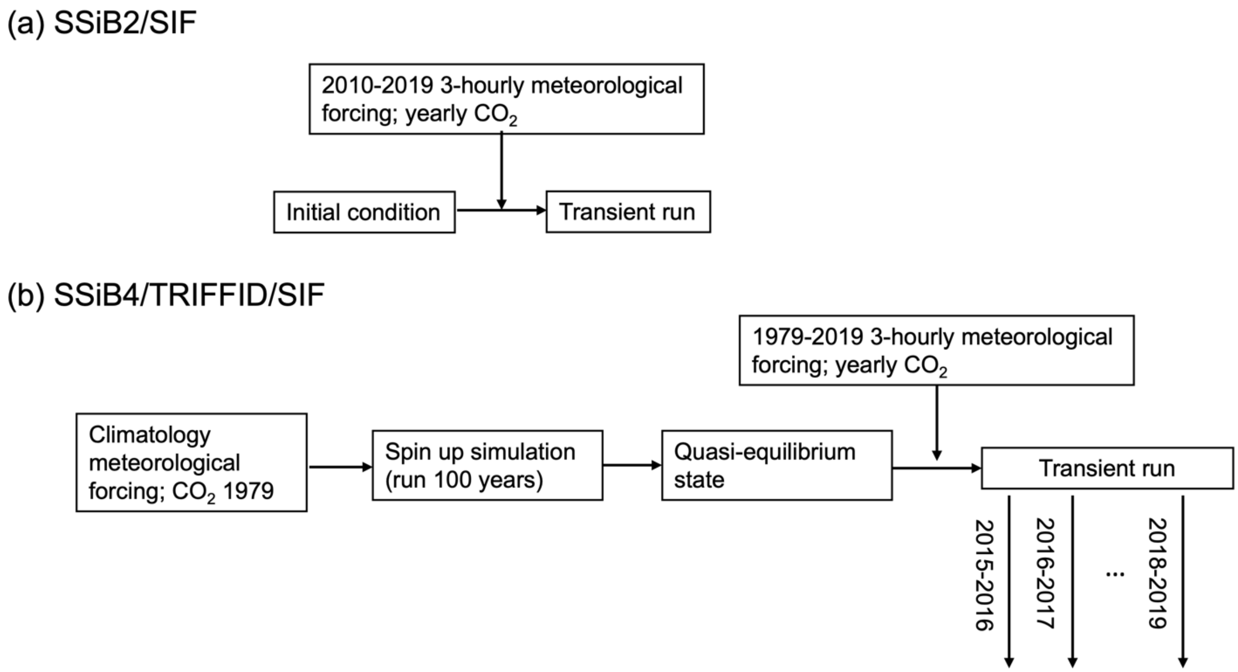


Figure 1. Experiment design for (a) SSiB2/SIF and (b) SSiB4/TRIFFID/SIF.

Studies have shown that soil properties substantially impact the soil moisture simulation in SSiB models, especially the parameterization of two key parameters, the B parameter and the hydraulic conductivity at saturation (K_s) (Xue et al., 1996; Qiu et al., 2018). The B parameter is an empirical constant that is dependent on the soil type. It represents the slope of the water retention curve and determines the relationship between the soil water potential and the volumetric soil water content through the following pedotransfer functions (Clapp and Hornberger, 1978):

$$\psi = \psi_s \left(\frac{\theta}{\theta_s}\right)^{-B} \tag{1}$$

where ψ is the soil water potential; ψ_s is the soil water potential at saturation; θ is the volumetric soil water content; and θ_s is the volumetric soil water content at saturation. The hydraulic conductivity at saturation (K_s) is the key coefficient in the soil water diffusion equation. This equation is used to calculate the transfer of water between the three soil layers in SSiB models. Both the B parameter and K_s affect the soil water diffusion (Xue et al., 1996):

$$Q = -K_s \left(\frac{\theta}{\theta_s}\right)^{(2B+3)}\left[\frac{\partial\psi}{\partial Z} + 1\right] \quad (2)$$

where Q is the soil water diffusion; and $\partial\psi/\partial Z$ is the soil water potential gradient.

In addition to these two parameters, Qiu et al. (2018) found that the wilting point is a parameter directly linked to stomatal resistance and consequently to photosynthesis processes, thus affecting soil moisture through transpiration and demonstrating the close link between the water and carbon cycles. The wilting point is defined as the soil water content below which the vegetation transpiration process tends to inhibit (Tolk, 2003). In the SSiB model, an empirical equation was developed to relate the soil moisture and stomatal conductance for each PFT (Xue et al., 1991), in which the wilting point is the natural logarithm of soil water potential at which the stomata close completely. In SSiB2/SIF and SSiB4/TRIFFID/SIF, the wilting point controls the stomata opening and affects the photosynthesis process through the β factor, the adjustment parameter on stomatal conductance:

$$\beta = 1 - \exp\{-C_2[C_1 - \ln(-\psi)]\} \quad (3)$$

where C_1 is the wilting point and C_2 is a slope factor that depends on the vegetation type.

The maximum Rubisco carboxylation rate (V_{max}) is a vegetation parameter that directly affects the photosynthesis rate (Zhan et al., 2003). The model simulated photosynthesis rates are controlled by three limitation factors related to Rubisco, electron transportation, and product sink. The vegetation parameter, V_{max}, plays a key role in this computation. It determines the photosynthetic limitations and serves as a link between the water and carbon cycles since it can also affect soil moisture through transpiration.

We have conducted a large number of experiments to test the parameters that affect the water and carbon cycle simulations in SSiB4/TRIFFID/SIF, and confirmed the importance of these four parameters mentioned above. The effects of the four parameters on soil moisture and SIF were tested through adjusting them within their normal ranges. Figure 2 shows the schematic flowchart of the SSiB4/TRIFFID/SIF model. The black boxes are the model components. The blue boxes are the satellite products used to evaluate the soil moisture and SIF simulations and to calibrate the parameters. The brown box and the green boxes represent the soil property parameters and the vegetation parameters tested and calibrated in this study, respectively.

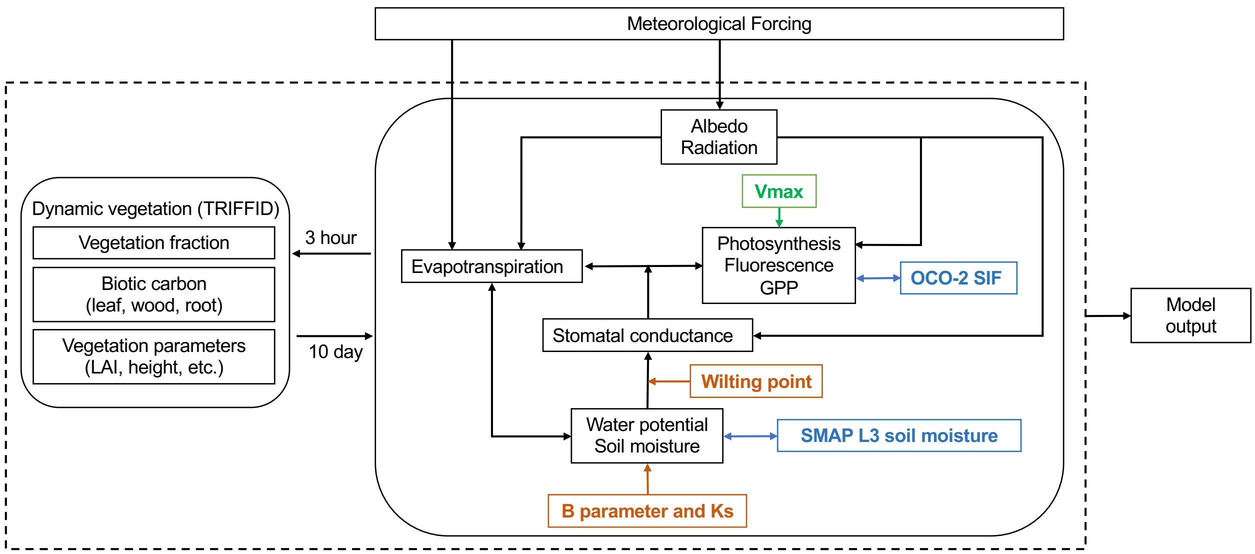


Figure 2. Overview flowchart of the SSiB4/TRIFFID/SIF model and the modified parameters in the model. The black boxes are the SSiB4/TRIFFID/SIF model components; the brown boxes represent the modified soil property parameters in the model; the green box represents the modified vegetation parameters in the model; and the blue boxes are the satellite data. SMAP

L3: Soil Moisture Active Passive enhanced Level 3; OCO-2: Orbiting Carbon Observatory 2; LAI: leaf area index.

We designed the following four sets of experiments to assess the effects of the four critical parameters on soil moisture and SIF simulation with the dynamic vegetation model coupled and for further calibration in SSiB4/TRIFFID/SIF (Table 1).

1. For the control run (CTL), the original values of the parameters were used.
2. For Test 1, the B parameter was modified. Our preliminary experiments suggested this parameter has a larger impact on soil moisture than other parameters.
3. For Test 2, the calibrated B parameter based on Test 1 was used, and the K_s was tested.
4. For Test 3, the wilting point was tested with the calibrated B parameter and K_s based on Test 2.
5. For Test 4, the V_{max} was tested with the calibrated B parameter, K_s, and wilting point based on Test 3.

Table 1. SSiB4/TRIFFID/SIF Experiment Design.

	Experiment description
CTL	Original parameters
Test 1	With modified B parameter
Test 2	Same as Test 1 but with hydraulic conductivity at saturation (K_s) modified
Test 3	Same as Test 2 but with wilting point (Wp) modified
Test 4	Same as Test 3 but with maximum RuBP carboxylation rate (V_{max}) modified

2.3 Data

The SSiB vegetation map and table based on ground survey and satellite-derived information are used as the initial condition for SSiB2/SIF simulation and SSiB4/TRIFFID/SIF quasi-equilibrium simulation (Dorman & Sellers, 1989; Xe et al., 1996, Zhang et al., 2015). Meteorological forcing data are used to drive the model. The observation-based soil moisture, SIF, and GPP products are used to evaluate the model simulation and calibrate the model parameterization. The regions at latitudes higher than 60°N were excluded from the analysis because of the scarce satellite records.

2.3.1 Meteorological forcing data

The three-hourly meteorological forcing data from 1948 to 2008 used for the quasi-equilibrium simulation in SSiB4/TRIFFID/SIF are from the Princeton global meteorological dataset for land surface modeling (Sheffield et al., 2006). The dataset combines global observation-based datasets with the NCEP/NCAR reanalysis. The spatial resolution is 1°×1°, and the temporal interval is 3 h. Its 60-year mean climatology with 3-h intervals was generated and interpolated bilinearly to 0.5°×0.5° to drive the quasi-equilibrium simulation. The hourly meteorological forcing data used for simulations in SSiB2/SIF and SSiB4/TRIFFID/SIF are the bias-corrected reconstruction of near-surface meteorological variables derived from the fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMRF) atmospheric reanalysis (ERA5) (Cucchi et al., 2022). This dataset has 0.5°×0.5° spatial resolution and a 1-h temporal interval. The 3-hour average was generated to drive the transient simulations. The variables included in the meteorological forcings are surface air temperature (K), pressure (Pa), specific humidity (g kg^{-1}), wind speed (m s^{-1}), downward shortwave radiation flux (W m^{-2}), downward longwave radiation flux (W m^{-2}), and precipitation (kg m^{-2} s^{-1}).

2.3.2 Observation-based data

There is no human activity included in the SSiB4 model simulation. Therefore, the potential vegetation distributions produced by the quasi-equilibrium run in SSiB4/TRIFFID/SIF are not the same as the vegetation map observed by satellite-derived products over some areas due to anthropogenic effects, such as the croplands in the Central US, Southern Brazil, Europe, India, and Eastern China. In this study, we used the Global Land Cover (GLC) database for the year 2000 (Bartholome and Belward, 2005) derived from Satellite Pour 1'Observation de la Terre (SPOT) to exclude the cultivated and managed areas in simulation, evaluation, and analysis.

The Soil Moisture Active Passive (SMAP) mission, launched by NASA on January 31, 2015, is the newest L-band satellite dedicated to providing global surface soil moisture measurements. This study used the SMAP Enhanced L3 Radiometer Global Daily 9 km EASE-Grid Soil Moisture dataset (SMAP L3). This dataset presents the volumetric surface soil moisture (m^3/m^3) at 0–5 cm and is superior to other satellite soil moisture products, including the Soil Moisture and Ocean Salinity (SMOS) and the ESA Climate Change Initiative (ESA CCI) in terms of capturing temporal trends compared with in-situ observations from global dense and sparse networks (Ma et al., 2019). The assessment of the SMAP L3 product using the in-situ measurements from the core validation sites (CVSs) shows that the average unbiased root mean square error (ubRMSE) is lower than 0.04 m^3/m^3 (Colliander et al., 2017; O'Neill et al., 2020). Zhang et al. (2019) validated the SMAP L3 product using extensive ground measurements from sparse networks and found that the retrievals from the descending (6:00 AM) product and ascending (6:00 PM) product do not show significant differences. In this study, the average of the descending and ascending products was bilinearly interpolated to 0.5°×0.5° for evaluation and calibration.

The SIF simulation was evaluated using the Orbiting Carbon Observatory-2 (OCO-2) SIF product. This mission, launched on July 2, 2014, measures SIF from the infilling of the Fraunhofer lines at 1:36 p.m. local time with a repeat frequency of approximately 16 days. The retrieval precision of OCO-2 is considerably improved over other existing satellite SIF products, including the Greenhouse Gases Observing Satellite (GOSAT) product and the Global Ozone Monitoring Experiment-2 product (GOME-2) (Sun et al., 2018). All soundings within a 1°×1° pixel were averaged and archived onto a 0.5° grid to generate OCO-2 SIF at 757 nm so that most of the pixels have sufficient soundings to retrieve the gridded monthly SIF (Qiu et al., 2020). To use this dataset to assess the model simulated SIF, the simulation at noon and 3 p.m. in each time zone was selected to obtain the one at 1 p.m. through interpolation.

Previous studies found that GPP and SIF had a strong linear relationship, and the satellite SIF data provide useful information on terrestrial GPP (Bacour et al., 2019; Joiner et al., 2013; Lee et al., 2015; Walther et al., 2016). Li et al. (2018) explored the relationship between OCO-2 SIF and tower GPP at 64 flux sites across the globe encompassing eight major biomes, confirming the strong correlation between SIF and GPP. Because of the significant uncertainty in the quantification of global GPP due to the lack of direct GPP observations at a global scale (Wang et al., 2021; Zhang and Ye, 2021), we selected three global GPP datasets derived from observation using different methods for comparison rather than evaluation or calibration. First is the GLASS (Global Land Surface Satellite) GPP product generated from the Eddy Covariance – Light Use Efficiency (EC-LUE) model (Yuan et al., 2007). The EC-LUE model has been validated widely throughout various ecosystems using the measurements from eddy covariance towers (Li et al., 2013; Yuan et al., 2014), and Jia et al. (2018) indicated that the EC-LUE model performed better than the MODIS algorithms. This dataset has 0.05°×0.05° horizontal resolution and 8-day time intervals. The second GPP product used for comparison is the FLUXCOM RS GPP product. It uses machine learning to merge the carbon flux measurements from the FLUXNET eddy covariance towers and remote sensing data (Tramontana et al., 2016). Zhang and Ye (2021) evaluated 45 global terrestrial GPP products by taking Model Ensemble GPP derived from observations as the reference dataset and recommended the RS product for global GPP comparison. Its resolution is 0.5°×0.5° and the time interval is 8 days. The last dataset is a global MODIS and FLUXNET-derived GPP product (FLUXSAT GPP) (Joiner and Yoshida, 2021). It used MODIS product as input to neutral networks to globally upscale GPP estimates from selected FLUXNET eddy covariance tower sites (Joiner and Yoshida, 2020). The product has a 0.05° spatial resolution and a daily temporal resolution.

3 Results

3.1 Assessment of the simulated vegetation distribution

The rate of change in vegetation fraction is less than 2% over the last 10 years of simulation, which means it reached a steady state after a 100-year spin-up (Liu et al., 2019) (Figure S1). For most PFTs, the rate is less than 1.5%. Using initial vegetation conditions derived from this quasi-equilibrium state, SSiB4/TRIFFID/SIF was driven with the historical meteorological forcing and yearly updated atmospheric CO_2 concentration from 1979 to 2019. The simulated vegetation spatial distribution was compared with that simulated in the previous study (Liu et al., 2019) to ensure that the simulated vegetation spatial distribution is reasonable, which is the base for other simulated variables in the model. The evergreen broadleaf trees in the Amazon, central Africa, and Indonesia, needleleaf trees in midlatitudes and high latitudes of North America and Eurasia, deciduous broadleaf trees in southeastern US, C_3 grasses in central

US, South America, Eurasian Steppe, Africa, and east Australia, C_4 plants in southeast US, South America, Africa, Southeast Asia, and northern Australia, and shrubs in the semi-arid areas are reasonably simulated (Figure S2). Overall, the simulated vegetated area covers 77.5% of the global land surface. The simulated tree, C_3 grass, C_4 plants, and shrubs cover 31.1%, 11.3%, 15.3%, and 14.5%, respectively. These fractions are consistent with those in the study of Liu et al. (2019).

3.2 Effects of dynamic vegetation processes on SM, SIF, and GPP simulations

The spatial distribution of the global SIF simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF were evaluated against the OCO-2 measurements in Figure 3. The SIF simulated in SSiB2/SIF shows a negative bias in the South American and African savanna regions, southeast China, and east US, while a positive bias in the boreal forest in North America and North and Central Asia. In SSiB4/TRIFFID/SIF, the simulated SIF bias is positive in most regions, especially in semi-arid regions such as the Western United States, southwest South America, Africa, Central Asia, and Australia. Its positive bias is smaller in boreal forests compared with that in SSiB2/SIF. Table 2 lists the global spatial correlation coefficient (SCC), bias (BIAS), and root-mean-square error (RMSE) of the simulated SIF in SSiB2/SIF and SSiB4/TRIFFID/SIF compared with the OCO-2 SIF data. The SCC increased by 10%, and the RMSE decreased by 12% in SSiB4/TRFFID/SIF, which shows an improvement in the spatial pattern of the simulated SIF in the run with dynamic vegetation included. However, the absolute value of the global mean SIF bias increased in SSiB4/TRIFFID/SIF. The improvement in SCC indicates that the vegetation spatial distribution simulated by SSiB4/TRIFFID/SIF is more realistic than the observation-based one used in SSiB2/SIF and further confirms the reasonability of the vegetation distribution simulation. The simulated SIF in different seasons was also compared with OCO-2 SIF data. The highest RMSE of simulation compared to OCO-2 occurs in summer both in SSiB2/SIF and SSiB4/TRIFFID/SIF. The most obvious improvement in

SSiB4/TRIFFID/SIF appears in spring, with the SCC increasing by 37% and the RMSE decreasing by 18%.

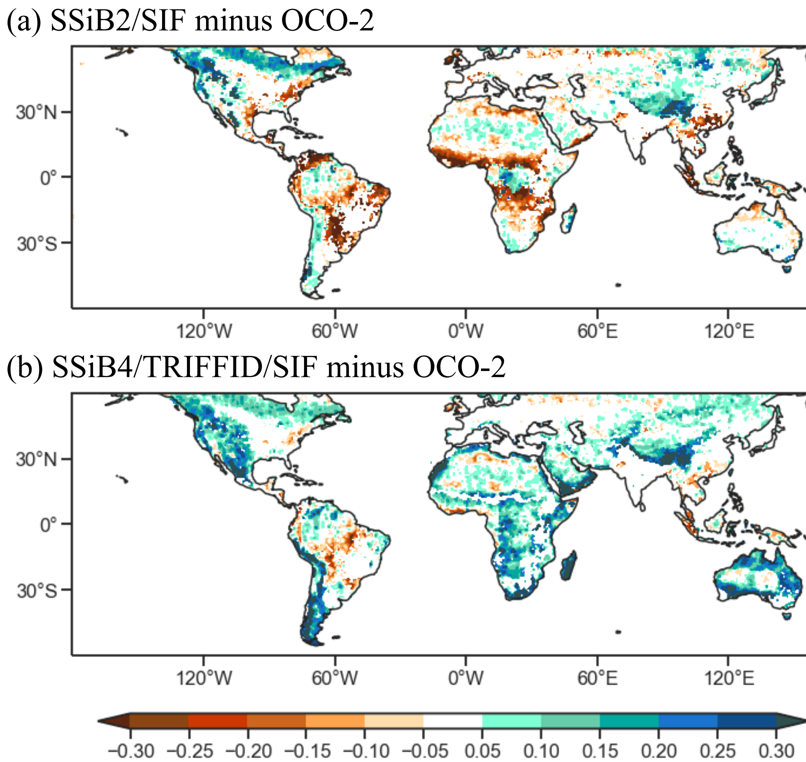


Figure 3. Global differences of solar-induced chlorophyll fluorescence (SIF) between simulations in (a) SSiB2/SIF, (b) SSiB4/TRIFFID/SIF and Orbiting Carbon Observatory 2 (OCO-2) data. Units: W/m^2/μm/sr.

Table 2. Spatial Correlation Coefficient (SCC), Mean Bias (BIAS), and Root-Mean-Square Error (RMSE) of annual SIF simulations compared to OCO-2 data. Units: W/m^2/μm/sr.

	SSiB2/SIF	SSiB4/TRIFFID/SIF
SCC	0.779	0.864
BIAS	-0.043	0.064
RMSE	0.169	0.143

The GPP simulation in SSiB2/SIF and SSiB4/TRIFFID/SIF was compared with observation-based estimated GPP in 2015, excluding the polar regions. In the three observation-based estimates, the global GPP ranges from 835.2 to 1088 g C/m^2/yr, with a median of 867.3 g C/m^2/yr. Figure 4 shows that the global GPP simulated by SSiB2/SIF is much lower than the observation-based estimations, with a value of 533.2 g C/m^2/yr. The simulated global GPP in SSiB4/TRIFFID/SIF is 875.2 g C/m^2/yr, which is close to the median value of the three observation-based estimates. Figure 5 further compared the latitudinal distribution of zonal mean GPP among the observation-based estimates and model simulations. The GLASS and FLUXSAT products demonstrate higher GPP values near the equator, while the FLUXCOM product has higher GPP values in subtropical regions in the Northern Hemisphere. The SSiB2/SIF GPP simulation is lower than the observation-based GPP products at all latitudes. The SSiB4/TRIFFID/SIF GPP simulation is close to the observation-based estimates except near the tropics, where the observation-based estimates show large discrepancies. Therefore, the SSiB4/TRIFFID/SIF simulation is within the range of various observations. Introducing the dynamic vegetation process can lead to significant improvement in GPP simulation throughout the globe. The plausible reason that may contribute to the improvement of GPP simulation in SSiB4/TRIFFID/SIF is the diversity of PFTs existing in a single grid box. In SSiB2/SIF, there is only one PFT in one grid box with the vegetation parameters, such as vegetation fraction cover (FRAC), LAI, and vegetation height (VH), specified based on a vegetation table (Sellers et al., 1996). In SSiB4/TRIFFID/SIF, each grid box consists of 7 PFTs, with the competition among them. The vegetation parameters are updated based on the carbon budget and related to the surface energy and water cycles. The improvement shows that the dynamic vegetation process can substantially improve the simulation of the carbon process and can help to provide a reasonable simulation of vegetation conditions and carbon fluxes.

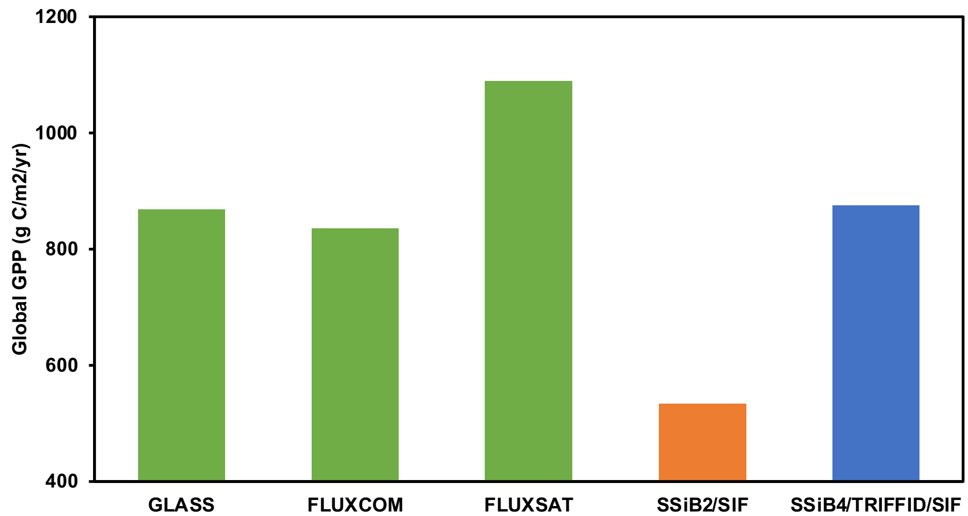


Figure 4. Comparison among observation-based estimated, SSiB2/SIF simulated, and SSiB4/TRIFFID/SIF simulated global GPP in 2015 (60°S–75°N). Units: g C/m^2/yr.

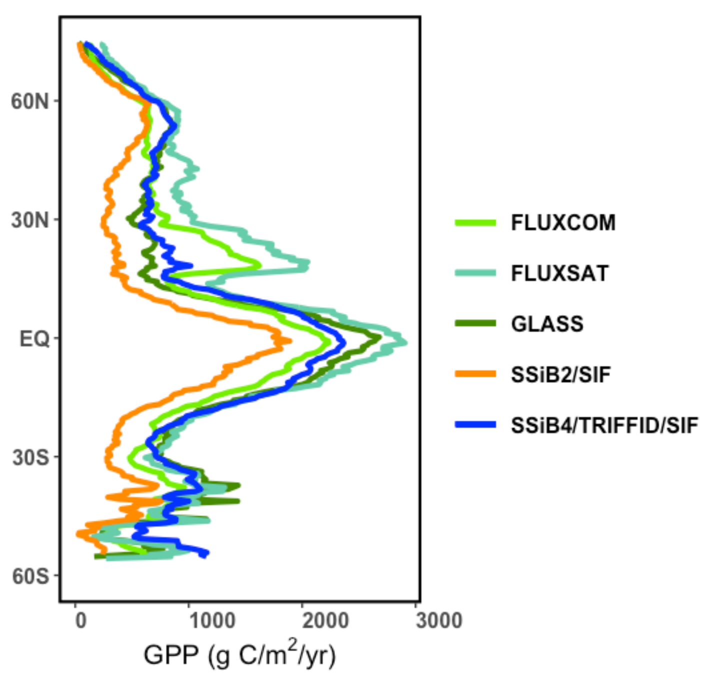


Figure 5. Comparisons of the latitudinal distribution of the zonal mean GPP among the observation-based estimates, SSiB2/SIF simulation, and SSiB4/TRIFFID/SIF simulation. Units: g C/m^2/yr.

Figure S3 compares the simulated soil moisture in SSiB2/SIF and SSiB4/TRIFFID/SIF with SMAP L3 soil moisture data. Over the globe, there was only marginal improvement in SSiB4/TRIFFID/SIF compared with SSiB2/SIF (Table S1). However, in SSiB4/TRIFFID/SIF, the global simulated SIF is higher, which represents higher photosynthesis and transpiration, the simulated soil evaporation rate is much lower, leading to a marginal change in simulated evapotranspiration. The spatial patterns of the soil moisture bias in SSiB2/SIF and SSiB4/TRIFFID/SIF are similar. The models underestimated the surface soil moisture in most areas, such as the North American boreal forest, Eastern United States, Amazon Basin, equatorial Africa, and Southeast Asia. The soil moisture was overestimated in the Eurasian boreal forest and central Asia. Calibration of the parameters directly related to soil property and affecting the vertical soil water distribution in SSiB4/TRIFFID/SIF is needed to improve the soil moisture simulation, which will be discussed in Section 3.4.

3.3 SIF−soil moisture relationship

Soil moisture plays a dominant role in determining dryness stress on ecosystem production over most vegetated areas (Liu et al., 2020). Several studies have analyzed the influence of soil water content limitation on vegetation productivity using various satellite products. Short Gianotti et al. (2019) found that the SIF−soil moisture relationship has increasing response strength with aridity, with little in the light-limited humid regions of the contiguous United States. Jonard et al. (2022) distinguished the water-limited and light-limited environments using the TROPOspheric Monitoring Instrument (TROPOMI) SIF data and the SMAP multitemporal dual channel algorithm (MT-DCA) soil moisture data in the growing season. We calculated the Pearson correlation coefficient between model-simulated SIF and soil moisture and evaluated it against that between OCO-2 SIF and SMAP L3 soil moisture. The SIF and soil moisture data used here are monthly data with seasonal cycles removed. Figure 6 shows the comparison of the correlation coefficient distribution between soil moisture and SIF in observation and simulation. The observed SIF−soil moisture correlation map shows a significant positive correlation over most regions, suggesting the water limitation on vegetation growth. Both SSiB2/SIF and SSiB4/TRIFFID/SIF simulations show a strong correlation between soil moisture and SIF anomalies in semi-arid regions, such as the Western United States, South American savanna, and South and East Africa. Meanwhile, both SSiB2/SIF and SSiB4/TRIFFID/SIF produce negative correlations over the Eastern United States, La Plata Basin, and south China, which is opposite to that in the observation. Over the Eurasian Steppe and coastal Australia, SSiB2/SIF and SSiB4/TRIFFID/SIF simulations show different correlation relationships. The SSiB4/TRIFFID/SIF model produced a positive relationship consistent with that derived from satellite data, while in SSiB2/SIF, the relationship is negative. The SIF−soil moisture correlation derived from the simulations in SSiB4/TRIFFID/SIF is more consistent with that derived from satellite data, showing that the coupling with the dynamic vegetation model helps to better capture the effects of monthly soil moisture dynamics on vegetation photosynthetic activities.

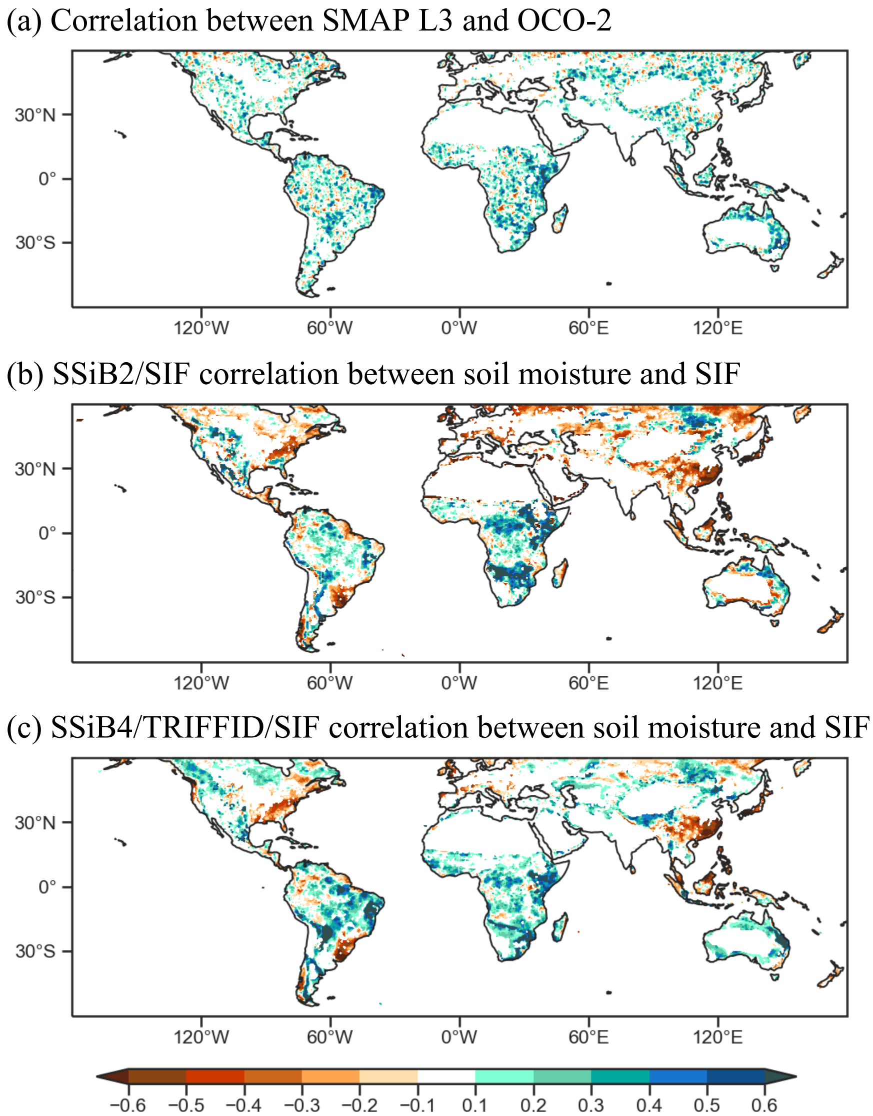


Figure 6. Comparisons of the correlations in the Northern Hemisphere summer between the monthly anomalies of (a) SMAP L3 soil moisture data and OCO-2 SIF data, (b) the SSiB2/SIF

simulated soil moisture and SIF, and (c) the SSiB4/TRIFFID/SIF simulated soil moisture and SIF.

3.4 Effects of key parameters on soil moisture and SIF simulation

The B parameter, K_s, wilting point, and V_{max} were changed within the normal range of soil and vegetation property variations to conduct experiments to show the model sensitivity to changes in the parameters (Beerling and Quick, 1995; Von Caemmerer and Furbank, 1999; Xue et al., 1996) (Table 3). The experiments covered the period from 2010 to 2019. The years from 2010 to 2014 were used for spin-up, and the annual results from 2015 to 2019 were analyzed.

Table 3. Soil and vegetation parameters used in the sensitivity experiments.

	Values
B parameter	3, 4, 5, 6, 7, 8, 9
K_s	2E-3, 2E-4, 2E-5, 2E-6, 2E-7
Wilting point	2, 4, 6, 8, 10, 12
V_{max}	20, 40, 60, 80, 100, 120, 140 ($\mu mol/m^2/s$)

3.4.1 Soil property parameters

Previous studies have shown that the soil property parameters are one of the key sources of uncertainties in soil moisture simulation in land surface models (Demaria et al., 2007; Qiu et al., 2018). According to previous work, carbon fluxes are also sensitive to soil parameters in the SSiB model (Prihodko et al., 2008). To improve the soil moisture and SIF simulation in SSiB4/TRIFFID/SIF and to better understand the role of the parameters determining the soil texture in the interactions between the water and carbon cycles, we examined the effects of B parameter, K_s, and wilting point on soil moisture and SIF simulation in SSiB4/TRIFFID/SIF (Figure 7).

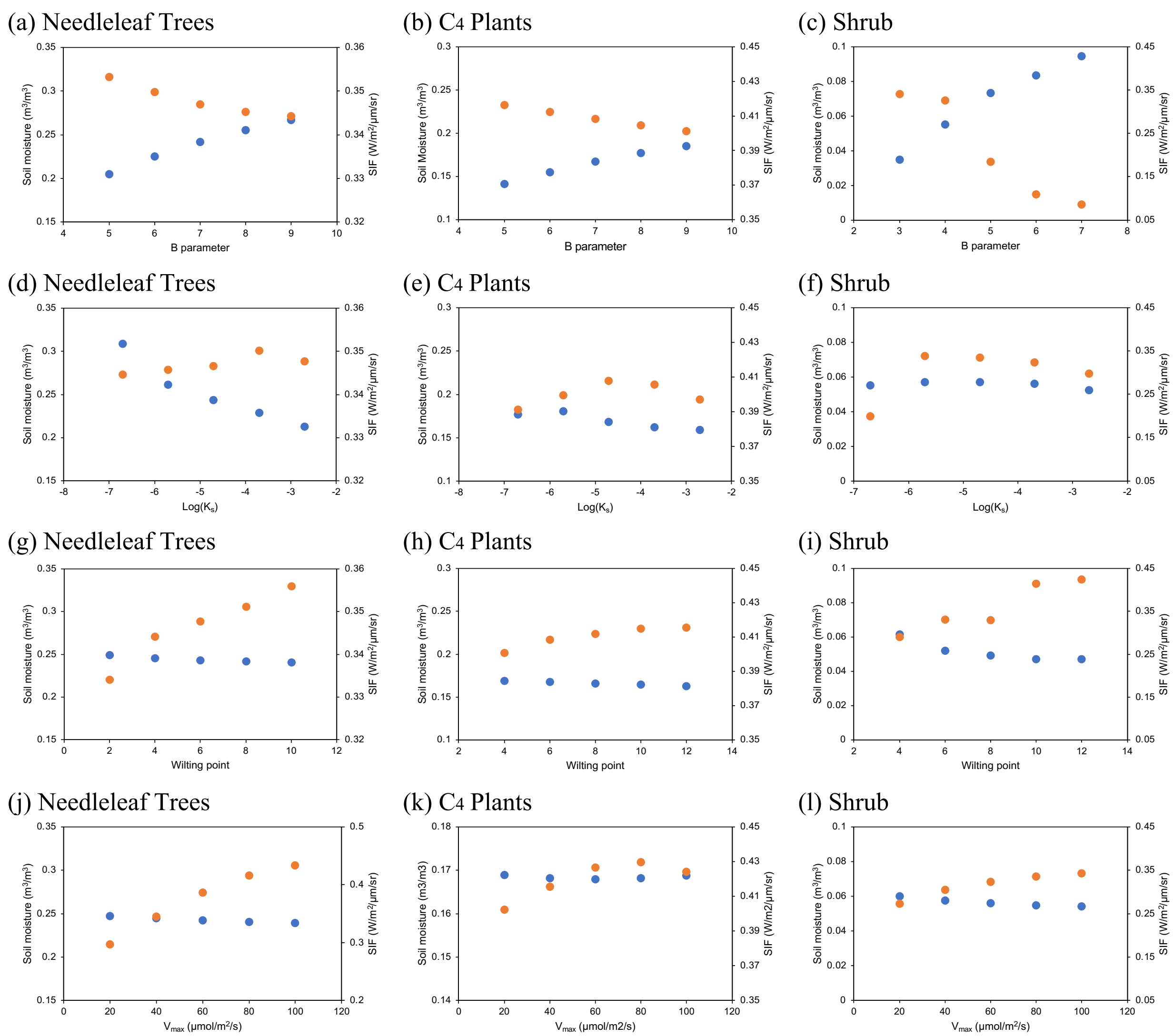


Figure 7. Calculated soil moisture (blue), SIF (orange) for (a, d, g, j) needleleaf trees, (b, e, h, k) C_4 plants, and (c, f, i, l) shrubs under different (a, b, c) B parameter; (d, e, f) logarithm of K_s; (g, h, i) wilting point, and (j, k, l) V_{max}.

The effects of the B parameter on water and carbon cycles are complex. With a higher B parameter, soil moisture increased, and SIF decreased (Figures 7a, 7b, 7c). A higher B parameter represents a soil texture closer to clay, which leads to more difficulty in soil evaporation and more soil moisture. Meanwhile, soil hydraulic conductivity decreased with increased B parameter (Eq. 2), which reduced the total runoff and may have increased evaporation; however, the change in evaporation was marginal. Overall, a higher B parameter is associated with more soil moisture. Moreover, the B parameter indirectly modifies SIF through its effect on the wilting point. The change in the B parameter modifies the relationship between soil water potential and soil water content through the retention curve. When the B parameter is higher, for a given amount of soil water content, the absolute value of water potential increases, and then the β factor in Eq. 3 is reduced, leading to stomata close and lower SIF and transpiration. In the tropics, the soil moisture increased with a larger B parameter while the SIF and transpiration almost stayed the same. The abundant soil water content in the rainforests keeps the β factor high in the change of the B parameter.

As for K_s, the soil moisture decreases when K_s is higher (Figures 7d, 7e, 7f). Higher K_s indicates that the soil texture is closer to sand, increasing surface infiltration and changing the vertical soil water content distribution. The hydraulic conductivity is larger with higher K_s, leading to larger drainage and decreased total soil water content. When K_s becomes very low, the surface infiltration becomes extremely low, leading to much larger runoff and low root zone soil moisture. The low root zone soil water potential under low K_s conditions in SSiB4/TRIFFID/SIF lead to lower β factor and SIF. Therefore, the SIF drops in SSiB4/TRIFFID/SIF when the K_s value is very small. In humid regions, it is hard for the soil water content to drop to a value at which photosynthesis weakens, so the SIF does not change obviously (Figure 7d).

For the wilting point, when it increases, the soil moisture, at which the stomata close completely, drops, leading to a higher β factor (Eq. 3), allowing more open stomata and higher stomatal conductance, which leads to higher SIF and photosynthesis and transpiration rates (Figures 7g, 7h, 7i). For example, in South Africa covered by savanna, when the wilting point increased from 4 to 10, the corresponding volumetric soil moisture at which β factor started to increase rapidly decreased from 0.30 to 0.13 m^3/m^3, and the simulated SIF increased from 0.40 to 0.42 $W/m^2/\mu m/sr$ (Figure 7h). Since a higher wilting point leads to higher transpiration rates, the soil moisture decreases with the increase of the wilting point. However, the effects of the wilting point on soil moisture are not as efficient as that of the B parameter and K_s. For example, the soil moisture in South Africa dropped slightly from 0.169 to 0.165 m^3/m^3 when the wilting point increased from 4 to 10 (Figure 7h).

3.4.2 Vegetation parameter

Photosynthesis is an important process of the terrestrial carbon cycle, and it is simulated in SSiB2/SIF and SSiB4/TRIFFID/SIF following the analytical solution approach developed by Zhan et al. (2003) based on the Collatz et al. (1991) and Collatz et al. (1992) model. The vegetation parameter directly related to photosynthesis, V_{max}, varies considerably among and within plant functional types (PFTs) (Kattge et al., 2009; Wang et al., 2021; Wullschleger, 1993), and it cannot be measured directly but must be inferred by model inversion from photosynthesis measurements. The terrestrial biosphere models demonstrate considerable sensitivity in carbon flux simulation given the uncertainty in V_{max} (Bonan et al., 2011; Piao et al., 2013). To further improve the carbon flux simulation in SSiB4/TRIFFID/SIF and to explore the effects of this vegetation parameter on water and carbon cycles, we examined the effects of V_{max} on soil moisture and SIF simulation in SSiB4/TRIFFID/SIF.

As demonstrated in Figure 7j, the photosynthesis rates of needleleaf trees are especially sensitive to the change in V_{max} in all the PFTs simulated in SSiB4/TRIFFID/SIF. When the V_{max} value increased from 20 to 100 $\mu mol/m^2/s$, the SIF simulation increased dramatically from 0.30 to 0.43 $W/m^2/\mu m/sr$, which is a much more marked increment compared with the changes in the B parameter, K_s, and wilting point as shown in Section 3.4.1. For other PFTs, the effects of V_{max} on SIF simulation are also significant. For example, with the V_{max} changing from 20 to 80 $\mu mol/m^2/s$, the SIF simulation increased from 0.40 to 0.43 $W/m^2/\mu m/sr$ in the South African savanna, and the SIF simulation increased from 0.27 to 0.34 $W/m^2/\mu m/sr$ in shrubland in the Western United States (Figure 7k). The effects of V_{max} on soil moisture simulation are similar to that of the wilting point. With the increasing V_{max}, the photosynthesis rates are higher, leading to higher SIF and transpiration rates, which results in lower soil moisture. For example, in the

Western United States, the soil moisture decreased from 0.060 to 0.054 m^3/m^3 when the V_{max} increased from 20 to 100 $\mu mol/m^2/s$ (Figure 7l).

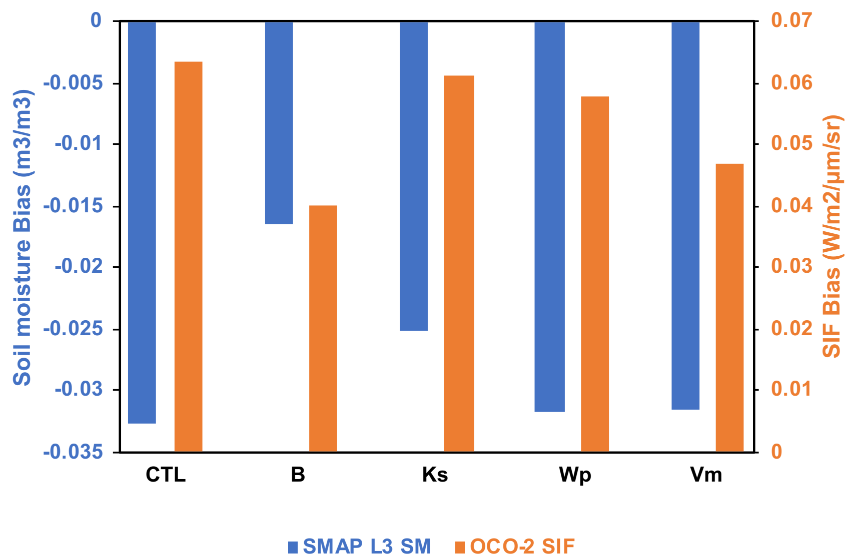
3.5 Improvement in soil moisture and SIF simulation after calibration

Based on the tests in section 3.4, we identified that the B parameter, K_s, wilting point, and V_{max} are the key parameters that significantly impact both soil moisture and SIF simulations in SSiB4/TRIFFID/SIF. To identify their impact on soil moisture and SIF simulation, we first conducted a set of experiments with individual parameters modified in each test. The B parameter, K_s, wilting point, and V_{max} were modified in Test B, Test K_s, Test Wp, and Test V_m. The range of these parameters is according to the sensitivity tests in section 3.4. The soil moisture and SIF in the control run and the four tests were calculated and compared with the SMAP L3 and OCO-2 data at global scales. In the tests with the modified soil parameters, the parameter set with minimum RMSE in soil moisture is identified as the optimized set, and the experiment with this set of parameters will be referred to as Test B opt, Test K_s opt, and Test Wp opt, while in the test with the modified vegetation parameter, the parameter set with minimum RMSE in SIF is identified as the optimized set, Test V_m opt.

Figure 8 shows the improvement in the global mean bias and RMSE of soil moisture and SIF simulations in each test with the optimized values relative to SMAP L3 soil moisture and OCO-2 SIF data. The most significant improvement in soil moisture and SIF simulations both occurred in Test B, and the most significant improvement in SIF simulation happened in Test V_m. The improvement in soil moisture simulation is also substantial in Test K_s, but the effects of K_s are less efficient than the B parameter. Through this set of tests, we found that the improvement of both soil moisture and SIF simulation is most with the change in the B parameter. The soil moisture simulation is most sensitive to the B parameter and K_s, while the SIF simulation is most sensitive to V_{max}. Based on these results, we designed another set of experiments listed in Table 1 to get optimal values of the four parameters in SSiB4/TRIFFID/SIF. The tests with the set of optimal parameters will be referred to as Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt. The soil moisture and SIF in the control run and four tests were evaluated at global scales and for the six PFTs, including the Evergreen Broadleaf

Trees (EBT), Needleleaf Trees (NT), C_3 Grasses (C_3), C_4 Plants (C_4), Shrub (SH), and Deciduous Broadleaf Trees (DBT).

(a) BIAS



(b) RMSE

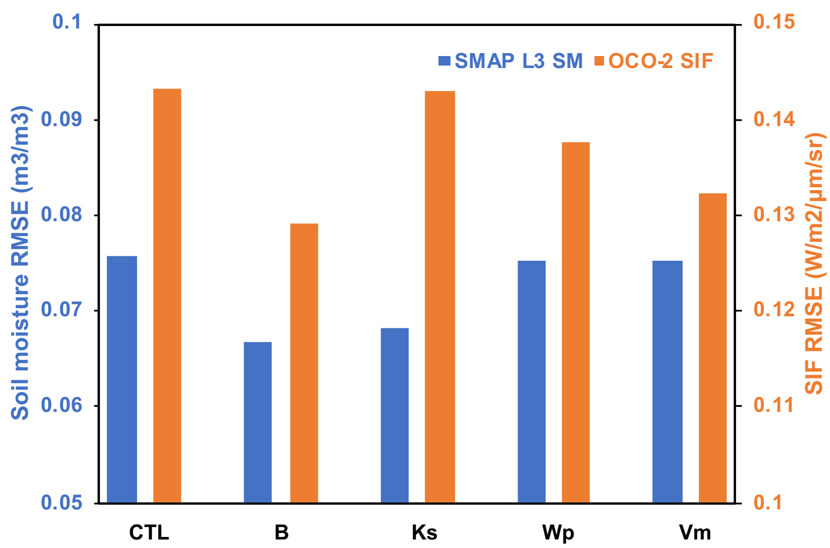
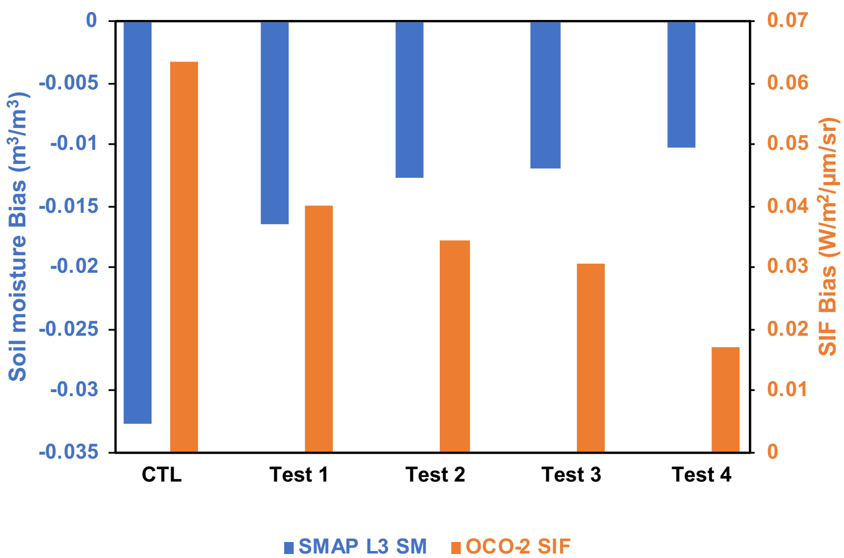


Figure 8. Global (a) mean bias (BIAS) and (b) root-mean-square error (RMSE) in the control run (CTL), Test B opt (B), Test K_s opt (Ks), Test Wp opt (Wp), and Test V_{max} opt (Vm) relative to SMAP L3 soil moisture and OCO-2 SIF data.

Figure 9 shows the global mean bias and RMSE of soil moisture and SIF relative to SMAP L3 soil moisture and OCO-2 SIF data in the control run, Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt. The optimal B parameter led to significant improvement in both soil moisture and SIF, with the global mean bias decreasing by 49.6% (from -0.033 to -0.0165 m^3/m^3) and by 37.0% (from 0.064 to 0.040 $W/m^2/\mu m/sr$), respectively, and with the RMSE decreasing by 11.9% (from 0.076 to 0.067 m^3/m^3) and by 9.9% (from 0.143 to 0.129 $W/m^2/\mu m/sr$), respectively. The optimal K_s also improved both soil moisture and SIF simulation but with reduced magnitude in SIF. The global mean bias decreased by 22.7% and 13.7%, respectively, and the global RMSE decreased by 4.6% and 0.3%, respectively. Wilting point calibration also improved the simulation but with less magnitude in soil moisture. It decreased the mean bias by 5.8% and 11.2%, respectively, and the RMSE by 0.3% and 3.1%, respectively. The calibrated V_{max} further improved the SIF simulation substantially by 44.0% on the global mean bias and

5.9% on the RMSE and improved the soil moisture simulation slightly by 14.6% on the global mean bias.

(a) BIAS



(b) RMSE

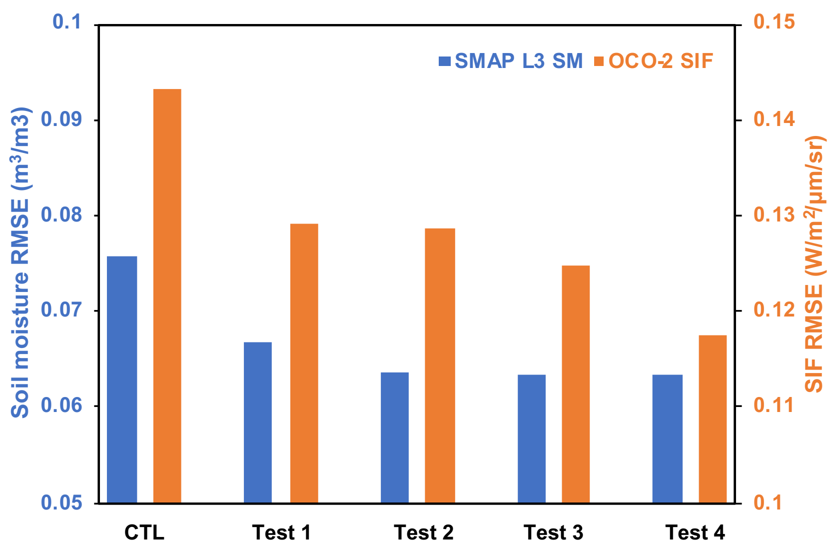


Figure 9. Global (a) mean bias (BIAS) and (b) root-mean-square error (RMSE) in the control run (CTL), Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt relative to SMAP L3 soil moisture and OCO-2 SIF data.

Figures 10a and 10b illustrate the spatial distribution of global differences between simulated and SMAP L3 soil moisture and between simulated and OCO-2 SIF. The SSiB4/TRIFFID/SIF model significantly underestimated the soil moisture in most regions, especially in the tropics and semi-arid regions, while overestimating the SIF throughout the globe, with the most significant overestimation occurring in the semi-arid regions covered by shrubs and savanna. To delineate the spatial distribution of improvement in each test, Figures 10c to 10j show the soil moisture and SIF differences between simulations and observations in the test runs and the control run, and Table 4 lists the spatial correlation coefficient (SCC), mean bias (BIAS), and RMSE of the soil moisture and SIF at the global scale and for different vegetation types in the test runs and the control run. The most significant improvement for soil moisture simulation was in tropical rainforests and semi-arid regions. In Test 1 opt, with the B parameter modified, the soil moisture increased substantially over the tropics in the Amazon basin and Central Africa and in semi-arid regions, such as the Western United States, south Argentina, Sahel, South Africa, and Australia (Figure 10c). The soil moisture BIAS of EBT decreased from -0.103 to -0.069 m^3/m^3 and the RMSE from 0.124 to 0.097 m^3/m^3. The BIAS and RMSE of SH decreased from 0.057 to 0.043 m^3/m^3 and from 0.057 to 0.043 m^3/m^3, respectively, in soil moisture simulation. The SIF simulation was improved together with soil moisture in Test 1 in semi-arid regions covered by shrubs, including the Western United States, South Africa, and coastal Australia (Figure 10d). The BIAS and RMSE of SIF simulation for SH decreased from 0.130 to 0.018 $W/m^2/\mu m/sr$, and from 0.174 to 0.096 $W/m^2/\mu m/sr$. With the modification of K_s in Test 2 opt, the soil moisture simulation in the tropics was further improved (Figure 10e), with the BIAS and RMSE of EBT further decreased to -0.043 m^3/m^3 and 0.082 m^3/m^3, and both the soil moisture and SIF simulations were improved in the savanna in Africa, the Sahel, and coastal Australia (Figure 10e and Figure 10f). In Test 3 opt, the soil moisture simulation was slightly improved for C_3 and DBT, and the SIF simulation was improved for most PFTs, including EBT, C_3, C_4, SH, and DBT (Table 4). In Test 4 opt, the V_{max} modification significantly improved SIF simulation in the boreal forests in North America and Siberia and the grassland in the central United States and South America (Figure 10j). The BIAS and RMSE of NT in SIF simulation decreased from 0.080 to 0.036 $W/m^2/\mu m/sr$ and from 0.128 to 0.099

W/m^2/μm/sr. For C_3, the BIAS and RMSE of SIF simulation decreased from 0.111 to 0.081 W/m^2/μm/sr and from 0.174 to 0.153 W/m^2/μm/sr.

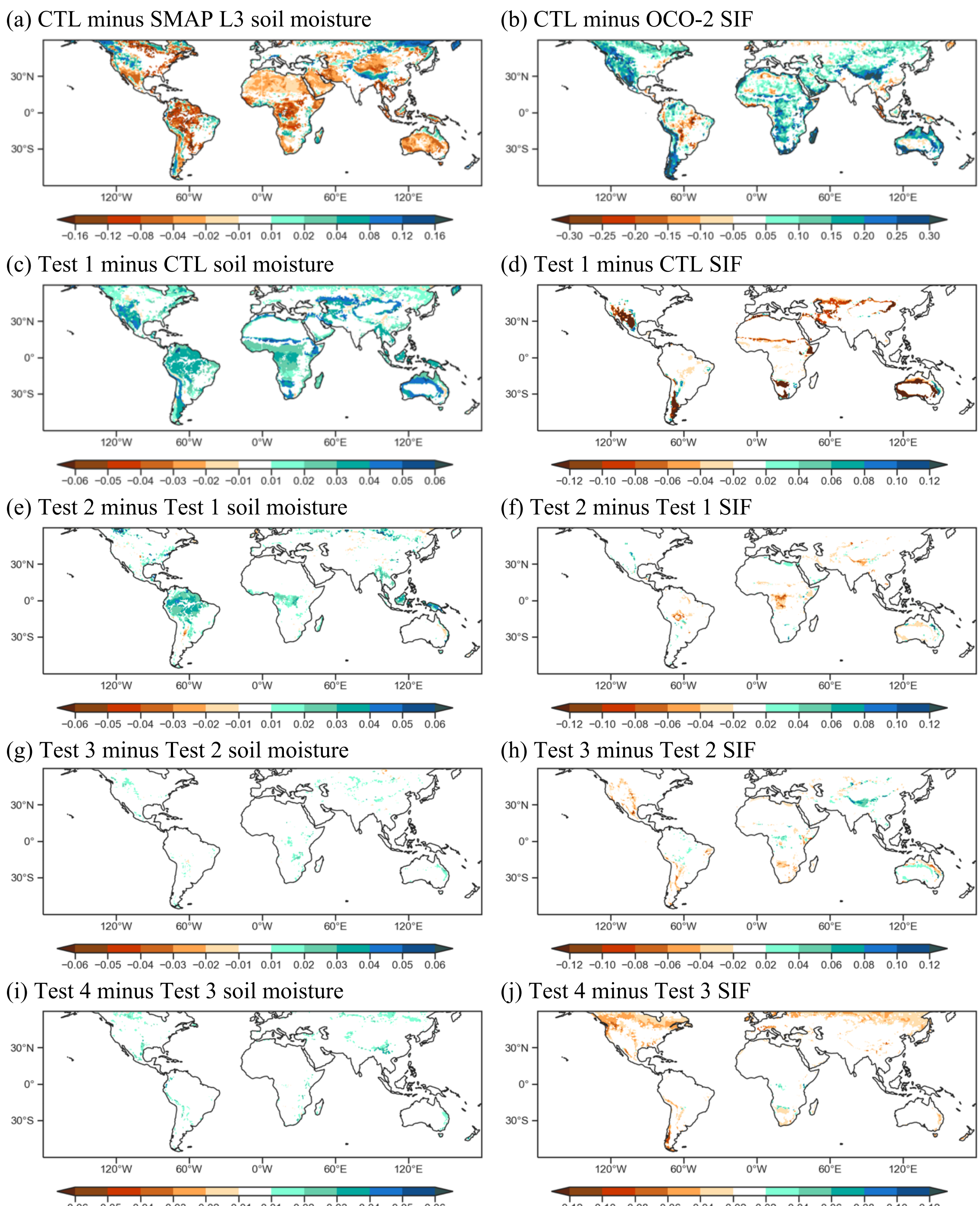


Figure 10. Global differences of simulated soil moisture and SIF in the control run compared to (a) SMAP L3 (units: m^3/m^3) and (b) OCO-2 (units: $W/m^2/\mu m/sr$). Global differences of simulated soil moisture (c, e, g, i) (units: m^3/m^3) and SIF (d, f, h, j) (units: $W/m^2/\mu m/sr$) in the control run and different tests. (c, d) Test 1 opt minus CTL, (e, f) Test 2 opt minus Test 1 opt, (g, h) Test 3 opt minus Test 2 opt, (i, j) Test 4 opt minus Test 3 opt.

Table 4. Spatial Correlation Coefficient (SCC), Mean Bias (BIAS), and Root-Mean-Square Error (RMSE) of the comparison between SSiB4/TRIFFID/SIF simulated and observation-based soil moisture and SIF. Units for soil moisture: m^3/m^3. Units for SIF: $W/m^2/\mu m/sr$.

Vegetation Type	Experiment	Soil Moisture			SIF		
		SCC	BIAS	RMSE	SCC	BIAS	RMSE
Evergreen Broadleaf Trees (EBT)	CTL	0.366	-0.103	0.124	0.150	-0.016	0.124
	Test 1 opt	0.366	-0.069	0.097	0.119	-0.023	0.128
	Test 2 opt	0.335	-0.043	0.082	0.120	-0.037	0.130
	Test 3 opt	0.332	-0.042	0.081	0.136	-0.035	0.128
	Test 4 opt	0.330	-0.042	0.081	0.141	-0.035	0.128
Needleleaf Trees (NT)	CTL	0.304	-0.012	0.087	0.411	0.082	0.130
	Test 1 opt	0.288	0.000	0.087	0.413	0.081	0.130
	Test 2 opt	0.302	0.003	0.086	0.402	0.078	0.128
	Test 3 opt	0.303	0.003	0.086	0.422	0.080	0.128
	Test 4 opt	0.312	0.006	0.086	0.439	0.036	0.099
C_3 Grasses (C_3)	CTL	0.489	0.012	0.070	0.407	0.124	0.187
	Test 1 opt	0.494	0.002	0.069	0.390	0.126	0.189
	Test 2 opt	0.498	-0.006	0.069	0.392	0.125	0.188
	Test 3 opt	0.498	-0.003	0.068	0.418	0.111	0.174
	Test 4 opt	0.508	0.008	0.069	0.406	0.081	0.153
C_4 Plants (C_4)	CTL	0.662	-0.042	0.080	0.491	0.055	0.151
	Test 1 opt	0.671	-0.022	0.071	0.514	0.044	0.145
	Test 2 opt	0.674	-0.017	0.069	0.518	0.036	0.142
	Test 3 opt	0.676	-0.016	0.069	0.542	0.026	0.138
	Test 4 opt	0.676	-0.014	0.069	0.550	0.020	0.136
Shrub (SH)	CTL	0.540	-0.034	0.057	0.368	0.130	0.174
	Test 1 opt	0.541	-0.000	0.043	0.612	0.018	0.096
	Test 2 opt	0.533	-0.001	0.043	0.617	0.008	0.098
	Test 3 opt	0.536	0.001	0.043	0.605	-0.001	0.091
	Test 4 opt	0.538	0.001	0.043	0.601	-0.005	0.090
Deciduous Broadleaf	CTL	0.858	-0.054	0.090	0.264	0.075	0.222
	Test 1 opt	0.861	-0.030	0.077	0.261	0.073	0.221

Trees (DBT)	Test 2 opt	0.864	-0.014	0.070	0.198	0.072	0.228
	Test 3 opt	0.866	-0.014	0.069	0.224	0.068	0.222
	Test 4 opt	0.864	-0.014	0.069	0.248	0.045	0.211

4 Discussion

This study shows that the B parameter is a key parameter that connects the water and carbon cycles in SSiB models and has significant effects on both soil moisture and SIF simulations. The B parameter has the largest impact on soil moisture for all PFTs, and its effect on SIF varies among different vegetation types. The impact on SIF simulation is larger over semi-arid regions where the soil water content is a key limitation factor on vegetation growth. The K_s can also affect both soil moisture and SIF simulations but with reduced magnitude. The wilting point and V_{max} have significant effects on SIF simulation, but their effects on soil moisture simulation are not substantial compared with the B parameter and K_s. Consistent with the previous study (Qiu et al., 2018) in SSiB2/SIF, the wilting point plays a role in connecting the carbon and water cycles in semiarid regions in SSiB4/TRIFFID/SIF. For humid regions, the role of the wilting point is limited, and V_{max} is more important in SIF simulation, especially for the boreal forests.

To evaluate the model performance in predicting the temporal variability of soil moisture and SIF, we created the time series of the monthly satellite observations and simulations in the control run and four tests with the optimal parameter values. Figure 11 demonstrates the monthly mean soil moisture and SIF at the global scale in the control run and the test runs together with the satellite observations from Jan 2016 to Dec 2019. After calibrating the four parameters, the simulated global mean soil moisture increased by about 0.02 m^3/m^3, and the simulated global mean SIF decreased by about 0.05 $W/m^2/\mu m/sr$. Among all the PFTs, the seasonality of soil moisture and SIF simulations for C_4 plants and shrubs was best simulated, and the simulated soil moisture and SIF values got the most improvement for these two PFTs (Figure 12). At the global scale, the most improvements in soil moisture were in Test 1 opt, and secondarily in Test 2 opt. The seasonality of soil moisture had a marginal change in four tests, and the increment happened throughout the year. The improved soil moisture simulation still has a considerable discrepancy compared with the SMAP L3 soil moisture, which means the model needs to be further improved. To pursue more improvement, forthcoming work can use the global high-resolution dataset of soil hydraulic properties instead of parameterization for each vegetation type in the soil moisture simulation (Dai et al., 2019). For the SIF simulation, the most improvement happened in Test 1 opt and Test 4 opt. The SIF simulation was improved in spring, fall, and winter, but got worse in summer. The higher B parameter value decreased the SIF simulation in each season while the change in V_{max} had more effect in summer. To improve the seasonality of SIF simulation, future work can test the parameters in the TRIFFID model to better simulate vegetation distribution, LAI, and SIF.

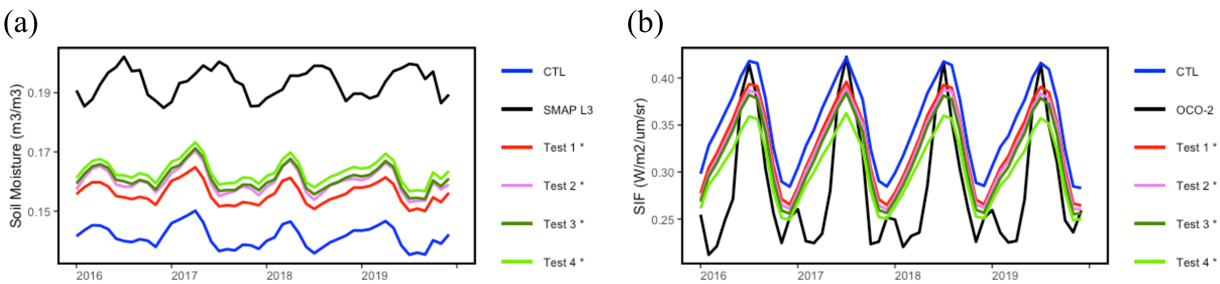


Figure 11. The monthly mean (a) soil moisture and (b) SIF at the global scale (60°S–60°N) in different experiments. * Indicates significant differences between different experiments (p<0.01).

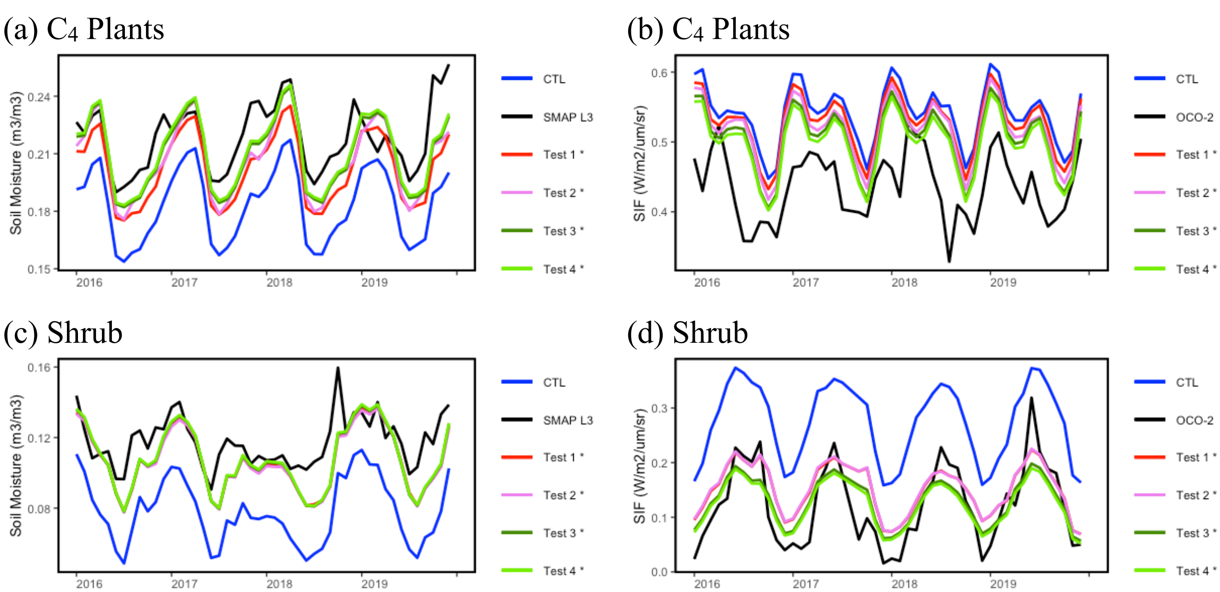


Figure 12. The monthly mean (a, c) soil moisture and (b, d) SIF of (a, b) C_4 plants in Africa and (c, d) shrubs in the Western United States in different experiments. * Indicates significant differences between different experiments (p<0.01).

Qiu et al. (2018) integrated the SMOS soil moisture data and GOSAT SIF data into SSiB2/SIF to understand the response of SIF to soil moisture dynamics. SSiB2/SIF largely overestimated the soil moisture and underestimated the SIF in most regions when evaluated against SMOS soil moisture and GOSAT SIF but underestimated both soil moisture and SIF in semiarid regions. Therefore, calibration of the B parameter and K_s in SSiB2/SIF based on the SMOS soil moisture resulted in better soil moisture simulation but poorer SIF simulation for regions covered by savanna, grass, and shrub. Ma et al. (2019) assessed several satellite surface soil moisture products using global ground-based observations and found that the SMOS products exhibited dry bias due to their underestimating surface temperature. In this study, we used SMAP L3 soil moisture data instead of SMOS to calibrate the B parameter and K_s, and the SIF simulation was evaluated against OCO-2 SIF data. Compared with the SMAP L3 product, SSiB4/TRIFFID/SIF underestimated the soil moisture in most regions. Also, the introduction of the dynamic vegetation processes made the SIF simulation higher than the satellite observation throughout the globe. These two aspects lead to improved soil moisture and SIF simulation in SSiB4/TRIFFID/SIF after calibrating the B parameter and K_s in semiarid regions, which differs from the previous results (Qiu et al., 2018). This study confirmed the importance of using satellite products with higher accuracy and precision, and better spatial and temporal resolution in the calibration of parameters in SSiB models and the exploration of the relationship between soil moisture and SIF. The SMAP products provide the high-resolution mapping of global soil moisture and have been widely validated against core validation sites (Burgin et al., 2017; Zhang et al., 2017). Zhang et al. (2019) assessed the SMAP L3 product using extensive ground measurements from sparse networks and found that the product showed better performance in temperate zones and grassland while negative bias in tropical climate zones and regions with high soil organic carbon contents. As for the OCO-2 SIF data, despite its high resolution, the satellite-observed SIF soundings are sparse, and we averaged the soundings in each 1°×1° pixel first to fulfill more grids with SIF retrieval. This methodology can induce uncertainties in the evaluation of SIF simulation. Those uncertainties in satellite observations can affect the parameter calibration and the understanding of water-carbon cycle interactions. The SMAP L4 product assimilates SMAP brightness temperature observations into a land surface model and provides both the 0-5 cm vertical averaged surface soil moisture and the 0-100 cm vertical averaged root zone soil moisture with complete spatial coverage. The Sentinel-5 Precursor/TROPOspheric Monitoring Instrument (TROPOMI) launched in 2017 provides SIF data with comparable quality but with largely improved spatial and temporal coverage, and Köhler et al. (2018) suggested tying TROPOMI to OCO-2 SIF data in overlapped regions to virtually fill the large gaps left by the OCO-2 product. Future work can include the SMAP L4 and TROPOMI products as further constraints in the model simulation improvement and the SIF−soil moisture relationship exploration.

This study was conducted by the offline models, SSiB2/SIF and SSiB4/TRIFFID/SIF, using meteorological forcing to drive soil moisture, SIF, and GPP simulation. With the coupling of the dynamic vegetation model, SSiB4/TRIFFID/SIF can reproduce the global distribution of dominant vegetation types, the vegetation fraction, and the LAI, including its seasonal, interannual, and decadal variabilities (Zhang et al., 2015; Liu et al., 2019), and can provide an improved simulation of photosynthesis and carbon flux. However, the offline model simulation is not able to include feedback to the atmosphere, which represents a lack of investigation on fully coupled two-way interaction. The simulated SIF and GPP in SSiB4/TRIFFID/SIF were much higher than that in SSiB2/SIF, which indicated higher transpiration. Since the same meteorological forcing was used, the simulated total evapotranspiration fluxes in the two models are consistent, with a lower simulated soil evaporation rate in SSiB4/TRIFFID/SIF. The higher vegetation fraction, LAI, transpiration, and photosynthesis rates in SSiB4/TRIFFID/SIF cannot lead to an obvious change in the soil moisture simulation. Zhang et al. (2021) coupled the SSiB2 model and the SSiB4/TRIFFID model to the NCEP Global Forecast System (GFS) to investigate vegetation-atmosphere feedback and found that the correlations between the simulated and observed monthly LAI, albedo, near-surface temperature, and precipitation were improved with the dynamic vegetation processes included. Therefore, it remains necessary to add the SIF module into the coupled GFS/SSiB4/TRIFFID model and to evaluate the soil moisture, SIF, and GPP simulated by it against satellite products. This fully coupled biophysical processes model has the potential to better reproduce the satellite-observed soil moisture and carbon flux and to contribute to the understanding of the interactions between water and carbon cycles through controls over evapotranspiration, vegetation phenology, and surface energy balance.

5 Conclusions

To investigate the role of dynamic vegetation processes on soil moisture and carbon flux simulations and to better understand the relationship between terrestrial carbon and soil moisture dynamics, this study incorporated the SIF module used in SSiB2/SIF into SSiB4/TRIFFID. The soil moisture, SIF, SIF−soil moisture relationship, and GPP simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF were evaluated against the SMAP L3 soil moisture data and the OCO-2 SIF data. The three soil property parameters, the B parameter, K_s, and wilting point, and the vegetation parameter, V_{max}, were tested within the normal range to confirm their important role in the water and carbon cycles in model simulation and to test their effects on soil moisture, SIF, and the interactions. The four parameters were calibrated using the SMAP L3 soil moisture and OCO-2 SIF to improve the soil moisture and SIF simulations in SSiB4/TRIFFID/SIF.

The coupling with the dynamic vegetation model, TRIFFID, led to substantial improvement in the SIF and GPP simulations. The global spatial correlation of SIF increased by 10%, and the global RMSE of SIF simulation decreased by 12%. The global mean GPP simulation increased from 533.2 g C/m^2/yr to 875.2 g C/m^2/yr, which is closer to the median of three observation-based GPP products (867.3 g C/m^2/yr). The global spatial distribution of the correlation coefficient between soil moisture and SIF was more properly simulated in SSiB4/TRIFFID/SIF, with the relationship switched from negative to positive over the Eurasian Steppe and coastal Australia.

The empirical coefficient, B parameter, has the largest impact on soil moisture simulation and efficiently affects the SIF simulation for plants in semi-arid regions through its effects on water potential and soil water diffusion. K_s also affects soil moisture and SIF simulation through the water diffusion in soil layers. The wilting point and V_{max} affect the stomatal opening and the photosynthesis process, thus changing the transpiration rates and SIF simulation. Their effects on soil moisture simulation exist but are less in magnitude than the B parameter and K_s.

The SMAP L3 and OCO-2 products improved soil moisture and SIF measurements with better quality, higher spatial and temporal resolution, and accuracy. They can help to improve the global performance of SSiB4/TRIFFID/SIF on soil moisture and SIF simulations and provide advances in understanding the global terrestrial coupled water-carbon cycles. The global RMSE of soil moisture and SIF decreased from 0.076 to 0.067 m^3/m^3 and from 0.143 to 0.129 $W/m^2/\mu m/sr$ with the B parameter optimization and further decreased to 0.063 m^3/m^3 and 0.125 $W/m^2/\mu m/sr$ with the K_s and wilting point optimized. Calibration of V_{max} further improved the SIF simulation, with the global RMSE decreased to 0.117 $W/m^2/\mu m/sr$.

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Understanding Interactions between Terrestrial Water and Carbon Cycles Using Integrated SMAP Soil Moisture and OCO-2 SIF Observations and Land Surface Models

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Key Points:

- Dynamic vegetation processes substantially improve of terrestrial carbon flux simulation.
- Satellite products lead to advances in simulation and understanding of water and carbon cycles and their interactions.
- The B parameter, representing the slope of water retention curve, shows the most significant effects on both water and carbon cycles.

Abstract

Recently, more advanced synchronous global-scale satellite observations, the Soil Moisture Active Passive enhanced Level 3 (SMAP L3) soil moisture product and the Orbiting Carbon Observatory 2 (OCO-2) solar-induced chlorophyll fluorescence (SIF) product, provide an opportunity to improve the simulations of both water and carbon cycles in land surface modeling. This study introduces a mechanistic representation of SIF to the Simplified Simple Biosphere Model version 4 (SSiB4) coupled with the Top-down Representation of Interactive Foliage and Flora Including Dynamics Model (TRIFFID). This newly developed model with the observed satellite data indicates that introducing dynamic processes can lead to substantial improvement in global carbon flux simulation. In the SSiB4/TRIFFID/SIF, four critical soil and vegetation parameters--B parameter, soil hydraulic conductivity at saturation (K_s), wilting point, and maximum Rubisco carboxylation rate (V_{max})--were identified through numerical sensitivity experiments. Among the four parameters, the B parameter has the most significant effects on both soil moisture and SIF simulations. With the optimized B parameter, both soil moisture and SIF simulations were improved substantially, with especially significant improvement for shrubs. The K_s and wilting point also affect both soil moisture and SIF but with reduced magnitude. The V_{max} directly affects photosynthesis, and its modification can substantially improve the SIF simulation of needleleaf trees and C_3 grasses. With all four calibrated parameters based on SMAP L3 and OCO-2 data, the root-mean-squared error (RMSE) of soil moisture and SIF simulations decreased from 0.076 to 0.063 m^3/m^3 and from 0.143 to 0.117 $W/m^2/\mu m/sr$, respectively.

1 Introduction

The terrestrial carbon and water cycles are tightly coupled by biological plant processes (Niyogi and Xue, 2006; Scholze et al., 2016). The interactions between soil moisture and carbon flux have been confirmed by previous studies (Koster et al., 2016; Qiu et al., 2018). Surface soil moisture plays a crucial role in land-atmosphere interactions (Humphrey et al., 2021; McColl et al., 2017; Seneviratne et al., 2010). It directly affects the photosynthesis and transpiration processes (Cox et al., 2002; Zhan et al., 2003) and indirectly affects carbon assimilation through modulating phenological processes (Zhang et al., 2015). The amount of available soil moisture is a key limiting factor on photosynthesis and transpiration since it affects both the water use and carbon uptake of the plant through the leaf stomata gas exchange (Manzoni et al., 2013), which makes the interactions between vegetation and soil moisture dynamics contribute significantly to the structure and function in arid and semiarid ecosystems (Walker et al., 1981; Bhark and Small, 2003; D'Odorico et al., 2007). The terrestrial ecosystem provides feedback on the water cycle through transpiration and vegetation structure (Xue et al., 2004; Kang et al., 2007).

Surface soil moisture has large uncertainty in spatiotemporal distribution, and great efforts have been devoted to improving measurements using active or passive microwave instruments (Font et al., 2001; Njoku et al., 2003; Entekhabi et al., 2010; Kerr et al., 2012). The assimilation of the remotely sensed surface soil moisture has the potential to improve land surface processes modeling (Wander et al., 2014; Scholze et al., 2016). Wu et al. (2020) found that the Soil Moisture and Ocean Salinity (SMOS) soil moisture data can be used to constrain the simulations of the terrestrial biosphere carbon cycle to optimize soil hydrological and biophysical parameters simultaneously. The Soil Moisture Active Passive (SMAP) mission is the most recent space-borne mission at L-band and has been considered one of the most promising satellites for surface soil moisture monitoring (Wigneron et al., 2017). Recent studies suggest that SMAP outperforms other satellite products compared to in situ soil moisture measurements (Ma et al., 2019; Beck et al., 2021). Zhang et al. (2022) used the direct insertion of SMAP soil moisture observation to improve the simulated land-surface carbon fluxes across a variety of timescales. The SMAP product can provide a better representation of soil moisture, which suggests its potential for improvement in coupled carbon-water dynamics in terrestrial ecosystem models.

In recent years, remote sensing of solar-induced chlorophyll fluorescence (SIF) has been a rapidly advancing front in investigating carbon dynamics and other applications (Frankenberg et al., 2011; Sun et al., 2018; Doughty et al., 2022; Leng et al., 2022). The SIF retrieved from spaceborne spectrometers has been extensively used as a proxy for terrestrial photosynthesis to understand terrestrial ecosystem dynamics (Sun et al., 2017; Helm et al., 2020). As a signal emitted by the photochemically active centers of plants, SIF is directly linked to the actual process of photosynthesis (Porcar-Castell et al., 2014). Gonsamo et al. (2019) found that the Orbiting Carbon Observatory-2 (OCO-2) SIF can accurately capture the control of soil moisture on photosynthetic activity, especially for regions with distinct seasonality of rainfall. Lee et al. (2015) incorporated equations coupling SIF to photosynthesis in a land surface model and confirmed that SIF has the potential to improve photosynthesis simulation. Qiu et al. (2018) incorporated this mechanistic representation of SIF and the Greenhouse gases Observing SATellite (GOSAT) and the Global Ozone Monitoring Experiment-2 (GOME-2) SIF measurements into a global terrestrial biosphere model, the Simplified Simple Biosphere Model version 2 (SSiB2/SIF), to evaluate and investigate the model-simulated relationships between soil moisture and SIF. In this study, we incorporated this existing SIF module into SSiB version 4 (SSiB4) to enable the fluorescence simulation, which is directly linked to photosynthetic activity and gross primary production (GPP).

In most studies, the vegetation conditions are specified based on observed and satellite-derived data, which suppresses the interactions between soil moisture and carbon cycle dynamics and indicates an important deficiency in the representation of terrestrial carbon processes in coupled carbon balance-based dynamic vegetation models. Dynamic vegetation models (DVMs) can simulate vegetation establishment, growth, competition, and mortality (Sitch et al., 2008). Studies suggest that the DVMs can be used at seasonal/interannual/decadal scales to simulate the land/atmosphere feedback (Lu et al., 2001; Levis and Bonan, 2004; Kim and Wang, 2012; Zhang et al., 2021). The Top-down Representation of Interactive Foliage and Flora Including Dynamics model (TRIFFID) uses the CO_2 fluxes at the land-atmosphere interface to update plant distributions and soil carbon, which allows the changes in biophysical properties to provide feedback onto the atmosphere (Cox et al., 2001; Hawkins et al., 2019). TRIFFID has been validated across spatial scales and ecosystems (Cox et al., 2000; Cox et al., 2004; Piao et al., 2009; Zhang et al., 2015; Liu et al., 2019). It serves as the foundation of the Joint UK Land Environment Simulator (JULES) for global carbon budget assessment (Clark et al., 2011; Le Quéré et al., 2016) and was coupled to SSiB4 to study the connections between vegetation dynamics and climate variability (Zhang et al., 2015). Liu et al. (2019) validated the vegetation distribution and leaf area index (LAI) simulated by SSiB4/TRIFFID against satellite products. With the coupling of TRIFFID, the relevant land-surface characteristics of vegetation cover and structure are modeled directly, which suggests SSiB4/TRIFFID can be used to investigate the role and mechanisms of the interactions between soil moisture and carbon cycle dynamics.

This study used the SMAP L3 soil moisture data, in conjunction with the OCO-2 SIF measurements, to evaluate the soil moisture and SIF simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF as well as the relationships between the soil moisture and SIF simulation to investigate the effects of dynamic vegetation processes on soil moisture and carbon flux estimates. We integrated the two satellite measurements into SSiB4/TRIFFID/SIF to improve the model parameterization and to investigate the broad-scale relationships between soil moisture and carbon cycle dynamics, providing the opportunity to better understand the mechanistic processes in the global terrestrial biosphere model that bridges water and carbon cycles. This paper is organized as follows: Section 2 presents the model structure, experimental design, and the satellite datasets used for evaluation and calibration. The effects of the dynamic vegetation processes and key parameters on SM, SIF, and GPP simulations and the performance after calibration are illustrated in Section 3. Discussions and concluding remarks are presented in Section 4 and Section 5, respectively.

2 Model description, experimental design, and data

2.1 Model description

SSiB is a biosphere model that intends to simulate the biophysical exchange processes realistically (Xue et al., 1991 and 1996). Zhan et al. (2003) developed an analytical solution approach from a photosynthesis model (Collatz et al., 1991, 1992) and incorporated it into SSiB to generate SSiB2, which improved the land surface CO_2 fluxes simulation. The dynamic vegetation model, TRIFFID, which has been widely used in vegetation-climate interaction studies (Cox et al., 2000; Harper et al., 2016), was coupled to SSiB4 (Xue et al., 2006) to calculate vegetation dynamics. In SSiB4/TRIFFID, SSiB4 provides net plant photosynthesis assimilation rate, autotrophic respiration, and other surface conditions such as canopy temperature and soil moisture for TRIFFID. TRIFFID updates the vegetation dynamics, including the plant functional type (PFT) fractional coverage, vegetation height, and LAI, for SSiB4. Equations coupling SIF to photosynthesis, which were incorporated into the Community Land Model version 4 (CLM4, Lee et al., 2015), were incorporated into SSiB2 by Qiu et al.

(2018). In this study, the SIF module was incorporated into SSiB4/TRIFFID, forming SSiB4/TRIFFID/SIF, to enable the chlorophyll fluorescence simulation in photosynthesis.

2.2 Experimental design

In this study, SSiB2/SIF and SSiB4/TRIFFID/SIF were used to simulate the global soil moisture, SIF, and GPP and to assess the effects of the dynamic vegetation process on the simulations. The SSiB2/SIF model was driven by atmospheric forcing from 2010 to 2019 (Figure 1a). For the SSiB4/TRIFFID/SIF model, we first conducted spin-up simulations driven with climatological forcing and 1979 CO_2 concentration for 100 years to reach a quasi-equilibrium state as done by Liu et al. (2019) and Huang et al. (2020). Using the quasi-equilibrium simulation results as the initial vegetation conditions, such as each plant functional type's (PFT) fraction coverage, leaf area index (LAI), etc., we performed transient runs driven with historical meteorological forcing and yearly updated atmospheric CO_2 concentration from 1979 to 2019 (Liu et al., 2019) (Figure 1b). The time step of model integration is 3 h, and the spatial resolution of the model is 0.5°×0.5°. The experiments covered the period from 2010 to 2019 in SSiB2/SIF and 1979 to 2019 in SSiB4/TRIFFID/SIF, and the results from April 2015 to

December 2019, when the soil moisture and SIF satellite data were both available, were analyzed.

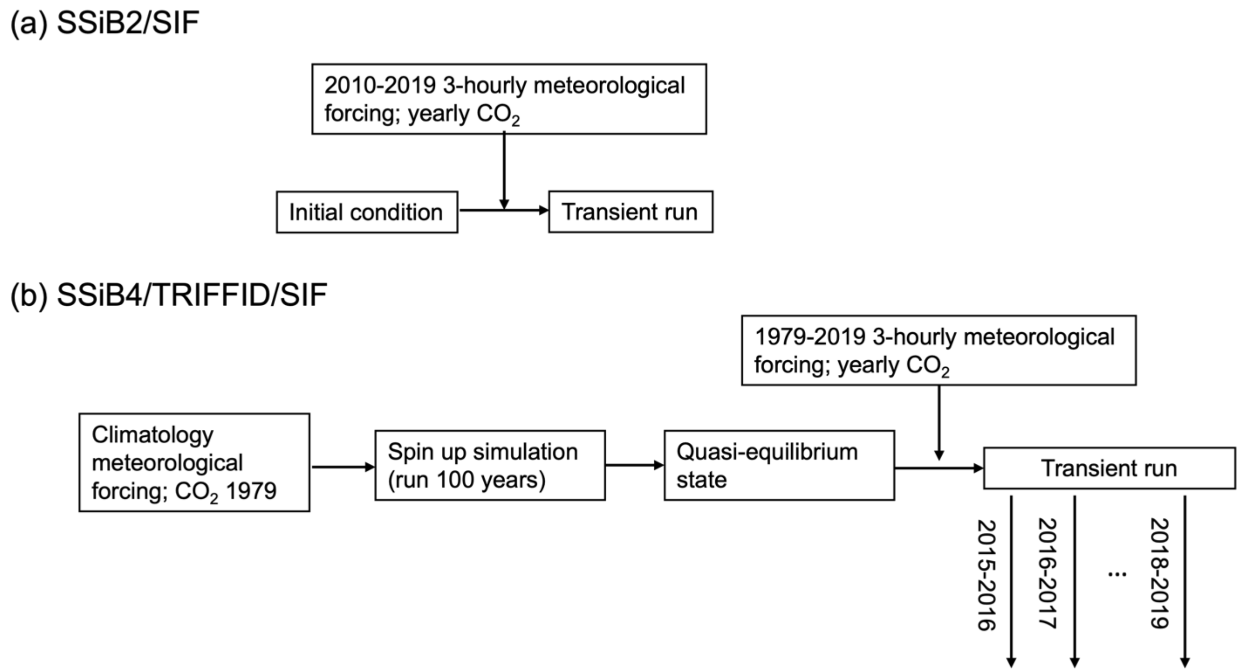

Figure 1. Experiment design for (a) SSiB2/SIF and (b) SSiB4/TRIFFID/SIF.

Studies have shown that soil properties substantially impact the soil moisture simulation in SSiB models, especially the parameterization of two key parameters, the B parameter and the hydraulic conductivity at saturation (K_s) (Xue et al., 1996; Qiu et al., 2018). The B parameter is an empirical constant that is dependent on the soil type. It represents the slope of the water retention curve and determines the relationship between the soil water potential and the volumetric soil water content through the following pedotransfer functions (Clapp and Hornberger, 1978):

$$\psi = \psi_s \left(\frac{\theta}{\theta_s}\right)^{-B} \tag{1}$$

where ψ is the soil water potential; ψ_s is the soil water potential at saturation; θ is the volumetric soil water content; and θ_s is the volumetric soil water content at saturation. The hydraulic conductivity at saturation (K_s) is the key coefficient in the soil water diffusion equation. This equation is used to calculate the transfer of water between the three soil layers in SSiB models. Both the B parameter and K_s affect the soil water diffusion (Xue et al., 1996):

$$Q = -K_s \left(\frac{\theta}{\theta_s}\right)^{(2B+3)} \left[\frac{\partial\psi}{\partial Z} + 1\right] \quad (2)$$

where Q is the soil water diffusion; and $\partial\psi/\partial Z$ is the soil water potential gradient.

In addition to these two parameters, Qiu et al. (2018) found that the wilting point is a parameter directly linked to stomatal resistance and consequently to photosynthesis processes, thus affecting soil moisture through transpiration and demonstrating the close link between the water and carbon cycles. The wilting point is defined as the soil water content below which the vegetation transpiration process tends to inhibit (Tolk, 2003). In the SSiB model, an empirical equation was developed to relate the soil moisture and stomatal conductance for each PFT (Xue et al., 1991), in which the wilting point is the natural logarithm of soil water potential at which the stomata close completely. In SSiB2/SIF and SSiB4/TRIFFID/SIF, the wilting point controls the stomata opening and affects the photosynthesis process through the β factor, the adjustment parameter on stomatal conductance:

$$\beta = 1 - \exp\{-C_2[C_1 - \ln(-\psi)]\} \quad (3)$$

where C_1 is the wilting point and C_2 is a slope factor that depends on the vegetation type.

The maximum Rubisco carboxylation rate (V_{max}) is a vegetation parameter that directly affects the photosynthesis rate (Zhan et al., 2003). The model simulated photosynthesis rates are controlled by three limitation factors related to Rubisco, electron transportation, and product sink. The vegetation parameter, V_{max}, plays a key role in this computation. It determines the photosynthetic limitations and serves as a link between the water and carbon cycles since it can also affect soil moisture through transpiration.

We have conducted a large number of experiments to test the parameters that affect the water and carbon cycle simulations in SSiB4/TRIFFID/SIF, and confirmed the importance of these four parameters mentioned above. The effects of the four parameters on soil moisture and SIF were tested through adjusting them within their normal ranges. Figure 2 shows the schematic flowchart of the SSiB4/TRIFFID/SIF model. The black boxes are the model components. The blue boxes are the satellite products used to evaluate the soil moisture and SIF simulations and to calibrate the parameters. The brown box and the green boxes represent the soil property parameters and the vegetation parameters tested and calibrated in this study, respectively.

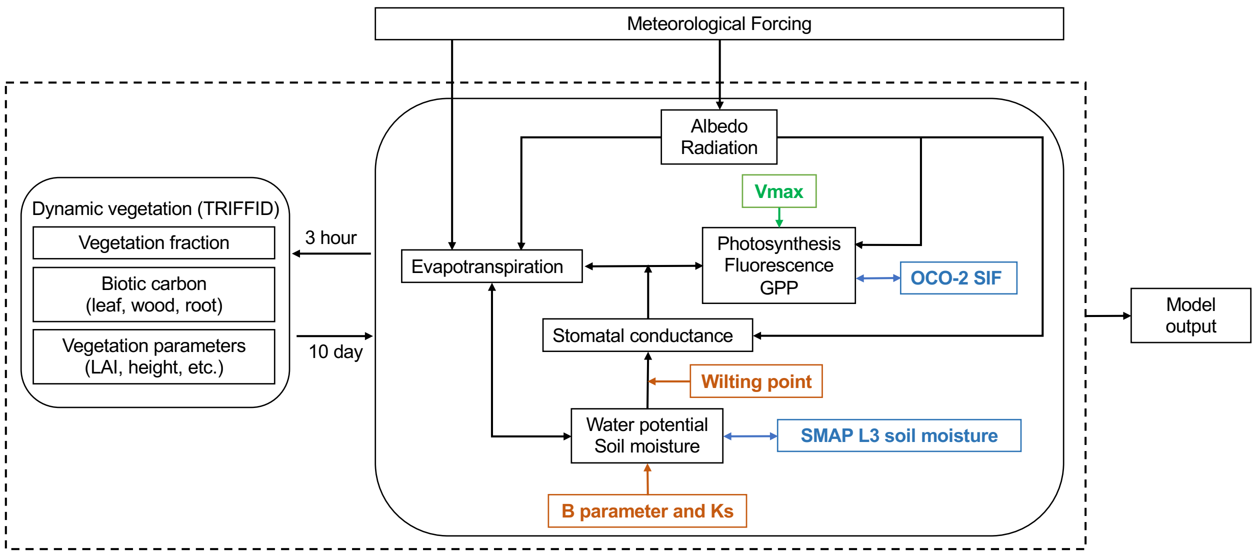

Figure 2. Overview flowchart of the SSiB4/TRIFFID/SIF model and the modified parameters in the model. The black boxes are the SSiB4/TRIFFID/SIF model components; the brown boxes represent the modified soil property parameters in the model; the green box represents the modified vegetation parameters in the model; and the blue boxes are the satellite data. SMAP

L3: Soil Moisture Active Passive enhanced Level 3; OCO-2: Orbiting Carbon Observatory 2; LAI: leaf area index.

We designed the following four sets of experiments to assess the effects of the four critical parameters on soil moisture and SIF simulation with the dynamic vegetation model coupled and for further calibration in SSiB4/TRIFFID/SIF (Table 1).

1. For the control run (CTL), the original values of the parameters were used.
2. For Test 1, the B parameter was modified. Our preliminary experiments suggested this parameter has a larger impact on soil moisture than other parameters.
3. For Test 2, the calibrated B parameter based on Test 1 was used, and the K_s was tested.
4. For Test 3, the wilting point was tested with the calibrated B parameter and K_s based on Test 2.
5. For Test 4, the V_{max} was tested with the calibrated B parameter, K_s, and wilting point based on Test 3.

Table 1. SSiB4/TRIFFID/SIF Experiment Design.

	Experiment description
CTL	Original parameters
Test 1	With modified B parameter
Test 2	Same as Test 1 but with hydraulic conductivity at saturation (K_s) modified
Test 3	Same as Test 2 but with wilting point (Wp) modified
Test 4	Same as Test 3 but with maximum RuBP carboxylation rate (V_{max}) modified

2.3 Data

The SSiB vegetation map and table based on ground survey and satellite-derived information are used as the initial condition for SSiB2/SIF simulation and SSiB4/TRIFFID/SIF quasi-equilibrium simulation (Dorman & Sellers, 1989; Xe et al., 1996, Zhang et al., 2015). Meteorological forcing data are used to drive the model. The observation-based soil moisture, SIF, and GPP products are used to evaluate the model simulation and calibrate the model parameterization. The regions at latitudes higher than 60°N were excluded from the analysis because of the scarce satellite records.

2.3.1 Meteorological forcing data

The three-hourly meteorological forcing data from 1948 to 2008 used for the quasi-equilibrium simulation in SSiB4/TRIFFID/SIF are from the Princeton global meteorological dataset for land surface modeling (Sheffield et al., 2006). The dataset combines global observation-based datasets with the NCEP/NCAR reanalysis. The spatial resolution is 1°×1°, and the temporal interval is 3 h. Its 60-year mean climatology with 3-h intervals was generated and interpolated bilinearly to 0.5°×0.5° to drive the quasi-equilibrium simulation. The hourly meteorological forcing data used for simulations in SSiB2/SIF and SSiB4/TRIFFID/SIF are the bias-corrected reconstruction of near-surface meteorological variables derived from the fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMRF) atmospheric reanalysis (ERA5) (Cucchi et al., 2022). This dataset has 0.5°×0.5° spatial resolution and a 1-h temporal interval. The 3-hour average was generated to drive the transient simulations. The variables included in the meteorological forcings are surface air temperature (K), pressure (Pa), specific humidity (g kg^{-1}), wind speed (m s^{-1}), downward shortwave radiation flux (W m^{-2}), downward longwave radiation flux (W m^{-2}), and precipitation (kg m^{-2} s^{-1}).

2.3.2 Observation-based data

There is no human activity included in the SSiB4 model simulation. Therefore, the potential vegetation distributions produced by the quasi-equilibrium run in SSiB4/TRIFFID/SIF are not the same as the vegetation map observed by satellite-derived products over some areas due to anthropogenic effects, such as the croplands in the Central US, Southern Brazil, Europe, India, and Eastern China. In this study, we used the Global Land Cover (GLC) database for the year 2000 (Bartholome and Belward, 2005) derived from Satellite Pour 1'Observation de la Terre (SPOT) to exclude the cultivated and managed areas in simulation, evaluation, and analysis.

The Soil Moisture Active Passive (SMAP) mission, launched by NASA on January 31, 2015, is the newest L-band satellite dedicated to providing global surface soil moisture measurements. This study used the SMAP Enhanced L3 Radiometer Global Daily 9 km EASE-Grid Soil Moisture dataset (SMAP L3). This dataset presents the volumetric surface soil moisture (m^3/m^3) at 0–5 cm and is superior to other satellite soil moisture products, including the Soil Moisture and Ocean Salinity (SMOS) and the ESA Climate Change Initiative (ESA CCI) in terms of capturing temporal trends compared with in-situ observations from global dense and sparse networks (Ma et al., 2019). The assessment of the SMAP L3 product using the in-situ measurements from the core validation sites (CVSs) shows that the average unbiased root mean square error (ubRMSE) is lower than 0.04 m^3/m^3 (Colliander et al., 2017; O'Neill et al., 2020). Zhang et al. (2019) validated the SMAP L3 product using extensive ground measurements from sparse networks and found that the retrievals from the descending (6:00 AM) product and ascending (6:00 PM) product do not show significant differences. In this study, the average of the descending and ascending products was bilinearly interpolated to 0.5°×0.5° for evaluation and calibration.

The SIF simulation was evaluated using the Orbiting Carbon Observatory-2 (OCO-2) SIF product. This mission, launched on July 2, 2014, measures SIF from the infilling of the Fraunhofer lines at 1:36 p.m. local time with a repeat frequency of approximately 16 days. The retrieval precision of OCO-2 is considerably improved over other existing satellite SIF products, including the Greenhouse Gases Observing Satellite (GOSAT) product and the Global Ozone Monitoring Experiment-2 product (GOME-2) (Sun et al., 2018). All soundings within a 1°×1° pixel were averaged and archived onto a 0.5° grid to generate OCO-2 SIF at 757 nm so that most of the pixels have sufficient soundings to retrieve the gridded monthly SIF (Qiu et al., 2020). To use this dataset to assess the model simulated SIF, the simulation at noon and 3 p.m. in each time zone was selected to obtain the one at 1 p.m. through interpolation.

Previous studies found that GPP and SIF had a strong linear relationship, and the satellite SIF data provide useful information on terrestrial GPP (Bacour et al., 2019; Joiner et al., 2013; Lee et al., 2015; Walther et al., 2016). Li et al. (2018) explored the relationship between OCO-2 SIF and tower GPP at 64 flux sites across the globe encompassing eight major biomes, confirming the strong correlation between SIF and GPP. Because of the significant uncertainty in the quantification of global GPP due to the lack of direct GPP observations at a global scale (Wang et al., 2021; Zhang and Ye, 2021), we selected three global GPP datasets derived from observation using different methods for comparison rather than evaluation or calibration. First is the GLASS (Global Land Surface Satellite) GPP product generated from the Eddy Covariance – Light Use Efficiency (EC-LUE) model (Yuan et al., 2007). The EC-LUE model has been validated widely throughout various ecosystems using the measurements from eddy covariance towers (Li et al., 2013; Yuan et al., 2014), and Jia et al. (2018) indicated that the EC-LUE model performed better than the MODIS algorithms. This dataset has 0.05°×0.05° horizontal resolution and 8-day time intervals. The second GPP product used for comparison is the FLUXCOM RS GPP product. It uses machine learning to merge the carbon flux measurements from the FLUXNET eddy covariance towers and remote sensing data (Tramontana et al., 2016). Zhang and Ye (2021) evaluated 45 global terrestrial GPP products by taking Model Ensemble GPP derived from observations as the reference dataset and recommended the RS product for global GPP comparison. Its resolution is 0.5°×0.5° and the time interval is 8 days. The last dataset is a global MODIS and FLUXNET-derived GPP product (FLUXSAT GPP) (Joiner and Yoshida, 2021). It used MODIS product as input to neutral networks to globally upscale GPP estimates from selected FLUXNET eddy covariance tower sites (Joiner and Yoshida, 2020). The product has a 0.05° spatial resolution and a daily temporal resolution.

3 Results

3.1 Assessment of the simulated vegetation distribution

The rate of change in vegetation fraction is less than 2% over the last 10 years of simulation, which means it reached a steady state after a 100-year spin-up (Liu et al., 2019) (Figure S1). For most PFTs, the rate is less than 1.5%. Using initial vegetation conditions derived from this quasi-equilibrium state, SSiB4/TRIFFID/SIF was driven with the historical meteorological forcing and yearly updated atmospheric CO_2 concentration from 1979 to 2019. The simulated vegetation spatial distribution was compared with that simulated in the previous study (Liu et al., 2019) to ensure that the simulated vegetation spatial distribution is reasonable, which is the base for other simulated variables in the model. The evergreen broadleaf trees in the Amazon, central Africa, and Indonesia, needleleaf trees in midlatitudes and high latitudes of North America and Eurasia, deciduous broadleaf trees in southeastern US, C_3 grasses in central

US, South America, Eurasian Steppe, Africa, and east Australia, C_4 plants in southeast US, South America, Africa, Southeast Asia, and northern Australia, and shrubs in the semi-arid areas are reasonably simulated (Figure S2). Overall, the simulated vegetated area covers 77.5% of the global land surface. The simulated tree, C_3 grass, C_4 plants, and shrubs cover 31.1%, 11.3%, 15.3%, and 14.5%, respectively. These fractions are consistent with those in the study of Liu et al. (2019).

3.2 Effects of dynamic vegetation processes on SM, SIF, and GPP simulations

The spatial distribution of the global SIF simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF were evaluated against the OCO-2 measurements in Figure 3. The SIF simulated in SSiB2/SIF shows a negative bias in the South American and African savanna regions, southeast China, and east US, while a positive bias in the boreal forest in North America and North and Central Asia. In SSiB4/TRIFFID/SIF, the simulated SIF bias is positive in most regions, especially in semi-arid regions such as the Western United States, southwest South America, Africa, Central Asia, and Australia. Its positive bias is smaller in boreal forests compared with that in SSiB2/SIF. Table 2 lists the global spatial correlation coefficient (SCC), bias (BIAS), and root-mean-square error (RMSE) of the simulated SIF in SSiB2/SIF and SSiB4/TRIFFID/SIF compared with the OCO-2 SIF data. The SCC increased by 10%, and the RMSE decreased by 12% in SSiB4/TRFFID/SIF, which shows an improvement in the spatial pattern of the simulated SIF in the run with dynamic vegetation included. However, the absolute value of the global mean SIF bias increased in SSiB4/TRIFFID/SIF. The improvement in SCC indicates that the vegetation spatial distribution simulated by SSiB4/TRIFFID/SIF is more realistic than the observation-based one used in SSiB2/SIF and further confirms the reasonability of the vegetation distribution simulation. The simulated SIF in different seasons was also compared with OCO-2 SIF data. The highest RMSE of simulation compared to OCO-2 occurs in summer both in SSiB2/SIF and SSiB4/TRIFFID/SIF. The most obvious improvement in

SSiB4/TRIFFID/SIF appears in spring, with the SCC increasing by 37% and the RMSE decreasing by 18%.

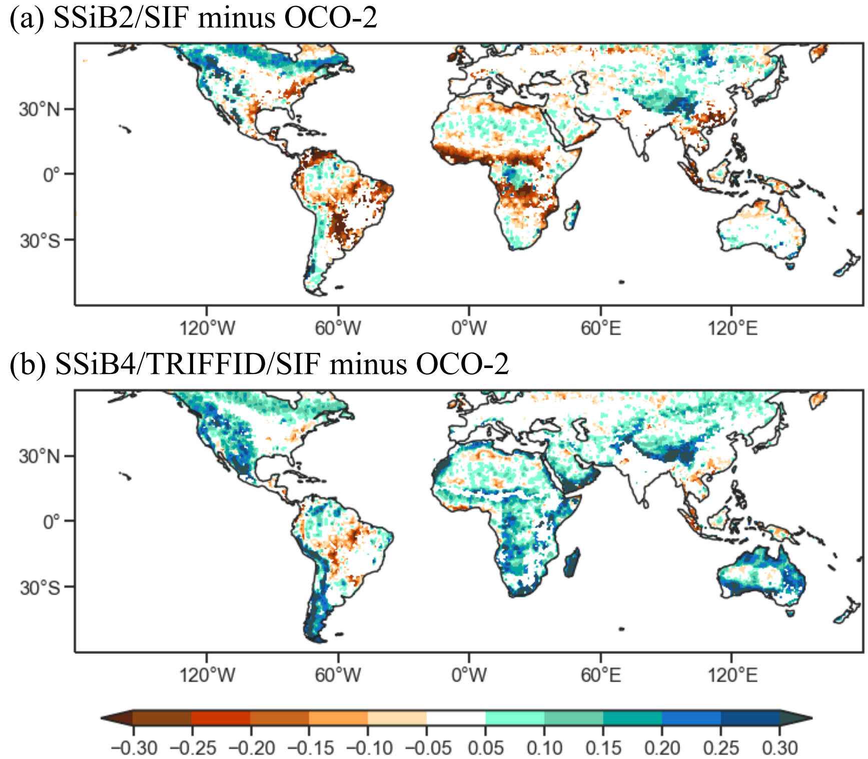

Figure 3. Global differences of solar-induced chlorophyll fluorescence (SIF) between simulations in (a) SSiB2/SIF, (b) SSiB4/TRIFFID/SIF and Orbiting Carbon Observatory 2 (OCO-2) data. Units: $W/m^2/\mu m/sr$.

Table 2. Spatial Correlation Coefficient (SCC), Mean Bias (BIAS), and Root-Mean-Square Error (RMSE) of annual SIF simulations compared to OCO-2 data. Units: $W/m^2/\mu m/sr$.

	SSiB2/SIF	SSiB4/TRIFFID/SIF
SCC	0.779	0.864
BIAS	-0.043	0.064
RMSE	0.169	0.143

The GPP simulation in SSiB2/SIF and SSiB4/TRIFFID/SIF was compared with observation-based estimated GPP in 2015, excluding the polar regions. In the three observation-based estimates, the global GPP ranges from 835.2 to 1088 g C/m^2/yr, with a median of 867.3 g C/m^2/yr. Figure 4 shows that the global GPP simulated by SSiB2/SIF is much lower than the observation-based estimations, with a value of 533.2 g C/m^2/yr. The simulated global GPP in SSiB4/TRIFFID/SIF is 875.2 g C/m^2/yr, which is close to the median value of the three observation-based estimates. Figure 5 further compared the latitudinal distribution of zonal mean GPP among the observation-based estimates and model simulations. The GLASS and FLUXSAT products demonstrate higher GPP values near the equator, while the FLUXCOM product has higher GPP values in subtropical regions in the Northern Hemisphere. The SSiB2/SIF GPP simulation is lower than the observation-based GPP products at all latitudes. The SSiB4/TRIFFID/SIF GPP simulation is close to the observation-based estimates except near the tropics, where the observation-based estimates show large discrepancies. Therefore, the SSiB4/TRIFFID/SIF simulation is within the range of various observations. Introducing the dynamic vegetation process can lead to significant improvement in GPP simulation throughout the globe. The plausible reason that may contribute to the improvement of GPP simulation in SSiB4/TRIFFID/SIF is the diversity of PFTs existing in a single grid box. In SSiB2/SIF, there is only one PFT in one grid box with the vegetation parameters, such as vegetation fraction cover (FRAC), LAI, and vegetation height (VH), specified based on a vegetation table (Sellers et al., 1996). In SSiB4/TRIFFID/SIF, each grid box consists of 7 PFTs, with the competition among them. The vegetation parameters are updated based on the carbon budget and related to the surface energy and water cycles. The improvement shows that the dynamic vegetation process can substantially improve the simulation of the carbon process and can help to provide a reasonable simulation of vegetation conditions and carbon fluxes.

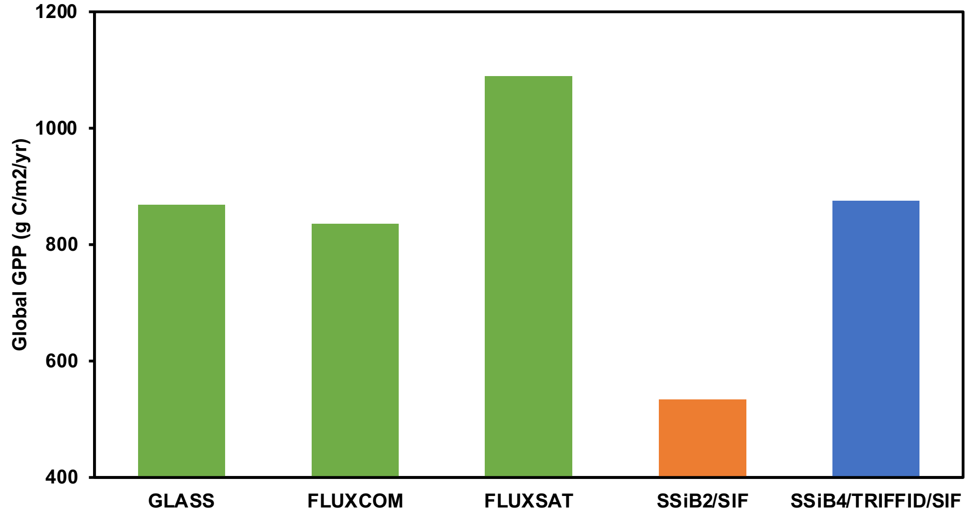

Figure 4. Comparison among observation-based estimated, SSiB2/SIF simulated, and SSiB4/TRIFFID/SIF simulated global GPP in 2015 (60°S–75°N). Units: g C/m^2/yr.

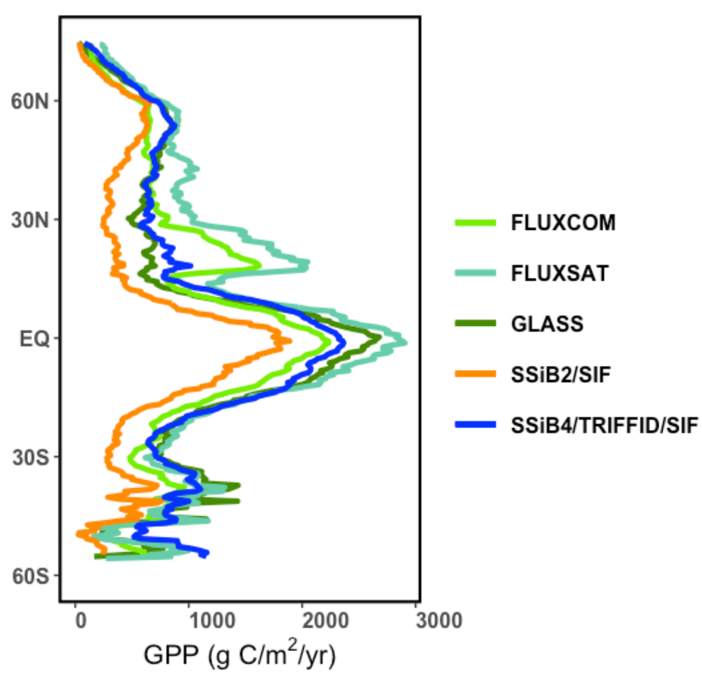

Figure 5. Comparisons of the latitudinal distribution of the zonal mean GPP among the observation-based estimates, SSiB2/SIF simulation, and SSiB4/TRIFFID/SIF simulation. Units: g C/m^2/yr.

Figure S3 compares the simulated soil moisture in SSiB2/SIF and SSiB4/TRIFFID/SIF with SMAP L3 soil moisture data. Over the globe, there was only marginal improvement in SSiB4/TRIFFID/SIF compared with SSiB2/SIF (Table S1). However, in SSiB4/TRIFFID/SIF, the global simulated SIF is higher, which represents higher photosynthesis and transpiration, the simulated soil evaporation rate is much lower, leading to a marginal change in simulated evapotranspiration. The spatial patterns of the soil moisture bias in SSiB2/SIF and SSiB4/TRIFFID/SIF are similar. The models underestimated the surface soil moisture in most areas, such as the North American boreal forest, Eastern United States, Amazon Basin, equatorial Africa, and Southeast Asia. The soil moisture was overestimated in the Eurasian boreal forest and central Asia. Calibration of the parameters directly related to soil property and affecting the vertical soil water distribution in SSiB4/TRIFFID/SIF is needed to improve the soil moisture simulation, which will be discussed in Section 3.4.

3.3 SIF−soil moisture relationship

Soil moisture plays a dominant role in determining dryness stress on ecosystem production over most vegetated areas (Liu et al., 2020). Several studies have analyzed the influence of soil water content limitation on vegetation productivity using various satellite products. Short Gianotti et al. (2019) found that the SIF−soil moisture relationship has increasing response strength with aridity, with little in the light-limited humid regions of the contiguous United States. Jonard et al. (2022) distinguished the water-limited and light-limited environments using the TROPOspheric Monitoring Instrument (TROPOMI) SIF data and the SMAP multitemporal dual channel algorithm (MT-DCA) soil moisture data in the growing season. We calculated the Pearson correlation coefficient between model-simulated SIF and soil moisture and evaluated it against that between OCO-2 SIF and SMAP L3 soil moisture. The SIF and soil moisture data used here are monthly data with seasonal cycles removed. Figure 6 shows the comparison of the correlation coefficient distribution between soil moisture and SIF in observation and simulation. The observed SIF−soil moisture correlation map shows a significant positive correlation over most regions, suggesting the water limitation on vegetation growth. Both SSiB2/SIF and SSiB4/TRIFFID/SIF simulations show a strong correlation between soil moisture and SIF anomalies in semi-arid regions, such as the Western United States, South American savanna, and South and East Africa. Meanwhile, both SSiB2/SIF and SSiB4/TRIFFID/SIF produce negative correlations over the Eastern United States, La Plata Basin, and south China, which is opposite to that in the observation. Over the Eurasian Steppe and coastal Australia, SSiB2/SIF and SSiB4/TRIFFID/SIF simulations show different correlation relationships. The SSiB4/TRIFFID/SIF model produced a positive relationship consistent with that derived from satellite data, while in SSiB2/SIF, the relationship is negative. The SIF−soil moisture correlation derived from the simulations in SSiB4/TRIFFID/SIF is more consistent with that derived from satellite data, showing that the coupling with the dynamic vegetation model helps to better capture the effects of monthly soil moisture dynamics on vegetation photosynthetic activities.

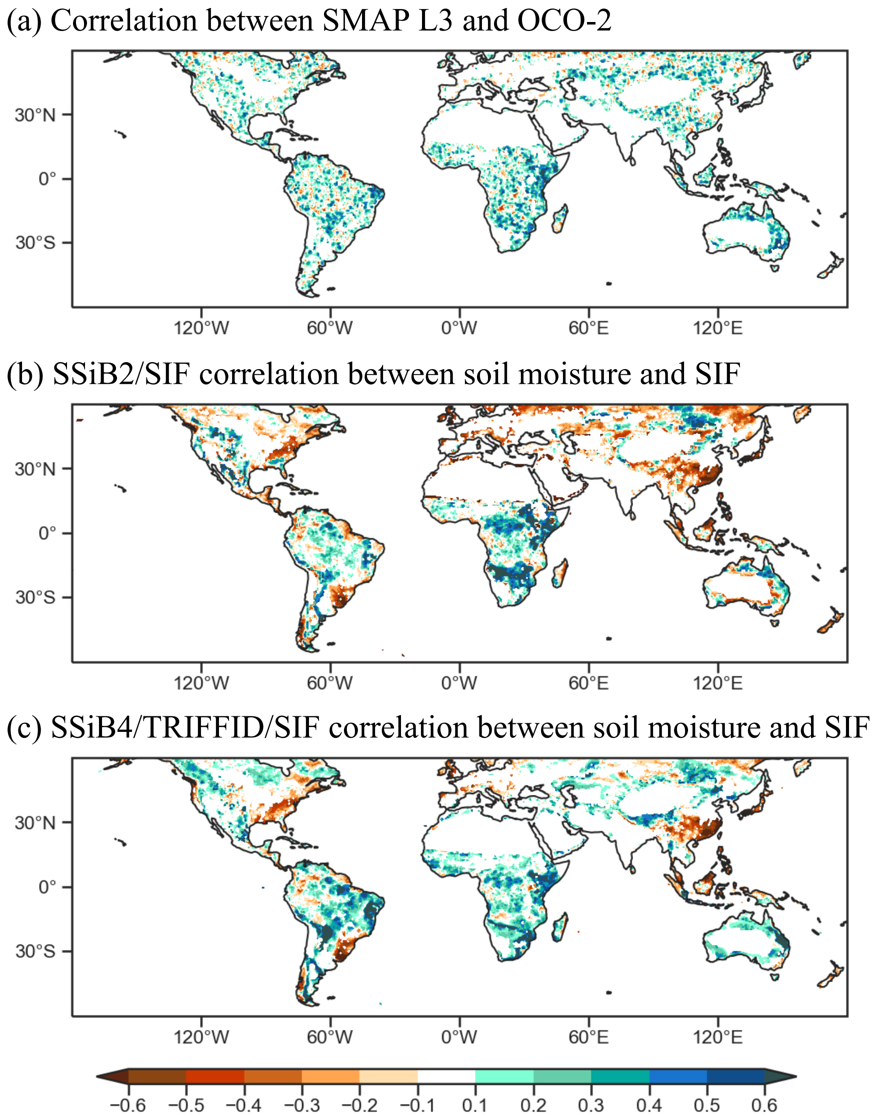

Figure 6. Comparisons of the correlations in the Northern Hemisphere summer between the monthly anomalies of (a) SMAP L3 soil moisture data and OCO-2 SIF data, (b) the SSiB2/SIF

simulated soil moisture and SIF, and (c) the SSiB4/TRIFFID/SIF simulated soil moisture and SIF.

3.4 Effects of key parameters on soil moisture and SIF simulation

The B parameter, K_s, wilting point, and V_{max} were changed within the normal range of soil and vegetation property variations to conduct experiments to show the model sensitivity to changes in the parameters (Beerling and Quick, 1995; Von Caemmerer and Furbank, 1999; Xue et al., 1996) (Table 3). The experiments covered the period from 2010 to 2019. The years from 2010 to 2014 were used for spin-up, and the annual results from 2015 to 2019 were analyzed.

Table 3. Soil and vegetation parameters used in the sensitivity experiments.

	Values
B parameter	3, 4, 5, 6, 7, 8, 9
K_s	2E-3, 2E-4, 2E-5, 2E-6, 2E-7
Wilting point	2, 4, 6, 8, 10, 12
V_{max}	20, 40, 60, 80, 100, 120, 140 (μmol/m^2/s)

3.4.1 Soil property parameters

Previous studies have shown that the soil property parameters are one of the key sources of uncertainties in soil moisture simulation in land surface models (Demaria et al., 2007; Qiu et al., 2018). According to previous work, carbon fluxes are also sensitive to soil parameters in the SSiB model (Prihodko et al., 2008). To improve the soil moisture and SIF simulation in SSiB4/TRIFFID/SIF and to better understand the role of the parameters determining the soil texture in the interactions between the water and carbon cycles, we examined the effects of B parameter, K_s, and wilting point on soil moisture and SIF simulation in SSiB4/TRIFFID/SIF (Figure 7).

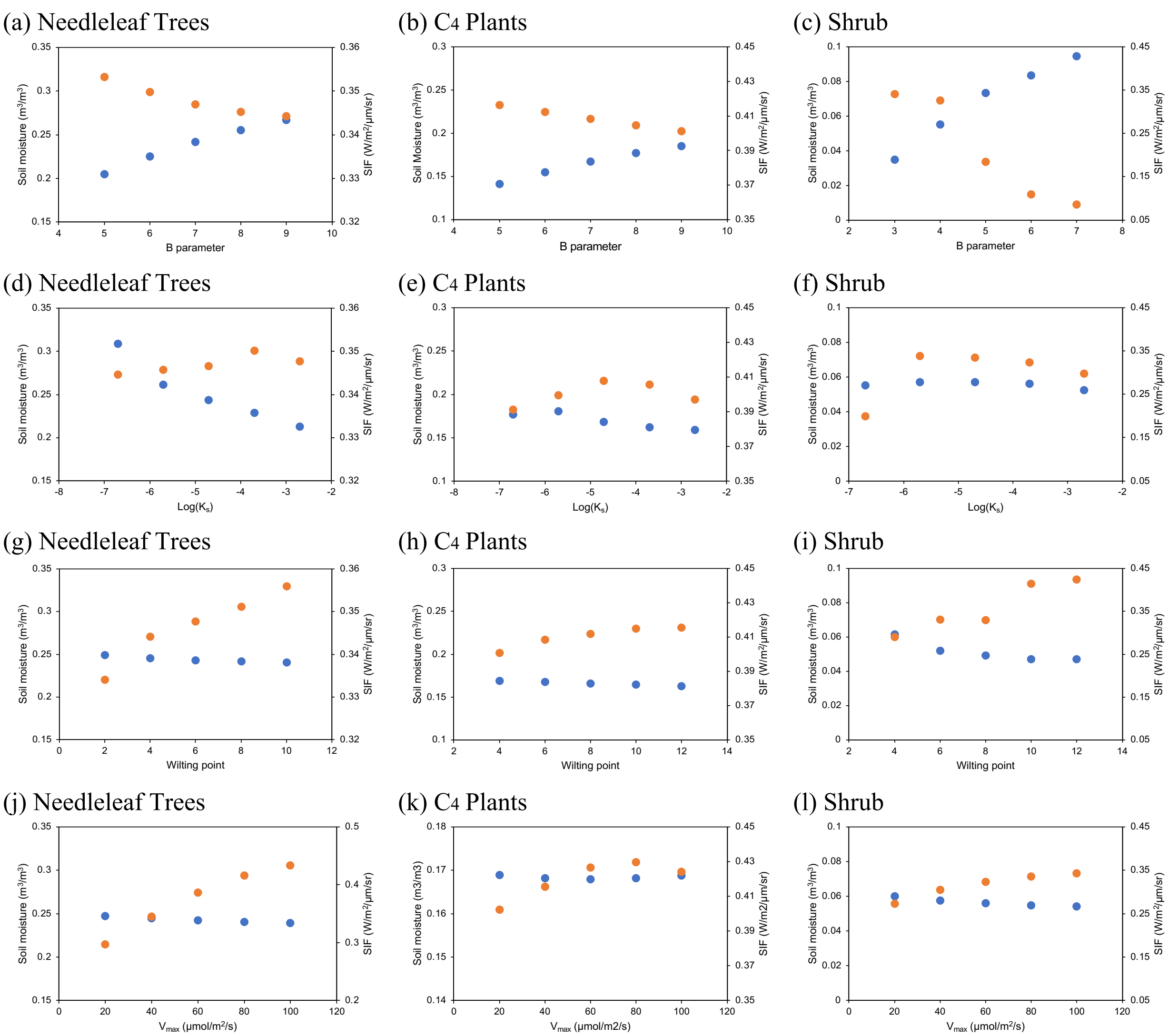

Figure 7. Calculated soil moisture (blue), SIF (orange) for (a, d, g, j) needleleaf trees, (b, e, h, k) C_4 plants, and (c, f, i, l) shrubs under different (a, b, c) B parameter; (d, e, f) logarithm of K_s; (g, h, i) wilting point, and (j, k, l) V_{max}.

The effects of the B parameter on water and carbon cycles are complex. With a higher B parameter, soil moisture increased, and SIF decreased (Figures 7a, 7b, 7c). A higher B parameter represents a soil texture closer to clay, which leads to more difficulty in soil evaporation and more soil moisture. Meanwhile, soil hydraulic conductivity decreased with increased B parameter (Eq. 2), which reduced the total runoff and may have increased evaporation; however, the change in evaporation was marginal. Overall, a higher B parameter is associated with more soil moisture. Moreover, the B parameter indirectly modifies SIF through its effect on the wilting point. The change in the B parameter modifies the relationship between soil water potential and soil water content through the retention curve. When the B parameter is higher, for a given amount of soil water content, the absolute value of water potential increases, and then the β factor in Eq. 3 is reduced, leading to stomata close and lower SIF and transpiration. In the tropics, the soil moisture increased with a larger B parameter while the SIF and transpiration almost stayed the same. The abundant soil water content in the rainforests keeps the β factor high in the change of the B parameter.

As for K_s, the soil moisture decreases when K_s is higher (Figures 7d, 7e, 7f). Higher K_s indicates that the soil texture is closer to sand, increasing surface infiltration and changing the vertical soil water content distribution. The hydraulic conductivity is larger with higher K_s, leading to larger drainage and decreased total soil water content. When K_s becomes very low, the surface infiltration becomes extremely low, leading to much larger runoff and low root zone soil moisture. The low root zone soil water potential under low K_s conditions in SSiB4/TRIFFID/SIF lead to lower β factor and SIF. Therefore, the SIF drops in SSiB4/TRIFFID/SIF when the K_s value is very small. In humid regions, it is hard for the soil water content to drop to a value at which photosynthesis weakens, so the SIF does not change obviously (Figure 7d).

For the wilting point, when it increases, the soil moisture, at which the stomata close completely, drops, leading to a higher β factor (Eq. 3), allowing more open stomata and higher stomatal conductance, which leads to higher SIF and photosynthesis and transpiration rates (Figures 7g, 7h, 7i). For example, in South Africa covered by savanna, when the wilting point increased from 4 to 10, the corresponding volumetric soil moisture at which β factor started to increase rapidly decreased from 0.30 to 0.13 m^3/m^3, and the simulated SIF increased from 0.40 to 0.42 $W/m^2/\mu m/sr$ (Figure 7h). Since a higher wilting point leads to higher transpiration rates, the soil moisture decreases with the increase of the wilting point. However, the effects of the wilting point on soil moisture are not as efficient as that of the B parameter and K_s. For example, the soil moisture in South Africa dropped slightly from 0.169 to 0.165 m^3/m^3 when the wilting point increased from 4 to 10 (Figure 7h).

3.4.2 Vegetation parameter

Photosynthesis is an important process of the terrestrial carbon cycle, and it is simulated in SSiB2/SIF and SSiB4/TRIFFID/SIF following the analytical solution approach developed by Zhan et al. (2003) based on the Collatz et al. (1991) and Collatz et al. (1992) model. The vegetation parameter directly related to photosynthesis, V_{max}, varies considerably among and within plant functional types (PFTs) (Kattge et al., 2009; Wang et al., 2021; Wullschleger, 1993), and it cannot be measured directly but must be inferred by model inversion from photosynthesis measurements. The terrestrial biosphere models demonstrate considerable sensitivity in carbon flux simulation given the uncertainty in V_{max} (Bonan et al., 2011; Piao et al., 2013). To further improve the carbon flux simulation in SSiB4/TRIFFID/SIF and to explore the effects of this vegetation parameter on water and carbon cycles, we examined the effects of V_{max} on soil moisture and SIF simulation in SSiB4/TRIFFID/SIF.

As demonstrated in Figure 7j, the photosynthesis rates of needleleaf trees are especially sensitive to the change in V_{max} in all the PFTs simulated in SSiB4/TRIFFID/SIF. When the V_{max} value increased from 20 to 100 $\mu mol/m^2/s$, the SIF simulation increased dramatically from 0.30 to 0.43 $W/m^2/\mu m/sr$, which is a much more marked increment compared with the changes in the B parameter, K_s, and wilting point as shown in Section 3.4.1. For other PFTs, the effects of V_{max} on SIF simulation are also significant. For example, with the V_{max} changing from 20 to 80 $\mu mol/m^2/s$, the SIF simulation increased from 0.40 to 0.43 $W/m^2/\mu m/sr$ in the South African savanna, and the SIF simulation increased from 0.27 to 0.34 $W/m^2/\mu m/sr$ in shrubland in the Western United States (Figure 7k). The effects of V_{max} on soil moisture simulation are similar to that of the wilting point. With the increasing V_{max}, the photosynthesis rates are higher, leading to higher SIF and transpiration rates, which results in lower soil moisture. For example, in the

Western United States, the soil moisture decreased from 0.060 to 0.054 m^3/m^3 when the V_{max} increased from 20 to 100 μmol/m^2/s (Figure 7l).

3.5 Improvement in soil moisture and SIF simulation after calibration

Based on the tests in section 3.4, we identified that the B parameter, K_s, wilting point, and V_{max} are the key parameters that significantly impact both soil moisture and SIF simulations in SSiB4/TRIFFID/SIF. To identify their impact on soil moisture and SIF simulation, we first conducted a set of experiments with individual parameters modified in each test. The B parameter, K_s, wilting point, and V_{max} were modified in Test B, Test K_s, Test Wp, and Test V_m. The range of these parameters is according to the sensitivity tests in section 3.4. The soil moisture and SIF in the control run and the four tests were calculated and compared with the SMAP L3 and OCO-2 data at global scales. In the tests with the modified soil parameters, the parameter set with minimum RMSE in soil moisture is identified as the optimized set, and the experiment with this set of parameters will be referred to as Test B opt, Test K_s opt, and Test Wp opt, while in the test with the modified vegetation parameter, the parameter set with minimum RMSE in SIF is identified as the optimized set, Test V_m opt.

Figure 8 shows the improvement in the global mean bias and RMSE of soil moisture and SIF simulations in each test with the optimized values relative to SMAP L3 soil moisture and OCO-2 SIF data. The most significant improvement in soil moisture and SIF simulations both occurred in Test B, and the most significant improvement in SIF simulation happened in Test V_m. The improvement in soil moisture simulation is also substantial in Test K_s, but the effects of K_s are less efficient than the B parameter. Through this set of tests, we found that the improvement of both soil moisture and SIF simulation is most with the change in the B parameter. The soil moisture simulation is most sensitive to the B parameter and K_s, while the SIF simulation is most sensitive to V_{max}. Based on these results, we designed another set of experiments listed in Table 1 to get optimal values of the four parameters in SSiB4/TRIFFID/SIF. The tests with the set of optimal parameters will be referred to as Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt. The soil moisture and SIF in the control run and four tests were evaluated at global scales and for the six PFTs, including the Evergreen Broadleaf

Trees (EBT), Needleleaf Trees (NT), C_3 Grasses (C_3), C_4 Plants (C_4), Shrub (SH), and Deciduous Broadleaf Trees (DBT).

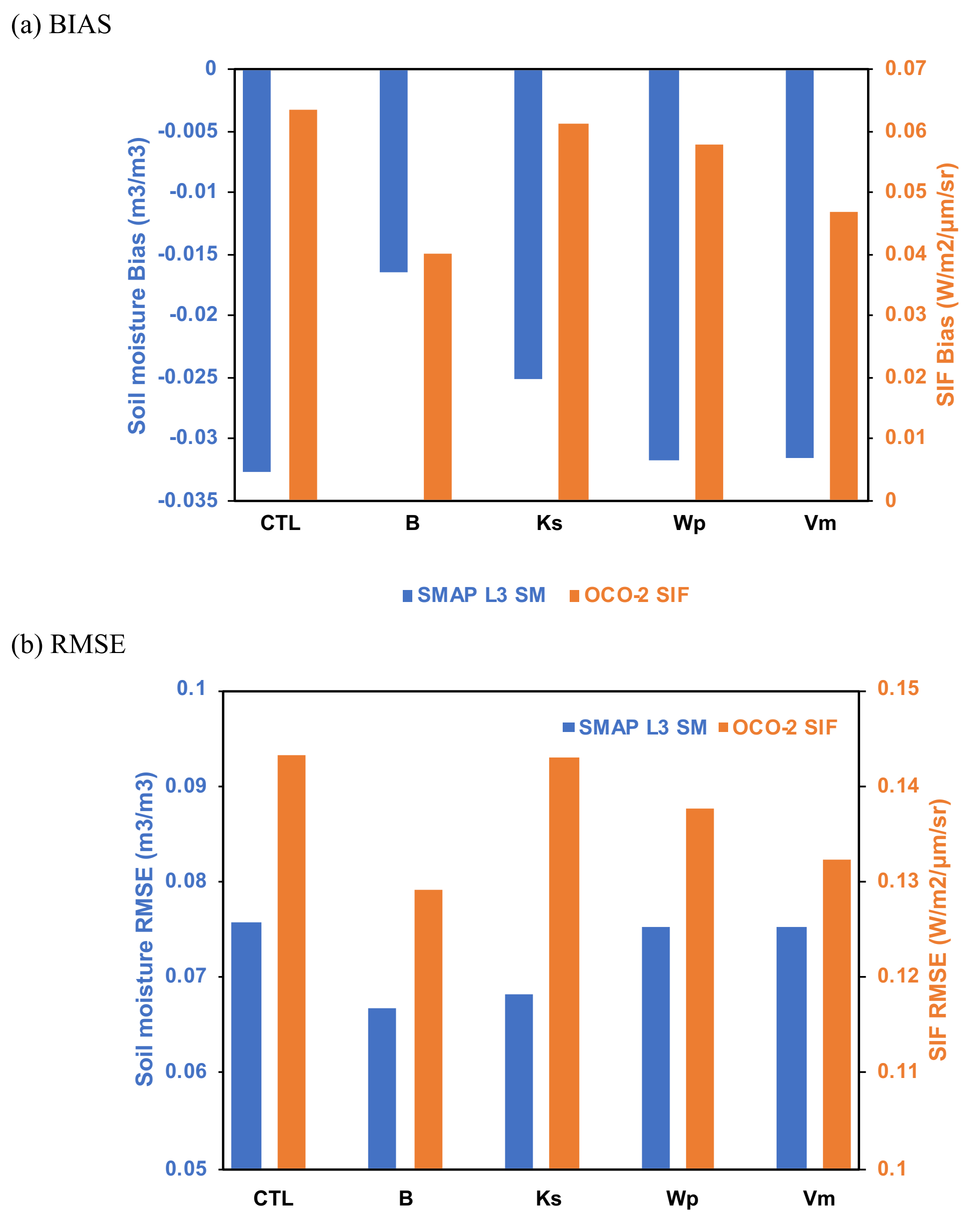

Figure 8. Global (a) mean bias (BIAS) and (b) root-mean-square error (RMSE) in the control run (CTL), Test B opt (B), Test K_s opt (Ks), Test Wp opt (Wp), and Test V_{max} opt (Vm) relative to SMAP L3 soil moisture and OCO-2 SIF data.

Figure 9 shows the global mean bias and RMSE of soil moisture and SIF relative to SMAP L3 soil moisture and OCO-2 SIF data in the control run, Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt. The optimal B parameter led to significant improvement in both soil moisture and SIF, with the global mean bias decreasing by 49.6% (from -0.033 to -0.0165 m^3/m^3) and by 37.0% (from 0.064 to 0.040 $W/m^2/\mu m/sr$), respectively, and with the RMSE decreasing by 11.9% (from 0.076 to 0.067 m^3/m^3) and by 9.9% (from 0.143 to 0.129 $W/m^2/\mu m/sr$), respectively. The optimal K_s also improved both soil moisture and SIF simulation but with reduced magnitude in SIF. The global mean bias decreased by 22.7% and 13.7%, respectively, and the global RMSE decreased by 4.6% and 0.3%, respectively. Wilting point calibration also improved the simulation but with less magnitude in soil moisture. It decreased the mean bias by 5.8% and 11.2%, respectively, and the RMSE by 0.3% and 3.1%, respectively. The calibrated V_{max} further improved the SIF simulation substantially by 44.0% on the global mean bias and

5.9% on the RMSE and improved the soil moisture simulation slightly by 14.6% on the global mean bias.

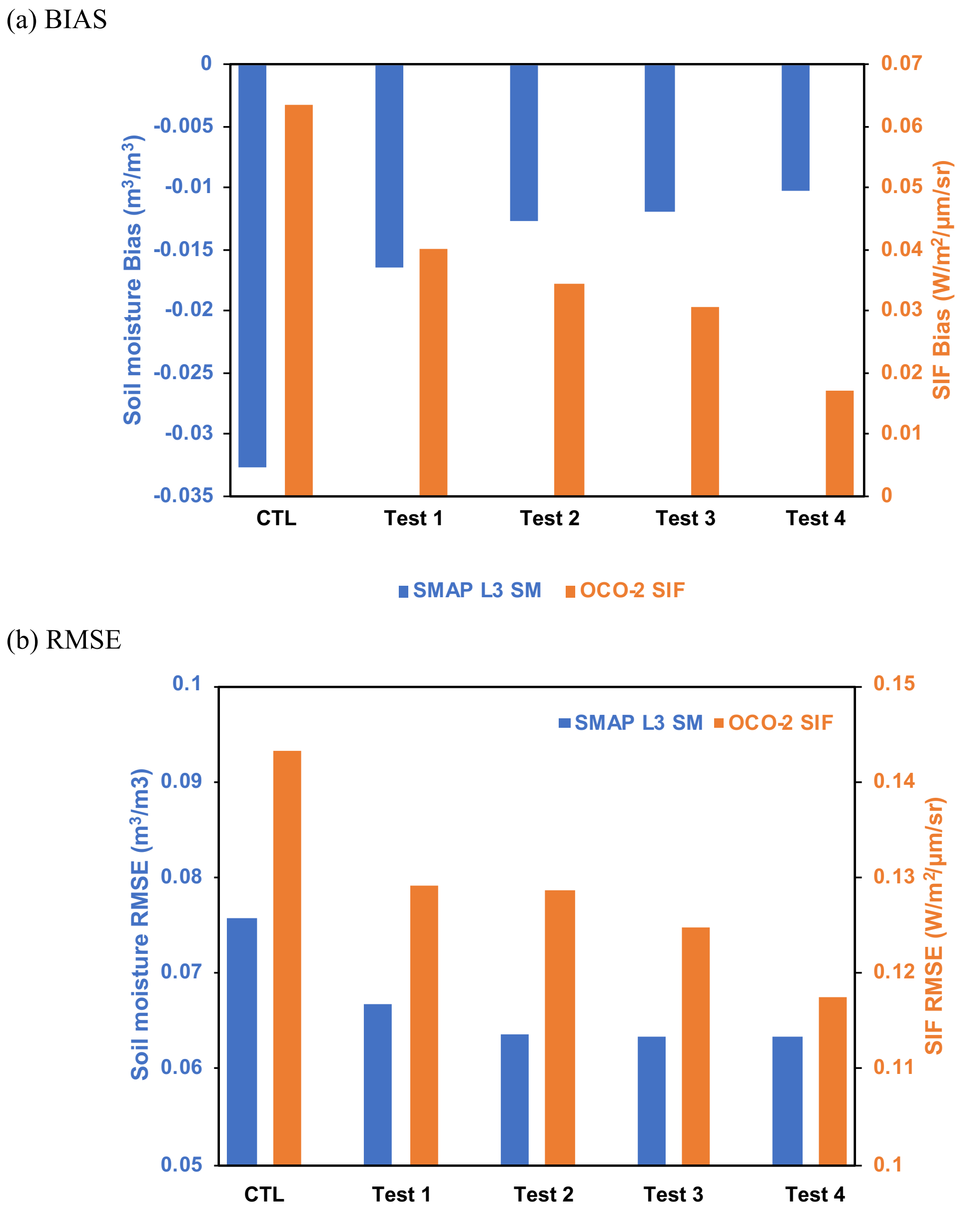

Figure 9. Global (a) mean bias (BIAS) and (b) root-mean-square error (RMSE) in the control run (CTL), Test 1 opt, Test 2 opt, Test 3 opt, and Test 4 opt relative to SMAP L3 soil moisture and OCO-2 SIF data.

Figures 10a and 10b illustrate the spatial distribution of global differences between simulated and SMAP L3 soil moisture and between simulated and OCO-2 SIF. The SSiB4/TRIFFID/SIF model significantly underestimated the soil moisture in most regions, especially in the tropics and semi-arid regions, while overestimating the SIF throughout the globe, with the most significant overestimation occurring in the semi-arid regions covered by shrubs and savanna. To delineate the spatial distribution of improvement in each test, Figures 10c to 10j show the soil moisture and SIF differences between simulations and observations in the test runs and the control run, and Table 4 lists the spatial correlation coefficient (SCC), mean bias (BIAS), and RMSE of the soil moisture and SIF at the global scale and for different vegetation types in the test runs and the control run. The most significant improvement for soil moisture simulation was in tropical rainforests and semi-arid regions. In Test 1 opt, with the B parameter modified, the soil moisture increased substantially over the tropics in the Amazon basin and Central Africa and in semi-arid regions, such as the Western United States, south Argentina, Sahel, South Africa, and Australia (Figure 10c). The soil moisture BIAS of EBT decreased from -0.103 to -0.069 m^3/m^3 and the RMSE from 0.124 to 0.097 m^3/m^3. The BIAS and RMSE of SH decreased from 0.057 to 0.043 m^3/m^3 and from 0.057 to 0.043 m^3/m^3, respectively, in soil moisture simulation. The SIF simulation was improved together with soil moisture in Test 1 in semi-arid regions covered by shrubs, including the Western United States, South Africa, and coastal Australia (Figure 10d). The BIAS and RMSE of SIF simulation for SH decreased from 0.130 to 0.018 $W/m^2/\mu m/sr$, and from 0.174 to 0.096 $W/m^2/\mu m/sr$. With the modification of K_s in Test 2 opt, the soil moisture simulation in the tropics was further improved (Figure 10e), with the BIAS and RMSE of EBT further decreased to -0.043 m^3/m^3 and 0.082 m^3/m^3, and both the soil moisture and SIF simulations were improved in the savanna in Africa, the Sahel, and coastal Australia (Figure 10e and Figure 10f). In Test 3 opt, the soil moisture simulation was slightly improved for C_3 and DBT, and the SIF simulation was improved for most PFTs, including EBT, C_3, C_4, SH, and DBT (Table 4). In Test 4 opt, the V_{max} modification significantly improved SIF simulation in the boreal forests in North America and Siberia and the grassland in the central United States and South America (Figure 10j). The BIAS and RMSE of NT in SIF simulation decreased from 0.080 to 0.036 $W/m^2/\mu m/sr$ and from 0.128 to 0.099

W/m^2/µm/sr. For C_3, the BIAS and RMSE of SIF simulation decreased from 0.111 to 0.081 W/m^2/µm/sr and from 0.174 to 0.153 W/m^2/µm/sr.

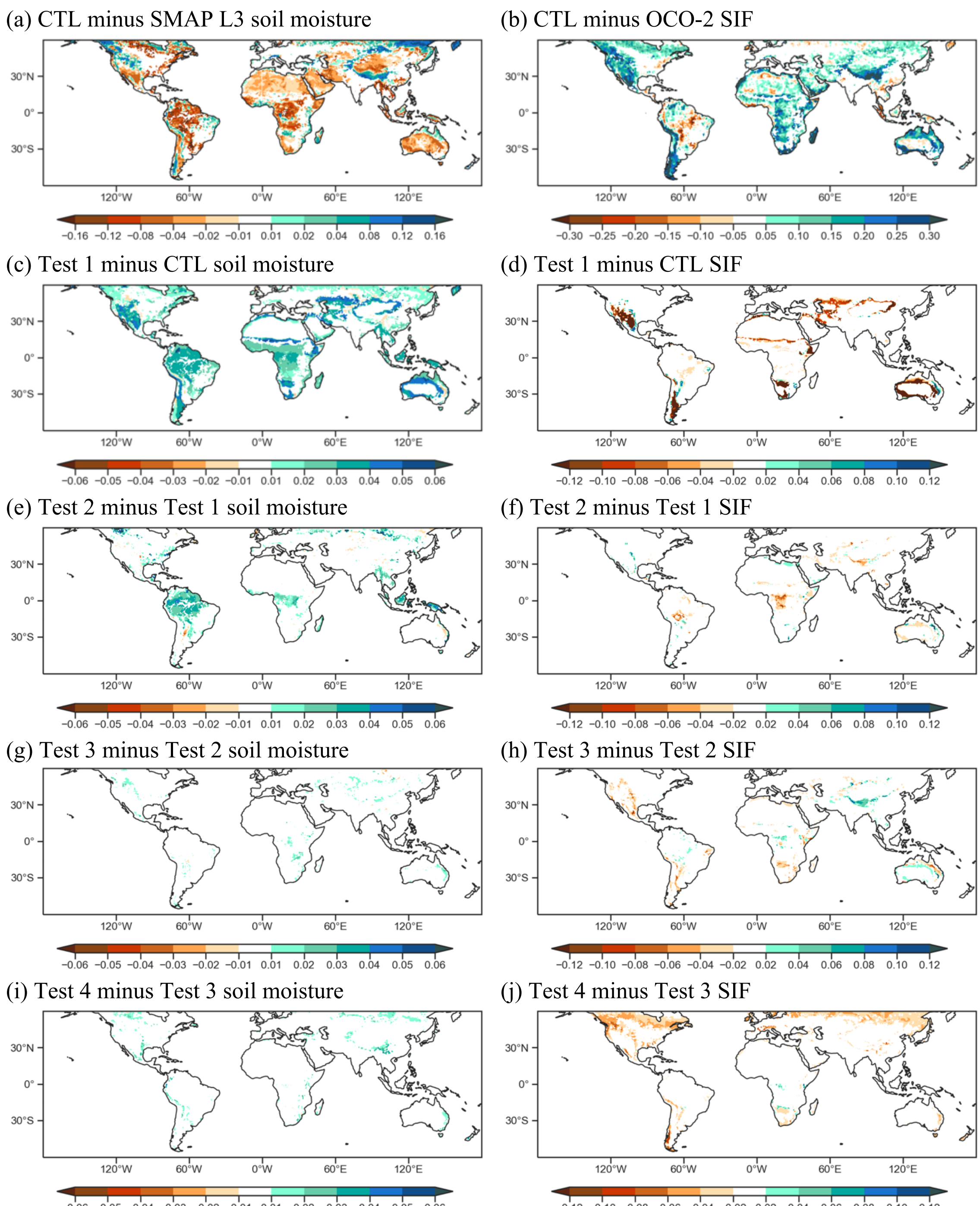

Figure 10. Global differences of simulated soil moisture and SIF in the control run compared to (a) SMAP L3 (units: m^3/m^3) and (b) OCO-2 (units: $W/m^2/\mu m/sr$). Global differences of simulated soil moisture (c, e, g, i) (units: m^3/m^3) and SIF (d, f, h, j) (units: $W/m^2/\mu m/sr$) in the control run and different tests. (c, d) Test 1 opt minus CTL, (e, f) Test 2 opt minus Test 1 opt, (g, h) Test 3 opt minus Test 2 opt, (i, j) Test 4 opt minus Test 3 opt.

Table 4. Spatial Correlation Coefficient (SCC), Mean Bias (BIAS), and Root-Mean-Square Error (RMSE) of the comparison between SSiB4/TRIFFID/SIF simulated and observation-based soil moisture and SIF. Units for soil moisture: m^3/m^3. Units for SIF: $W/m^2/\mu m/sr$.

Vegetation Type	Experiment	Soil Moisture			SIF		
		SCC	BIAS	RMSE	SCC	BIAS	RMSE
Evergreen Broadleaf Trees (EBT)	CTL	0.366	-0.103	0.124	0.150	-0.016	0.124
	Test 1 opt	0.366	-0.069	0.097	0.119	-0.023	0.128
	Test 2 opt	0.335	-0.043	0.082	0.120	-0.037	0.130
	Test 3 opt	0.332	-0.042	0.081	0.136	-0.035	0.128
	Test 4 opt	0.330	-0.042	0.081	0.141	-0.035	0.128
Needleleaf Trees (NT)	CTL	0.304	-0.012	0.087	0.411	0.082	0.130
	Test 1 opt	0.288	0.000	0.087	0.413	0.081	0.130
	Test 2 opt	0.302	0.003	0.086	0.402	0.078	0.128
	Test 3 opt	0.303	0.003	0.086	0.422	0.080	0.128
	Test 4 opt	0.312	0.006	0.086	0.439	0.036	0.099
C_3 Grasses (C_3)	CTL	0.489	0.012	0.070	0.407	0.124	0.187
	Test 1 opt	0.494	0.002	0.069	0.390	0.126	0.189
	Test 2 opt	0.498	-0.006	0.069	0.392	0.125	0.188
	Test 3 opt	0.498	-0.003	0.068	0.418	0.111	0.174
	Test 4 opt	0.508	0.008	0.069	0.406	0.081	0.153
C_4 Plants (C_4)	CTL	0.662	-0.042	0.080	0.491	0.055	0.151
	Test 1 opt	0.671	-0.022	0.071	0.514	0.044	0.145
	Test 2 opt	0.674	-0.017	0.069	0.518	0.036	0.142
	Test 3 opt	0.676	-0.016	0.069	0.542	0.026	0.138
	Test 4 opt	0.676	-0.014	0.069	0.550	0.020	0.136
Shrub (SH)	CTL	0.540	-0.034	0.057	0.368	0.130	0.174
	Test 1 opt	0.541	-0.000	0.043	0.612	0.018	0.096
	Test 2 opt	0.533	-0.001	0.043	0.617	0.008	0.098
	Test 3 opt	0.536	0.001	0.043	0.605	-0.001	0.091
	Test 4 opt	0.538	0.001	0.043	0.601	-0.005	0.090
Deciduous Broadleaf	CTL	0.858	-0.054	0.090	0.264	0.075	0.222
	Test 1 opt	0.861	-0.030	0.077	0.261	0.073	0.221

Trees (DBT)	Test 2 opt	0.864	-0.014	0.070	0.198	0.072	0.228
	Test 3 opt	0.866	-0.014	0.069	0.224	0.068	0.222
	Test 4 opt	0.864	-0.014	0.069	0.248	0.045	0.211

4 Discussion

This study shows that the B parameter is a key parameter that connects the water and carbon cycles in SSiB models and has significant effects on both soil moisture and SIF simulations. The B parameter has the largest impact on soil moisture for all PFTs, and its effect on SIF varies among different vegetation types. The impact on SIF simulation is larger over semi-arid regions where the soil water content is a key limitation factor on vegetation growth. The K_s can also affect both soil moisture and SIF simulations but with reduced magnitude. The wilting point and V_{max} have significant effects on SIF simulation, but their effects on soil moisture simulation are not substantial compared with the B parameter and K_s. Consistent with the previous study (Qiu et al., 2018) in SSiB2/SIF, the wilting point plays a role in connecting the carbon and water cycles in semiarid regions in SSiB4/TRIFFID/SIF. For humid regions, the role of the wilting point is limited, and V_{max} is more important in SIF simulation, especially for the boreal forests.

To evaluate the model performance in predicting the temporal variability of soil moisture and SIF, we created the time series of the monthly satellite observations and simulations in the control run and four tests with the optimal parameter values. Figure 11 demonstrates the monthly mean soil moisture and SIF at the global scale in the control run and the test runs together with the satellite observations from Jan 2016 to Dec 2019. After calibrating the four parameters, the simulated global mean soil moisture increased by about 0.02 m^3/m^3, and the simulated global mean SIF decreased by about 0.05 $W/m^2/\mu m/sr$. Among all the PFTs, the seasonality of soil moisture and SIF simulations for C_4 plants and shrubs was best simulated, and the simulated soil moisture and SIF values got the most improvement for these two PFTs (Figure 12). At the global scale, the most improvements in soil moisture were in Test 1 opt, and secondarily in Test 2 opt. The seasonality of soil moisture had a marginal change in four tests, and the increment happened throughout the year. The improved soil moisture simulation still has a considerable discrepancy compared with the SMAP L3 soil moisture, which means the model needs to be further improved. To pursue more improvement, forthcoming work can use the global high-resolution dataset of soil hydraulic properties instead of parameterization for each vegetation type in the soil moisture simulation (Dai et al., 2019). For the SIF simulation, the most improvement happened in Test 1 opt and Test 4 opt. The SIF simulation was improved in spring, fall, and winter, but got worse in summer. The higher B parameter value decreased the SIF simulation in each season while the change in V_{max} had more effect in summer. To improve the seasonality of SIF simulation, future work can test the parameters in the TRIFFID model to better simulate vegetation distribution, LAI, and SIF.

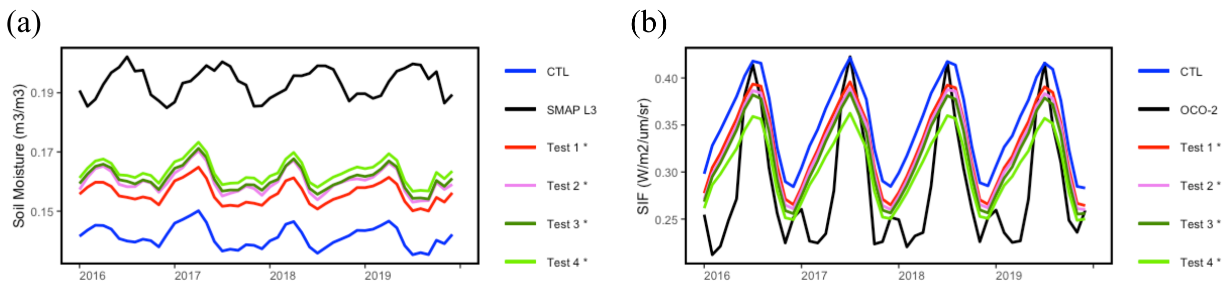

Figure 11. The monthly mean (a) soil moisture and (b) SIF at the global scale (60°S–60°N) in different experiments. * Indicates significant differences between different experiments (p<0.01).

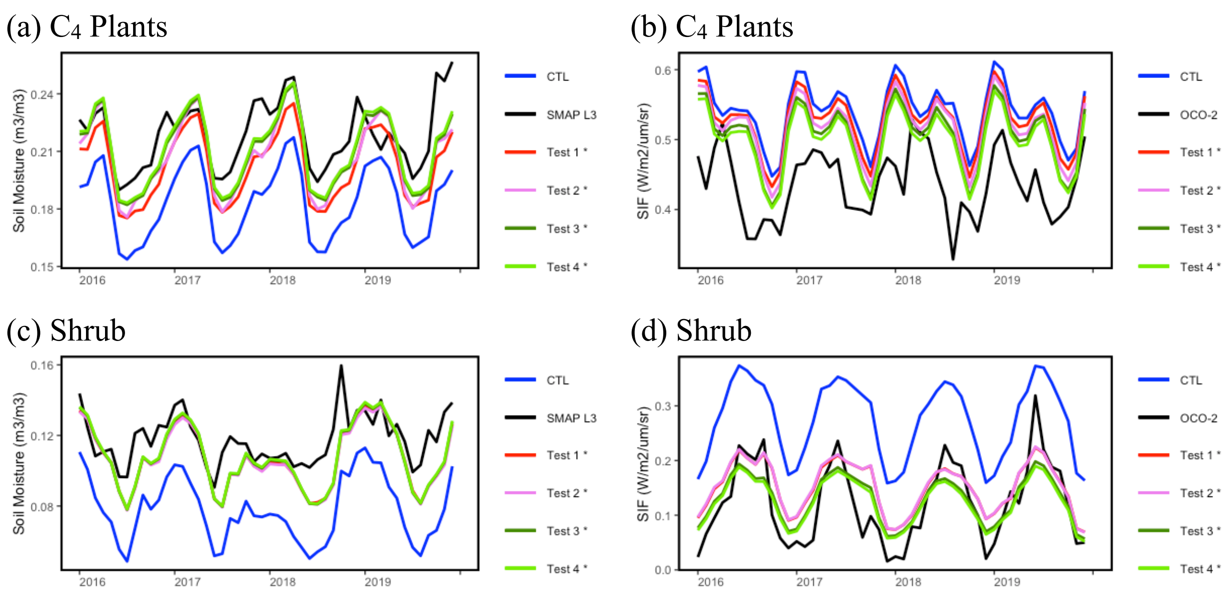

Figure 12. The monthly mean (a, c) soil moisture and (b, d) SIF of (a, b) C_4 plants in Africa and (c, d) shrubs in the Western United States in different experiments. * Indicates significant differences between different experiments (p<0.01).

Qiu et al. (2018) integrated the SMOS soil moisture data and GOSAT SIF data into SSiB2/SIF to understand the response of SIF to soil moisture dynamics. SSiB2/SIF largely overestimated the soil moisture and underestimated the SIF in most regions when evaluated against SMOS soil moisture and GOSAT SIF but underestimated both soil moisture and SIF in semiarid regions. Therefore, calibration of the B parameter and K_s in SSiB2/SIF based on the SMOS soil moisture resulted in better soil moisture simulation but poorer SIF simulation for regions covered by savanna, grass, and shrub. Ma et al. (2019) assessed several satellite surface soil moisture products using global ground-based observations and found that the SMOS products exhibited dry bias due to their underestimating surface temperature. In this study, we used SMAP L3 soil moisture data instead of SMOS to calibrate the B parameter and K_s, and the SIF simulation was evaluated against OCO-2 SIF data. Compared with the SMAP L3 product, SSiB4/TRIFFID/SIF underestimated the soil moisture in most regions. Also, the introduction of the dynamic vegetation processes made the SIF simulation higher than the satellite observation throughout the globe. These two aspects lead to improved soil moisture and SIF simulation in SSiB4/TRIFFID/SIF after calibrating the B parameter and K_s in semiarid regions, which differs from the previous results (Qiu et al., 2018). This study confirmed the importance of using satellite products with higher accuracy and precision, and better spatial and temporal resolution in the calibration of parameters in SSiB models and the exploration of the relationship between soil moisture and SIF. The SMAP products provide the high-resolution mapping of global soil moisture and have been widely validated against core validation sites (Burgin et al., 2017; Zhang et al., 2017). Zhang et al. (2019) assessed the SMAP L3 product using extensive ground measurements from sparse networks and found that the product showed better performance in temperate zones and grassland while negative bias in tropical climate zones and regions with high soil organic carbon contents. As for the OCO-2 SIF data, despite its high resolution, the satellite-observed SIF soundings are sparse, and we averaged the soundings in each $1°\times1°$ pixel first to fulfill more grids with SIF retrieval. This methodology can induce uncertainties in the evaluation of SIF simulation. Those uncertainties in satellite observations can affect the parameter calibration and the understanding of water-carbon cycle interactions. The SMAP L4 product assimilates SMAP brightness temperature observations into a land surface model and provides both the 0-5 cm vertical averaged surface soil moisture and the 0-100 cm vertical averaged root zone soil moisture with complete spatial coverage. The Sentinel-5 Precursor/TROPOspheric Monitoring Instrument (TROPOMI) launched in 2017 provides SIF data with comparable quality but with largely improved spatial and temporal coverage, and Köhler et al. (2018) suggested tying TROPOMI to OCO-2 SIF data in overlapped regions to virtually fill the large gaps left by the OCO-2 product. Future work can include the SMAP L4 and TROPOMI products as further constraints in the model simulation improvement and the SIF−soil moisture relationship exploration.

This study was conducted by the offline models, SSiB2/SIF and SSiB4/TRIFFID/SIF, using meteorological forcing to drive soil moisture, SIF, and GPP simulation. With the coupling of the dynamic vegetation model, SSiB4/TRIFFID/SIF can reproduce the global distribution of dominant vegetation types, the vegetation fraction, and the LAI, including its seasonal, interannual, and decadal variabilities (Zhang et al., 2015; Liu et al., 2019), and can provide an improved simulation of photosynthesis and carbon flux. However, the offline model simulation is not able to include feedback to the atmosphere, which represents a lack of investigation on fully coupled two-way interaction. The simulated SIF and GPP in SSiB4/TRIFFID/SIF were much higher than that in SSiB2/SIF, which indicated higher transpiration. Since the same meteorological forcing was used, the simulated total evapotranspiration fluxes in the two models are consistent, with a lower simulated soil evaporation rate in SSiB4/TRIFFID/SIF. The higher vegetation fraction, LAI, transpiration, and photosynthesis rates in SSiB4/TRIFFID/SIF cannot lead to an obvious change in the soil moisture simulation. Zhang et al. (2021) coupled the SSiB2 model and the SSiB4/TRIFFID model to the NCEP Global Forecast System (GFS) to investigate vegetation-atmosphere feedback and found that the correlations between the simulated and observed monthly LAI, albedo, near-surface temperature, and precipitation were improved with the dynamic vegetation processes included. Therefore, it remains necessary to add the SIF module into the coupled GFS/SSiB4/TRIFFID model and to evaluate the soil moisture, SIF, and GPP simulated by it against satellite products. This fully coupled biophysical processes model has the potential to better reproduce the satellite-observed soil moisture and carbon flux and to contribute to the understanding of the interactions between water and carbon cycles through controls over evapotranspiration, vegetation phenology, and surface energy balance.

5 Conclusions

To investigate the role of dynamic vegetation processes on soil moisture and carbon flux simulations and to better understand the relationship between terrestrial carbon and soil moisture dynamics, this study incorporated the SIF module used in SSiB2/SIF into SSiB4/TRIFFID. The soil moisture, SIF, SIF−soil moisture relationship, and GPP simulated by SSiB2/SIF and SSiB4/TRIFFID/SIF were evaluated against the SMAP L3 soil moisture data and the OCO-2 SIF data. The three soil property parameters, the B parameter, K_s, and wilting point, and the vegetation parameter, V_{max}, were tested within the normal range to confirm their important role in the water and carbon cycles in model simulation and to test their effects on soil moisture, SIF, and the interactions. The four parameters were calibrated using the SMAP L3 soil moisture and OCO-2 SIF to improve the soil moisture and SIF simulations in SSiB4/TRIFFID/SIF.

The coupling with the dynamic vegetation model, TRIFFID, led to substantial improvement in the SIF and GPP simulations. The global spatial correlation of SIF increased by 10%, and the global RMSE of SIF simulation decreased by 12%. The global mean GPP simulation increased from 533.2 g C/m^2/yr to 875.2 g C/m^2/yr, which is closer to the median of three observation-based GPP products (867.3 g C/m^2/yr). The global spatial distribution of the correlation coefficient between soil moisture and SIF was more properly simulated in SSiB4/TRIFFID/SIF, with the relationship switched from negative to positive over the Eurasian Steppe and coastal Australia.

The empirical coefficient, B parameter, has the largest impact on soil moisture simulation and efficiently affects the SIF simulation for plants in semi-arid regions through its effects on water potential and soil water diffusion. K_s also affects soil moisture and SIF simulation through the water diffusion in soil layers. The wilting point and V_{max} affect the stomatal opening and the photosynthesis process, thus changing the transpiration rates and SIF simulation. Their effects on soil moisture simulation exist but are less in magnitude than the B parameter and K_s.

The SMAP L3 and OCO-2 products improved soil moisture and SIF measurements with better quality, higher spatial and temporal resolution, and accuracy. They can help to improve the global performance of SSiB4/TRIFFID/SIF on soil moisture and SIF simulations and provide advances in understanding the global terrestrial coupled water-carbon cycles. The global RMSE of soil moisture and SIF decreased from 0.076 to 0.067 m^3/m^3 and from 0.143 to 0.129 $W/m^2/\mu m/sr$ with the B parameter optimization and further decreased to 0.063 m^3/m^3 and 0.125 $W/m^2/\mu m/sr$ with the K_s and wilting point optimized. Calibration of V_{max} further improved the SIF simulation, with the global RMSE decreased to 0.117 $W/m^2/\mu m/sr$.

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AGU PUBLICATIONS

Global Biogeochemical Cycles

Supporting Information for

Understanding Interactions between Terrestrial Water and Carbon Cycles Using Integrated SMAP Soil Moisture and OCO-2 SIF Observations and Land Surface Models

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Figures S1 to S3

Introduction

This supporting information provides the ancillary figures mentioned in the article.

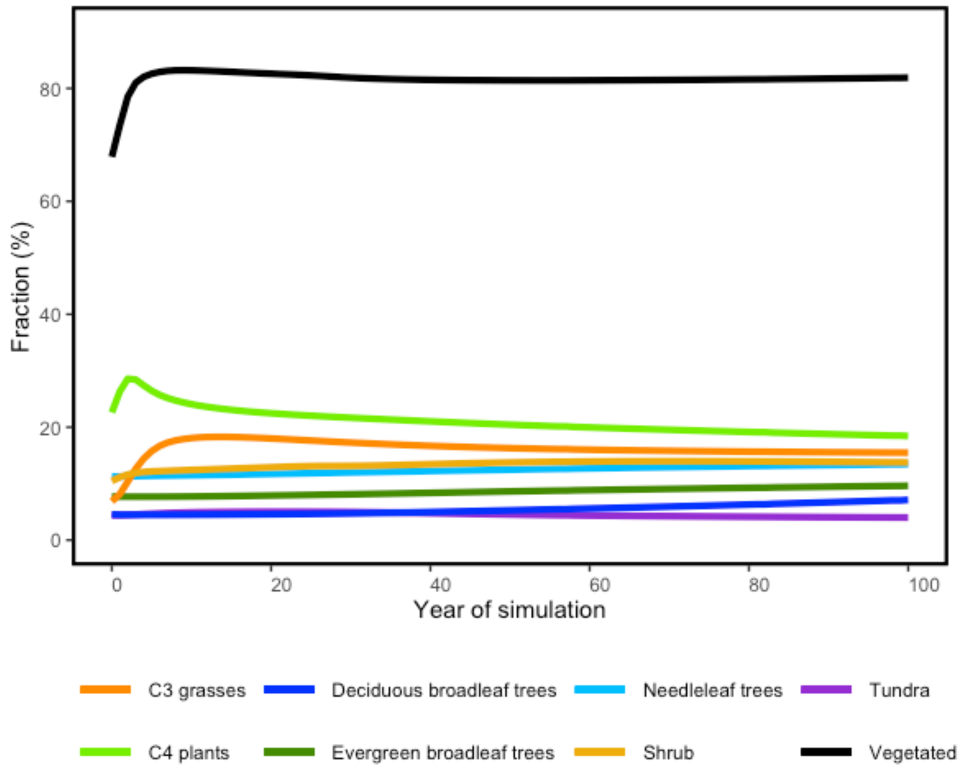

Figure S1. Fractional coverage of each plant functional type (PFT) in the equilibrium experiment in SSiB4/TRIFFID/SIF.

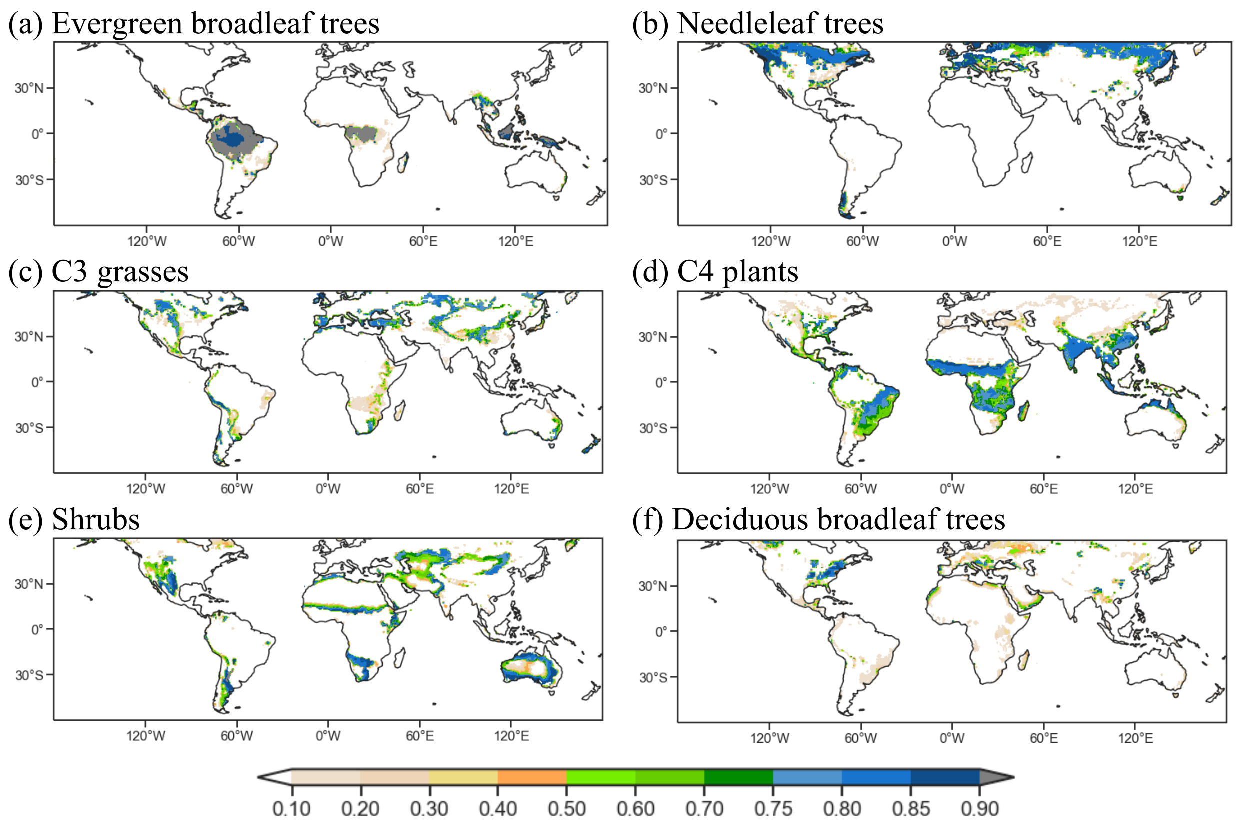

Figure S2. 2015-2019 averaged vegetation fractional coverage (Frac) distribution for (a) Evergreen broadleaf trees, (b) Needleleaf trees, (c) C_3 grasses, (d) C_4 plants, (e) Shrubs, and (f) Deciduous broadleaf trees in SSiB4/TRIFFID/SIF.

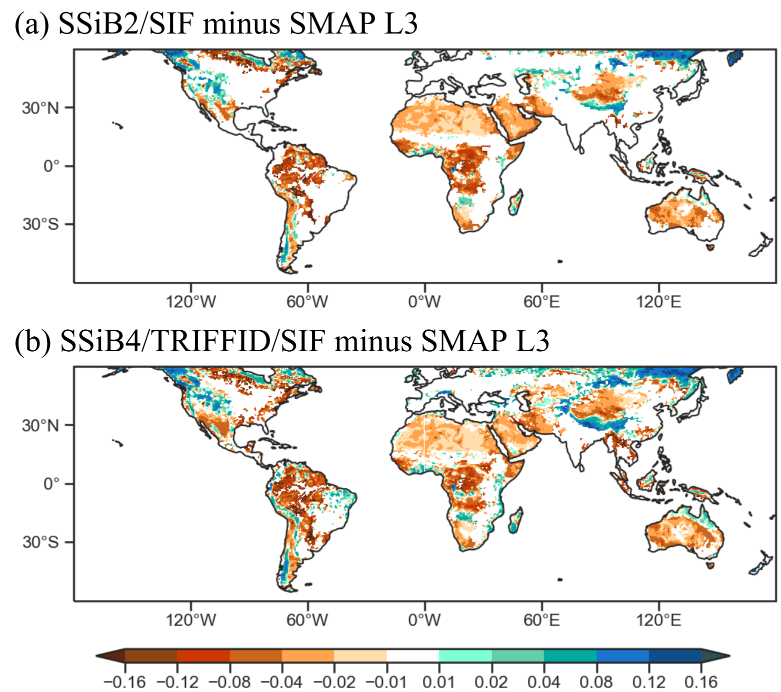

Figure S3. Global differences of soil moisture between simulations in (a) SSiB2/SIF, (b) SSiB4/TRIFFID/SIF and Soil Moisture Active Passive enhanced Level 3 (SMAP L3) data, units: m^3/m^3.

AGU PUBLICATIONS

Global Biogeochemical Cycles

Supporting Information for

Understanding Interactions between Terrestrial Water and Carbon Cycles Using Integrated SMAP Soil Moisture and OCO-2 SIF Observations and Land Surface Models

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Tables S1 to S4

Introduction

This supporting information provides the ancillary tables mentioned in the article.

Table S1. Spatial Correlation Coefficient (SCC), Mean Bias (BIAS), and Root-Mean-Square Error (RMSE) of annual soil moisture simulations compared to SMAP L3 data, units: m^3/m^3.

	SSiB2/SIF	SSiB4/TRIFFID/SIF
SCC	0.849	0.831
BIAS	-0.037	-0.033
RMSE	0.076	0.076

Table S2. Descriptions for the vegetation types in SSiB4/TRIFFID/SIF

Type	Description
1	Evergreen broadleaf trees (EBT)
2	Needleleaf trees (NT)
3	C_3 grasses (C_3)
4	C_4 plants (C_4)
5	Shrubs (SH)
6	Tundra
7	Deciduous broadleaf trees (DBT)
8	Bare soil
9	Crops
10	Ice

Table S3. The original and new values of soil property parameters

	Original B parameter	New B parameter	Original K_s	New K_s	Original wilting point	New wilting point
EBT	7.12	10.0	2.0×10^{-5}	1.0×10^{-6}	5.85	8.35
NT	7.12	7.82	2.0×10^{-5}	1.0×10^{-5}	5.53	4.00
C_3	7.12	5.62	2.0×10^{-5}	2.0×10^{-4}	5.80	4.15
C_4	7.12	9.12	2.0×10^{-5}	1.0×10^{-5}	5.67	4.05
SH	4.05	6.80	1.8×10^{-4}	1.0×10^{-4}	5.01	4.00
DBT	7.12	10.0	2.0×10^{-5}	1.0×10^{-6}	5.57	4.10

Table S4. The original and new values of vegetation parameter, units: μmol/m^2/s

	Original V_{max}	New V_{max}
EBT	100	100
NT	60	30
C_3	60	30
C_4	30	30
SH	60	60
DBT	100	80