Simulating carbon and water fluxes using a coupled process-based terrestrial biosphere model and joint assimilation of leaf area index and surface soil moisture

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Abstract:

Reliable modeling of carbon and water fluxes is essential for understanding the terrestrial carbon and water cycles and informing policy strategies aimed at constraining carbon emissions and improving water use efficiency. We designed an assimilation framework (LPJ-Vegetation and soil moisture Joint Assimilation, or LPJ-VSJA) to improve gross primary production (GPP) and evapotranspiration (ET) estimates globally. ~~The terrestrial biosphere model we used to be the~~ The integrated model, LPJ-PM as the underlying model, coupled from the Lund-Potsdam-Jena Dynamic Global Vegetation Model (LPJ-DGVM version 3.01) and a hydrology module (i.e., the updated Priestley–Taylor Jet Propulsion Laboratory model, $PT\text{-}JPL_{SM}$). Satellite-based soil moisture products derived from the Soil Moisture and Ocean Salinity (SMOS) and Soil Moisture Active and Passive (SMAP) and leaf area index (LAI) from the global Land and Ground satellite (GLASS) product were assimilated into LPJ-PM to improve GPP and ET simulations using a Proper Orthogonal Decomposition-based ensemble four-dimensional variational assimilation method (PODEn4DVar). The joint assimilation framework LPJ-VSJA achieved the best model performance (with an R^2 of 0.91and 0.81 and an ubRMSD reduced by ~~50.4~~40.3% and ~~38.4~~29.9% for GPP and ET, respectively, compared with those of LPJ-DGVM at the monthly scale). The assimilated GPP and ET demonstrated a better performance in the arid and semi-arid regions (GPP: R^2=0.73, ubRMSD=1.05 g C m^{-2} d^{-1}; ET: R^2=0.73, ubRMSD= 0.61 mm d^{-1}) than in the humid and sub-dry humid regions (GPP: R^2=0.61, ubRMSD=1.23 g C m^{-2} d^{-1}; ET: R^2=0.66; ubRMSD=0.67 mm d^{-1}). The ET simulated by LPJ-PM that assimilated SMAP or SMOS had a slight difference, and the SMAP soil moisture data performed better than that SMOS data. Our global simulation modeled by LPJ-VSJA was compared with several global GPP and ET products (e.g., GLASS GPP, GOSIF GPP, GLDAS ET, GLEAM ET) using the triple collocation (TC) method. Our products, especially ET, exhibited advantages in the overall error distribution (estimated error (μ): 3.4 mm month^{-1}; estimated standard deviation of μ: 1.91 mm month^{-1}). Our research showed that the assimilation of multiple datasets could reduce model uncertainties, while the model performance differed across regions and plant functional types. Our assimilation framework (LPJ-VSJA) can improve the model simulation performance of daily GPP and ET globally, especially in water-limited regions.

Keywords: Data Assimilation; SMOS; SMAP; Gross primary production (GPP); evapotranspiration (ET); GLASS LAI

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1. Introduction

Gross primary production (GPP) and evapotranspiration (ET) are essential components of the carbon and water cycles. Carbon and water fluxes are inherently coupled on multiple spatial and temporal scales (Law et al. 2002; Sun et al. 2019; Waring and Running 2010). Terrestrial biosphere models Land surface models (LSMs) are the most sophisticated approach for providing a relatively detailed description of such interdependent relationships regarding water and carbon fluxes and understanding the response of terrestrial ecosystems to changes in atmospheric CO_2 and climate (Kaminski et al. 2017). The dynamic global vegetable models (DGVMs) are process-based dynamic terrestrial biosphere models, which can simulate material exchange between vegetation and different conditions from the perspective of vegetation physiological processes, and ~~is~~ are widely used to estimate carbon and water fluxes of terrestrial vegetation. However, there are still large uncertainties in carbon and water flux estimates at regional to global scales. Both diagnostic and prognostic models show substantial differences in the magnitude and spatiotemporal patterns of GPP and ET. For example, the global annual GPP estimates exhibited a large range (130–169 Pg C yr^{-1}) among 16 process~~-~~-based terrestrial biosphere models (Anav et al. 2015). The global ET ranged from 70,000 to 75,000 km^{3} yr^{-1}, and the uncertainty of regional or global ET estimates was up to 50% of the annual mean ET value, especially in the semi-arid regions (Miralles et al. 2016). These uncertainties mainly arise from the forcing datasets, simplification of mechanisms or imperfect assumptions in processes, and uncertain parameters in the processed models and assimilation methods (Xiao et al. 2019).

In the last two decades, remote sensing products have been assimilated into DGVMs to reduce the uncertainty in modeled carbon and water fluxes (MacBean et al. 2016; Scholze et al. (2017); Exbrayat et al. (2019)). Data assimilation (DA) is an effective approach to reduce uncertainties in terrestrial biosphere models by integrating satellite products with models to constrain related parameters or state variables. A DA system contains ~~three~~ four main components: a set of observations, an observation operator, an underlying model, and an assimilation method. The assimilation method considers the errors from both models ~~LSMs~~ and observations, and reduces model uncertainties by minimizing a cost function. The Ensemble Kalman Filter (EnKF) has been widely applied in land surface process models for parameter optimization, ~~—~~which significantly improve simulations by periodically updating state variables (e.g., LAI and soil moisture) using remote sensing data without altering the model structure

(Ines et al. 2013; Li et al. 2017; Ma et al. 2013). Yet, the EnKF relies on the instantaneous observations to update the state variable at the current time, and gives the predicted value at the next time based on the forward integration of the updated state variable. The four-dimensional variational method (4DVar) assimilation method can obtain the dynamic balance of the estimation in the time window when it is applied to the long-series forecast model (Barth et al. 2014；Zhang et al. 2014). In particular, the Proper Orthogonal Decomposition (POD)-based ensemble 4DVAR assimilation method (referred to as PODEn4DVar) (Tian and Feng 2015) requires relatively less computation and can simultaneously assimilate the observations at different time intervals. Meanwhile, it maintains the structural information of the four-dimensional space. This method has a satisfactory performance in land DA for carbon and water variables (Tian et al. 2009; Tian et al. 2010) and can better estimate GPP and ET than ~~ENKF~~EnKF (Ma et al. 2017).

Multiple sources of remote sensing data streams have been used to constrain models for assimilation. As a critical biophysical parameter of the land, leaf area index (LAI) is closely related to many land processes, such as photosynthesis, respiration, precipitation interception, ET, and surface energy exchange (Fang et al. 2019). LAI is highly sensitive to the simulation of carbon and water fluxes (Liu et al. 2018), and accurate LAI estimates can improve the simulations of the carbon and water fluxes (Bonan et al. 2014; ~~Liu et al. 2018~~; Mu et al. 2007). ~~Soil moisture (SM) controls the process of surface infiltration and runoff, determines the amount of water that can be extracted from plant roots, and distributes the input energy into sensible heat flux and latent heat flux (Trugman et al. 2018). More accurate SM data can improve the simulation of hydrologic parameters (SM, Streamflow, etc.) (e.g., Brocca et al. 2012;~~

~~Draper et al. 2011; Lee et al. 2011; Li and Rodell 2013).~~ Soil moisture is a major driving factor affecting vegetation production in arid ecosystems, especially, in semi-arid areas (Liu et al. 2020). Introducing surface soil moisture (SSM) into the model can significantly improve GPP and ET simulation, particularly in water-limited areas (He et al. 2017; Li et al. 2020).

The advancement of earth observation, machine learning, inversion algorithms, and computer technology has improved the accuracy of global LAI products and boosted model-data fusion studies (Fang et al. 2019; Kganyago et al. 2020; Xiao et al. 2017). The Advanced Very High-Resolution Radiometer (AVHRR) generates global LAI products with the longest historic record (since the early 1980s). The GLASS LAI product has been verified to have a better accuracy than that of MODIS and CYCLOPES and is more temporally continuous and spatially complete (Xiao et al. 2013). Several recent studies showed that the assimilation of GLASS LAI into ~~terrestrial biosphere models~~DGVMs enhanced the performance of the models in simulating carbon cycling (e.g., GPP, Net Ecosystem Exchange (NEE)) and hydrological (e.g., ET, SM) processes (Ling et al. 2019; Ma et al. 2017; Yan et al. 2016).

Microwave remote sensors are considered effective tools for measuring SM globally (Petropoulos et al. 2015). For example, surface SM products have been derived from the Soil Moisture and Ocean Salinity (SMOS) and Soil Moisture Active and Passive (SMAP) satellites equipped with an L-band microwave instrument. The products from these satellites have been evaluated against in-situ observations and other SM products and overall have high accuracy(Burgin et al. 2017; Cui et al. 2018). Additionally, the SMAP performs better than SMOS and other SM products (e.g., Advanced Scatterometer (ASCAT), Advanced Microwave Scanning Radiometer 2 (AMSR2)) with an overall lower error and a higher correlation based on the verification with in-situ SM data from 231 sites (Cui et al. 2018; Kim et al. 2018). The assimilation of SMAP data can improve the simulation accuracy of carbon and water fluxes (He et al. 2017; Li et al. 2020) and hydrological variables (surface soil moisture, root-zoon soil moisture, and streamflow) (Blyverket et al. 2019; Koster et al. 2018; Reichle et al. 2017). In addition, the assimilation of SMAP data performed slightly better than that of SMOS and ESA CCI data (Blyverket et al. 2019).

In the nonlinear model or nonlinear observation operator, only simultaneous assimilation makes optimal use of observations (MacBean et al. 2016). Therefore, a joint assimilation of soil moisture and LAI can make full use of the two variables. ~~–~~From site (Albergel et al. (2010);Rüdiger et al. (2010); Wu et al.,2018) to regional assimilation (Ines et al. (2013)), many studies have proposed that joint assimilation of vegetation parameters and soil moisture is a potential improvement in modeling the carbon-water cycle. For instance, ~~Ines et al. (2013) found that the joint assimilation of soil moisture and LAI achieved better results than the assimilation of one of the two variables~~. joint assimilation of soil moisture and leaf area index can improve the accuracy of crop yield estimation (Xie et al.,2018; Pan et al.,2019), with small region and high spatial resolution, which adopting observation data from stations or high-resolution satellites (e.g. Sentinel-1 and 2). ~~On~~At a large regional scale, Bonan et al. (2020) assimilated LAI and SM together into the Interactions between Soil, Biosphere and Atmosphere (ISBA) land model and improved the modeled GPP, ET, and runoff in the Mediterranean region. Rahman et al. (2022) jointly assimilates GLASS LAI and SMAP soil moisture to improve water and carbon flux ~~simulaitons~~simulations within the Noah-MP model over the CONUS domain. Albergel et al.(2020) jointly assimilates the ASCAT soil moisture index (SM~~W~~I) and LAI GEOV1 into ISBA (Interaction between Soil Biosphere and Atmosphere) surface model through the Global Offline Land Data assimilation system LDAS-Model to monitor extreme events such as drought and Heatwave events. In conclusion, Kalman Filter and its variant methods are mostly used~~ in regional scale~~ joint assimilation methods at regional scale, which requires many ~~various~~kinds of observation data ~~were chosen~~ and ~~the~~ their ~~its~~ accuracy directly affects the assimilation performance. ~~However, no studies have examined the performance of assimilation of LAI and SM into terrestrial biosphere models for improving the simulation of carbon and water fluxes at the global scale.~~

~~In this study, we assimilated the SM products from both SMAP and SMOS and a LAI product (GLASS) derived from AVHRR and MODIS into the LPJ-PM to improve the GPP and ET using the PODEn4DVar method. We designed a new assimilation framework, LPJ-VSJA, which consists of three assimilation schemes: (1) assimilation of LAI only, (2) assimilation of SM only, and (3) joint assimilation of LAI and SM. Then, four experiments were performed based on global flux sites to evaluate the assimilation performance.~~ This study stems from the researches discussed above and further explored the potential of joint assimilating satellite LAI and soil moisture products globally. Specifically, it was the first time that an updated LPJ-DGVM model was used to jointly assimilate GLASS LAI and SMAP soil moisture for ~~and~~ simulating~~e~~ global water and carbon fluxes. The latest global soil moisture datasets (SMOS and SMAP) were used, and the assimilation performance of these two observations was analyzed. Since previous work showed the ~~vital~~importance of surface soil moisture in the semi-arid and arid areas, one of t~~T~~he specific objectives of our study ~~are~~is to~~: (1) evaluate the assimilation performance of three assimilation schemes for estimating GPP and ET and further to select the optimal assimilation scheme;~~

~~(2)~~ compare the assimilation effect ~~of the optimal assimilation scheme~~ in the humid and arid areas and improve~~d~~ the understanding of the effect of surface soil moisture on vegetation activity in wet and dry zones. ~~; (3) compare the assimilation capability in ET assimilation based on two microwave soil moisture products (SMOS and SMAP) (scheme 2); and (4) apply our LPJ-VSJA framework to simulate global carbon and water fluxes.~~ In addition, compared with the assimilation methods in previous studies (mostly using Kalman Filter variants), the POD-En4DVar method is used, which greatly improves the computational efficiency.

2. LPJ-VSJA framework and assimilation strategy

2.1. Coupled- model (LPJ-PM) for assimilation

In this study, a coupled terrestrial biosphere model, LPJ-PM, was used to simulate daily GPP and ET by assimilating satellite-derived LAI and SM. The LPJ-PM is coupled from LPJ-DGVM and PT-JPL_{SM}. The original input data in PT-JPL_{SM} were all inherited from LPJ-DGVM, with the exception of relative humidity (RH) and surface soil moisture (SMOS and SMAP), including the initial LAI calculated by the LPJ-DGVM or assimilated LAI obtained through the LAI assimilation scheme, canopy height, and the fraction of absorbed photosynthetic effective radiation (fAPAR). The detailed processes of the LPJ-PM have been described in Li et al. (2020), and the flow chart for the coupling is shown in Figure 1.

Table 1. Description of the models and outputs in this study

acronyms	Full name	Description	Output

LPJ-DGVM (Sitch et al. 2003)	Lund-Potsdam-Jena Dynamic Global Vegetation Model	This model is used as a model operator to simulated initial ET	GPP_{LPJ}, ET_{LPJ}
PT-JPL_{SM} (Purdy et al. (2018))	Updated Priestley–Taylor Jet Propulsion Laboratory model	The model is used as a module of the LPJ-PM and establishes a connection between SMAP SM and ET	N/A
LPJ-PM (Li et al. (2020))	Lund-Potsdam-Jena and Updated Priestley–Taylor Jet Propulsion Laboratory coupled model	An integrated model coupled from the PT-JPL_{SM} and LPJ-DGVM	GPP_{SM}, ET_{PM}
LPJ-VSJA (this study)	Lund-Potsdam-Jena Vegetation-Soil moisture-Joint - Assimilation system	A process-based assimilation framework for assimilating LAI and SSM jointly into LPJ-~~DGVM~~ PM	GPP_{LAI}, ET_{LAI}; GPP_{SM}, ET_{SM}; GPP_{CO}; ET_{CO}

2.1.1 LPJ-DGVM

The LPJ-DGVM is a process-oriented dynamic model, which considers mutual interaction of carbon and water cycling and is designed to simulate vegetation distribution and carbon, soil and atmosphere fluxes (Sitch et al. 2003). For each plant functional type (PFT), the GPP is calculated by implementing coupled photosynthesis and water balance

The canopy GPP is updated daily:

$$\mathrm{GPP} = \frac{(J_E + J_c - \sqrt{(J_E + J_c)^2 - 4\theta J_E J_c})}{2\theta} \qquad (2.1)$$

where J_C is the Rubisco limiting rate of photosynthesis, J_E is the light limiting rate of photosynthesis, and the empirical parameter θ represents the common limiting effect between the two terms. J_E is related to APAR (absorbed photosynthetic radiation, product of FPAR and PAR), while J_C is related to Vcmax (canopy maximum carboxylation capacity, μ mol CO^2/m ^{2}/s):

$$J_E = C_1 \mathrm{APAR} \qquad (2.2)$$

$$J_C = C_2 V_{C\,max} \qquad (2.3)$$

where C_1 and C_2 are determined by a variety of photosynthetic parameters and the intercellular partial pressure of CO_2, which is related to atmospheric CO_2 content and further altered by leaf stomatal conductance (Sitch et al. 2003). APAR and FPAR are directly related to LAI.

In the water cycle module, ET is calculated as the minimum of a plant- and soil-limited supply function (E_{supply}) and the atmospheric demand (E_{demand}) (Haxeltine and Prentice 1996; Sitch et al. 2003). The soil structure is simplified to a “two-layer bucket” model (the top soil layer at a 0-50 cm depth and the bottom layer at a 50-100 cm depth) .

$$E_S = Ep \times Wr_{20} \times (1 - fv) \quad (2.4)$$

In this module, it is assumed that the soil layer above 20 cm produces water through evaporation, and Wr_{20} is the relative water content of the soil above 20 cm, which is used as the only soil water limit for calculating vegetation transpiration and soil evaporation. In the evapotranspiration estimation, the over-simplification of soil structure and soil water limitation lead to a large error (Sitch et al. 2003), while LPJ-DGVM cannot directly assimilate surface soil water due to the limitation of soil layer stratification..

The soil structure is simplified to a "two-layer bucket" model (the top soil layer at a 0-50 cm depth and the bottom layer at a 50-100 cm depth), and therefore, the satellite-derived surface SM cannot be assimilated into LPJ-DGVM directly. The oversimplified soil structure and single soil moisture limitation inevitably lead to sizeable uncertainty in ET simulation. Additionally, the monthly input caused a daily variation of the modeled SM, which was also not transmitted to the calculation of GPP and ET. Thus, the updated PT-JPL model (hereafter referred to as PT-JPL_{SM}) was coupled with LPJ-DGVM and the model structure was modified so that surface SM can be directly assimilated into the coupled model at the daily time step.

2.1.2 PT-JPL_{SM}

In PT-JPL_{SM}, three ET components are modelled: soil evaporation (E), vegetation transpiration (T), and leaf evaporation (I). The PT-JPL_{SM} introduced a constraint (0–1, C_{RSM}) of surface SM for T and E, which was used to avoid the implicit soil water control (represented by $f_{SM}=RH^{VPD}$) in the PT-JPL model.

The constraint is determined by the amount of soil water available that depends on soil properties, surface SM, atmospheric conditions, potential ET (PET), and canopy height.

Vegetation transpiration:

$$C_{RSM} = (1 - RH^{4(1-VWC)(1-RH)})C_{SM} + (RH^{4(1-VWC)(1-RH)})C_{TRSM} \quad (2.5)$$

$$C_{TRSM} = 1 - \left(\frac{w_{CR} - w_{obs}}{w_{CR} - w_{pwp\_CH}}\right)^{\sqrt{CH}}, \quad (2.6)$$

where w_{obs} is the SMAP SM, w_{pwp} is the water content at the wilting point, and w_{fc} is the water content at field capacity, which is determined by the properties of the soil. W_{CR} is a crucial parameter in characterizing the extent of SM restriction on ET; w_{pwp_CH} is the canopy height (CH) and is related to the potential of roots capturing water from deeper sources to limit the transpiration rate and characterize the SM availability (Purdy et al., 2018; Evensen 2003; Serraj et al., 1999). The specific formula is given in Purdy et al. (2018).

Soil evaporation:

$$C_{RSM} = \frac{w_{obs} - w_{pwp}}{w_{fc} - w_{pwp}} \quad (2.7)$$

The proportion of available water limits the soil evapotranspiration to the maximum available water. This scalar was formulated to represent the relatively accurate extractable water content for the vegetation, determined by soil properties and the water available for evaporation, which is estimated via surface water constraints.

–The SMAP SM as surface SM data was applied to model global ET using PT-JPL$_{SM}$ and the results demonstrated the largest improvements for ET estimates in dry regions (Purdy et al. 2018). Due to the limitation of soil stratification in LPJ-DGVM, the model was coupled with an updated remote-sensing ET algorithm in the PT-JPL$_{SM}$ that could better simulate ET in water-limited regions than in humid regions (Purdy et al. 2018).

2.2. Assimilation scheme and experiment procedure

To improve the prediction capability of LPJ-PM, we designed three assimilation schemes: assimilating LAI only(scheme 1, **output: ET$_{LAI}$, GPP$_{LAI}$**), assimilating ~~ET~~ SSM only (scheme 2, **output: GPP$_{SM}$, ET$_{SM}$**), and joint assimilation of LAI and ~~ET~~ SSM (~~(~~scheme 3, **output: ET$_{CO}$, GPP$_{CO}$**), i.e., LPJ-VSJA framework) to test the assimilation performance for simulating GPP and ET.

The proposed LPJ-VSJA framework consists of four main components: the model operator (the LPJ-PM), the observation operator (to establish the relation between the assimilation variable and the observed variable), the observation series (GLASS LAI and SMOS or SMAP products), and the assimilation algorithm (POD4DVar). With the surface soil moisture constraint in the PT-JPL$_{SM}$, the LPJ-VSJA corrects the output fluxes (GPP and ET in this study).

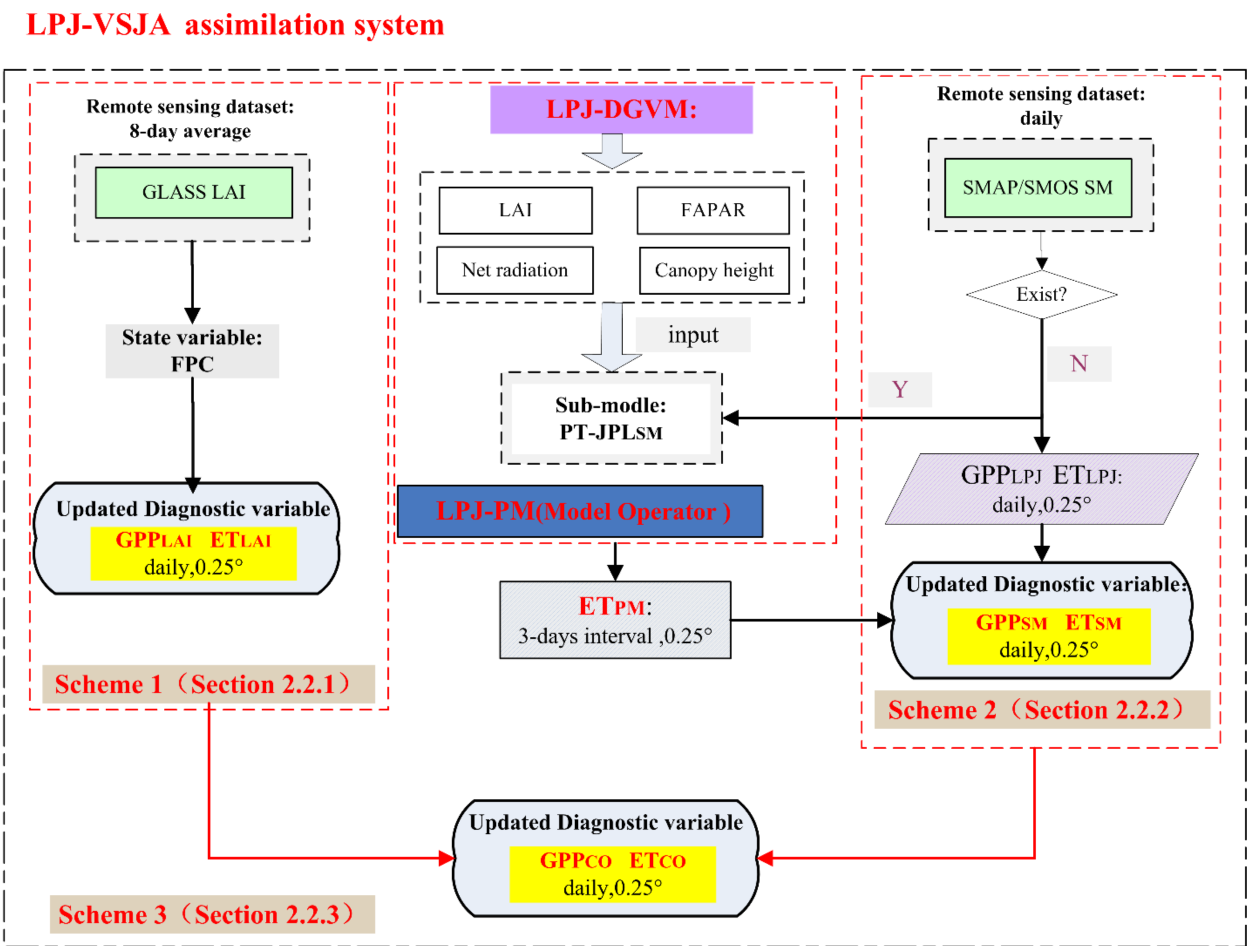


Figure 1. Flowchart of the LPJ-VSJA assimilation scheme: three assimilation schemes and the coupled model: LPJ-PM. (adapted from Li et al., 2020). The abbreviation of model and assimilation framework is explained in Table 1.

The experiment consisted of six steps:

(1)Step 1: initialize the LPJ-DGVM and output the reference state variables without assimilation over the experimental period (2010–2018), referred to as the “Control run” scenario;.

Step 2: (2) implement schemes 1, 2, and 3, respectively, and the results represent the assimilation integration state (daily GPP and ET assimilation results are referred to as the “GPP_{LAI}” and “ET_{LAI}” in scheme 1,;“GPP_{SM}” and “ET_{SM}” in scheme 2 and “GPP_{CO}” and “ET_{CO}” in scheme 3;. This scenario used the same input data and model parameter scheme with the “Control run” scenario;.

Step 3(3): evaluate GPP and ET results (schemes 1, 2 and 3) by comparing the parameters, R^2 (correlation coefficient), RMSD (root mean square deviation), BIAS, and ubRMSD (unbiased root mean square deviation), for conditions of without-DA (“Control run” scenario) and with-DA states, and assess the assimilation performance of separate assimilation (schemes 1 and 2) and joint assimilation (scheme 3) to determine the optimal assimilation scheme for GPP and ET, respectively;.

Step 4: (4) evaluate the in-situ assimilated GPP and ET results where the sites are located in wet or dry regions by dividing these validation sites into four parts (humid, sub-dry humid, semi-arid, and arid regions), and this step was designed to assess the superiority of the proposed assimilation scheme in water-limited areas;.

Step 5:(5) compare the ET assimilation performance by assimilating the SMOS data with that by assimilating the SMAP data.

Step 6:and (6) evaluate the simulated GPP and ET maps based on the optimal assimilation scheme against existing global flux products.

2.2.1 DA scheme 1: LAI assimilation

In assimilation scheme 1, the observation operator determines the relationship between LAI and foliage projective cover (FPC) in the process model (equation 2.1), and the assimilated LAI will be propagated by energy transmission and ecosystem processes (e.g. photosynthesis, transpiration of vegetative process) in the dynamic model to improve GPP and ET simulations (Bonan et al. 2014; Mu et al. 2007). FPC, the vertically projected percentage of the land covered by foliage, regulates the rate of photosynthate conversion and transpiration. In this study, the GLASS LAI with 8-day interval for the period 2010–2018 was selected as the observation dataset for assimilation, and the FPC state variable was updated daily through running the LPJ-PM (GPP_{LAI}, ET_{LAI} in this study) as shown below:

$$FPC = 1 - e^{-0.5LAI} \quad (2.1)$$

We set the model and observation errors at a given time as 20% and 10% (scale factor) of the LAI value and the observed LAI value, respectively. By verifying the assimilation performance (R, RMSD, BIAS) for different scale factors(f) of model simulation and observations in the range of 0.05 to 0.40, taking a step size of 0.05 (a total of 64 combinations), the optimal scale factors (0.2 and 0.1) were determined (Bonan et al., 2020). The model and observation errors was the LAI value multiply by f. The model integration generation method described by Pipunic et al. (2008) was used to determine the minimum number of ensemble members required to achieve maximum efficiency, and the number of sets was 20.

2.2.2 DA scheme 2: SSM assimilation

In this scheme, the surface SM products (SMOS or SMAP) were assimilated to LPJ-PM to obtain more accurate ET (ET_{SM}) estimates in water-limited areas. The observation series was the SMOS or SMAP SSM product, and the observation operator was the PT-JPL$_{SM}$ model. The ET_{PM} estimated by the coupled model (LPJ-PM) introducing surface SM was directly assimilated as a diagnostic variable. The assimilated ET was applied to compute the top layer SM (50 cm) at the next time step (a nonlinear soil water availability function described by Zhao et al. (2013), providing feedback for subsequent hydrologic and carbon cycle processes. Then, the updated SM values regulated the GPP simulation (output: GPP_{SM}). Different from other "constant" ET observations, the ET_{PM} ("observation") at each time *t* were adjusted by absorbing intermediate variables updated after assimilation at time *t*-1. The ET_{PM} was shown to be better than ET simulated by LPJ-DGVM but not as good as that simulated by the model with SMAP SM assimilated (Li et al. 2020). Thus, it is proven that this SM assimilation schemes could improve the accuracy of ET simulations.

All assimilation simulations were conducted between January 2010 and December 2018. Between January 2010 and April 2015, SMOS data were used for assimilation;, and after May 2015, both SMOS and SMAP data were used for assimilation. An assimilation scheme was conducted when RH and SMOS or SMAP SM data existed simultaneously; otherwise, the original simulation of the LPJ-DGVM was conducted directly without adjustment of assimilation.

Similar to the LAI assimilation scheme, the model and observation errors were set as 15% and 5% of ET_{LPJ} and ET_{PM}, respectively (LPJ-PM was adopted before assimilation). The number of ensembleset members was set to 50.~~-~~The ET_{PM} must be rescaled to the ET_{LPJ} distribution via their corresponding cumulative probabilities using the cumulative distribution function (CDF) matching to avoid introducing any bias in the LPJ-VSJA system (Li et al. 2020).

2.2.3 DA scheme 3: joint assimilation of LAI and SSM

In this scheme, both LAI from GLASS and SM from SMOS or SMAP were the observation datasets. The GLASS LAI was assimilated by scheme 1 to obtain the FPC_{DA} and ET_{LAI}, and then the FPC_{DA} served as input to LPJ-PM to simulate optimized ET_{PM}, and the ET_{LAI} was further assimilated with ET_{PM} to generate $ET_{CO.}$ Then, the SM (referred to as SM_{CO} in Figure S1) updated by ET_{CO} and the FPC_{DA} were used as input to correct GPP (GPP$_{CO}$).~~. Finally, GPP_{CO} and ET_{CO} were output by joint assimilation based on the POD-En4DVar method.~~

Here, we applied the error regulation in scheme 1 and maintained the error setting of the LAI observation and model simulation. Considering the transmission of integrated model error, we recalculated the model error of LPJ-PM after the LAI assimilation and set model and observation errors of ET_{LAI} and ET_{PM} to be 15 and 10%, respectively. ~~The number of set members was set to 70.~~

2.3. POD-Based Ensemble 4D Variational Assimilation Method

~~The PODEn4DVar~~The Proper Orthogonal Decomposition (POD)-based ensemble four-dimensional variational (4DVar) assimilation method (referred to as PODEn4DVar) (Tian and Feng 2015)~~(Tian et al. 2011) method~~ has the advantage of avoiding the calculation of adjoint patterns as its incremental analysis field, which can be represented linearly by the POD base (Transformed OP (Observing Perturbation) and MP (Model Perturbation))~~, and then saving computation~~. Moreover, the PODEn4DVar can simultaneously assimilate multiple-time observation data and provide flow-dependent (the flow-dependent is the ensembles of forecasting statistical characteristics in the t time) error estimates of the background errors. It has shown advantages in terrestrial assimilation, Tan-Tracker joint DA, and Radar assimilation (Tian et al. 2010; Tian et al. 2009; Tian et al. 2014; Zhang and Weng 2015).

By minimizing the following initial incremental format of the cost function in the 4DVar algorithm, an analysis field can be obtained:

$$\boldsymbol{J}(\boldsymbol{x'}) = \frac{\boldsymbol{1}}{\boldsymbol{2}}(\boldsymbol{x'})\boldsymbol{B}^{-\boldsymbol{1}}(\boldsymbol{x'}) + \frac{\boldsymbol{1}}{\boldsymbol{2}}[\boldsymbol{y'}(\boldsymbol{x'}) - \boldsymbol{y'}_{\boldsymbol{obs}}]^{\boldsymbol{T}}\boldsymbol{R}^{-\boldsymbol{1}}[\boldsymbol{y'}(\boldsymbol{x'}) - \boldsymbol{y'}_{\boldsymbol{obs}}]$$

Here, the $x' = x - x_b$, $y'(x') = y(x' + x_b) - y(x_b)$, $y'_{obs} = y_{obs} - y(x_b)$, $y = H[M_{to\rightarrow tk}(x)]$. $x'(x'_1, x'_2, \ldots\ldots, x'_N)$ is the model perturbation (MP) matrix and $y'(y'_1, y'_2, \ldots\ldots, y'_N)$ is the observation perturbation (OP) matrix with N samples. Following Rüdiger et al. (2010), the LAI perturbation was set to a fraction (0.001) of the LAI itself. The perturbation of ET_{PM} and ET_{LPJ} conforms to a Gaussian distribution with a mean of 0 and a specified covariance (10 and 5% of the ET_{PM} and ET_{LPJ} at time t). The subscript b represents the background field, the superscript T represents a transpose, H is the observation operator of scheme 1 as described in section ~~2.3~~2.2.1, and scheme 2 is the $PT\text{-}JPL_{SM}$ (described in ~~Purdy et al. (2018)~~2.1.2). M is the forecast model (LPJ-PM in this study), B is the background error covariance, R is the observation error covariance, and obs denotes observation.

Assuming the approximately linear relationship between OP(y') and MP(x'), POD decomposition and transformation were successively conducted for OP and MP. The transformed OP samples ($\Phi_y = y'_1, y'_2, \ldots\ldots, y'_n$) are orthogonal and independent, and the transformed MP samples ($\Phi_x = x'_1, x'_2, \ldots\ldots, x'_n$) are orthogonal to the corresponding OP samples, where n is the number of POD modes.

The manifestation of the background error covariance is the same as the Ensemble Kalman filter (EnKF, Evensen (2004)), and the incremental analysis x'_a was expressed by the $\Phi_{x,n}$, and $\widetilde{\Phi}_y(\widetilde{\Phi}_y = \left[(n-1)I_{n\times n} + \Phi_{y,n}^T R^{-1}\Phi_{y,n}\right]^{-1}\Phi_{y,n}^T R^{-1})$. Finally, the ~~final~~ optimal analysis x_a is calculated as $x_a = x_b + \Phi_{x,n}\widetilde{\Phi}_y y'_{obs}$. The detailed derivation process of the algorithm is described by a previous study (Tian et al. 2011).

In the ensemble-based method (Evensen et al.,2004), the number of ensemble members is usually fewer than that of the observation data and the degrees of freedom of the model variables, and spurious long-range correlations occur between observation locations and model variables. A practical method, the localization technique, is applied to address this issue (Mitchell et al. 2002). The final incremental analysis is rewritten as:

$$x'_a = \Phi_{x,n}\widetilde{\Phi}_y y'_{obs} C_0\left(\frac{d_h}{d_{h,0}}\right) \cdot C_0\left(\frac{d_v}{d_{v,0}}\right)$$

where d_h and d_v are the horizontal and vertical distances between the spatial positions of state and observed variables, respectively; and $d_{h,0}$ and $d_{v,0}$ are the horizontal and vertical covariance localization Schur radii, respectively. The filtering function C_0 is expressed as:

$$C_0(r) = \begin{cases} -\frac{1}{4}r^5 + \frac{1}{2}r^4 + \frac{5}{8}r^3 - \frac{5}{3}r^2 + 1, & 0 \le r \le 1, \\ \frac{1}{12}r^5 - \frac{1}{2}r^4 + \frac{5}{8}r^3 + \frac{5}{3}r^2 - 5r + 4 - \frac{2}{3}r^{-1}, & 1 \le r \le 2, \\ 0, & 2 < r \end{cases}$$

where r is the radius of the filter.

The assimilation algorithm is mainly divided into two steps: (1) prediction: run LPJ-PM in the current assimilation window and generate simulation results and background field vectors; (2) update: the algorithm is used to calculate the optimal assimilation increment x'_a and analysis solution x_a, and the simulation results and the initial conditions of the model in the current window are updated using the analysis solution. The updated initial conditions were applied for model LPJ-PM prediction, and the above process was repeated.

2.4. Validation method for assimilation performance

The R^2 (correlation coefficient), ~~RMSD (root mean square deviation),~~ Bias, and ubRMSD (unbiased root mean square deviation) between simulation and tower-based observations were applied for evaluation. In addition, a Taylor chart was also used to demonstrate the performance of two ET estimations with different SM observations in terms of R, ubRMSD, and Normalized Standard Deviation (NSD) on 2D plots, to display how closely the datasets matched observations in one diagram (Taylor 2001). In the Taylor diagram, SD represents the radial distance from the origin point and the correlation with the site observations as an angle in the polar plot. The ubRMSD is the distance between the observation and the model and is represented in the figure as a green semi-circular arc with point A as the center of the circle. The closer the model point to the reference point (Point A), the better the performance. This diagram is convenient and visual in evaluating multiple aspects of various models.

The error variance of GPP and ET products was estimated using the triple collocation (TC) approach (Stoffelen 1998) to validate the global simulation in this study. The method has been extensively applied in the study of hydrology and oceanography (Caires and Sterl 2003; Khan et al. 2018; O'Carroll et al. 2008; Stoffelen 1998), particularly in SM studies (Chan et al. 2016; Kim et al. 2018). The TC provides a reliable platform for comparison of spatial assimilation results and in-situ measurements. In this experiment, no calculation was performed on the non-vegetated areas where the correlation was lower than 0.2 to have independent datasets and avoid correlated errors (crucial assumptions in TC) (Yilmaz and Crow 2014).

In this study, the five products were divided into three product categories, including satellite product (MODIS, GOSIF GPP), reanalysis product (GLASS, GLDAS) and data assimilation product (GLEAM ET, LPJ-VSJA) (Li et al.,2018). One product in each category was selected to form a group to calculate their error. The LPJ-VSJA product was set as the reference data.

For GPP products, GOSIF, GLASS, and LPJ-VSJA were treated as a group, and MODIS, GLASS and LPJ-VSJA were treated as another group to calculate the errors; the final errors were determined by the average of these two.

Similarly, to calculate the errors for ET, GLEAM, GLASS, and MODIS were chosen as a group; LPJ-VSJA, GLDAS, and MODIS were treated as a group; LPJ-VSJA, GLASS and MODIS were considered as a group. In order to reduce the influence of orthogonality hypothesis of error, the first and third groups are for indirect and effective comparison between LPJ-VSJA product and GLEAM product.

3. Experiment sites and data

3.1. Description of flux tower sites

We screened over 300 EC flux sites across the globe from the FLUXNET2015 (https://fluxnet.fluxdata.org/data/fluxnet2015-dataset/), AmeriFlux (http://public.ornl.gov/ameriflux), and the HeiHe river basin (Liu et al. (2018), http://www.heihedata.org)(Li et al. 2013) for the evaluation of assimilation performance over the period from January 2010 to December 2018. The in-situ half-hourly LE and GPP data from the sites were aggregated into daily data. The daily gap-filled data were excluded if the percentage of gap-filled half-hourly values was more than 20%. Then we corrected the data of energy non-closure by using the Bowen ratio closure method (Twine et al. 2000) to improve the energy closure rate (Huang et al. 2015; Yang et al. 2020). The data were selected to cover the 2010–2018 period with at least one year of reliable data, and the result from the error of assimilation is relative to the LE value and seasonal variation (Purdy et al. 2018; Zou et al. 2017). It is essential to have available data every month during a one-year period, and only days with less than 25% missing data were processed per month (Feng et al. 2015). In addition, for flux tower data, the data were also excluded for the analysis if the SMAP/SMOS SM data were not of good quality.

Finally, we identified a total of 105 sites across the globe encompassing five major biomes: grassland (18 for GPP and 19 for ET), savanna (11), shrubland (4), forest (49 and 53), and cropland (13 and 14). In the comparative analysis of the performance for simulating ET by assimilating SMOS and SMAP SM data separately, we selected 46 AmeriFlux sites (Figure S3) with at least one year of reliable data from 2015 to 2018 based on the simultaneous availability of SMAP and SMOS data, including grassland (19), savanna (11), shrubland (5), forest (23), and cropland (7). Figure S2 and S3 illustrate the location and distribution of the 105 and 46 EC flux tower sites, respectively. A more detailed description is summarized in the Supporting Information Table S1.

3.2. Remote sensing datasets: LAI and SM

The GLASS LAI product with an 8-day time step and 5 km resolution was derived from MODIS and CYCLOPES surface reflectance and ground observations using general regression neural networks (GRNNs) (Liang et al. 2013; Xiao et al. 2016). The verification of the product using the mean values of high-resolution LAI maps showed that the GLASS LAI values were closer to these high-resolution LAI maps (RMSD= 0.78 and R^2= 0.81). Therefore, the GLASS LAI product has satisfactory performance and can be assimilated into terrestrial biosphere models.

The SMAP mission (Entekhabi et al. 2010) and SMOS mission (Jacquette et al. 2010), the two dedicated soil moisture satellites currently in orbit equipped with L-band microwave instruments, provide surface SM retrievals. We chose the SMOS-L2 product and the SMAP-L3-Enhanced product, which both provide global coverage every three days for soil depth of 5 cm. Only good-quality SMAP and SMOS data were used. The grid cells with water areas larger than 10% and those with less than 50% good-quality data in one year were masked out, which alleviates the undesirable model simulations caused by the decrease in SMAP retrieval accuracy (Chan et al. 2016; O'Neill et al. 2010). We only adopted the data with an uncertainty below 0.1 m^3 m^{-3}, in the actual range (0.00–0.6 m^3 m^{-3}), and the temperature of the LSM observation layer (the second layer) was higher than 2 °C (Blyverket et al. 2019).

Both tThe GLASS LAI, SMOS and SMAP observations was resampled to 9 km for site simulation and 0.25° for spatial simulation.

3.3. Model-forcing and validation datasets

In this study, the meteorological, soil property, and CO_2 concentration datasets were used to drive the LPJ-PM. For site simulation, in order to maintain consistency with the SMAP Enhanced 3 Level product (Entekhabi et al. 2010), model-forcing data were resampled to a 9 km spatial resolution based on EASE-2 projection grid. In the global spatial simulation, the model-forcing datasets were interpolated to 0.25° based on the bilinear method to ensure the consistency of spatial representation. Table 2 provides the spatial and temporal characteristics of the model-forcing datasets in the LPJ-PM (submodule: LPJ-DGVM and PT-JPL$_{SM}$).

Table 2. List of the selected forcing and remote-sensing datasets used in this study

Datasets	Variable	Period	Spatial resolution	References
CRU TS v4.1[a]	Cloud cover,	1901-	0.5°× 0.5°	New et al.

	temperature, precipitation, wet day	1930		(2000), https://crudata.uea.ac.uk/cru/data/hrg/
Ice-core measurements and atmospheric observations at the Mauna Loa Observatory [a]	Atmospheric CO_2 concentrations	1901-2018	NA	(Etheridge et al. (1996); Keeling et al. (1995)) , https://scrippsco2.ucsd.edu/data/atmospheric_co2/
MERRA-2 [a]	Precipitation, surface temperature, cloud fraction, relative humidity	2010-2018	0.5°× 0.625°	Rienecker et al. (2011) （https://www.esrl.noaa.gov/psd/）
HWSD (v121)[b]	Soil texture data	NA	1 km×1 km	Wieder et al. (2014) （http://daac.ornl.gov）

SPL3SMP_E[b]	Surface soil moisture	2015.4–present	9 km×9 km	Entekhabi et al. (2010), (https://smap.jpl.nasa.gov/)
GLASS LAI [a,b]	Leaf area index	2010-2018	5 km×5 km	Xiao et al. (2016), (http://www.glass.umd.edu/Download.html)
SMOS_L3 CATDS[b]	Surface soil moisture	2010-present	25km×25 km	Jacquette et al. (2010),(https://earth.esa.int/eogateway/missions/smos)

452 [a]: forcing dataset for LPJ-DGVM

453 [b]: external input dataset for PT-JPL$_{SM}$

We used four global ET products and three global GPP products (Li et al. 2018; Li and Xiao 2019; Wang et al. 2017) that was resample to 0.25° to evaluate the performance of the model with the joint assimilation scheme. Table 3 shows the details of these GPP and ET products.

Table 3. Global GPP and ET products for comparison in this study

Product	Dataset	Temporal resolution	Spatial resolution	Retrieval algorithm	References
MOD17A2	GPP and ET	8-day average	1 km × 1 km	GPP: Based on the light use efficiency (LUE) model ET: Improved Penman formula	Running et al. (2004)
GLASS	GPP and ET	8-day average	5 km × 5 km	GPP: EC-LUE model ET: Combining five Bayesian averages based on process models (BMA)	Yuan et al. (2010)
GOSIF GPP	GPP	8-day average	0.05° × 0.05°	Estimated from solar-induced chlorophyll	Li and Xiao (2019)

				fluorescence with GPP-SIF relationships	
GLDAS ET	ET	daily	0.25°× 0.25°	Processed model assimilation	Fang et al. (2009)
GLEAM v3a ET	ET	daily	0.25°× 0.25°	Processed model assimilation	Martens et al. (2017)

4. Results

4.1. Performance of LPJ-PM for simulating GPP and ET with the assimilation of LAI and soil moisture

4.1.1 Accuracy assessment of GPP for separate and joint assimilation

In general, the R^2 between GPP_{LPJ} and GPP_{OBS} was above 0.4 at most of the sites (62 sites) and were relatively weak for some sites~~ (R^2<0.4)~~. The LAI assimilation improved the simulations at most sites (R^2 value increased at 82 sites), particularly for sites in the U.S. and Europe (Figure 2). The R^2 improvement from the LAI assimilation (scheme 1) was superior to that from the SM assimilation (Figure 2-R^2 (b) and (c)). The performance of the joint assimilation (scheme 3) was similar to that of scheme 1. ~~The GPP assimilation performance in terms of RMSD between scheme 1 and scheme 2 was not significantly different. For sites with no improvement in the separate assimilation (schemes 1 and 2), the RMSD, however, was improved in the joint assimilation (scheme 3) (Figure 2)~~. Sites (Figure 2-

BIAS (a)) showed positive bias (GPP_{OBS}-GPP_{LPJ}) were mainly distributed in the humid and dry-sub humid forest, grassland, and arid cropland regions, showing an underestimation for GPP_{OBS}. The assimilation improved the accuracy for overestimated sites, but there was no significant improvement for underestimated sites. The ubRMSD implied that the SM assimilation alone had a better performance than the LAI assimilation alone, especially for sites in arid areas. The analysis of the above ~~four~~ three statistical measures (R^2, ~~RMSD,~~ BIAS, and ubRMSD) indicated that the accuracy of joint assimilation was much better than that of separate assimilation.

At the seasonal scale, all three assimilation schemes corrected the model trajectory and significantly improved the growing season simulations, especially for peak values (IT-Tor, US-NR1, US-NE1)(Figure 3). In addition, the linear fitting of GPP_{CO} and GPP_{OBS} on a monthly scale was closer to 1:1 (y= 0.92 + 21.66 $p < 0.001$) than that of GPP_{LAI} (y= 0.89 + 28.3, $p < 0.001$) and GPP_{SM} (y= 0.86 + 41.70, $p < 0.001$) (Figure S5). The results in Table S2 support the above analysis, and the joint assimilation showed advantages in overall accuracy in both arid and humid areas.

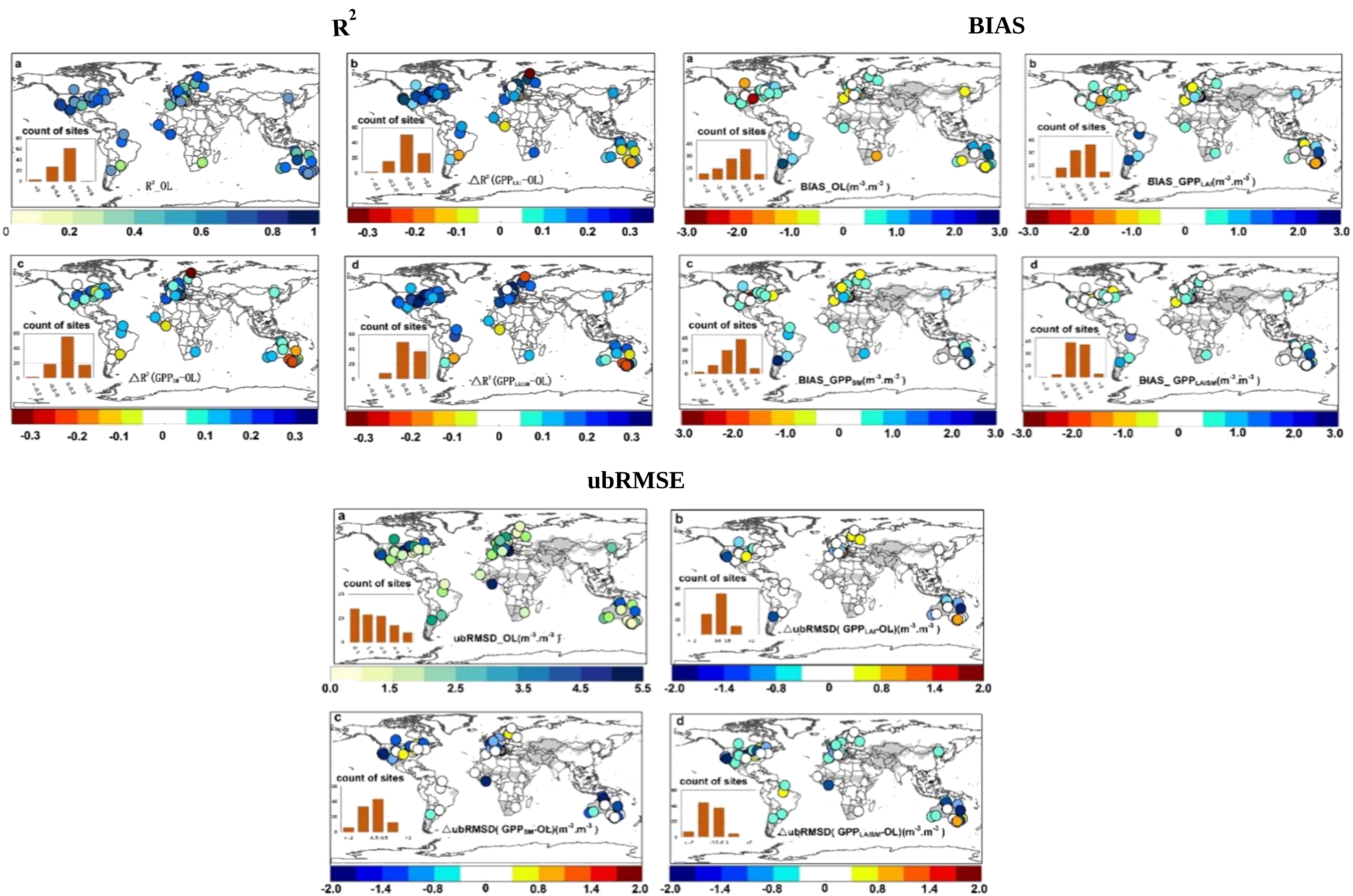


Figure 2 (a) The correlation coefficient (R^2),Bias and the Unbiased Root Mean Square Error (ubRMSE) between the GPP(GPP_{LPJ}) simulated by the LPJ-DGVM and the site observations, the yellow/blue indicating low/high correlation ;(b) △R^2(correlation difference between GPP_{LAI} and GPP_{LPJ}), BIAS（GPP_{LAI}）and △ubRMSD（GPP_{LAI}- GPP_{LPJ}）;(c) △R^2（correlation difference between GPP_{SM} and GPP_{LPJ}）, △ BIAS（GPP_{SM}）and △ubRMSD（GPP_{SM}- GPP_{LPJ}）; (d) △R^2（The correlation difference between GPP_{CO} and GPP_{LPJ}）, △ BIAS（GPP_{CO}）and △ubRMSD（GPP_{CO}- GPP_{LPJ}） , blue/red represent positive/negative values.

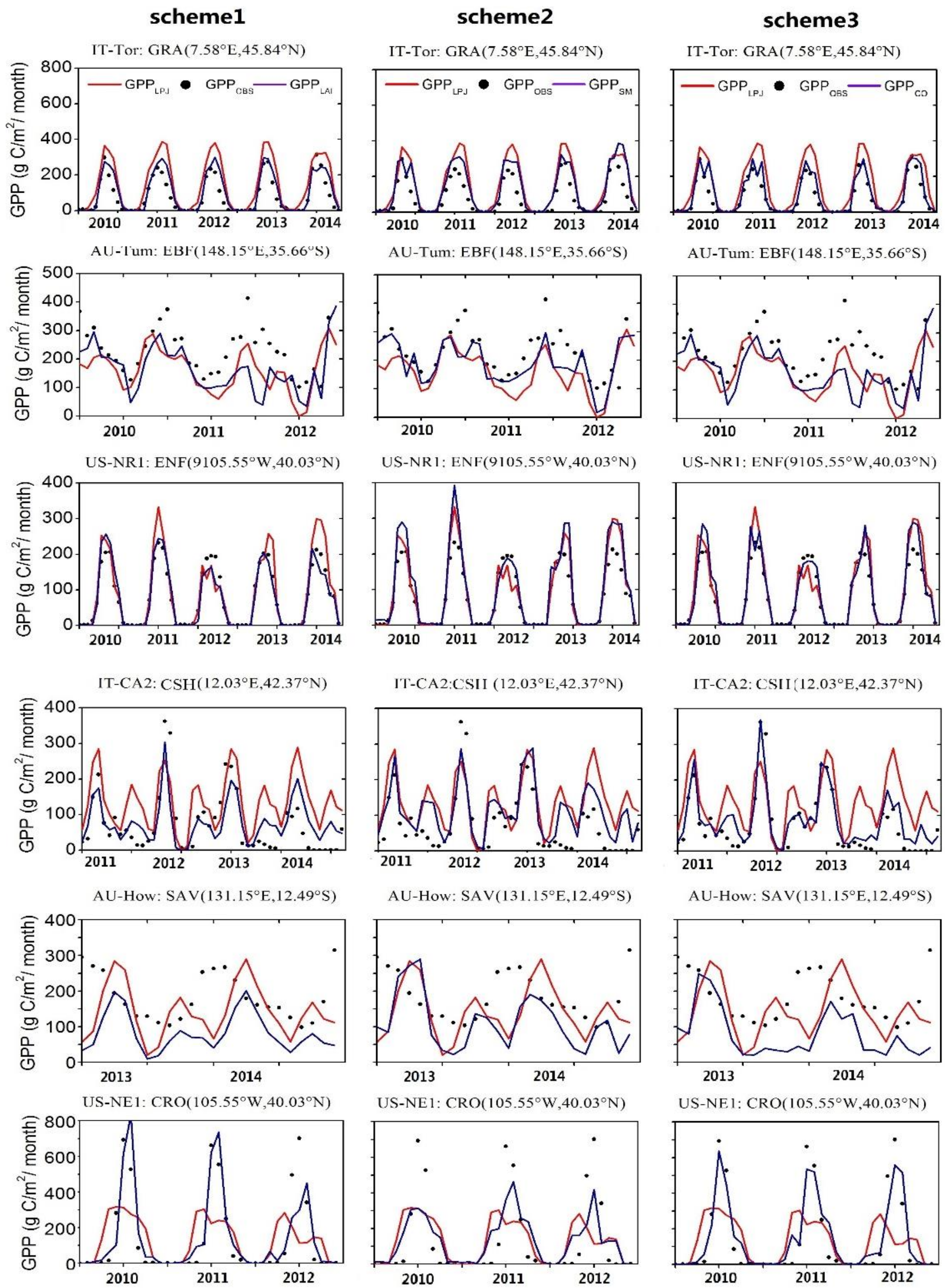


Figure 3. Seasonal cycles of tower GPP and simulated gross primary productivity (GPP) from Lund-Potsdam-Jena (LPJ), GLASS LAI assimilation (scheme 1), SMOS assimilation (scheme 2) and joint

assimilation (scheme 3) for six sites representing six PFTs.

The residual analysis indicated that the three assimilation schemes for GPP (Figure S7 (left)) were different. For the assimilation results, most of the errors were distributed around –70 ~ 60 g C m^{-2} $month^{-1}$. The high GPP_{OBS} values were considerably underestimated. The maximum negative error reached 100 g C m^{-2} $month^{-1}$. The error distribution of GPP_{SM} was more dispersed than that of GPP_{LAI} and GPP_{CO}. Among the residuals of these three schemes, GPP_{SM} significantly overestimated the GPP_{OBS}, mainly distributed in the 0–200 g C m^{-2} $month^{-1}$ range. GPP_{LAI} showed significant improvement in the overestimation of GPP_{OBS} compared with GPP_{CO}. In general, the GPP_{CO} with the most concentrated error distribution had significant improvement.

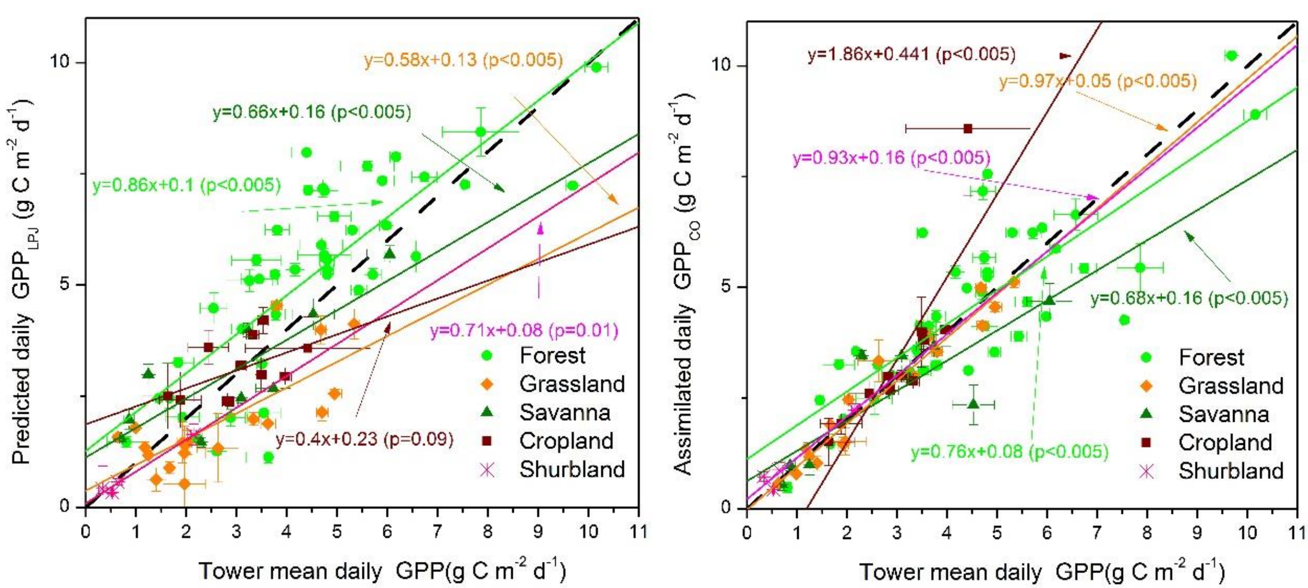


Figure 4. Scatterplots of daily GPP_{LPJ} (left) and GPP_{CO} (right) versus tower GPP for different PFTs.

After determining the optimal assimilation scheme (scheme 3), we evaluated the GPP_{LPJ} and GPP_{CO}

at the site level (Fig.4). The results showed that GPP_{CO} performed better (R^2= 0.83, ubRMSD= 1.15 g C m^{-2} d^{-1}) than GPP_{LPJ} (R^2= 0.69, ubRMSD= ~~2.15~~1.91 g C m^{-2} d^{-1}). The noticeable underestimation in all PFTs and overestimation at most forest sites for GPP_{LPJ} were corrected by joint assimilation (GPP_{CO}). Our joint assimilation methods had better performance in forests, shrublands, and grasslands than in croplands and savannas. Except for the cropland, the linear fitting results of other types were all below the 1:1 line, showing the overall underestimation. Superior performance in both original simulation and assimilation occurred at shrubland (R^2= 0.93, ubRMSD= ~~0.27~~0.89 g C m^{-2} d^{-1}) and grassland (R^2= 0.97, ubRMSD= 0.~~38~~ 83 g C m^{-2} d^{-1}) sites. However, the standard deviation of GPP_{CO} and GPP_{OBS} at savanna sites was relatively large, and the assimilated GPP at several savanna sites was significantly underestimated.

4.1.2 Accuracy assessment of ET for separate and ~~conjunct~~ joint assimilation

In general, the coefficient of determination (R^2) between ET_{LPJ} and ET_{OBS} was generally over 0.4 (the simulations were superior to GPP_{LPJ}) (Figure 5). ET_{LAI} showed slightly higher R^2, while some sites showed reduced values (41 sites). The ET_{SM} and ET_{CO} were significantly improved compared with the ET_{LAI}. The R^2 increased considerably in Australia but declined at some sites in the United States after assimilation. For ~~RMSD and~~ ubRMSD, ET_{CO} performed better than ET_{SM} and ET_{LAI}. The SM assimilation improved more in humid regions, while ~~the RMSD of ET_{LAI} only slightly improved in Australia and~~ the ubRMSD of ET_{SM} was slightly higher in South America. ~~According to the bar chart (Fig.5-RMSD(b)), the LAI assimilation increased the ET simulation error.~~ In the original LPJ-DGVM simulation, the sites with a negative bias were mostly located in the humid and dry-sub humid regions, while most of the sites in arid and semi-arid regions had underestimation (Fig. 5-BIAS(a), Table S3). The assimilation improved ET at some of the overestimated sites, but the underestimation over these sites showed little improvement.

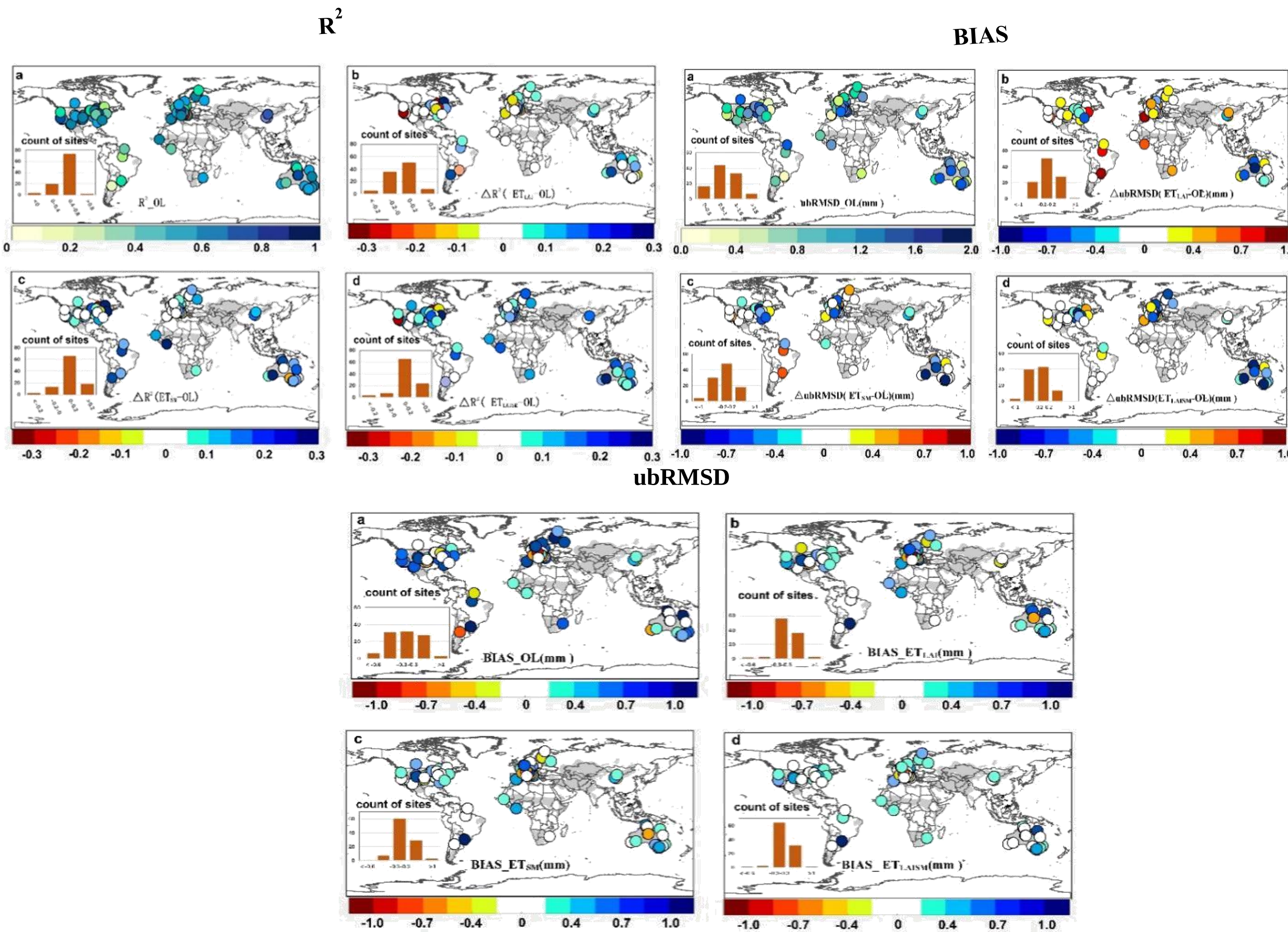


Figure 5 (a) The correlation coefficient), BIAS and the Unbiased Root Mean Square Error (ubRMSE) between the ET(GPP_{LPJ}) simulated by the LPJ-DGVM and the site observations, with yellow/blue indicating low/high correlation or ubRMSE; (b) △R^2(correlation difference between ET_{LAI} and ET_{LPJ}) , BIAS（ET_{LAI}） and △ubRMSD（ET_{LAI}- ET_{LPJ}）;(c) △R^2（correlation difference between ET_{SM} and ET_{LPJ}）, BIAS（ET_{SM}） and △ubRMSD（ET_{SM}- ET_{LPJ}）; (d) △R^2（The correlation difference between ET_{CO} and ET_{LPJ}）, BIAS（ET_{CO}） and △ubRMSD（ET_{CO}- ET_{LPJ}）, blue/red represent positive/negative value.

At the seasonal scale, the model simulations were able to capture the temporal trend of ET_{OBS}, and joint assimilation significantly improved the simulation in the growing season (US-NR1, US-NE1); overall underestimation was observed for ET_{OBS}, especially in winter (Figure ~~Fig.~~6). Overall, the linear fitting of monthly ET_{CO} and ET_{OBS} was closer to 1:1 than that of ET_{LAI} and ET_{SM} (Figure S6). The simulation accuracy of joint assimilation was better than that of separate assimilation, and the performance of the SM assimilation was better than that of the LAI assimilation.

The ET residual analysis (Figure S7 (right)) indicated that the three assimilation scheme errors showed underestimation for ET_{OBS}. In general, the error distribution of separate assimilations was more dispersed than that of the joint assimilation. Similar to the assimilation performance of GPP, ET_{CO} and ET_{SM} significantly improved the overestimation of ET_{OBS}, but did not significantly improve the underestimation. For the ET_{CO}, most of the errors were distributed around -30–18 mm month^{-1}. The region with high ET_{OBS} was considerably underestimated, and the maximum negative error reached –~~-~~57 mm month^{-1}.

We also evaluated the ET assimilation results at the PFT scale (Figure 7). The results showed that our assimilated ET performed better at the site level (R^2= 0.77, ubRMSD= 0.~~28~~ 65 mm d^{-1}) than that of ET_{LPJ} (R^2= 0.67, ubRMSD=0.~~98~~ 95 mm d^{-1}). Joint assimilation significantly reduced the errors of those shrubland sites with overestimation for ET_{OBS}, and the site distribution was closer to the 1:1 line. Our assimilation methods had better performance in forest, savanna, and grassland ecosystems than in cropland and shrubland (Table S3). The linear fitting results of grassland and shrubland were all above the 1:1 line, showing overall overestimation. Although the original simulation and assimilation performance were superior at savanna sites (R^2= 0.95, ubRMSD= 0.~~33~~ 78 mm d^{-1}), the standard deviations of ET_{CO} and ET_{OBS} at savanna sites were relatively large, which was similar to the GPP results at savanna sites.

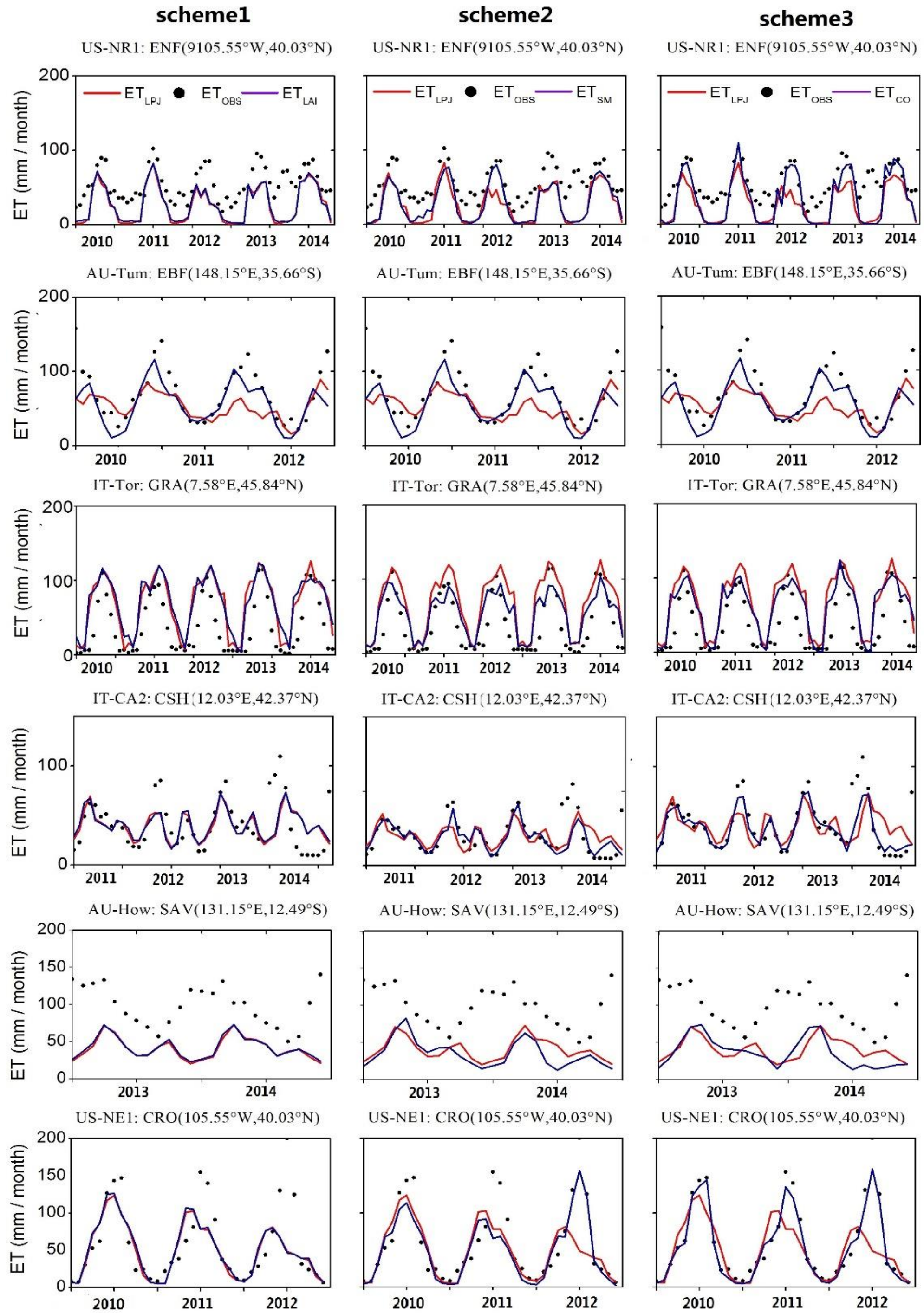

scheme1
scheme2
scheme3
US-NR1: ENF(9105.55°W,40.03°N)
ET_{LPJ} ET_{OBS} ET_{LAI}
ET_{LPJ} ET_{OBS} ET_{SM}
ET_{LPJ} ET_{OBS} ET_{CO}
AU-Tum: EBF(148.15°E,35.66°S)
IT-Tor: GRA(7.58°E,45.84°N)
IT-CA2: CSH(12.03°E,42.37°N)
AU-How: SAV(131.15°E,12.49°S)
US-NE1: CRO(105.55°W,40.03°N)
ET (mm / month)
2010
2011
2012
2013
2014

Figure 6. Seasonal cycles of tower-based and simulated ET from Lund-Potsdam-Jena (LPJ), GLASS LAI assimilation (scheme 1), SMOS assimilation (scheme 2) and joint assimilation (scheme 3) for the six sites representing six PFTs during the study period.

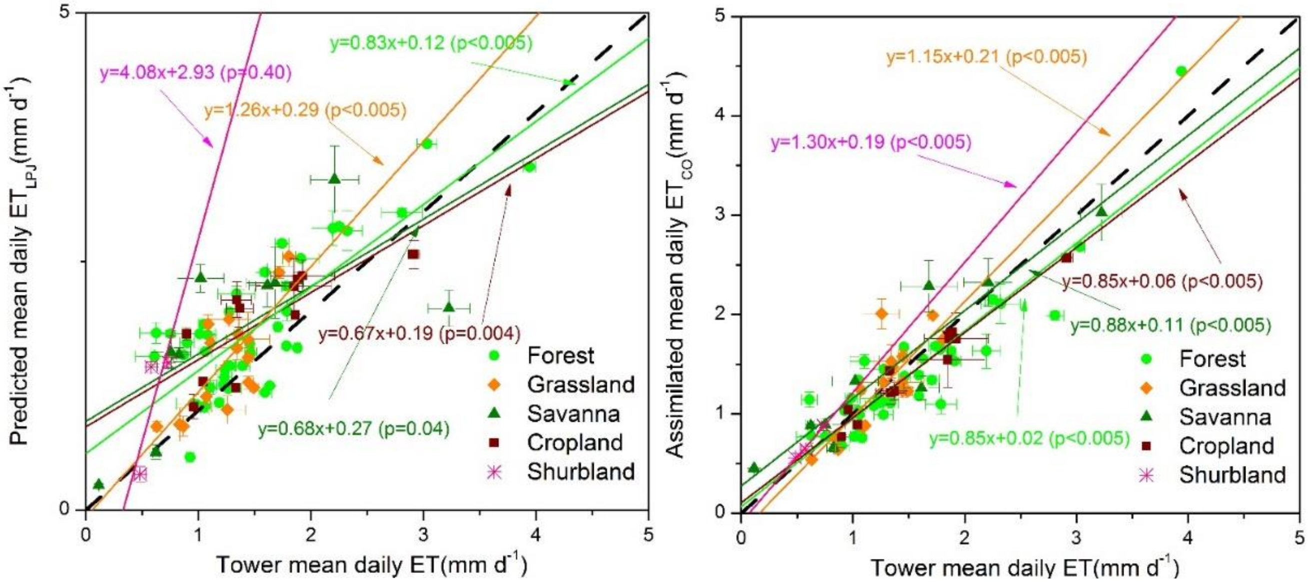


Figure 7. Scatter plots of daily ET_{CO} versus tower ET under different PFTs.

4.2. Comparison of assimilation performance in semi-arid and arid regions with that in humid and dry-sub humid regions

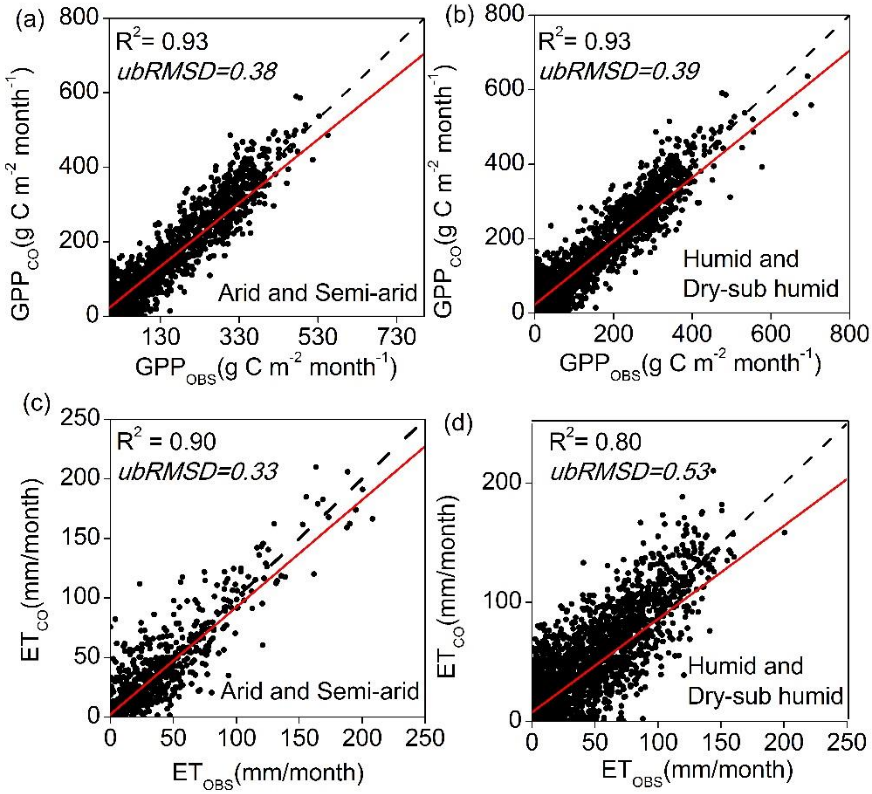


Figure 8. Scatter plots of daily tower GPP and ET versus GPP_{CO} and ET_{CO} under ~~different~~ arid and humid sites: (a) and (c) are the fitting results of GPP and ET in arid and semi-arid regions, respectively; (b) and (d) are the fitting results of GPP and ET in humid and dry sub-humid zone, respectively.

During the period 2010–2014, monthly GPP_{CO} and ET_{CO} performed differently in humid and sub-dry humid regions and semi-arid and arid regions (Figure 8, Table S2,3). Overall, the GPP and ET simulations had good consistency with the tower data in the two regions. For GPP_{CO}, there was no significant difference in the correlation and fitting coefficients between the two regions. ~~Due to the higher standard deviation and GPP_{OBS} values in the humid and sub-dry humid regions than in the semi-~~

arid and arid regions, the higher RMSD of the humid and sub-dry humid regions did not reflect higher accuracy in semi-arid and arid regions. As for ET_{CO}, the fitting results and R^2 values in the semi-arid and arid regions performed better than those in the humid and sub-dry humid regions, which also suggested the importance of surface SM for ET estimation in water-limited areas.

On the daily scale, the original GPP simulations (GPP_{LPJ}) performed better in the semi-arid and arid regions than in the humid and sub-dry humid regions with higher R^2 and lower ubRMSD (Table S2). the R^2 and bias implied that the LAI assimilation alone had a better performance than the SM assimilation alone. However, for sites in arid and semi-arid areas, the RMSD and ubRMSD showed that the GPP_{SM} improved better than GPP_{LAI}, which both demonstrated SM data are essential in water-limited regions. For GPP_{CO}, the shrubland in the semi-arid and arid regions had the lowest R^2 values and the second lowest ubRMSD. The forest in the semi-arid and arid regions had the largest improvement after assimilation. In the humid and sub-dry humid regions, the GPP_{CO} of the savanna and cropland showed the largest improvement (R^2 increased by 64.7% and 71.1%, respectively; ubRMSD decreased by 47.0% and 31.8%, respectively). The grassland in the semi-arid and arid regions had the highest R^2, and the savanna by combining all indicators had the best assimilation results compared to other types in both regions.

Similar to ET_{CO}, the ET_{LPJ} in the semi-arid and arid regions was better than that in humid and sub-dry humid regions in terms of four evaluation indicators (RMSD decreased by 32.7%, ubRMSD decreased by 34.4% in semi-arid and arid regions and RMSD decreased by 26.4%, and the ubRMSD decreased by 30.9% in humid and sub-dry humid regions compared with ET_{LPJ}). The R^2 and ubRMSD implied that the SM assimilation alone had a better performance than the LAI assimilation alone, especially for sites in arid areas. and the bias showed that the ET_{LAI} improved better than ET_{SM} for sites in humid and sub-dry humid areas. The performance of the original simulation and assimilation of grassland sites in the semi-arid and arid regions was the best among all five PFTs.

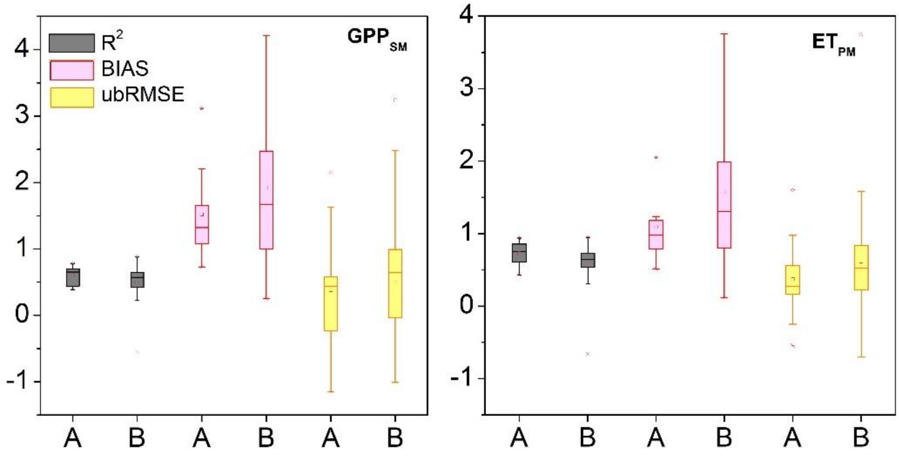


Figure 9. Boxplots of R^2, ubRMSD and BIAS for GPP_{SM} (left) and ET_{PM} (right). A represents the sites in arid and semi-arid areas, and B represents the sites in humid and dry sub-humid areas.

To investigate the reasons for better assimilation performance in water-limited regions, we evaluated the GPP and ET simulated by the LPJ-PM according to R^2, ubRMSD, ~~RMSD,~~ and BIAS (Figure 7). Compared with the semi-arid and arid regions, the humid and sub-dry humid region had smaller R^2 mean, larger BIAS ~~and RMSD mean~~, and no significant difference in mean ubRMSD for GPP_{SM}. In general, the evaluation results of joint assimilation for ET_{PM} were generally consistent with those for GPP_{SM} and GPP_{SM}. ET_{PM} showed underestimation, which was consistent with the underestimation in SM assimilation.

These results indicated that, both GPP and ET modeled by LPJ-PM with joint assimilation were less stable and had a lower performance in the humid and sub-dry regions than in the semi-arid and arid regions.

4.3. Comparison of assimilation performance in assimilating SMOS and SMAP soil moisture data

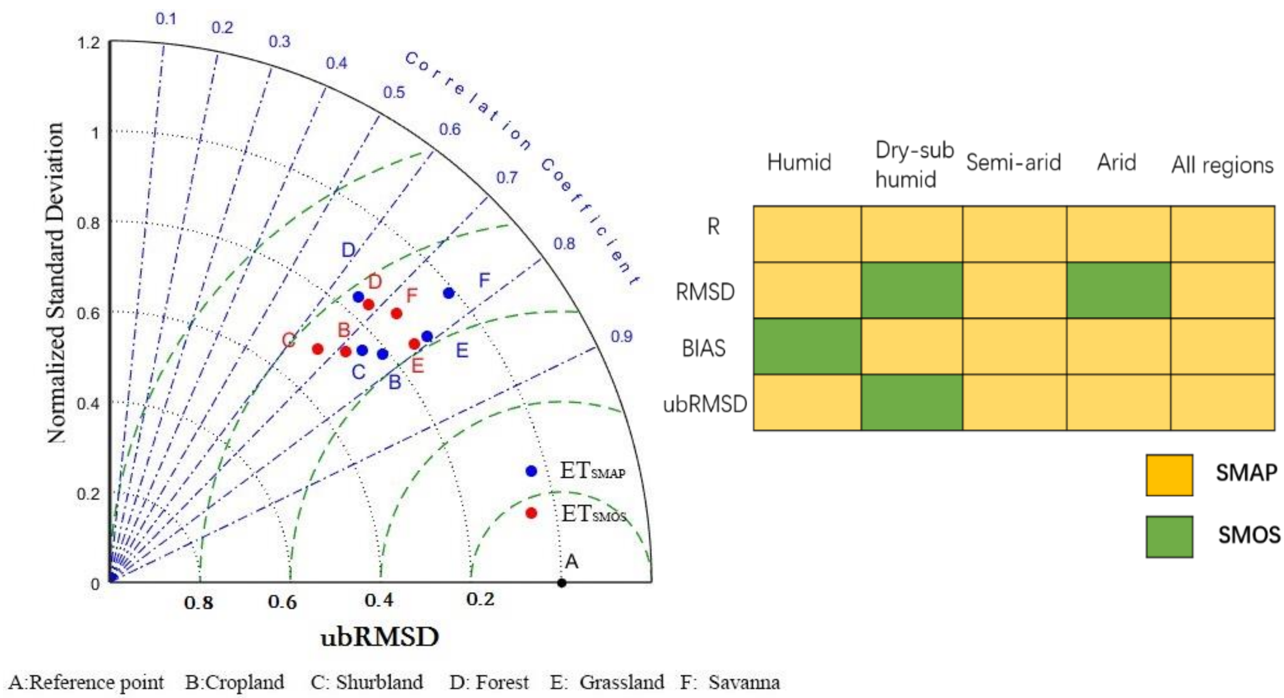


Figure 10. Taylor diagram (left) comparing ET simulations with observations at all 46 AmeriFlux sites at the daily time step between April 2015 and December 2018. Blue dots represent results based on assimilation with SMAP SM only and red dots represent results based on assimilation with SMOS SM only. Reference points A and B-F correspond to the vegetation functional types (PFTs). The grid diagram (right) compares the evaluation indices of ET simulations with those of the observed values at all 46 AmeriFlux sites with different wet and dry zones at the daily time step; the yellow cells indicate that ET_{SMAP} performs better in the metric, and green cells indicate that ET_{SMOS} performs better in the metric.

The Taylor chart was used to compare the assimilation performance of ET_{SMAP} and ET_{SMOS} at 46 AmeriFux sites (Figure 10-left). The results showed that ET_{SMAP} performed better than ET_{SMOS} for all PFTs. Both ET_{SMAP} and ET_{SMOS} performed well for grassland (closer to point A), and there was little difference between R^2 and standardized RMSD. The NSD of ET_{SMAP} in grassland was 0.88, which was closer to 1 than that of ET_{SMOS}. The assimilation of ET in the forest had a lower R and higher standardized RMSD (0.7-0.8) than those of other PFTs, and the NSD of cropland and shrubland was lower than that of other PFTs (0.6-0.8), indicating that the assimilation for cropland and shrubland could not reproduce the variations in ET effectively. However, ET_{SMAP} showed significant improvement in R^2 compared with ET_{SMOS} for shrubland and cropland. The assimilation performance of ET_{SMAP} and ET_{SMOS} for savanna showed the greatest difference. In general, the ET_{SMAP} and ET_{SMOS} were slightly different, and the ET_{SMAP} was more improved than ET_{SMOS}.

Figure 10 (right) shows the assimilation accuracy of ET_{SMOS} and ET_{SMAP} in different humid and arid regions. The ET_{SMAP} had significant advantages for the four indicators. The R of ET_{SMAP} was higher than that of ET_{SMOS} in all the areas. However, ET_{SMOS} in some evaluation indicators showed a better performance than ET_{SMAP} (BIAS in the humid region; ~~RMSD and~~ ubRMSD in the sub-dry humid region). This may be due to the overall more humid nature of SMOS SM than the SMAP SM. Moreover, the sensitivity of deep soil moisture contributed more to the ET in humid areas than in the water-limited areas.

4.4. Global simulations of GPP and ET with joint assimilation of LAI and soil moisture data

To assess the spatial scalability of the LPJ-VSJA assimilation scheme, we simulated the global daily GPP and ET for 2010–2018 with a spatial resolution of 0.25°. The original results simulated by the LPJ-

DGVM and LPJ-VSJA were referred to as LPJ-DGVM GPP(ET) and LPJ-VSJA GPP(ET), respectively. We compared the annual spatial GPP and ET values and the error standard deviation of the LPJ-VSJA with several existing flux products.

Figures 11 and 12 depict the spatial distribution of the annual mean and the differences between our simulation results and the global independent satellite-based products. The developed LPJ-VSJA GPP was the closest to GOSIF GPP (Li and Xiao 2019) in most regions with the lowest spatial mean deviation (LPJ-VSJA-GOSIF) (27.9 g C m^{-2} yr^{-1}), followed by GLASS GPP (51.2 g C m^{-2} yr^{-1}) (Yuan et al. 2010), LPJ-DGVM (-73.4 g C m^{-2} yr^{-1}), and MODIS GPP (93.1 g C m^{-2} yr^{-1}). LPJ-VSJA had higher GPP values than GOSIF GPP in tropical regions, such as Amazonia, Central Africa, and Southeast Asia. In general, the annual mean and differences between MODIS, GOSIF GPP, LPJ-DGVM, and our LPJ-VSJA were in broad agreement (with higher R^2 ranging from 0.74 to 0.95).

LPJ-VSJA ET was the closest to GLEAM ET on the spatial average with the least spatial average deviation (-13.9 mm yr^{-1}) and highest R^2 (0.88), followed by GLASS ET (-23.1 mm $yr^{-1}$and 0.82), GLDAS ET (-34.7 mm yr^{-1} and 0.73), LPJ-DGVM (-48.7 and 0.66 mm yr^{-1}), and MODIS ET (-122.1and 0.54 mm yr^{-1}).

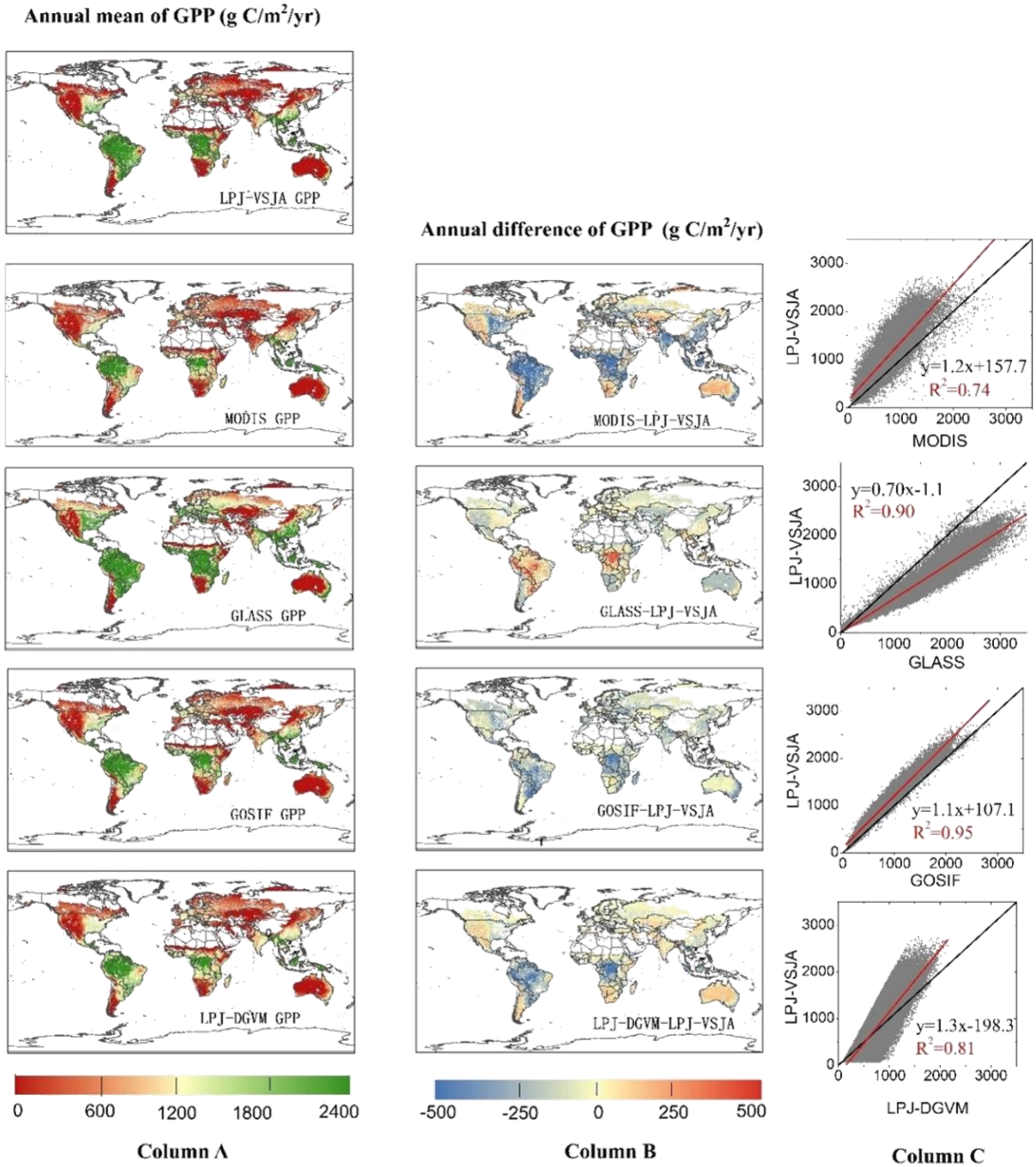
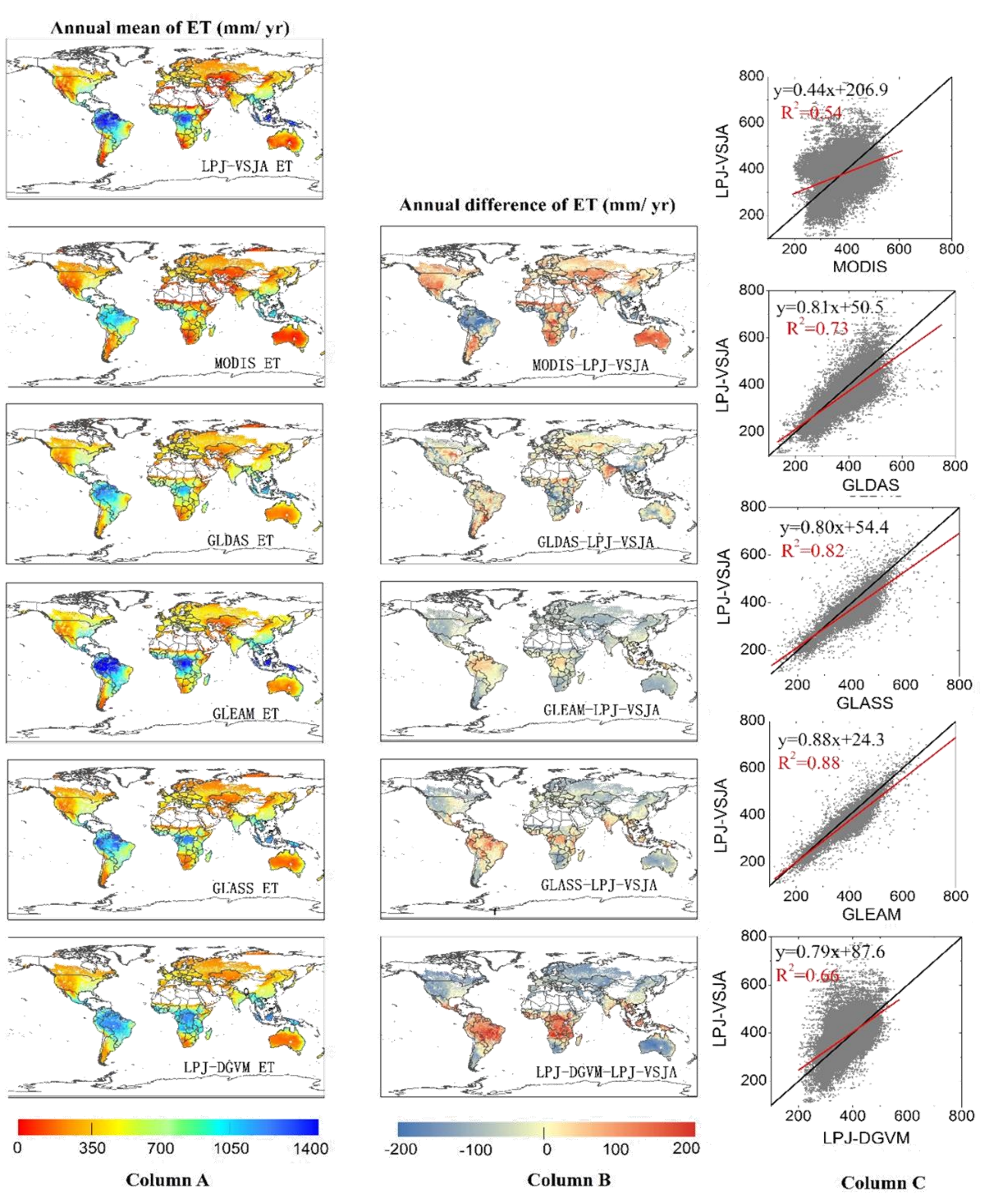


Figure 11. Column A: Spatial distribution of annual LPJ-VSJA GPP and other independent satellite-based datasets (a: MODIS GPP; b: GLASS GPP; c: GOSIF GPP; e: LPJ-DGVM). Column B: Spatial distribution of the difference between annual LPJ-VSJA GPP and other independent satellite-based

datasets. Column C: Scatter plots between these products. Black lines show the 1:1-line, red lines show the regression fit.



Annual mean of ET (mm/ yr)
Annual difference of ET (mm/ yr)
LPJ-VSJA ET
MODIS ET
GLDAS ET
GLEAM ET
GLASS ET
LPJ-DGVM ET
MODIS-LPJ-VSJA
GLDAS-LPJ-VSJA
GLEAM-LPJ-VSJA
GLASS-LPJ-VSJA
LPJ-DGVM-LPJ-VSJA
y=0.44x+206.9
R²=0.54
y=0.81x+50.5
R²=0.73
y=0.80x+54.4
R²=0.82
y=0.88x+24.3
R²=0.88
y=0.79x+87.6
R²=0.66
LPJ-VSJA
MODIS
GLDAS
GLASS
GLEAM
LPJ-DGVM
0 350 700 1050 1400
-200 -100 0 100 200
Column A
Column B
Column C

650

Figure 12. Column A: Spatial distribution of annual LPJ-VSJA ET and other independent satellite-based datasets (a: MODIS GPP; b: GLDAS ET; c: GLEAM ET; d: GLASS ET; e: LPJ-DGVM ET). Column B: Spatial distribution of the difference between annual LPJ-VSJA ET and other independent satellite-based datasets. Column C: Scatter plots between these products are provided on the right of the difference maps. Black lines show the 1:1-line, red lines show the regression fit.

Figure 13 (a)–(e) represent the spatial error standard deviation (σ) distribution of MODIS, GLASS, GOSIF, and LPJ-VSJA GPP, respectively. The graphs on the right side depict the corresponding histograms. The σ of the MODIS GPP was evenly distributed between 30 and 60 g C m^{-2} $month^{-1}$~~g C/m^2/month~~, while the average σ of other products was concentrated in 0–20 g C m^{-2} $month^{-1}$ (90%). The high errors of all products were concentrated in the high temperature and humid areas of southern North America, eastern South America, humid and dry sub-humid areas of South Asia, and the savannas of Africa and Australia. The error histogram of GOSIF GPP and LPJ-DGVM GPP were in line with the normal distribution, with an average value of 8.3 g C m^{-2} $month^{-1}$ and 22.4 g C m^{-2} $month^{-1}$. The GLASS GPP product had the lowest mean value (3.6 g C m^{-2} $month^{-1}$), followed by LPJ-VSJA (4.7 g C m^{-2} $month^{-1}$), but the error variance of the LPJ-VSJA product was the lowest, indicating a stability of the regional error (Table S4). Compared to the LPJ-DGVM, the joint assimilation results showed improvement in all regions (the average error reduced by 17.7 g C m^{-2} $month^{-1}$), especially in the humid regions of South Asia, Australia, and the United States. Our LPJ-VSJA GPP was generally proven to have high accuracy and stability for spatial analysis and could provide a reference for other model products.

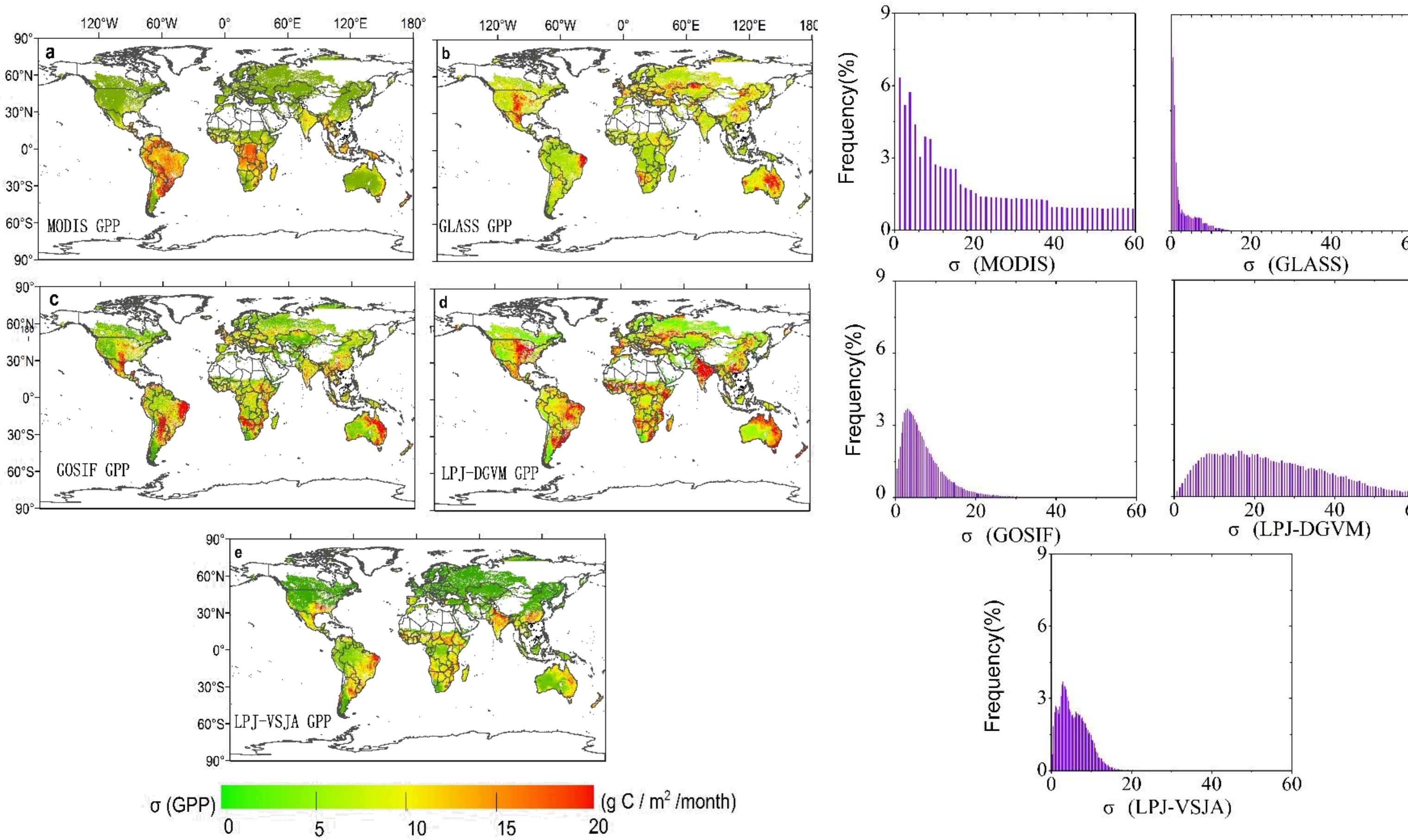


Figure 13. Spatial distribution and histograms of error standard deviation (σ) for global GPP products: MODIS (a), GOSIF (b), GLASS (c), LPJ-DGVM (d), and LPJ-VSJA (e).

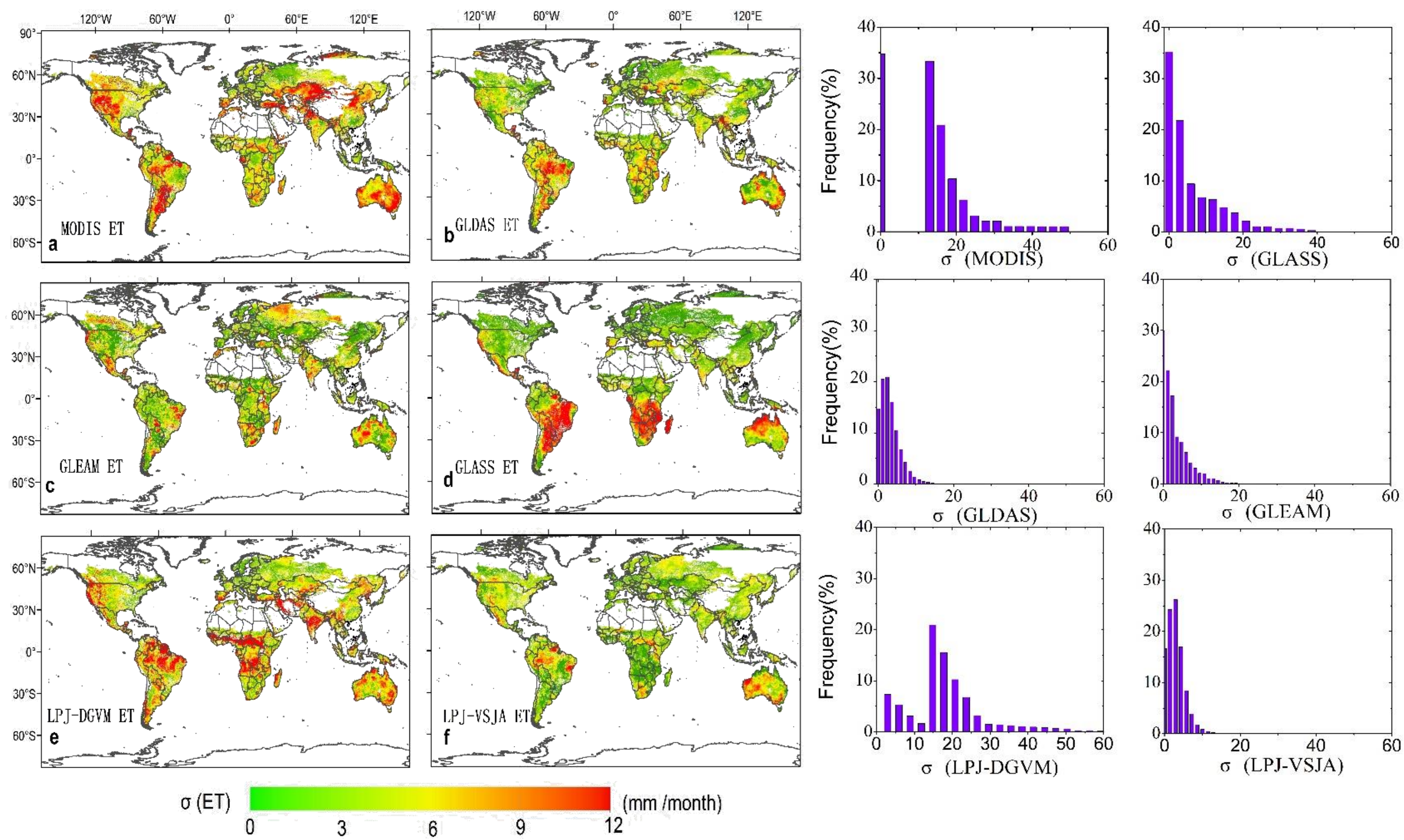


Figure14. Spatial distribution and histograms of error standard deviation (σ) for global ET products: MODIS (a),GLDAS (b),GLEAM (c), GLASS (d), LPJ-DGVM (e), and LPJ-VSJA (f).

Figures 14 (a)–(f) show the σ of MODIS, GLDAS, GLEAM, GLASS, and LPJ-VSJA ET (the units are mm/month), and the right graphs are the corresponding histograms. The σ values of GLDAS and LPJ-VSJA represented a normal distribution trend. Except for MODIS, GLASS, and LPJ-DGVM (0–60 mm $month^{-1}$), the σ of other products was generally between 0-20 mm $month^{-1}$. The simulation error was relatively smaller in the Northern Hemisphere than in the Southern Hemisphere, especially for GLASS ET and GLDAS ET. Significant improvements in joint assimilation were observed in the northern hemisphere (especially in the semi-arid areas of the western United States and savanna and cropland areas of central India) and African savanna areas, and the average error was reduced by 15.1 mm $month^{-1}$. In general, the error mean and variance of LPJ-VSJA and GLEAM products were relatively low (Table S4), and there was no apparent extremely high value region in the error distribution. Among the five products, LPJ-VSJA had the lowest error mean and variance and the highest accuracy.

5. Discussion

5.1 Advantage of joint assimilation for GPP and ET

The benefit of employing multiple data flows in an assimilation system is the complementarity of the data, which enables constraints on different components of the underlying process-based terrestrial biosphere model. Due to the interaction and feedback between the internal components of the model, the assimilation of multiple observations has a synergistic effect, and the integrated constraints are greater than the individual constraint (Kato et al. (2013)). The advantage of our joint assimilation is that it can improve the simulation accuracy of both GPP and ET, especially ET, in arid and semi-arid regions.

In the GPP assimilation experiment, the performance of the LAI assimilation was better than that of the SSM assimilation possibly for two reasons: (1) the LPJ-VSJA is more controlled by LAI data because the ratio of assimilated LAI (daily input) to SSM observations (3-day interval input) is approximately 3:1, which makes the likelihood function biased to LAI data; (2) the SM directly influences the simulation of ET, and the corresponding time function (computes the top layer SM (50 cm)) used here by Zhao et al. (2013)~~(section 2.4)~~ will result in the error of the updated top SM and propagating the error to the GPP_{SM}. ~~Moreover, GPP is not only directly affected by LAI but also by other vegetation and environmental conditions. These multiple dependencies (direct and indirect) make GPP less likely to respond to transient changes in LAI (Zobitz et al. 2014).~~ In addition, ~~the LAI dynamic variability varies depending on the ecosystem type. For instance, the LAI for coniferous forest has less dynamic variability than for cropland and the deciduous forest (Turner et al. 2006; Turner et al. 2005).~~, the 8-day interval LAI has the capability to capture the temporal variability of phenology. ~~The LAI assimilation with different time scales (e.g., 8-day interval, monthly, annual) for different ecosystems may achieve better results.~~

Current studies on terrestrial water and carbon flux assimilation mostly focus on the assimilation between a single model framework and observation results, lacking the fusion and comparison between multiple models. The processed models used in DA are simplifications and approximations of reality, and different models focus on different ecological processes. In this study, the updated ET module was integrated to compensate for the simplification of soil stratification and the lack of SM information in the hydrological module of the LPJ-DGVM. Therefore, the integration of multiple types of models and multi-source observation data (remotely sensed data, ecological inventory data (National Ecological Observatory Network, NEON (Keller et al. 2008)), and other measurements (Desai et al. 2011; Hayes et al. 2012) is expected to more objectively and effectively simulate the real state of ecosystems.

5.2 Comparison of joint assimilation (LPJ-VSJA) and other models for GPP and ET across regions and vegetation types

Global GPP and ET for different products were calculated by multiplying the global mean GPP density flux with the global vegetation area (122.4 million km^2) originated from the MODIS land cover product (Friedl et al. 2010). The mean global GPP of the LPJ-VSJA (130.2 Pg C yr^{-1}) was approximately 12% lower than that of PML-V2 (145.8 Pg C yr^{-1}) and 18% higher than that of GLASS and MODIS, respectively (Table S6). The GPP values of LPJ-VSJA and GOSIF were the most similar. The GOSIF GPP was developed from gridded SIF using simple linear relationships between SIF and

GPP. Our global LPJ-VSJA GPP estimates were within the currently most plausible 110–150 Pg C/yr range.

As for ET, our results were similar to those of GLEAM ET and lower than those of PML-V2, GLDAS-2, and GLASS ET (~72000 mm yr^{-1}). Joint assimilation improved the overestimation of LPJ-DGVM ET. At the daily scale, the estimation accuracy of PML-V2 and GLDAS-2 products, calibrated with flux tower data, was better than that of our estimates, which suggests an underestimation of LPJ-VSJA ET in wet regions. It is likely because the SM of SMAP or SMOS was underestimated in the wet region or the influence of deep SM was under-represented. According to Seneviratne et al. (2010), satellite-based ET estimation approaches often overestimate ET in areas of arid and semi-arid climatic regimes in the magnitude of 0.50 to 3.00 mm d^{-1}. The poor performance of these models can largely be attributed to the lack of constraints of SM and more accurate vegetation parameters (Gokmen et al. 2012; Pardo et al. 2014). For instance, the monthly estimated ET modeled by the Penman-Monteith-Leuning (PML) model agreed with flux tower data well ($R^2 = 0.77$; bias = − 9.7%, approximately 0.2 mm d^{-1}). Our annual ET simulations were lower than other products and slightly underestimated tower ET with a bias of 0.19 mm d^{-1} (ET_{OBS}-ET_{CO}).

In general, GPP and ET had better assimilation performance in arid and semi-arid regions than in humid and semi-humid regions likely because of the following reasons. First, the incorporation of surface SM is more important for vegetation growth in water-limited areas. The module PT-JPL_{SM} has been proven to have better performance in semi-arid and arid regions (Purdy et al. 2018). Our integrated model LPJ-PM also performed better in semi-arid and arid regions by assimilating SMAP soil moisture (Li et al.

2020). Second, the input performance, including SMOS and SMAP SM products, is better in arid and temperate regions than in cold and humid regions (Zhang et al. 2019). Third, the vegetation types in humid regions are more complex and relatively less accurately simulated by the LPJ-DGVM within a single grid cell. For comparison, Zhang et al. (2020) used a data-driven upscaling approach to estimate GPP and ET in global semi-arid regions. This data-driven approach (R^2 = 0.79, RMSD = 1.13 g C m^{-2} d^{-1}) had slightly higher performance in estimating GPP than our LPJ-VSJA (R^2 =0.73 and RMSD= 1.14 g C m^{-2} d^{-1}) and~~;~~ the data-driven method (R^2 = 0.72 and RMSD = 0.72mm d^{-1}) had identical performance for estimating ET with our LPJ-VSJA(R^2 =0.73 and RMSD= 0.72 mm d^{-1}).

Our assimilation performance varied with PFT. The GPP and ET assimilation results of savanna sites performed well in both dry and wet regions, and those of shrubland sites showed the most remarkable improvement for simulations of LPJ-DGVM. The original simulation and assimilation performance of grassland sites in the semi-arid and arid regions were the best for all five PFTs. Consistent with our research, previous studies also showed better GPP or ET simulations for grassland, savannas, and shrublands biomes. For instance, Feng et al. (2015) validated five satellite-based ET algorithms for semi-arid ecosystems and concluded that all the models produced acceptable and relatively better results for most grassland, savanna, and shrubland sites. Yang et al. (2017) demonstrated that he GLEAM ET had a superior performance for the grassland sites. The GOSIF GPP demonstrated better simulation for grassland and woody savannas sites at 8-day time steps with higher R^2 (0.77 and 0.83, respectively) and lower RMSD (1.48 g C m^{-2} d^{-1} and 1.1 g C m^{-2} d^{-1}) (Li and Xiao 2019). In contrast, our LPJ-VSJA GPP showed an R^2 of 0.87 for grassland and 0.75 for savannas and an RMSD of 1.11 g C m^{-2} d^{-1} and 1.1 g C m^{-2} d^{-1}, respectively, in semi-arid and arid regions.

5.3 Uncertainty analysis of joint assimilation

Our validation results at both site and regional scales indicated that uncertainty existed in LPJ-VSJA daily GPP and ET estimates. The errors from the tower EC observations, model-driven data, model structure, error of satellite-based observations (e.g., LAI and SM), and the spatial scale mismatch between the ground observed footprint size and satellite-derived footprint size were the vital factors affecting assimilation performance.

First, recent studies have revealed errors in the GLASS LAI and SMOS or SMAP SM compared with ground measurements. By computing the RMSD and R^2 of each product, the GLASS LAI accuracy was clearly superior to that of MODIS and Four-Scale Geometric Optical Model based LAI (FSGOM) in forests and GLASS and FSGOM led to in much higher annual GPP and ET estimates compared to MCD15(Liu et al. 2018). The vegetation type (or land cover) misclassification caused 15–50% differences in LAI retrieval (Fang and Liang 2005; Gonsamo and Chen 2011). Yan et al. (2016) calculated a RMSD of 0.18 for the GLASS LAI over a range of HeiHe drainage basin sites and used the error to improve the simulation of LAI and fluxes by assimilating GLASS LAI data. Previous studies reported an improvement in the performance of the SMOS and SMAP products (Lievens et al. 2015; Miernecki et al. 2014), which both provide an accuracy of 0.04 m^3 m^{-3} (Zhang et al. 2019). However, the actual observation error of these two products typically depends on the spatial location and time of the year (RMSD varying between

0.035 and 0.056 m^3 m^{-3} for several retrieval configurations) (Brocca et al. 2012). According to Purdy et al. (2018), the ET simulated by PT-JPL_{SM} using the 9 km SM_L3_P_E data showed an inferior agreement (R^2= 0.47) but a relatively low RMSD (0.77 mm d^{-1}), due to the SMAP errors in the grid cell with soil heterogeneity and the climatological differences between model SM forecasts and SMAP SM (Reichle and Koster 2004). We rescaled the ET_{PM} to the probability distribution of the ET_{LPJ} through a cumulative distribution function (CDF) to correct the potential seasonal biases of ET_{PM} before assimilation.

Second, there is large uncertainty in the influence of root zone SM as the source of water available to plants (Albergel et al. 2008; Bonan et al. 2020). Our GPP results of cropland sites were largely influenced by US-Ne1, an irrigate site. This site maintained high annual GPP in 2012 despite the drought (Figure S4). However, the SMOS SM in 2012 had a lower surface SM annual mean than the site observations likely because the detected soil layer (0-50 cm) of the site observation is deeper than that of the satellite retrieval and the cumulative deep soil moisture due to the regular irrigation was higher than the surface SM that could easily be vaporized during the drought period (Figure S4). Therefore, the influence of deep SM of some cropland sites during the drought years induced large simulation errors and unsatisfactory assimilation performance. Moreover, some deep-rooted forests maintain a high LAI during drought by absorbing deep SM (>2 m) and groundwater (Zhang et al. 2016). Thus, joint assimilation of the LAI and SM may eliminate a portion of the underestimation of GPP of such vegetation in drought periods. Therefore, further research is needed on how to optimally utilize satellite SM data for improving GPP and ET simulations.

Third, the problem of mixed pixels and mismatches in the observation footprints may also have an influence on the accuracy of estimated GPP and ET. The 5 km spatial resolution of the GLASS LAI ,9 km of SMAP, and 25 km of SMOS products cannot capture the sub-grid-scale condition, especially in grid cells for complex land surfaces or strong soil heterogeneity. To ensure the consistency of the grid-cell representativeness for the LAI and SM, the interpolation result in errors that propagate through the modeling and assimilation, causing the accumulation of output errors (Nijssen and Lettenmaier 2004). Moreover, the shrubland in the LPJ-DGVM was most likely simulated as C4 grassland in the hydrothermal condition of semi-arid and arid regions. In contrast, the shrubland tended to be hybrid vegetation types (grassland mixed with other types of forest vegetation) in the hydrothermal condition of humid and sub-dry humid regions, and the simulated canopy height is closer to the real condition of shrubland. This might also be the reason for the superior performance of ET_{LPJ} and assimilation results of shrubland sites in humid and sub-dry humid regions.

When assimilating multiple data streams, all data streams could be in the same optimization (simultaneous assimilation) or use a sequential (step-by-step) approach. Mathematically, simultaneous optimization is optimal because strong parametric connections are maintained between different processes. However, complications may arise due to computational constraints related to the inversion of large matrices or the requirement of numerous simulations, particularly for global datasets (e.g. Peylin et al.,2016), and due to the “weight” of different data streams in the optimization (e.g. Wutzler and Carvalhais, 2014). This is particularly true when considering a regional-to-global-scale, multiple site optimization of a complex model that contains many parameters, and which typically takes on the order of minutes to an hour to run a one-year simulation. In practice, it is very difficult to define a probability distribution that properly characterizes the model structural uncertainty and observation errors accounting for biases and non-Gaussian distributions. Nevertheless, a step-wise assimilation may be useful in dealing with possible inconsistencies on a temporary basis, since parameter error covariance matrix must be propagated at each step. It's worth noting that the deviation between the model and observational data should be solved in the process of step-wise assimilation, such as the joint assimilation in this study, the satellite observations and model simulation were fitting through the CDF method so that the first step assimilation will strongly constrain the uncertainty of parameters related to phenology and carbon flux and propagate to the second step . Alternative solutions were found for water -related parameters through soil moisture, providing a better fit for all data streams.

The sequence of assimilation is essential in the step-wise assimilation, and if the first observation contains a strong bias, then the associated error correlation will also propagate through the first assimilation. If the autocorrelation in the observation error, or the correlation between the data stream errors is not considered, it is likely that the posterior simulation has been overturned. That is, we overestimate the reduction in parametric uncertainty. If two observational data are less uncertainty (i.e., high precision of observation data), and the model of deviation is smaller (depend on the spatial scale and inversion method). Moreover, the correlation of these observations is stronger, and contain enough spatio-temporal information to limit all the parameters optimization accurately, the step-wise assimilation performance is basically the same as that of simultaneous assimilation.

6. Conclusions

We developed an assimilation system LPJ-VSJA that integrates GLASS LAI, SMOS SM, and SMAP SM data to improve GPP and ET estimates globally. The system was designed to assimilate two SM products (SMOS and SMAP) into the integrated model - LPJ-PM for both dry and humid regions through separate and joint assimilation. The results show that the joint constraints provided by vegetation and soil variable strategies improve model simulations. Both the original and joint assimilation results for GPP and ET in semi-arid and arid regions performed better than those in humid and dry-sub humid regions, and the LPJ-PM that emphasized the SM information is more suitable for the water-limited regions. For ET assimilation, the different SM products influence assimilation performance, and SMAP SM possesses a slight advantage in most vegetation types and in both dry and humid regions. Our global LPJ-VSJA GPP and ET products have relatively higher accuracy than other products, especially in water-limited regions with lower ET values.

Data availability

The LPJ-DGVM v4.1 version code (LPJ-ML) and example configurations are public available via the project homepage (https://github.com/PIK-LPJmL/LPJmL). We used the 3.01 version of LPJ-DGVM, which removed the agricultural management module. The access of all the input and validation dataset of assimilation system have been described in article. The assimilation method code configurated by Fortran platform could be provided by contacting the X.T co-author. The modified code of LPJ-PM model and the underlying and global LPJ-VSJA GPP and ET data can be obtained by contacting the lead author of this manuscript.

Author contributions

S.L. and L.Z. designed the experiment and wrote the paper with support from all coauthors. S.L. and R.M. implemented the codes necessary for the experiments. J.X. contributed to the structure of the article and comparison of assimilation performance between the SMOS and SMAP experiments. X.T provided the POD-En4DVAR method and the code. M.Y contributed to the validation and analysis of the results. All the authors contributed to the synthesis of results and key conclusions.

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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