



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

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20 **Abstract:**

21 Reliable modeling of carbon and water fluxes is essential for understanding the terrestrial carbon
22 and water cycles and informing policy strategies aimed at constraining carbon emissions and improving
23 water use efficiency. We used an assimilation framework (LPJ-Vegetation and soil moisture Joint
24 Assimilation, or LPJ-VSJA) to improve gross primary production (GPP) and evapotranspiration (ET)
25 estimates globally. The terrestrial biosphere model that we used is the integrated model - LPJ-PM coupled
26 from the Lund-Potsdam-Jena Dynamic Global Vegetation Model (LPJ-DGVM) and a hydrology module
27 (i.e., the updated Priestley–Taylor Jet Propulsion Laboratory model, PT-JPL_{SM}). Satellite-based soil
28 moisture products derived from the Soil Moisture and Ocean Salinity (SMOS) and Soil Moisture Active
29 and Passive (SMAP) and leaf area index (LAI) from the global Land and Ground satellite (GLASS)
30 product were assimilated into LPJ-PM to improve GPP and ET simulations using a Proper Orthogonal
31 Decomposition-based ensemble four-dimensional variational assimilation method (POD_{En4DVar}). The
32 joint assimilation framework LPJ-VSJA achieved the best model performance (with an R^2 of 0.91 and
33 0.81 and an RMSD reduced by 50.4% and 38.4% for GPP and ET, respectively, compared with those of
34 LPJ-DGVM at the monthly scale). The assimilated GPP and ET demonstrated a better performance in the
35 arid and semiarid regions (GPP: $R^2=0.73$, ubRMSD=1.05 g C m⁻² d⁻¹; ET: $R^2=0.73$, ubRMSD= 0.61 mm
36 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: $R^2=0.66$;
37 ubRMSD=0.67 mm d⁻¹). The ET simulated by LPJ-PM that assimilated SMAP or SMOS had a slight
38 difference, and the ET that assimilated SMAP soil moisture data was more improved than that assimilated
39 SMOS data. Our global simulation modeled by LPJ-VSJA was compared with several global GPP and



40 ET products (e.g., GLASS GPP, GOSIF GPP, GLDAS ET, GLEAM ET) using the triple collocation (TC)
41 method. Our products, especially ET, exhibited advantages in the overall error distribution (estimated
42 error (μ): 3.4 mm month⁻¹; estimated standard deviation of μ : 1.91 mm month⁻¹). Our research showed
43 that the assimilation of multiple datasets could reduce model uncertainties, while the model performance
44 differed across regions and plant functional types. Our assimilation framework (LPJ-VSJA) can improve
45 the model simulation performance of daily GPP and ET globally, especially in water-limited regions.

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

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49 1. Introduction

50 Gross primary production (GPP) and evapotranspiration (ET) are essential components of the carbon
51 and water cycles, respectively. Carbon and water fluxes are inherently coupled on multiple spatial and
52 temporal scales (Law et al. 2002; Sun et al. 2019; Waring and Running 2010). Land surface models
53 (LSMs) are the most sophisticated approach for providing a relatively detailed description of such
54 interdependent relationships regarding water and carbon fluxes and understanding the response of
55 terrestrial ecosystems to changes in atmospheric CO₂ and climate (Kaminski et al. 2017). However, there
56 are still large uncertainties in carbon and water flux estimates at regional to global scales. Both diagnostic
57 and prognostic models show substantial differences in the magnitude and spatiotemporal patterns of GPP
58 and ET. For example, the global annual GPP estimates exhibited a large range (130–169 Pg C yr⁻¹) among



59 16 Earth System Models (Anav et al. 2015). The global ET ranged from 70,000 to 75,000 km³ yr⁻¹, and
60 the uncertainty of regional or global ET estimates was up to 50% of the annual mean ET value, especially
61 in the semi-arid regions (Miralles et al. 2016). These uncertainties mainly arise from the forcing datasets,
62 simplification of mechanisms or imperfect assumptions in processes, and uncertain parameters in the
63 LSMs and assimilation methods (Xiao et al. 2019).

64 In the last two decades, remote sensing products have been assimilated into LSMs to reduce the
65 uncertainty in modeled carbon and water fluxes (MacBean et al. 2016). Data assimilation (DA) is an
66 effective approach to reduce uncertainties in terrestrial biosphere models by integrating satellite products
67 with models to constrain related parameters or state variables. A DA system contains three main
68 components: a set of observations, an observation operator, and an assimilation method. The assimilation
69 method considers the errors from both LSMs and observations and reduces model uncertainties by
70 minimizing a cost function. The Ensemble Kalman Filter (EnKF) has been widely applied in land surface
71 process models for parameter optimization, and can also significantly improve simulations by periodically
72 updating state variables (e.g., LAI and soil moisture) and without altering the model's structure based on
73 remote sensing observations (Ines et al. 2013; Li et al. 2017; Ma et al. 2013). However, ENKF cannot
74 obtain the dynamic balance of the estimation in the time window like the four-dimensional variational
75 method (4DVar) assimilation method. In particular, the Proper Orthogonal Decomposition (POD)-based
76 ensemble 4DVAR assimilation method (referred to as PODEn4DVar) (Tian and Feng 2015) requires
77 relatively less computation and can simultaneously assimilate the observations at different time intervals.
78 Meanwhile, it maintains the structural information of the four-dimensional space. This method has a



79 satisfactory performance in land DA (Tian et al. 2019; Tian et al. 2010) and can better estimate GPP and
80 ET than ENKF (Ma et al. 2017).

81 Multiple sources of remote sensing data streams have been used to constrain models for assimilation.
82 As a critical biophysical parameter of the land, leaf area index (LAI) is closely related to many land
83 processes, such as photosynthesis, respiration, precipitation interception, ET, and surface energy
84 exchange (Fang et al. 2019). More accurate LAI estimates can improve the simulations of the carbon and
85 water fluxes (Bonan et al. 2014; Liu et al. 2018; Mu et al. 2007). Soil moisture (SM) controls the process
86 of surface infiltration and runoff, determines the amount of water that can be extracted from plant roots,
87 and distributes the input energy into sensible heat flux and latent heat flux (Trugman et al. 2018). More
88 accurate SM data can improve the simulation of hydrologic parameters (SM, Streamflow, etc.) in regions
89 of interest or on a global scale (e.g., (Brocca et al. 2012; Draper et al. 2011; Lee et al. 2011; Li and Rodell
90 2013). Soil moisture is a major driving factor affecting vegetation production in arid ecosystems,
91 especially, in semi-arid areas (Liu et al. 2020). Introducing surface soil moisture (SSM) into the model
92 can significantly improve GPP and ET simulation, particularly in water-limited areas (He et al. 2017; Li
93 et al. 2020).

94 The advancement of earth observation, machine learning, inversion algorithms, and computer
95 technology has improved the accuracy of global LAI products and boosted model-data fusion studies
96 (Fang et al. 2019; Kganyago et al. 2020; Xiao et al. 2017). The Advanced Very High-Resolution
97 Radiometer (AVHRR) generates global LAI products with the longest historic record (since the early
98 1980s). The GLASS LAI product has been verified to have a better accuracy than that of MODIS and



99 CYCLOPES and is more temporally continuous and spatially complete (Xiao et al. 2013). Several recent
100 studies showed that the assimilation of GLASS LAI into terrestrial biosphere models enhanced the
101 performance of the models in simulating carbon cycling (e.g., GPP, net ecosystem exchange or NEE) and
102 hydrological (e.g., ET, SM) processes (Ling et al. 2019; Ma et al. 2017; Yan et al. 2016).

103 Microwave remote sensors are considered effective tools for measuring SM globally (Petropoulos et
104 al. 2015). For example, surface SM products have been derived from the Soil Moisture and Ocean Salinity
105 (SMOS) and Soil Moisture Active and Passive (SMAP) satellites equipped with an L-band microwave
106 instrument. The products from these satellites have been evaluated against in-situ observations and other
107 SM products and overall have high accuracy (Burgin et al. 2017; Cui et al. 2018). Additionally, the SMAP
108 performed better than SMOS and other SM products (e.g., Advanced Scatterometer (ASCAT), Advanced
109 Microwave Scanning Radiometer 2 (AMSR2)) with an overall lower error and a higher correlation based
110 on the verification with in-situ SM data from 231 sites (Cui et al. 2018; Kim et al. 2018). The assimilation
111 of SMAP data can improve the simulation accuracy of carbon and water fluxes (He et al. 2017; Li et al.
112 2020) and hydrological variables (surface soil moisture, root-zone soil moisture, and streamflow)
113 (Blyverket et al. 2019; Koster et al. 2018; Reichle et al. 2017) on a regional or global scale. For example,
114 one recent study showed that the assimilation of SMAP data performed slightly better than that of SMOS
115 and ESA CCI data (Blyverket et al. 2019).

116 In the nonlinear model or nonlinear observation operator, only simultaneous assimilation makes
117 optimal use of observations (MacBean et al. 2016). Therefore, a joint assimilation of soil moisture and
118 LAI can make use of information on these two variables separately and their interactions. For instance,



119 Ines et al. (2013) found that the joint assimilation of soil moisture and LAI achieved better results than
120 the assimilation of one of the two variables. Bonan et al. (2020) assimilated LAI and SM together into
121 the Interactions between Soil, Biosphere and Atmosphere (ISBA) land model and improved the modeled
122 GPP, ET, and runoff in the Mediterranean region. However, no studies have examined how the
123 assimilation of LAI and SM into terrestrial biosphere models can improve the simulation of carbon and
124 water fluxes at the global scale and how the performance vary across different regions.

125 In this study, we assimilated the SM products from both SMAP and SMOS and a LAI product
126 (GLASS) derived from AVHRR and MODIS into the LPJ-PM to improve the GPP and ET using the
127 PODEn4DVar method. We designed a new assimilation framework, LPJ-VSJA, which consists of three
128 assimilation schemes: (1) assimilation of LAI only, (2) assimilation of SM only, and (3) joint assimilation
129 of LAI and SM. Then, four experiments were performed based on global flux sites to evaluate the
130 assimilation performance. The specific objectives of our study are to: (1) evaluate the assimilation
131 performance of three assimilation schemes for estimating GPP and ET to select the optimal assimilation
132 scheme; (2) compare the assimilation effect of the optimal assimilation scheme in humid and arid areas;
133 (3) compare the assimilation capability in ET assimilation based on two microwave soil moisture products
134 (SMOS and SMAP) (scheme 2); and (4) apply our LPJ-VSJA framework to the globe to evaluate its
135 accuracy and robustness.

136 **2. LPJ-VSJA framework and assimilation strategy**

137 *2.1. Coupled- model (LPJ-PM) for assimilation*



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

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

acronyms	Full name	Description	Output
LPJ-DGVM	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}	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	Lund-Potsdam-Jena coupled model	An integrated model coupled from the PT-JPL _{SM} and LPJ-DGVM	GPP _{SM} , ET _{PM}
LPJ-VSJA	Lund-Potsdam-Jena Vegetation-Soil	A process-based assimilation framework for assimilating LAI	GPP _{LAI} , ET _{LAI} ; GPP _{SM} , ET _{SM} ; GPP _{CO} ; ET _{CO}



moisture-Joint - and SSM jointly into LPJ-DGVM
Assimilation system

146

147 Due to the limitation of soil stratification in LPJ-DGVM, the model was coupled with an updated
148 remote-sensing ET algorithm in the PT-JPL_{SM} that could better simulate ET in water-limited regions than
149 in humid regions (Purdy et al. 2018). The LPJ-DGVM is a process-oriented dynamic model, which
150 considers mutual interaction of carbon and water cycling and is designed to simulate vegetation
151 distribution and carbon, soil and atmosphere fluxes (Sitch et al. 2003). For each plant functional type
152 (PFT), the GPP is calculated by implementing coupled photosynthesis and water balance. In the water
153 cycle module, ET is calculated as the minimum of a plant- and soil-limited supply function (E_{supply}) and
154 the atmospheric demand (E_{demand}) (Haxeltine and Prentice 1996; Sitch et al. 2003). The soil structure is
155 simplified to a “two-layer bucket” model (the top soil layer at a 0-50 cm depth and the bottom layer at a
156 50-100 cm depth), and therefore the satellite-derived surface SM cannot be assimilated into LPJ-DGVM
157 directly. The oversimplified soil structure and single soil moisture limitation inevitably lead to sizeable
158 uncertainty in ET simulation. Additionally, the monthly input caused a daily variation of the modeled SM,
159 which was also not transmitted to the calculation of GPP and ET. Thus, the updated PT-JPL model
160 (hereafter referred to as PT-JPL_{SM}) was coupled with LPJ-DGVM and the model structure was modified
161 so that surface SM can be directly assimilated into the coupled model at the daily time step.

162 In both LPJ-DGVM and PT-JPL, three ET components are modelled: soil evaporation (E),
163 vegetation transpiration (T), and leaf evaporation (I). The PT-JPL_{SM} introduced a constraint (0–1) of



164 surface SM for transpiration and soil evaporation, which was used to avoid the implicit soil water control
165 (represented by $f_{SM}=RH^{VPD}$) in the PT-JPL model. The constraint is determined by the amount of soil
166 water available that depends on soil properties, surface SM, atmospheric conditions, potential ET (PET),
167 and canopy height. The SMAP SM was applied to model global ET using PT-JPL_{SM} and the results
168 demonstrated the largest improvements for ET estimates in dry regions (Purdy et al. 2018).

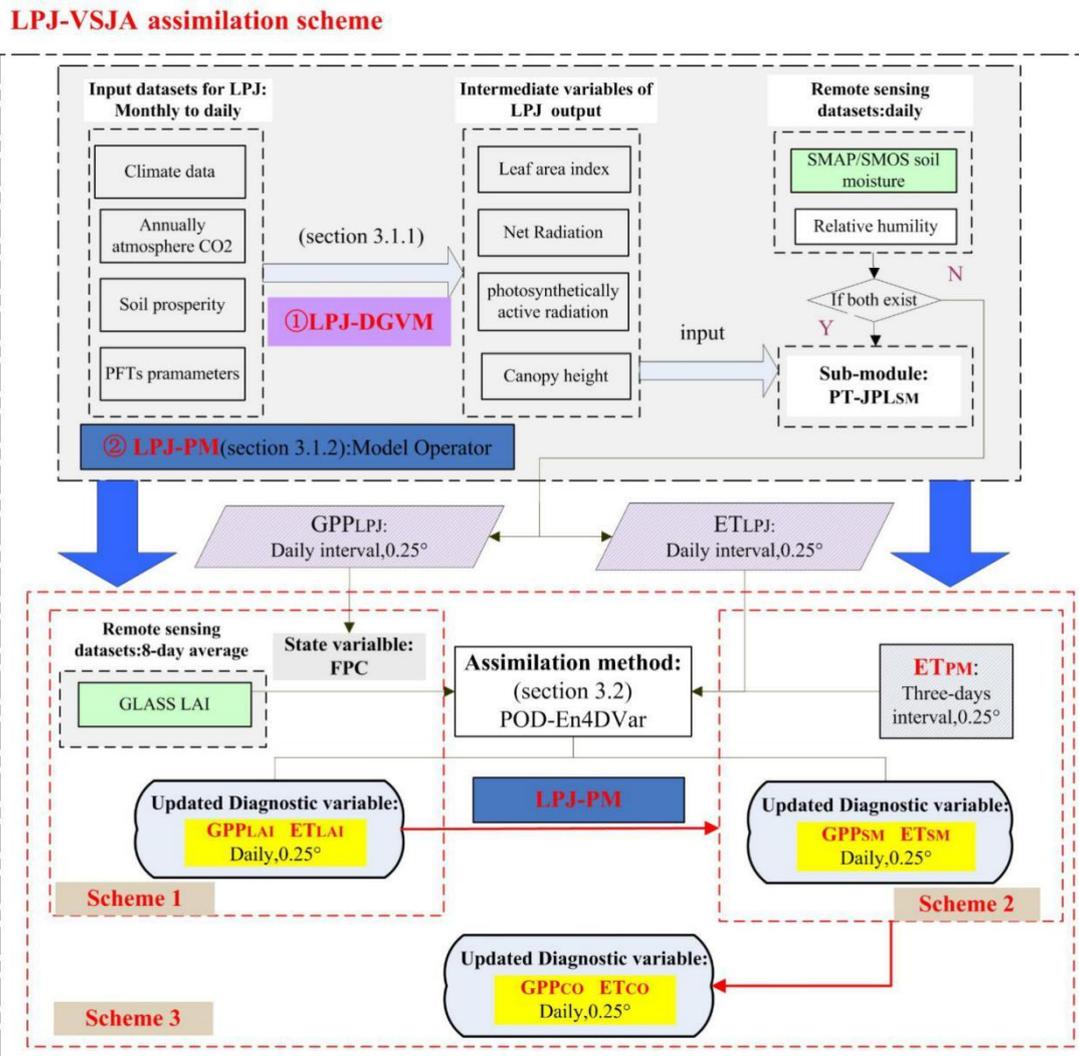
169 The ET_{PM} estimated by the coupled model (LPJ-PM) introducing surface SM is regarded as the "truth
170 value" of the surface SM assimilation scheme (scheme 2). Subsequently, assimilated ET (ET_{SM}) was
171 converted to the top soil moisture (surface layer of 0–50 cm) through the soil water conversion function,
172 providing feedback for subsequent hydrologic and carbon cycle processes. Different from other
173 "constant" ET observations, the ET_{SM} ("observation") at each time t were adjusted by absorbing
174 intermediate variables updated after assimilation at time $t-1$. The ET_{PM} was shown to be better than ET
175 simulated by LPJ-DGVM but was as not as good as that simulated by the model with SMAP SM
176 assimilated (Li et al. 2020).

177 *2.2. Assimilation scheme and experiment procedure*

178 To improve the prediction capability of LPJ-PM, we designed three assimilation schemes:
179 assimilating LAI only (scheme 1, **output: ET_{LAI} , GPP_{LAI}**), assimilating ET only (scheme 2, **output:**
180 **GPP_{SM} , ET_{SM}**), and joint assimilation of LAI and ET ((scheme 3, **output: ET_{CO} , GPP_{CO}**), i.e., LPJ-
181 VSJA framework) to test the assimilation performance for simulating GPP and ET. The proposed LPJ-
182 VSJA framework consists of four main components: the model operator (the LPJ-PM), the observation



183 operator (to establish the relation between the assimilation variable and the observed variable), the
 184 observation series (GLASS LAI and SMOS or SMAP products), and the assimilation algorithm
 185 (POD4DVar). With the surface soil moisture constraint in the PT-JPL_{SM}, the LPJ-VSJA corrects the
 186 output fluxes (GPP and ET in this study).



187



188 **Figure 1. Flowchart of the LPJ-VSJA assimilation scheme: three assimilation schemes and the coupled**
189 **model: LPJ-PM. (adapted from Li et al., 2020)**

190 The experiment consisted of six steps: (1) initialize the LPJ-DGVM and output the reference state
191 variables without assimilation over the experimental period (2010–2018), referred to as the “Control run”
192 scenario; (2) implement schemes 1, 2, and 3, respectively, and the results represent the assimilation
193 integration state (daily GPP and ET assimilation results are referred to as the “GPP_{LAI}” and “ET_{LAI}” in
194 scheme 1, “GPP_{SM}” and “ET_{SM}” in scheme 2 and “GPP_{CO}” and “ET_{CO}” in scheme 3; This scenario used
195 the same input data and model parameter scheme with the “Control run” scenario; (3) evaluate GPP and
196 ET results (schemes 1, 2 and 3) by comparing the parameters, R^2 (correlation coefficient), RMSD (root
197 mean square deviation), BIAS, and ubRMSD (unbiased root mean square deviation), for conditions of
198 without-DA (“Control run” scenario) and with-DA states, and assess the assimilation performance of
199 separate assimilation (schemes 1 and 2) and joint assimilation (scheme 3) to determine the optimal
200 assimilation scheme for GPP and ET, respectively; (4) evaluate the in-situ assimilated GPP and ET results
201 where the sites are located in wet or dry regions by dividing these validation sites into four parts (humid,
202 sub-dry humid, semi-arid, and arid regions), and this step was designed to assess the superiority of the
203 proposed assimilation scheme in water-limited areas; (5) compare the ET assimilation performance by
204 assimilating the SMOS data with that by assimilating the SMAP data; and (6) evaluate the simulated GPP
205 and ET maps based on the optimal assimilation scheme against existing global flux products.

206



207 2.2.1 DA scheme 1: LAI assimilation

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

$$215 \quad FPC = 1 - e^{-0.5LAI} \quad (2.1)$$

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

222 2.2.2 DA scheme 2: SM assimilation

223 In this scheme, the surface SM products (SMOS or SMAP) were assimilated to LPJ-PM to obtain
224 more accurate ET (ET_{SM}) estimates in water-limited areas. The observation series was the SMOS or
225 SMAP SSM product, and the observation operator was the PT-JPL_{SM} model. The ET_{PM} was directly



226 assimilated as a diagnostic variable. The assimilated ET was applied to compute the top layer SM (50 cm)
227 at the next time step (a nonlinear soil water availability function described by Zhao et al. (2013)). Then,
228 the updated SM values regulated the GPP simulation (output: GPP_{SM}).

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

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

239 2.2.3 DA scheme 3: joint assimilation of LAI and SSM

240 In this scheme, both LAI from GLASS and SM from SMOS or SMAP were the observation datasets.
241 The GLASS LAI was assimilated by scheme 1 to obtain the FPC_{DA} and ET_{LAI} , and then the FPC_{DA} served
242 as input to LPJ-PM to simulate optimized ET_{PM} , and the ET_{LAI} was further assimilated with ET_{PM} to
243 generate ET_{CO} . Then, the SM (referred to as SM_{CO} in Figure S1) updated by ET_{CO} and the FPC_{DA} were



244 used as input to correct GPP. Finally, GPP_{CO} and ET_{CO} were output by joint assimilation based on the
245 POD-En4DVar method.

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

250 2.3. *POD-Based Ensemble 4D Variational Assimilation Method*

251 The PODEn4DVar (Tian et al. 2011) method has the advantage of avoiding the calculation of adjoint
252 patterns as its incremental analysis field, which can be represented linearly by the POD base, and then
253 saving computation. Moreover, the PODEn4DVar can simultaneously assimilate multiple-time
254 observation data and provide flow-dependent error estimates of the background errors. It has shown
255 advantages in terrestrial assimilation, Tan-Tracker joint DA, and Radar assimilation (Tian et al. 2010;
256 Tian et al. 2009; Tian et al. 2014; Zhang and Weng 2015).

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

$$259 \quad J(\mathbf{x}') = \frac{1}{2}(\mathbf{x}')\mathbf{B}^{-1}(\mathbf{x}') + \frac{1}{2}[\mathbf{y}'(\mathbf{x}') - \mathbf{y}'_{obs}]^T \mathbf{R}^{-1}[\mathbf{y}'(\mathbf{x}') - \mathbf{y}'_{obs}]$$

260 Here, the $\mathbf{x}' = \mathbf{x} - \mathbf{x}_b$, $\mathbf{y}'(\mathbf{x}') = \mathbf{y}(\mathbf{x}' + \mathbf{x}_b) - \mathbf{y}(\mathbf{x}_b)$, $\mathbf{y}'_{obs} = \mathbf{y}_{obs} - \mathbf{y}(\mathbf{x}_b)$, $\mathbf{y} = H[M_{t_o \rightarrow t_k}(\mathbf{x})]$.
261 $\mathbf{x}'(\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_N)$ is the model perturbation (MP) matrix and $\mathbf{y}'(\mathbf{y}'_1, \mathbf{y}'_2, \dots, \mathbf{y}'_N)$ is the



262 observation perturbation (OP) matrix with N samples. Following Rüdiger et al. (2010), the LAI
263 perturbation was set to a fraction (0.001) of the LAI itself. The perturbation of ET_{PM} and ET_{LPJ} conforms
264 to a Gaussian distribution with a mean of 0 and a specified covariance (10 and 5% of the ET_{PM} and ET_{LPJ}
265 at time t). The subscript b represents the background field, the superscript T represents a transpose, H is
266 the observation operator of scheme 1 as described in section 2.3, and scheme 2 is the PT-JPL_{SM} (described
267 in Purdy et al. (2018)). M is the forecast model (LPJ-PM in this study), B is the background error
268 covariance, R is the observation error covariance, and obs denotes observation.

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

273 The manifestation of the background error covariance is the same as the Ensemble Kalman filter
274 (EnKF, Evensen (2004)), and the incremental analysis x'_a was expressed by the $\Phi_{x,n}$, and $\tilde{\Phi}_y$ ($\tilde{\Phi}_y =$
275 $[(n-1)I_{n \times n} + \Phi_{y,n}^T R^{-1} \Phi_{y,n}]^{-1} \Phi_{y,n}^T R^{-1}$). Finally, the final analysis x_a is calculated as $x_a = x_b +$
276 $\Phi_{x,n} \tilde{\Phi}_y y'_{obs}$. The detailed derivation process of the algorithm is described by a previous study (Tian et
277 al. 2011).

278 In the ensemble-based method, the number of ensemble members is usually fewer than that of the
279 observation data and the degrees of freedom of the model variables, and spurious long-range correlations



280 occur between observation locations and model variables. A practical method, the localization technique,
281 is applied to address this issue (Mitchell et al. 2002). The final incremental analysis is rewritten as:

$$282 \quad x'_a = \Phi_{x,n} \tilde{\Phi}_y y'_{obs} C_0 \left(\frac{d_h}{d_{h,0}} \right) \cdot C_0 \left(\frac{d_v}{d_{v,0}} \right)$$

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

$$286 \quad C_0(r) = \begin{cases} -\frac{1}{4}r^5 + \frac{1}{2}r^4 + \frac{5}{8}r^3 - \frac{5}{3}r^2 + 1, & 0 \leq r \leq 1, \\ \frac{1}{12}r^5 - \frac{1}{2}r^4 + \frac{5}{8}r^3 + \frac{5}{3}r^2 - 5r + 4 - \frac{2}{3}r^{-1}, & 1 \leq r \leq 2, \\ 0, & 2 < r \end{cases}$$

287 where r is the radius of the filter.

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

294 *2.4. Validation method for assimilation performance*



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

305 The error variance of GPP and ET products was estimated using the triple collocation (TC) approach
306 (Stoffelen 1998) to validate the global simulation in this study. The method has been extensively applied
307 in the study of hydrology and oceanography (Caires and Sterl 2003; Khan et al. 2018; O'Carroll et al.
308 2008; Stoffelen 1998), particularly in SM studies (Chan et al. 2016; Kim et al. 2018). The TC provides a
309 reliable platform for comparison of spatial assimilation results and in-situ measurements. In this
310 experiment, no calculation was performed on the non-vegetated areas where the correlation was lower
311 than 0.2 to have independent datasets and avoid correlated errors (crucial assumptions in TC) (Yilmaz
312 and Crow 2014).

313



314 **3. Experiment sites and data**

315 *3.1. Description of flux tower sites*

316 We screened over 300 EC flux sites across the globe from the FLUXNET2015
317 (<https://fluxnet.fluxdata.org/data/fluxnet2015-dataset/>), AmeriFlux (<http://public.ornl.gov/ameriflux/>),
318 and the HeiHe river basin (Li et al. 2013) for the evaluation of assimilation performance over the period
319 from January 2010 to December 2018. The in-situ half-hourly LE and GPP data from the sites were
320 aggregated into daily data. The daily gap-filled data were excluded if the percentage of gap-filled half-
321 hourly values was more than 20%. Then we corrected the data of energy non-closure by using the Bowen
322 ratio closure method (Twine et al. 2000) to improve the energy closure rate (Huang et al. 2015; Yang et
323 al. 2020). The data were selected to cover the 2010–2018 period with at least one year of reliable data,
324 and the result from the error of assimilation is relative to the LE value and seasonal variation (Purdy et al.
325 2018; Zou et al. 2017). It is essential to have available data every month during a one-year period, and
326 only days with less than 25% missing data were processed per month (Feng et al. 2015). In addition, for
327 flux tower data, the data were also excluded for the analysis if the SMAP/SMOS SM data were not of
328 good quality.

329 Finally, we identified a total of 105 sites across the globe encompassing five major biomes: grassland
330 (18 for GPP and 19 for ET), savanna (11), shrubland (4), forest (49 and 53), and cropland (13 and 14). In
331 the comparative analysis of the performance for simulating ET by assimilating SMOS and SMAP SM
332 data separately, we selected 46 AmeriFlux sites (Figure S3) with at least one year of reliable data from



333 2015 to 2018 based on the simultaneous availability of SMAP and SMOS data, including grassland (19),
334 savanna (11), shrubland (5), forest (23), and cropland (7). Figure S2 and S3 illustrate the location and
335 distribution of the 105 and 46 EC flux tower sites, respectively. A more detailed description is
336 summarized in the Supporting Information Table S1.

337 *3.2. Remote sensing datasets: LAI and SM*

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

344 The SMAP mission (Entekhabi et al. 2010) and SMOS mission (Jacquette et al. 2010), the two
345 dedicated soil moisture satellites currently in orbit equipped with L-band microwave instruments, provide
346 surface SM retrievals. We chose the SMOS-L2 product and the SMAP-L3-Enhanced product, which both
347 provide global coverage every three days for soil depth of 5 cm. Only good-quality SMAP and SMOS
348 data were used. The grid cells with water areas larger than 10% and those with less than 50% good-quality
349 data in one year were masked out, which alleviates the undesirable model simulations caused by the
350 decrease in SMAP retrieval accuracy (Chan et al. 2016; O'Neill et al. 2010). We only adopted the data



351 with an uncertainty below $0.1 \text{ m}^3 \text{ m}^{-3}$, in the actual range ($0.00\text{--}0.6 \text{ m}^3 \text{ m}^{-3}$), and the temperature of the
352 LSM observation layer (the second layer) was higher than $2 \text{ }^\circ\text{C}$ (Blyverket et al. 2019).

353

354 3.3. Model-forcing and validation datasets

355 In this study, the meteorological, soil property, and CO_2 concentration datasets were used to drive
356 the LPJ-PM. The model-forcing datasets were interpolated to 0.25° based on the bilinear method to ensure
357 the consistency of spatial representation. Table 2 provides the spatial and temporal characteristics of the
358 model-forcing datasets in the LPJ-PM (submodule: LPJ-DGVM and PT-JPL_{SM}).

359

360 **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,			
	temperature,	1901-	$0.5^\circ \times 0.5^\circ$	New et al. (2000)
	precipitation, wet	1930		
day				
Ice-core measurements and atmospheric	Atmospheric CO_2 concentrations	1901-2018	NA	(Etheridge et al. (1996); Keeling et al.



observations at the				(1995))
Mauna Loa				
Observatory ^a				
	Precipitation, surface			
MERRA-2 ^a	temperature, cloud fraction, relative humidity	2010- 2018	0.5°× 0.625°	Rienecker et al. (2011)
HWSD (v121) ^b	Soil texture data	NA	1 km×1 km	Wieder et al. (2014)
SPL3SMP_E ^b	Surface soil moisture	2015.4– present	9 km×9 km	Entekhabi et al. (2010)
GLASS LAI ^{a,b}	Leaf area index	2010- 2018	5 km×5 km	Xiao et al. (2016)
SMOS_L3 CATDS ^b	Surface soil moisture	2010- present	25km×25 km	Jacquette et al. (2010)

^a: forcing dataset for LPJ-DGVM

^b: external input dataset for PT-JPL_{SM}

361
362
363

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



367

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 fluorescence with GPP-SIF relationships	Li and Xiao (2019)
GLDAS ET	ET	daily	0.25° × 0.25°	Processed model assimilation	Fang et al. (2009)



GLEAM				Processed model	Martens et
v3a ET	ET	daily	0.25° × 0.25°	assimilation	al. (2017)

368

369 4. Results

370 4.1. Performance of LPJ-PM for simulating GPP and ET with the assimilation of LAI and soil moisture

371 4.1.1 Accuracy assessment of GPP for separate and joint assimilation

372 In general, the R^2 between GPP_{LPJ} and GPP_{OBS} was above 0.4 at most of the sites (62 sites) and
373 were relatively weak for some sites ($R^2 < 0.4$). The LAI assimilation improved the simulations at most
374 sites (R^2 value increased at 82 sites), particularly for sites in the U.S. and Europe (Figure 2). The R^2
375 improvement from the LAI assimilation (scheme 1) was superior to that from the SM assimilation
376 (Figure 2- R^2 (b) and (c)). The performance of the joint assimilation (scheme 3) was similar to that of
377 scheme 1. The GPP assimilation performance in terms of RMSD between scheme 1 and scheme 2 was
378 not significantly different. For sites with no improvement in the separate assimilation (schemes 1 and
379 2), the RMSD, however, was improved in the joint assimilation (scheme 3) (Figure 2). More sites
380 (Figure 2-BIAS (a)) showed positive bias ($GPP_{OBS} - GPP_{LPJ}$), which were mainly distributed in the
381 humid and dry-sub humid forest, grassland, and arid cropland regions, showing underestimation for
382 GPP_{OBS} . The assimilation improved the accuracy for overestimated sites, but there was no significant
383 improvement for underestimated sites. The ubRMSD implied that the SM assimilation alone had a



384 better performance than the LAI assimilation alone, especially for sites in arid areas. The analysis of the
385 above four statistical measures (R^2 , RMSD, BIAS, and ubRMSD) indicated that the accuracy of joint
386 assimilation was better than that of separate assimilation.

387 At the seasonal scale, all three assimilation schemes corrected the model trajectory and
388 significantly improved the growing season simulations, especially for peak values (IT-Tor, US-NR1,
389 US-NE1). In addition, the linear fitting of GPP_{CO} and GPP_{OBS} on a monthly scale was closer to 1:1 ($y =$
390 $0.92 + 21.66 p < 0.001$) than that of GPP_{LAI} ($y = 0.89 + 28.3, p < 0.001$) and GPP_{SM} ($y = 0.86 + 41.70, p$
391 < 0.001) (Figure S5). The results in Table S2 support the above analysis, and the joint assimilation
392 showed advantages in overall accuracy in both arid and humid areas.

393

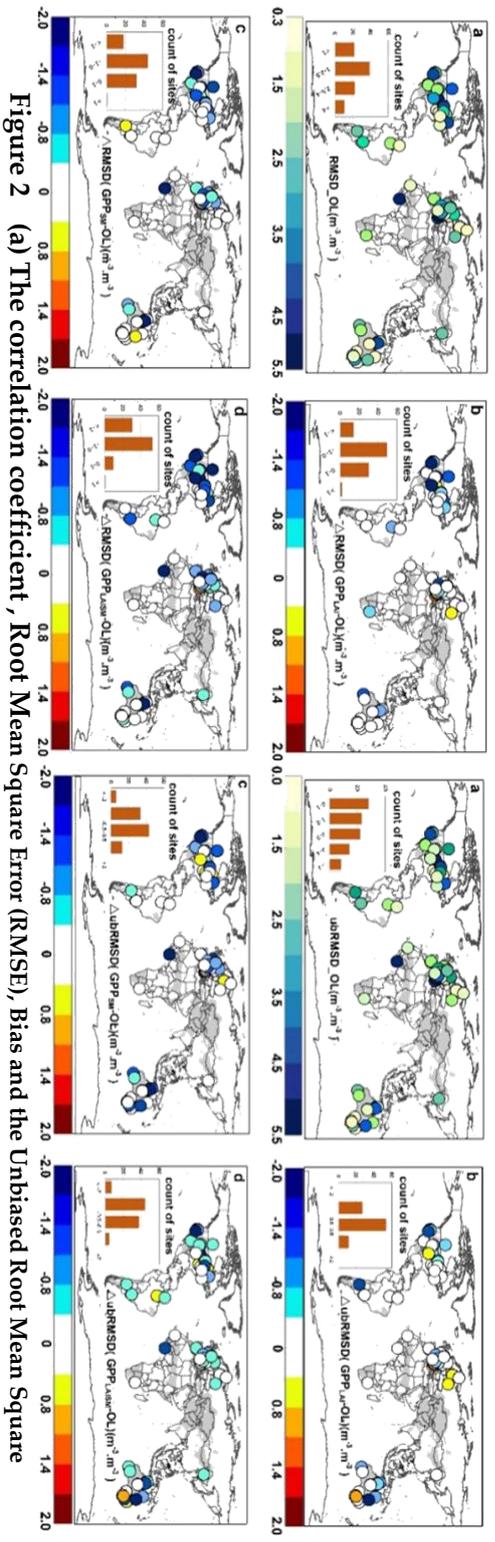
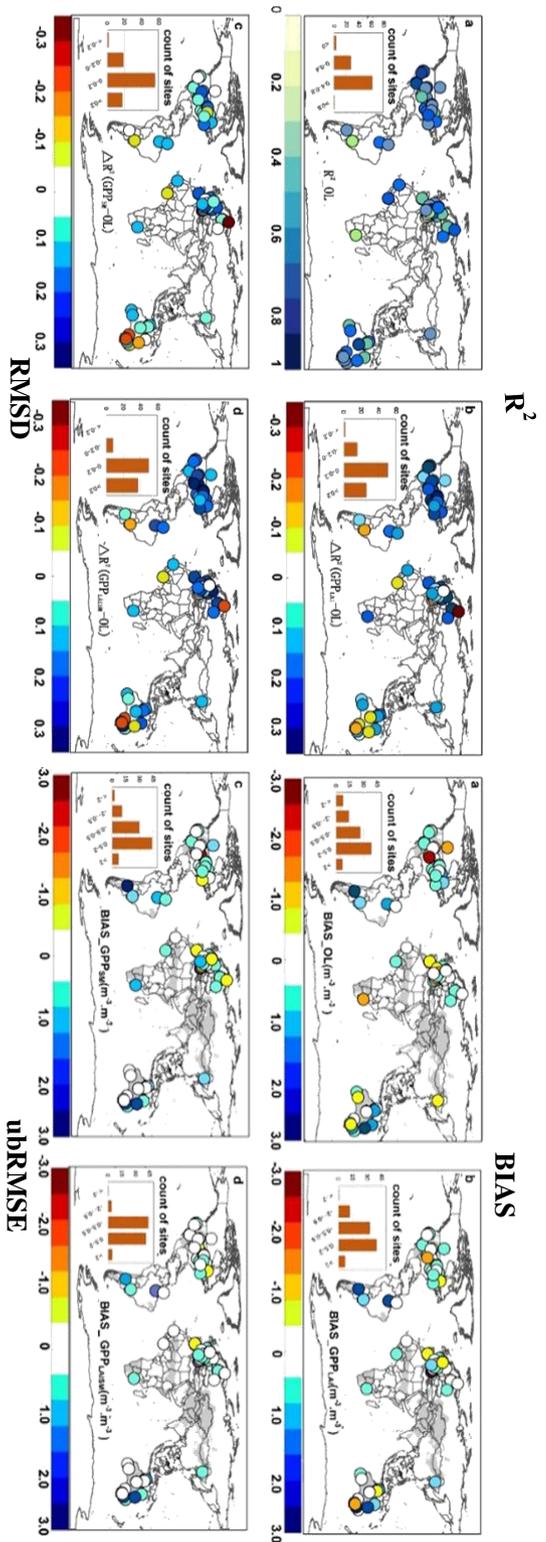


Figure 2 (a) The correlation coefficient, Root Mean Square Error (RMSE), Bias and the Unbiased Root Mean Square

Error (ubRMSE) between the GPP(GPP_{LPI}) simulated by the LPI-DGVM and the site observations, the yellow/blue indicating low/high correlation r ; (b) ΔR (correlation difference between GPP_{LAI} and GPP_{LPI}), $\Delta RMSE$ ($GPP_{LAI} - GPP_{LPI}$), $BIAS$ (GPP_{LAI}) and $\Delta ubRMSE$ ($GPP_{LAI} - GPP_{LPI}$); (c) ΔR (correlation difference between GPP_{SM} and GPP_{LPI}), $\Delta RMSE$ ($GPP_{SM} - GPP_{LPI}$), $BIAS$ (GPP_{SM}) and $\Delta ubRMSE$ ($GPP_{SM} - GPP_{LPI}$); (d) ΔR (The correlation difference between GPP_{CO_2} and GPP_{LPI}), $\Delta RMSE$ ($GPP_{CO_2} - GPP_{LPI}$), $BIAS$ (GPP_{CO_2}) and $\Delta ubRMSE$ ($GPP_{CO_2} - GPP_{LPI}$), blue/red represent positive/negative values.

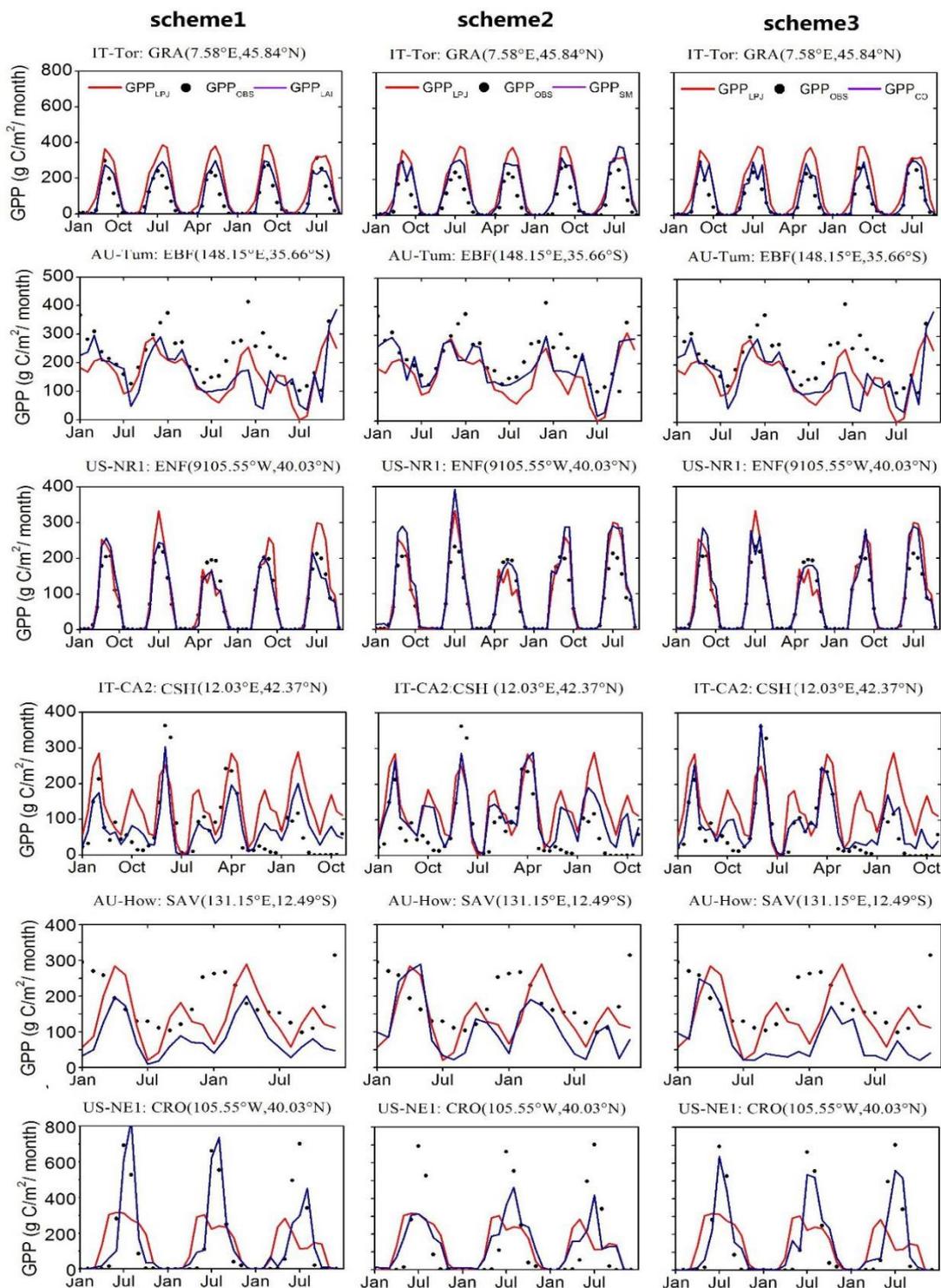
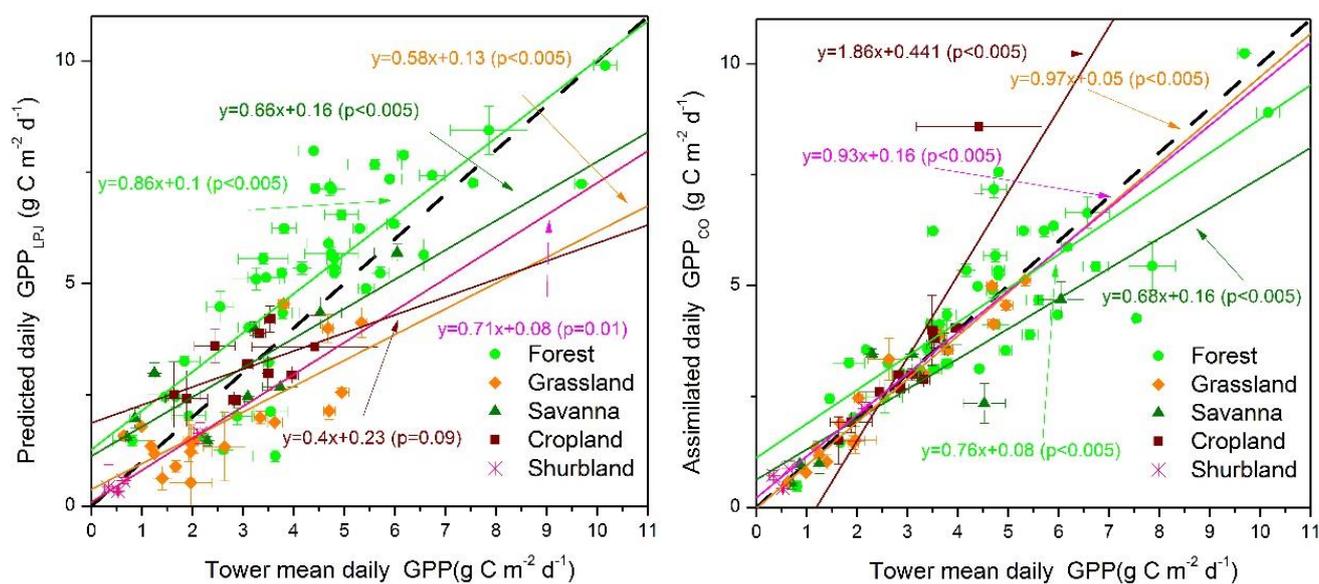




Figure 3. Seasonal cycles of tower GPP and simulated gross primary productivity (GPP) from Lund-Potsdam-Jena (LPJ), GLASS LAI assimilation (scheme 1), SMOS assimilation (scheme 2) and joint assimilation (scheme 3) for six sites representing six PFTs.

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 $-70 \sim 60 \text{ g C m}^{-2} \text{ month}^{-1}$. The high GPP_{OBS} values were considerably underestimated. The maximum negative error reached $100 \text{ g C m}^{-2} \text{ month}^{-1}$. 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 $0\text{--}200 \text{ g C m}^{-2} \text{ month}^{-1}$ 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.



408



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

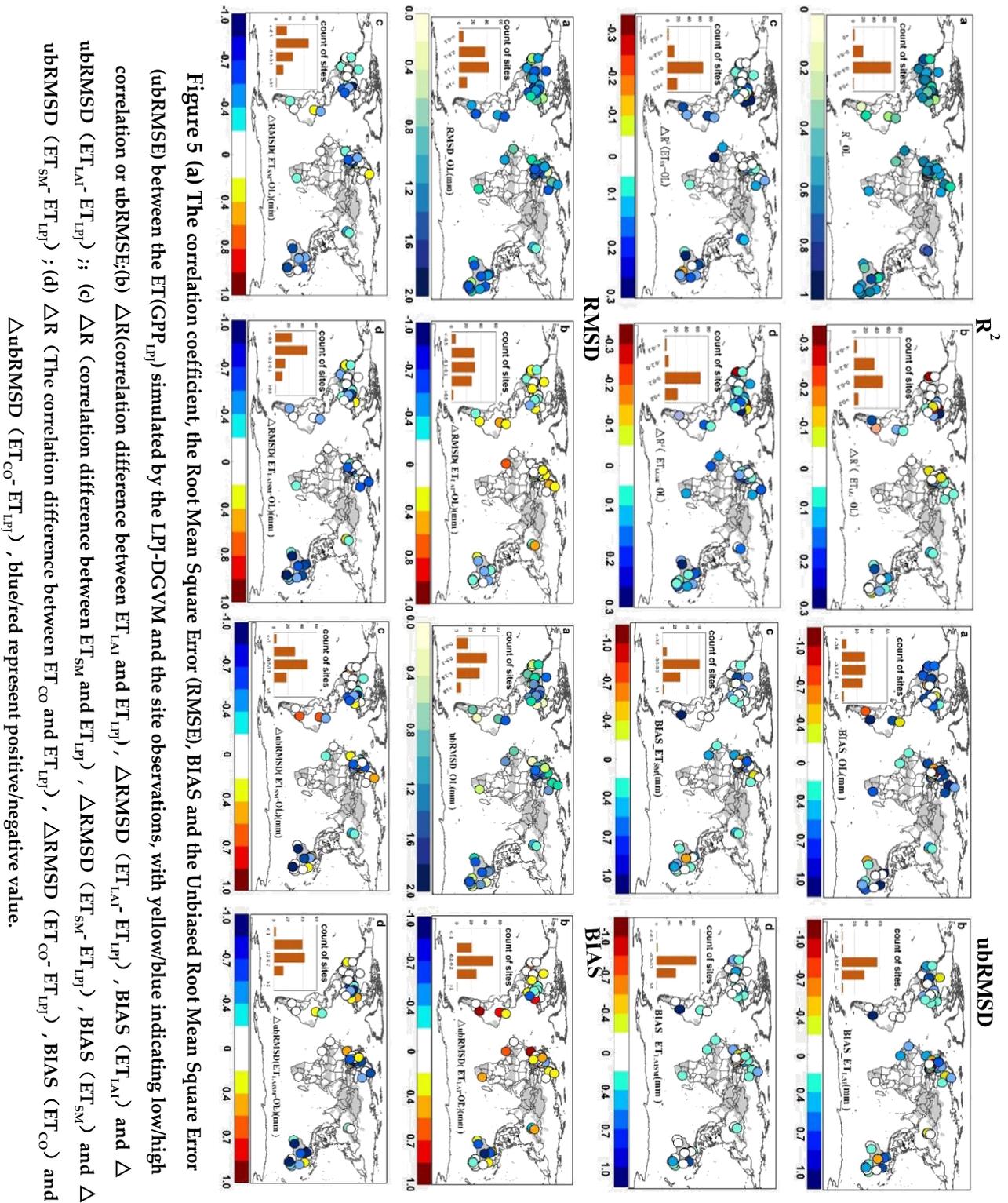
410 After determining the optimal assimilation scheme (scheme 3), we evaluated the GPP_{LPJ} and GPP_{CO}
411 at the site level (Fig.4). The results showed that GPP_{CO} performed better ($R^2= 0.83$, $RMSD= 1.05 \text{ g C m}^{-2}$
412 d^{-1}) than GPP_{LPJ} ($R^2= 0.69$, $RMSD= 2.15 \text{ g C m}^{-2} \text{ d}^{-1}$). The noticeable underestimation in all PFTs and
413 overestimation at most forest sites for GPP_{LPJ} were corrected by joint assimilation (GPP_{CO}). Our joint
414 assimilation methods had better performance in forests, shrublands, and grasslands than in croplands and
415 savannas. Except for the cropland, the linear fitting results of other types were all below the 1:1 line,
416 showing the overall underestimation. Superior performance in both original simulation and assimilation
417 occurred at shrubland ($R^2= 0.93$, $RMSD= 0.27 \text{ g C m}^{-2} \text{ d}^{-1}$) and grassland ($R^2= 0.97$, $RMSD= 0.38 \text{ g C}$
418 $\text{m}^{-2} \text{ d}^{-1}$) sites. However, the standard deviation of GPP_{CO} and GPP_{OBS} at savanna sites was relatively large,
419 and the assimilated GPP at several savanna sites was significantly underestimated.

420 4.1.2 Accuracy assessment of ET for separate and conjunct assimilation

421 In general, the coefficient of determination (R^2) between ET_{LPJ} and ET_{OBS} was generally over 0.4
422 (the simulations were superior to GPP_{LPJ}) (Figure 5). ET_{LAI} showed slightly higher R^2 , while some sites
423 showed reduced values (41 sites). The ET_{SM} and ET_{CO} were significantly improved compared with the
424 ET_{LAI} . The R^2 increased considerably in Australia but declined at some sites in the United States after
425 assimilation. For RMSD and ubRMSD, ET_{CO} performed better than ET_{SM} and ET_{LAI} . The SM
426 assimilation improved more in humid regions, while the RMSD of ET_{LAI} only slightly improved in
427 Australia and the ubRMSD of ET_{SM} was slightly higher in South America. According to the bar chart



428 (Fig.5-RMSD(b)), the LAI assimilation increased the ET simulation error. In the original LPJ-DGVM
429 simulation, the sites with a negative bias were mostly located in the humid and dry-sub humid regions,
430 while most of the sites in arid and semi-arid regions had underestimation (Fig. 5-BIAS(a), Table S3).
431 The assimilation improved ET at some of the overestimated sites, but the underestimation over these
432 sites showed little improvement.





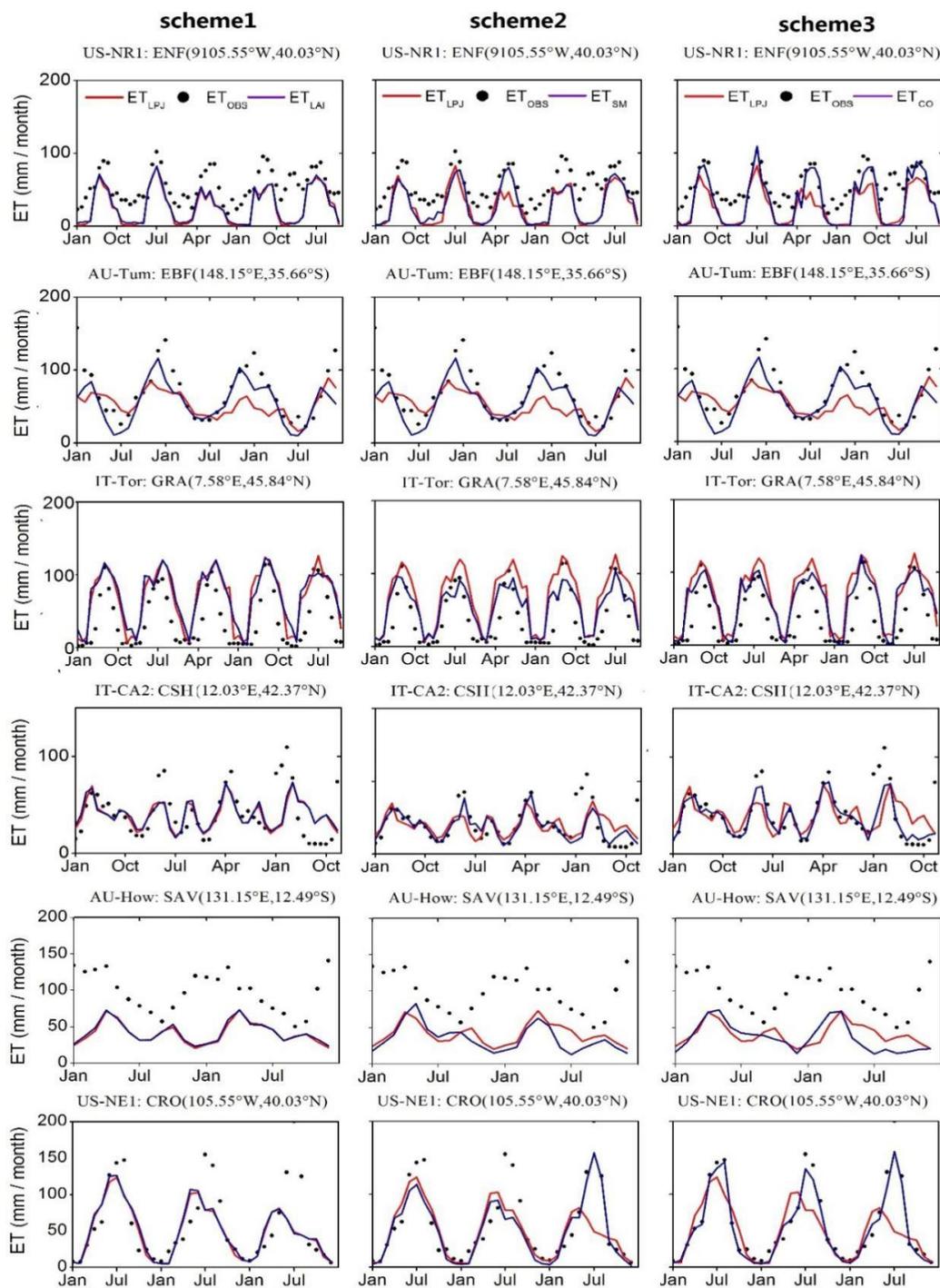
434 At the seasonal scale, the model simulations were able to capture the temporal trend of ET_{OBS} , and
435 joint assimilation significantly improved the simulation in the growing season (US-NR1, US-NE1);
436 overall underestimation was observed for ET_{OBS} , especially in winter (Fig.6). Overall,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

440 The ET residual analysis (Figure S7 (right)) indicated that the three assimilation scheme errors
441 showed underestimation for ET_{OBS} . In general, the error distribution of separate assimilations was more
442 dispersed than that of the joint assimilation. Similar to the assimilation performance of GPP, ET_{CO} and
443 ET_{SM} significantly improved the overestimation of ET_{OBS} , but did not significantly improve the
444 underestimation. For the ET_{CO} , most of the errors were distributed around -30 – 18 $mm\ month^{-1}$. The region
445 with high ET_{OBS} was considerably underestimated, and the maximum negative error reached -57 mm
446 $month^{-1}$.

447 We also evaluated the ET assimilation results at the PFT scale (Figure 7). The results showed that
448 our assimilated ET performed better at the site level ($R^2= 0.77$, $RMSD= 0.28$ $mm\ d^{-1}$) than that of ET_{LPI}
449 ($R^2= 0.67$, $RMSD=0.98$ $mm\ d^{-1}$). Joint assimilation significantly reduced the errors of those shrubland
450 sites with overestimation for ET_{OBS} , and the site distribution was closer to the 1:1 line. Our assimilation
451 methods had better performance in forest, savanna, and grassland ecosystems than in cropland and
452 shrubland (Table S3). The linear fitting results of grassland and shrubland were all above the 1:1 line,
453 showing overall overestimation. Although the original simulation and assimilation performance were
454 superior at savanna sites ($R^2= 0.95$, $RMSD= 0.33$ $mm\ d^{-1}$), the standard deviations of ET_{CO} and ET_{OBS} at

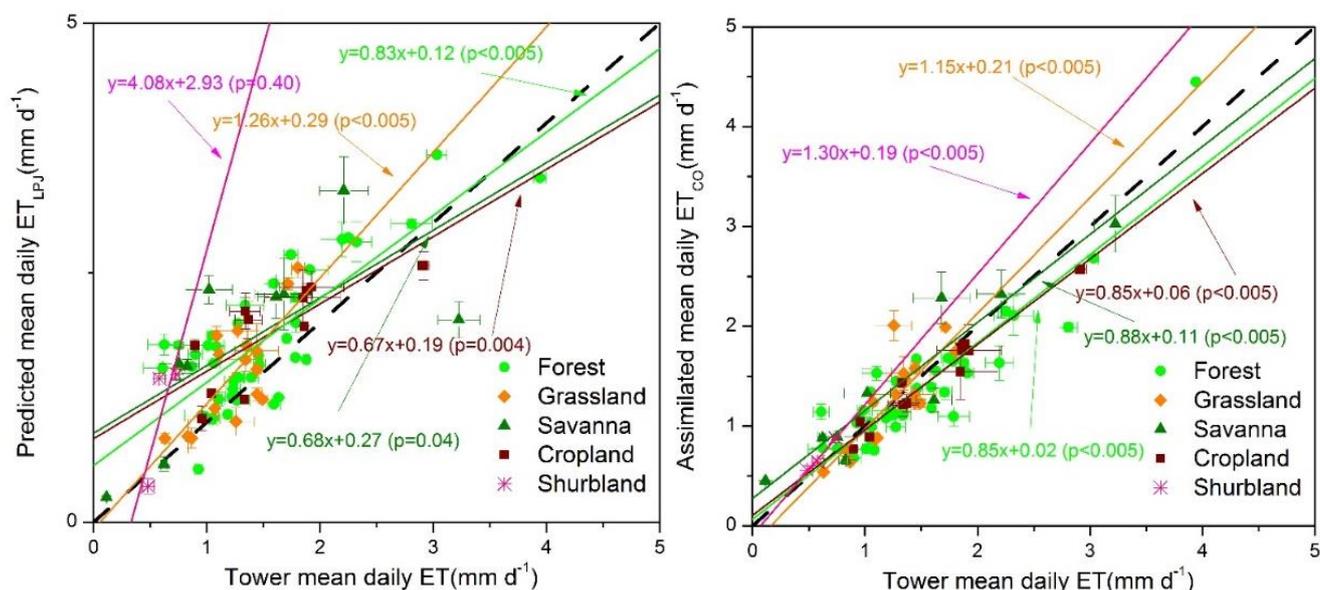


455 savanna sites were relatively large, which was similar to the GPP results at savanna sites.



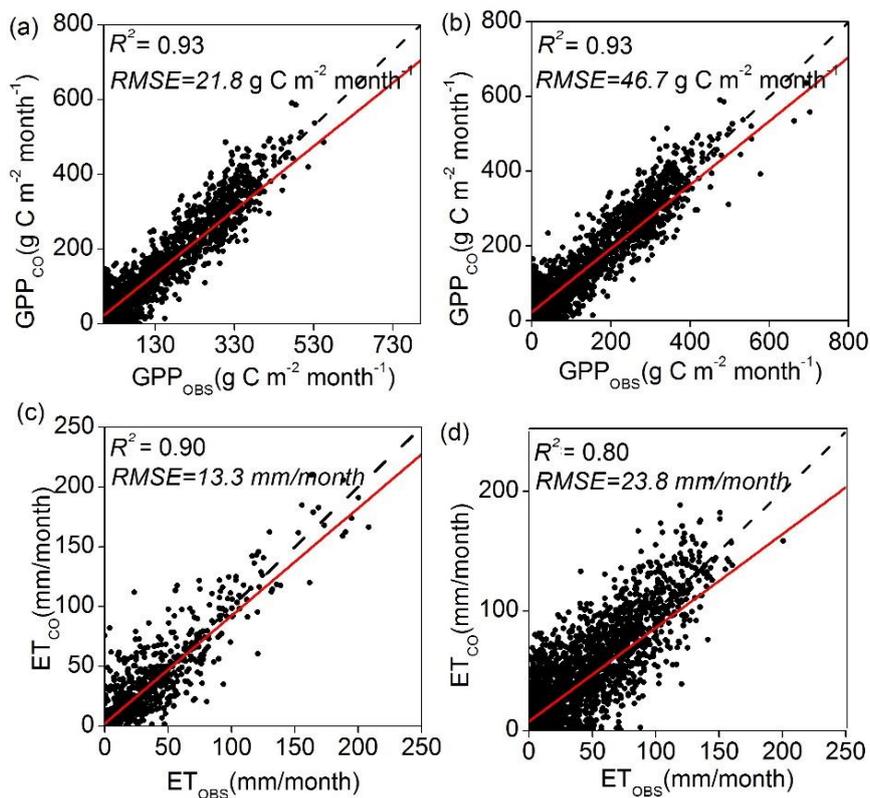


457 **Figure 6. Seasonal cycles of tower-based and simulated ET from Lund-Potsdam-Jena (LPJ), GLASS LAI**
458 **assimilation (scheme 1), SMOS assimilation (scheme 2) and joint assimilation (scheme 3) for the six sites**
459 **representing six PFTs during the study period.**



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

462 *4.2. Comparison of assimilation performance in semi-arid and arid regions with that in humid and dry-*
463 *sub humid regions*



464

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

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

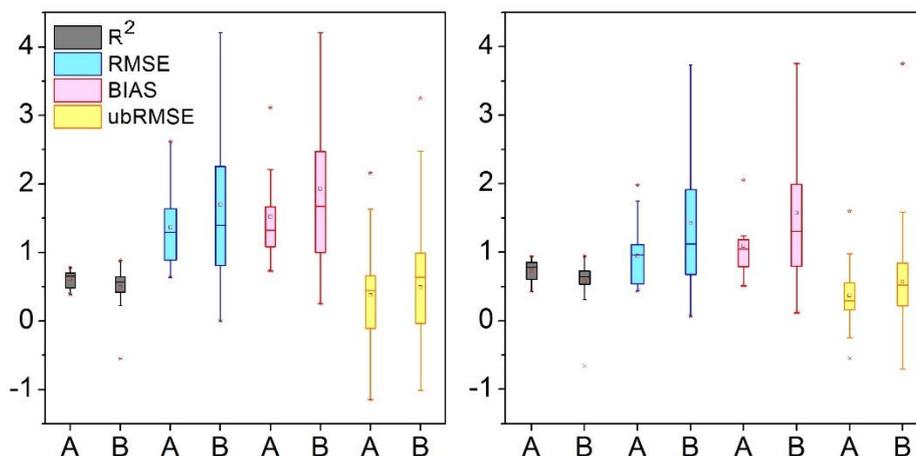


473 arid and arid regions, the higher RMSD of the humid and sub-dry humid regions did not reflect higher
474 accuracy in semi-arid and arid regions. As for ET_{CO} , the fitting results and R^2 values in the semi-arid
475 and arid regions performed better than those in the humid and sub-dry humid regions,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

477 On the daily scale, the original GPP simulations (GPP_{LPJ}) performed better in the semi-arid and
478 arid regions than in the humid and sub-dry humid regions with higher R^2 and lower ubRMSD (Table S2).
479 For GPP_{CO} , the shrubland in the semi-arid and arid regions had the lowest R^2 values and the second lowest
480 ubRMSD. The forest in the semi-arid and arid regions had the largest improvement after assimilation. In
481 the humid and sub-dry humid regions, the GPP_{CO} of the savanna and cropland showed the largest
482 improvement (R^2 increased by 64.7% and 71.1%, respectively; ubRMSD decreased by 47.0% and 31.8%,
483 respectively). The grassland in the semi-arid and arid regions had the highest R^2 , and the savanna by
484 combining all indicators had the best assimilation results compared to other types in both regions.

485 Similar to ET_{CO} , the ET_{LPJ} in the semi-arid and arid *regions* was better than that in humid and sub-
486 dry humid regions in terms of four evaluation indicators (RMSD decreased by 32.7%, ubRMSD decreased
487 by 34.4% in semi-arid and arid regions and RMSD decreased by 26.4%, and the ubRMSD decreased by
488 30.9% in humid and sub-dry humid regions compared with ET_{LPJ}). The performance of the original
489 simulation and assimilation of grassland sites in the semi-arid and arid regions was the best among all
490 five PFTs.

491

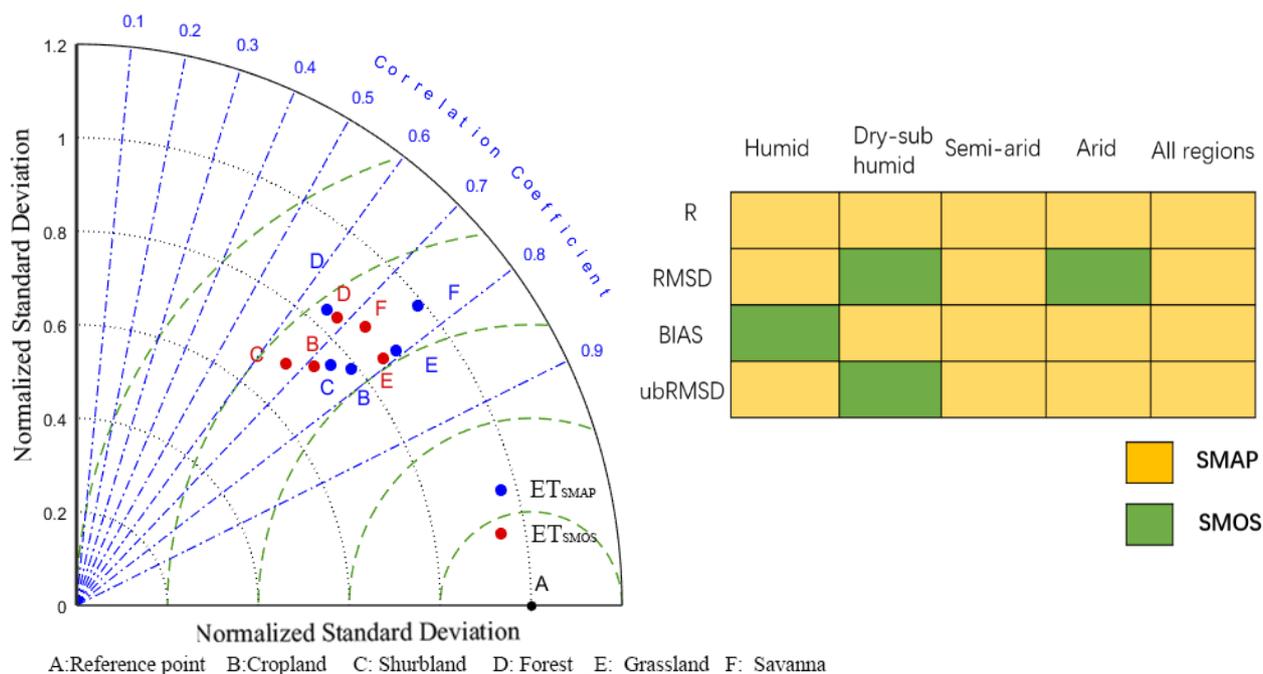


492

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

495 To investigate the reasons for better assimilation performance in water-limited regions, we evaluated
496 the GPP and ET simulated by the LPJ-PM according to R^2 , ubRMSD, RMSD, and BIAS (Figure 7).
497 Compared with the semi-arid and arid regions, the humid and sub-dry humid region had smaller R^2 mean,
498 larger BIAS and RMSD mean, and no significant difference in mean ubRMSD for GPP_{SM} . In general, the
499 evaluation results of joint assimilation for ET_{PM} were generally consistent with those for GPP_{SM} and
500 GPP_{SM} . ET_{PM} showed underestimation, which was consistent with the underestimation in SM assimilation.
501 These results indicated that, both GPP and ET modeled by LPJ-PM with joint assimilation were less stable
502 and had a lower performance in the humid and sub-dry regions than in the semi-arid and arid regions.

503 *4.3. Comparison of assimilation performance in assimilating SMOS and SMAP soil moisture data*



504

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

512

513 The Taylor chart was used to compare the assimilation performance of ET_{SMAP} and ET_{SMOS} at 46



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

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

530 4.4. Global simulations of GPP and ET with joint assimilation of LAI and soil moisture data

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



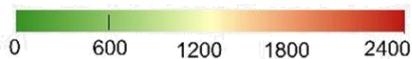
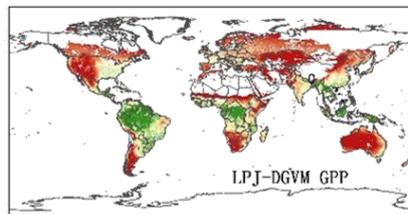
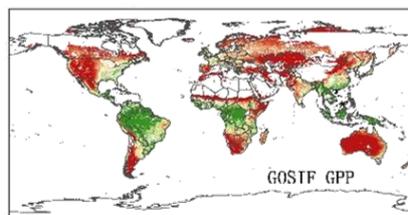
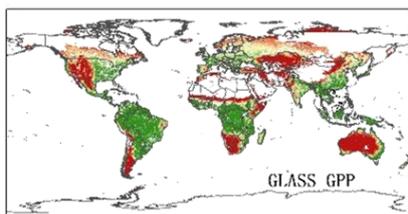
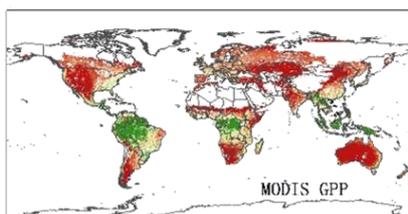
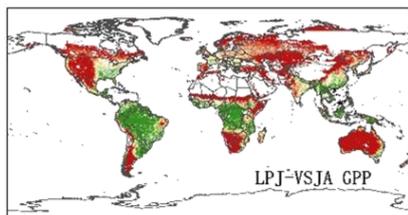
533 DGVM and LPJ-VSJA were referred to as LPJ-DGVM GPP(ET) and LPJ-VSJA GPP(ET), respectively.
534 We compared the annual spatial GPP and ET values and the error standard deviation of the LPJ-VSJA
535 with several existing flux products.

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

544 LPJ-VSJA ET was the closest to GLEAM ET on the spatial average with the least spatial average
545 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
546 ET (-34.7 mm yr^{-1} and 0.73), LPJ-DGVM (-48.7 and 0.66 mm yr^{-1}), and MODIS ET (-122.1 and 0.54 mm
547 yr^{-1}).

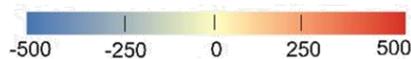
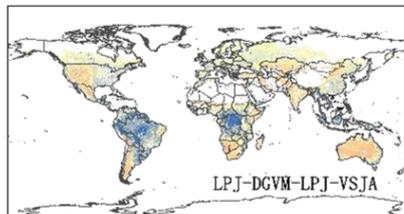
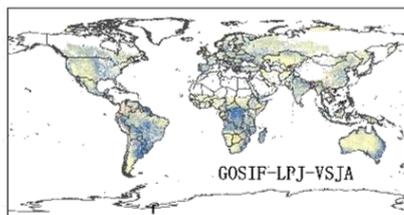
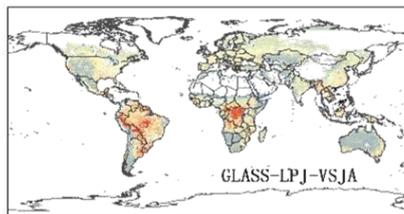
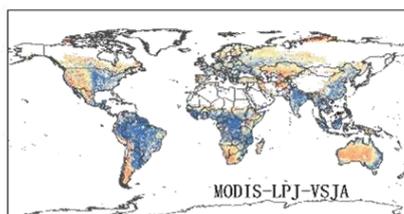


Annual mean of GPP (g C/m²/yr)

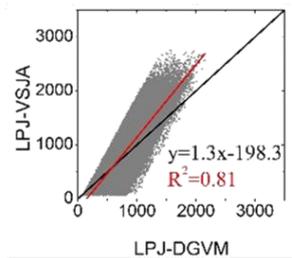
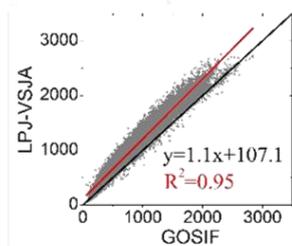
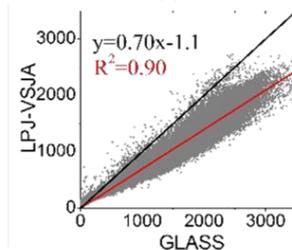
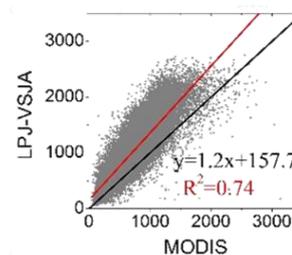


Column A

Annual difference of GPP (g C/m²/yr)



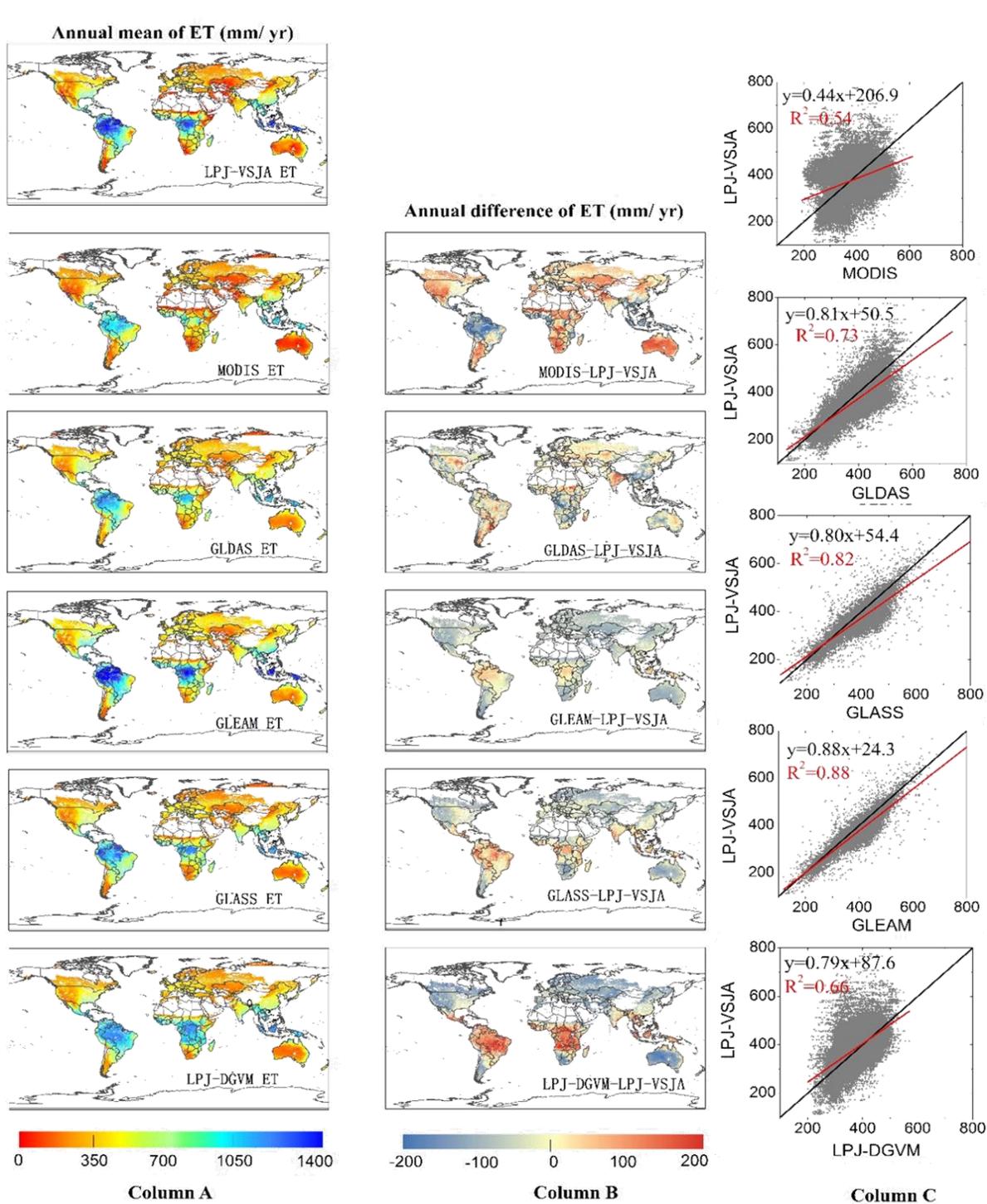
Column B



Column C



549 **Figure 11. Column A: Spatial distribution of annual LPJ-VSJA GPP and other independent satellite-based**
550 **datasets (a: MODIS GPP; b: GLASS GPP; c: GOSIF GPP; e: LPJ-DGVM). Column B: Spatial**
551 **distribution of the difference between annual LPJ-VSJA GPP and other independent satellite-based**
552 **datasets. Column C: Scatter plots between these products. Black lines show the 1:1-line, red lines show the**
553 **regression fit.**





555 **Figure 12. Column A: Spatial distribution of annual LPJ-VSJA ET and other independent satellite-**
556 **based datasets (a: MODIS GPP; b: GLDAS ET; c: GLEAM ET; d: GLASS ET; e: LPJ-DGVM ET).**
557 **Column B: Spatial distribution of the difference between annual LPJ-VSJA ET and other independent**
558 **satellite-based datasets. Column C: Scatter plots between these products are provided on the right of the**
559 **difference maps. Black lines show the 1:1-line, red lines show the regression fit.**
560

561 Figure 13 (a)–(e) represent the spatial error standard deviation (σ) distribution of MODIS, GLASS,
562 GOSIF, and LPJ-VSJA GPP, respectively. The graphs on the right side depict the corresponding
563 histograms. The σ of the MODIS GPP was evenly distributed between 30 and 60 g C/m²/month, while
564 the average σ of other products was concentrated in 0–20 g C m⁻² month⁻¹ (90%). The high errors of all
565 products were concentrated in the high temperature and humid areas of southern North America, eastern
566 South America, humid and dry sub-humid areas of South Asia, and the savannas of Africa and Australia.
567 The error histogram of GOSIF GPP and LPJ-DGVM GPP were in line with the normal distribution, with
568 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
569 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
570 variance of the LPJ-VSJA product was the lowest, indicating a stability of the regional error (Table S4).
571 Compared to the LPJ-DGVM, the joint assimilation results showed improvement in all regions (the
572 average error reduced by 17.7 g C m⁻² month⁻¹), especially in the humid regions of South Asia, Australia,
573 and the United States. Our LPJ-VSJA GPP was generally proven to have high accuracy and stability for
574 spatial analysis and could provide a reference for other model products.

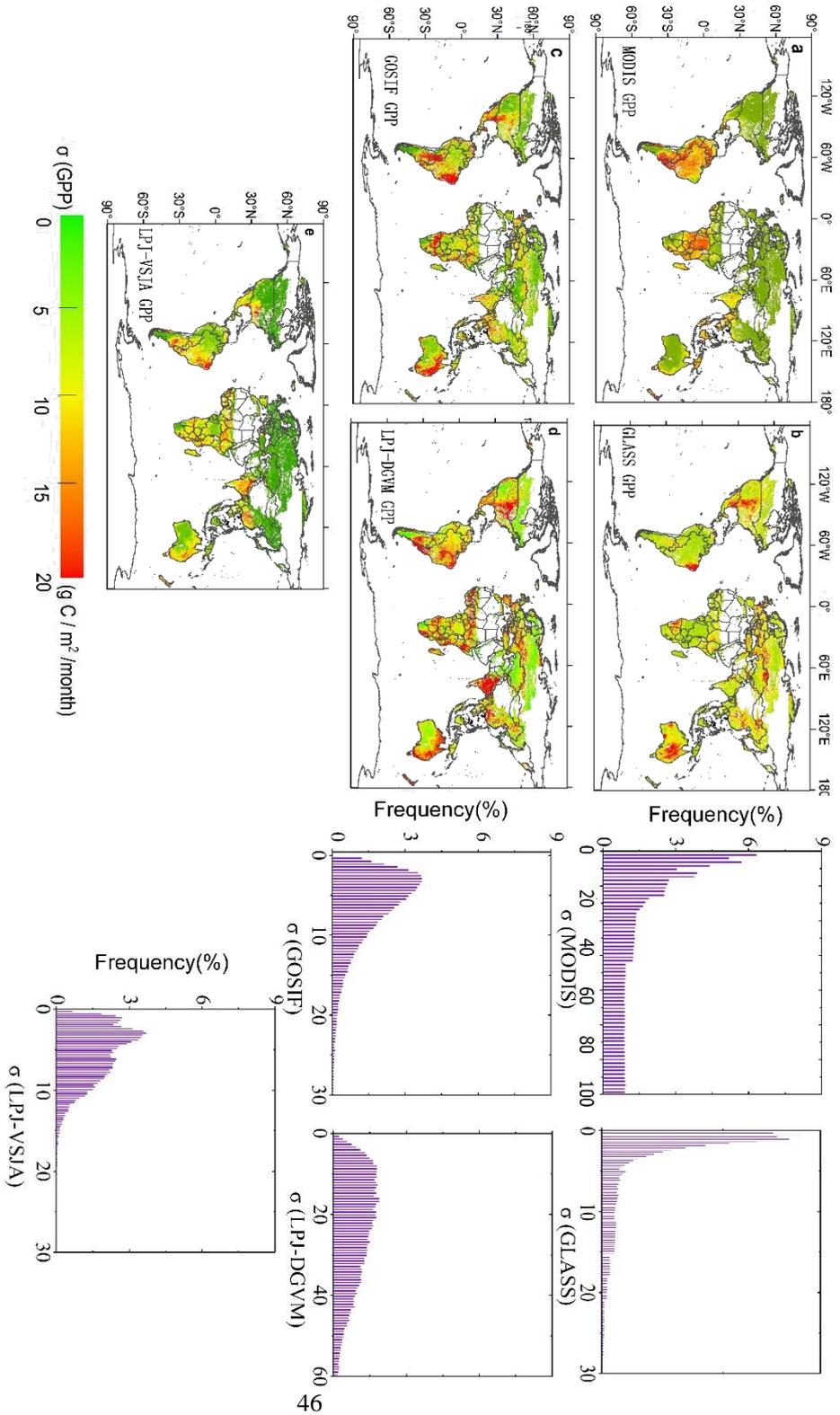
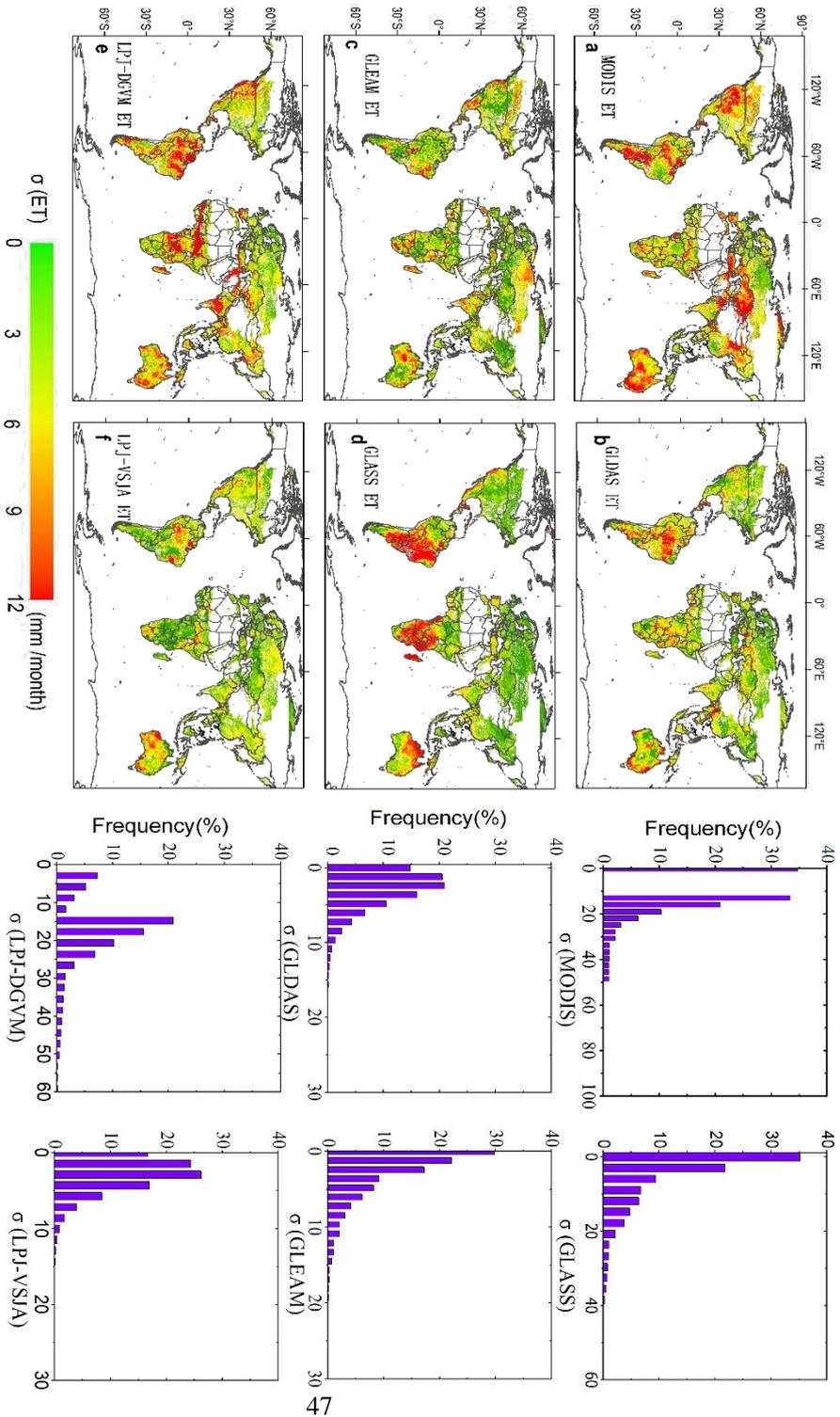


Figure 13. Spatial distribution and histograms of error standard deviation (σ) for global GPP products: MODIS (a), GOSIF (b), GLASS (c), LPJ-DGVM (d), and LPJ-VSJA (e).





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



588 **5. Discussion**

589 *5.1 Advantage of joint assimilation for GPP and ET*

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

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



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

617 *5.2 Comparison of joint assimilation (LPJ-VSJA) and other models for GPP and ET across regions and*
618 *vegetation types*

619 Global GPP and ET for different products were calculated by multiplying the global mean GPP
620 density flux with the global vegetation area (122.4 million km²) originated from the MODIS land cover
621 product (Friedl et al. 2010). The mean global GPP of the LPJ-VSJA (130.2 Pg C yr⁻¹) was
622 approximately 12% lower than that of PML-V2 (145.8 Pg C yr⁻¹) and 18% higher than that of GLASS
623 and MODIS, respectively (Table S6). The GPP values of LPJ-VSJA and GOSIF were the most similar.
624 The GOSIF GPP was developed from gridded SIF using simple linear relationships between SIF and
625 GPP. Our global LPJ-VSJA GPP estimates were within the currently most plausible 110–150 Pg C/yr
626 range.



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

640 In general, GPP and ET had better assimilation performance in arid and semi-arid regions than in
641 humid and semi-humid regions likely because of the following reasons. First, the incorporation of surface
642 SM is more important for vegetation growth in water-limited areas. The module PT-JPL_{SM} has been
643 proven to have better performance in semi-arid and arid regions (Purdy et al. 2018). Our integrated model
644 LPJ-PM also performed better in semi-arid and arid regions by assimilating SMAP soil moisture (Li et al.
645 2020). Second, the input performance, including SMOS and SMAP SM products, is better in arid and
646 temperate regions than in cold and humid regions (Zhang et al. 2019). Third, the vegetation types in humid



647 regions are more complex and relatively less accurately simulated by the LPJ-DGVM within a single grid
648 cell. For comparison, Zhang et al. (2020) used a data-driven upscaling approach to estimate GPP and ET
649 in global semi-arid regions. This data-driven approach ($R^2 = 0.79$, $\text{RMSD} = 1.13 \text{ g C m}^{-2} \text{ d}^{-1}$) had slightly
650 higher performance in estimating GPP than our LPJ-VSJA ($R^2 = 0.73$ and $\text{RMSD} = 1.14 \text{ g C m}^{-2} \text{ d}^{-1}$); the
651 data-driven method ($R^2 = 0.72$ and $\text{RMSD} = 0.72 \text{ mm d}^{-1}$) had identical performance for estimating ET
652 with our LPJ-VSJA ($R^2 = 0.73$ and $\text{RMSD} = 0.72 \text{ mm d}^{-1}$).

653 Our assimilation performance varied with PFT. The GPP and ET assimilation results of savanna sites
654 performed well in both dry and wet regions, and those of shrubland sites showed the most remarkable
655 improvement for simulations of LPJ-DGVM. The original simulation and assimilation performance of
656 grassland sites in the semi-arid and arid regions were the best for all five PFTs. Consistent with our
657 research, previous studies also showed better GPP or ET simulations for grassland, savannas, and
658 shrublands biomes. For instance, Feng et al. (2015) validated five satellite-based ET algorithms for semi-
659 arid ecosystems and concluded that all the models produced acceptable and relatively better results for
660 most grassland, savanna, and shrubland sites. Yang et al. (2017) demonstrated that the GLEAM ET had a
661 superior performance for the grassland sites. The GOSIF GPP demonstrated better simulation for
662 grassland and woody savannas sites at 8-day time steps with higher R^2 (0.77 and 0.83, respectively) and
663 lower RMSD ($1.48 \text{ g C m}^{-2} \text{ d}^{-1}$ and $1.1 \text{ g C m}^{-2} \text{ d}^{-1}$) (Li and Xiao 2019). In contrast, our LPJ-VSJA GPP
664 showed an R^2 of 0.87 for grassland and 0.75 for savannas and an RMSD of $1.11 \text{ g C m}^{-2} \text{ d}^{-1}$ and 1.1 g C
665 $\text{m}^{-2} \text{ d}^{-1}$, respectively, in semi-arid and arid regions.



666 *5.3 Uncertainty analysis of joint assimilation*

667 Our validation results at both site and regional scales indicated that uncertainty existed in LPJ-VSJA
668 daily GPP and ET estimates. The errors from the tower EC observations, model-driven data, model
669 structure, error of satellite-based observations (e.g., LAI and SM), and the spatial scale mismatch between
670 the ground observed footprint size and satellite-derived footprint size were the vital factors affecting
671 assimilation performance. First, recent studies have revealed errors in the GLASS LAI and SMOS or
672 SMAP SM compared with ground measurements. By computing the RMSD and R^2 of each product, the
673 GLASS LAI accuracy was clearly superior to that of MODIS and Four-Scale Geometric Optical Model
674 based LAI (FSGOM) in forests and GLASS and FSGOM led to in much higher annual GPP and ET
675 estimates compared to MCD15(Liu et al. 2018). The vegetation type (or land cover) misclassification
676 caused 15–50% differences in LAI retrieval (Fang and Liang 2005; Gonsamo and Chen 2011). Yan et al.
677 (2016) calculated a RMSD of 0.18 for the GLASS LAI over a range of HeiHe drainage basin sites and
678 used the error to improve the simulation of LAI and fluxes by assimilating GLASS LAI data. Previous
679 studies reported an improvement in the performance of the SMOS and SMAP products (Lievens et al.
680 2015; Miernecki et al. 2014), which both provide an accuracy of $0.04 \text{ m}^3 \text{ m}^{-3}$ (Zhang et al. 2019). However,
681 the actual observation error of these two products typically depends on the spatial location and time of
682 the year (RMSD varying between 0.035 and $0.056 \text{ m}^3 \text{ m}^{-3}$ for several retrieval configurations) (Brocca et
683 al. 2012). According to Purdy et al. (2018), the ET simulated by PT-JPL_{SM} using the 9 km SM_L3_P_E
684 data showed an inferior agreement ($R^2 = 0.47$) but a relatively low RMSD (0.77 mm d^{-1}), due to the SMAP
685 errors in the grid cell with soil heterogeneity and the climatological differences between model SM



686 forecasts and SMAP SM (Reichle and Koster 2004). We rescaled the ET_{PM} to the probability distribution
687 of the ET_{LPJ} through a cumulative distribution function (CDF) to correct the potential seasonal biases of
688 ET_{PM} before assimilation.

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

702 Third, the problem of mixed pixels and mismatches in the observation footprints may also have an
703 influence on the accuracy of estimated GPP and ET. The 5 km spatial resolution of the GLASS LAI, 9
704 km of SMAP, and 25 km of SMOS products cannot capture the sub-grid-scale condition, especially in



705 grid cells for complex land surfaces or strong soil heterogeneity. To ensure the consistency of the grid-
706 cell representativeness for the LAI and SM, the interpolation result in errors that propagate through the
707 modeling and assimilation, causing the accumulation of output errors (Nijssen and Lettenmaier 2004).
708 Moreover, the shrubland in the LPJ-DGVM was most likely simulated as C4 grassland in the
709 hydrothermal condition of semi-arid and arid regions. In contrast, the shrubland tended to be hybrid
710 vegetation types (grassland mixed with other types of forest vegetation) in the hydrothermal condition of
711 humid and sub-dry humid regions, and the simulated canopy height is closer to the real condition of
712 shrubland. This might also be the reason for the superior performance of ET_{LPJ} and assimilation results
713 of shrubland sites in humid and sub-dry humid regions.

714 **6. Conclusions**

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



724 GPP and ET products have relatively higher accuracy than other products, especially in water-limited
725 regions with lower ET values.

726 **Data availability**

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

734 **Author contributions**

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

740 **Competing interests**



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

743

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747

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