

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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19 **Abstract:**

20 Reliable modeling of carbon and water fluxes is essential for understanding the terrestrial carbon
21 and water cycles and informing policy strategies aimed at constraining carbon emissions and improving
22 water use efficiency. We designed an assimilation framework (LPJ-Vegetation and soil moisture Joint
23 Assimilation, or LPJ-VSJA) to improve gross primary production (GPP) and evapotranspiration (ET)
24 estimates globally. The integrated model, LPJ-PM (LPJ-PT-JPL_{SM} Model) as the underlying model, was
25 coupled from the Lund-Potsdam-Jena Dynamic Global Vegetation Model (LPJ-DGVM version 3.01) and
26 a hydrology module (i.e., the updated Priestley–Taylor Jet Propulsion Laboratory model, PT-JPL_{SM}).
27 Satellite-based soil moisture products derived from the Soil Moisture and Ocean Salinity (SMOS) and
28 Soil Moisture Active and Passive (SMAP) and leaf area index (LAI) from the global Land and Ground
29 satellite (GLASS) product were assimilated into LPJ-PM to improve GPP and ET simulations using a
30 Proper Orthogonal Decomposition-based ensemble four-dimensional variational assimilation method
31 (PODEn4DVar). The joint assimilation framework LPJ-VSJA achieved the best model performance (with
32 an R^2 of 0.91 and 0.81 and an ubRMSD reduced by 40.3% and 29.9% for GPP and ET, respectively,
33 compared with those of LPJ-DGVM at the monthly scale). The GPP and ET resulting from the
34 assimilation demonstrated a better performance in the arid and semi-arid regions (GPP: $R^2=0.73$,
35 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
36 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
37 simulated by LPJ-PM that assimilated SMAP or SMOS had a slight difference, and the SMAP soil
38 moisture data performed better than that of SMOS data. Our global simulation modeled by LPJ-VSJA

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

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

48

49 **1. Introduction**

50 Gross primary production (GPP) and evapotranspiration (ET) are essential components of the carbon
51 and water cycles. Carbon and water fluxes are inherently coupled on multiple spatial and temporal scales
52 (Law et al. 2002; Sun et al. 2019; Waring and Running 2010). Terrestrial biosphere models are the most
53 sophisticated approach for providing a relatively detailed description of such interdependent relationships
54 regarding water and carbon fluxes and understanding the response of terrestrial ecosystems to changes in
55 atmospheric CO₂ and climate (Kaminski et al. 2017). The dynamic global vegetation models (DGVMs)
56 are process-based dynamic terrestrial biosphere models, which can simulate water, carbon, and energy
57 exchange between vegetation and the atmosphere under different conditions accounting for vegetation

58 physiological processes, and are widely used to estimate carbon and water fluxes of terrestrial vegetation.
59 However, there are still large uncertainties in carbon and water flux estimates at regional to global scales.
60 Both diagnostic and prognostic models show substantial differences in the magnitude and spatiotemporal
61 patterns of GPP and ET. For example, the global annual GPP estimates exhibited a large range (130–169
62 Pg C yr⁻¹) among 16 process-based terrestrial biosphere models (Anav et al. 2015). The global ET ranged
63 from 70,000 to 75,000 km³ yr⁻¹, and the uncertainty of regional or global ET estimates was up to 50% of
64 the annual mean ET value, especially in the semi-arid regions (Miralles et al. 2016). These uncertainties
65 mainly arise from the forcing datasets, simplification of mechanisms or imperfect assumptions in
66 processes, and uncertain parameters in the processed models and assimilation methods (Xiao et al. 2019).

67 In the last two decades, remote sensing products have been assimilated into DGVMs to reduce the
68 uncertainty in modeled carbon and water fluxes (MacBean et al. 2016; Scholze et al. (2017); Exbrayat
69 et al. (2019)). Data assimilation (DA) is an effective approach to reduce uncertainties in terrestrial
70 biosphere models by integrating satellite products with models to constrain related parameters or state
71 variables. A DA system contains four main components: a set of observations, an observation operator,
72 an underlying model, and an assimilation method. The assimilation method considers the errors from both
73 models and observations, and reduces model uncertainties by minimizing a cost function. The Ensemble
74 Kalman Filter (EnKF) has been widely applied in land surface process models for parameter optimization,
75 which significantly improve simulations by periodically updating state variables (e.g., LAI and soil
76 moisture) using remote sensing data without altering the model structure (Rahman et al. 2021; Bonan et
77 al. 2020; Xu et al. 2021). Yet, the EnKF relies on the instantaneous observations to update the state

78 variable at the current time, and gives the predicted value at the next time based on the forward integration
79 of the updated state variable. The four-dimensional variational method (4DVar) assimilation method can
80 obtain the dynamic balance of the estimation in the time window when it is applied to the long-series
81 forecast model (Bateni et al. 2014; Xu et al. 2019). In particular, the Proper Orthogonal Decomposition
82 (POD)-based ensemble 4DVAR assimilation method (referred to as PODEn4DVar) (Tian and Feng 2015)
83 requires relatively less computation and can simultaneously assimilate the observations at different time
84 intervals. Meanwhile, it maintains the structural information of the four-dimensional space. This method
85 has a satisfactory performance in land DA for carbon and water variables (Tian et al. 2009; Tian et al.
86 2010) and can better estimate GPP and ET than EnKF (Ma et al. 2017).

87 Multiple sources of remote sensing data streams have been used to constrain models for assimilation.
88 As a critical biophysical parameter of the land, leaf area index (LAI) is closely related to many land
89 processes, such as photosynthesis, respiration, precipitation interception, ET, and surface energy
90 exchange (Fang et al. 2019). LAI has a lot of impact on the simulation of carbon and water fluxes (Liu et
91 al. 2018), and accurate LAI estimates can improve the simulations of the carbon and water fluxes (Bonan
92 et al. 2014;; Mu et al. 2007). He et al. (2021) assimilated land surface temperature and LAI observations
93 into the 4DVar framework and improved ET and GPP estimates. Soil moisture is a major driving factor
94 affecting vegetation production in arid ecosystems, especially, in semi-arid areas (Liu et al. 2020).
95 Introducing surface soil moisture (SSM) into the model can significantly improve GPP and ET simulation,
96 particularly in water-limited areas (He et al. 2017; Li et al. 2020).

97 The advancement of earth observation, machine learning, inversion algorithms, and computer

98 technology has improved the accuracy of global LAI products and boosted model-data fusion studies
99 (Fang et al. 2019; Kganyago et al. 2020; Xiao et al. 2017). The Advanced Very High-Resolution
100 Radiometer (AVHRR) generates global LAI products with the longest historic record (since the early
101 1980s). The GLASS LAI product has been verified to have a better accuracy than that of MODIS and
102 CYCLOPES and is more temporally continuous and spatially complete (Xiao et al. 2013). Several recent
103 studies showed that the assimilation of GLASS LAI into DGVMs enhanced the performance of the
104 models in simulating carbon cycling (e.g., GPP, Net Ecosystem Exchange (NEE)) and hydrological (e.g.,
105 ET, SM) processes (Ling et al. 2019; Ma et al. 2017; Yan et al. 2016).

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

118 al. 2019).

119 In the nonlinear model or nonlinear observation operator, only simultaneous assimilation makes
120 optimal use of observations (MacBean et al. 2016). Therefore, a joint assimilation of SM and LAI can
121 make full use of the two variables. From site (Albergel et al. (2010);Rüdiger et al. (2010); Wu et al.,2018)
122 to regional assimilation (Ines et al. (2013)), many studies showed that joint assimilation of vegetation
123 parameters and SM can improve the simulation of the carbon and water cycles. Over small regions and
124 at high spatial resolution, Xie et al. (2018) and Pan et al. (2019) showed that the joint assimilation of SM
125 and LAI improved the accuracy of crop yield estimation using high-resolution satellites products from
126 Sentinel-1 and -2. At a large regional scale, Bonan et al. (2020) assimilated LAI and SSM together into
127 the Interactions between Soil, Biosphere and Atmosphere (ISBA) land model and improved the modeled
128 GPP, ET, and runoff in the Mediterranean region. Rahman et al. (2022) jointly assimilates GLASS LAI
129 and SMAP soil moisture to improve water and carbon flux simulations within the Noah-MP model over
130 the Continental United States domain. Albergel et al.(2020) jointly assimilates the ASCAT soil moisture
131 index (SMI) and LAI GEOV1 into ISBA through the Global Offline Land Data assimilation system
132 LDAS-Monde to monitor extreme events such as drought and Heatwave events. In conclusion, Kalman
133 Filter and its variant methods are mostly used to implement joint assimilation methods at regional scale,
134 which requires many kinds of observation data and their accuracy directly affects the assimilation
135 performance.

136 This study stems from the researches discussed above and further explored the potential of jointly
137 assimilating satellite LAI and soil moisture products globally. Specifically, it was the first time that an

138 updated LPJ-DGVM model was used to jointly assimilate GLASS LAI and SMAP soil moisture for
139 simulating global water and carbon fluxes. The latest global soil moisture datasets (SMOS and SMAP)
140 were used, and the assimilation performance of these two observations was analyzed. Since previous work
141 showed the importance of surface soil moisture in the semi-arid and arid areas, one of the specific
142 objectives of our study is to compare the assimilation effect in the humid and arid areas and improve the
143 understanding of the effect of surface soil moisture on vegetation activity in wet and dry zones. In addition,
144 compared with the assimilation methods in previous studies (mostly using Kalman Filter variants), the
145 POD-En4DVar method is used, which greatly improves the computational efficiency.

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

147 *2.1. Coupled- model (LPJ-PM) for assimilation*

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

155 **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 corresponding to the coupling of 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-PM	GPP _{LAI} , ET _{LAI} ; GPP _{SM} , ET _{SM} ; GPP _{joint} ; ET _{joint}

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157 2.1.1 LPJ-DGVM

158 The LPJ-DGVM is a process-oriented dynamic model, which considers mutual interaction of carbon
159 and water cycling and is designed to simulate vegetation distribution and carbon, soil and atmosphere

160 fluxes (Sitch et al. 2003). For each plant functional type (PFT), the GPP is calculated by implementing
161 coupled photosynthesis and water balance

162 The canopy GPP is updated daily:

$$163 \quad GPP = \frac{(J_E + J_C - \sqrt{(J_E + J_C)^2 - 4\theta J_E J_C})}{2\theta} \quad (2.1)$$

164 where J_C is the Rubisco limiting rate of photosynthesis, J_E is the light limiting rate of photosynthesis, and
165 the empirical parameter θ represents the common limiting effect between the two terms. J_E is related to
166 APAR (absorbed photosynthetic radiation, product of FPAR and PAR), while J_C is related to V_{Cmax}
167 (canopy maximum carboxylation capacity, $\mu \text{ mol CO}_2/\text{m}^2/\text{s}$):

$$168 \quad J_E = C_1 APAR \quad (2.2)$$

$$169 \quad J_C = C_2 V_{Cmax} \quad (2.3)$$

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

173 In the water cycle module, ET is calculated as the minimum of a plant- and soil-limited supply
174 function (E_{supply}) and the atmospheric demand (E_{demand}) (Haxeltine and Prentice 1996; Sitch et al.
175 2003). The soil structure is simplified to a “two-layer bucket” model (the top soil layer at a 0-50 cm depth
176 and the bottom layer at a 50-100 cm depth).

$$177 \quad E_S = E_p \times W_{r20} \times (1 - f_v) \quad (2.4)$$

178 In this module, it is assumed that the soil layer above 20 cm produces water through evaporation,
 179 and W_{r20} is the relative water content of the soil above 20 cm, which is used as the only soil water limit
 180 for calculating vegetation transpiration and soil evaporation. In the evapotranspiration estimation, the
 181 over-simplification of soil structure and soil water limitation lead to a large error (Sitch et al. 2003), while
 182 LPJ-DGVM cannot directly assimilate surface soil water due to the limitation of soil layer stratification
 183 , and therefore, the satellite-derived SSM cannot be assimilated into LPJ-DGVM directly. The
 184 oversimplified soil structure and single soil moisture limitation inevitably lead to sizeable uncertainty in
 185 ET simulation. Additionally, the monthly input caused a daily variation of the modeled SM, which was
 186 also not transmitted to the calculation of GPP and ET. Thus, the updated PT-JPL model (hereafter referred
 187 to as PT-JPL_{SM}) was coupled with LPJ-DGVM and the model structure was modified so that SSM can be
 188 directly assimilated into the coupled model at the daily time step.

189 2.1.2 PT-JPL_{SM}

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

193 Vegetation transpiration:

$$194 \quad C_{RSM} = (1 - RH^{4(1-VWC)(1-RH)})C_{SM} + (RH^{4(1-VWC)(1-RH)})C_{TRSM} \quad (2.5)$$

195

$$C_{TRSM} = 1 - \left(\frac{W_{CR} - W_{obs}}{W_{CR} - W_{pwp_CH}} \right) \sqrt{CH} \quad , \quad (2.6)$$

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where w_{obs} is the SMAP SSM, w_{pwp} is the water content at the wilting point, and VWC is volumetric water content. W_{CR} is a crucial parameter in characterizing the extent of SM restriction on ET; w_{pwp_CH} is the canopy height (CH) adjusted surface soil moisture wilting point 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).

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Soil evaporation:

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

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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.

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The SMAP SSM 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).

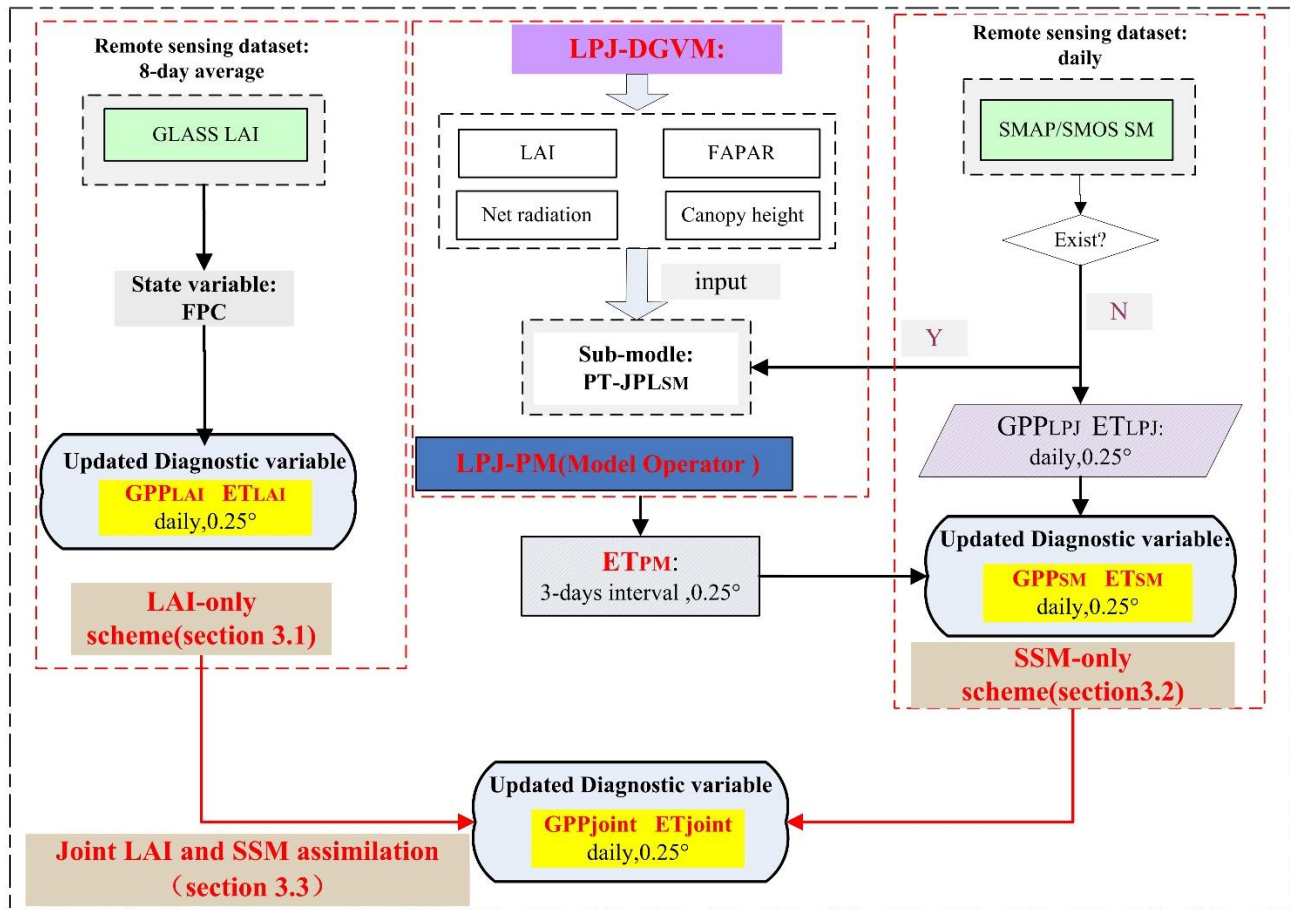
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2.2. Assimilation scheme and experiment procedure

212 To improve the prediction capability of LPJ-PM, we designed three assimilation schemes:
213 assimilating LAI only (LAI-only, **output: ET_{LAI} , GPP_{LAI}**), assimilating SSM only (SSM-only, **output:**
214 **GPP_{SSM} , ET_{SSM}**), and joint assimilation of LAI and SSM (Joint LAI and SSM assimilation, **output: ET_{joint} ,**
215 **GPP_{joint}**), i.e., LPJ-VSJA framework) to test the assimilation performance for simulating GPP and ET.

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

LPJ-VSJA assimilation system



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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:

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

229 Step 2: implement three assimilation schemes respectively, and the results represent the assimilation
230 integration state (daily GPP and ET assimilation results are referred to as the “GPP_{LAI}” and “ET_{LAI}” in
231 LAI-only scheme; “GPP_{SSM}” and “ET_{SSM}” in SSM-only scheme and “GPP_{joint}” and “ET_{joint}” in Joint LAI
232 and SSM assimilation scheme. This scenario used the same input data and model parameter scheme with
233 the “Control run” scenario.

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

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

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

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

247 2.2.1 LAI-only assimilation scheme

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

$$256 \quad FPC = 1 - e^{-0.5LAI} \quad (2.1)$$

257 We set the model and observation errors at a given time as 20% and 10% (scale factor) of the LAI
258 value and the observed LAI value, respectively. By verifying the assimilation performance (R^2 , RMSD,
259 BIAS) for different scale factors(f) of model simulation and observations in the range of 0.05 to 0.40,
260 taking a step size of 0.05 (a total of 64 combinations), the optimal scale factors (0.2 and 0.1) were
261 determined (Bonan et al., 2020).The model and observation errors was the LAI value multiplied by f . The
262 model integration generation method described by Pipunic et al. (2008) was used to determine the

263 minimum number of ensemble members required to achieve maximum efficiency, and the number of sets
264 was 20.

265 2.2.2 SSM-only assimilation scheme

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

278 All assimilation simulations were conducted between January 2010 and December 2018. Between
279 January 2010 and April 2015, SMOS data were used for assimilation; and after May 2015, both SMOS
280 and SMAP data were used for assimilation. An assimilation scheme was conducted when RH and SMOS

281 or SMAP SSM data existed simultaneously; otherwise, the original simulation of the LPJ-DGVM was
282 conducted directly without adjustment of assimilation.

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

288 2.2.3 Joint LAI and SSM assimilation scheme

289 In this scheme, both LAI from GLASS and SSM from SMOS or SMAP were the observation datasets.
290 The GLASS LAI was assimilated to obtain the FPC_{DA} and ET_{LAI} , and then the FPC_{DA} served as input to
291 LPJ-PM to simulate optimized ET_{PM} , and the ET_{joint} was generated using ET_{LAI} and ET_{PM} . Then, the SM
292 (referred to as SM_{CO} in Figure S1) updated by ET_{joint} and the FPC_{DA} were used as input to correct GPP
293 (ET_{joint}).

294 Here, we applied the error regulation in the LAI-only scheme and maintained the error setting of the
295 LAI observation and model simulation. Considering the transmission of integrated model error, we
296 recalculated the model error of LPJ-PM after the LAI assimilation and set model and observation errors
297 of ET_{LAI} and ET_{PM} to be 15 and 10%, respectively.

298 2.3. POD-Based Ensemble 4D Variational Assimilation Method

299 The Proper Orthogonal Decomposition (POD)-based ensemble four-dimensional variational (4DVar)
300 assimilation method (referred to as PODEn4DVar) ([Tian and Feng 2015](#)) has the advantage of avoiding
301 the calculation of adjoint patterns as its incremental analysis field, which can be represented linearly by
302 the POD base (Transformed OP (Observing Perturbation) and MP (Model Perturbation)). Moreover, the
303 PODEn4DVar can simultaneously assimilate multiple-time observation data and provide flow-dependent
304 (the flow-dependent is the ensembles of forecasting statistical characteristics in the t time) error estimates
305 of the background errors. It has shown advantages in terrestrial assimilation, Tan-Tracker system (a
306 Chinese carbon cycle data-assimilation system; in Chinese, “Tan” means carbon), and Radar assimilation
307 (Tian et al. 2010; Tian et al. 2009; Tian et al. 2014; Zhang and Weng 2015).

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

310
$$J(\mathbf{x}') = \frac{1}{2}(\mathbf{x}')\mathbf{B}^{-1}(\mathbf{x}') + \frac{1}{2}[\mathbf{y}'(\mathbf{x}') - \mathbf{y}'_{obs}]^T \mathbf{R}^{-1}[\mathbf{y}'(\mathbf{x}') - \mathbf{y}'_{obs}]$$

311 Here, the $\mathbf{x}' = \mathbf{x} - \mathbf{x}_b$, $\mathbf{y}'(\mathbf{x}') = \mathbf{y}(\mathbf{x}' + \mathbf{x}_b) - \mathbf{y}(\mathbf{x}_b)$, $\mathbf{y}'_{obs} = \mathbf{y}_{obs} - \mathbf{y}(\mathbf{x}_b)$, $\mathbf{y} = H[M_{t_o \rightarrow t_k}(\mathbf{x})]$.
312 $\mathbf{x}'(\mathbf{x}'_1, \mathbf{x}'_2, \dots, \mathbf{x}'_N)$ is the model perturbation (MP) matrix and $\mathbf{y}'(\mathbf{y}'_1, \mathbf{y}'_2, \dots, \mathbf{y}'_N)$ is the
313 observation perturbation (OP) matrix with N samples. Following Rüdiger et al. (2010), the LAI
314 perturbation was set to a fraction (0.001) of the LAI itself. The perturbation of ET_{PM} and ET_{LPJ} conforms
315 to a Gaussian distribution with a mean of 0 and a specified covariance (10 and 5% of the ET_{PM} and ET_{LPJ}

316 at time t). The subscript b represents the background field, the superscript T represents a transpose, H is
 317 the observation operator of the LAI-only assimilation scheme as described in section 2.2.1, and the SSM-
 318 only assimilation scheme is the PT-JPL_{SM} (described in 2.1.2). M is the forecast model (LPJ-PM in this
 319 study), B is the background error covariance, R is the observation error covariance, and obs denotes
 320 observation.

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

325 The manifestation of the background error covariance is the same as the Ensemble Kalman filter
 326 (EnKF, Evensen (2004)), and the incremental analysis x'_a was expressed by the $\Phi_{x,n}$, and $\tilde{\Phi}_y$ ($\tilde{\Phi}_y =$
 327 $[(n-1)I_{n \times n} + \Phi_{y,n}^T R^{-1} \Phi_{y,n}]^{-1} \Phi_{y,n}^T R^{-1}$). Finally, the optimal analysis x_a is calculated as $x_a = x_b +$
 328 $\Phi_{x,n} \tilde{\Phi}_y y'_{obs}$. The detailed derivation process of the algorithm is described by a previous study (Tian et
 329 al. 2011).

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

335

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

336

where d_h and d_v are the horizontal and vertical distances between the spatial positions of state and

337

observed variables, respectively; and $d_{h,0}$ and $d_{v,0}$ are the horizontal and vertical covariance localization

338

Schur radii, respectively. The filtering function C_0 is expressed as:

339

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

340

where r is the radius of the filter.

341

The assimilation algorithm is mainly divided into two steps: (1) prediction: run LPJ-PM in the

342

current assimilation window and generate simulation results and background field vectors; (2) update: the

343

algorithm is used to calculate the optimal assimilation increment x'_a and analysis solution x_a , and the

344

simulation results and the initial conditions of the model in the current window are updated using the

345

analysis solution. The updated initial conditions were applied for model LPJ-PM prediction, and the above

346

process was repeated.

347

2.4. Validation method for assimilation performance

348

The R^2 (coefficient of determination), BIAS, and ubRMSD (unbiased root mean square deviation)

349

between simulation and tower-based observations were applied for evaluation. In addition, a Taylor chart

350

was also used to demonstrate the performance of two ET estimations with different SSM observations in

351 terms of R, ubRMSD, and Normalized Standard Deviation (NSD) on 2D plots, to display how closely the
352 datasets matched observations in one diagram (Taylor 2001). In the Taylor diagram, NSD represents the
353 radial distance from the origin point and the correlation with the site observations as an angle in the polar
354 plot. The ubRMSD is the distance between the observation and the model and is represented in the Taylor
355 chart as a green semi-circular arc with point A as the center of the circle. The closer the model point to
356 the reference point (Point A), the better the performance. This diagram is convenient and visual in
357 evaluating multiple aspects of various models.

358 The error variance of GPP and ET products was estimated using the triple collocation (TC) approach
359 (Stoffelen 1998) to validate the global simulation in this study. The method has been extensively applied
360 in the study of hydrology and oceanography (Caires and Sterl 2003; Khan et al. 2018; O'Carroll et al.
361 2008; Stoffelen 1998), particularly in SM studies (Chan et al. 2016; Kim et al. 2018). The TC provides a
362 reliable platform for comparison of spatial assimilation results and in-situ measurements. In this
363 experiment, no calculation was performed on the non-vegetated areas where the correlation was lower
364 than 0.2 to have independent datasets and avoid correlated errors (crucial assumptions in TC) (Yilmaz
365 and Crow 2014).

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

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

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

377 **3. Experiment sites and data**

378 *3.1. Description of flux tower sites*

379 We screened over 300 EC flux sites across the globe from the FLUXNET2015
380 (<https://fluxnet.fluxdata.org/data/fluxnet2015-dataset/>), AmeriFlux (<http://public.ornl.gov/ameriflux>),
381 and the HeiHe river basin (Liu et al. (2018), <http://www.heihedata.org>) for the evaluation of assimilation
382 performance over the period from January 2010 to December 2018. The in-situ half-hourly LE and GPP
383 data from the sites were aggregated into daily data. The daily gap-filled data were excluded if the
384 percentage of gap-filled half-hourly values was more than 20%. Then we corrected the data of energy
385 non-closure by using the Bowen ratio closure method (Twine et al. 2000) to improve the energy closure
386 rate (Huang et al. 2015; Yang et al. 2020). The data were selected to cover the 2010–2018 period with at
387 least one year of reliable data, and the result from the error of assimilation is relative to the LE value and
388 seasonal variation (Purdy et al. 2018; Zou et al. 2017). It is essential to have available data every month
389 during a one-year period, and only days with less than 25% missing data were processed per month (Feng

390 et al. 2015). In addition, for flux tower data, the data were also excluded for the analysis if the
391 SMAP/SMOS SSM data were not of good quality.

392 Finally, we identified a total of 105 sites across the globe encompassing five major biomes: grassland
393 (18 for GPP and 19 for ET), savanna (11), shrubland (4), forest (49 and 53), and cropland (13 and 14). In
394 the comparative analysis of the performance for simulating ET by assimilating SMOS and SMAP SSM
395 data separately, we selected 46 AmeriFlux sites (Figure S3) with at least one year of reliable data from
396 2015 to 2018 based on the simultaneous availability of SMAP and SMOS data, including grassland (19),
397 savanna (11), shrubland (5), forest (23), and cropland (7). Figure S2 and S3 illustrate the location and
398 distribution of the 105 and 46 EC flux tower sites, respectively. A more detailed description is
399 summarized in the Supporting Information Table S1.

400 *3.2. Remote sensing datasets: LAI and SSM*

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

407 The SMAP mission (Entekhabi et al. 2010) and SMOS mission (Jacquette et al. 2010), the two
408 dedicated soil moisture satellites currently in orbit equipped with L-band microwave instruments, provide

409 SSM retrievals. We chose the SMOS-L2 product and the SMAP-L3-Enhanced product, which both
410 provide global coverage every three days for soil depth of 5 cm. Only good-quality SMAP and SMOS
411 data were used. The grid cells with water areas larger than 10% and those with less than 50% good-quality
412 data in one year were masked out, which alleviates the undesirable model simulations caused by the
413 decrease in SMAP retrieval accuracy (Chan et al. 2016; O'Neill et al. 2010). We only adopted the data
414 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
415 LSM observation layer (the second layer) was higher than $2 \text{ }^\circ\text{C}$ (Blyverket et al. 2019).

416 The GLASS LAI, SMOS and SMAP observations were resampled to 9 km for site simulation and
417 0.25° for regional simulation. The 8- day average of GLASS LAI were assimilated for each day, and the
418 SMAP or SMOS SSM was assimilated every 3 days.

419 *3.3. Model-forcing and validation datasets*

420 In this study, the meteorological, soil property, and CO_2 concentration datasets were used to drive
421 the LPJ-PM. The climate-driven datasets used for the initialization of the LPJ-DGVM are the atmospheric
422 CO_2 concentrations (1901-2018) of ice-core measurements and atmospheric observations at the Mauna
423 Loa Observatory and CRU TS4.03 version Climate data from 1901 to 1930 provided by the Climatic
424 Research Unit (CRU) of the Climate Laboratory, University of East Anglia, UK, including monthly
425 precipitation, surface temperature, cloud cover and wet day. In the simulation period of 2010-2018, the
426 Modern Era Retrospective-Analysis for Research and Applications Version 2 (MERRA-2) was adopted,
427 and the variables used included precipitation, temperature, cloud cover and relative humidity. Soil

428 properties (including limited water content of vegetation at wilting points, field capacity and Soil porosity)
 429 from Harmonized World Soil Database (HWSD) V1.2 dataset (Wieder et al. 2014) were selected as inputs
 430 to the PT-JPLSM model. Table 2 provides the spatial and temporal characteristics of the model-forcing
 431 datasets in the LPJ-PM (submodule: LPJ-DGVM and PT-JPL_{SM}).

432 The GLASS LAI product, SMOS-L2 product and the SMAP-L3-Enhanced product were assimilated
 433 to simulate GPP and ET. For site simulation, in order to maintain consistency with the SMAP Enhanced
 434 3 Level product (Entekhabi et al. 2010), model-forcing data were resampled to a 9 km spatial resolution
 435 based on EASE-2 projection grid. In the global spatial simulation, the model-forcing datasets were
 436 resampled to 0.25° based on the bilinear method to ensure the consistency of spatial representation.

437

438 **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, precipitation, wet day	1901- 1930	0.5° × 0.5°	New et al. (2000), https://crudat.a.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://scrippsc.o2.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/pod/)
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/u/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)

^a: forcing dataset for LPJ-DGVM

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

446

447 **4. Results**

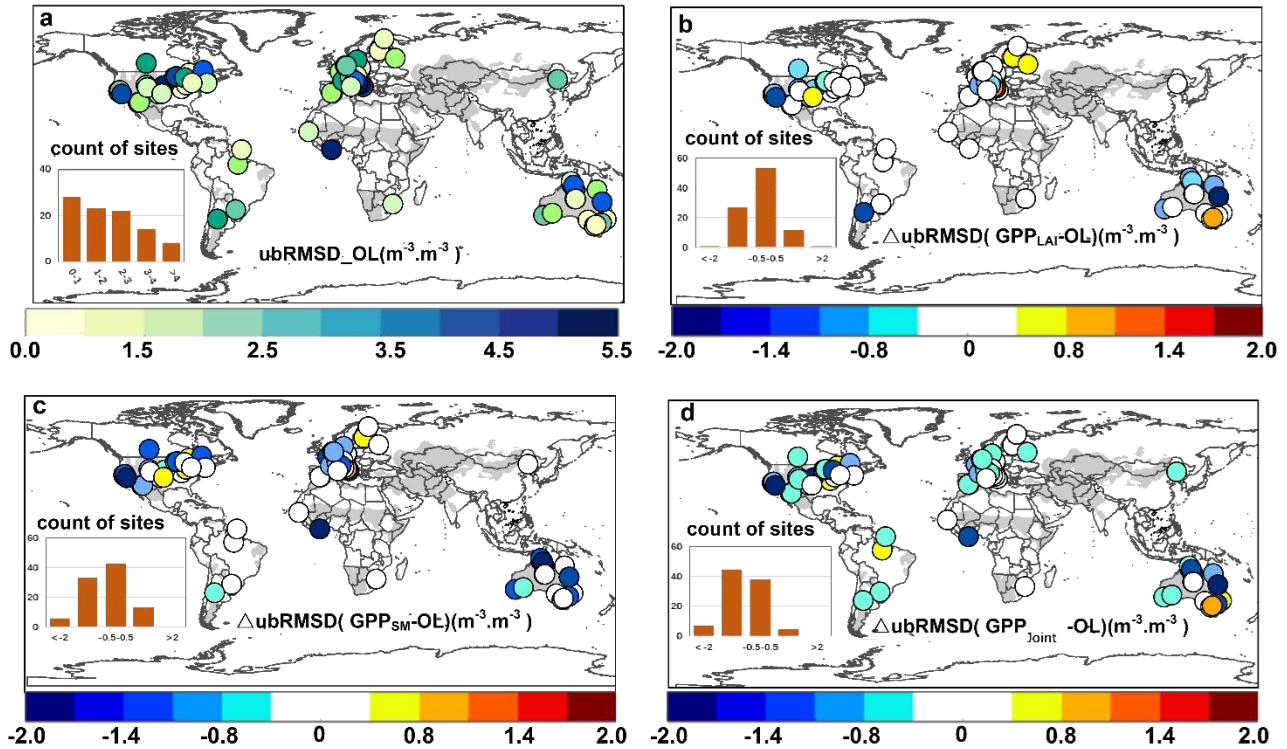
448 *4.1. Performance of LPJ-PM for simulating GPP and ET with the assimilation of LAI and soil moisture*

449 4.1.1 Accuracy assessment of GPP for separate and joint assimilation

450 In general, the R^2 between GPP_{LPJ} and GPP_{OBS} was above 0.4 at most of the sites (62 sites) and
451 were relatively weak for some sites. The LAI assimilation improved the simulations at most sites (R^2
452 value increased at 82 sites), particularly for sites in the U.S. and Europe (Figure S4). The R^2
453 improvement from the LAI assimilation (LAI-only assimilation) was superior to that from the SSM
454 assimilation (Figure S4- (b) and (c)). The performance of the joint assimilation was similar to that of
455 LAI-only assimilation. Sites (Figure S5 (a)) showed positive BIAS ($GPP_{OBS}-GPP_{LPJ}$) were mainly
456 distributed in the humid and sub-dry humid forest, grassland, and arid cropland regions, showing an
457 underestimation for GPP_{OBS} . The assimilation improved the accuracy for overestimated sites, but there
458 was no significant improvement for underestimated sites. The ubRMSD implied that the SSM
459 assimilation alone had a better performance than the LAI assimilation alone, especially for sites in arid
460 areas(Figure 2). The analysis of the above three statistical measures (R^2 , BIAS, and ubRMSD) indicated
461 that the accuracy of joint assimilation was much better than that of separate assimilation.

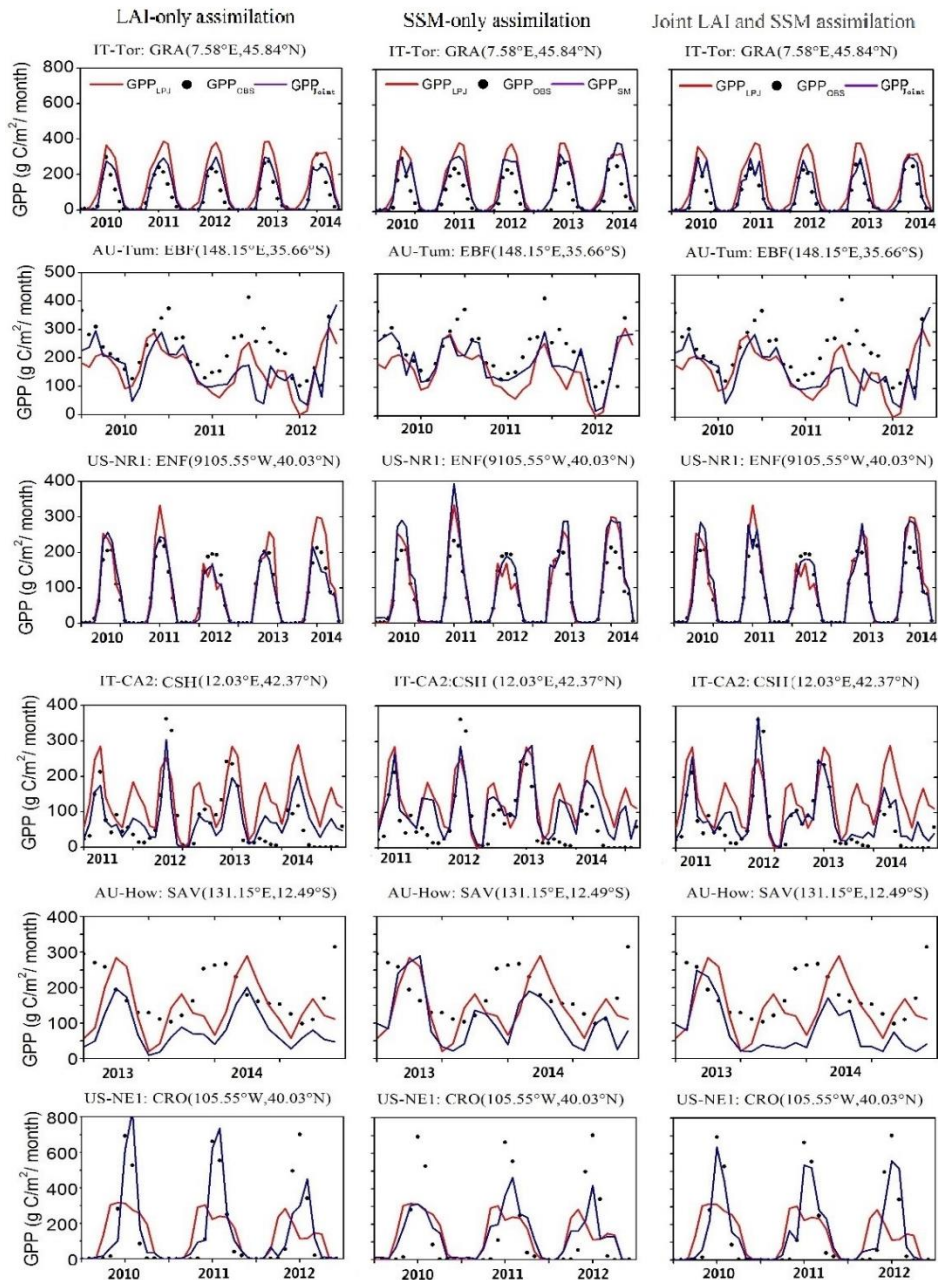
462 At the seasonal scale, all three assimilation schemes corrected the model trajectory and
463 significantly improved the growing season simulations, especially for peak values (IT-Tor, US-NR1,

464 US-NE1) (Figure 3). In addition, the linear fitting of GPP_{joint} and GPP_{OBS} on a monthly scale was closer
 465 to 1:1 ($y=0.92x+21.66$, $p<0.001$) than that of GPP_{LAI} ($y=0.89x+28.3$, $p<0.001$) and GPP_{SM} ($y=$
 466 $0.86x+41.70$, $p<0.001$) (Figure S9). The results in Table S2 support the above analysis, and the joint
 467 assimilation showed advantages in overall accuracy in both arid and humid areas.



468

Figure 2 (a)The Unbiased Root Mean Square Error (ubRMSD) between the GPP_{LPJ} and the site observations, the yellow/blue indicating low/high $ubRMSD_z$; (b) $\Delta ubRMSD(GPP_{\text{LAI}}-GPP_{\text{LPJ}})$; (c) $\Delta ubRMSD(GPP_{\text{SM}}-GPP_{\text{LPJ}})$; (d) $\Delta ubRMSD(GPP_{\text{Joint}}-GPP_{\text{LPJ}})$, blue/red represent positive/negative values.



469

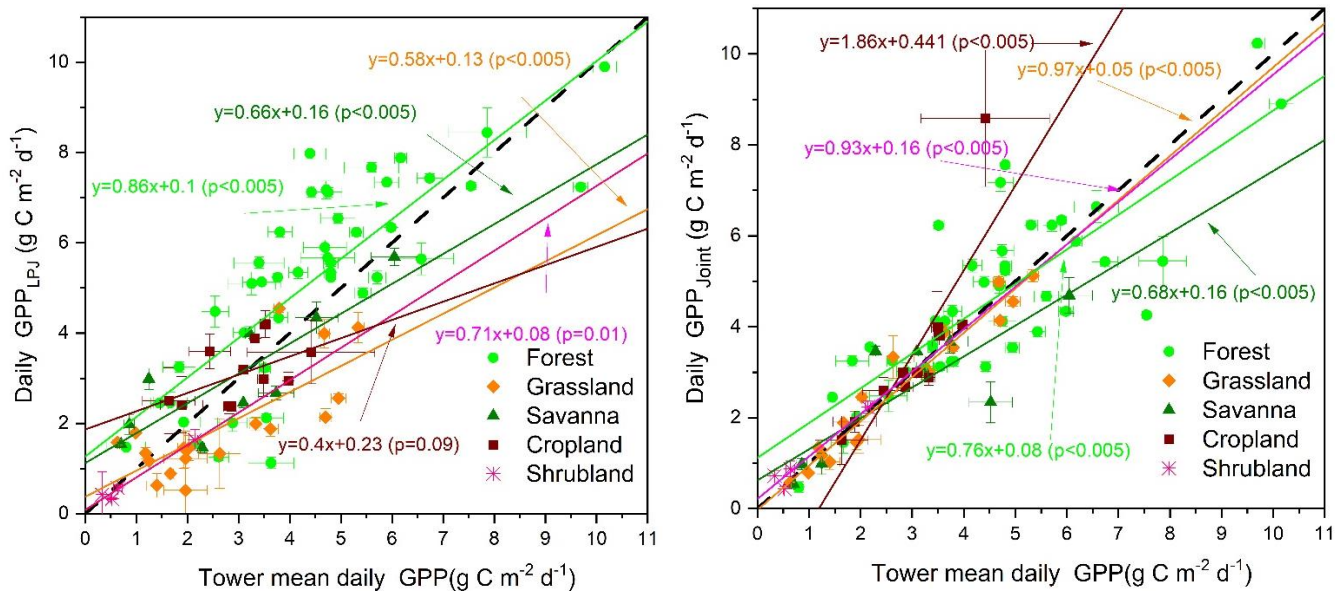
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471

472

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

473 The residual analysis indicated that the three assimilation schemes for GPP (Figure S11 (left)) were
 474 different. For the assimilation results, most of the errors were distributed around $-70 \sim 60 \text{ g C m}^{-2} \text{ month}^{-1}$
 475 1 . The high GPP_{OBS} values were considerably underestimated. The maximum negative error reached 100
 476 $\text{g C m}^{-2} \text{ month}^{-1}$. The error distribution of GPP_{SM} was more dispersed than that of GPP_{LAI} and $\text{GPP}_{\text{joint}}$.
 477 Among the residuals of these three schemes, GPP_{SM} significantly overestimated the GPP_{OBS} , mainly
 478 distributed in the $0\text{--}200 \text{ g C m}^{-2} \text{ month}^{-1}$ range. GPP_{LAI} showed significant improvement in the
 479 overestimation of GPP_{OBS} compared with $\text{GPP}_{\text{joint}}$. In general, the $\text{GPP}_{\text{joint}}$ with the most concentrated
 480 error distribution had significant improvement.



481

482 **Figure 4. Scatterplots of daily GPP_{LPJ} (left) and $\text{GPP}_{\text{joint}}$ (right) versus tower GPP for different PFTs.**

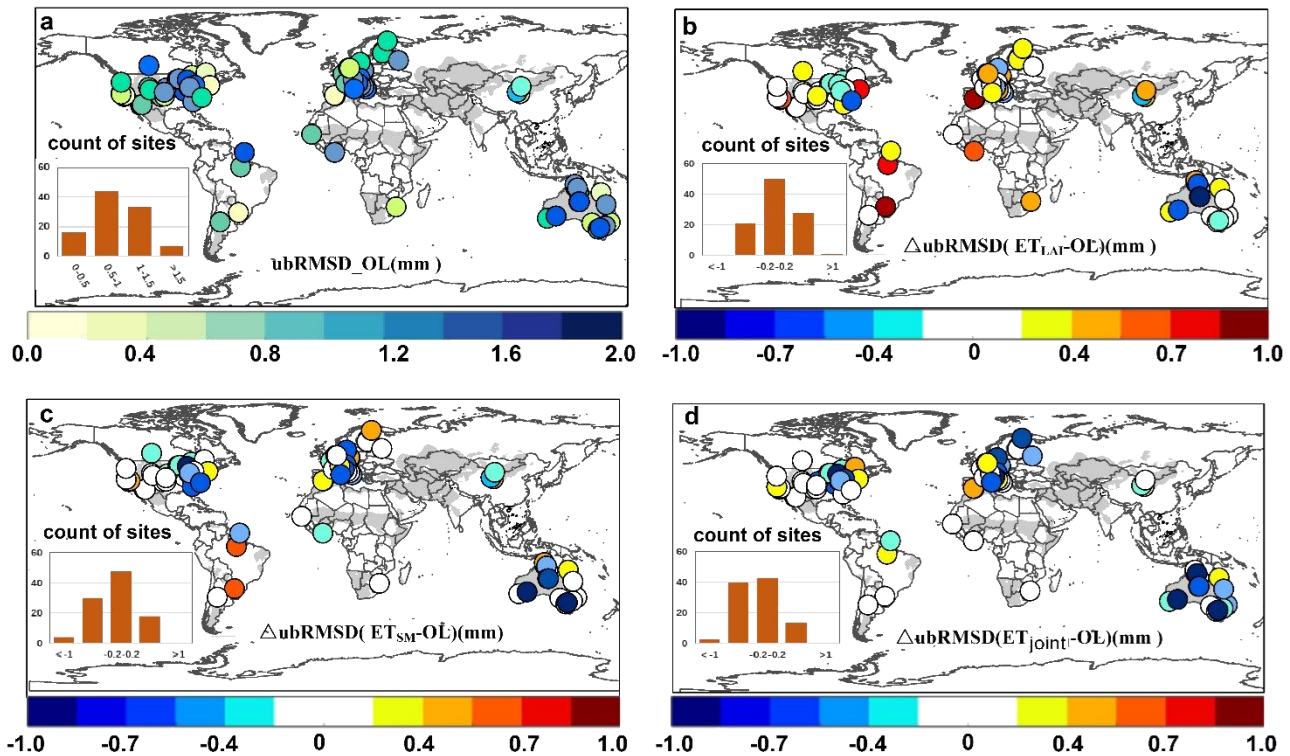
483 After determining the optimal assimilation scheme (Joint LAI and SSM assimilation scheme), we

484 evaluated the GPP_{LPJ} and GPP_{joint} at the site level (Figure.4). The results showed that GPP_{joint} performed
485 better ($R^2= 0.83$, $ubRMSD= 1.15 \text{ g C m}^{-2} \text{ d}^{-1}$) than GPP_{LPJ} ($R^2= 0.69$, $ubRMSD= 1.91 \text{ g C m}^{-2} \text{ d}^{-1}$). The
486 noticeable underestimation in all PFTs and overestimation at most forest sites for GPP_{LPJ} were corrected
487 by joint assimilation (GPP_{joint}). Our joint assimilation methods had better performance in forests,
488 shrublands, and grasslands than in croplands and savannas. Except for the cropland, the linear fitting
489 results of other types were all below the 1:1 line, showing the overall underestimation. Superior
490 performance in both original simulation and assimilation occurred at shrubland ($R^2= 0.93$, $ubRMSD=$
491 $0.89 \text{ g C m}^{-2} \text{ d}^{-1}$) and grassland ($R^2= 0.97$, $ubRMSD= 0.83 \text{ g C m}^{-2} \text{ d}^{-1}$) sites. However, the standard
492 deviation of GPP_{joint} and GPP_{OBS} at savanna sites was relatively large, and the GPP_{joint} at several savanna
493 sites was significantly underestimated.

494 4.1.2 Accuracy assessment of ET for separate and joint assimilation

495 In general, the coefficient of determination (R^2) between ET_{LPJ} and ET_{OBS} was generally over 0.4
496 (the simulations were superior to GPP_{LPJ}) (Figure S6). ET_{LAI} showed slightly higher R^2 , while some
497 sites showed reduced values (41 sites). The ET_{SM} and ET_{joint} were significantly improved compared
498 with the ET_{LAI} . The R^2 increased considerably in Australia but declined at some sites in the United
499 States after assimilation. For $ubRMSD$, ET_{joint} performed better than ET_{SM} and ET_{LAI} . The SSM
500 assimilation improved more in humid regions, while the $ubRMSD$ of ET_{SM} was slightly higher in South
501 America (Figure 5). In the original LPJ-DGVM simulation, the sites with a negative BIAS were mostly

502 located in the humid and sub-dry humid regions, while most of the sites in arid and semi-arid regions
 503 had underestimation (Figure. S7- (a), Table S3). The assimilation improved ET at some of the
 504 overestimated sites, but the underestimation over these sites showed little improvement.



505

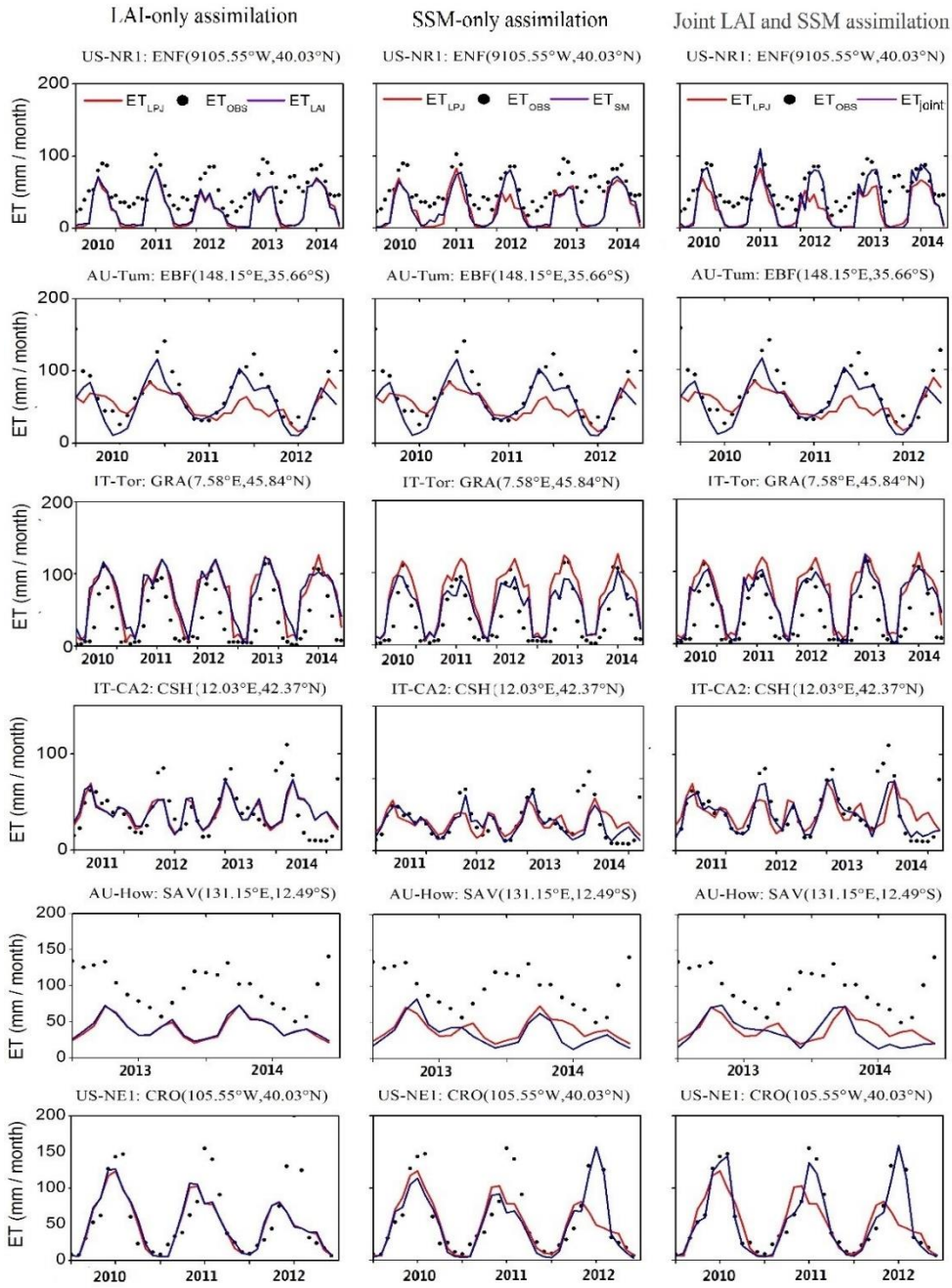
Figure 5 (a) The Unbiased Root Mean Square Error (ubRMSE) between the ET simulated by the LPJ-DGVM and the site observations, with yellow/blue indicating low/high ubRMSD; (b) $\Delta\text{ubRMSD} (ET_{\text{LAI}} - ET_{\text{LPJ}})$; (c) $\Delta\text{ubRMSD} (ET_{\text{SM}} - ET_{\text{LPJ}})$; (d) $\Delta\text{ubRMSD} (ET_{\text{Joint}} - ET_{\text{LPJ}})$, blue/red represent positive/negative value.

507 At the seasonal scale, the model simulations were able to capture the temporal trend of ET_{OBS} , and
508 joint assimilation significantly improved the simulation in the growing season (US-NR1, US-NE1);
509 overall underestimation was observed for ET_{OBS} , especially in winter (Figure 6). Overall, the linear fitting
510 of monthly ET_{joint} and ET_{OBS} was closer to 1:1 than that of ET_{LAI} and ET_{SM} (Figure S10). The simulation
511 accuracy of joint assimilation was better than that of separate assimilation, and the performance of the
512 SSM assimilation was better than that of the LAI assimilation.

513 The ET residual analysis (Figure S11 (right)) indicated that the three assimilation scheme errors
514 showed underestimation for ET_{OBS} . In general, the error distribution of separate assimilations was more
515 dispersed than that of the joint assimilation. Similar to the assimilation performance of GPP, ET_{joint} and
516 ET_{SM} significantly improved the overestimation of ET_{OBS} , but did not significantly improve the
517 underestimation. For the ET_{joint} , most of the errors were distributed around -30–18 mm month⁻¹. The
518 region with high ET_{OBS} was considerably underestimated, and the maximum negative error reached -57
519 mm month⁻¹.

520 We also evaluated the ET assimilation results at the PFT scale (Figure 7). The results showed that
521 our ET values resulting from the assimilation performed better at the site level ($R^2= 0.77$, ubRMSD= 0.65
522 mm d⁻¹) than that of ET_{LPJ} ($R^2= 0.67$, ubRMSD=0.95 mm d⁻¹). Joint assimilation significantly reduced
523 the errors of those shrubland sites with overestimation for ET_{OBS} , and the site distribution was closer to
524 the 1:1 line. Our assimilation methods had better performance in forest, savanna, and grassland
525 ecosystems than in cropland and shrubland (Table S3). The linear fitting results of grassland and
526 shrubland were all above the 1:1 line, showing overall overestimation. Although the original simulation

527 and assimilation performance were superior at savanna sites ($R^2= 0.95$, ubRMSD= 0.78 mm d^{-1}), the
528 standard deviations of ET_{joint} and ET_{OBS} at savanna sites were relatively large, which was similar to the
529 GPP results at savanna sites.

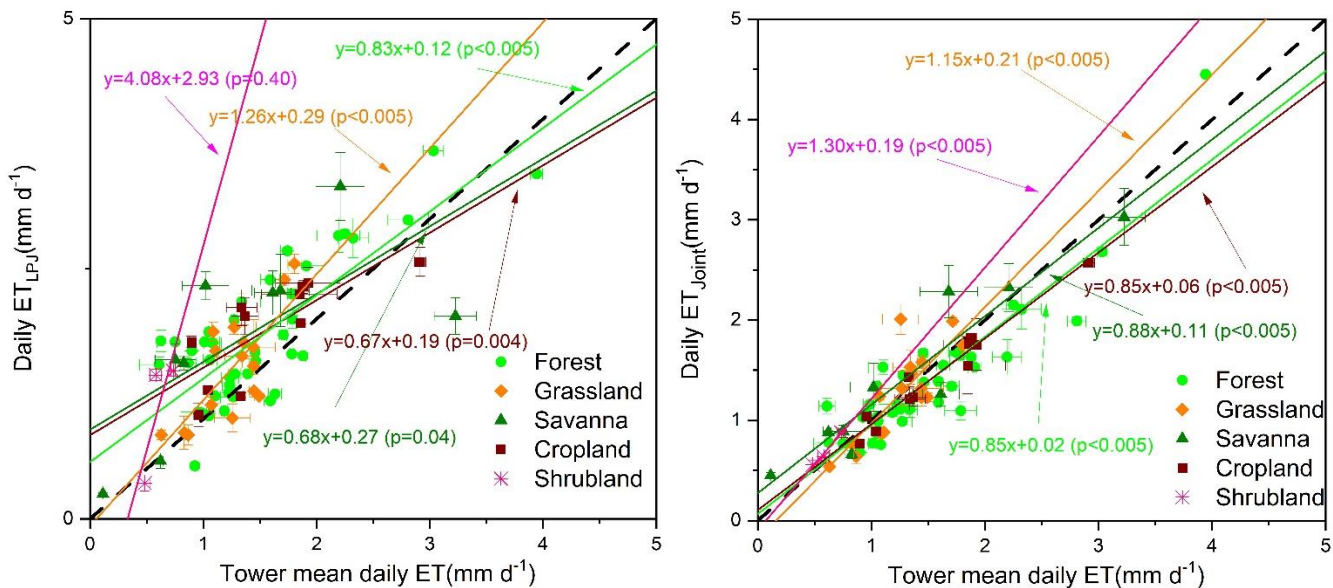


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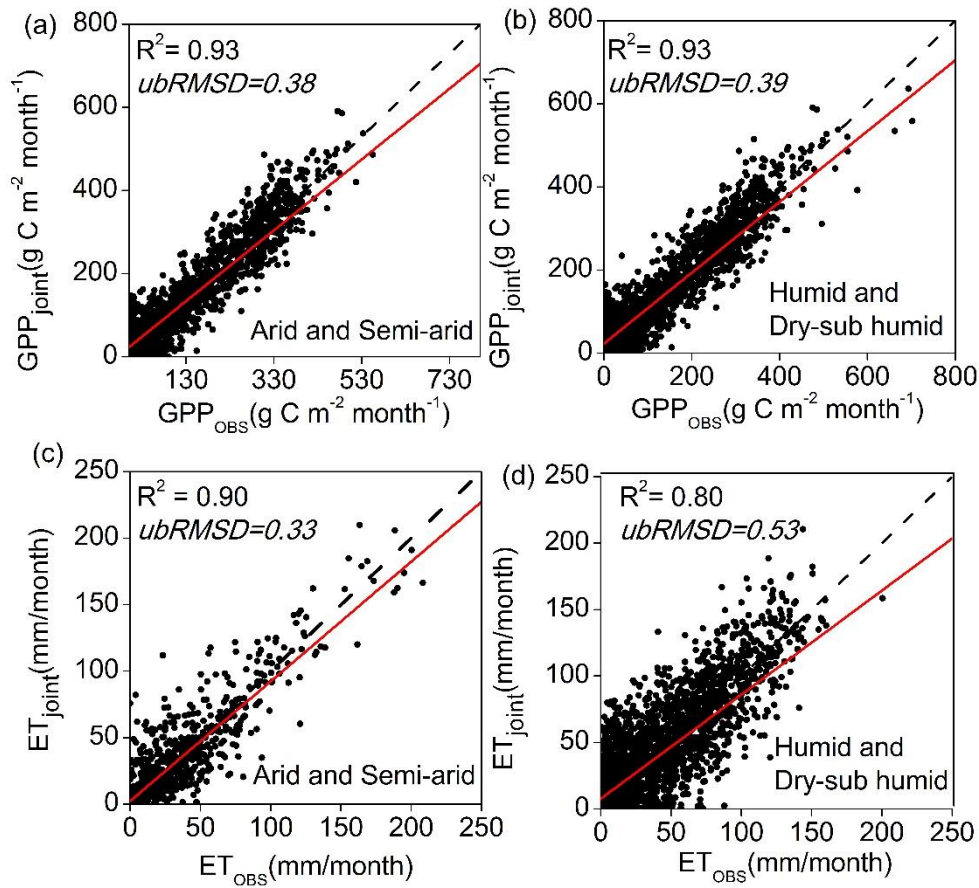
Figure 6. Seasonal cycles of tower-based and simulated ET from Lund-Potsdam-Jena (LPJ), LAI-only

532 assimilation, SSM-only assimilation and joint assimilation for the six sites representing six PFTs during the
533 study period.



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

536 4.2. Comparison of assimilation performance in semi-arid and arid regions with that in humid and sub-
537 dry humid regions



538

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

542

543

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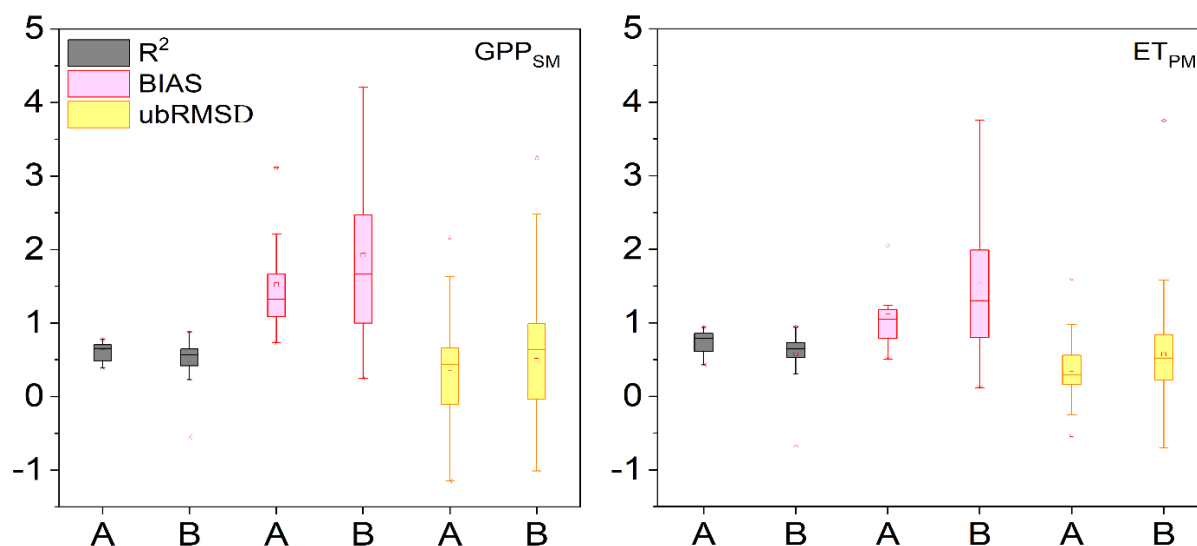
During the period 2010–2014, monthly GPP_{joint} and ET_{joint} performed differently in humid and sub-dry humid regions and semi-arid and arid regions (Figure 8, Table S2,3). Overall, the GPP and ET simulations had good consistency with the tower data in the two regions. For GPP_{joint}, there was no

545 significant difference in the correlation and fitting coefficients between the two regions. As for ET_{joint},
546 the fitting results and R² values in the semi-arid and arid regions performed better than those in the
547 humid and sub-dry humid regions, which also suggested the importance of SSM for ET estimation in
548 water-limited areas.

549 On the daily scale, the original GPP simulations (GPP_{LPI}) performed better in the semi-arid and
550 arid regions than in the humid and sub-dry humid regions with higher R² and lower ubRMSD (Table S2).
551 the R² and BIAS implied that the LAI assimilation alone had a better performance than the SSM
552 assimilation alone. However, for sites in arid and semi-arid areas, the ubRMSD showed that the GPP_{SM}
553 improved better than GPP_{LAI}, which both demonstrated SSM data are essential in water-limited regions.
554 For GPP_{joint}, the shrubland in the semi-arid and arid regions had the lowest R² values and the second
555 lowest ubRMSD. The forest in the semi-arid and arid regions had the largest improvement after
556 assimilation. In the humid and sub-dry humid regions, the GPP_{joint} of the savanna and cropland showed
557 the largest improvement (R² increased by 64.7% and 71.1%, respectively; ubRMSD decreased by 47.0%
558 and 31.8%, respectively). The grassland in the semi-arid and arid regions had the highest R², and the
559 savanna by combining all indicators had the best assimilation results compared to other types in both
560 regions.

561 Similar to ET_{joint}, the ET_{LPI} in the semi-arid and arid regions was better than that in humid and sub-
562 dry humid regions in terms of four evaluation indicators (ubRMSD decreased by 34.4% in semi-arid and
563 arid regions and the ubRMSD decreased by 30.9% in humid and sub-dry humid regions compared with

564 ET_{LPJ}). The R^2 and ubRMSD implied that the SSM assimilation alone had a better performance than the
 565 LAI assimilation alone, especially for sites in arid areas. and the BIAS showed that the ET_{LAI} improved
 566 better than ET_{SM} for sites in humid and sub-dry humid areas. The performance of the original simulation
 567 and assimilation of grassland sites in the semi-arid and arid regions was the best among all five PFTs.
 568

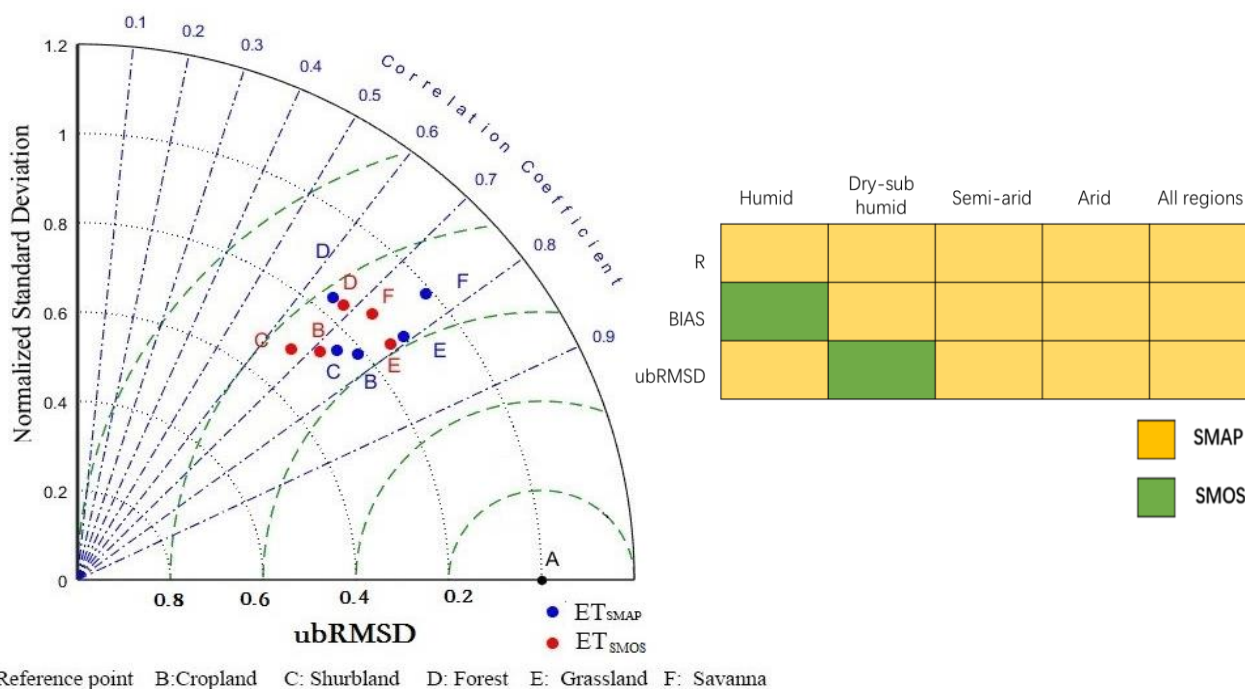


569
 570 **Figure 9. Boxplots of R^2 , ubRMSD and BIAS for GPP_{SM} (left) and ET_{PM} (right). A represents the sites in arid**
 571 **and semi-arid areas, and B represents the sites in humid and dry sub-humid areas.**

572 To investigate the reasons for better assimilation performance in water-limited regions, we evaluated
 573 the GPP and ET simulated by the LPJ-PM according to R^2 , ubRMSD, and BIAS (Figure 9). Compared
 574 with the semi-arid and arid regions, the humid and sub-dry humid region had smaller R^2 mean, larger
 575 BIAS, and no significant difference in mean ubRMSD for GPP_{SM} . In general, the evaluation results of

576 joint assimilation for ET_{PM} were generally consistent with those for GPP_{SM} and GPP_{SM} . ET_{PM} showed
 577 underestimation, which was consistent with the underestimation in SSM assimilation. These results
 578 indicated that, both GPP and ET modeled by LPJ-PM with joint assimilation were less stable and had a
 579 lower performance in the humid and sub-dry regions than in the semi-arid and arid regions.

580 *4.3. Comparison of assimilation performance in assimilating SMOS and SMAP soil moisture data*



581
 582 **Figure 10. Taylor diagram (left) comparing ET simulations with observations at all 46 AmeriFlux sites**
 583 **at the daily time step between April 2015 and December 2018. Blue dots represent results based on**
 584 **assimilation with SMAP SSM only and red dots represent results based on assimilation with SMOS SSM**
 585 **only. ubRMSD refers to the dashed green lines. Reference points A and B-F correspond to the vegetation**
 586 **functional types (PFTs). The grid diagram (right) compares the evaluation indices of ET simulations with**

587 **those of the observed values at all 46 AmeriFlux sites with different wet and dry zones at the daily time step;**
588 **the yellow cells indicate that ET_{SMAP} performs better in the metric, and green cells indicate that ET_{SMOS}**
589 **performs better in the metric.**

590 The Taylor chart was used to compare the assimilation performance of ET_{SMAP} and ET_{SMOS} at 46
591 AmeriFlux sites (Figure 10-left). The results showed that ET_{SMAP} performed better than ET_{SMOS} for most
592 PFTs, except forest. Both ET_{SMAP} and ET_{SMOS} performed well for grassland (closer to point A), and there
593 was little difference between R^2 and ubRMSD. The NSD of ET_{SMAP} in grassland was 0.88, which was
594 closer to 1 than that of ET_{SMOS} . The assimilation of ET in the forest had a lower R^2 and higher ubRMSD
595 (0.7-0.8) than those of other PFTs, and the NSD of cropland and shrubland was lower than that of other
596 PFTs (0.6-0.8), indicating that the assimilation for cropland and shrubland could not reproduce the
597 variations in ET effectively. However, ET_{SMAP} showed significant improvement in R^2 compared with
598 ET_{SMOS} for shrubland and cropland. The assimilation performance of ET_{SMAP} and ET_{SMOS} for savanna
599 showed the greatest difference. In general, the ET_{SMAP} and ET_{SMOS} were slightly different, and the ET_{SMAP}
600 was more improved than ET_{SMOS} .

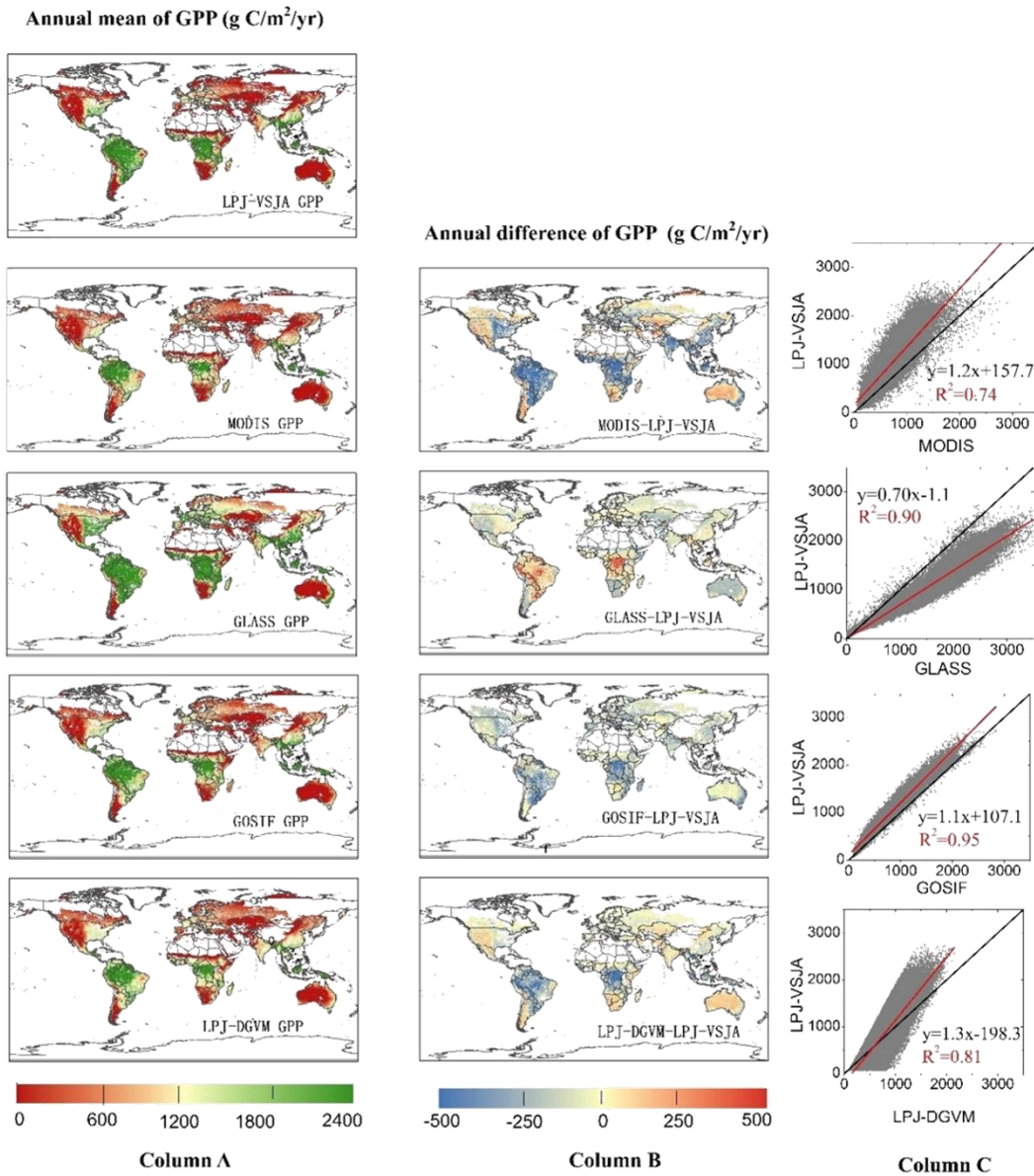
601 Figure 10 (right) shows the assimilation accuracy of ET_{SMOS} and ET_{SMAP} in different humid and arid
602 regions. The ET_{SMAP} had significant advantages for the four indicators. The R^2 of ET_{SMAP} was higher than
603 that of ET_{SMOS} in all the areas. However, ET_{SMOS} in some evaluation indicators showed a better
604 performance than ET_{SMAP} (BIAS in the humid region; ubRMSD in the sub-dry humid region). This may
605 be due to the overall more humid nature of SMOS SSM than the SMAP SSM. Moreover, the sensitivity
606 of deep soil moisture contributed more to the ET in humid areas than in the water-limited areas.

607 *4.4. Global simulations of GPP and ET with joint assimilation of LAI and soil moisture data*

608 To assess the spatial scalability of the LPJ-VSJA assimilation scheme, we simulated the global daily
609 GPP and ET for 2010–2018 with a spatial resolution of 0.25°. The original results simulated by the LPJ-
610 DGVM and LPJ-VSJA were referred to as LPJ-DGVM GPP(ET) and LPJ-VSJA GPP(ET), respectively.
611 We compared the annual spatial GPP and ET values and the error standard deviation of the LPJ-VSJA
612 with several existing flux products.

613 Figures 11 and 12 depict the spatial distribution of the annual mean and the differences between our
614 simulation results and the global independent satellite-based products. The developed LPJ-VSJA GPP
615 was the closest to GOSIF GPP (Li and Xiao 2019) in most regions with the lowest spatial mean deviation
616 (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),
617 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
618 than GOSIF GPP in tropical regions, such as Amazonia, Central Africa, and Southeast Asia. In general,
619 the annual mean and differences between MODIS, GOSIF GPP, LPJ-DGVM, and our LPJ-VSJA were
620 in broad agreement (with higher R^2 ranging from 0.74 to 0.95).

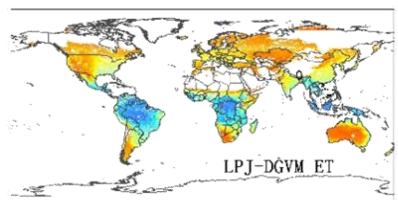
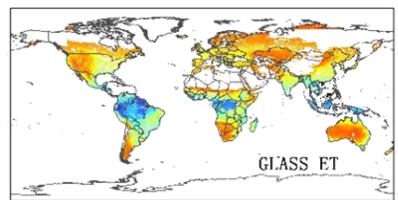
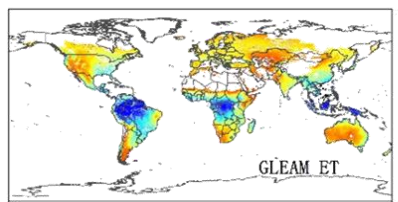
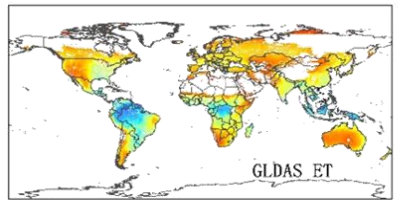
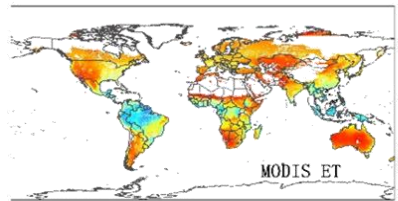
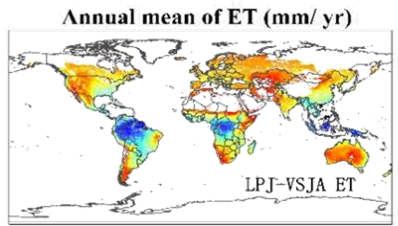
621 LPJ-VSJA ET was the closest to GLEAM ET on the spatial average with the least spatial average
622 deviation (-13.9 mm yr^{-1}) and highest R^2 (0.88), followed by GLASS ET (-23.1 mm yr^{-1} and 0.82), GLDAS
623 ET (-34.7 mm yr^{-1} and 0.73), LPJ-DGVM (-48.7 and 0.66 mm yr^{-1}), and MODIS ET (-122.1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



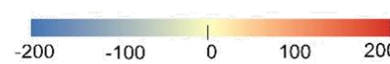
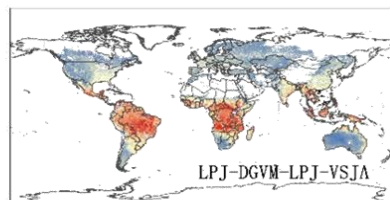
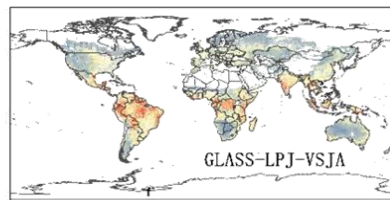
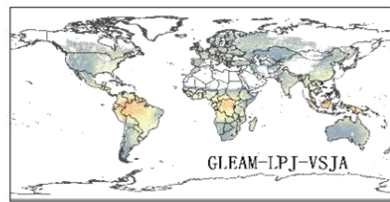
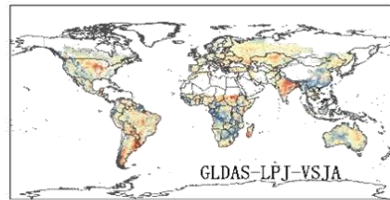
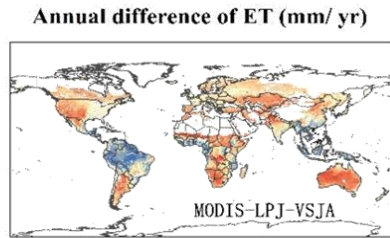
625

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

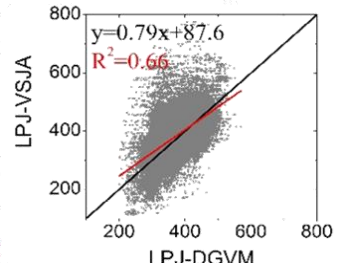
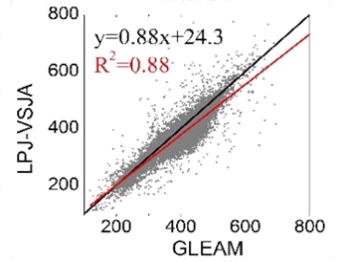
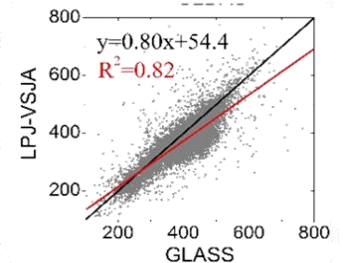
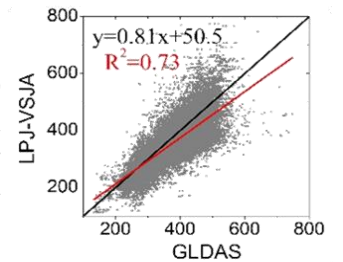
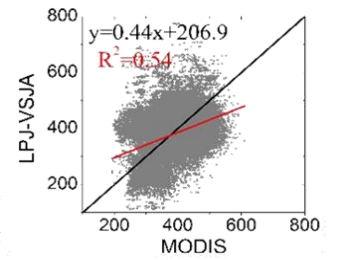
629 **datasets. Column C: Scatter plots between these products. Black lines show the 1:1-line, red lines show the**
630 **regression fit.**



Column A



Column B



Column C

632 **Figure 12. Column A: Spatial distribution of annual LPJ-VSJA ET and other independent satellite-**
633 **based datasets (a: MODIS GPP; b: GLDAS ET; c: GLEAM ET; d: GLASS ET; e: LPJ-DGVM ET).**
634 **Column B: Spatial distribution of the difference between annual LPJ-VSJA ET and other independent**
635 **satellite-based datasets. Column C: Scatter plots between these products are provided on the right of the**
636 **difference maps. Black lines show the 1:1-line, red lines show the regression fit.**
637

638 Figure 13 (a)–(e) represent the spatial error standard deviation (σ) distribution of MODIS, GLASS,
639 GOSIF, and LPJ-VSJA GPP, respectively. The graphs on the right side depict the corresponding
640 histograms. The σ of the MODIS GPP was evenly distributed between 30 and 60 g C m⁻² month⁻¹, while
641 the average σ of other products was concentrated in 0–20 g C m⁻² month⁻¹ (90%). The high errors of all
642 products were concentrated in the high temperature and humid areas of southern North America, eastern
643 South America, humid and dry sub-humid areas of South Asia, and the savannas of Africa and Australia.
644 The error histogram of GOSIF GPP and LPJ-DGVM GPP were in line with the normal distribution, with
645 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
646 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
647 variance of the LPJ-VSJA product was the lowest, indicating a stability of the regional error (Table S4).
648 Compared to the LPJ-DGVM, the joint assimilation results showed improvement in all regions (the
649 average error reduced by 17.7 g C m⁻² month⁻¹), especially in the humid regions of South Asia, Australia,
650 and the United States. Our LPJ-VSJA GPP was generally proven to have high accuracy and stability for
651 spatial analysis and could provide a reference for other model products.

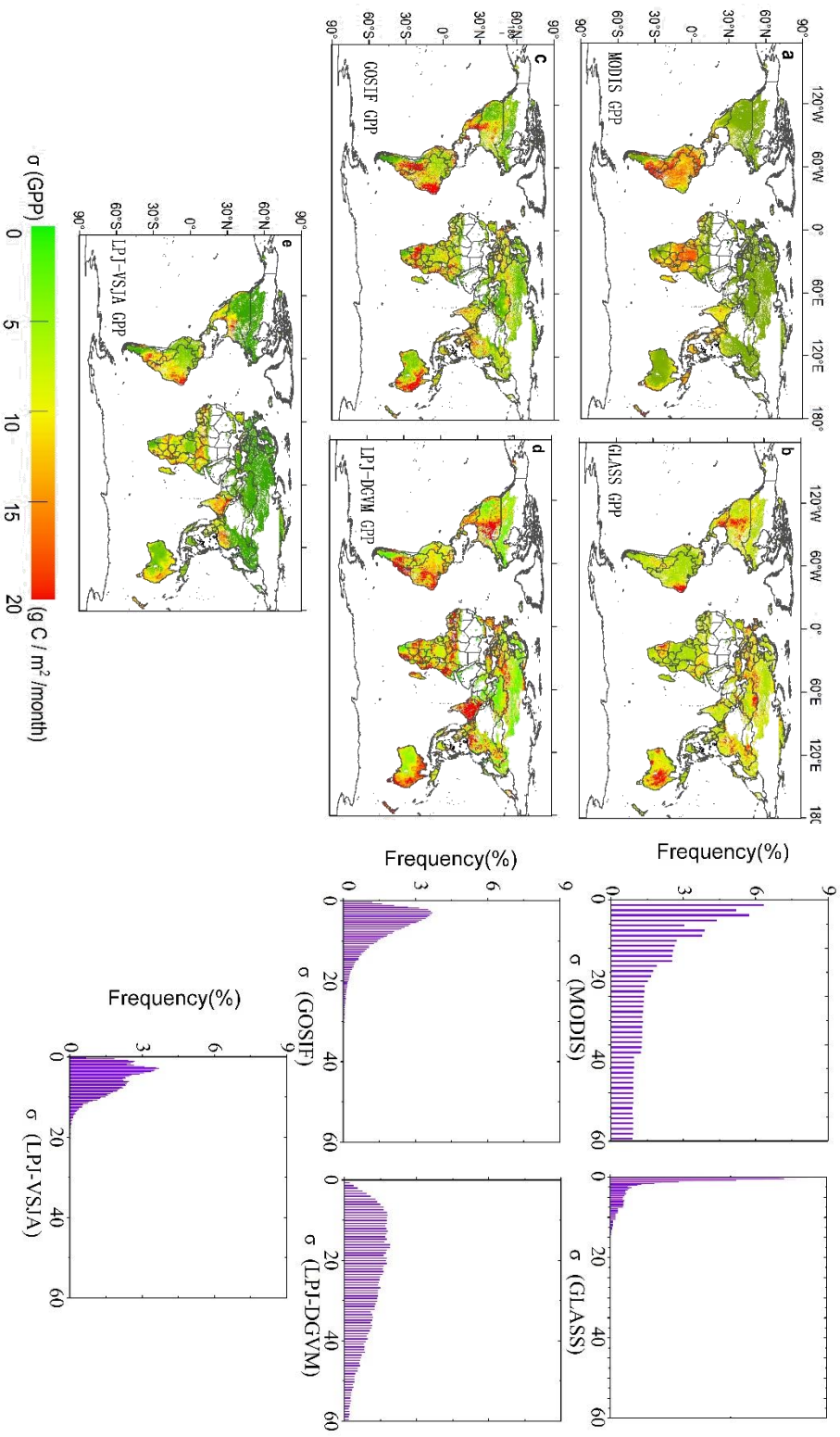


Figure 13. Spatial distribution and histograms of error standard deviation (σ) for global GPP products: MODIS (a), GOSIF (b), GLASS (c), LPJ-DGVM (d), and LPJ-VSJA (e).

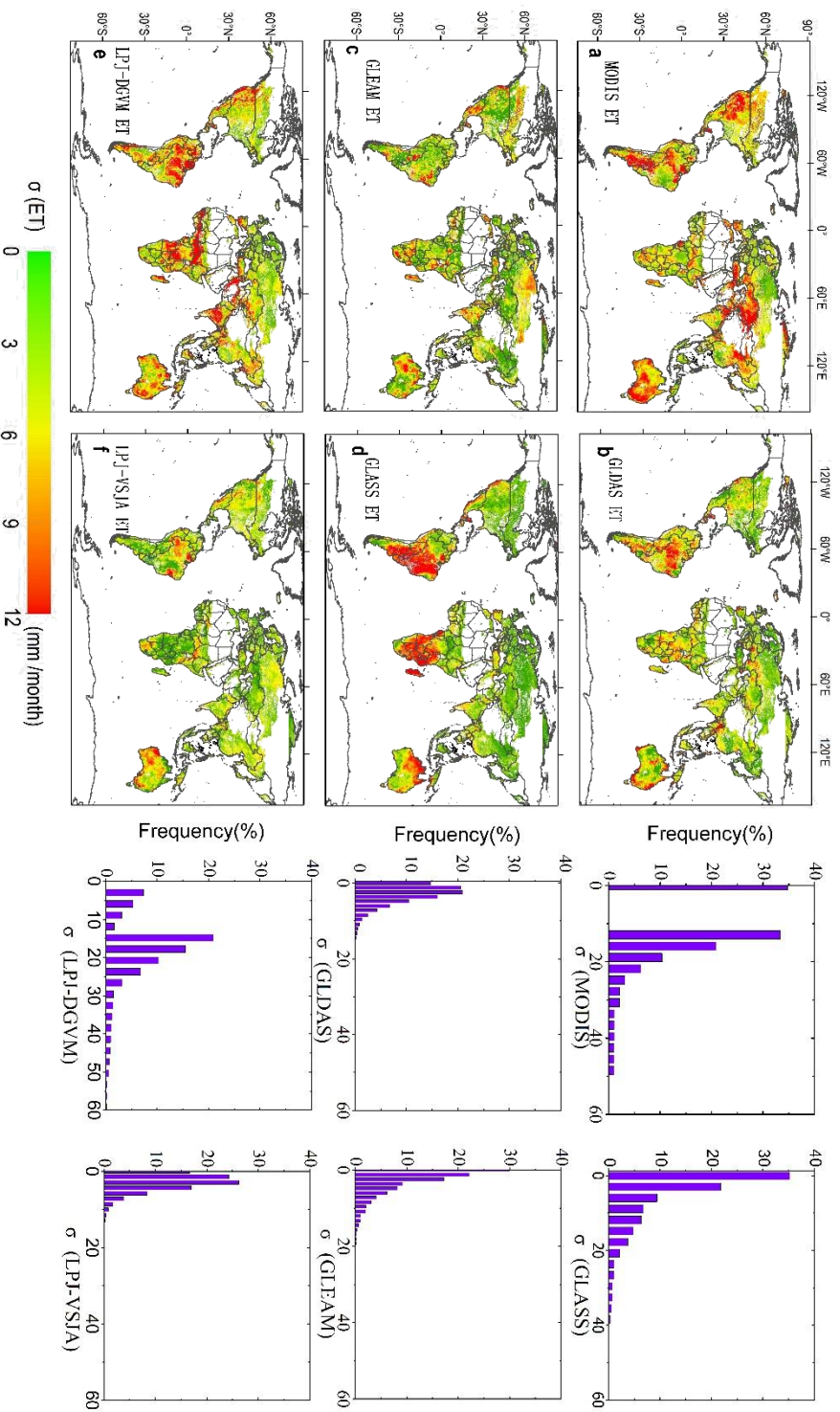


Figure 4. Spatial distribution and histograms of error standard deviation (σ) for global ET products:

MODIS (a),GLDAS (b),GLEAM (c), GLASS (d), LPJ-DGVM (e), and LPJ-VSJA (f).

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

665 **5. Discussion**

666 *5.1 Advantage of joint assimilation for GPP and ET*

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

673 In the GPP assimilation experiment, the performance of the LAI assimilation was better than that of
674 the SSM assimilation possibly for two reasons: (1) the LPJ-VSJA is more controlled by LAI data because
675 the ratio of assimilated LAI (daily input) to SSM observations (3-day interval input) is approximately 3:1,
676 which makes the likelihood function biased to LAI data; (2) the SM directly influences the simulation of
677 ET, and the corresponding time function (computes the top layer SM (50 cm)) used here by Zhao et al.
678 (2013) will result in the error of the updated top SM and propagating the error to the GPP_{SM} . In addition,
679 the 8-day interval LAI has the capability to capture the temporal variability of phenology.

680 Current studies on terrestrial water and carbon flux assimilation mostly focus on the assimilation
681 between a single model framework and observation results, lacking the fusion and comparison between
682 multiple models. The processed models used in DA are simplifications and approximations of reality, and
683 different models focus on different ecological processes. In this study, the updated ET module was

684 integrated to compensate for the simplification of soil stratification and the lack of SM information in the
685 hydrological module of the LPJ-DGVM. Therefore, the integration of multiple types of models and multi-
686 source observation data (remotely sensed data, ecological inventory data (National Ecological
687 Observatory Network, NEON (Keller et al. 2008)), and other measurements (Desai et al. 2011; Hayes et
688 al. 2012) is expected to more objectively and effectively simulate the real state of ecosystems.

689 *5.2 Comparison of joint assimilation (LPJ-VSJA) and other models for GPP and ET across regions and* 690 *vegetation types*

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

699 As for ET, our results were similar to those of GLEAM ET and lower than those of PML-V2,
700 GLDAS-2, and GLASS ET (~72000 km² yr⁻¹). Joint assimilation improved the overestimation of LPJ-
701 DGVM ET. At the daily scale, the estimation accuracy of PML-V2 and GLDAS-2 products, calibrated
702 with flux tower data, was better than that of our estimates, which suggests an underestimation of LPJ-

703 VSJA ET in wet regions. It is likely because the SSM of SMAP or SMOS was underestimated in the wet
704 region or the influence of deep SM was under-represented. According to Seneviratne et al. (2010),
705 satellite-based ET estimation approaches often overestimate ET in areas of arid and semi-arid climatic
706 regimes in the magnitude of 0.50 to 3.00 mm d⁻¹. The poor performance of these models can largely be
707 attributed to the lack of constraints of SSM or RZSM and more accurate vegetation parameters (Gokmen
708 et al. 2012; Pardo et al. 2014). For instance, the monthly estimated ET modeled by the Penman-Monteith-
709 Leuning (PML) model agreed with flux tower data well ($R^2 = 0.77$; BIAS = - 9.7%, approximately 0.2
710 mm d⁻¹). Our annual ET simulations were lower than other products and slightly underestimated tower
711 ET with a BIAS of 0.19 mm d⁻¹ ($ET_{OBS} - ET_{joint}$).

712 In general, GPP and ET had better assimilation performance in arid and semi-arid regions than in
713 humid and sub-dry humid regions likely because of the following reasons. First, the incorporation of SSM
714 is more important for vegetation growth in water-limited areas. The module PT-JPL_{SM} has been proven
715 to have better performance in semi-arid and arid regions (Purdy et al. 2018). Our integrated model LPJ-
716 PM also performed better in semi-arid and arid regions by assimilating SMAP soil moisture (Li et al.
717 2020). Second, the input performance, including SMOS and SMAP SSM products, is better in arid and
718 temperate regions than in cold and humid regions (Zhang et al. 2019). Third, the vegetation types in humid
719 regions are more complex and relatively less accurately simulated by the LPJ-DGVM within a single grid
720 cell. For comparison, Zhang et al. (2020) used a data-driven upscaling approach to estimate GPP and ET
721 in global semi-arid regions. This data-driven approach ($R^2 = 0.79$, RMSD = 1.13 g C m⁻² d⁻¹) had slightly
722 higher performance in estimating GPP than our LPJ-VSJA ($R^2 = 0.73$ and RMSD = 1.14 g C m⁻² d⁻¹) and

723 the data-driven method ($R^2 = 0.72$ and $\text{RMSD} = 0.72\text{mm d}^{-1}$) had identical performance for estimating
724 ET with our LPJ-VSJA ($R^2 = 0.73$ and $\text{RMSD} = 0.72\text{ mm d}^{-1}$).

725 Our assimilation performance varied with PFT. The GPP and ET assimilation results of savanna sites
726 performed well in both dry and wet regions, and those of shrubland sites showed the most remarkable
727 improvement for simulations of LPJ-DGVM. The original simulation and assimilation performance of
728 grassland sites in the semi-arid and arid regions were the best for all five PFTs. Consistent with our
729 research, previous studies also showed better GPP or ET simulations for grassland, savannas, and
730 shrublands biomes. For instance, Feng et al. (2015) validated five satellite-based ET algorithms for semi-
731 arid ecosystems and concluded that all the models produced acceptable and relatively better results for
732 most grassland, savanna, and shrubland sites. Yang et al. (2017) demonstrated that the GLEAM ET had a
733 superior performance for the grassland sites. The GOSIF GPP demonstrated better simulation for
734 grassland and woody savannas sites at 8-day time steps with higher R^2 (0.77 and 0.83, respectively) and
735 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
736 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
737 $\text{m}^{-2}\text{ d}^{-1}$, respectively, in semi-arid and arid regions.

738 *5.3 Uncertainty analysis of joint assimilation*

739 Our validation results at both site and regional scales indicated that uncertainty existed in LPJ-VSJA
740 daily GPP and ET estimates. The errors from the tower EC observations, model-driven data, model
741 structure, error of satellite-based observations (e.g., LAI and SSM), and the spatial scale mismatch

742 between the ground observed footprint size and satellite-derived footprint size were the vital factors
743 affecting assimilation performance.

744 First, recent studies have revealed errors in the GLASS LAI and SMOS or SMAP SSM compared
745 with ground measurements. By computing the RMSD and R^2 of each product, the GLASS LAI accuracy
746 was clearly superior to that of MODIS and Four-Scale Geometric Optical Model based LAI (FSGOM) in
747 forests and GLASS and FSGOM led to in much higher annual GPP and ET estimates compared to
748 MCD15(Liu et al. 2018). The vegetation type (or land cover) misclassification caused 15–50% differences
749 in LAI retrieval (Fang and Liang 2005; Gonsamo and Chen 2011). Yan et al. (2016) calculated a RMSD
750 of 0.18 for the GLASS LAI over a range of HeiHe river basin sites and used the error to improve the
751 simulation of LAI and fluxes by assimilating GLASS LAI data. Previous studies reported an improvement
752 in the performance of the SMOS and SMAP products (Lievens et al. 2015; Miernecki et al. 2014), which
753 both provide an accuracy of $0.04 \text{ m}^3 \text{ m}^{-3}$ (Zhang et al. 2019). However, the actual observation error of
754 these two products typically depends on the spatial location and time of the year (RMSD varying between
755 0.035 and $0.056 \text{ m}^3 \text{ m}^{-3}$ for several retrieval configurations) (Brocca et al. 2012). According to Purdy et
756 al. (2018), the ET simulated by PT-JPL_{SM} using the 9 km SM_L3_P_E data showed an inferior agreement
757 ($R^2= 0.47$) but a relatively low RMSD (0.77 mm d^{-1}), due to the SMAP errors in the grid cell with soil
758 heterogeneity and the climatological differences between model SM forecasts and SMAP SSM (Reichle
759 and Koster 2004). We rescaled the ET_{PM} to the probability distribution of the ET_{LPJ} through a cumulative
760 distribution function (CDF) to correct the potential seasonal biases of ET_{PM} before assimilation.

761 Second, there is large uncertainty in the influence of RZSM as the source of water available to plants
762 (Albergel et al. 2008; Bonan et al. 2020). Our GPP results of irrigated sites were largely influenced by
763 US-Ne1, an irrigate site. This site maintained high annual GPP in 2012 despite the drought (Figure S8).
764 However, the SMOS SSM in 2012 had a lower SSM annual mean than the site observations likely because
765 the detected soil layer (0-50 cm) of the site observation is deeper than that of the satellite retrieval and the
766 cumulative deep soil moisture due to the regular irrigation was higher than the SSM that could easily be
767 vaporized during the drought period (Figure S8). Therefore, the influence of deep SM of some cropland
768 sites during the drought years induced large simulation errors and unsatisfactory assimilation performance.
769 Moreover, some deep-rooted forests maintain a high LAI during drought by absorbing deep SM (>2 m)
770 and groundwater (Zhang et al. 2016). Thus, joint assimilation of the LAI and SSM may eliminate a portion
771 of the underestimation of GPP of such vegetation in drought periods. Therefore, further research is needed
772 on how to optimally utilize satellite SM data for improving GPP and ET simulations.

773 Third, the problem of mixed pixels and mismatches in the observation footprints may also have an
774 influence on the accuracy of estimated GPP and ET. The 5 km spatial resolution of the GLASS LAI ,9
775 km of SMAP, and 25 km of SMOS products cannot capture the sub-grid-scale condition, especially in
776 grid cells for complex land surfaces or strong soil heterogeneity. To ensure the consistency of the grid-
777 cell representativeness for the LAI and SSM, the interpolation result in errors that propagate through the
778 modeling and assimilation, causing the accumulation of output errors (Nijssen and Lettenmaier 2004).
779 Moreover, the shrubland in the LPJ-DGVM was most likely simulated as C4 grassland in the
780 hydrothermal condition of semi-arid and arid regions. In contrast, the shrubland tended to be hybrid

781 vegetation types (grassland mixed with other types of forest vegetation) in the hydrothermal condition of
782 humid and sub-dry humid regions, and the simulated canopy height is closer to the real condition of
783 shrubland. This might also be the reason for the superior performance of ET_{LPJ} and assimilation results
784 of shrubland sites in humid and sub-dry humid regions.

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

801 and propagate to the second step . Alternative solutions were found for water -related parameters through
802 soil moisture, providing a better fit for all data streams. The sequence of assimilation is essential in the
803 step-wise assimilation, and if the first observation contains a strong BIAS, then the associated error
804 correlation will also propagate through the first assimilation. If the autocorrelation in the observation error,
805 or the correlation between the data stream errors is not considered, it is likely that the posterior simulation
806 has been overturned. That is, we overestimate the reduction in parametric uncertainty. If two observational
807 data are less uncertainty (i.e., high precision of observation data), and the model of deviation is smaller
808 (depend on the spatial scale and inversion method). Moreover, the correlation of these observations is
809 stronger, and contain enough spatio-temporal information to limit all the parameters optimization
810 accurately, the step-wise assimilation performance is basically the same as that of simultaneous
811 assimilation.

812 **6. Conclusions**

813 We developed an assimilation system LPJ-VSJA that integrates GLASS LAI, SMOS SSM, and
814 SMAP SSM data to improve GPP and ET estimates globally. The system was designed to assimilate two
815 SSM products (SMOS and SMAP) into the integrated model - LPJ-PM for both dry and humid regions
816 through separate and joint assimilation. The results show that the joint constraints provided by vegetation
817 and soil variable strategies improve model simulations. Both the original and joint assimilation results for
818 GPP and ET in semi-arid and arid regions performed better than those in humid and sub-dry humid regions,
819 and the LPJ-PM that emphasized the SSM information is more suitable for the water-limited regions. For

820 ET assimilation, the different SSM products influence assimilation performance, and SMAP SSM
821 possesses a slight advantage in most vegetation types and in both dry and humid regions. Our global LPJ-
822 VSJA GPP and ET products have relatively higher accuracy than other products, especially in water-
823 limited regions with lower ET values.

824 **Data availability**

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

832 **Author contributions**

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

838 **Competing interests**

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

841

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