

Optimizing Phenology Parameters Drastically Improves Terrestrial Biosphere Model Underestimates of Dryland Net CO₂ Flux Inter-Annual Variability

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November 30, 2022

Abstract

Dryland ecosystems occupy ~40% of the land surface and are thought to dominate the inter-annual variability (IAV) and long-term trend of the global carbon (C) cycle. Therefore, it is imperative that global terrestrial biosphere models (TBMs), which form the land component of IPCC earth system models, are able to accurately simulate dryland vegetation and biogeochemical processes. However, compared to more mesic ecosystems, TBMs have not been widely tested or optimized against in situ dryland ecosystem CO₂ fluxes. Here, we address this gap using a Bayesian data assimilation system and 89 site-years of daily net CO₂ flux (net ecosystem exchange - NEE) data from 12 southwest US Ameriflux sites spanning forest, shrub and grass dryland ecosystems to evaluate and optimize the C cycle related parameters of the ORCHIDEE TBM. We find that the default (prior) model simulations drastically underestimate both the mean annual NEE and the NEE IAV. By testing different assimilation scenarios, we showed that optimizing phenology parameters dramatically improves the model ability across all sites to capture both the magnitude and sign of the NEE IAV. At high elevation forested sites, which are a mean C sink, optimizing parameters related to C allocation, respiration and turnover reduces the underestimate in simulated mean annual NEE. Our study demonstrates that all TBMs need to be calibrated specifically for dryland ecosystems before they are used to determine dryland contributions to global C cycle variability and long-term carbon-climate feedbacks.

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17 **Key Points:**

- 18 • ORCHIDEE terrestrial biosphere model drastically underestimates dryland mean annual
19 net CO₂ fluxes and their inter-annual variability (IAV)
20 • Optimizing phenology, carbon allocation, and respiration parameters are crucial for
21 capturing net CO₂ flux mean and IAV
22 • Models need to be optimized against dryland CO₂ flux data to achieve accurate
23 predictions of dryland's role in global C cycle variability

24 **Abstract**

25 Dryland ecosystems occupy ~40% of the land surface and are thought to dominate the inter-
26 annual variability (IAV) and long-term trend of the global carbon (C) cycle. Therefore, it is
27 imperative that global terrestrial biosphere models (TBMs), which form the land component of
28 IPCC earth system models, are able to accurately simulate dryland vegetation and
29 biogeochemical processes. However, compared to more mesic ecosystems, TBMs have not been
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31 gap using a Bayesian data assimilation system and 89 site-years of daily net CO₂ flux (net
32 ecosystem exchange - NEE) data from 12 southwest US Ameriflux sites spanning forest, shrub
33 and grass dryland ecosystems to evaluate and optimize the C cycle related parameters of the
34 ORCHIDEE TBM. We find that the default (prior) model simulations drastically underestimate
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37 sites to capture both the magnitude and sign of the NEE IAV. At high elevation forested sites,
38 which are a mean C sink, optimizing parameters related to C allocation, respiration and turnover
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40 need to be calibrated specifically for dryland ecosystems before they are used to determine
41 dryland contributions to global C cycle variability and long-term carbon-climate feedbacks.

42 **1 Introduction**

43 Terrestrial ecosystems currently take up ~30% of anthropogenic CO₂ emissions, thus
44 acting as a substantial global carbon (C) sink (Fu et al., 2017) and providing a critical reduction
45 in the rate of global warming. However, while we know the magnitude of the global C sink to a
46 good degree of certainty, our knowledge of other components of the global C cycle are more
47 uncertain. One such knowledge gap is which ecosystems, and/or which processes, are driving
48 inter-annual variability (IAV) in land net C uptake (Fu et al., 2017). Improving our
49 understanding of the IAV characteristics of the global terrestrial C cycle is key to being able to
50 forecast the future of the land C sink and long-term biosphere-climate feedback (Cox et al.,
51 2013).

52 Recent studies have pointed to drylands (arid and semi-arid ecosystems) as the dominant
53 driver of global terrestrial C cycle IAV (Ahlström et al., 2015; Cleverly et al., 2016; Haverd et

54 al., 2017; Poulter et al., 2014). High annual variability in net CO₂ exchange in response to plant-
55 available moisture is observed in site-based flux studies in these regions (Biederman et al., 2017;
56 Cleverly et al., 2016; Haverd et al., 2017; Scott et al., 2015). However, the global terrestrial
57 biosphere models (TBMs) used in the recent C cycle IAV regional attribution studies have often
58 only been extensively evaluated against data in more mesic ecosystems (e.g. (Peng et al., 2015;
59 Piao et al., 2013; Raczka et al., 2013; Schaefer et al., 2012)), although studies have evaluated
60 models against eddy covariance flux data from Australian dryland sites (Haverd et al., 2013a;
61 Whitley et al., 2016a). TBM optimization (parameter calibration) has also only typically been
62 carried out using temperate and boreal site data (Haverd et al., 2013a; Kuppel et al., 2014).
63 Therefore, there remains a relative gap in model benchmarking and optimization using dryland C
64 cycle related data.

65

66 Model benchmarking and optimization studies that have been performed in dryland
67 regions indicate considerable model-data discrepancies in vegetation dynamics, C and water
68 fluxes (Haverd et al., 2013b; MacBean et al., 2015; Renwick et al., 2019; Trudinger et al., 2016;
69 Whitley et al., 2016b; Traore et al., 2014). A recent study by MacBean et al. (submitted) has
70 demonstrated that global TBMs participating in the TRENDY v7 model intercomparison project
71 dramatically underestimate both the mean annual net ecosystem exchange (NEE) and its IAV at
72 a suite of southwestern (SW) US dryland sites due to weak sensitivity of gross primary
73 productivity (GPP) to changing water availability. This analysis is corroborated by (Renwick et
74 al., 2019) who also showed that a semi-deciduous phenology scheme was necessary to accurately
75 predict the magnitude of GPP in dryland shrublands. SW US hydrology modeling studies have
76 also suggested that parameter calibration is needed to realistically represent semi-arid water
77 fluxes because the default parameters diminish model performance (Natasha MacBean et al.,
78 2020; Hogue et al., 2005; Unland et al., 1996). Given the lack of model parameter calibration
79 studies that have included dryland sites in their optimizations, it remains to be seen whether
80 model-data discrepancies in dryland ecosystem NEE simulations are due to inaccurate model
81 processes or uncertain parameters. Parameter uncertainty may be higher for dryland ecosystems
82 given parameter values were initially measured in the field and/or optimized for more mesic
83 temperate and boreal ecosystems.

84 To address the gap in dryland site model parameter optimization, and to determine if
85 parameter optimization can account for dryland model-data discrepancies in NEE, we used a
86 Bayesian data assimilation (DA) framework to optimize the photosynthesis, phenology, C
87 allocation and turnover, and respiration parameters of the ORCHIDEE TBM using 89 site-years
88 of daily NEE observations of 12 Ameriflux sites spanning SW US semi-arid grass, shrub and
89 forest ecosystems. Following (Biederman et al., 2017, MacBean et al, submitted), we categorize
90 sites based on their mean annual NEE: US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses
91 are mostly tree-dominated C sink sites; shrub and grass-dominated sites US-Wkg, US-SRG, US-
92 Seg, US-SRM, and US-Whs “pivot” between a mean annual C sink and source; and the US-Aud
93 grassland is a mean source of C. We used the well-established DA system designed for
94 ORCHIDEE (ORCHIDAS: <https://orchidas.lsce.ipsl.fr>) (Kuppel et al., 2014; MacBean et al.,
95 2018; Peylin et al., 2016), in which a cost function that represents the misfit between the model
96 and the data - taking into account uncertainty in both - is iteratively minimized using the genetic
97 algorithm (GA; see Methods and Data).

98 We performed multiple optimization tests with combinations of parameters related to
99 different model processes in order to identify which processes were most influential in
100 improving the model mean annual NEE and IAV. We focus in particular on which processes are
101 responsible for model failure to capture NEE IAV. We focus on improving NEE IAV partly
102 because of the dominant role dryland ecosystems are thought to play in controlling global C
103 cycle IAV, and partly because we expect that, with the exception of sites that are a strong C sink,
104 eddy covariance estimates of mean annual NEE may be impacted by uncertainties in CO₂ flux
105 partitioning. We identified three main groups of parameters: parameters related to 1) phenology;
106 2) parameters related to photosynthesis; and 3) parameters related to all process calculations that
107 occur after gross C uptake (i.e. C allocation, autotrophic and heterotrophic respiration and
108 biomass and soil C turnover; hereafter grouped as “post C uptake” parameters). We split the
109 parameters into these three groups because GPP has been shown to be the dominant control on
110 dryland NEE IAV (MacBean et al., submitted); therefore, we expect that optimizing parameters
111 related to one of both of these main two processes controlling GPP (i.e., phenology and
112 photosynthesis) will result in the strongest improvements in NEE IAV. However, optimizing all
113 parameters related to processes that occur after gross C uptake can also influence NEE;
114 therefore, we include these parameters as a third category. The parameters included in each

115 assimilation scenario are: P1 - all parameters, including all three phenology, photosynthesis and
116 post C uptake parameter groups; P2 - phenology and photosynthesis parameters; P3 - phenology
117 and post C uptake; P4 - photosynthesis and post C uptake; P5 - phenology parameters only; P6 -
118 photosynthesis only; and P7 - post C uptake only. See **Table 2** for a description of all parameters
119 and to which category they belong. We compared the prior simulation (before parameter
120 optimization) to the posterior simulations (after parameter optimization, with different parameter
121 groupings for the different assimilation scenarios) by evaluating the simulations against the site
122 data using standard goodness of fit metrics (root mean square error, RMSE and correlation
123 coefficient, r) at daily, monthly and inter-annual timescales. We further attributed what might be
124 causing model-data misfits by decomposing the daily mean squared deviation (MSD) into its
125 component phase, variance and bias contributions. The bias, variance and phase indicate the
126 mean difference in flux magnitude, the mismatch in terms of the magnitude of fluctuations, and
127 the seasonality in flux time series, respectively (Kobayashi & Salam, 2000).

128 **2 Methods and Data**

129 **2.1 Study sites**

130 Twelve semi-arid sites in the southwestern US (SW US) have been utilized in this study.
131 These sites have a range of different vegetation types, climates and have been described in detail
132 by (Biederman et al., 2017), so we only provide a brief description here. We summarized the
133 sites' description, dominant vegetation species, mean climate and corresponding vegetation plant
134 functional types (PFTs), together with the observation period and disturbance history (**Table 1**).
135 The major regional IGBP vegetation classes represented include evergreen needleleaf forest,
136 woody savanna, open and closed shrubland, and grassland. These sites typically experience
137 monsoon rainfall during July to October, preceded by a hot, dry period in May and June. The SW
138 US is characterized by water limitation at the annual scale, i.e. potential ET is greater than
139 precipitation. The sites have large spatial gradients in mean annual precipitation (MAP 250–724
140 mm) and temperature (MAT 2.9 to 17.7°C) due to interactions among topography, latitude, wind
141 patterns, and distance from oceans. For further site details, see references in **Table 1** and
142 individual site pages on www.ameriflux.lbl.gov.

143 **Table 1.** Site descriptions, mean climate, observation years and corresponding vegetation plant
 144 functional types (PFTs) used in ORCHIDEE optimization. Simulation period corresponds to the
 145 period of available site data. PFT acronyms: BS = Bare soil (PFT=1); TeNE = Temperate
 146 Needleleaved Evergreen forest (PFT=4); TeBE = Temperate Broadleaved Evergreen forest
 147 (PFT=5); TeBD = Temperate Broadleaved Deciduous forest (PFT=6); C4G = C4 grass
 148 (PFT=11). Sites are given in order from largest mean annual C sink (US-Vcm) to mean annual C
 149 source (US-Aud).

Site ID	Description	Dominant species	IGBP class	PFT fractions	Köppen climate	Elevation (m)	MAP (mm)	MA T (°C)	Period of site data	Disturbance History	Site reference
US-Vcm	Valles Caldera mixed conifer forest	<i>Picea engelmannii</i> , <i>Picea</i> pugnans, <i>Abies lasiocarpa</i> var. <i>lasiocarpa</i> , <i>Abies concolor</i>	Evergreen needleleaf forest	100% TeNE	Dfb	3042	724	2.9	2007–2012	Harvest 1960s	(Anderson-Teixeira et al., 2011)
US-Vcp	Valles Caldera ponderosa forest	<i>Pinus ponderosa</i> , <i>Quercus gambeli</i>	Evergreen needleleaf forest	100% TeNE	Dfb	2501	547	5.7	2007–2014	-	(Anderson-Teixeira et al., 2011)
US-Mpj	Heritage Land Conservancy pinyon-juniper	<i>Pinus edulis</i> , <i>Juniperus monosperma</i>	Savanna	20% BS; 60% TeNE ; 20% C4G	Bsk	2200	423	9.6	2008–2014	-	(Anderson-Teixeira et al., 2011)
US-Fuf	Flagstaff unmanaged ponderosa	<i>Pinus ponderosa</i>	Evergreen needleleaf forest	100% TeNE	Csb	2215	607	7.1	2006–2010	Harvest 1910	(Dore et al., 2012)

US- Wjs	Tablelands juniper savanna	Juniperus monosperma, Bouteloua gracilis	Savanna	15% TeNE ; 85% C4G	Bsk	1931	349	10. 9	2008– 2014	-	(Anderson- Teixeira et al., 2011)
US- Ses	Sevilleta creosote shrubland	Larrea tridentata, G. sarothrae	Open shrubland	20% BS; 55% TeBE ; 25% C4G	Bsk	1610	252	12. 6	2007– 2014	-	(Petrie et al., 2015)
US- Wkg	Walnut Gulch Kendall grassland	Eragrostis lehmanniana, Bouteloua spp. Calliandra erriophylla	Grassland	60% BS; 3% TeBE; 37% C4G	Bsk	1529	386	15. 8	2004– 2013	Drought 2003- 2005, non-native grass replacement 2007 onward, light grazing ongoing	(Scott, 2010)
US- SRG	Santa Rita grassland	Eragrostis lehmanniana	Savanna	45% BS; 11% TeBD ; 44% C4G	Bsh	1292	494	16. 7	2009– 2014	Mesquite removal 1957, ongoing light grazing	(Scott et al., 2009, 2015)
US- Seg	Sevilleta grassland: burned 2009	Bouteloua eriopoda, Gutierrezia sarothrae, Ceratooides lanata	Grassland	40% BS; 60% C4G	Bsk	160	250	12. 6	2007– 2014	Burned 2009	(Petrie et al., 2015)
US- SRM	Santa Rita mesquite savanna	Prosopis velutina, Eragrostis lehmanniana	Woody savanna	50% BS; 35% TeBD ; 15% C4G	Bsk	1122	421	17. 7	2004– 2014	Light grazing	(Scott et al., 2009)
US- Whs	Walnut Gulch Lucky Hills shrubland	Larrea tridentata, Parthenium incanum, Acacia constricta, Rhus microphylla	Open shrubland	57% BS; 40% TeBE ; 3% C4G	Bsk	1376	352	16. 8	2008– 2014	Drought 2005- 2006	(Scott, 2010)

US- Aud	Audubo n grasslan d	Boutelou agracilis, B. curtipendula, Eragrostis spp.	Grasslan d	30% BS; 70% <u>C4G</u>	Bsk	1496	348	15. 7	2004– 2009	Burned 2002	(Krishna n et al., 2012)
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150 2.1 ORCHIDEE terrestrial biosphere model

151 We use the ORCHIDEE (ORganizing Carbon and Hydrology In Dynamic EcosystEms)
152 process-oriented land surface model version 2.2 that has been developed at the IPSL (Institut
153 Pierre Simon Laplace, France). The model is a state-of-the-art mechanistic terrestrial biosphere
154 model (Krinner et al., 2005) and is the land surface component of the IPSLCM5 Earth System
155 Model (Dufresne et al., 2013). The model describes the exchanges of water, carbon, and energy
156 between biosphere and atmosphere at the smallest time scale (30 min), while the slow
157 components of the terrestrial carbon cycle (including carbon allocation, autotrophic respiration,
158 foliar onset and senescence, mortality and soil organic matter decomposition) are computed on a
159 daily to annual basis. Version 2.2 is virtually identical to version 2.0, which is being used in the
160 ongoing Coupled Modeling Intercomparison Project 6 (CMIP6) simulations, but includes few
161 recent bug corrections and code enhancements. It has been updated since the “AR5” version used
162 in CMIP5 (see (Krinner et al., 2005)) with the following developments: i) an 11-layer
163 mechanistic description of soil hydrology and associated modifications as described in
164 (MacBean et al., 2020); ii) addition of a coupled carbon-nitrogen scheme (Vuichard et al., 2019);
165 iii) an analytical solution for the set of equations for photosynthesis, stomatal conductivity and
166 internal CO₂ concentration in the leaf (described in (Vuichard et al., 2019)), following (Yin and
167 Struik, 2009); iv) an update of the soil thermal properties and extension of the soil depth for heat
168 diffusion (Wang et al., 2016); v) a 3-layer snow scheme (Wang et al., 2013); vi) a spatially
169 explicit observation-derived estimate for background albedo and optimized vegetation and snow
170 albedo coefficients;; vii) a new reconstruction of global land cover history and wood harvest
171 accounting following LUH2v2h maps (Hurtt et al., 2020) and PFT maps based the European
172 Space Agency Climate Change Initiative Land Cover product (Poulter et al., 2015).

173 As in most TBMs, the vegetation is grouped into several plant functional types (PFTs),
174 with 14 different types of vegetation plus bare soil in the case of ORCHIDEE v2.2. The original
175 13 PFTs are reported in (Krinner et al., 2005). Since ORCHIDEE v2.0 there are now two extra

176 PFTs included: C3 grasses are now split into three groups - tropical, temperate and boreal. The
 177 equations governing individual processes are generic with PFT specific parameters, except for
 178 the phenology models (see Appendix A in (MacBean et al., 2015)). In this study, ORCHIDEE is
 179 mainly used in a “grid-point mode” at each site location and forced with the corresponding local
 180 30-minute gap-filled meteorological forcing data. Before performing the optimizations the
 181 modelled C stocks are brought to equilibrium in the spin-up phase by cycling the available site
 182 meteorological forcing over a long period (1300 years) with the default parameters of the model,
 183 which ensures a net carbon flux close to zero over annual-to-decadal time scales.

184 2.2 ORCHIDEE data assimilation system

185 The ORCHIDEE Data Assimilation System (ORCHIDAS) has been described in detail in
 186 previous studies (Bastrikov et al., 2018; Kuppel et al., 2014; MacBean et al., 2018; Peylin et al.,
 187 2016), and hence we only briefly define the method here. ORCHIDAS uses a variational data
 188 assimilation method to optimize the model parameters, accounting for uncertainties regarding the
 189 observations, the model, and the prior parameters. It relies on a Bayesian framework with the
 190 assumption of Gaussian errors, and the optimized parameters corresponds to the minimization of
 191 the following cost function $J(x)$ (Tarantola, 2005):

$$192 \quad J(x) = \frac{1}{2} [(H(x) - y)^T \cdot R^{-1} \cdot (H(x) - y) + (x - x^b)^T \cdot B^{-1} (x - x^b)] \quad (1)$$

193 where x represents the parameters and $H(x)$ the model contingent on the parameters, and
 194 y the observations. The cost function contains both the misfit between observations, and
 195 corresponding model outputs (first term on the right hand side of Eq. 1), and the misfit between a
 196 priori parameter values x_b and optimized parameters x (*second term on the right hand side of the*
 197 *Eq. 1* R is the observation error covariance matrix (including measurement and model errors),
 198 and B is the prior parameter error covariance matrix. Both matrices (B and R) are diagonal since
 199 observation and model errors are assumed to be uncorrelated in space and time, and parameters
 200 are assumed to be independent. The cost function is iteratively minimized using the genetic
 201 algorithm (GA), which is a meta-heuristic optimization algorithm and follows the principles of
 202 genetics and natural selection (Goldberg et al., 1989; Haupt et al., 2004). The GA algorithm has
 203 been applied previously with ORCHIDAS tool and described in details by (Bastrikov et al.,

204 2018). Briefly, the algorithm works iteratively and considers the vector of parameters as a
 205 chromosome and each parameter as a gene on that chromosome. The method fills a set of n
 206 chromosomes at every iteration, having the starting pool as a randomly perturbed parameter
 207 pool. The chromosomes at each subsequent iteration are chosen from randomly selected
 208 chromosomes of the previous iteration by either “crossover” or “mutation” process. (Santaren et
 209 al., 2014) showed that the performance of the algorithm is highly sensitive to its specific
 210 configuration and found the best configuration based on computational efficiency after testing
 211 different options. Here, we used the same configuration (i.e. number of chromosomes in the pool
 212 total number of parameters optimized; the number of iterations is 40; crossover/mutation ratio is
 213 4:1; the number of gene blocks exchanged during crossover is 2 and the number of genes
 214 perturbed during mutation is 1) applied by (Santaren et al., 2014) and (Bastrikov et al., 2018).
 215 The algorithm does not assume prior knowledge of Gaussian PDFs for the observation and
 216 parameter uncertainties. Given we do not fully know the model uncertainty, we set the prior
 217 observation uncertainty as the RMSE between the model and the observations following (Kuppel
 218 et al., 2014). The prior parameter uncertainty is listed in Table S1.

219 The posterior error covariance matrix of the parameters (A) can be estimated by:

$$220 \quad \mathbf{A} = [\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{B}^{-1}]^{-1} \quad (2)$$

221 This computes error correlations between parameters with the assumption of Gaussian
 222 prior errors and linearity of the model in the vicinity of the solution.

223 2.3 Flux measurements

224 We used twelve eddy covariance flux sites (measurement period ranging between 2003
 225 and 2014) representing the various climate, elevation, and semi-arid ecosystems of SW US.
 226 Study sites are listed consecutively based on their mean annual C balance (Table 1). Flux tower
 227 instruments collect 30-minutes measurements of meteorological forcing data and eddy
 228 covariance measurements of net surface energy and carbon exchanges, which are available from
 229 the AmeriFlux data portal (<http://ameriflux.lbl.gov>). Meteorological forcing data included air
 230 temperature and surface pressure, precipitation, incoming long and shortwave radiation, wind
 231 speed, and specific humidity. To run the ORCHIDEE model, we partitioned the in-situ

232 precipitation into rain and snowfall using a temperature threshold of 0°C. The site-level
233 meteorological forcing data were gap filled utilizing downscaled and corrected ERA-Interim data
234 following the approach of (Vuichard & Papale, 2015). Gross primary productivity (GPP) and the
235 ecosystem respiration (R_{eco}) were estimated from the net ecosystem exchange (NEE) via the flux
236 partitioning method described in (Biederman et al., 2016). We acknowledge that GPP and R_{eco}
237 are not fully independent data with respect to NEE and are essentially model-derived estimates,
238 but these concerns have been largely discussed in previous studies e.g., (Desai et al., 2008). Note
239 that in this study, negative NEE refers to net CO₂ uptake into the ecosystem. In order to exclude
240 the influence of the short-term variations in the fluxes on the model optimization, the daily
241 averaged observations smoothed with a 15-day running mean have been used for the data
242 assimilation.

243 2.4 Parameters optimized

244 The optimized parameters are described in Table S1 with their prior values, uncertainty
245 and bounds for different plant functional types. Prior values are the default parameter values
246 used in all non-optimized ORCHIDEE simulations. In the most past ORCHIDAS studies with
247 previous versions of ORCHIDEE, only subsets of ORCHIDEE C cycle parameters have been
248 optimized (Bastrikov et al., 2018; Kuppel et al., 2012, 2014; MacBean et al., 2015; MacBean et
249 al., 2018; Santaren et al., 2007; Verbeeck et al., 2011). In this study, we considered all possible C
250 cycle related ORCHIDEE parameters and hence contribute towards the correct representation of
251 net and gross CO₂ fluxes. We selected all 102 parameters and divided them into four classes,
252 controlling the main C cycle and plant physiological processes i.e. photosynthesis, conductance,
253 phenology and post C uptake. This resulted in 31 parameters related to photosynthesis, 42 to
254 phenology, 16 to post C uptake (C allocation, respiration, biomass and soil turnover), and 13
255 related to conductance. In a preliminary study, we tested at several SW US sites (US-Vcp, US-
256 Mpj, US-Fuf, US-Wkg, US-Whs, US-Seg) the sensitivity of the ecosystem fluxes (NEE, GPP
257 and R_{eco}) when optimizing all model parameters and when we just optimized subsets of the
258 parameters related to each of the main processes. This test showed no significant optimization
259 improvement by adding the conductance related parameters (results not shown here), and thus
260 we did not include those parameters for all final optimizations presented in this study, leaving a
261 total of 89 optimized parameters for each site. The parameter names, descriptions, bounds and

262 prior uncertainties used in this study (Table S1) were derived from literature analysis, parameter
 263 databases and expert knowledge of the model equations. Documentation on the parameters can
 264 be accessed via ORCHIDEE webpage
 265 (<https://forge.ipsl.jussieu.fr/orchidee/wiki/Documentation/OrchideeParameters>, last access: 04
 266 January 2021). The prior uncertainty is set to 40% of the range of variation for each parameter
 267 following previous ORCHIDAS studies (Kuppel et al., 2012; MacBean et al., 2015).

268 2.5 Assimilation Scenarios

269 We conducted several different optimizations to identify which processes (and their
 270 related parameters) are potentially causing model-data discrepancies (listed in Table 2). We
 271 grouped the optimizations based on various parameters set to optimize; therefore, we tested 7
 272 assimilation scenarios (P1 – P7): P1 included all 89 parameters, whereas each consecutive
 273 scenario (P2 – P7) optimized different subsets of parameters related to each of the main C cycle
 274 processes (Table 2). The parameters that were not optimized were set to their default (prior)
 275 value. Comparing the P1 to P7 assimilation scenarios allows us to determine which sets of
 276 parameters (i.e. specific processes) are contributing most to the improvement in fluxes as a result
 277 of the parameter optimizations. See Table S1 for groupings of model parameters according to
 278 specific processes.

279 **Table 2.** Description of the different assimilation scenarios conducted in this study. The included
 280 parameter group(s) and numbers of parameters for each assimilation scenario are given.
 281 Parameters of each subgroup are listed in Table S1.

Optimization	Parameters included	Number of parameters
P1	All parameters (Phenology, Photosynthesis and Post C uptake)	~85
P2	Phenology and Photosynthesis	~70
P3	Phenology and Post C uptake	~50
P4	Photosynthesis and Post C uptake	~60
P5	Phenology only	~30
P6	Photosynthesis only	~45
P7	Post C uptake only	~15

282 2.6 Post-optimization analysis

283 We assessed the goodness of fit of the different assimilation scenarios by the mean square
 284 deviation (MSD) (in addition root mean squared error, RMSE or correlation coefficients, R or
 285 slope of linear least-square regression). Model evaluation metrics are presented in one of three
 286 ways: i) for each site; ii) grouped across all sites; and iii) sites grouped according to their mean
 287 net annual CO₂ flux characteristics across the time period identified in (Biederman et al., 2017).
 288 For the latter, the net CO₂ “sink” sites are US-Vcm, US-Vcp, US-Mpj, US-Fuf and US-Wjs; the
 289 “pivot” sites are US-Ses, US-Wkg, US-SRG, US-SRM, US-Whs, US-Seg; and the “source” site
 290 is US-Aud. We follow the approach of (Kobayashi & Salam, 2000) to quantify the differences
 291 between the simulations and observation in terms of bias, variance and phasing. We calculate the
 292 MSD between daily observation and each of the simulations and decompose it following the
 293 below equation:

$$294 \quad MSD = \frac{1}{n} \sum_{i=1}^n (x_i - y_i)^2 = (\bar{x} - \bar{y})^2 + (\sigma_x - \sigma_y)^2 + 2\sigma_x\sigma_y(1 - R) \quad (3)$$

295 where x is the model and y is the observations, σ is the standard deviation and R is the
 296 correlation coefficient.

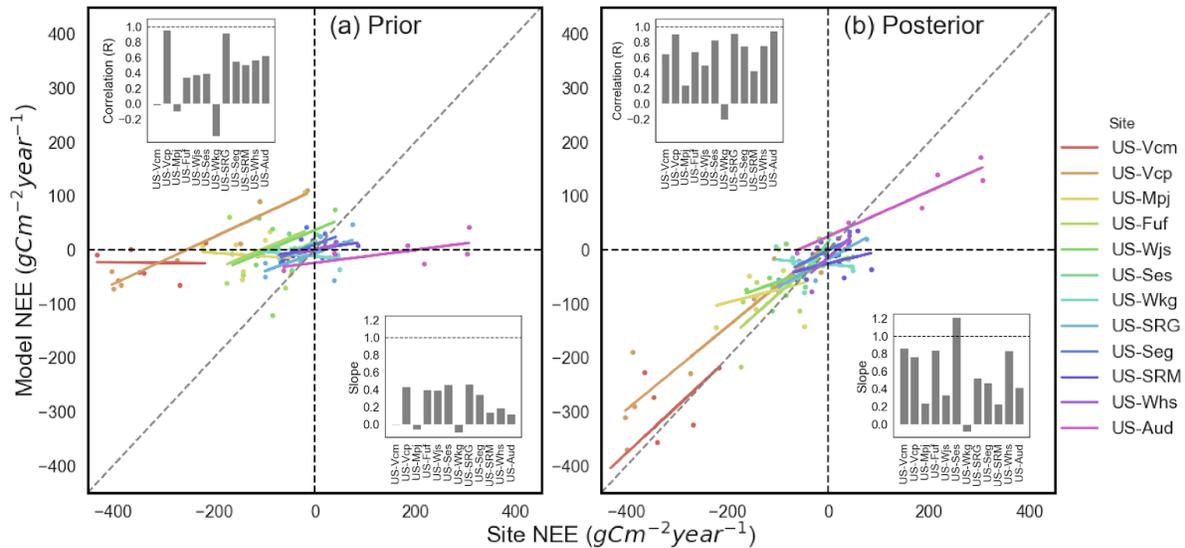
297 The first term specifies the bias between model simulation and observation (squared).
 298 The second term “variance” measures their differences in terms of variability (i.e., the difference
 299 between the magnitude of the modeled and observed fluctuations). And the third term generally
 300 demonstrates the lack of correlation between them weighted by their standard deviations, which
 301 can be deemed as a measure of their disagreement in terms of phase (Bacour et al., 2019; Gauch
 302 et al., 2003). However, the second and third terms are partially dependent on each other (Bacour

303 et al., 2019; Gauch et al., 2003). We further calculated the contribution of each component (bias,
304 variance and phase) to the overall MSD by dividing each component by the total MSD.

305 **3 Results**

306 3.1 Impact of optimization of all parameters on model net and gross CO₂ fluxes

307 Across all sites, the prior ORCHIDEE simulations (i.e. before parameter optimization)
308 fail to capture both the mean annual NEE and its IAV (**Figure 1a**) - as also seen for all
309 TRENDY TBMs in MacBean et al (submitted). Across all sites, optimizing all C cycle-related
310 parameters (phenology, photosynthesis and post C uptake - assimilation scenario P1) with NEE
311 data dramatically increases the ability of the model to capture both the mean C source/sink
312 behavior and the IAV (**Figure 1b**). C sink and source sites show significant improvement in
313 terms of both mean annual NEE and IAV. There is not a strong bias in the model simulations at
314 pivot sites whose mean annual NEE is close to zero; therefore, the optimization results in an
315 improvement mainly in IAV (as represented by the correlation and slope values shown in inset
316 figures in Figures 1 a and b). Improvement of the model-data fit resulting from the assimilation
317 of NEE and optimizing all parameters (P1) is evident across all sites, with a reduction of daily
318 NEE RMSE between 0.05 to 0.65 gCm⁻²d⁻¹ (**Figure S1**), with a similar reductions in daily GPP
319 and R_{eco} RMSE (Table S2). Moreover, the temporal dynamics are well captured for all the sites:
320 when optimizing all parameters, the median pearson correlation coefficients (R) increase by
321 0.45, 0.45, and 0.25 for daily, monthly and annual modeled NEE, respectively and posterior
322 median slope values ≥ 0.5 (**Figure S2a and d**). GPP temporal dynamics are also much improved
323 by the P1 assimilation with a higher and tighter range in posterior R and slope values than NEE
324 (**Figure S2b and e**). In contrast, there is less improvement in R_{eco} temporal dynamics although
325 the median R and slope values are higher after the optimization (**Figure S2c and f**).



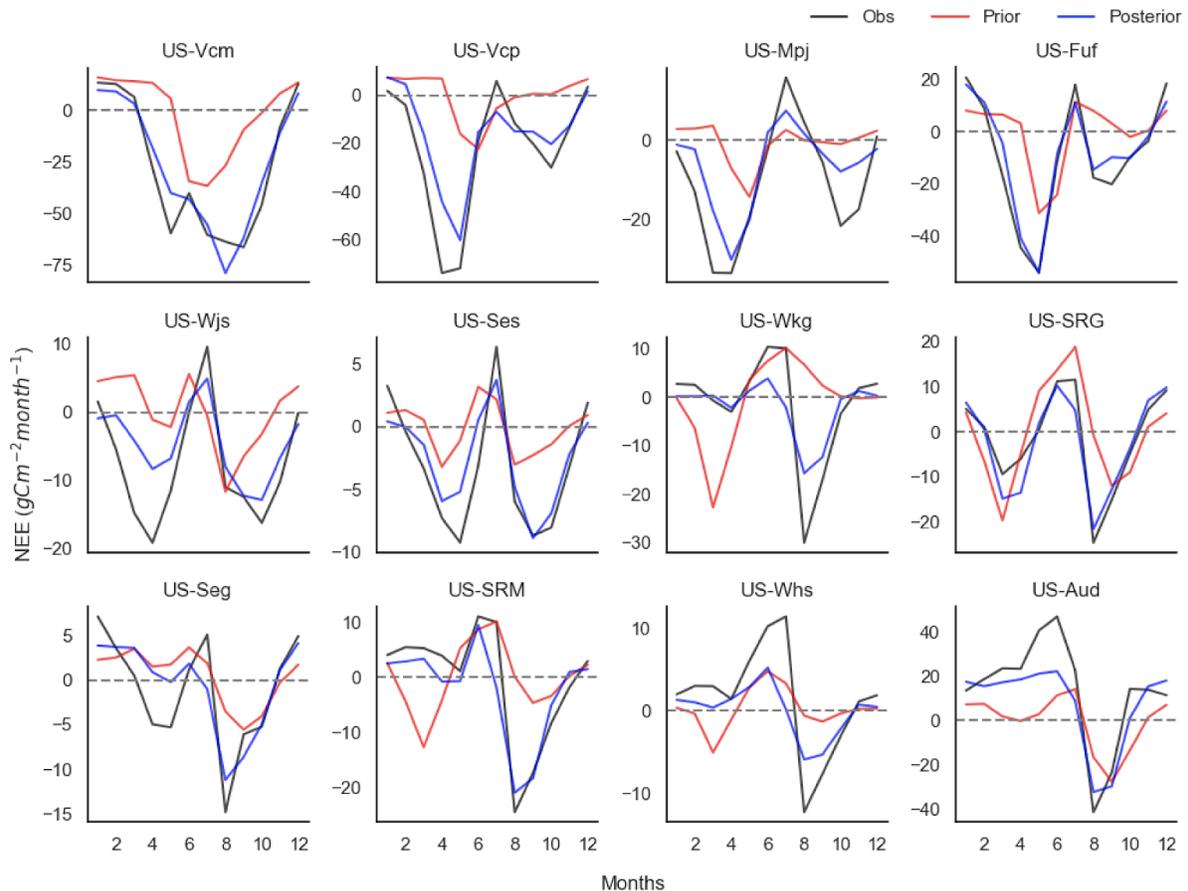
326

327 **Figure 1.** Comparison between modeled and observed annual NEE when assimilating NEE data
 328 and optimizing all phenology, photosynthesis and post C uptake parameters (P1) in the same
 329 assimilation. **(a)** Prior annual NEE simulation before parameter optimization, and **(b)** Posterior
 330 annual NEE after optimization. The trendline and slope value for the linear regression between
 331 the model and observations (bottom right inset figures) is shown for each site, together with their
 332 Pearson correlation coefficient, r (top left inset figures). The middle of the trend line should sit
 333 on the 1:1 line if the accurate mean annual source/sink behavior for a site is well captured by the
 334 model. A slope value close to or equal to 1 demonstrates the model is better at capturing the
 335 IAV. Colored points and trend lines represent all twelve sites, ordered from the largest mean sink
 336 (US-Vcm) to the largest mean source (US-Aud). The sink sites are: US-Vcm, US-Vcp, US-Mpj,
 337 US-Fuf, US-Wjs and US-Ses; the pivot sites are: US-Wkg, US-SRG, US-Seg, US-SRM and US-
 338 Whs; and the only source site is: US-Aud.

339

340 Across the majority of SW US dryland sites, the prior model simulates a depressed
 341 seasonal NEE amplitude and/or is unable to capture the observed bi-modal seasonality (**Figure**
 342 **2**). The NEE amplitude and bi-modal seasonality generally improve when optimizing all
 343 parameters (P1 - blue curves in **Figure 2**), although the posterior simulations struggles to reach
 344 the exact magnitude of the spring and monsoon NEE troughs (net CO₂ uptake) for several sites
 345 (e.g. US-Mpj, US-Wjs, US-Ses, US-Seg, US-Wkg and US-Whs). Accurately capturing the

346 seasonal peaks and troughs is important for NEE IAV because summer monsoon season fluxes
 347 are the dominant driver of NEE IAV (MacBean et al., submitted). While posterior seasonal NEE
 348 peaks and troughs are generally well captured, the assimilation of NEE alone often fails to
 349 capture the correct peaks in gross CO₂ fluxes (**Figure S3**), likely due to compensating errors in
 350 both GPP and R_{eco}. At the C source site (US-Aud) the model also fails to simulate the accurate
 351 peaks in springtime net carbon release (**Figure 2**). As also identified in MacBean et al
 352 (submitted), this is due to the fact that at US-Aud, TBMs tend to overestimate spring GPP and
 353 underestimate the earlier rise in spring R_{eco} (**Figure S3**). The optimization only partially corrects
 354 these model biases, suggesting that other missing processes may ultimately be responsible for the
 355 model-data misfit (such as disturbance following a fire that occurred at the site in 2002, which is
 356 not implemented in the current version of ORCHIDEE).



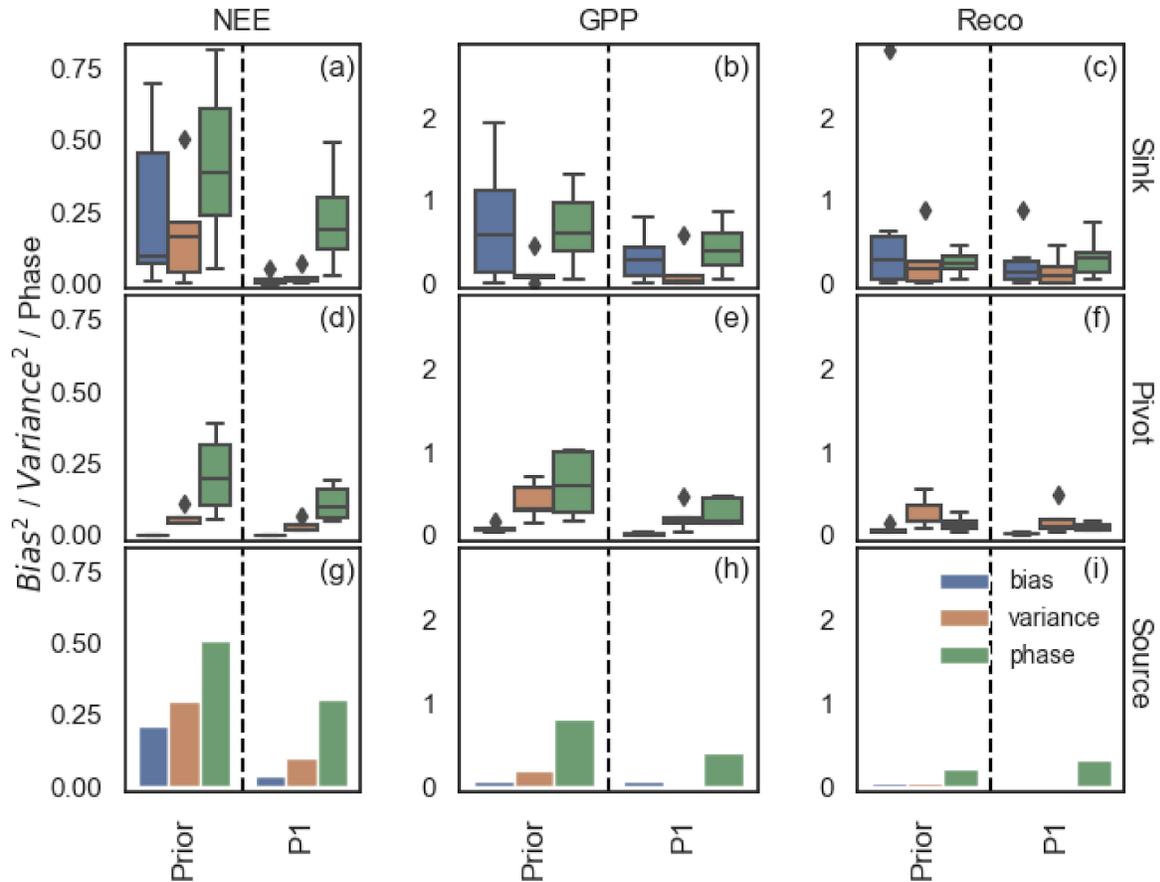
357

358 **Figure 2.** Mean monthly NEE seasonal cycles for each site comparing prior (red curve) and
 359 posterior (blue curve) ORCHIDEE simulations with observations (black curve). Posterior

360 simulation after assimilation of NEE data and optimization of all parameters: phenology,
361 photosynthesis and post C uptake (P1). The sites are listed in order from largest mean annual C
362 sink (US-Vcm) to mean annual C source (US-Aud).

363

364 Decomposing the daily NEE mean square deviations (MSD) between model and
365 observations into bias, variance and phase components shows that across all sites, bias, variance
366 and phase all contribute to prior NEE model-data discrepancies (**Figure 3a** left of vertical dashed
367 line). The prior daily NEE MSD at the C sink sites are dominated by both phase and bias
368 components (**Figure 3a** top panel). The fact that sink site MSD is also dominated by bias is
369 unsurprising given that at those sites the prior model does not capture the mean annual C sink
370 (**Figure 1a**). Note that, if we decompose the annual NEE MSD into the constituent bias, phase
371 and variance components then bias overwhelmingly dominates the MSD at sink (and source)
372 sites given their large underestimate of mean annual NEE (**Figure S4** top and bottom rows). In
373 contrast, at the C pivot and source sites, the highest contribution to the prior daily NEE MSD is
374 from the phase component (**Figure 3a** middle and bottom panel), indicating the default model
375 does a poor job of representing the timing of dryland C cycle related processes. Across all sites,
376 optimizing all parameters (P1) dramatically reduces the bias, variance and phase components of
377 the daily NEE MSD, with phase remaining the strongest contributor to daily NEE MSD (**Figure**
378 **3a** right of dashed line).



379

380 **Figure 3.** Daily NEE, GPP and R_{eco} mean square deviation (MSD) decomposition into bias,
 381 variance, and phase between simulations and observations for assimilating NEE observations and
 382 optimizing all phenology, photosynthesis and post C uptake parameters (P1). Blue, orange and
 383 green boxplots for bias, variance and phase components, respectively. Different rows separate
 384 the sites as sink (a-c), pivot (d-f) and source (g-i) based on total annual C flux. The sink sites are:
 385 US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses; the pivot sites are: US-Wkg, US-
 386 SRG, US-Seg, US-SRM and US-Whs; and the source site ia: US-Aud. The x axes display the
 387 optimization scenarios (Prior and P1). The box whiskers show the spread of bias, variance and
 388 phase for all 12 sites considered in this study. The bias, variance and phase indicate the mean
 389 difference in flux magnitude, the mismatch in terms of flux fluctuation magnitude scales with the
 390 mean seasonal amplitude, and the seasonality in flux time series, respectively. Note that the y
 391 axis limits for both gross fluxes (GPP and R_{eco}) are the same.

392

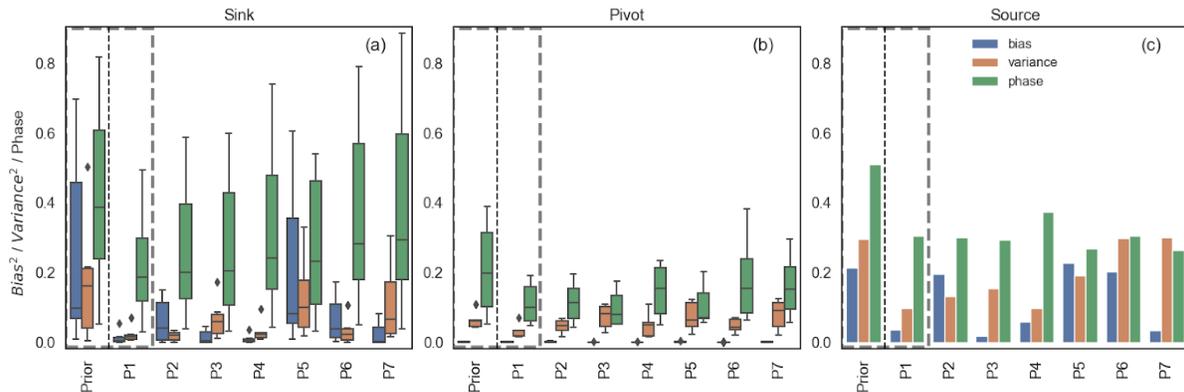
393 As for the NEE, bias and phase are the dominant contributors to prior daily GPP MSD for
394 the sink sites (left of vertical dashed line in **Figure 3b**), and phase only for the pivot and source
395 sites (**Figures 3e and h**) For R_{eco} , a different MSD component is dominant depending on the
396 mean C behavior of a site: bias dominates the prior daily R_{eco} MSD at the sink sites, variance at
397 the pivot sites, and phase at the source sites (**Figures 3c, f and i**). Overall, assimilating NEE data
398 in the P1 scenario reduces all gross CO₂ flux MSD components (right of dashed line in **Figure 3**
399 middle and left columns), with phase remaining the strongest contributor to daily gross CO₂ flux
400 MSD. However, unlike for the NEE, at the C sink sites phase *and* bias remain strong contributors
401 to posterior GPP MSD (**Figure 3b**).

402

403 3.2 Impact of different processes (assimilation scenarios) on optimization results

404 Across all sites, modeled annual and seasonal NEE are improved the most in the P1
405 assimilation scenario compared to the other assimilation scenarios (P2 to P7), although all
406 scenarios result in some improvement (**Figures S5, S6a and d**, and seasonal cycles in **Figure**
407 **S7**). In general, there is less improvement in R_{eco} compared to NEE and GPP (**Figure S6**).

408 Comparing the MSD decomposition results for the various assimilation scenarios (P1-
409 P7) can help to identify which processes may be causing the prior model-discrepancies in mean
410 annual NEE and NEE IAV. At the source and sink sites, the bias component (blue bars in **Figure**
411 **4a and c**) is reduced dramatically by all optimization tests that include the post C uptake
412 parameters related to C allocation, respiration, and biomass and soil C turnover (P1, P3, P4 and
413 P7). For the sink sites, assimilation scenarios that also include photosynthesis parameters (P2 and
414 P6) also result in a strong reduction in bias. This decrease in mean bias is also shown by the fact
415 that the midpoints of the linear regression trendline between model and observations at forested
416 sink sites (US-Vcm, US-Vcp, US-Mpj, and US-Fuf) and low-elevation source site (US-Aud)
417 with optimization scenarios P1 to P4, P6 and P7 parameters all lie much closer to the 1:1 (grey
418 dashed) line compared to P5 (**Figure S5**).



419

420 **Figure 4.** Daily NEE MSD decomposition into bias, variance, and phase components when
 421 assimilating NEE observations for different assimilation scenarios (P1-P7). Different panels
 422 separate the sites as sink (a), pivot (b) and source (c) based on total annual C flux. The C sink
 423 sites are: US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses; the C pivot sites are: US-
 424 Wkg, US-SRG, US-Seg, US-SRM and US-Whs; and the C source site is: US-Aud. The grey
 425 dashed boxes highlight results repeated from **Figure 3(a,d,g)** to have better comparison of
 426 different process parameters side-by-side. The parameters included in each optimization are: P1:
 427 all parameters; P2: phenology and photosynthesis; P3: phenology and post C uptake; P4:
 428 photosynthesis and post C uptake; P5: phenology; P6: photosynthesis and P7: post C uptake. The
 429 boxplots show the median and interquartile range of the bias, variance and phase across all 12
 430 sites considered in this study. US-Aud is the only C source site; therefore, the barplots in (c)
 431 show the bias, phase, and variance components of the MSD for that one site. The bias, variance
 432 and phase indicate the mean difference in flux magnitude, the difference in the magnitude of flux
 433 variations, and the difference in the correlations weighted by the standard deviations,
 434 respectively (see Methods).

435

436 Across all sites the difference in phase between the model and observations (green bars in
 437 **Figure 4**), which, as already noted, is the largest contribution to the prior NEE MSD across all
 438 sites, is mostly reduced by assimilation scenarios that include phenology parameters (i.e. P1, P2,
 439 P3 and P5). However, the phase component is not reduced as much as the bias in any of the
 440 assimilation scenarios; thus, for all sites and all assimilation scenarios the phase remains the
 441 largest component of the posterior daily NEE MSD (**Figure 4**). Including parameters related to

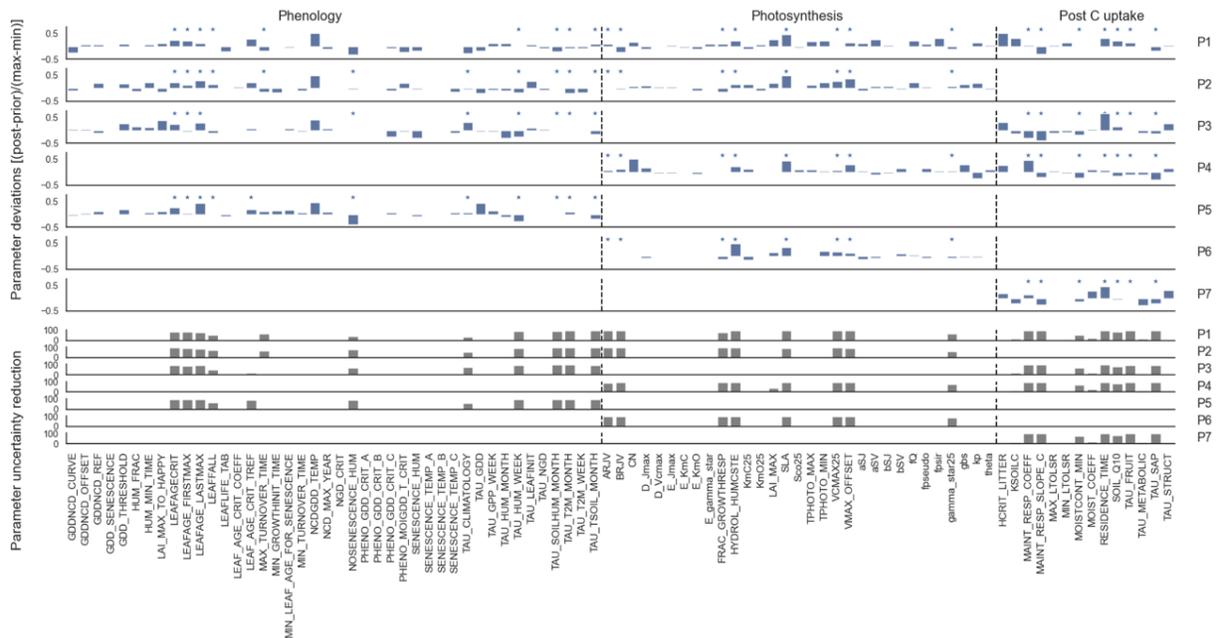
442 photosynthesis or post C uptake with the phenology parameters (i.e. assimilation scenarios P2
443 and P3) helps to slightly reduce the phase discrepancy at sink sites compared with phenology
444 parameters alone (P5) (as seen above for the improvement in slope values at the sink sites).
445 Examining the spread in slope and R values across all sites, we see that the annual variability
446 (median slope and R values) is improved the most for assimilation scenarios with at least two
447 parameter sets (P1 to P4 - **Figure S6a and d**). The persistence of phase as the dominant
448 component of the posterior daily NEE suggests further model improvement in dryland phenology
449 models is needed before TBMs can correctly reproduce NEE seasonality and IAV.

450 The variance component of the daily NEE MSD (orange bars in **Figure 4**), which also
451 shows a modest contribution to daily NEE MSD at the sink and source sites, is mostly reduced at
452 the sink sites with assimilation scenarios that include photosynthesis parameters (i.e. P1, P2, P4
453 and P6). At US-Aud the variance component was reduced most by assimilation scenarios that
454 included two or more sets of parameters (i.e. P1 - P4) (**Figure 4c**).

455 While the post C uptake parameters are key for reducing bias in forested sink site NEE,
456 biases in GPP and R_{eco} at these sites are reduced by optimizing photosynthesis parameters (P1,
457 P2, P4, and P6 - blue boxes **Figure S8b and c**). The GPP and R_{eco} bias components at the sink
458 sites are not reduced as strongly as NEE biases for any assimilation scenario; thus, bias remains a
459 key contributor to posterior gross CO_2 flux MSD. Similarly to NEE, parameter subsets that
460 include phenology parameters (P1, P2, P3 and P5) are key for reducing the daily GPP MSD
461 phase component at pivot sites (green boxes in **Figure S8e**; however, in contrast with the NEE
462 results, at sink sites the GPP phase component tends to be reduced by all assimilation scenarios
463 except P7 (see also median GPP slope and R values in **Figures S6b and e**). With the exception
464 of P1 and P2 for GPP, the GPP and R_{eco} variance components are not reduced much by any of
465 the assimilation scenarios and remain a considerable component of the MSD for both GPP and
466 R_{eco} at the pivot sites, and for R_{eco} at the sink sites (**Figures S8b,c,e,f**). We note that the GPP and
467 R_{eco} reductions in MSD components tend to be similar, suggesting model-deficiencies in R_{eco} are
468 mainly influenced by those in GPP. Addressing GPP model-data deficiencies is therefore a high
469 priority.

470 3.3 Constraint on parameters

471 For all assimilation scenarios, we found significant parameter deviations from prior
 472 values for numerous phenology, photosynthesis and post C uptake related parameters (**Figure 5**),
 473 which is consistent with the fact that we find all parameter subsets are needed to improve model
 474 mean annual NEE and IAV. We do not find that parameters deviate more, or the uncertainty
 475 reduction much different, when only one subset or two parameter subsets are included in the
 476 optimization instead of all three (e.g. cf. P2 with P1), although posterior values are different for
 477 each assimilation scenario (**Figure 5**). In particular, most of the post C uptake parameters deviate
 478 strongly from the prior median deviations (>20% of total parameter bound). There are also
 479 significant uncertainty reductions (>50%) for most of the parameters which show strong
 480 deviations from their prior value: 10 for phenology (out of 42), 7 for photosynthesis (out of 31)
 481 and 7 for post C uptake (out of 16) (**Figure 5**). The error correlations between the estimated
 482 parameters are usually minimal except between post C uptake parameters (see example for one
 483 site in **Figure S9**).



484
 485 **Figure 5.** Optimized median parameter deviations $[(\text{posterior} - \text{prior}) / (\text{max} - \text{min})]$ (blue bars)
 486 and associated median parameter uncertainty reductions (grey bars) for all parameters controlling
 487 phenology, photosynthesis and post C uptake assimilating NEE data (P1-P7). Bars represent the
 488 median across all 12 sites. The asterisks above blue bars indicate the parameters that have larger
 489 than 50% uncertainty reduction. Each line corresponds to a specific optimization test (shown on
 490 the right axis). The parameters are given on the bottom axis. The vertical dashed lines separate

491 the different parameter subsets (phenology, photosynthesis and post C uptake). **Table S1** details
492 the prior and posterior parameter values and their uncertainty for all parameters together with the
493 maximum and minimum bounds used in the optimizations.

494

495 Looking at the individual parameter plots for the P1 assimilation scenario (**Figure S10**),
496 we find that at some sites several posterior parameters are “edge-hitting” (e.g. soil Q10). Given
497 we chose weak prior constraints (wide bounds) in all optimizations, the fact that some posterior
498 parameters are hitting their bounds suggests that the optimization may be aliasing model
499 structural error onto the parameters (MacBean et al., 2016) and/or that the model cannot improve
500 further via parameter optimization. Instead, further model developments are likely needed to
501 address structural uncertainties and missing processes. Hypotheses as to what (missing)
502 processes might be responsible for these remaining model errors have been discussed in
503 MacBean et al (submitted). For example, it is possible that model inability to capture peak GPP
504 fluxes for some sites (see Section 3.1) is due to too weak a response of model vegetation growth
505 to pulses of moisture availability, an issue which is not fully alleviated by using only NEE to
506 optimize model parameters.

507

508 **4 Conclusions**

509 While improvement in modeled NEE is best when all parameters are optimized, our
510 assimilation scenario experiments have shown that post C uptake and phenology parameters are
511 key for correcting model underestimates in dryland mean annual NEE and IAV, respectively.
512 Remaining model-data discrepancies indicate that additional model developments are needed. .
513 The specific DA configuration (e.g. the number of parameters, and the processes with which they
514 are related) can lead to different posterior values and degree of improvement in model-data fit.
515 Therefore, further tests of different DA configurations and optimizations at other locations are
516 needed to explore the potential of Bayesian DA systems for quantifying and reducing error in
517 dryland ecosystem C fluxes. However, our study demonstrates that dryland C cycle parameters
518 and processes in TBMs need optimizing and/or further development before we can reliably use
519 these models to accurately simulate dryland ecosystem contributions to global C cycle
520 variability.

521

522 Acknowledgments

523 This work was supported by the Department of Geography at Indiana University.

524

525 Code availability

526 The ORCHIDEE model is under a free software license (CeCILL; see

527 <http://www.cecill.info/index.en.html>) and the source code is visible here:

528 <https://forge.ipsl.jussieu.fr/orchidee/browser/tags/ORCHIDEE>. The ORCHIDEE model code is

529 written in Fortran 90 and is maintained and developed under an SVN version control system at

530 the Institute Pierre Simon Laplace (IPSL) in France. The ORCHIDAS code is currently in the

531 process of being put on a GitHub repository but for now it is available on request to

532 vladislav.bastrikov@lsce.ipsl.fr.

533

534 Data availability

535 Meteorological forcing data and eddy covariance measurements of net surface energy and

536 carbon exchanges at 30-minutes intervals are available from the AmeriFlux data portal

537 (<http://ameriflux.lbl.gov>). The model outputs from ORCHIDEE simulations and post-processing

538 python scripts for manuscript figures and tables are freely available in a Git repository

539 (https://github.com/kashifmahmud/SW_US_semiarid).

540

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Optimizing Phenology Parameters Drastically Improves Terrestrial Biosphere Model Underestimates of Dryland Net CO₂ Flux Inter-Annual Variability

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Parameter Name	Description (Unit)	Plant functional type			
		TeNE	TeBE	TeBD	GC4
Photosynthesis parameters					
ARJV	a coefficient of the linear regression (a+bT) defining the J_{max25}/V_{cmax25} ratio ($\mu\text{ mol e}^- (\mu\text{ mol CO}_2)^{-1}$)	2.59 ± 0.4 2, 3	2.59 ± 0.4 2, 3	2.59 ± 0.4 2, 3	1.715 ± 0.48 1, 2, 2
aSJ	a coefficient of the linear regression (a+bT) defining the Entropy term for J_{max} ($\text{J K}^{-1}\text{ mol}^{-1}$)	659.7 ± 264 330, 990	659.7 ± 264 330, 990	659.7 ± 264 330, 990	630 ± 252 315, 945
aSV	a coefficient of the linear regression (a+bT) defining the Entropy term for V_{cmax} ($\text{J K}^{-1}\text{ mol}^{-1}$)	668.39 ± 267.6 334, 1003	668.39 ± 267.6 334, 1003	668.39 ± 267.6 334, 1003	641.64 ± 256.4 321, 962
BRJV	b coefficient of the linear regression (a+bT) defining the J_{max25}/V_{cmax25} ratio ($\mu\text{ mol e}^- (\mu\text{ mol CO}_2)^{-1}$)	-0.035 ± 0.028 -0.07, 0	-0.035 ± 0.028 -0.07, 0	-0.035 ± 0.028 -0.07, 0	-0.01 ± 0.028 -0.035, 0.035
bSJ	b coefficient of the linear regression (a+bT) defining the Entropy term for J_{max} ($\text{J K}^{-1}\text{ C}^{-1}$)	-0.75 ± 0.6 -1.5, 0	-0.75 ± 0.6 -1.5, 0	-0.75 ± 0.6 -1.5, 0	0.01 ± 0.6 -0.75, 0.75
bSV	b coefficient of the linear regression (a+bT) defining the Entropy term for V_{cmax} ($\text{J K}^{-1}\text{ C}^{-1}$)	-1.07 ± 0.8 -2, 0	-1.07 ± 0.8 -2, 0	-1.07 ± 0.8 -2, 0	0.1 ± 0.856 -1.07, 1.07
CN	C/N ratio	40 ± 32 20, 100	40 ± 32 20, 100	40 ± 32 20, 100	-
D_Jmax	Energy of deactivation for J_{max} (J/mol)	200000 ± 16000 180000, 220000	200000 ± 16000 180000, 220000	200000 ± 16000 180000, 220000	192000 ± 15200 173000, 211000
D_Vcmax	Energy of deactivation for V_{cmax} (J/mol)	200000 ± 16000 180000, 220000	200000 ± 16000 180000, 220000	200000 ± 16000 180000, 220000	192000 ± 15200 173000, 211000
E_gamma_star	Energy of activation for γ_{star} (J mol^{-1})	37830 ± 8000 27830, 47830			
E_Jmax	Energy of activation for J_{max} (J mol^{-1})	49884 ± 8000 39884, 59884	49884 ± 8000 39884, 59884	49884 ± 8000 39884, 59884	77900 ± 8000 67900, 87900
E_KmC	Energy of activation for K_mC (J mol^{-1})	79430 ± 8000 69430, 89430			
E_KmO	Energy of activation for K_mO (J mol^{-1})	36380 ± 8000 26380, 46380			
fpseudo	Fraction of electrons at PSI that follow pseudocyclic transport	-	-	-	0.1 ± 0.032 0.06, 0.14
fpsir	Fraction of PSII e ⁻ transport rate partitioned to the C4 cycle	-	-	-	0.4 ± 0.16 0.4, 0.6
FRAC_GROWTHRESP	Fraction of GPP which is lost as growth respiration	0.28 ± 0.064 0.2, 0.36			

fQ	Fraction of electrons at reduced plastoquinone that follow the Q-cycle	-	-	-	1 ± 0.24 0.7, 1.3
gamma_star25	Ci-based CO ₂ compensation point in the absence of Rd at 25C (ubar)	42.75 ± 8 22.75, 62.75	42.75 ± 8 22.75, 62.75	42.75 ± 8 22.75, 62.75	42.75 ± 8 22.75, 62.75
gbs	Bundle-sheath conductance (mol m ⁻² s ⁻¹ bar ⁻¹)	-	-	-	0.003 ± 0.0008 0.001, 0.005
HYDROL_HUMCSTE	Root profile (m) in empirical plant water stress function calculation	1 ± 1.5 0.25, 4	0.8 ± 1.12 0.2, 3	0.8 ± 1.12 0.2, 3	1 ± 1.5 0.25, 4
KmC25	Michaelis-Menten constant of Rubisco for CO ₂ at 25C (ubar)	404.9 ± 160 204.9, 604.9	404.9 ± 160 204.9, 604.9	404.9 ± 160 204.9, 604.9	650 ± 160 450, 850
KmO25	Michaelis-Menten constant of Rubisco for O ₂ at 25C (ubar)	278400 ± 80000 178400, 378400	278400 ± 80000 178400, 378400	278400 ± 80000 178400, 378400	450000 ± 80000 350000, 550000
kp	Initial carboxylation efficiency of the PEP carboxylase (mol m ⁻² s ⁻¹ bar ⁻¹)	-	-	-	0.7 ± 0.24 0.4, 1
LAI_MAX	Maximum LAI (m ² /m ²)	5 ± 2 3, 8	5 ± 2 3, 8	5 ± 2 3, 8	2.5 ± 0.8 4, 10
Sco25	Relative CO ₂ /O ₂ specificity factor for Rubisco at 25C (bar bar ⁻¹)	2800 ± 800 1800, 3800	2800 ± 800 1800, 3800	2800 ± 800 1800, 3800	2590 ± 800 1590, 3590
SLA	Specific leaf area (m ² /gC)	0.00926 ± 0.005 0.004, 0.02	0.02 ± 0.012 0.01, 0.04	0.026 ± 0.0148 0.013, 0.05	0.026 ± 0.0148 0.013, 0.05
theta	Convexity factor for response of J to irradiance	0.7 ± 0.18 0.5, 0.95			
TPHOTO_MAX	Maximum photosynthesis temperature (deg C)	55 ± 4 50, 60			
TPHOTO_MIN	Minimum photosynthesis temperature (deg C)	-4 ± 4 -9, 1			
VCMAX25	Maximum rate of Rubisco activity-limited carboxylation at 25C (micromol/m ² /s)	35 ± 10 19, 51	45 ± 16 25, 65	55 ± 20 30, 80	70 ± 25.6 38, 102
VMAX_OFFSET	Offset (minimum relative v _{max})	0.3 ± 0.048 0.24, 36			
Post C uptake parameters - autotrophic and heterotrophic respiration, C allocation, biomass and soil C turnover					
HCRIT_LITTER	Scaling depth for litter humidity (m)	0.08 ± 0.192 0.02, 0.5			
KSOILC	Scalar on the active soil C pool content (to account for uncertainty in spin-up)	1 ± 0.6 0.5, 2			
MAINT_RES_P_COEFF	Coefficient to calculate maintenance respiration as a fraction of biomass	1.4 ± 0.84 0.7, 2.4			
MAINT_RES_P_SLOPE_C	Slope of maintenance respiration coefficient (1/K), constant c of aT ² +bT+c, tabulated	0.16 ± 0.064 0.08, 0.24	0.16 ± 0.064 0.08, 0.24	0.16 ± 0.064 0.08, 0.24	0.12 ± 0.06 0.04, 0.2
MAX_LTOLSR	Extrema of leaf allocation fraction	0.5 ± 0.08 0.4, 0.6			
MIN_LTOLSR	Extrema of leaf allocation fraction	0.2 ± 0.08 0.1, 0.3			
MOIST_COEFF_1	Coefficient to calculate moisture control for litter and soil C decomposition	1.1 ± 0.24 0.8, 1.4			
MOIST_COEFF_2	Coefficient to calculate moisture control for litter and soil C decomposition	2.4 ± 0.24 2.1, 2.7			
MOIST_COEFF_3	Coefficient to calculate moisture control for litter and soil C decomposition	0.29 ± 0.232 0.01, 0.59			
MOISTCON_T_MIN	Minimum soil wetness to limit the heterotrophic respiration	0.25 ± 0.2 0.1, 0.6			

RESIDENCE_TIME	Residence time of trees (years)	40 ± 24 30, 90	40 ± 24 30, 90	40 ± 24 30, 90	0 ± 0 0,0
SOIL_Q10	Temperature dependency factor for heterotrophic respiration (Note: actual Q10 = $\exp^{\text{SOIL_Q10}}$)	0.69 ± 0.44 0, 1.1			
TAU_FRUIT	Fruit lifetime (days)	90 ± 24 60, 120	90 ± 24 60, 120	90 ± 24 60, 120	-
TAU_META_BOLIC	A coefficient to calculate residence times in metabolic litter pools (days)	0.066 ± 0.0112 0.052, 0.08			
TAU_SAP	Sapwood heartwood conversion time (days)	730 ± 144 550, 910	730 ± 144 550, 910	730 ± 144 550, 910	-
TAU_STRUCT	A coefficient to calculate residence times in structural litter pools (days)	0.245 ± 0.04 0.2, 0.3			
Phenology parameters					
GDD_THRESHOLD	Temperature threshold used in the calculation of number of growing degree day, GDD (days)	5 ± 0.8 4, 6			
GDDNCD_CURVE	Constant in the computation of critical GDD	0.0091 ± 0.00112 0.0072, 0.01			
GDDNCD_OFFSET	Constant in the computation of critical GDD (days)	64 ± 11.2 50, 78			
GDDNCD_REFERENCE	Reference value used in the computation of critical GDD (days)	603 ± 96.8 482, 724			
HUM_FRAC	Critical humidity (relative to min/max) for phenology (%)	-	-	-	0.5 ± 0.2 0.25, 0.75
HUM_MIN_TIME	Minimum time elapsed since moisture minimum (days)	-	-	-	35 ± 12 20, 50
LAI_MAX_THRESHOLD_HAPPY	Threshold of LAI below which plant uses carbohydrate reserves	0.5 ± 0.14 0.35, 0.7	0.5 ± 0.14 0.35, 0.7	0.5 ± 0.14 0.35, 0.7	0.5 ± 0.14 0.35, 0.7
LEAF_AGE_CRIT_COEFF_1	A coefficient to calculate critical leaf age (days)	1.5 ± 0.24 1.2, 1.8			
LEAF_AGE_CRIT_COEFF_2	A coefficient to calculate critical leaf age (days)	0.75 ± 0.12 0.6, 0.9			
LEAF_AGE_CRIT_COEFF_3	A coefficient to calculate critical leaf age (days)	10 ± 1.6 12, 8			
LEAF_AGE_CRIT_TREF	Reference temperature used to calculate of critical leaf age (days)	20 ± 4 15, 25			
LEAFAGE_FIRSTMAT	Leaf age at which v _{max} attains v _{max_opt} (in fraction of critical leaf age)	0.03 ± 0.0048 0.024, 0.036			
LEAFAGE_LASTMAT	Leaf age at which v _{max} falls below v _{max_opt} (in fraction of critical leaf age)	0.5 ± 0.08 0.4, 0.6			
LEAFAGE_CRITICAL	Critical leaf age, tabulated (days)	910 ± 200 610, 1210	730 ± 192 490, 970	180 ± 60 120, 240	120 ± 60 30, 180
LEAFFALL	Length of death of leaves, tabulated (days)	-	-	10 ± 4 5, 15	10 ± 4 5, 15
LEAFLIFE_TABLE	Leaf longevity (years)	0.33 ± 0.1 0.2, 0.75	1 ± 0.668 0.33, 2	2 ± 0.9 0.75, 3	2 ± 0.9 0.75, 3
MAX_TURNOVER_TIME	Maximum turnover time for grass (days)	-	-	-	80 ± 4 75, 85
MIN_GROWTH_INITIAL_TIME	Minimum time since last beginning of a growing season (days)	300 ± 24 270, 330			
MIN_LEAF_AGE_FOR_SENESCENCE	minimum leaf age to allow senescence (days)	-	-	90 ± 8 80, 100	30 ± 4 25, 35
MIN_TURNOVER_TIME	Minimum turnover time for grass (days)	-	-	-	10 ± 4 5, 15

NCD_MAX_YEAR	A coefficient to calculate maximum possible number of chilling days (NCD)	3 ± 0.8 2, 4			
NCDGDD_T EMP	Critical temperature for the ncd vs. gdd function in phenology (C)	-	-	5 ± 4 0, 10	-
NOSENESCE NCE_HUM	Relative moisture availability above which there is no humidity-related senescence	-	-	-	0.3 ± 0.12 0.15, 0.45
PHENO_GD D_CRIT_A	Critical gdd tabulated constant a	-	-	-	0 ± 0 0, 0
PHENO_GD D_CRIT_B	Critical gdd constant b	-	-	-	0 ± 0 0, 0
PHENO_GD D_CRIT_C	Critical gdd constant c	-	-	-	400 ± 64 320, 480
PHENO_MOI GDD_T_CRI T	Average temperature threshold for C4 grass used (C)	-	-	-	22 ± 8 12, 32
SENESENC E_HUM	Critical relative moisture availability for senescence	-	-	-	0.2 ± 0.08 0.1, 0.3
SENESENC E_TEMP_A	Critical temperature for senescence (C), constant a of aT ² +bT+c, tabulated	-	-	0 ± 0 0, 0	0 ± 0 0, 0
SENESENC E_TEMP_B	Critical temperature for senescence (C), constant b of aT ² +bT+c, tabulated	-	-	0 ± 0 0, 0	0 ± 0 0, 0
SENESENC E_TEMP_C	Critical temperature for senescence (C), constant c of aT ² +bT+c, tabulated	-	-	12 ± 8 2, 22	5 ± 4.8 -1, 11
TAU_CLIMA TOLOGY	tau for climatologic variables (days)	20 ± 8 10, 30			
TAU_GDD	Time scales for phenology and other processes (days)	40 ± 16 20, 60			
TAU_GPP_ WEEK	Time scales for phenology and other processes (days)	6 ± 1 5, 7			
TAU_HUM_ MONTH	Time scales for phenology and other processes (days)	20 ± 8 10, 30			
TAU_HUM_ WEEK	Time scales for phenology and other processes (days)	6 ± 1 5, 7			
TAU_LEAFI NIT	Time to attain the initial foliage using the carbohydrate reserve (days)	10 ± 10 5, 30	10 ± 10 5, 30	10 ± 10 5, 30	10 ± 10 5, 30
TAU_NGD	Time scales for phenology and other processes (days)	50 ± 20 25, 75			
TAU_SOILH UM_MONTH	Time scales for phenology and other processes (days)	20 ± 8 10, 30			
TAU_T2M_ MONTH	Time constant for the “monthly” 2-meter temperature (days)	20 ± 8 10, 30			
TAU_T2M_ WEEK	Time constant for the “weekly” 2-meter temperature (days)	6 ± 1 5, 7			
TAU_TSOIL _MONTH	Time constant for the “monthly” soil temperature (days)	20 ± 8 10, 30			
Conductance parameters - included in initial optimization sensitivity test but not in final optimizations					
A1	empirical factor involved in the calculation of fvpd	0.85 ± 0.04 0.8, 0.9	0.85 ± 0.04 0.8, 0.9	0.85 ± 0.04 0.8, 0.9	0.85 ± 0.04 0.8, 0.9
B1	empirical factor involved in the calculation of fvpd	0.14 ± 0.032 0.1, 0.18	0.14 ± 0.032 0.1, 0.18	0.14 ± 0.032 0.1, 0.18	0.2 ± 0.032 0.15, 0.25
CHOISNEL_ RSOL_CSTE	Constant in the computation of resistance for bare soil evaporation (s/m ²)	3.3E4 ± 19400 1.75E4, 6.6E4			
CONDVEG_ Z0	Surface roughness (m)	0.15 ± 0.12 0, 0.3			
DEFC_MUL T	Constant in the computation of surface resistance (KW ⁻¹)	1.5 ± 0.9 0.75, 3			
DEFC_PLUS	Constant in the computation of surface resistance (KW ⁻¹)	0.023 ± 0.016 0.003, 0.043			

g0	Residual stomatal conductance when irradiance approaches zero (mol m ⁻² s ⁻¹ bar ⁻¹)	0.00625 ± 0.00048 0.00565, 0.00685	0.00625 ± 0.00048 0.00565, 0.00685	0.00625 ± 0.00048 0.00565, 0.00685	0.01875 ± 0.0016 0.01675, 0.02075
GB_REF	Leaf bulk boundary layer resistance (s m ⁻¹)	0.04 ± 0.032 0, 0.08			
KZERO	A vegetation dependent constant used in the calculation of the surface resistance (kg/m ² /s)	0.00012 ± 0.000016 0.0001, 0.00014	0.00012 ± 0.000016 0.0001, 0.00014	0.00025 ± 0.00004 0.0002, 0.0003	0.0003 ± 0.00004 0.00025, 0.00035
RATIO_Z0M_Z0H	Ratio between z0m and z0h	1 ± 0.4 0.5, 1.5	1 ± 0.4 0.5, 1.5	1 ± 0.4 0.5, 1.5	1 ± 0.4 0.5, 1.5
Z_DECOMP	Scaling depth for soil activity	0.2 ± 0.6 0, 1.5			
Z0_BARE	Bare soil roughness length (m)	0.01 ± 0.0016 0.008, 0.012			
Z0_OVER_H EIGHT	To get z0 from height	0.0625 ± 0.032 0.02, 0.1			

Table S1. Prior information for all ORCHIDEE parameters optimized in this study: prior value, uncertainty and maximum and minimum bounds for the different plant functional types (temperate needleleaf/broadleaf evergreen (TeNE, TeBE) forests, temperate broadleaf deciduous (TeBD) forest, C4 grassland (GC4)).

Site	Daily root mean square error (RMSE)			
	GPP		Reco	
	Prior	Posterior	Prior	Posterior
US-Vcm	1.392	1.366	2.009	1.315
US-Vcp	1.822	1.116	0.979	0.927
US-Mpj	1.312	0.903	1.051	0.867
US-Fuf	1.074	0.828	0.534	0.629
US-Wjs	0.995	0.73	0.778	0.672
US-Ses	0.259	0.229	0.233	0.255
US-Wkg	1.177	0.809	0.617	0.49
US-SRG	1.345	0.982	0.95	0.825
US-Seg	0.699	0.449	0.441	0.324
US-SRM	1.158	0.617	0.8	0.572
US-Whs	0.698	0.531	0.507	0.437
US-Aud	1.028	0.707	0.561	0.602

Table S2. Daily GPP and ecosystem respiration (R_{eco}) model-data fit when assimilating NEE observations with all parameters (P1) in terms of prior and posterior root mean square error (RMSE) for all twelve sites. The reduction in daily GPP RMSE varies between 0.03 to $0.7 \text{ gCm}^{-2}\text{d}^{-1}$, and the reduction in daily R_{eco} RMSE varies between 0 to $0.7 \text{ gCm}^{-2}\text{d}^{-1}$. The sites are listed in order from largest mean annual C sink (US-Vcm) to mean annual C source (US-Aud).

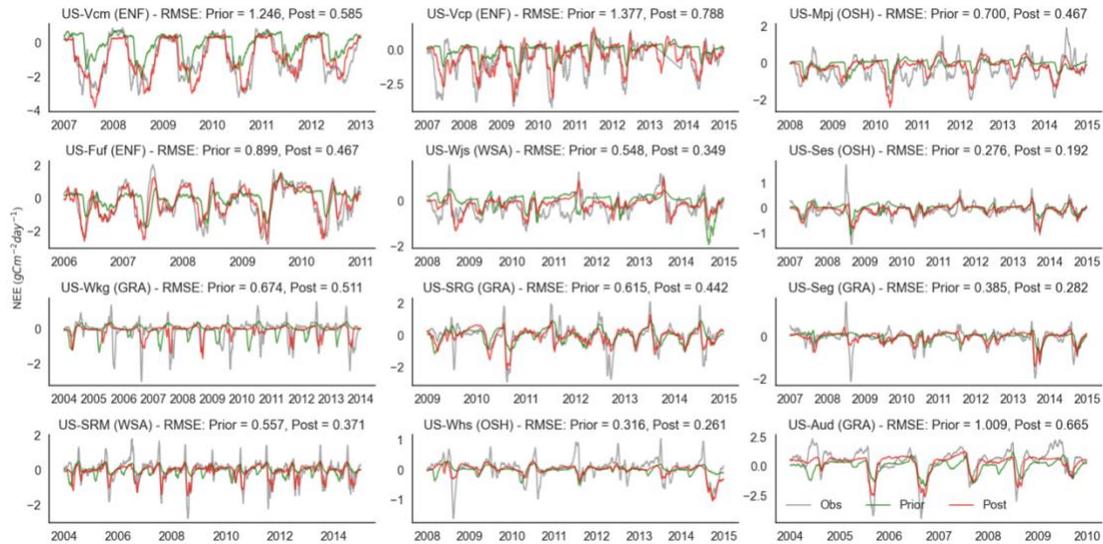


Figure S1. Comparison of NEE observations (grey) with corresponding ORCHIDEE model simulations before (green line) and after assimilation (red line) for assimilating NEE observations with all parameters (P1). The vegetation types are listed within brackets for each site. The RMSE measures the fit of the model prior and posterior simulations with the corresponding observations. Across all sites, the prior and posterior NEE RMSEs vary between 0.291-1.377 and 0.196-0.788, respectively. The sites are listed in order from largest mean annual C sink (US-Vcm) to mean annual C source (US-Aud).

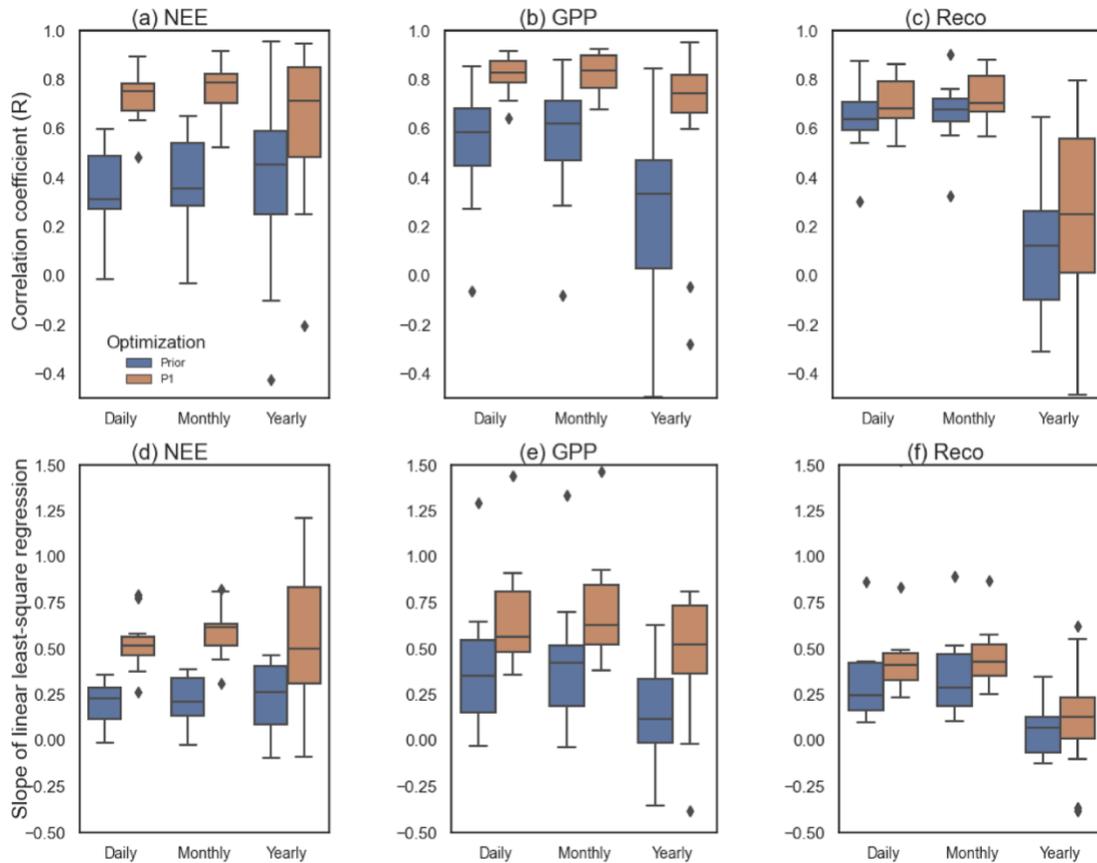


Figure S2. Daily, monthly and annual NEE (a, d), GPP (b, e) and R_{eco} (c, f) prior and posterior Pearson correlation coefficients (R) and slope values for the linear regression between model and observed fluxes for assimilating NEE observations and optimizing all phenology, photosynthesis and post C uptake parameters (P1). The R between observed and modeled NEE at daily, monthly and annual timescales for optimizing all parameters (P1) increase by up to 0.50, 0.55, 0.65 respectively. Note that the y axis limits for both R and slope are the same and therefore 3 sites fall outside the y-axis upper limit for the R_{eco} slope.

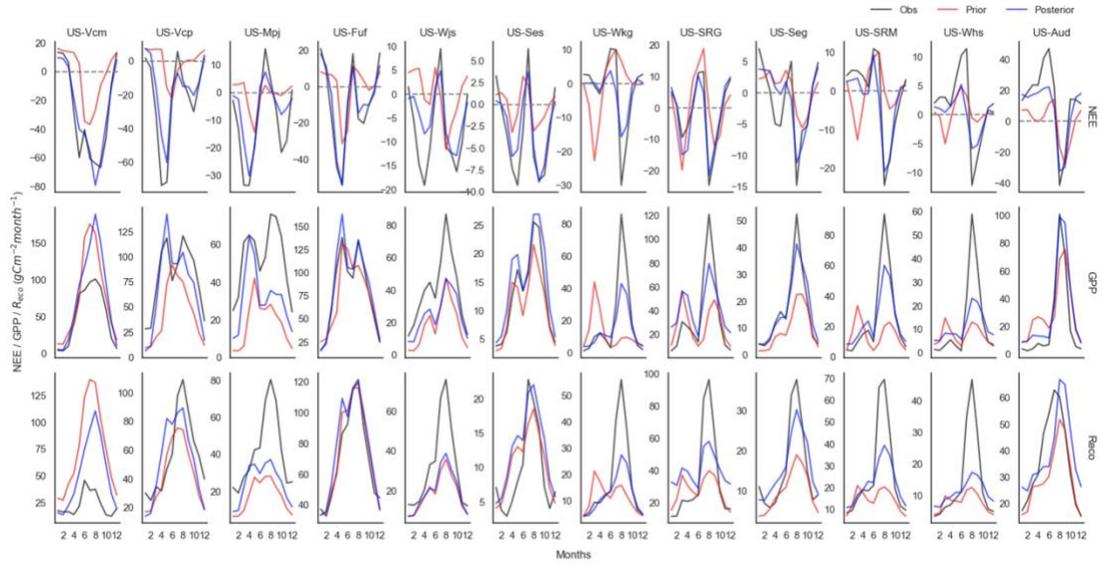


Figure S3. Seasonal cycle with mean monthly total fluxes. Comparison of flux observations with corresponding ORCHIDEE model simulations (prior and posterior) for assimilating NEE observations and optimizing all phenology, photosynthesis and post C uptake parameters (P1). The sites are listed from left to right according to C sink to source.

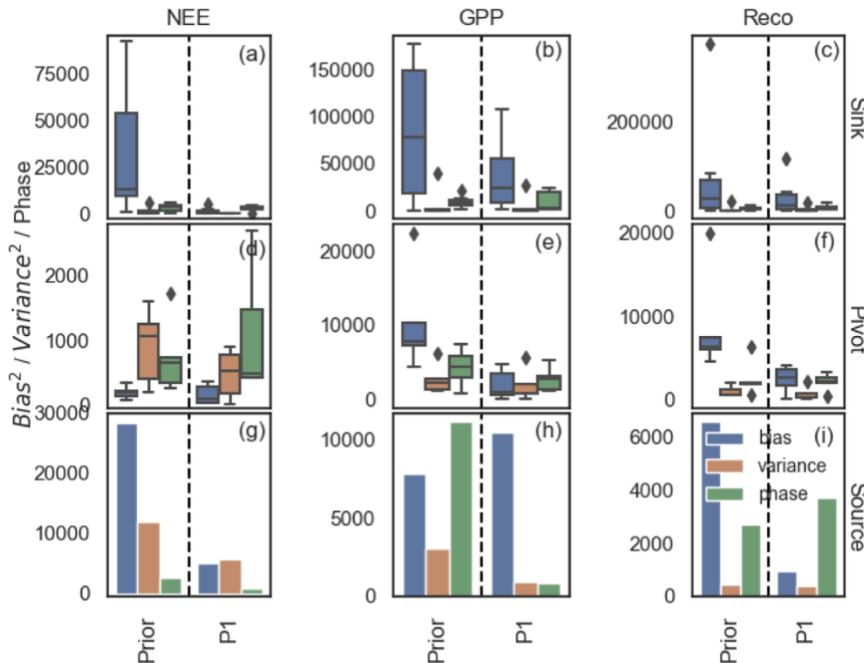


Figure S4. Annual NEE, GPP and R_{eco} mean square deviation (MSD) decomposition into bias, variance, and phase between simulations and observations for assimilating NEE observations and optimizing all phenology, photosynthesis and post C uptake parameters (P1). Different rows separate the sites as sink (a-c), pivot (d-f) and source (g-i)

based on total annual C flux. The sink sites are: US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses; the pivot sites are: US-Wkg, US-SRG, US-Seg, US-SRM and US-Whs; and the source site is: US-Aud. The x axes display the optimization scenarios (Prior and P1). The box whiskers show the spread of bias, variance and phase for all 12 sites considered in this study. The bias, variance and phase indicate the mean difference in flux magnitude, the mismatch in terms of flux fluctuation magnitude scales with the mean seasonal amplitude, and the seasonality in flux time series, respectively. Note that the y axis limits are different for all fluxes and site types.

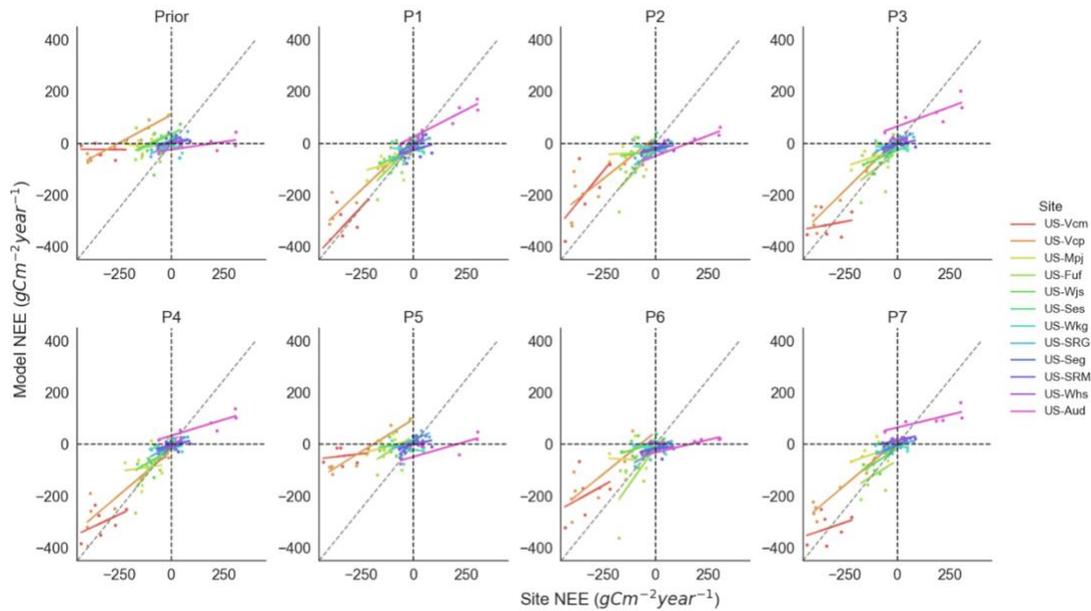


Figure S5. Annual NEE scatter plots for prior and all posterior simulations for assimilating NEE observations with various parameter sets (P1-P7). Different colour legends represent various sites, ordered from the largest mean sink (US-Vcm) to the largest mean source (US-Aud). The middle of the trend line should sit on the 1:1 line if the accurate mean annual source/sink behavior for a site is well captured by the model. A slope value close to or equal to 1 demonstrates the model is better at capturing the IAV. The sink sites are: US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses; the pivot sites are: US-Wkg, US-SRG, US-Seg, US-SRM and US-Whs; and the source site is: US-Aud.

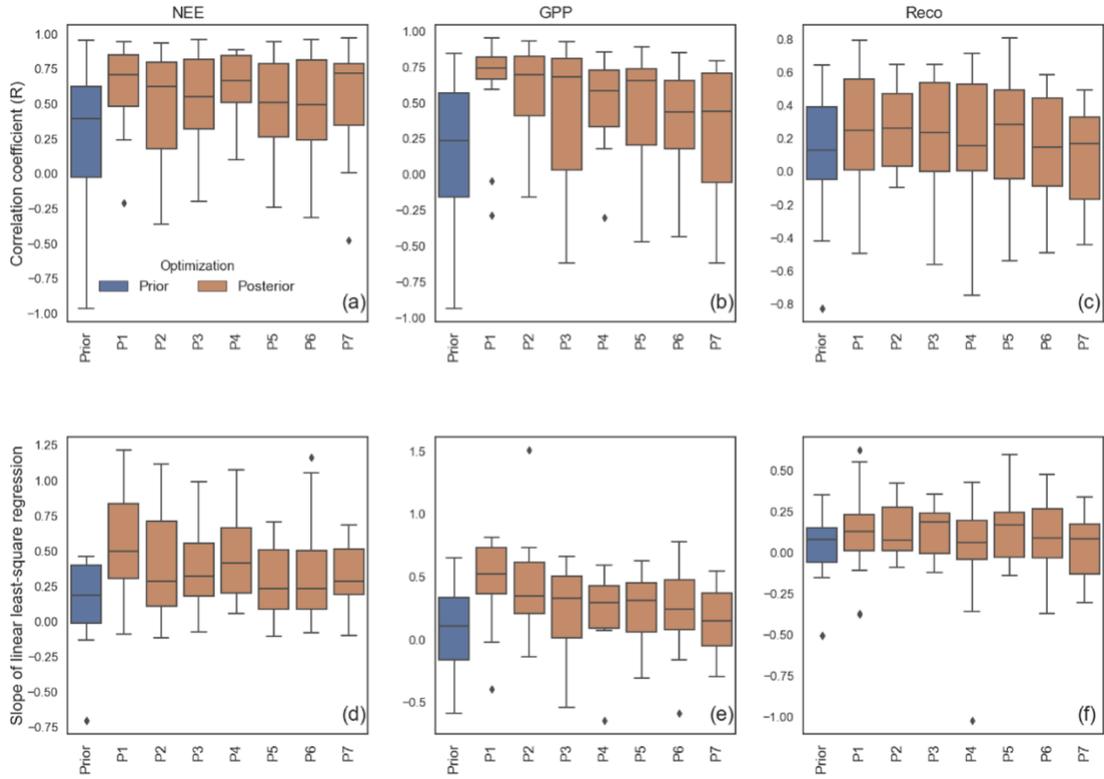


Figure S6. NEE (a, d), GPP (b, e) and R_{eco} (c, f) annual anomaly prior and posterior Pearson correlation coefficients (R) and slope values for the linear regression between model and observed fluxes across all assimilation scenarios with different parameter combinations (P1-P7). The legend represents various assimilation scenarios (Prior - blue bars, and posterior P1-P7 - orange bars).

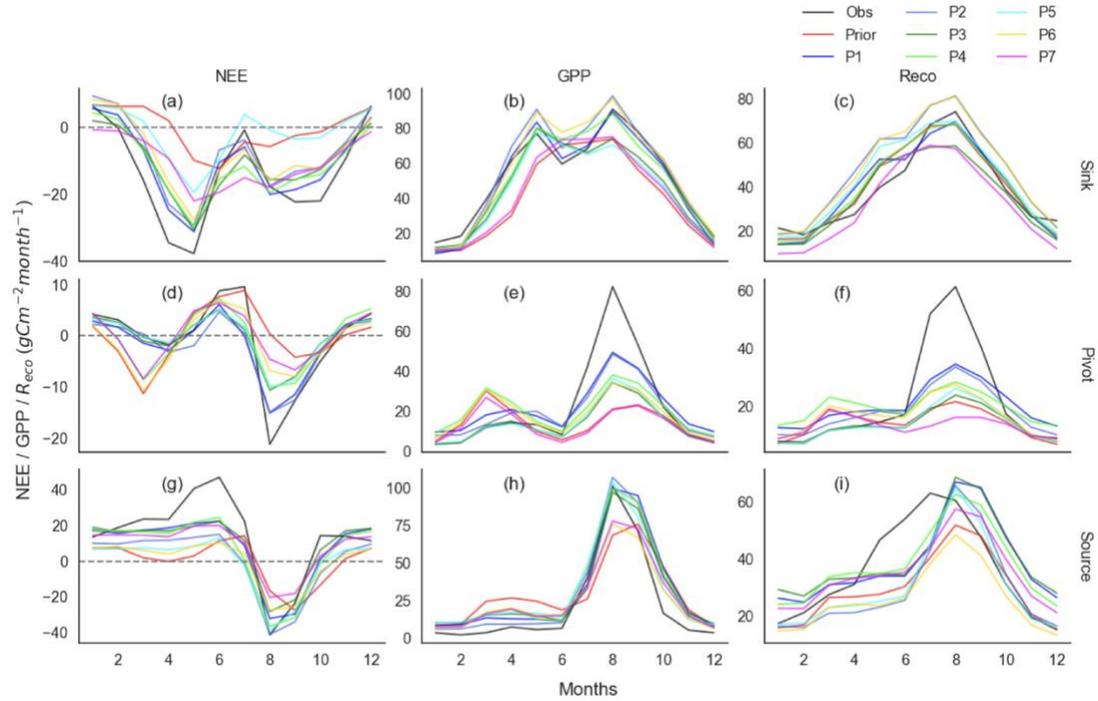


Figure S7. Mean monthly seasonal cycles comparing observations (black curve), prior (red curve), and posterior simulations for assimilation scenarios (P1 to P7 - blue to magenta curves) for NEE (left column), GPP (middle column), and R_{eco} (right column) averaged across site C balance types (sink - top row; pivot - middle row; and the source site, US-Aud, on the bottom row).

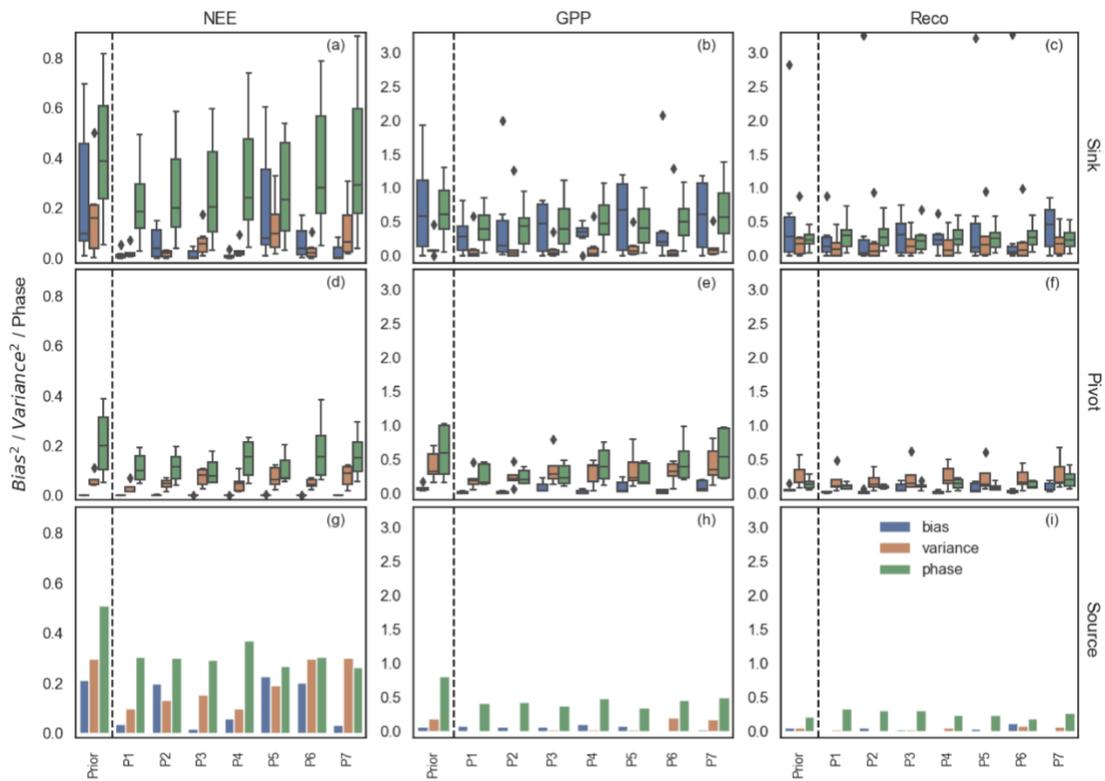


Figure S8. Daily NEE, GPP and R_{eco} mean square deviation (MSD) decomposition into bias, variance, and phase between simulations and observations for assimilating NEE observations with various parameter sets (P1-P7). Different rows separate the sites as sink (a-c), pivot (d-f) and source (g-i) based on total annual C flux. The sink sites are: US-Vcm, US-Vcp, US-Mpj, US-Fuf, US-Wjs and US-Ses; the pivot sites are: US-Wkg, US-SRG, US-Seg, US-SRM and US-Whs; and the only source site is: US-Aud. The x axes display various optimization scenarios (Prior, P1-P7). The parameters included in each optimization are: P1: all parameters; P2: phenology and photosynthesis; P3: phenology and post C uptake; P4: photosynthesis and post C uptake; P5: phenology; P6: photosynthesis and P7: post C uptake. The box whiskers show the spread of bias, variance and phase for all 12 sites considered in this study. The bias, variance and phase indicate the mean difference in flux magnitude, the mismatch in terms of flux fluctuation magnitude scales with the mean seasonal amplitude, and the seasonality in flux time series, respectively. Note that the y axis limits for both gross fluxes are the same.

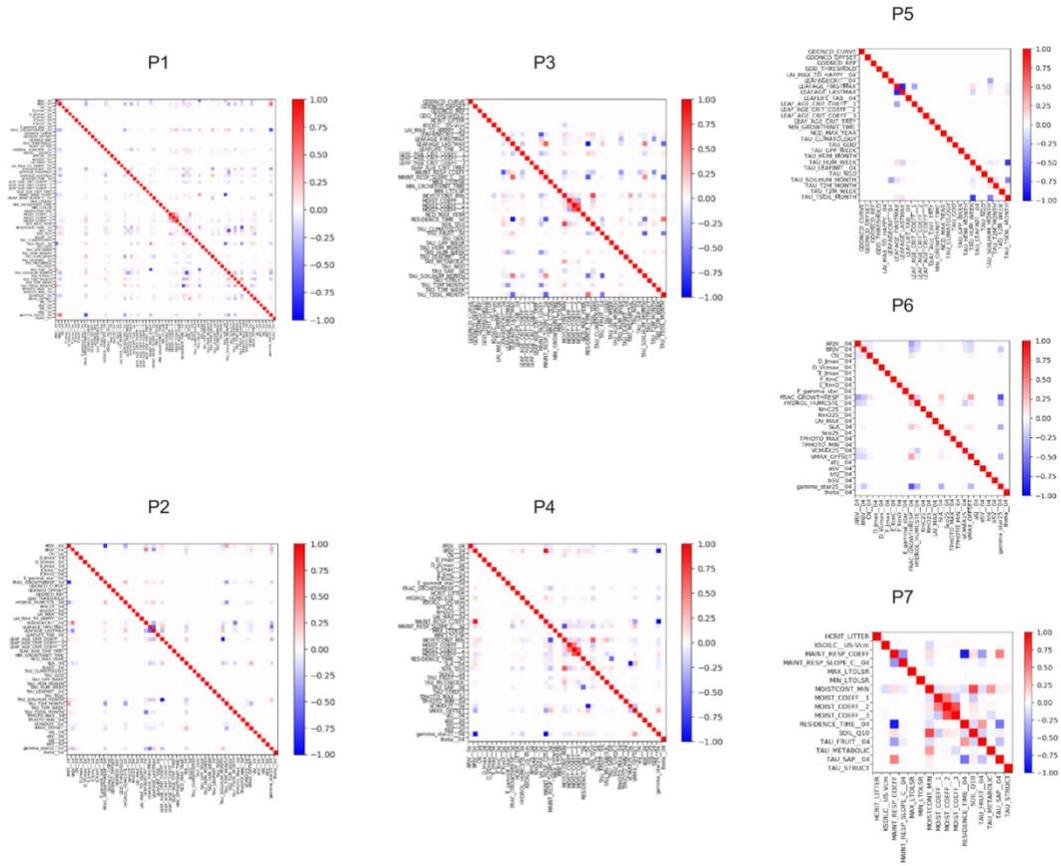


Figure S9. Parameter posterior error covariance matrix for US-Vcm for various assimilation scenarios (P1-P7).

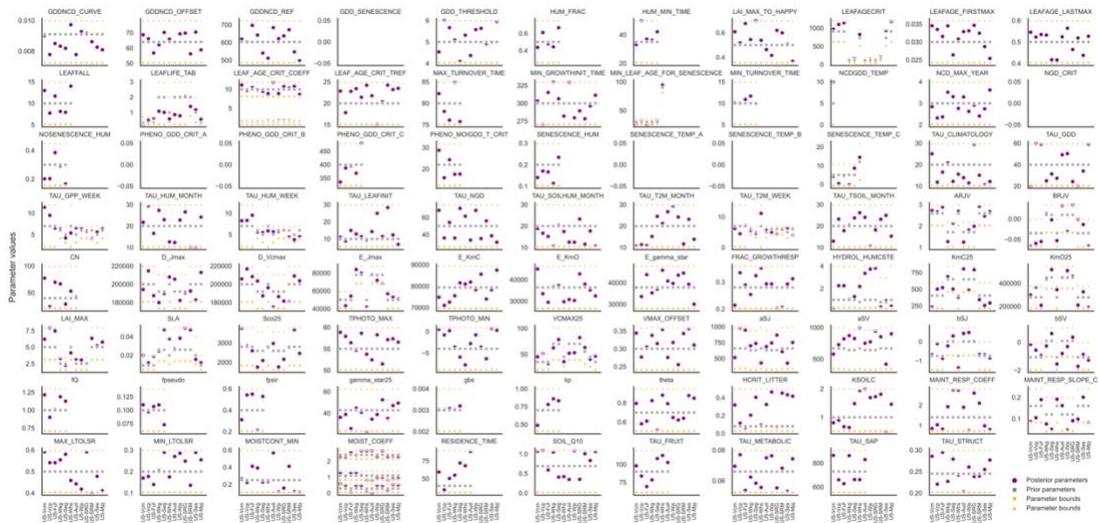


Figure S10. Values of all optimized parameters related to phenology, photosynthesis and post C uptake when assimilating NEE and optimizing all parameters (P1) for all 12 sites. For each parameter, the range of variation (corresponding to yellow arrows), the

prior and the posterior values are provided for all sites. For the mixed-PFT sites, only the parameters for the majority PFT fraction are presented, although the other PFT parameters are also optimized. For example, this figure shows the parameters associated with PFT=4 (TeNE) for site US-Mpj, however the optimization is performed with all the parameters of both PFT=4 (TeNE) and 11 (C4G). Note that the soil Q10 parameter is the exponent of the actual Q10 value used to calculate heterotrophic respiration temperature sensitivity (see **Table S1** for more information).