

1 **Optimizing Carbon Cycle Parameters Drastically Improves Terrestrial Biosphere**
2 **Model Underestimates of Dryland Mean Net CO₂ Flux and its Inter-Annual**
3 **Variability**

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18 **Key Points:**

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

25 Abstract

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

44 1 Introduction

45 Terrestrial ecosystems currently take up ~30% of anthropogenic CO₂ emissions, thus
46 acting as a substantial global carbon (C) sink (Fu et al., 2017) and providing a critical reduction
47 in the rate of global warming. However, while we know the magnitude of the global C sink to a
48 good degree of certainty, our knowledge of other components of the global C cycle are more
49 uncertain. One such knowledge gap is which ecosystems, and/or which processes, are driving
50 inter-annual variability (IAV) in land net C uptake (Fu et al., 2017). Improving our
51 understanding of the IAV characteristics of the global terrestrial C cycle is key to being able to
52 forecast the future of the land C sink and long-term biosphere-climate feedback (Cox et al.,
53 2013).

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

Model benchmarking and optimization studies that have been performed in dryland regions indicate considerable model-data discrepancies in vegetation dynamics, C and water fluxes (Haverd et al., 2013b; MacBean et al., 2015; Renwick et al., 2019; Trudinger et al., 2016; Whitley et al., 2016; Traore et al., 2014). MacBean et al. (2015) showed that calibrating the phenology parameters of the ORCHIDEE TBM (vAR5) using satellite NDVI at global scales could not account for model errors in semi-arid region seasonal cycle and long-term trends in vegetation dynamics. A recent study by MacBean et al. (in review) has demonstrated that global TBMs participating in the TRENDY v7 model intercomparison project drastically underestimate both the mean annual net ecosystem exchange (NEE) and its IAV at a suite of southwestern (SW) US dryland sites due to weak sensitivity of gross primary productivity (GPP) to changing water availability. This analysis is corroborated by (Renwick et al., 2019) who also showed that a semi-deciduous phenology scheme was necessary to accurately predict the magnitude of GPP in a dryland shrubland. SW US hydrology modeling studies have also suggested that parameter calibration is needed to realistically represent semi-arid water fluxes because the default parameters hamper model performance (Natasha MacBean et al., 2020; Hogue et al., 2005; Unland et al., 1996). Given the lack of model parameter calibration studies that have included dryland sites in their optimizations, it remains to be seen whether model-data discrepancies in dryland ecosystem NEE simulations are due to inaccurate model processes or uncertain parameters. Parameter uncertainty may be higher for dryland ecosystems given parameter values

85 were initially measured in the field and/or optimized for more mesic temperate and boreal
86 ecosystems.

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

101 Beyond investigating if the DA system could account for model-data discrepancies in
102 dyland NEE simulations, our second objective was to identify which parameters (therefore,
103 which processes) may be responsible for model errors. To address this objective, we performed
104 multiple optimization tests with combinations of parameters related to different model processes
105 in order to identify which processes were most influential in improving the model mean annual
106 NEE and IAV. We focused in particular on which processes are responsible for model failure to
107 capture NEE IAV. Our focus on improving NEE IAV was partly because of the dominant role
108 dryland ecosystems are thought to play in controlling global C cycle IAV, and partly because we
109 expected that, with the exception of sites that are a strong C sink, eddy covariance estimates of
110 mean annual NEE may be impacted by uncertainties in CO₂ flux partitioning. We identified three
111 main groups of parameters: parameters related to 1) phenology; 2) parameters related to
112 photosynthesis; and 3) parameters related to all process calculations that occur after gross C
113 uptake (i.e. C allocation, autotrophic and heterotrophic respiration, biomass and soil C turnover
114 and a scalar on the active soil C pool; hereafter grouped as “post C uptake” parameters). We split
115 the parameters into these three groups because GPP has been shown to be the dominant control

116 on dryland NEE IAV (MacBean et al., in review); therefore, we expected that optimizing
117 parameters related to one or both of the main two processes controlling GPP (i.e., phenology and
118 photosynthesis) will result in the strongest improvements in NEE IAV. However, optimizing all
119 parameters related to processes that occur after gross C uptake can also influence NEE;
120 therefore, we included these parameters as a third category. The parameters included in each
121 assimilation scenario are: P1 - all parameters, including all three phenology, photosynthesis and
122 post C uptake parameter groups; P2 - phenology and photosynthesis parameters; P3 - phenology
123 and post C uptake; P4 - photosynthesis and post C uptake; P5 - phenology parameters only; P6 -
124 photosynthesis only; and P7 - post C uptake only. See **Table 2** for a description of all parameters
125 and to which category they belong.

126 For all assimilation scenarios we compared the prior simulation (before parameter
127 optimization) to the posterior simulations (after parameter optimization, with different parameter
128 groupings for the different assimilation scenarios) by evaluating the simulations against the site
129 data using standard goodness of fit metrics (root mean square error, RMSE and correlation
130 coefficient, r) at daily, monthly and inter-annual timescales. We further attributed what might be
131 causing model-data misfits by decomposing the daily mean squared deviation (MSD) into its
132 component phase, variance and bias contributions. The bias, variance and phase indicate the
133 mean difference in flux magnitude, the mismatch in terms of the magnitude of fluctuations, and
134 the seasonality in flux time series, respectively (Kobayashi & Salam, 2000). All methods and
135 data are described in Section 2 and the results are presented and discussed in Section 3.

136 **2 Methods and Data**

137 **2.1 Study sites**

138 Twelve semi-arid eddy covariance flux sites in the southwestern US (SW US) have been
139 utilized in this study, with a measurement period ranging between 2003 and 2014. These sites
140 have a range of different vegetation types, climates, elevation and have been described in detail
141 by Biederman et al. (2017), so we only provide a brief description here. We summarize the sites'
142 description, dominant vegetation species, mean climate and corresponding vegetation plant
143 functional types (PFTs), together with the observation period and disturbance history (**Table 1**).
144 The sites are listed consecutively based on their mean annual C balance in Table 1. The major

145 regional IGBP vegetation classes represented include evergreen needleleaf forest, woody
 146 savanna, open and closed shrubland, and grassland. These sites typically experience monsoon
 147 rainfall during July to October, preceded by a hot, dry period in May and June. The SW US is
 148 characterized by water limitation at the annual scale, i.e. potential ET is greater than
 149 precipitation. The sites have large spatial gradients in mean annual precipitation (MAP 250–724
 150 mm) and temperature (MAT 2.9 to 17.7°C) due to interactions among topography, latitude, wind
 151 patterns, and distance from oceans. For further site details, see references in **Table 1** and
 152 individual site pages on www.ameriflux.lbl.gov.

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

Site ID	Description	Dominant species	IGBP class	PFT fractions	Koppen climate	Elevation (m)	MA P (mm)	MA T (°C)	Period of site data	Disturbance History	Site reference
US-Vcm	Valles Caldera mixed conifer forest	Picea engelmannii, Picea pungens, Abies lasiocarpa var. lasiocarpa, Abies concolor	Evergreen needleleaf forest	100% TeNE	Dfb	3042	724	2.9	2007–2012	Harvest 1960s	(Anderso n-Teixeira et al., 2011)
US-Vep	Valles Caldera ponderosa forest	Pinus ponderosa, Quercus gambeli	Evergreen needleleaf forest	100% TeNE	Dfb	2501	547	5.7	2007–2014	-	(Anderso n-Teixeira et al., 2011)
US-Mpj	Heritage Land Conservancy pinyon-juniper	Pinus edulis, Juniperus monosperma	Savanna	20% BS; 60% TeNE ; 20% C4G	Bsk	2200	423	9.6	2008–2014	-	(Anderso n-Teixeira et al., 2011)

US-Fuf	Flagstaff unmanaged ponderosa	Pinus ponderosa	Evergreen needleleaf forest	100% <u>TeNE</u>	Csb	2215	607	7.1	2006–2010	Harvest 1910	(Dore et al., 2012)
US-Wjs	Tablelands juniper savanna	Juniperus monosperma, Bouteloua gracilis	Savanna	15% <u>TeNE</u> ; 85% <u>C4G</u>	Bsk	1931	349	10.9	2008–2014	-	(Andersson-Teixeira et al., 2011)
US-Ses	Sevilleta creosote shrubland	Larrea tridentata, G. sarotheiae	Open shrubland	20% BS; 55% <u>TeBE</u> ; 25% <u>C4G</u>	Bsk	1610	252	12.6	2007–2014	-	(Petrie et al., 2015)
US-Wkg	Walnut Gulch Kendall grassland	Eragrostis lehmanniana, Bouteloua spp. Calliandra eriophylla	Grassland	60% BS; 3% TeBE; 37% <u>C4G</u>	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% <u>TeBD</u> ; 44% <u>C4G</u>	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 sarotheiae, Ceratoides lanata	Grassland	40% BS; 60% <u>C4G</u>	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% <u>TeBD</u> ; 15% <u>C4G</u>	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% <u>TeBE:</u> 3% C4G	Bsk	1376	352	16. 8	2008–2014	Drought 2005–2006	(Scott, 2010)
US-Aud	Audubon grassland	Bouteloua gracilis, B. curtipendula, Eragrostis spp.	Grassland	30% BS; 70% <u>C4G</u>	Bsk	1496	348	15. 7	2004–2009	Burned 2002	(Krishnan et al., 2012)

160 2.2 ORCHIDEE terrestrial biosphere model

161 We used the ORCHIDEE (ORganizing Carbon and Hydrology In Dynamic EcosystEms)
 162 process-oriented land surface model version 2.2 that has been developed at the IPSL (Institut
 163 Pierre Simon Laplace, France). The model is a state-of-the-art mechanistic terrestrial biosphere
 164 model (Krinner et al., 2005) and is the land surface component of the IPSLCM5 Earth System
 165 Model (Dufresne et al., 2013). The model describes the exchanges of water, carbon, and energy
 166 between biosphere and atmosphere at the smallest time scale (30 min), while the slow
 167 components of the terrestrial carbon cycle (including carbon allocation, autotrophic respiration,
 168 foliar onset and senescence, mortality and soil organic matter decomposition) are computed on a
 169 daily to annual basis. Version 2.2 is virtually identical to version 2.0, which is being used in the
 170 ongoing Coupled Modeling Intercomparison Project 6 (CMIP6) simulations, but includes few
 171 recent bug corrections and code enhancements. It has been updated since the “AR5” version used
 172 in CMIP5 (see Krinner et al., 2005) with the following developments: i) an 11-layer mechanistic
 173 description of soil hydrology and associated modifications as described in MacBean et al.
 174 (2020); ii) addition of a coupled carbon-nitrogen scheme (Vuichard et al., 2019); iii) an
 175 analytical solution for the set of equations for photosynthesis, stomatal conductivity and internal
 176 CO₂ concentration in the leaf (described in Vuichard et al., 2019), following (Yin and Struik,
 177 2009); iv) an update of the soil thermal properties and extension of the soil depth for heat
 178 diffusion (Wang et al., 2016); v) a 3-layer snow scheme (Wang et al., 2013); vi) a spatially
 179 explicit observation-derived estimate for background albedo and optimized vegetation and snow
 180 albedo coefficients;; vii) a new reconstruction of global land cover history and wood harvest

181 accounting following LUH2v2h maps (Hurtt et al., 2020) and PFT maps based the European
 182 Space Agency Climate Change Initiative Land Cover product (Poulter et al., 2015).

183 As in most TBMs, the vegetation is grouped into several plant functional types (PFTs),
 184 with 14 different types of vegetation plus bare soil in the case of ORCHIDEE v2.2. The original
 185 13 PFTs are reported in Krinner et al. (2005). Since ORCHIDEE v2.0 there are now two extra
 186 PFTs included: C3 grasses are now split into three groups - tropical, temperate and boreal. The
 187 equations governing individual processes are generic with PFT specific parameters, except for
 188 the phenology models (see Appendix A in MacBean et al., 2015)). In this study, ORCHIDEE
 189 was mainly used in a “grid-point mode” at each site location and forced with the corresponding
 190 local 30-minute gap-filled meteorological forcing data. Before performing the optimizations the
 191 modelled C stocks were brought to equilibrium in the spin-up phase by cycling the available site
 192 meteorological forcing over a long period (1300 years) with the default parameters of the model,
 193 which ensures a net carbon flux close to zero over annual-to-decadal time scales.

194 2.3 ORCHIDEE data assimilation system

195 The ORCHIDEE Data Assimilation System (ORCHIDAS) has been described in detail in
 196 previous studies (Bastrikov et al., 2018; Kuppel et al., 2014; MacBean et al., 2018; Peylin et al.,
 197 2016), and hence we only briefly define the method here. ORCHIDAS uses a variational data
 198 assimilation method to optimize the model parameters, accounting for uncertainties regarding the
 199 observations, the model, and the prior parameters. It relies on a Bayesian framework with the
 200 assumption of Gaussian errors, and the optimized parameters corresponds to the minimization of
 201 the following cost function $J(x)$ (Tarantola, 2005):

$$202 J(\mathbf{x}) = \frac{1}{2} [(\mathbf{H}(\mathbf{x}) - \mathbf{y})^T \cdot \mathbf{R}^{-1} \cdot (\mathbf{H}(\mathbf{x}) - \mathbf{y}) + (\mathbf{x} - \mathbf{x}^b)^T \cdot \mathbf{B}^{-1} \cdot (\mathbf{x} - \mathbf{x}^b)] \quad (1)$$

203 where x represents the parameters and $H(x)$ the model contingent on the parameters, and
 204 y the observations. The cost function contains both the misfit between observations, and
 205 corresponding model outputs (first term on the right hand side of Eq. 1), and the misfit between a
 206 priori parameter values x_b and optimized parameters x (*second term on the right hand side of the*
 207 *Eq. 1*). R is the observation error covariance matrix (including measurement and model errors),
 208 and B is the prior parameter error covariance matrix. Both matrices (B and R) are diagonal since

observation and model errors are assumed to be uncorrelated in space and time, and parameters are assumed to be independent. The cost function is iteratively minimized using the genetic algorithm (GA), which is a meta-heuristic optimization algorithm and follows the principles of genetics and natural selection (Goldberg et al., 1989; Haupt et al., 2004). The GA algorithm has been applied previously with ORCHIDAS tool and described in details by Bastrikov et al. (2018). Briefly, the algorithm works iteratively and considers the vector of parameters as a chromosome and each parameter as a gene on that chromosome. The method fills a set of n chromosomes at every iteration, having the starting pool as a randomly perturbed parameter pool. The chromosomes at each subsequent iteration are chosen from randomly selected chromosomes of the previous iteration by either “crossover” or “mutation” process. Santaren et al. (2014) showed that the performance of the algorithm is highly sensitive to its specific configuration and found the best configuration based on computational efficiency after testing different options. Here, we used the same configuration (i.e. number of chromosomes in the pool total number of parameters optimized; the number of iterations is 40; crossover/mutation ratio is 4:1; the number of gene blocks exchanged during crossover is 2 and the number of genes perturbed during mutation is 1) applied by Santaren et al. (2014) and Bastrikov et al. (2018). The algorithm does not assume prior knowledge of Gaussian PDFs for the observation and parameter uncertainties. Given we do not fully know the model uncertainty, we set the prior observation uncertainty as the RMSE between the model and the observations following Kuppel et al. (2014). The prior parameter uncertainty is listed in Table S1.

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

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

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

2.4 Flux measurements

At all twelve SW US sites, flux tower instruments collect 30-minutes measurements of meteorological forcing data and eddy covariance measurements of net surface energy and carbon exchanges, which are available from the AmeriFlux data portal (<http://ameriflux.lbl.gov>).

237 Meteorological forcing data included air temperature and surface pressure, precipitation,
238 incoming long and shortwave radiation, wind speed, and specific humidity. To run the
239 ORCHIDEE model, we partitioned the in-situ precipitation into rain and snowfall using a
240 temperature threshold of 0°C. The site-level meteorological forcing data were gap filled utilizing
241 downscaled and corrected ERA-Interim data following the approach of Vuichard & Papale
242 (2015). Gross primary productivity (GPP) and the ecosystem respiration (R_{eco}) were estimated
243 from the net ecosystem exchange (NEE) via the flux partitioning method described in Biederman
244 et al. (2016). We acknowledge that GPP and R_{eco} are not fully independent data with respect to
245 NEE and are essentially model-derived estimates, but these concerns have been largely discussed
246 in previous studies e.g., Desai et al. (2008). Note that in this study, negative NEE refers to net
247 CO₂ uptake into the ecosystem. In order to exclude the influence of the short-term variations in
248 the fluxes on the model optimization, the daily averaged observations smoothed with a 15-day
249 running mean were used in the assimilation as per Bastrikov et al. (2018).

250 2.5 Parameters optimized

251 The optimized parameters are described in Table S1 with their prior values, prior
252 uncertainty, and upper and lower bounds for different plant functional types based on literature
253 analysis, parameter databases and expert knowledge of the model equations. Prior values are the
254 default parameter values used in all non-optimized ORCHIDEE simulations. In the most past
255 ORCHIDAS studies with previous versions of ORCHIDEE, only subsets of ORCHIDEE C cycle
256 parameters have been optimized (Bastrikov et al., 2018; Kuppel et al., 2012, 2014; MacBean et
257 al., 2015; MacBean et al., 2018; Santaren et al., 2007; Verbeeck et al., 2011). In this study, we
258 considered all possible C cycle related ORCHIDEE parameters to fully explore all sources of
259 parameter uncertainty that is contributing to uncertainties in modeled net and gross CO₂ fluxes.
260 We further allowed weak constraints in the DA system (i.e., large prior parameter bounds, albeit
261 within realistic limits) because the main objective of our study was to determine if parameter
262 calibration can account for model-data errors and to use our assimilation scenario tests to identify
263 which processes are responsible for model-data errors. We selected all 102 parameters and
264 divided them into four classes, controlling the main C cycle and plant physiological processes
265 i.e. photosynthesis, conductance, phenology and post C uptake. This resulted in 31 parameters
266 related to photosynthesis, 42 to phenology, 16 to post C uptake (C allocation, respiration,

267 biomass and soil turnover), and 13 related to conductance. In a preliminary study, we tested at
 268 several SW US sites (US-Vcp, US-Mpj, US-Fuf, US-Wkg, US-Whs, US-Seg) the sensitivity of
 269 the ecosystem fluxes (NEE, GPP and R_{eco}) when optimizing all model parameters and when we
 270 just optimized subsets of the parameters related to each of the main processes. This test showed
 271 no significant optimization improvement by adding the conductance related parameters (results
 272 not shown here), and thus we did not include those parameters for all final optimizations
 273 presented in this study, leaving a total of 89 optimized parameters for each site. Documentation
 274 on the parameters can be accessed via ORCHIDEE webpage
 275 (<https://forge.ipsl.jussieu.fr/orchidee/wiki/Documentation/OrechideeParameters>, last access: 04
 276 January 2021). The prior uncertainty was set to 40% of the bounds for each parameter following
 277 previous ORCHIDAS studies (Kuppel et al., 2012; MacBean et al., 2015).

278 2.6 Assimilation Scenarios

279 We conducted several different assimilation scenarios to identify which processes (and
 280 their related parameters) are potentially causing model-data discrepancies (listed in Table 2). We
 281 grouped the optimizations based on various parameters set to optimize; therefore, we tested 7
 282 assimilation scenarios (P1 – P7): P1 included all 89 parameters, whereas each consecutive
 283 scenario (P2 – P7) optimized different subsets of parameters related to each of the main C cycle
 284 processes (Table 2). The parameters that were not optimized were set to their default (prior)
 285 value. Comparing the P1 to P7 assimilation scenarios allows us to determine which sets of
 286 parameters (i.e. specific processes) are contributing most to the improvement in fluxes as a result
 287 of the parameter optimizations and therefore provides insight into which model processes may
 288 need further modification or development. See Table S1 for groupings of model parameters
 289 according to specific processes.

290 **Table 2.** Description of the different assimilation scenarios conducted in this study. The included
 291 parameter group(s) and numbers of parameters for each assimilation scenario are given.
 292 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

293 2.7 Post-optimization analysis

294 We assessed the goodness of fit of the different assimilation scenarios by the mean square
 295 deviation (MSD) (in addition root mean squared error, RMSE or correlation coefficients, R and
 296 the slope of linear least-square regression). Model evaluation metrics are presented in one of
 297 three ways: i) for each site; ii) grouped across all sites; and iii) sites grouped according to their
 298 mean net annual CO₂ flux characteristics across the observed time period as in Biederman et al.
 299 (2017). For the latter, the net CO₂ “sink” sites are US-Vcm, US-Vcp, US-Mpj, US-Fuf and US-
 300 Wjs; the “pivot” sites are US-Ses, US-Wkg, US-SRG, US-SRM, US-Whs, US-Seg; and the
 301 “source” site is US-Aud. We followed the approach of Kobayashi & Salam (2000) to quantify
 302 the differences between the simulations and observation in terms of bias, variance and phase
 303 contributions to the overall mean squared deviation (MSD). We calculated the MSD between
 304 daily model and observed time series and decompose it following the below equation:

$$305 \quad MSD = \frac{1}{n} \sum_{i=1}^n (x_i - y_i)^2 = (\bar{x} - \bar{y})^2 + (\sigma_x - \sigma_y)^2 + 2\sigma_x\sigma_y(1 - R) \quad (3)$$

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

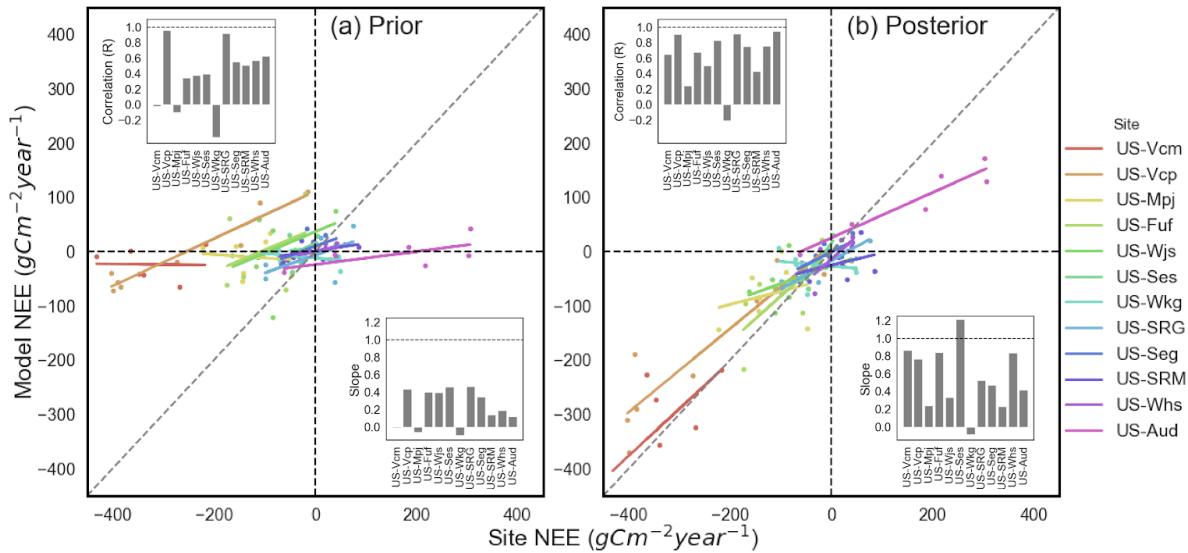
308 The first term specifies the bias between model simulation and observation (squared).
 309 The second “variance” term measures their differences in terms of variability (i.e., the difference
 310 between the magnitude of the modeled and observed fluctuations). The third term in Eq. 3
 311 generally demonstrates the lack of correlation between model and observations weighted by their
 312 standard deviations, which can be deemed a measure of their disagreement in terms in phase
 313 (Bacour et al., 2019; Gauch et al., 2003). We further calculated the contribution of each

314 component (bias, variance and phase) to the overall MSD by dividing each component by the
315 total MSD.

316 **3 Results**

317 **3.1 Impact of optimization of all parameters (P1) on model net and gross CO₂ fluxes**

318 Across all sites, the prior ORCHIDEE simulations (i.e. before parameter optimization)
319 fail to capture both the mean annual NEE at mean C sink and source sites and the NEE IAV
320 across all sites (**Figure 1a**) - as also seen for all TRENDY TBMs in MacBean et al (in review).
321 Across all sites, optimizing all C cycle-related parameters (phenology, photosynthesis and post C
322 uptake - assimilation scenario P1) with NEE data dramatically increases the ability of the model
323 to capture both the mean C source/sink behavior and the IAV (**Figure 1b**). C sink and source
324 sites show significant improvement in terms of both mean annual NEE and IAV. There is not a
325 strong bias in the model simulations at pivot sites whose mean annual NEE is close to zero;
326 therefore, the optimization results in an improvement mainly in IAV (as represented by the
327 correlation and slope values shown in inset figures in Figures 1 a and b). Improvement of the
328 model-data fit resulting from the assimilation is evident across all sites, with a reduction of daily
329 NEE RMSE between 0.05 to 0.65 gCm⁻²d⁻¹ (**Figure S1**), with a similar reductions in daily GPP
330 and R_{eco} RMSE (Table S2). Moreover, the temporal dynamics are well captured for all the sites:
331 when optimizing all parameters, the median pearson correlation coefficients (R) increase by
332 0.45, 0.45, and 0.25 for daily, monthly and annual modeled NEE, respectively and posterior
333 median slope values ≥ 0.5 (**Figure S2a and d**). GPP temporal dynamics are also much improved
334 by the P1 assimilation with a higher and tighter range in posterior R and slope values than NEE
335 (**Figure S2b and e**). In contrast, there is less improvement in R_{eco} temporal dynamics although
336 the median R and slope values are higher after the optimization (**Figure S2c and f**).



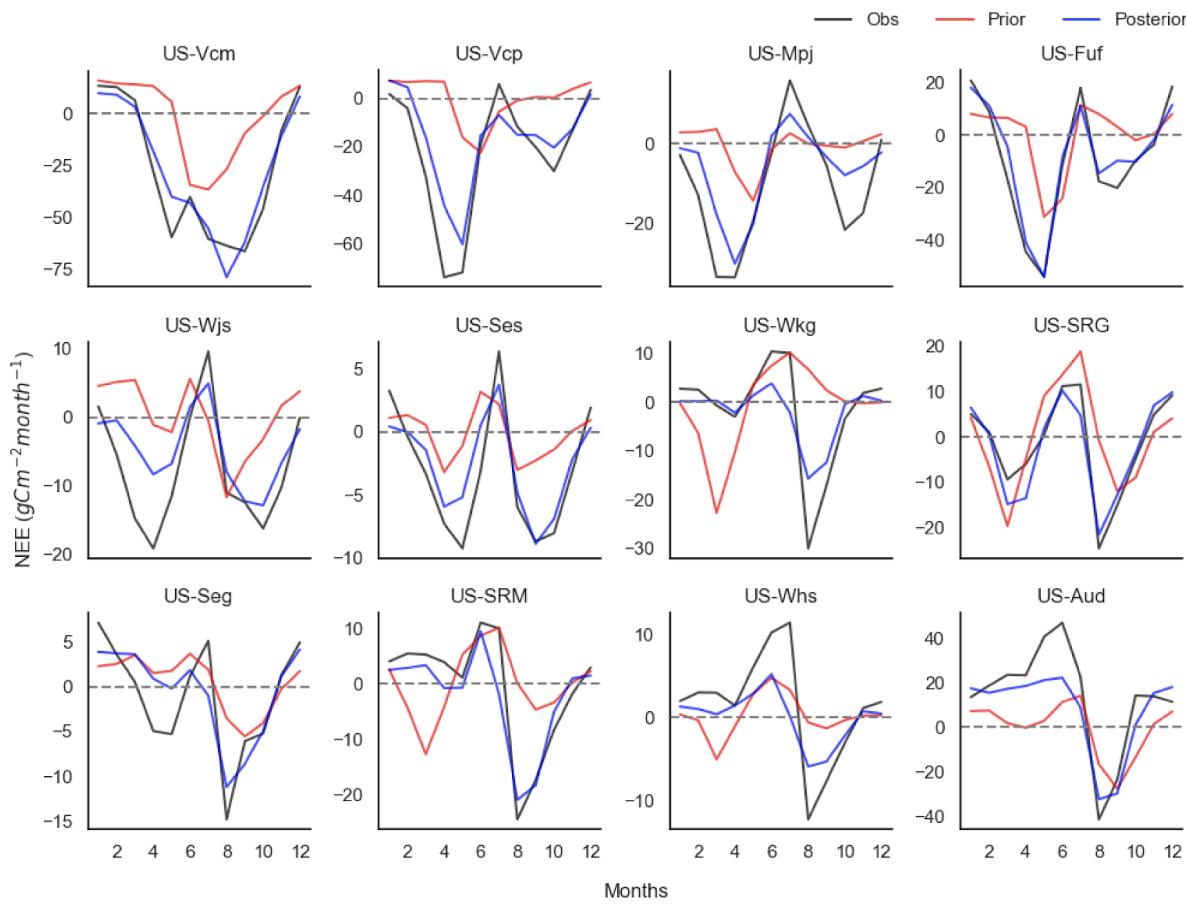
337

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

350

351 Across the majority of the sites, the prior model simulates a depressed seasonal NEE
 352 amplitude and/or is unable to capture the observed bi-modal seasonality (**Figure 2**). The NEE
 353 amplitude and bi-modal seasonality generally improved when optimizing all parameters (blue
 354 curves in **Figure 2**), although the posterior simulations struggle to reach the exact magnitude of
 355 the spring and monsoon NEE troughs (net CO_2 uptake) for several sites (e.g. US-Mpj, US-Wjs,
 356 US-Ses, US-Seg, US-Wkg and US-Whs). Accurately capturing the seasonal peaks and troughs is
 357 important for replicating observed NEE IAV because variability in summer monsoon season
 358 fluxes are the dominant driver of NEE IAV (MacBean et al., in review). While posterior seasonal
 359 NEE peaks and troughs are generally well captured, the assimilation of NEE alone often fails to
 360 capture the correct peaks in gross CO_2 fluxes (**Figure S3**), likely due to compensating errors in

361 both GPP and R_{eco} . At the C source site (US-Aud) the model also fails to simulate the accurate
 362 peaks in springtime net carbon release (**Figure 2**). This is due to the fact that at US-Aud, TBMs
 363 tend to overestimate spring GPP and underestimate the earlier rise in spring R_{eco} (**Figure S3**).
 364 The optimization only partially corrects these model biases, suggesting that other missing
 365 processes may ultimately be responsible for the model-data misfit (such as disturbance following
 366 a fire that occurred at the site in 2002, which is not implemented in the current version of
 367 ORCHIDEE).

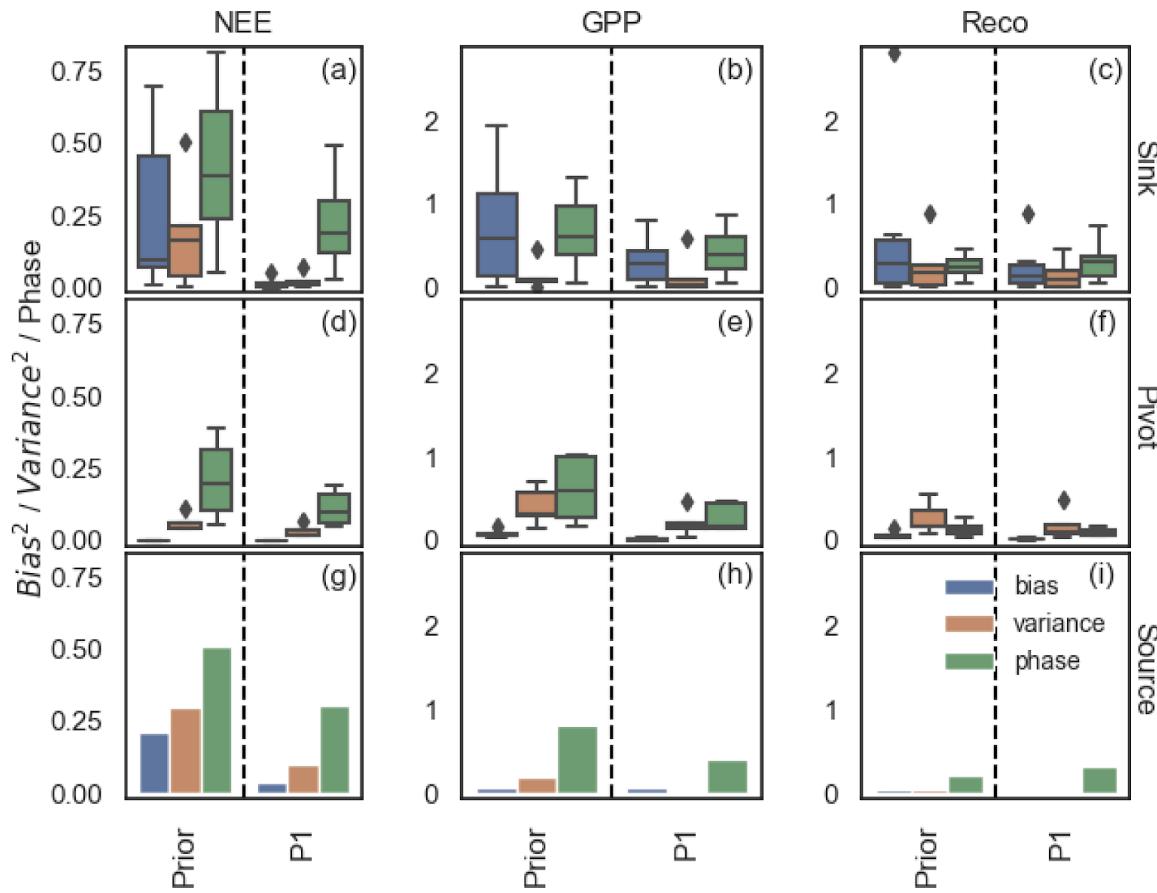


368

369 **Figure 2.** Mean monthly NEE seasonal cycles for each site comparing prior (red curve) and
 370 posterior (blue curve) ORCHIDEE simulations with observations (black curve). Posterior
 371 simulation after assimilation of NEE data and optimization of all parameters: phenology,
 372 photosynthesis and post C uptake (P1). The sites are listed in order from largest mean annual C
 373 sink (US-Vcm) to mean annual C source (US-Aud).

374

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



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

402

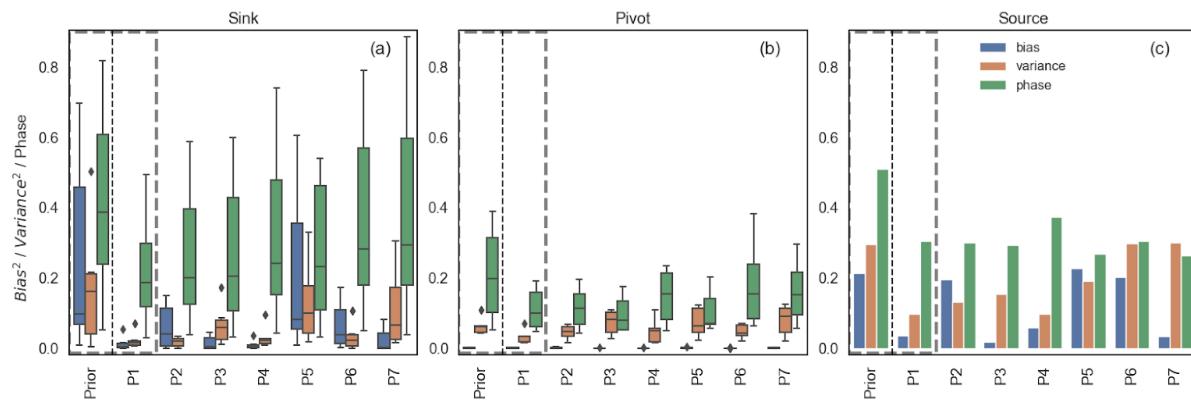
403 As for the NEE, bias and phase are the dominant contributors to prior daily GPP MSD for
 404 the sink sites (left of vertical dashed line in **Figure 3b**), and phase only for the pivot and source
 405 sites (**Figures 3e and h**). For R_{eco} , a different MSD component is dominant depending on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

412

413 3.2 Impact of different processes (assimilation scenarios) on optimization results

414 Across all sites, modeled annual and seasonal NEE are improved the most in the P1
 415 assimilation scenario compared to the other assimilation scenarios (P2 to P7), although all
 416 scenarios result in some improvement (**Figures S5, S6a and d**, and seasonal cycles in **Figure**
 417 **S7**). In general, there is less improvement in R_{eco} compared to NEE and GPP (**Figure S6**).
 418 Comparing the MSD decomposition results for the various assimilation scenarios (P1-P7) can
 419 help to identify which processes may be causing the prior model-discrepancies in mean annual
 420 NEE and NEE IAV. At the source and sink sites, the bias component (blue bars in **Figure 4a**
 421 **and c**) is reduced dramatically by all optimization tests that include the post C uptake parameters
 422 related to C allocation, respiration, and aboveground biomass and soil C turnover (P1, P3, P4 and
 423 P7). For the sink sites, assimilation scenarios that also include photosynthesis parameters (P2 and

424 P6) also result in a strong reduction in bias. This decrease in mean bias is also shown by the fact
 425 that the midpoints of the linear regression trendline between model and observations at forested
 426 sink sites (US-Vcm, US-Vcp, US-Mpj, and US-Fuf) and low-elevation source site (US-Aud)
 427 with optimization scenarios P1 to P4, P6 and P7 parameters all lie much closer to the 1:1 (grey
 428 dashed) line compared to P5 (**Figure S5**).



429

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

445

446 Across all sites the difference in phase between the model and observations (green bars in
 447 **Figure 4**), which, as already noted, is the largest contribution to the prior NEE MSD across all
 448 sites, is mostly reduced by assimilation scenarios that include phenology parameters (i.e. P1, P2,
 449 P3 and P5). The P4 assimilation (photosynthesis and post C uptake parameters) also does well in
 450 reducing phase contributions to NEE MSD at forested C sink sites (Figure 4a). However, the
 451 phase component is not reduced as much as the bias in any of the assimilation scenarios; thus, for

452 all sites and all assimilation scenarios the phase remains the largest component of the posterior
453 daily NEE MSD (**Figure 4**). Including parameters related to photosynthesis or post C uptake
454 with the phenology parameters (i.e. assimilation scenarios P2 and P3) helps to slightly reduce the
455 phase discrepancy at sink sites compared with phenology parameters alone (P5) (as seen above
456 for the improvement in slope values at the sink sites). Examining the spread in slope and R
457 values across all sites, we see that the annual variability (median slope and R values) is improved
458 the most for assimilation scenarios with at least two parameter sets (P1 to P4 - **Figure S6a and**
459 **d**). The persistence of phase as the dominant component of the posterior daily NEE suggests
460 further model improvement in processes related to dryland vegetation temporal dynamics (e.g.
461 phenology and all associated processes) is needed before TBMs can correctly reproduce NEE
462 seasonality and IAV.

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

468 While the post C uptake parameters are key for reducing bias in forested sink site NEE,
469 biases in GPP and R_{eco} at these sites are reduced by optimizing photosynthesis parameters (P1,
470 P2, P4, and P6 - blue boxes **Figure S8b and c**). The GPP and R_{eco} bias components at the sink
471 sites are not reduced as strongly as NEE biases for any assimilation scenario; thus, bias remains a
472 key contributor to posterior gross CO₂ flux MSD. Similarly to NEE, parameter subsets that
473 include phenology parameters (P1, P2, P3 and P5) are key for reducing the daily GPP MSD
474 phase component at pivot sites (green boxes in **Figure S8e**; however, in contrast with the NEE
475 results, at sink sites the GPP phase component tends to be reduced by all assimilation scenarios
476 except P7 (see also median GPP slope and R values in **Figures S6b and e**). With the exception
477 of P1 and P2 for GPP, the GPP and R_{eco} variance components are not reduced much by any of
478 the assimilation scenarios and remain a considerable component of the MSD for both GPP and
479 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
480 R_{eco} reductions in MSD components tend to be similar, suggesting model-deficiencies in R_{eco} are
481 mainly influenced by those in GPP. Addressing GPP model-data deficiencies is therefore a high
482 priority.

483 3.3 Constraint on parameters

484 For all assimilation scenarios, we found significant parameter deviations from prior
485 values for numerous phenology, photosynthesis and post C uptake related parameters (**Figure 5**),
486 which is consistent with the fact that all parameter subsets are needed to improve model mean
487 annual NEE and IAV. Parameter deviation was calculated using the difference between the
488 posterior and prior parameter value normalized by the total parameter variation used in the
489 optimization. Finally, the median value was taken as the mean deviation from all 12 sites. We
490 did not find that parameters deviate more, or the uncertainty reduction (calculated as $1 -$
491 (posterior parameter uncertainty / prior parameter uncertainty)) was much different, when only
492 one subset or two parameter subsets were included in the optimization instead of all three (e.g.
493 cf. P2 with P1), although posterior values are different for each assimilation scenario (**Figure 5**).
494 In particular, most of the post C uptake parameters deviate strongly from the prior median
495 deviations (>20% of total parameter bound). There are also significant uncertainty reductions
496 (>50%) for most of the parameters which show strong deviations from their prior value: 10 for
497 phenology (out of 42), 7 for photosynthesis (out of 31) and 7 for post C uptake (out of 16)
498 (**Figure 5**). The error correlations between the estimated parameters are usually minimal except
499 between post C uptake parameters (see example for one site in **Figure S9**).
500

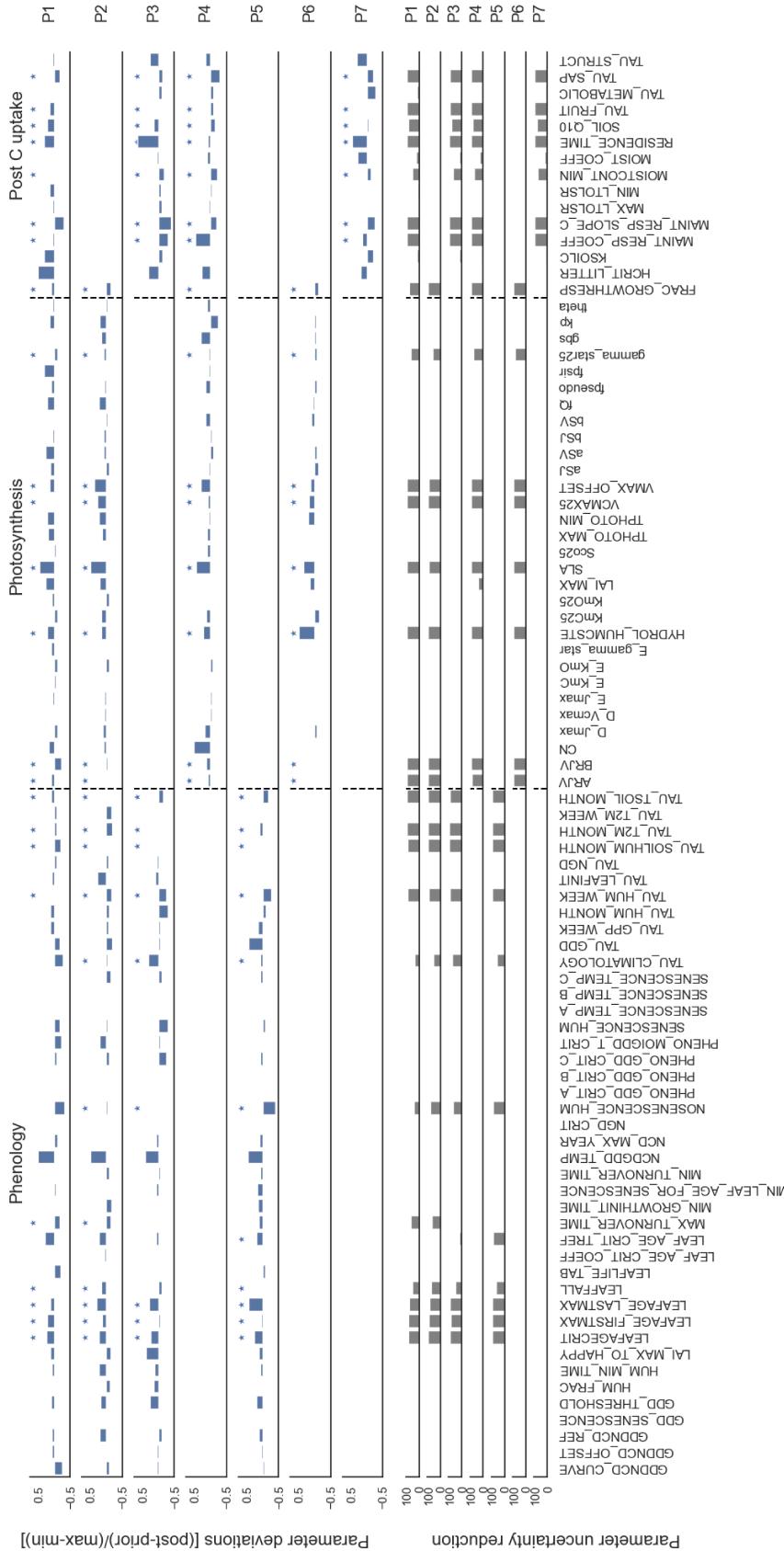


Figure 5. Optimized median parameter deviations [$(\text{posterior} - \text{prior}) / (\text{max} - \text{min})$] (blue bars) and associated median parameter uncertainty reductions (grey bars) for all parameters controlling phenology, photosynthesis and post C uptake assimilating NEE data (P1-P7). Bars represent the median across all 12 sites. The asterisks above blue bars indicate the parameters that have larger than 50% uncertainty reduction. Each line corresponds to a specific optimization test (shown on the right axis). The parameters are given on the bottom axis. The vertical dashed lines separate the different parameter subsets (phenology, photosynthesis and post C uptake). **Table S1** details the prior and posterior parameter values and their uncertainty for all parameters together with the maximum and minimum bounds used in the optimizations.

502 Certain phenology parameters are important across all assimilation scenarios: i)
503 parameters related to leaf age; ii) a parameter related to the critical temperature threshold for the
504 start of deciduous shrub leaf growth (ncdgdd_temp); iii) moisture thresholds that govern C4
505 grass senescence (nosenescence_hum); and iv) various parameters that control the time scales
506 used in phenology schemes (e.g. tau_climatology, tau_hum_week) (**Figure 5**). The phenology
507 models are highly dependent on such empirical parameters, which likely need to be optimized
508 for each site. Key photosynthesis related parameters are SLA, parameters involved in the
509 calculation of $V_{c,max}$ (the maximum carboxylation rate, which has been shown to be a highly
510 sensitive model parameter in previous studies, e.g. Kuppel et al., 2014), and the parameter that
511 represents the root profile in the empirical calculation of leaf water stress (hydrol_humcste),
512 which downregulates photosynthesis and stomatal conductance in the dry season. The most
513 important post C uptake parameters are fairly similar across assimilation scenario tests, and are
514 related to: i) the calculation of the maintenance respiration as a fraction of biomass; ii)
515 aboveground biomass residence time and various turnover rates for biomass and litter pools; and
516 finally, iii) the Q10 parameter involved in the temperature dependence of soil C decomposition
517 (**Figure 5**).

518 **4 Discussion and Conclusions**

519 In this study, we have shown that it is possible to account for model discrepancies in both
520 the mean annual NEE and NEE IAV at a range of semi-arid SW US sites via optimization of C
521 cycle parameters within a Bayesian DA framework. We used weak prior constraints (i.e. large
522 prior parameter bounds) to give the assimilation the maximum chance to correct any model
523 errors. Our goal was not to identify the ideal “correct” set of C cycle parameters for capturing
524 semi-arid vegetation and C cycle dynamics, but rather to identify whether, within the current
525 model representation, we could account for model-data mismatches. Looking at the individual
526 parameter plots for the P1 assimilation scenario (**Figure S10**), we find that at some sites several
527 posterior parameters are “edge-hitting” (e.g. soil Q10). Given we chose weak prior constraints in
528 the assimilation, the fact that some posterior parameters are hitting their bounds suggests that the
529 optimization may be aliasing model structural error onto the parameters (as demonstrated in
530 MacBean et al., 2016) and/or that the model cannot improve further via parameter optimization.

531 This suggests that further model developments are likely needed to address structural
532 uncertainties and missing processes.

533 Hypotheses as to which processes might be responsible for model inability to capture
534 semi-arid CO₂ fluxes are numerous and will take time to explore fully (MacBean et al., in
535 review). Here, we aimed to speed up that process by using the different assimilation scenarios as
536 tests of which parameter sets (and therefore, which processes) may be responsible for model
537 errors. The assimilation with all C cycle and vegetation parameters (P1) performed the best in
538 terms of correcting underestimates in modeled mean annual NEE and IAV. However, the
539 additional assimilation scenarios (P2 to P7) further demonstrated that phenology parameters are
540 likely key for improving semi-arid ecosystem NEE IAV. Issues with semi-arid phenology in
541 TBMs have been documented elsewhere (Traore et al., 2014; Dahlin et al., 2015; MacBean et al.,
542 2015; Renwick et al., 2019; Whitley et al., 2016; Teckentrup et al., in review). Further evidence
543 for inadequate TBM phenology schemes comes from MacBean et al. (2020), who noted that
544 while the ORCHIDEE model can capture evapotranspiration (ET) fluxes extremely well, even
545 without parameter optimization, the model simulates a delayed increase in transpiration/ET
546 (T/ET) ratios during the summer monsoon when compared to two independent T/ET estimates.
547 This suggests that the model is getting ET right for the wrong reasons – i.e. the partitioning of
548 ET into its component fluxes of T and bare soil evaporation is incorrect. This lagged response of
549 T to increasing rainfall is consistent with the results of MacBean et al. (in review) who found
550 across a suite of TBMs (TRENDY v7) too weak ecosystem-scale water use efficiency (WUE) –
551 i.e. a too weak response of GPP to increasing ET – during the monsoon was likely the cause of
552 their inability to capture NEE IAV. Put simply, the models simulate too weak a response of
553 vegetation growth to pulses of moisture availability. Thus, the evidence from all these studies,
554 including our results presented here, is pointing to issues with phenology, plant hydraulics,
555 and/or the fraction of vegetation prescribed in the model. As noted by MacBean et al. (2020), the
556 static PFT fractions prescribed in the models likely prevent monsoon season growth of summer
557 annual C4 grasses in the interstitial bare soil patches. Errors in PFT fractions in sparsely
558 vegetated regions have also been shown to propagate into large model errors in simulated
559 carbon, water and energy fluxes (Hartley et al., 2017). The optimization of numerous phenology
560 parameters with weak constraints in this study could be partially accounting for such a model
561 error. But it is also possible that this issue of static PFT fractions explains even the posterior

562 model's inability to capture peak GPP fluxes for some sites (see Section 3.1), and the fact that in
563 the posterior simulations, the phase remains the strongest contribution to the NEE MSD.

564 The same Bayesian DA system was used by MacBean et al (2015) to correct phenology
565 model issues in a previous version of ORCHIDEE that was nonetheless identical in its
566 representation of phenology. However, while they were able to correct the seasonal leaf
567 dynamics in temperate and boreal ecosystems, they found the parameter optimization was unable
568 to correct for phenology model issues in semi-arid ecosystems. While the data they used were
569 different – normalized difference vegetation index (NDVI) from the MODIS satellite instrument
570 as opposed to the flux tower NEE used here – they also used stronger prior constraints and fewer
571 phenology parameters, suggesting that the additional degrees of freedom in the assimilations in
572 this study (from weaker prior constraints and a greater number of phenology parameters) may
573 have resulted in the improvements from the parameter optimization. Still, as we noted above, the
574 combination of weak prior constraints and edge-hitting posterior parameters suggests the
575 assimilations are accounting for other structural errors in the model, and phase errors remain a
576 strong source of NEE MSD even after optimization. As also noted, the phenology schemes in
577 these models are highly dependent on a number of empirical parameters that require site
578 calibration and which were typically not developed for dryland ecosystems. Future developments
579 in this area should take account of the variety of different strategies in dryland plants for dealing
580 with water stress (Smith et al., 2012).

581 MacBean et al. (in review) also presented a range of other hypotheses as to which
582 processes might be causing model errors in capturing semi-arid phenology other than the need to
583 represent summer annual C4 grass fractional cover and phenology, including: the lack of
584 drought-deciduous shrub phenology schemes in TBMs; the lack of deep tap shrub and tree roots
585 that draw up groundwater needed for growth during drier periods; and the lack of dynamic root
586 growth as moisture becomes more available. Future studies need to systematically test all of the
587 proposed hypotheses to determine which, if any, can explain the observed model-data
588 discrepancies.

589 Our assimilation tests also showed that so-called “post C uptake” parameters related to
590 maintenance respiration, biomass and litter turnover, and soil C decomposition are mainly
591 responsible for reducing the strong model underestimate of mean annual NEE, particularly at the

higher elevation forested C sink sites. We did not focus on correcting mean annual NEE, and instead focused more on correcting errors in NEE IAV, because the variability in eddy covariance measurements of NEE are more trusted than the absolute values due to errors in flux partitioning. Furthermore, for the semi-arid sites that pivot between a C source and sink, their mean sink versus source behavior may be a function of a time period involved. In particular, the only mean C source site (US-Aud) is likely a source because of a fire in 2002 from which the site was still recovering during the measurement period. As discussed, we know that even TBMs that include wildfire modules will likely not reproduce the specific impacts of an individual fire. Nevertheless, while we do not focus on the C source site, we do know that the high elevation forested sites in this study are consistently sinks of C, even during the drought period that has been affecting the SW US for most of this century (Scott et al., 2015). It is important that we are able to capture this dryland forested site C sink, particularly given these ecosystems have been shown to contribute to long-term trends in the global C cycle (Ahlstrom et al., 2015). Drylands are vulnerable to future increases in drought, which may reduce the C sink (Bodner and Robles, 2017). On the other hand, drought impacts on dryland vegetation could be mitigated by increases in WUE and vegetation growth under elevated CO₂ (e.g. Donohue et al., 2013). Thus, it is an important contribution that parameter optimizations presented here can account for these biases in modeling C sinks at high elevation forested sink sites. MacBean et al. (in review) postulated that TRENDY TBM underestimates in mean annual NEE at these sites was due to underestimates in spring GPP, possibly due to issues with model snow melt not providing enough moisture for spring growth. In contrast, the results presented here suggest that the issues at the high elevation forested sink sites may be more linked to processes that occur after the gross uptake of CO₂, such as maintenance respiration, biomass turnover, and temperature limitation on soil C decomposition (**Figure S11**). If true, it may be that the processes in TBMs can accurately capture dryland forested site photosynthesis if the parameters are better adapted for dryland PFTs, which simply requires more careful calibration across a range of dryland forest sites.

As discussed in the introduction, we have focused on correcting parameters related to GPP because MacBean et al. (in review) found that GPP, and particularly summer monsoon season GPP, is the dominant driver of NEE IAV. We also are obliged to focus on GPP parameters because the number of model parameters is higher for GPP. In a follow up study, we

623 are assessing how the number of parameters linked to each different process affects the ability of
624 the optimization to correct for errors in those processes. We may find, for example, that the sheer
625 number of parameters related to phenology that are included here results in those parameters
626 being the more important for correcting NEE IAV. This then becomes an issue of wider model
627 development because we can only include in the optimization that are in the model. Still, the fact
628 that the relatively few “post C uptake” parameters included in the assimilation tests carried out in
629 this study can account for biases in mean annual NEE suggests that the number of parameters
630 linked to each process does not prevent us from identifying which set of parameters (and
631 processes) are mostly causing model-data discrepancies. It is still possible that those parameters
632 are accounting for other structural errors in the model, as we have discussed above. The specific
633 DA configuration (e.g. type of data included – e.g. net or gross CO₂ fluxes, the number of
634 parameters included, and to which processes they are related) can lead to different posterior
635 values and degree of improvement in model-data fit. Therefore, further tests of different DA
636 configurations and optimizations at other locations are needed to explore the potential of
637 Bayesian DA systems for quantifying and reducing error in semi-arid ecosystem C fluxes. While
638 we have particularly highlighted one key area of the model that needs improvement (dryland
639 phenology schemes and associated processes related to plant water availability), we have also
640 shown that all C cycle model parameters and processes in semi-arid ecosystems need either
641 optimizing or further development by TBM groups. Only by addressing these issues will we be
642 able to reliably use these models to accurately simulate dryland contributions to IAV and long-
643 term trends in the global C cycle.

644

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658 providing the ORCHIDEE version used in this study.

659

660 **Code availability**

661 The ORCHIDEE model is under a free software license (CeCILL; see
662 <http://www.cecill.info/index.en.html>) and the source code is visible here:
663 <https://forge.ipsl.jussieu.fr/orchidee/browser/tags/ORCHIDEE>. The ORCHIDEE model code is
664 written in Fortran 90 and is maintained and developed under an SVN version control system at
665 the Institute Pierre Simon Laplace (IPSL) in France. The ORCHIDAS code is currently in the
666 process of being put on a GitHub repository but for now it is available on request to
667 vladislav.bastrikov@lsce.ipsl.fr.

668

669 **Data availability**

670 Meteorological forcing data and eddy covariance measurements of net surface energy and
671 carbon exchanges at 30-minutes intervals are available from the AmeriFlux data portal
672 (<http://ameriflux.lbl.gov>). The model outputs from ORCHIDEE simulations and post-processing
673 python scripts for manuscript figures and tables are freely available in a Git repository
674 (https://github.com/kashifmahmud/SW_US_semiarid).

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