Supplementary information for Evaluation of carbonyl sulfide biosphere exchange in the Simple Biosphere Model (SiB4)

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Table S1. Site information of long-term CO_2 flux measurements from FLUXNET, AmeriFlux or ICOS, including mean annual temperature (MAT) and mean annual precipitation (mm).

	Network	Lat (°N), Lon (°E)	Years	MAT (°C)	MAP (mm)	Reference
Hyytiälä, Finland (FI-HYY)	ICOS	61.8, 24.3	1996-2018	3.8	709	Kolari et al. (2009)
Sorø, Denmark (DK-SOR)	ICOS	55.5, 11.6	1996-2018	8.2	660	Pilegaard et al. (2011); Wu et al. (2013).
Neustift, Austria (AT-NEU)	FLUXNET-2015	47.1, 11.3	2002-2012	6.5	852	Wohlfahrt et al. (2008) DOI:10.18140/FLX/1440121
Harvard Forest, US (US-HA1)	FLUXNET-2015	42.5, -72.2	1991-2012	6.6	1071	DOI:10.18140/FLX/1440071
Fermilab, US (US-IB2)	FLUXNET-2015	41.8, -88.2	2004-2011	9.0	930	Matamala et al. (2008) DOI:10.17190/AMF/1246066
Bondville, US (US-BO1)	AMERI-FLUX	40.0, -88.3	1996-2008	11.0	991	DOI:10.17190/AMF/1246036
Majadas, Spain (ES-LM1)	ICOS	39.9, -5.8	2014-2018	16.0	700	El-Madany et al. (2018)
ARM Southern Great Plains, US (US-ARM)	FLUXNET-2015	36.6, -97.5	2003-2012	14.8	843	DOI:10.18140/FLX/1440066

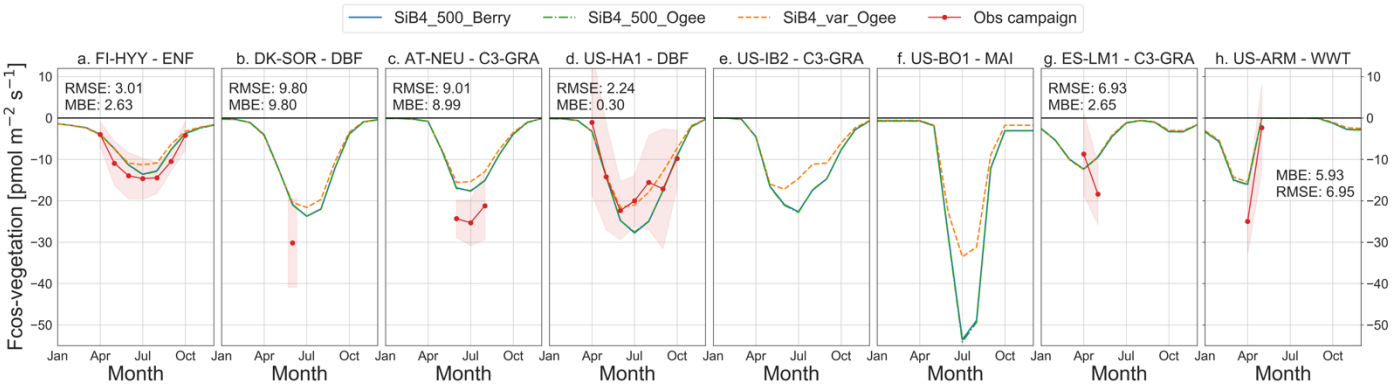


Figure S1. Comparison of COS vegetation flux seasonal cycles of observations (red) with different SiB4 model runs: SiB4_500_Berry (blue, solid), SiB4_var_Ogee (orange, dashed), SiB4_500_Ogee (green, dot-dash). Monthly averages are shown with the 1σ spread around the mean of observations. Negative values indicate uptake of COS by the ecosystem while positive values indicate COS emissions. The model simulations are from the same year(s) in which observations were made. The MBE and RMSE (pmol m^{-2} s^{-1}) are given for monthly average fluxes. Sites are presented from high to low latitude.

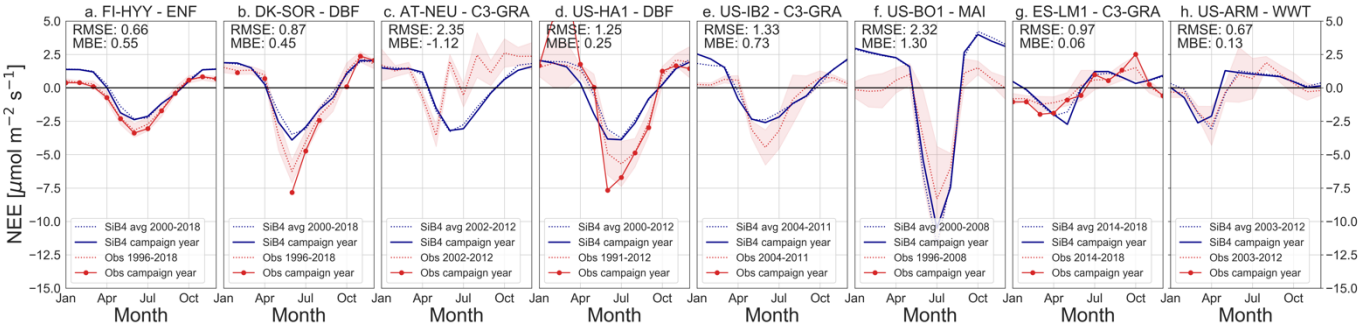


Figure S2. Comparison of NEE seasonal cycles of SiB4 model simulations (blue) with observations from either FLUXNET, AmeriFlux or ICOS (indicated in legend) (red). Monthly averages are shown with the 1σ spread around the mean of observations. Negative values indicate uptake of CO_2 by the ecosystem while positive values indicate CO_2 emissions. The model simulations represent the years in which observations were made from 2000 onwards. The MBE and RMSE (μmol m^{-2} s^{-1}) are given for monthly average fluxes.

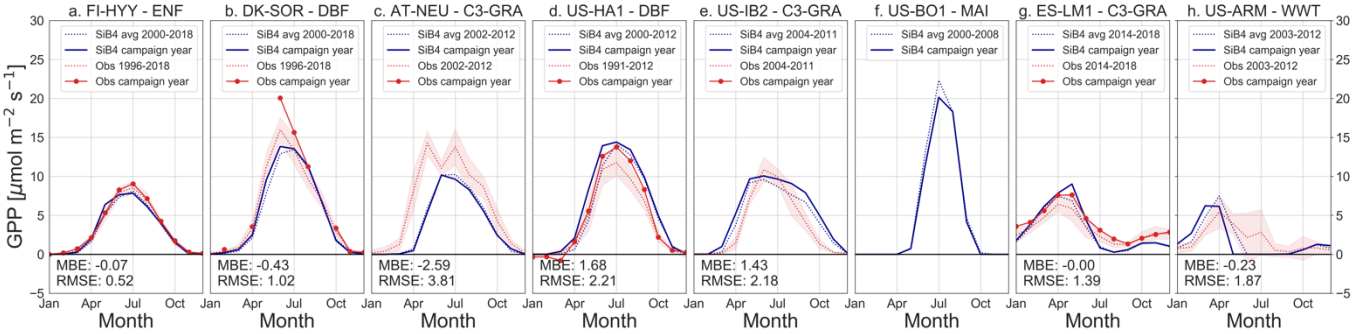


Figure S3. Comparison of GPP seasonal cycles of SiB4 model simulations (blue) with observations from either FLUXNET, AmeriFlux or ICOS (indicated in legend) (red). Monthly averages are shown with the 1σ spread around the mean of observations. The model simulations represent the years in which observations were made from 2000 onwards. The MBE and RMSE (μmol m^{-2} s^{-1}) are given for monthly average fluxes.

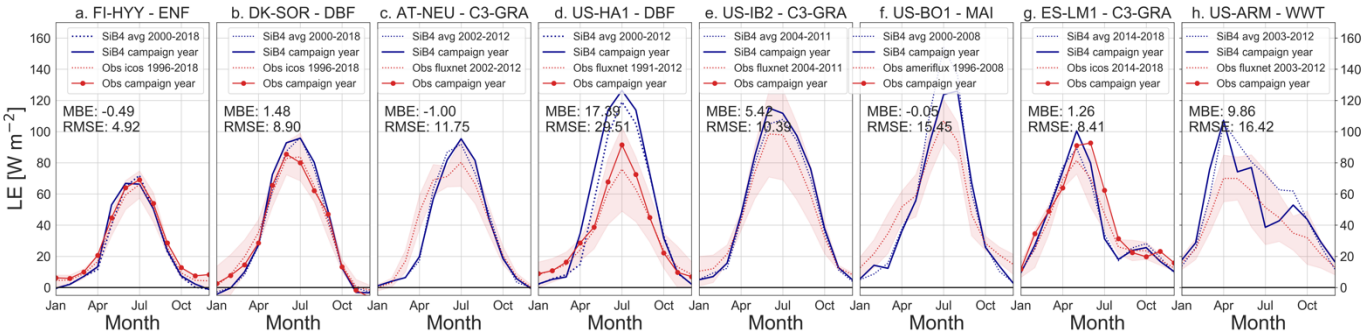


Figure S4. Comparison of LE seasonal cycles of SiB4 model simulations (blue) with observations from either FLUXNET, AmeriFlux or ICOS (indicated in legend) (red). The model simulations represent the years in which observations were made from 2000 onwards. The MBE and RMSE (W m^{-2}) are given for monthly average fluxes.

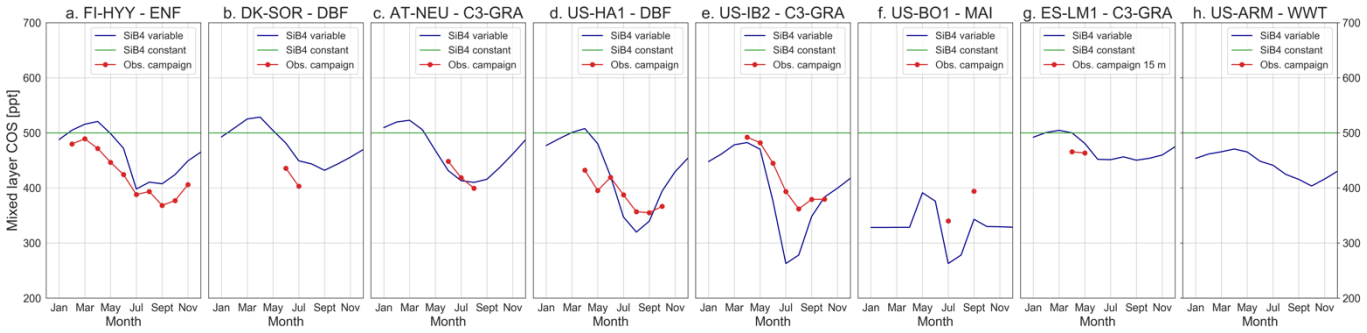


Figure S5: Seasonal cycles of COS mole fractions as used in the SiB4 simulations (blue and green) together with observed COS mole fractions above or in the canopy. No COS mole fraction observations are available for US-ARM.

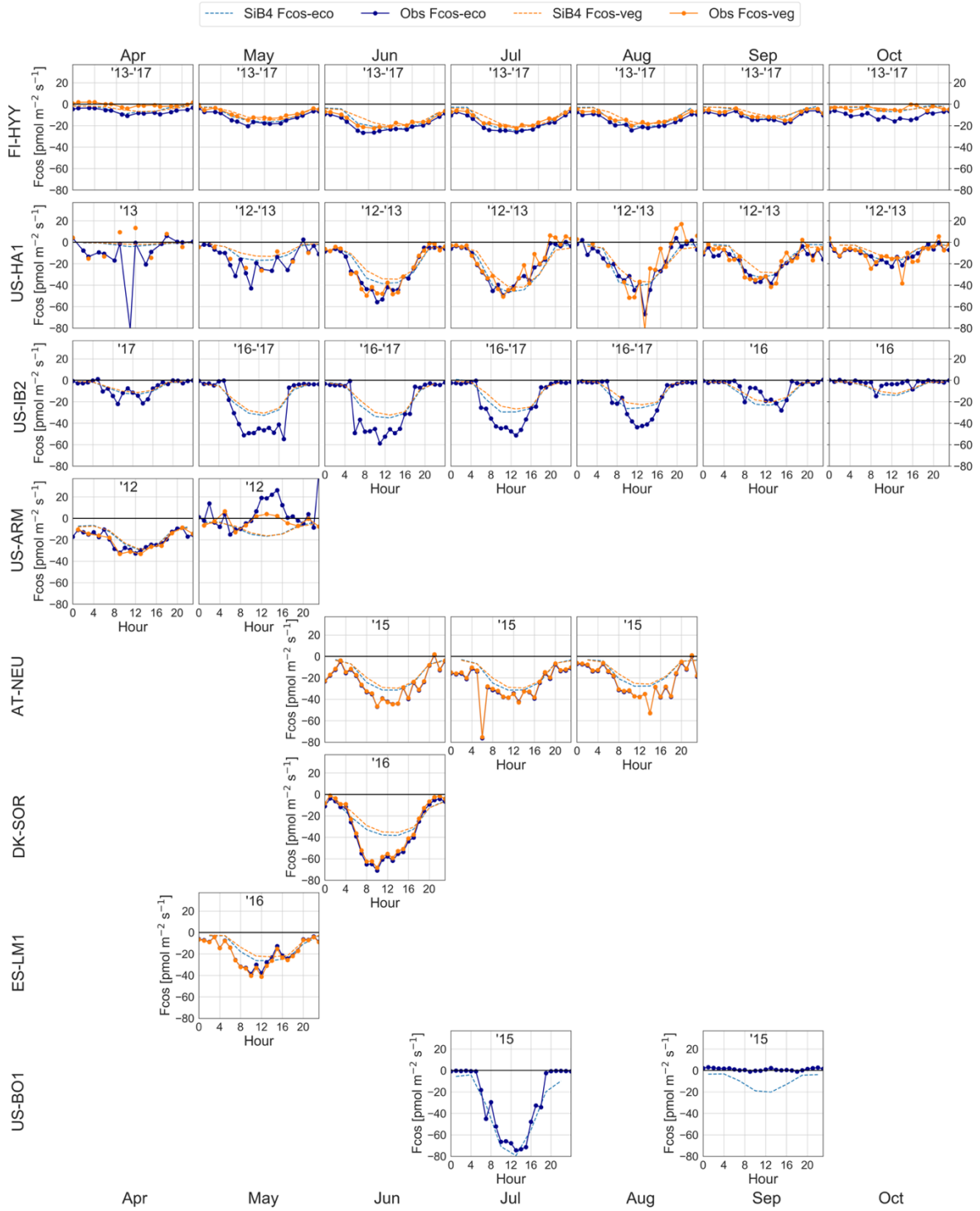
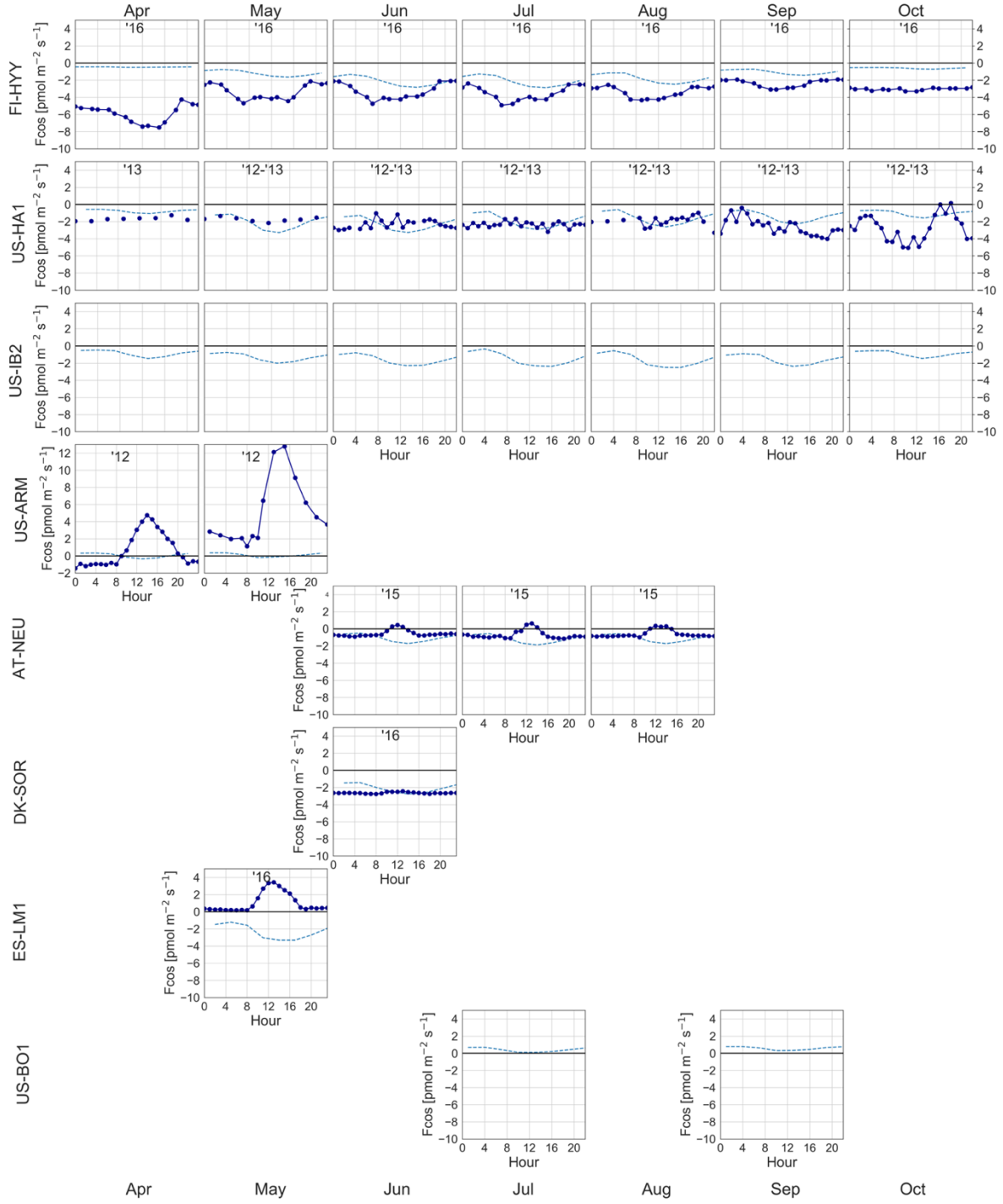


Figure S6. Diurnal cycles of COS ecosystem (blue) and vegetation (orange) fluxes as observed (dotted line) and simulated (dashed line) per month and per site. Model results represent settings from SiB4_var_Ogee. Negative values indicate uptake of COS by the ecosystem while positive values indicate COS emissions.



50 **Figure S7. Diurnal cycles of COS *soil* fluxes as observed (dotted line) and simulated (dashed line) per month and per site. Model results represent settings from SiB4_var_Ogee. Positive fluxes represent uptake by the soil. Negative values indicate uptake of COS by the ecosystem while positive values indicate COS emissions.**

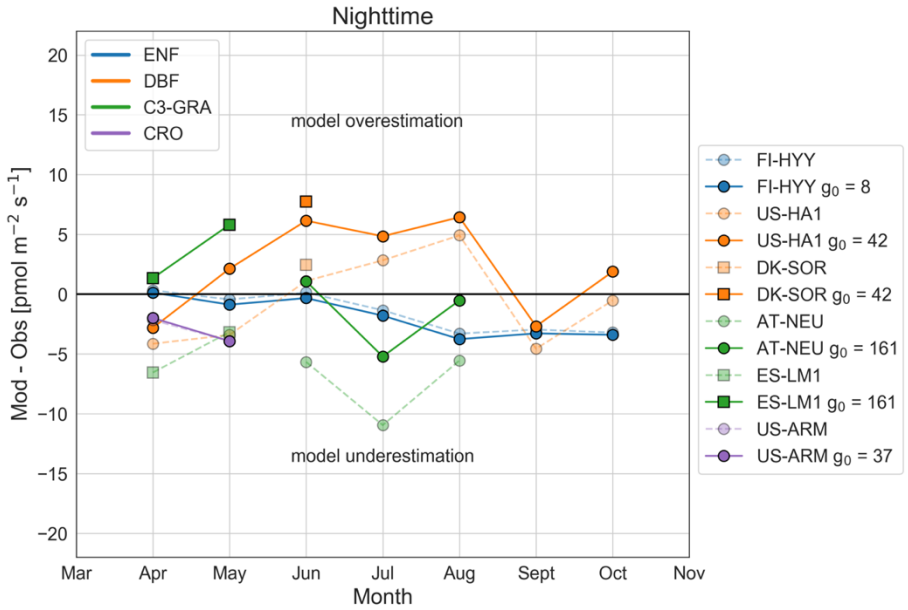


Figure S8. Difference between model simulations and observations of monthly average COS vegetation fluxes (ecosystem – soil) for nighttime data (21 – 03 hr) based on two different minimum stomatal conductance settings. The runs with original SiB4 minimum stomatal conductance values (10 mmol m^{-2} s^{-1} for most PFTs, and 40 mmol m^{-2} s^{-1} for C4 plants and crops) are shown as transparent dashed lines (equal to those shown in Fig. 3 of the main text). The runs with modified minimum stomatal conductance as adopted by Lombardozzi et al. (2017) (values indicated in the legend, unit in mmol m^{-2} s^{-1}, see also Table S2) are shown as solid lines. All runs are done with settings following SiB4_var_Ogee.

Table S2. Minimum stomatal conductance (g_0) values used as default in SiB4 and those adopted from Lombardozzi et al. (2017). Units are in mmol m^{-2} s^{-1}.

PFT	Sites	Default SiB4 g_0	Adjusted g_0
ENF	FI-HYY	10	8
DBF	US-HA1, DK-SOR	10	42
C3-GRA	AT-NEU, ES-LM1	10	161
WWT	US-ARM	40	37

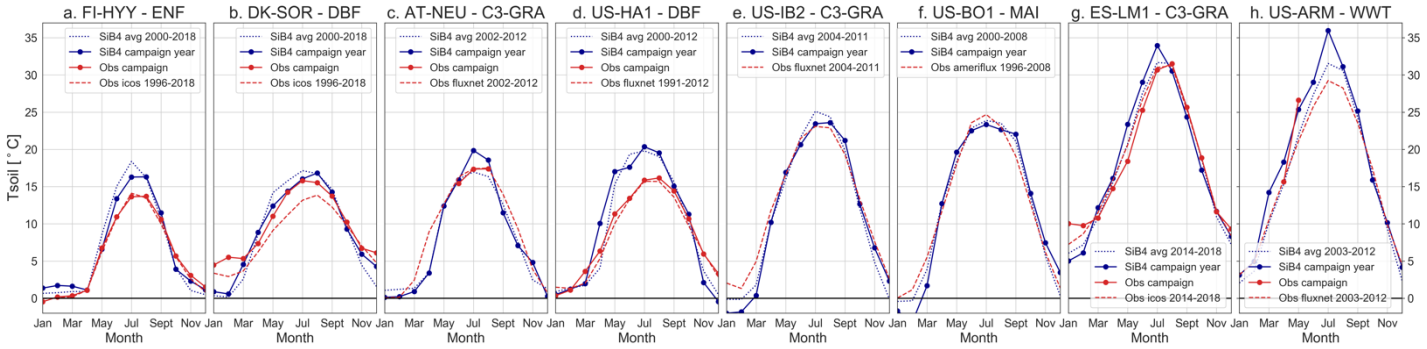


Figure S9. Comparison of soil temperature seasonal cycles as measured by the FLUXNET, AmeriFlux or ICOS network at 0.05 m (red) and simulated in the upper two soil layers (0-0.13 m by the SiB4 model (blue). The model simulations are from the same year(s) in which observations were made.

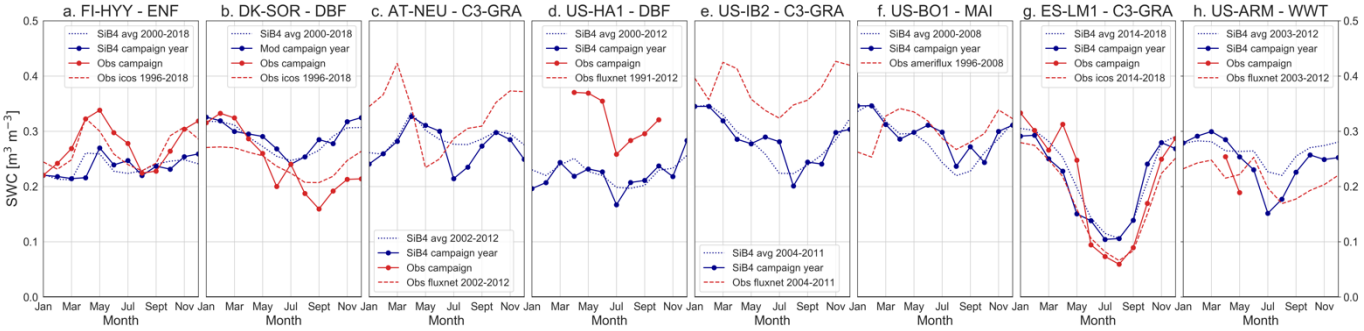


Figure S10. Comparison of soil moisture as measured by the FLUXNET, AmeriFlux or ICOS network at 0.05 m (red) and simulated in the upper two soil layers (0-0.13 m) by the SiB4 model (blue). The model simulations are from the same year(s) in which observations were made.

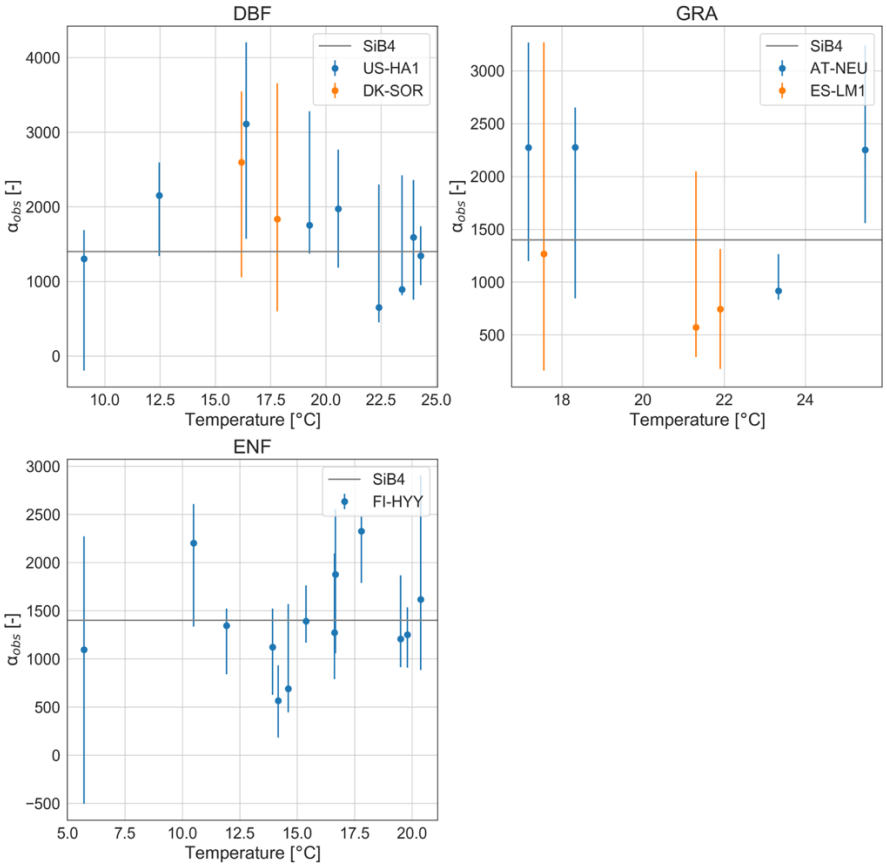


Figure S11. Correlation of α_{obs} against air temperature based on two-weekly medians, separated by PFT. Error bars represent the 25th-75th percentiles.

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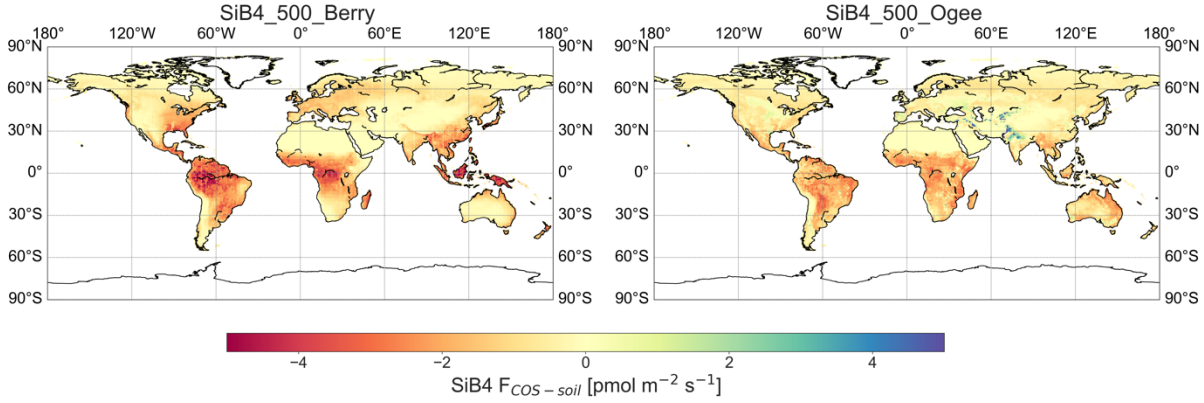

Figure S12. Global distribution of the COS soil flux as simulated by SiB4_500_Berry (left) and SiB4_500_Ogee. Negative values indicate uptake of COS by the biosphere while positive values indicate COS emissions.

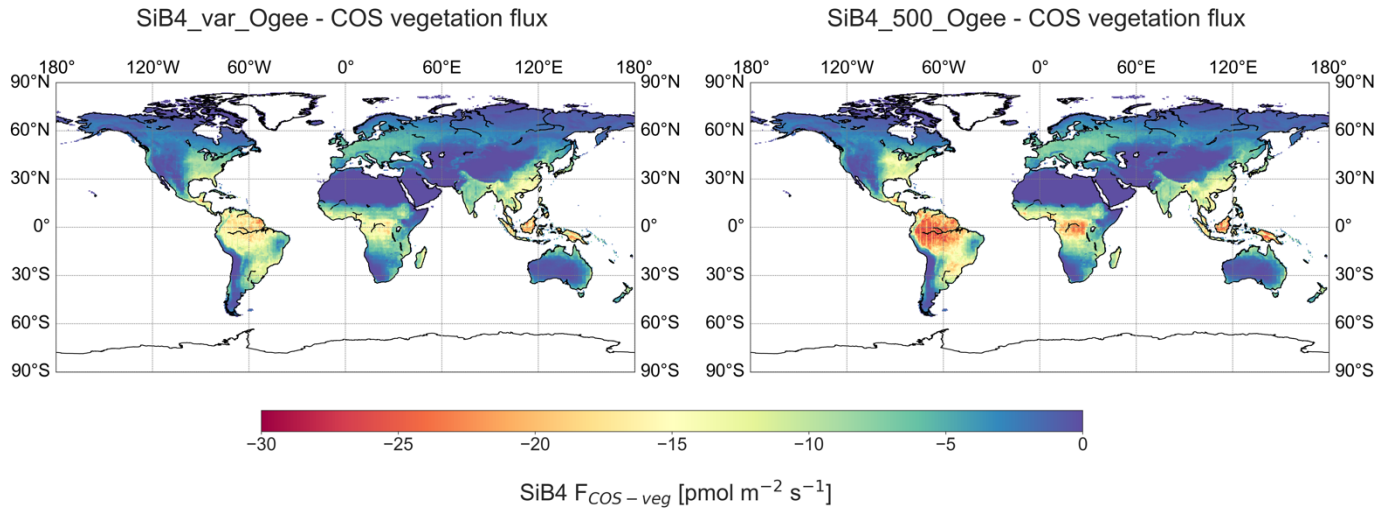

Figure S13. Global distribution of the COS vegetation flux as simulated by SiB4_var_Ogee (left) and SiB4_500_Ogee (right). Negative values indicate uptake of COS by the biosphere while positive values indicate COS emissions.

References in supplementary information

El-Madany, T. S., Reichstein, M., Perez-Priego, O., Carrara, A., Moreno, G., Pilar Martín, M., Pacheco-Labrador, J., Wohlfahrt, G., Nieto, H., Weber, U., Kolle, O., Luo, Y.-P., Carvalhais, N. and Migliavacca, M.: Drivers of spatio-temporal variability of carbon dioxide and energy fluxes in a Mediterranean savanna ecosystem, Agric. For. Meteorol., 262, 258–278, doi:https://doi.org/10.1016/j.agrformet.2018.07.010, 2018.

Kolari, P., Kulmala, L., Pumpanen, J., Launiainen, S., Ilvesniemi, H., Hari, P. and Nikinmaa, E.: CO2 exchange and component CO2 fluxes of a boreal Scots pine forest, Boreal Environ. Res., 14, 761–783, 2009.

Lombardozzi, D. L., Zeppel, M. J. B., Fisher, R. A. and Tawfik, A.: Representing nighttime and minimum conductance in CLM4.5: global hydrology and carbon sensitivity analysis using observational constraints, Geosci. Model Dev., 10(1), 321–331, doi:10.5194/gmd-10-321-2017, 2017.

Matamala, R., Jastrow, J. D., Miller, R. M. and Garten, C. T.: Temporal changes in C and N stocks of restored prairie: Implications for C sequestration strategeies, Ecol. Appl., 18(6), 1470–1488, doi:https://doi.org/10.1890/07-1609.1, 2008.

Pilegaard, K., Ibrom, A., Courtney, M. S., Hummelshøj, P. and Jensen, N. O.: Increasing net CO2 uptake by a Danish beech forest during the period from 1996 to 2009, Agric. For. Meteorol., 151(7), 934–946, doi:https://doi.org/10.1016/j.agrformet.2011.02.013, 2011.

Wohlfahrt, G., Hammerle, A., Haslwanter, A., Bahn, M., Tappeiner, U. and Cernusca, A.: Seasonal and inter-annual variability of the net ecosystem CO2 exchange of a temperate mountain grassland: Effects of weather and management, J. Geophys. Res. Atmos., 113(D8), doi:https://doi.org/10.1029/2007JD009286, 2008.

Wu, J., Larsen, K. S., van der Linden, L., Beier, C., Pilegaard, K. and Ibrom, A.: Synthesis on the carbon budget and cycling in a Danish, temperate deciduous forest, Agric. For. Meteorol., 181, 94–107, doi:https://doi.org/10.1016/j.agrformet.2013.07.012, 2013.

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