Supplement of

Assimilation of Carbonyl Sulfide (COS) fluxes within the adjoint-based data assimilation system—Nanjing University Carbon Assimilation System (NUCAS v1.0)

Huajie Zhu et al.

Correspondence to: Mousong Wu (mousongwu@nju.edu.cn)

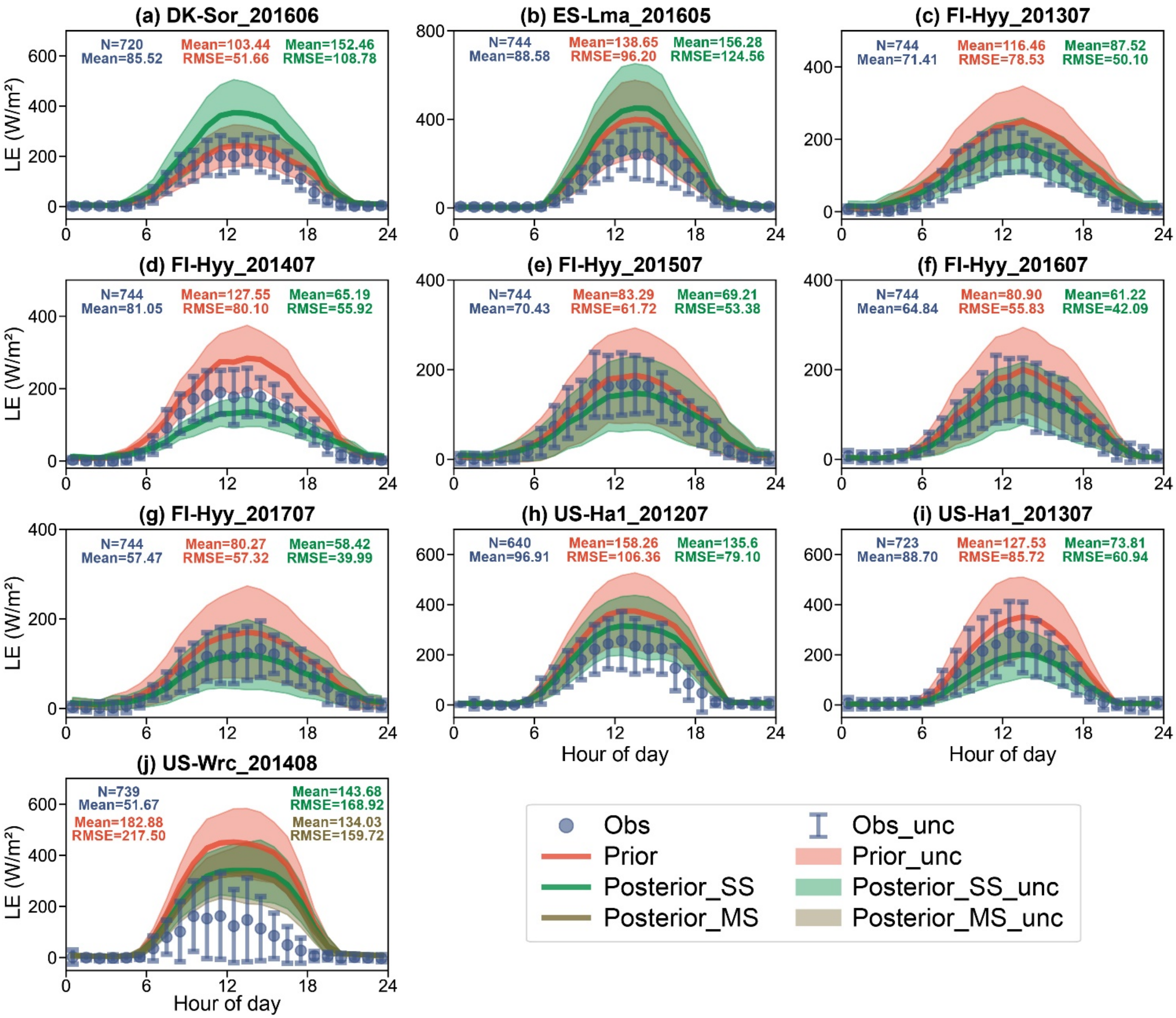

Figure S1. The diurnal cycle of observed (blue) and simulated LE using prior parameters (red), single-site (green) and multi-site (brown) posterior parameters. The size of the circle indicates the number of observations within each circle, and the error bars depict the standard deviations in the mean of observations from the variability within each circle. Lines connect the mean values of simulations and pale bands depict the standard deviation in the mean of simulations from the variability within each bin.

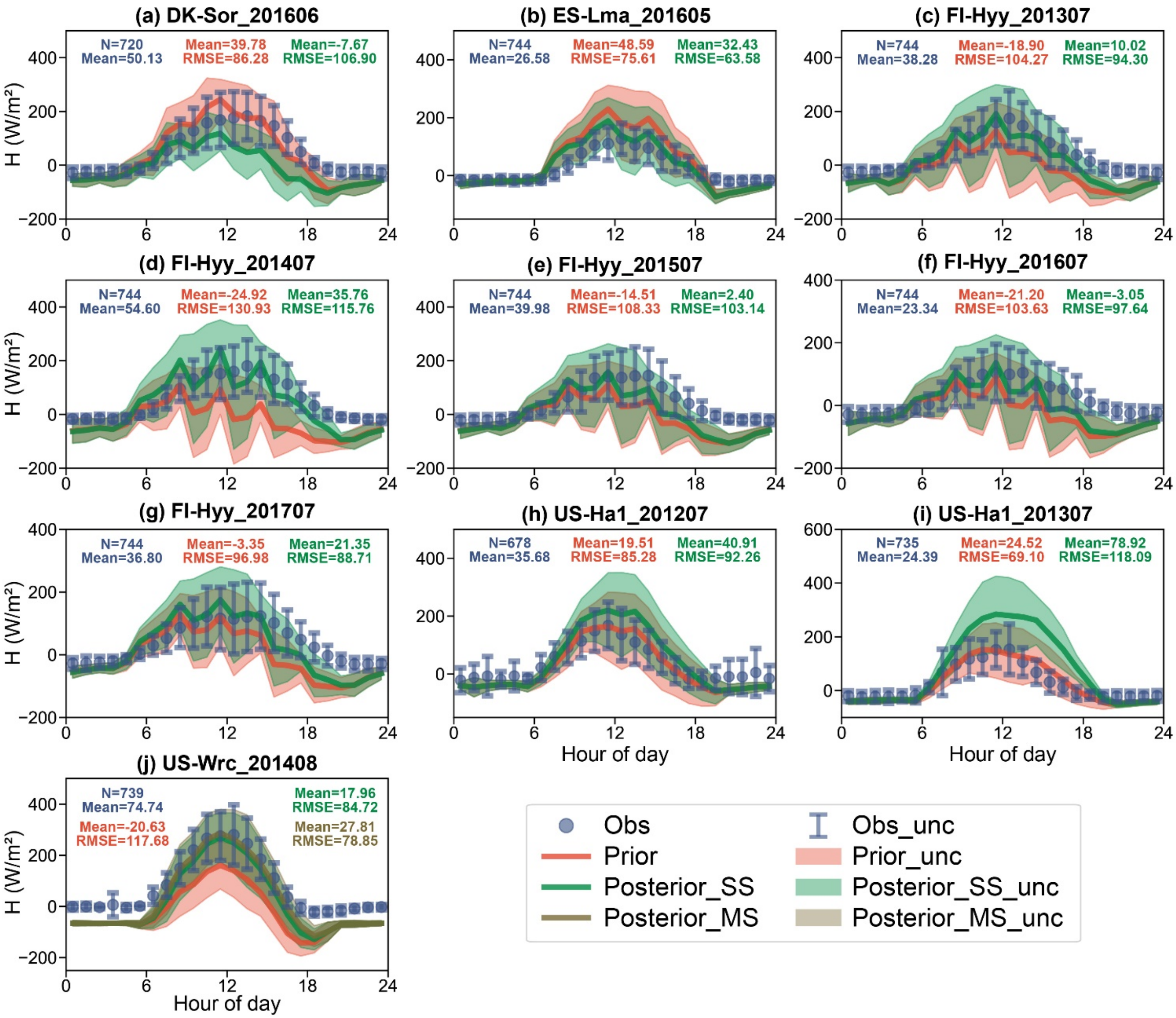

Figure S2. The diurnal cycle of observed (blue) and simulated H using prior parameters (red), single-site (green) and multi-site (brown) posterior parameters. The size of the circle indicates the number of observations within each circle, and the error bars depict the standard deviations in the mean of observations from the variability within each circle. Lines connect the mean values of simulations and pale bands depict the standard deviation in the mean of simulations from the variability within each bin.

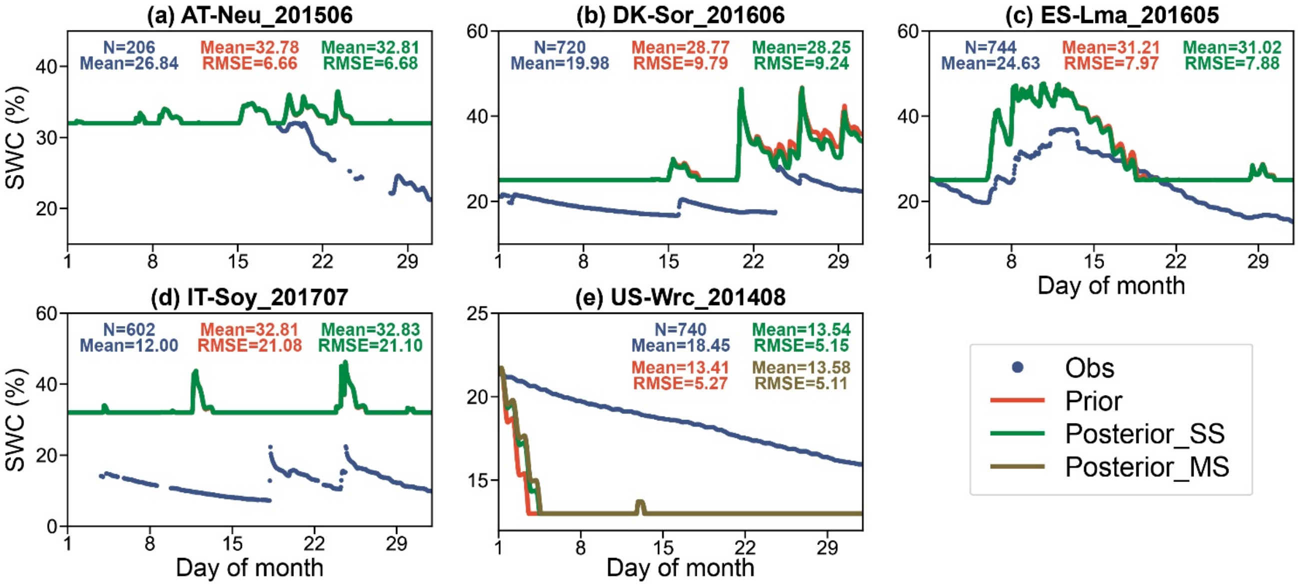

Figure S3. Observed (blue point) and simulated SWC (%). Results show SWC simulated using prior parameters (red line), single-site (green line) and multi-site (brown line) posterior parameters.

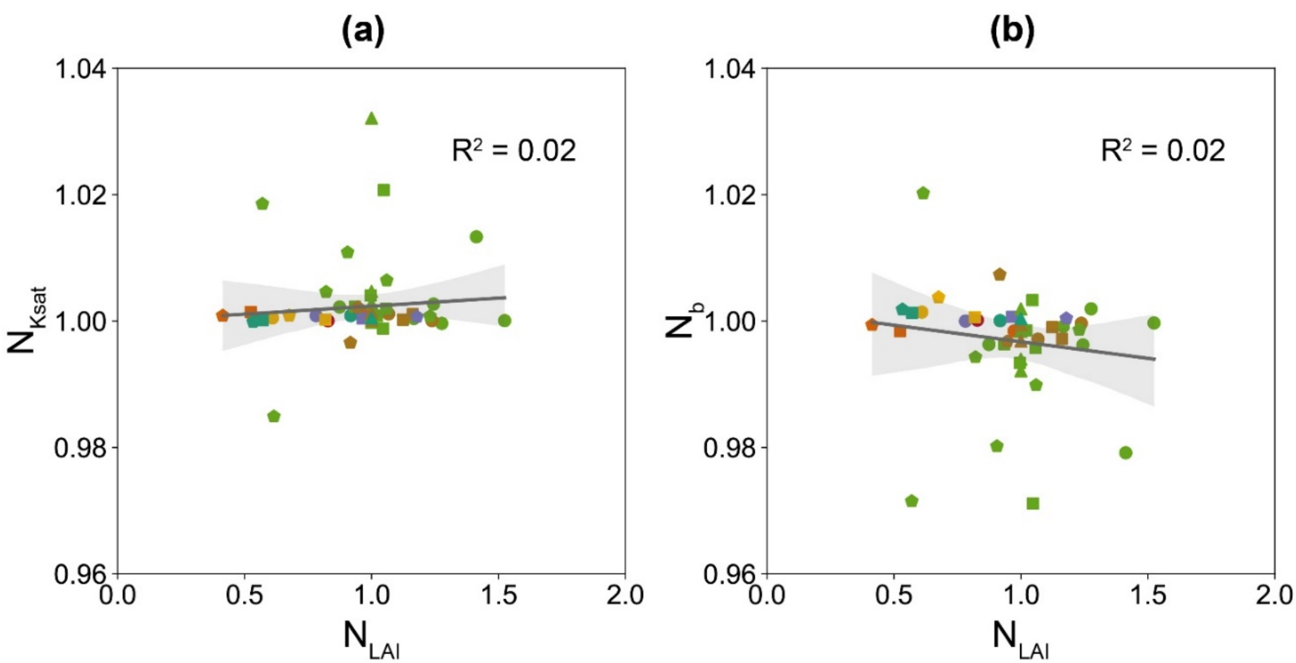

Figure S4. Influence of LAI on the posterior Ksat (a), the posterior b (b) obtained by the single-site experiments conducted at seven sites and driven by four LAI data. The posterior Ksat, the posterior b and the LAI were represented by their normalized values N_{Ksat}, N_b and N_{LAI}, respectively. The posterior parameters were normalized by their prior values and the LAI were normalized by the in situ values.

Table S1. PFT and Soil Texture descriptions in BEPS model.

PFT No.	Descriptions
1	Evergreen needleleaf forest
2	Deciduous needleleaf forest
3	Deciduous broadleaf forest
4	Evergreen broadleaf forest
5	Mixed forest
6	Shrub
7	Grass
8	Crop
9	C4 Grass
10	C4 Crop
Soil texture No.	**Description**
1	Sand
2	Loamy sand
3	Sandy loam
4	Loam
5	Silty loam
6	Sandy clay loam
7	Clay loam
8	Silty clay loam
9	Sandy clay
10	Silty clay
11	Clay

Table S2. Description of parameters used for optimizations within the Nanjing University Carbon Assimilation System (NUCAS). Parameters are either specified per PFT, per soil texture, or globally, i.e all PFTs and textures share one value, as indicated in column 2.

No.	Parameter	Dependent	Unit	Description	Prior Value	Prior Uncertainty
1	V_{cmax25}	PFT	$\mu mol/m^2/s$	maximum carboxylation rate at 25°C	62.5	15.625
2					39.1	9.775
3					57.7	14.425
4					29	7.25
5					66	16.5
6					57.85	14.4625
7					48	12
8					84.5	21.125
9					30	7.5
10					30	7.5
11	VJ_slope	PFT	-		2.39	0.5975

12					2.39	0.5975
13					2.39	0.5975
14					2.39	0.5975
15					2.39	0.5975
16				Slope of the V_{cmax} and J_{max} (maximum electron transport rate) relationship	2.39	0.5975
17					2.39	0.5975
18					2.39	0.5975
19					2.39	0.5975
20					2.39	0.5975
21					0.046	0.0115
22					0.046	0.0115
23					0.046	0.0115
24					0.046	0.0115
25					0.046	0.0115
26	Q10	PFT	-	Soil respiration temperature factor	0.046	0.0115
27					0.046	0.0115
28					0.046	0.0115
29					0.046	0.0115
30					0.046	0.0115
31					6.2473	1.561825
32					6.2473	1.561825
33					6.2473	1.561825
34					6.2473	1.561825
35					6.2473	1.561825
36	SIF_alpha	PFT	W/m^2	Quadratic term coefficient for the relationship between additional heat dissipation under light adapted conditions and relative reduction of photochemical yield	6.2473	1.561825
37					6.2473	1.561825
38					6.2473	1.561825
39					6.2473	1.561825
40					6.2473	1.561825
41					0.5994	0.14985
42					0.5994	0.14985
43					0.5994	0.14985
44					0.5994	0.14985
45					0.5994	0.14985
46	SIF_beta	PFT	W/m^2	Primary term coefficient for the relationship between additional heat dissipation under light adapted conditions and relative reduction of photochemical yield	0.5994	0.14985
47					0.5994	0.14985
48					0.5994	0.14985
49					0.5994	0.14985
50					0.5994	0.14985
51	Ksat	texture	m/s	Saturated hydraulic conductivity	1	0.25
52					1	0.25

53					1	0.25
54					1	0.25
55					1	0.25
56					1	0.25
57					1	0.25
58					1	0.25
59					1	0.25
60					1	0.25
61					1	0.25
62					1	0.25
63					1	0.25
64					1	0.25
65					1	0.25
66					1	0.25
67	b	texture	-	Campbell parameter (the exponential parameter of Campbell's soil moisture retention model)	1	0.25
68					1	0.25
69					1	0.25
70					1	0.25
71					1	0.25
72					1	0.25
73	f_leaf	global	-	The ratio of photosynthetically active radiation to shortwave radiation	0.5	0.125
74	kc25	global	μbar	Michaelis–Menten constants for CO_2 in 25℃	274.6	68.65
75	ko25	global	$mbar$	Michaelis–Menten constants for O_2 in 25℃	419.8	104.95
76	tau25	global	-	the CO_2/O2 specificity factor, which reflects the carbon assimilation efficiency of Rubisco	2904.12	726.03

Table S3. Summary of configurations of twin experiments, the variation of D_x during assimilation ($D_{initial}$, D_{max}, D_{final}), and the relative changes of the parameters. The suffix "*" indicates the multi-site experiment.

Site name	Data duration	D_{itial}	D_{max}	D_{final}	Relative changes of parameters (%)				
					V_{cmax25}	VJ_slope	Ksat	b	f_leaf
AT-Neu	June 2015	1.39E+01	7.60E+03	1.48E-07	-1.70E-07	3.15E-07	4.62E-07	5.38E-07	1.19E-07
DK-Sor	June 2016	1.39E+01	7.60E+03	1.70E-08	-5.95E-10	6.23E-09	5.39E-08	4.83E-08	1.03E-08
ES-Lma	May 2016	1.39E+01	3.93E+03	8.80E-10	2.18E-09	-1.64E-09	-1.53E-08	-1.12E-08	-1.09E-08
FI-Hyy	July 2013	6.97E+00	7.60E+03	2.57E-08	2.92E-09	1.71E-08	-1.24E-07	6.56E-08	-1.36E-08
	July 2014	6.97E+00	7.60E+03	4.74E-09	1.11E-08	-3.58E-08	6.80E-08	4.69E-08	-2.17E-09
	August 2014	6.97E+00	7.60E+03	1.02E-09	1.61E-09	-4.43E-09	6.25E-09	-5.00E-09	-1.17E-09
	July 2015	6.97E+00	7.60E+03	7.58E-10	1.34E-10	-2.84E-10	-8.87E-09	1.58E-08	-4.31E-10
	July 2016	6.97E+00	7.60E+03	4.53E-08	-9.19E-08	7.42E-08	7.07E-07	-7.50E-07	1.74E-07
	July 2017	6.97E+00	7.60E+03	2.45E-08	-4.00E-09	6.98E-08	-3.71E-07	4.80E-07	-3.68E-08
IT-Soy	July 2017	1.39E+01	7.60E+03	6.98E-08	8.20E-08	1.52E-06	8.19E-08	4.43E-08	-8.42E-07

US-Ha1	July 2012	1.39E+01	7.60E+03	1.63E-07	2.89E-08	3.37E-08	-4.38E-07	-1.83E-07	-1.13E-07
	July 2013	1.39E+01	7.60E+03	2.36E-08	5.28E-09	-1.19E-08	9.98E-09	1.43E-07	-1.95E-08
US-Wrc	August 2014	6.97E+00	7.60E+03	2.84E-08	-6.84E-08	7.98E-09	1.49E-07	2.86E-08	2.03E-07
FI-Hyy*	August 2014	6.97E+00	7.60E+03	2.01E-08	-6.62E-08	3.60E-07	1.24E-07	-1.82E-07	-1.60E-07
US-Wrc*							-1.02E-07	1.67E-07	