



Supplement of

Improved estimation of net ecosystem CO₂ exchange over North America using LSTM-based flux upscaling (2001–2021)

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FIGURES

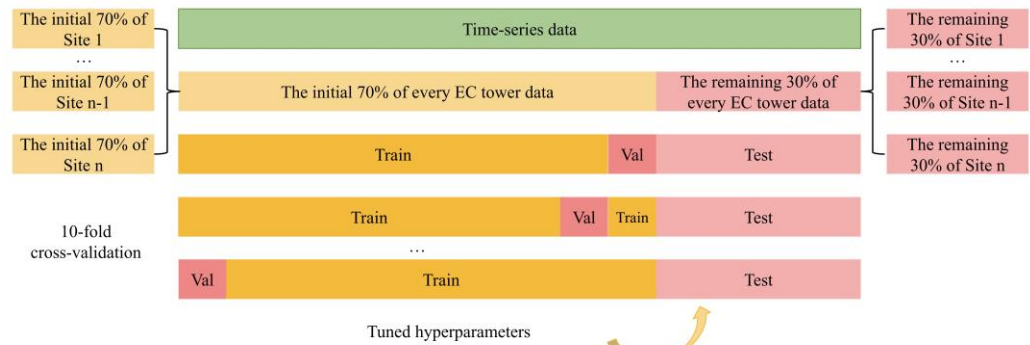


Figure S1. Schematic of the nested ten-fold cross-validation strategy employed to develop the model in this study.

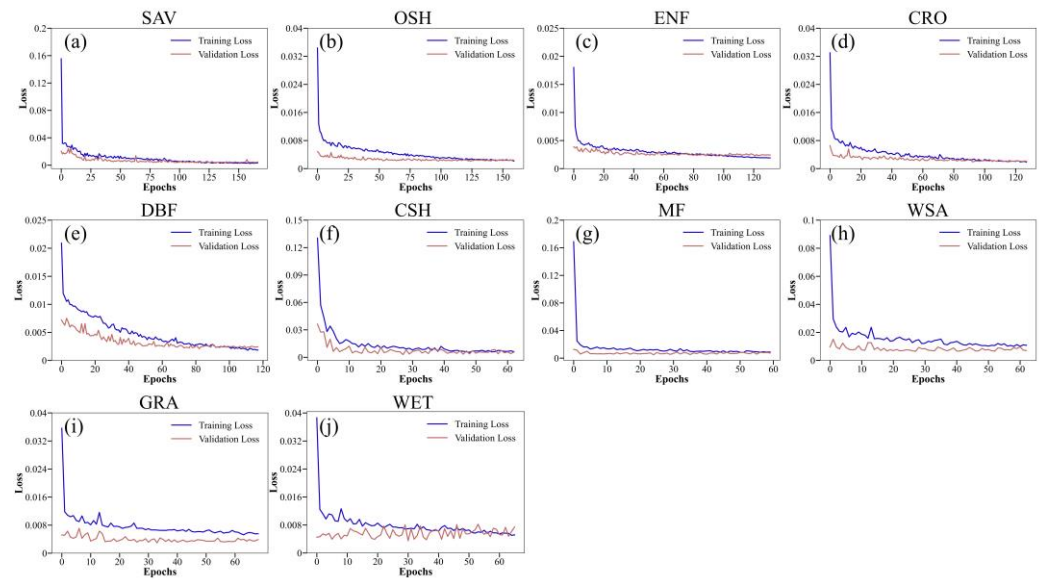


Figure S2. Loss curve of LSTM models at the site level across the 10 considered PFT. Note that the learning procedure was stopped by the early stopping technology.

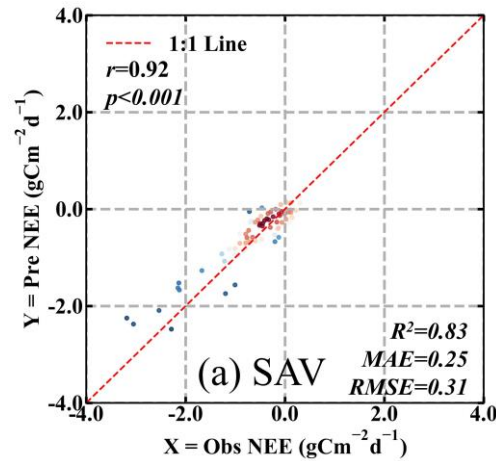
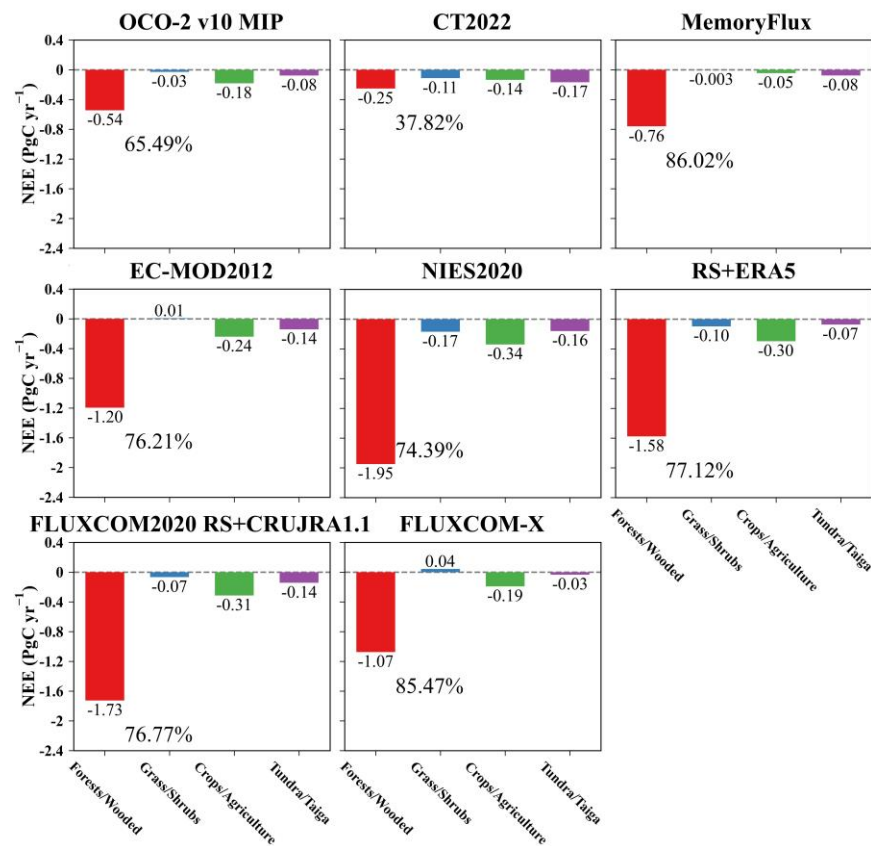
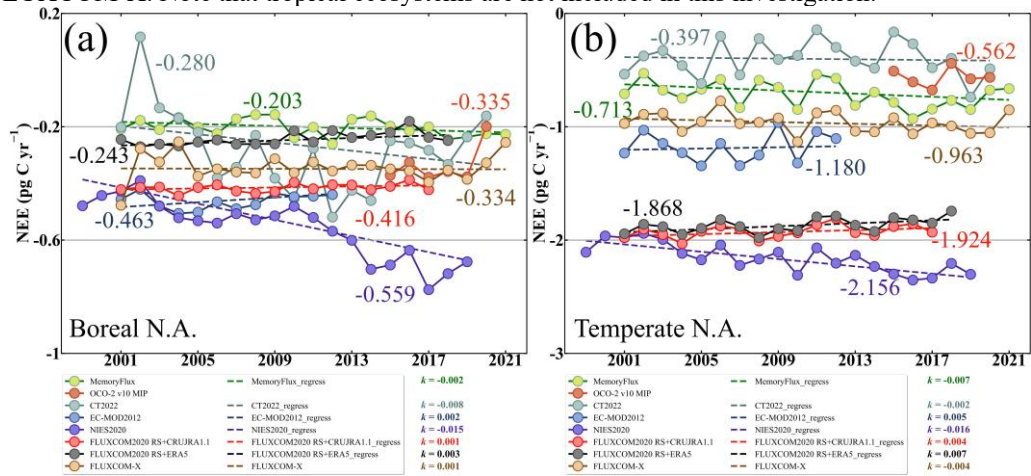


Figure S3. Scatter plots of the predicted NEE by LSTM models against the observed NEE across SAV sites.



27 **Figure S4.** Mean annual net ecosystem CO₂ exchange (NEE) for each biome across the boreal and temperate North America of
28 MemoryFlux, EC-MOD2012, CT2022, OCO-2 v10 MIP, NIES2020, FLUXCOM2020 RS+CRUJRA1.1, FLUXCOM2020
29 RS+ERA5, and FLUXCOM-X. Note that tropical ecosystems are not included in this investigation.



31 **Figure S5.** Interannual variations of the (a) boreal and (b) temperate North America NEE estimated by OCO-2 v10 MIP ensemble
32 mean, CT2022, EC-MOD2012, MemoryFlux, NIES2020, FLUXCOM2020 RS+ERA5, FLUXCOM2020 RS+CRUJRA, and
33 FLUXCOM-X. The dashed lines represent the long-term trend, calculated using the Mann–Kendall test and the Theil–Sen slope
34 method. Due to the limited data, we did not estimate a slope for OCO-2 v10 MIP.

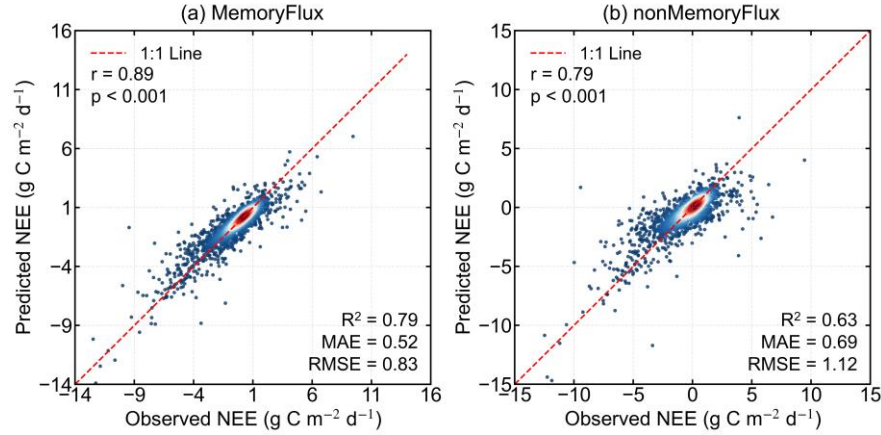


Figure S6. Comparative evaluation of monthly NEE predicted by the LSTM models used to generate (a) MemoryFlux and (b) nonMemoryFlux against the corresponding observed NEE. The units of RMSE and MAE are $\text{g C m}^{-2} \text{d}^{-1}$.

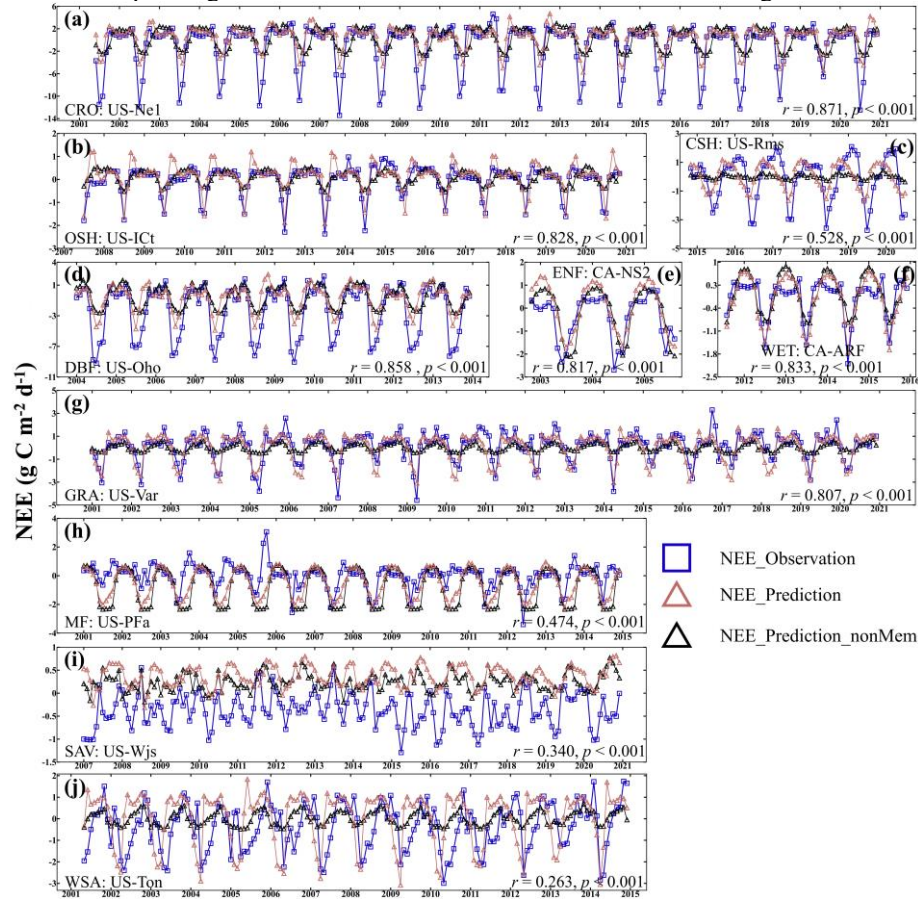


Figure S7. Comparison between the upscaled NEE from our estimates (MemoryFlux), the nonmemory variant, nonMemoryFlux, and the observed NEE for representative sites having long-term data across each PFT.

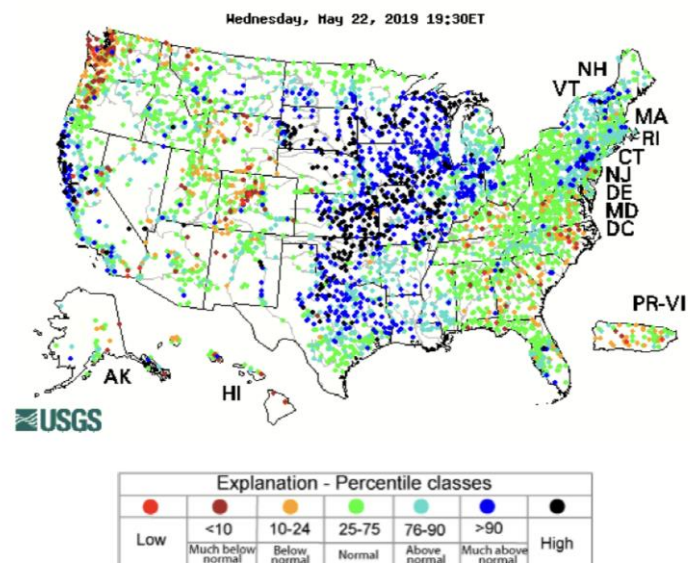


Figure S8. The 2019 Midwest American floods. Stream gauges levels in percentiles for Wednesday, May 22, 2019. From USGS: <https://waterwatch.usgs.gov/index.php?id=ww%20past>. U.S. Geological Survey (USGS) © 2019.

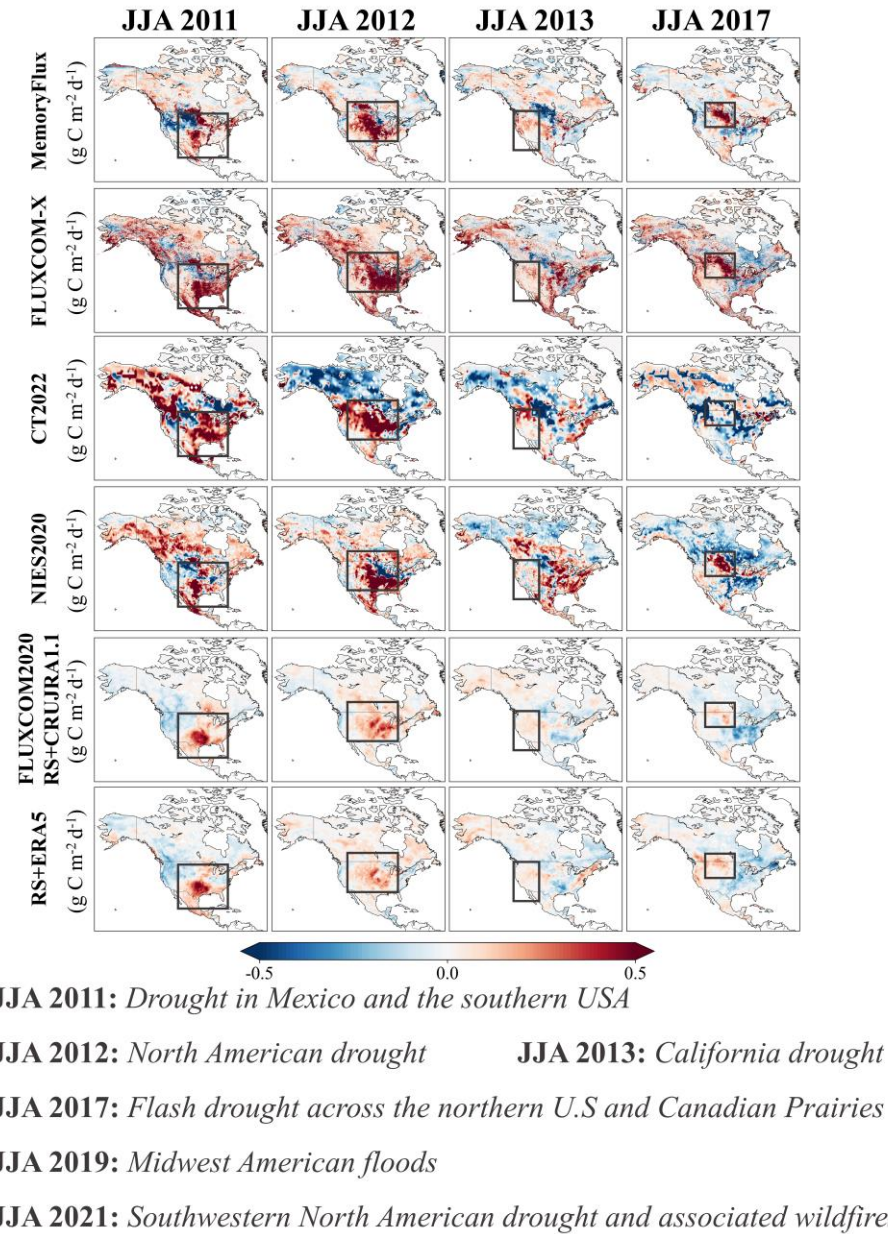


Figure S9. Spatial anomalies of JJA NEE associated with major drought and flood events in North America, calculated using a common 2011–2017 reference period for MemoryFlux, CT2022, NIES2020, FLUXCOM2020 RS+CRUJRA1.1, FLUXCOM2020 RS+ERA5, and FLUXCOM-X. Black rectangles indicate the regions most strongly affected by the selected extreme climate events.

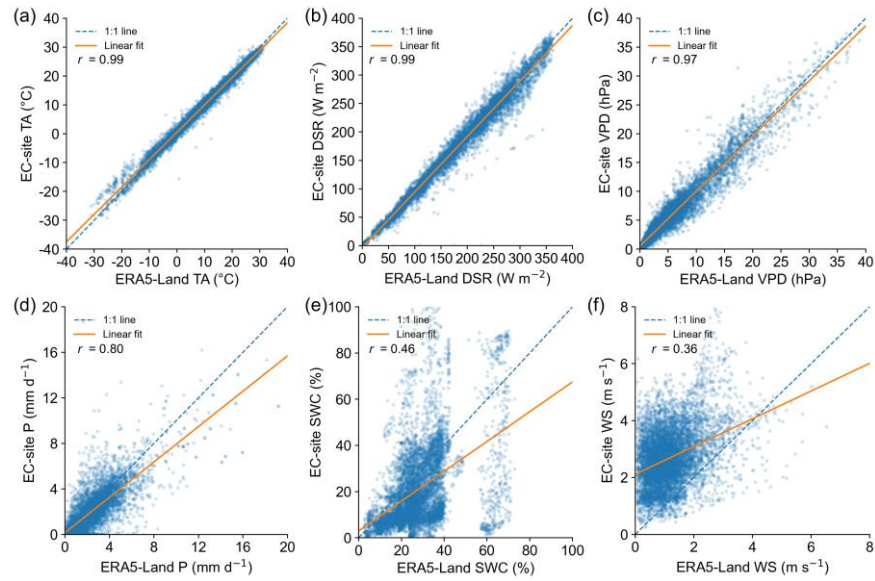


Figure S10. Comparison of ERA5-Land gridded meteorological variables with concurrent observations from EC flux-tower sites. Scatterplots show (a) air temperature (TA), (b) downward shortwave radiation (DSR), (c) vapor pressure deficit (VPD), (d) precipitation (P), (e) soil water content (SWC), and (f) wind speed (WS). Dashed lines indicate the 1:1 relationship, and solid lines indicate linear regression fits.

TABLES

Table S1. Details of FLUXNET2015 and AmeriFlux network sites.

Sites name	Network	Latitude	Longitude	Study period	PFT
CA-LP1	AmeriFlux	55.11	-122.84	2007 – 2017	ENF
CA-NS1	FLUXNET	55.88	-98.48	2002 – 2005	ENF
CA-NS2	FLUXNET	55.91	-98.52	2002 – 2005	ENF
CA-NS3	FLUXNET	55.91	-98.38	2002 – 2005	ENF
CA-NS4	FLUXNET	55.91	-98.38	2002 – 2005	ENF
CA-Qfo	FLUXNET	49.69	-74.34	2003 – 2010	ENF
CA-SF1	AmeriFlux	54.49	-105.82	2003 – 2006	ENF
CA-SF2	FLUXNET	54.25	-105.88	2001 – 2005	ENF
CA-TP1	FLUXNET	42.66	-80.56	2003 – 2014	ENF
CA-TP2	FLUXNET	42.77	-80.46	2002 – 2007	ENF
CA-TP3	AmeriFlux	42.71	-80.35	2002 – 2017	ENF
CA-TP4	FLUXNET	42.71	-80.36	2002 – 2014	ENF
US-BIo	FLUXNET	38.90	-120.63	2000 – 2007	ENF
US-BZS	AmeriFlux	64.70	-148.32	2015 – 2020	ENF
US-GLE	AmeriFlux	41.37	-106.24	2005 – 2020	ENF
US-Me2	AmeriFlux	44.45	-121.56	2002 – 2020	ENF
US-Me3	AmeriFlux	44.32	-121.61	2004 – 2009	ENF
US-Me5	FLUXNET	44.44	-121.57	2000 – 2002	ENF
US-Me6	FLUXNET	44.32	-121.61	2010 – 2014	ENF
US-NC1	AmeriFlux	35.81	-76.71	2005 – 2012	ENF
US-NR1	AmeriFlux	40.03	-105.55	2002 – 2016	ENF
US-Prr	FLUXNET	65.12	-147.49	2010 – 2014	ENF
PA-SPs	FLUXNET	9.31	-79.63	2007 – 2009	GRA
US-A32	AmeriFlux	36.82	-97.82	2015 – 2017	GRA
US-AR1	FLUXNET	36.43	-99.42	2009 – 2012	GRA
US-AR2	FLUXNET	36.64	-99.60	2009 – 2012	GRA
US-ARb	FLUXNET	35.55	-98.04	2005 – 2006	GRA
US-ARc	FLUXNET	35.55	-98.04	2005 – 2006	GRA
US-Cop	FLUXNET	38.09	-109.39	2001 – 2003	GRA
US-Goo	FLUXNET	34.25	-89.87	2002 – 2006	GRA
US-Hn2	AmeriFlux	46.69	-119.46	2016 – 2018	GRA
US-KFS	AmeriFlux	39.06	-95.19	2007 – 2018	GRA
US-KLS	AmeriFlux	38.77	-97.57	2012 – 2019	GRA
US-NGC	AmeriFlux	64.86	-163.70	2017 – 2019	GRA
US-ONA	AmeriFlux	27.38	-81.95	2016 – 2020	GRA
US-Ro4	AmeriFlux	44.68	-93.07	2016 – 2020	GRA
US-SRG	FLUXNET	31.79	-110.83	2008 – 2014	GRA
US-Var	AmeriFlux	38.41	-120.95	2001 – 2020	GRA
US-Wkg	AmeriFlux	31.74	-109.94	2004 – 2020	GRA
CA-Cbo	AmeriFlux	44.32	-79.93	2005 – 2020	DBF
CA-TPD	AmeriFlux	42.64	-80.56	2012 – 2017	DBF
MX-Tes	AmeriFlux	27.84	-109.30	2004 – 2008	DBF
PA-SPn	FLUXNET	9.32	-79.63	2007 – 2009	DBF
US-MMS	AmeriFlux	39.32	-86.41	2000 – 2020	DBF
US-MOz	AmeriFlux	38.74	-92.20	2004 – 2019	DBF
US-Oho	FLUXNET	41.55	-83.84	2004 – 2013	DBF

Sites name	Network	Latitude	Longitude	Study period	PFT
US-UMB	FLUXNET	45.56	-84.71	2001 – 2014	DBF
US-UMd	AmeriFlux	45.56	-84.70	2007 – 2020	DBF
US-WCr	FLUXNET	45.81	-90.08	2000– 2006	DBF
US-xBR	AmeriFlux	44.06	-71.29	2017 – 2020	DBF
CA-NS6	FLUXNET	55.92	-98.96	2002 – 2005	OSH
CA-NS7	FLUXNET	56.64	-99.95	2002 – 2005	OSH
CA-SF3	FLUXNET	54.09	-106.01	2001 – 2006	OSH
US-ICt	AmeriFlux	68.61	-149.30	2007 – 2020	OSH
US-Jo1	AmeriFlux	32.58	-106.64	2010 – 2020	OSH
US-Jo2	AmeriFlux	32.58	-106.60	2010 – 2020	OSH
US-Rws	AmeriFlux	43.17	-116.71	2015 – 2020	OSH
US-SRC	AmeriFlux	31.91	-110.84	2008 – 2014	OSH
US-Sta	FLUXNET	41.40	-106.80	2007 – 2009	OSH
US-Whs	AmeriFlux	31.74	-110.05	2007 – 2020	OSH
US-ARM	AmeriFlux	36.61	-97.49	2003 – 2020	CRO
US-Bi1	AmeriFlux	38.10	-121.50	2016 – 2020	CRO
US-Bi2	AmeriFlux	38.11	-121.54	2017 – 2020	CRO
US-CF2	AmeriFlux	46.78	-117.09	2017 – 2020	CRO
US-CRT	FLUXNET	41.63	-83.35	2011 – 2013	CRO
US-Ne1	AmeriFlux	41.17	-96.48	2001 – 2020	CRO
US-Ro5	AmeriFlux	44.69	-93.06	2017 – 2020	CRO
US-Ro6	AmeriFlux	44.69	-93.06	2017 – 2020	CRO
US-Tw3	AmeriFlux	38.12	-121.65	2013 – 2018	CRO
CA-ARB	AmeriFlux	52.70	-83.95	2011 – 2015	WET
CA-ARF	AmeriFlux	52.70	-83.69	2011 – 2015	WET
US-BZB	AmeriFlux	64.70	-148.32	2013 – 2020	WET
US-BZF	AmeriFlux	64.70	-148.31	2014 – 2020	WET
US-BZo	AmeriFlux	64.69	-148.33	2018 – 2020	WET
US-ICs	AmeriFlux	68.61	-149.31	2011 – 2020	WET
US-NC4	AmeriFlux	35.79	-75.90	2009 – 2020	WET
US-KS2	FLUXNET	28.61	-80.67	2003 – 2006	CSH
US-Rms	AmeriFlux	43.06	-116.75	2014 – 2020	CSH
US-PFa	FLUXNET	45.95	-90.27	2000 – 2014	MF
US-Syv	FLUXNET	46.24	-89.35	2001 – 2007	MF
US-SRM	FLUXNET	31.82	-110.87	2004 – 2014	WSA
US-Ton	FLUXNET	38.43	-120.97	2001 – 2014	WSA
US-LS2	AmeriFlux	31.57	-110.13	2002 – 2007	SAV
US-Wjs	AmeriFlux	34.43	-105.86	2007 – 2020	SAV

Table S2. Number of flux-tower sites and corresponding monthly NEE observations for each PFT.

	All	ENF	GRA	DBF	OSH	CRO	WET	CSH	MF	WSA	SAV
Number of sites	84	22	17	11	10	9	7	2	2	2	2
Number of monthly NEE observations	7711	2058	1182	1353	878	763	572	116	253	296	240

Table S3. Mean and standard deviation of the seasonal cycle of NEE (Pg C month⁻¹) estimated by seven products (EC-MOD2012 data unavailable) mentioned in this study across North America during 2015–2017. The standard deviation represents interannual variability.

Month	MemoryFlux	OCO-2 v10 MIP	CT2022	NIES2020	FLUXCOM20 20 RS+CRUJRA 1.1	FLUXCOM20 20 RS+ERA5	FLUXCOM-X
January	0.195±0.02	0.173±0.01	0.189±0.03	0.091±0.01	0.065±0.00	0.066±0.00	0.203±0.01
February	0.144±0.01	0.156±0.00	0.177±0.01	0.051±0.02	0.040±0.01	0.038±0.01	0.171±0.02
March	0.045±0.01	0.146±0.01	0.134±0.01	0.003±0.01	-0.005±0.00	-0.008±0.00	0.122±0.00
April	-0.078±0.01	0.023±0.02	0.031±0.02	-0.178±0.01	-0.159±0.01	-0.161±0.01	-0.050±0.01
May	-0.232±0.02	-0.287±0.02	-0.187±0.00	-0.541±0.01	-0.508±0.01	-0.482±0.00	-0.399±0.01
June	-0.479±0.02	-0.664±0.01	-0.611±0.03	-1.009±0.03	-0.902±0.02	-0.840±0.01	-0.839±0.03
July	-0.715±0.02	-0.764±0.04	-0.805±0.10	-1.170±0.02	-0.952±0.01	-0.883±0.02	-1.002±0.03
August	-0.554±0.01	-0.447±0.06	-0.441±0.08	-0.842±0.04	-0.565±0.03	-0.494±0.02	-0.591±0.02
September	-0.205±0.01	-0.002±0.01	0.011±0.03	-0.310±0.02	-0.171±0.00	-0.132±0.00	-0.089±0.01
October	0.064±0.01	0.253±0.02	0.285±0.02	0.033±0.02	0.017±0.00	0.049±0.01	0.216±0.01
November	0.197±0.02	0.279±0.02	0.357±0.06	0.131±0.02	0.083±0.01	0.098±0.01	0.280±0.02
December	0.209±0.01	0.238±0.01	0.288±0.01	0.121±0.01	0.084±0.01	0.092±0.01	0.251±0.01

Table S4. Mean and standard deviation of NEE over the season scale (Pg C season⁻¹) estimated by seven products (EC-MOD2012 data unavailable) mentioned in this study in whole North America during 2015–2017. The standard deviation represents interannual variability.

Season	MemoryFlux	OCO-2 v10 MIP	CT2022	NIES2020	FLUXCOM20 20 RS+CRUJRA 1.1	FLUXCOM20 20 RS+ERA5	FLUXCOM-X
MAM	-0.261±0.05	-0.122±0.06	-0.040±0.01	-0.719±0.01	-0.675±0.01	-0.654±0.01	-0.343±0.02
JJA	-1.757±0.01	-1.812±0.06	-1.725±0.07	-3.000±0.00	-2.390±0.03	-2.195±0.02	-2.414±0.04
SON	0.056±0.00	0.524±0.04	0.663±0.12	-0.114±0.02	-0.061±0.00	0.027±0.01	0.428±0.02
DJF	0.521±0.01	0.577±0.02	0.682±0.02	0.287±0.00	0.195±0.00	0.203±0.00	0.644±0.02

Table S5. Interannual variation (Pg C yr⁻¹) of NEE estimated by eight products and nonMemoryFlux mentioned in this study across North America.

Year	MemoryFlux	nonMemoryFlux	OCO-2 v10 MIP	CT2022	EC-MOD2012	NIES2020	FLUXCOM2020 RS+CRUJRA 1.1	FLUXCOM2020 RS+ERA5	FLUXCOM-X
1999						-3.181			
2000						-2.997			
2001	-1.259	-1.147		-0.781	-1.843	-2.975	-3.111	-2.857	-1.815
2002	-1.050	-1.098		-0.266	-1.596	-2.901	-3.017	-2.784	-1.537
2003	-1.238	-1.201		-0.505	-1.783	-3.045	-3.072	-2.791	-1.565
2004	-1.264	-1.299		-0.666	-1.908	-3.235	-3.191	-2.879	-1.664
2005	-1.226	-1.291		-0.839	-2.016	-3.259	-3.040	-2.782	-1.663
2006	-1.166	-1.161		-0.570	-1.782	-3.163	-2.992	-2.709	-1.483
2007	-1.351	-1.305		-0.916	-2.012	-3.319	-3.049	-2.792	-1.713
2008	-1.095	-1.262		-0.494	-1.900	-3.290	-3.153	-2.879	-1.688
2009	-1.153	-1.199		-0.831	-1.566	-3.206	-3.091	-2.811	-1.606
2010	-1.447	-1.396		-0.812	-1.948	-3.374	-3.033	-2.750	-1.839
2011	-1.092	-1.194		-0.415	-1.655	-3.168	-2.978	-2.678	-1.560
2012	-1.191	-1.167		-0.869	-1.721	-3.380	-2.915	-2.658	-1.616
2013	-1.344	-1.325		-0.855		-3.291	-3.031	-2.728	-1.741
2014	-1.208	-1.393		-0.979		-3.527	-3.073	-2.783	-1.757
2015	-1.322	-1.371	-0.817	-0.428		-3.584	-2.962	-2.637	-1.640
2016	-1.496	-1.535	-0.877	-0.510		-3.578	-2.920	-2.620	-1.799
2017	-1.407	-1.524	-0.993	-0.777		-3.698	-3.041	-2.715	-1.742
2018	-1.375	-1.381	-0.736	-0.744		-3.516		-2.636	-1.733
2019	-1.424	-1.544	-0.870	-1.008		-3.568			-1.826
2020	-1.253	-1.315	-0.659	-0.659					-1.735
2021	-1.250	-1.249							-1.495
mean±std	-1.267±0.12	-1.303±0.12	-0.825±0.11	-0.696±0.20	-1.811±0.15	-3.298±0.22	-3.039±0.07	-2.750±0.08	-1.677±0.11

Table S6. Model performance across different PFTs for the LSTM models incorporating historical information used to generate the MemoryFlux dataset. The units of RMSE and MAE are g C m⁻² d⁻¹.

PFT	All	ENF	GRA	DBF	OSH	CRO	WET	CSH	MF	WSA	SAV
R ²	0.79	0.71	0.56	0.88	0.76	0.77	0.69	0.93	0.51	0.65	0.83
MAE	0.52	0.56	0.49	0.61	0.20	0.95	0.42	0.34	0.41	0.39	0.25
RMSE	0.83	0.83	0.73	0.92	0.28	1.47	0.63	0.39	0.62	0.53	0.31

Table S7. Model performance across different PFTs for the LSTM models using only contemporaneous predictor information to generate the nonMemoryFlux dataset. The units of RMSE and MAE are g C m⁻² d⁻¹.

PFT	All	ENF	GRA	DBF	OSH	CRO	WET	CSH	MF	WSA	SAV
R ²	0.63	0.32	0.44	0.83	0.58	0.57	0.50	0.93	0.40	0.64	0.68
MAE	0.69	0.86	0.59	0.73	0.27	1.28	0.55	0.33	0.52	0.38	0.32
RMSE	1.12	1.27	0.82	1.11	0.36	2.02	0.81	0.39	0.68	0.53	0.42