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Breathing storms: Enhanced ecosystem respiration during storms in a heterotrophic headwater stream

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S1. Stream metabolic calculations: model specifications and performance.

Data preparation

To ensure that temporal patterns of environmental variables were accurate and realistic, we removed noise and outliers using the *loess* R package. Specifically, we applied a locally estimated scatterplot smoothing (LOESS) model with a *span* parameter of 0.03 to dissolved oxygen (DO), water temperature (T), light intensity (PAR), water depth (h), and oxygen saturation (DO.sat) variables, effectively smoothing fluctuations and replacing outliers. To address data gaps in the DO time series, we applied imputation using the *miceRanger* R package. This was done for 6 storm events for which some parts of the DO record were missing. The imputation was applied only to the missing days. In total, 48 days of DO data were imputed across the following events: event 5 (5 days), event 11 (6 days), event 24 (11 days), event 34 (11 days), event 35 (9 days), and event 41 (6 days). The process involved generating 5 imputations over 5 iterations to ensure accurate reconstruction of missing data while preserving variability.

Model description and specifications

We estimated stream metabolism using the single-station open-channel method described by Odum (1956). Daily fluxes of the normalized gas transfer coefficient (K_{600}, in d^{-1}), gross primary production (GPP), and ecosystem respiration (ER) (in g O_2 m^{-2} d^{-1}) were calculated by fitting a Bayesian model to DO dynamics using the *streamMetabolizer* R package (Appling et al., 2018). In particular, we used the model *b_Kb_oipi_tr_plrckm.stan*, which incorporates both observational and process errors. In the model, K_{600} and GPP were assumed to vary linearly with discharge (Q) and light intensity (van de Bogert et al., 2007), respectively, while ER was constant over 24 hours. Model fitting involved running four parallel Markov Chain Monte Carlo (MCMC) chains on four cores. Each chain included 1500 warmup iterations, followed by 2000 saved steps.

The model was fitted for each 24-hour window starting at 23:00 on the preceding day. Prior probability distributions for GPP and ER were set based on previously reported values (0.5 ± 10 and -5 ± 10 g O_2 $m^{-2}d^{-1}$ for GPP and ER, respectively) (Acuña et al., 2004; Bernal et al., 2022). Prior probability distributions for K_{600} were strongly constrained based on a deterministic, hand-pooled K_{600} derived from the relationship between binned Q and K_{600} estimates obtained from 11 propane additions using a mixed tracer injection method (Jin et al., 2012, Fig. S1). This approach involves fitting a relationship between daily K_{600} and mean daily Q as a series of linearly connected nodes at fixed intervals of natural log units, covering the observed Q range. For our model, the interval between nodes (n) was set at 0.2 natural log units. Constraining K_{600} based on empirical values minimized potential equifinality problems (Appling et al., 2018, Fig. S2) and overall improved the goodness of fit of the model. Further details on model parameters and specifications can be found in Table S2.

Diagnosis of model outputs

Modelled metabolism estimates were subjected to a thorough quality control process to identify impossible values, adequate model convergence, and a good fit between modelled and observed DO dynamics (Table S2). First, we removed days with biologically impossible values (i.e., negative GPP or positive ER) as well as days with unrealistic high ER (i.e., ER < -40 g O_2 $m^{-2}d^{-1}$) and K_{600} values (i.e., K_{600} > 100 d^{-1}). Further, model convergence was evaluated using the $\hat{R}$-hat statistic and the number of effective samples (n_eff). The $\hat{R}$-hat statistic measures consistency across MCMC chains, with values = 1 indicating good convergence and values >1 suggesting low convergence (Appling et al., 2018b). Days with $\hat{R}$-hat > 1.2 for GPP, ER, or K_{600} were excluded. Additionally, the n_eff quantifies the estimation power of the MCMC method in terms of its equivalence to a number of independent samples, which should be lower than the product of the number of chains run and the number of saved steps (in our case, n_eff < 8000 indicates good model performance). Finally, the goodness of fit of modelled vs observed DO curves was assessed with three metrics: the coefficient of determination (R^2), the residual root mean square error (RMSE) and the mean absolute error (MAE). We considered R^2 > 0.50, and RMSE and MAE < 0.4 as indicators of a good fit between measured and predicted DO curves.

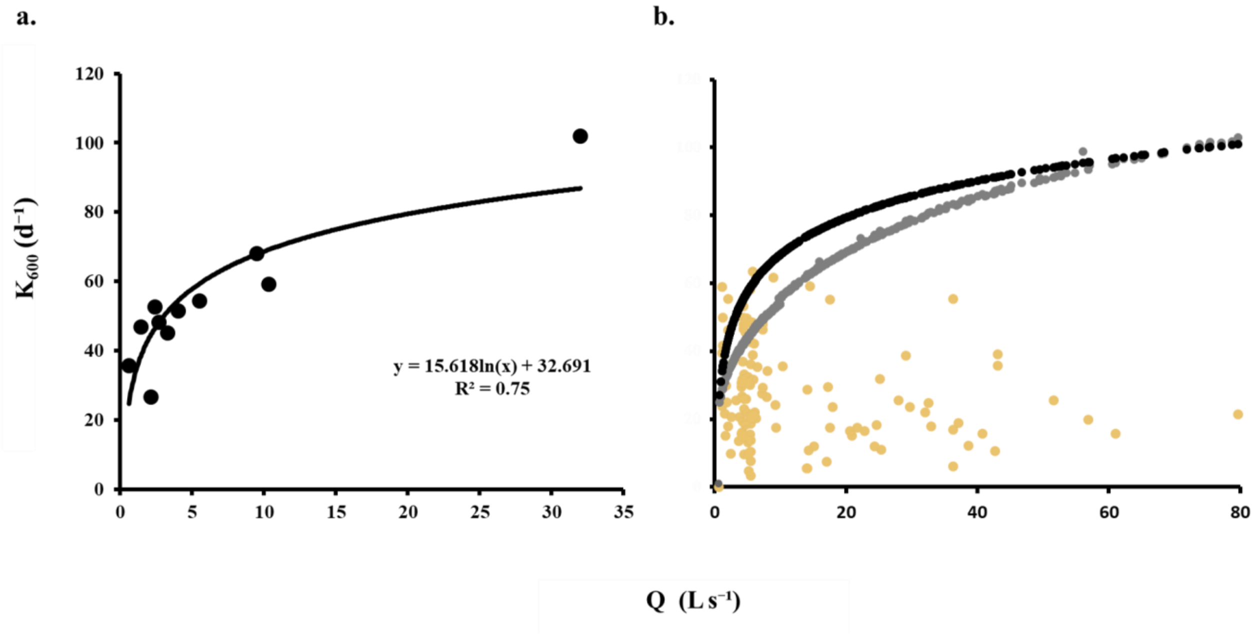

Figure S1. Mean daily discharge (Q) and gas exchange coefficient (*K_{600}*). (a) *K_{600}*estimates from 11 propane tracer additions using a mixed tracer injection method (Jin et al., 2012). A logarithmic relationship between Q and *K_{600}* was derived from these measurements. (b) *K_{600}* estimates for all days before, during, and after storm events using three methods: night-time regression (yellow dots, n = 417), hydraulic geometry following Raymond et al. (2012) (grey dots, n = 774), and modeled *K_{600}* values (black dots) calculated using the Q–*K_{600}* relationship derived from panel (a).

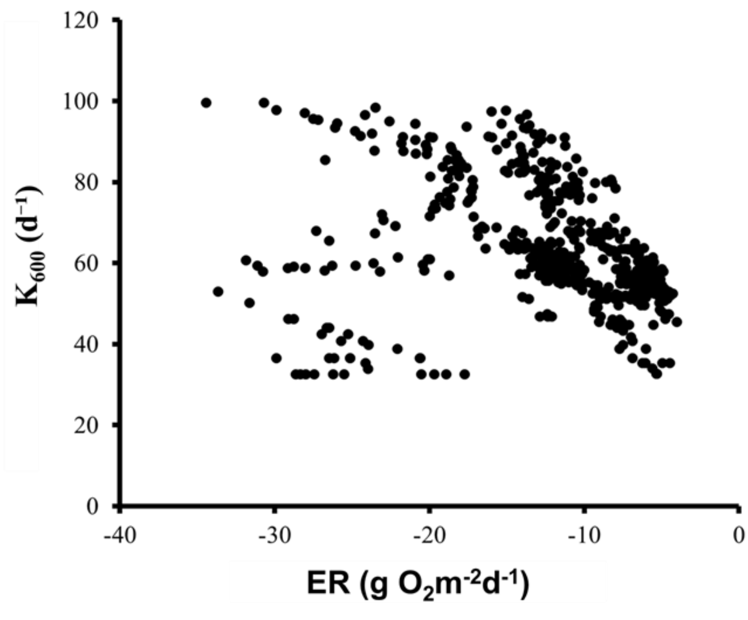

Figure S2. Relationship between daily ecosystem respiration (ER) and final estimates of *K_{600}*.

Table S1. Hydrological descriptors of each storm event identified from October 2018 to February 2023. Start date, rainfall amount (P), and maximum rainfall intensity (PI_{max}) are indicated for each event, as well as the duration of the hydrological event (D), discharge at baseflow conditions before the event (Q_{prior}), maximum discharge (Q_{max}), change in discharge (ΔQ), and the runoff coefficient (RC). Average light inputs (PAR) during each event are also included. Events marked with * are those for which metabolic rates were available.

Event	**Start date**	**P**	**PI_{max}**	**D**	**Q_{prior}**	**Q_{max}**	**Δ Q**	**RC**	**PAR**
	dd/mm/yyyy	mm	mm h^{-1}	days	L s^{-1}	L s^{-1}	L s^{-1}	%	mol m^{-2} d^{-1}
1*	13/10/2018	98.8	21.3	13	10.6	157.2	146.6	4.29	3.41 ± 0.6
2*	25/10/2018	39.6	6.3	6	20.7	49.4	28.7	4.34	3.83 ± 1.2
3*	30/10/2018	53.7	9.5	6	40.6	158.6	118	7.94	3.62 ± 0.8
4*	08/11/2018	23.7	8.7	6	48.5	94.2	45.7	13.7	3.88 ± 0.7
5	14/11/2018	53.2	15.9	4	50.7	356.4	305.7	11.6	2.1 ± 0.8
6*	17/11/2018	77.5	12.7	17	164.6	1037	872.4	33.3	4.49 ± 0.5
7*	19/01/2019	12.4	1.3	5	9.7	11.3	1.6	3.66	7.35 ± 1.3
8*	09/03/2019	9.6	7.9	23	5.9	7.3	1.4	12.1	11.6 ± 1.4
9*	03/04/2019	36.8	5.8	17	4.9	7.3	2.4	2.03	7.7 ± 0.8
10*	01/05/2019	26.1	4.8	12	3.8	5.1	1.3	1.52	9.05 ± 0.7
11*	12/05/2019	10.6	2.6	10	3.6	4.3	0.7	3.1	6.29 ± 1.0
12*	21/05/2019	10.6	1.7	14	3	3.6	0.6	3.22	5.02 ± 0.8
13*	09/06/2019	22.5	3	12	2.1	3.7	1.6	0.99	4.9 ± 0.5
14	22/10/2019	93.6	31.4	5	0	14.4	14.4	0.22	3.87 ± 1.1
15	21/11/2019	31.9	7.8	8	4.6	10.1	5.5	1.66	3.3 ± 0.2
16	01/12/2019	126	15	19	7.5	1374	1367	17.4	2.6 ± 0.2
17	19/12/2019	14.5	2.4	19	13.5	14.5	1	10.8	2.65 ± 0.1
18	07/01/2020	15.9	5.9	5	6.1	7.5	1.4	1.74	2.72 ± 0.2
19	19/01/2020	235	18.8	31	6.4	3508	3501	26.2	5.4 ± 0.4
20*	15/03/2020	24	6.3	8	3.8	15.6	11.8	2.67	9.28 ± 1.8
21*	22/03/2020	38.9	8	10	9	46.7	37.7	7.37	6.21 ± 1.1
22*	31/03/2020	15.4	2.3	13	33.2	80.4	47.2	32.5	14.7 ± 1.8
23	12/04/2020	48.3	8.4	7	35.2	193.2	158	13	12 ± 2.5
24*	18/04/2020	185	12.3	21	112	3884	3772	39.4	9.86 ± 1.2
25*	13/05/2020	37.7	19.2	16	31.9	35.1	3.3	7.96	8.53 ± 0.6
26*	03/06/2020	29.3	13.8	5	14.7	18.4	3.7	2.38	5.75 ± 0.8
27*	07/06/2020	50.8	6.3	17	16.9	26.7	9.8	5.09	6.11 ± 0.5
28*	01/07/2020	34.1	15.7	18	9.9	29.8	19.9	5.52	6.14 ± 0.3
29*	01/08/2020	29.6	13.2	11	6.1	8.3	2.2	1.88	6.16 ± 0.2
30*	28/08/2020	72.6	30.1	12	4	9.7	5.7	0.83	4.92 ± 0.5
31	08/09/2020	32.2	7.9	7	5.4	6.2	0.8	1.08	4.44 ± 0.7
32	06/10/2020	72.2	25.5	8	4.8	388.9	384.1	7.37	4.06 ± 0.6
33	13/10/2020	15.4	9.9	7	9.3	15.5	6.2	3.49	3.8 ± 0.5
34*	23/11/2020	77.4	14.3	25	3.4	71.8	68.4	3.4	3.07 ± 0.1
35*	17/12/2020	8.6	6.6	11	3.5	7.5	4	5.66	3.05 ± 0.2
36*	08/01/2021	16.8	2.5	11	3.7	6.3	2.6	2.83	3.4 ± 0.3

37*	06/02/2021	24.4	11.8	7	4.2	10.9	6.7	2.05	5.48	±	0.8
38*	12/02/2021	34.6	18.6	20	6.9	8.2	1.3	3.51	5.06	±	0.5
39*	16/03/2021	26	4.6	21	5.3	8.9	3.6	4.15	11.2	±	0.6
40*	09/04/2021	48.9	12.2	17	4.9	9.3	4.4	1.77	8	±	1.0
41*	30/04/2021	19.1	8.2	10	4.3	6.6	2.3	2.41	7.59	±	1.0
42*	27/10/2021	37	12.6	14	2.3	22.2	19.9	2.52	1.95	±	0.5
43*	09/11/2021	51.9	14.1	14	4.8	7.6	2.8	1.26	2.38	±	0.3
44*	22/11/2021	44.9	10	32	4.5	68.4	63.9	6.65	3.79	±	0.2
45*	11/03/2022	61.4	7	7	2.9	98.5	95.6	6.1	5.46	±	2.3
46*	19/03/2022	33.4	6.3	10	60.3	108.2	47.9	13.2	19.9	±	3.5
47*	29/03/2022	46.9	7.4	14	25.8	68	42.2	8.18	28.6	±	2.8
48*	19/04/2022	62.9	6	27	22.5	259.5	237	15.7	16.2	±	1.3
49*	22/05/2022	17.2	6.4	11	6.2	7.3	1.1	3.03	8.81	±	1.2
50	15/09/2022	41.7	28.7	8	0	113.2	113.2	4.26	7.06	±	0.5
51*	16/11/2022	24.8	16.4	17	0.7	1.3	0.6	0.62	3.58	±	0.2
52*	11/12/2022	26.7	6.4	8	1.8	3.7	1.9	0.62	2.8	±	0.3
53*	03/02/2023	56.3	8.9	22	3.9	10.4	6.5	1.99	5.2	±	0.1

Table S2. Specifications (*specs*) of the used model for estimating metabolic rates with *StreamMetabolizer*. Node centers and associated K_{600} are shown in Figure S1. Other *specs* not defined here were set as default.

Model specifications	**Values**
burning_steps	1500
saved_steps	2000
n_cores	4
n_chains	4
K_{600}_lnQ_nodes_centers	vector (Fig. S1)
K_{600}_lnQ_nodediffs_sdlog	0.01
K_{600}_lnQ_nodes_meanlog	vector (Fig. S1)
K_{600}_lnQ_nodes_sdlog	0.001
K_{600}_daily_sigma_sigma	0.01
GPP_daily_mu	1
GPP_daily_sigma	10
ER_daily_mu	-5
ER_daily_sigma	10
day_start	-1
day_end	23

Table S3. Diagnostics assessing model performance, detailing the total number of days analyzed (including storm days and days prior to each storm event) and the number of storm events affected by each diagnostic criterion. The table includes the total available data, the number of imputed days using *miceRanger*, and occurrences of both biologically implausible values (i.e., negative GPP or positive ER) and implausible values of K_{600} (K_{600} > 110 d^{-1}). It also reports instances of unsuccessful model convergence (R̂-hat > 1.2 and n_eff < 8000) and days with poor model fit (R^2 < 0.5, RMSE > 0.4). Finally, the number of days that passed all quality checks is indicated. The same diagnostics are shown for different ranges of discharge during storm events.

Quality test	Days analyzed	Number of storm events	Discharge Range During Storm Events (L/s)			
			0.7–10	10.1–40	40.1–100	>100
Total data	698	53	347	135	57	26
Imputed data	48	6	32	0	2	14
GPP < 0, ER > 0	53	18	8	11	9	14
K_{600} > 110	18	8	0	0	0	18
R̂-hat > 1.2	48	9	18	10	0	0
n_eff > 8000	0	0	0	0	0	0
R^2 < 0.50	147	31	56	18	7	19
RMSE > 0.4	92	26	30	23	7	19
Passed quality check	542	35	274	106	37	0
% Success	72%	66%	79%	79%	65%	0%

Table S4. Comparison of linear and logarithmic regression model performance comparing hydrological, environmental, and biological variables. Each row shows a pair of variables tested as predictors and responses. For each model type, the Akaike Information Criterion (AIC), p-value, and coefficient of determination (R^2) are reported. Predictor variables include maximum rainfall intensity (PI_{max}), storm duration (D), runoff coefficient (RC), change in discharge (ΔQ), daily discharge (Q), temperature (T), and light (PAR). Response variables include gross primary production (GPP), ecosystem respiration (ER), metabolic resistance as the change in metabolic rates between the storms and pre-storm conditions (ΔGPP, ΔER), and metabolic resilience as recovery time (RT_{GPP}, RT_{ER}). In bold are the models that were finally selected based on AIC and p-values (p-value < 0.01). When the difference in AIC between the two models was less than 2, we considered them equally supported. Missing values (--) indicate cases where logarithmic transformation was not possible.

			Linear model			Logarithmic model		
Relationship explored			**AIC**	**R^2**	**p value**	**AIC**	**R^2**	**p value**
PI_{max}	vs	GPP	126	0.1	0.035	129	0.1	0.183
PI_{max}	vs	ER	232	0.2	0.015	234	0.1	0.034
D	vs	GPP	131	0	0.632	130	0	0.424
D	vs	ER	236	0.1	0.104	237	0.1	0.157
RC	vs	GPP	131	0	0.775	131	0	0.659
RC	vs	ER	238	0	0.386	239	0	0.65
ΔQ	vs	GPP	130	0	0.312	131	0	0.66
ΔQ	vs	ER	237	0.1	0.212	236	0.1	0.143
Q	vs	GPP	1405	0	0.025	1409	0	0.803
Q	vs	**ER**	**2549**	**0.2**	**< 0.001**	2586	0.1	<0.001
T	vs	GPP	1903	0	0.06	1902	0	0.04
T	vs	ER	**3554**	**0.1**	**<0.001**	**3552**	**0.1**	**<0.001**
PAR	vs	GPP	128	0.1	0.097	125	0.2	0.017
PAR	vs	ER	239	0	0.734	239	0	0.753
PI_{max}	vs	ΔGPP	391	0	0.477	391	0	0.539
PI_{max}	vs	ΔER	341	0	0.352	342	0	0.862
D	vs	ΔGPP	391	0	0.672	391	0	0.526
D	vs	ΔER	342	0	0.936	342	0	0.928
RC	vs	ΔGPP	391	0	0.663	391	0	0.739
RC	vs	ΔER	340	0.1	0.216	339	0.1	0.103
ΔQ	vs	ΔGPP	387	0.1	0.034	388	0.1	0.071
ΔQ	vs	**ΔER**	**325**	**0.4**	**<0.001**	**325**	**0.4**	**<0.001**
PI_{max}	vs	RT_{GPP}	153	0	0.427	152	0.1	0.184
PI_{max}	vs	RT_{ER}	150	0	0.864	150	0	0.563
D	vs	RT_{GPP}	151	0.1	0.11	151	0.1	0.161
D	vs	RT_{ER}	148	0	0.246	149	0	0.352
RC	vs	RT_{GPP}	153	0	0.38	153	0	0.93
RC	vs	RT_{ER}	147	0.1	0.132	148	0.1	0.221
ΔQ	vs	RT_{GPP}	153	0	0.49	153	0	0.822
ΔQ	vs	**RT_{ER}**	**126**	**0.5**	**<0.001**	**128**	**0.5**	**<0.001**
RT_{GPP}	vs	ΔGPP	387	0.1	0.046	--	--	--
RT_{ER}	vs	**ΔER**	**321**	**0.5**	**<0.001**	--	--	--

Table S5. Results of the reanalysis of storm days with daily discharge above 100 L s⁻¹ using *StreamMetabolizer* with constrained K_{600} to 100 d⁻¹. For each date, the table shows daily discharge (Q), model fit metrics (R^2, RMSE), and daily estimates of gross primary production (GPP, g O_2 m^{-2} d^{-1}), ecosystem respiration (ER, g O_2 m^{-2} d^{-1}), and reareation rates (K_{600}, d^{-1}). Values in bold indicate days that passed the quality check. Missing values (NA) indicate cases where reliable metabolic estimates could not be obtained.

date	**Q**	**R^2**	**RMSE**	**GPP**	**ER**	**K600**
dd/mm/yyyy	L s^{-1}			g O_2 m^{-2} d^{-1}	g O_2 m^{-2} d^{-1}	d^{-1}
15/10/2018	157.2	98.40	6.74	-0.03	-20.34	99.99
01/11/2018	158.6	6.67	57.93	0.62	-20.44	100.00
15/11/2018	104	-54.44	69.32	0.19	-20.63	100.00
16/11/2018	356.4	-186.36	98.23	-1.30	-37.59	100.00
17/11/2018	218.8	-16.32	61.90	0.53	-33.13	100.00
18/11/2018	744.1	-16009.87	714.99	-3.95	-67.99	99.86
19/11/2018	1037	-2748.18	295.03	4.86	-106.70	99.86
20/11/2018	283.2	80.42	24.05	-1.85	-54.05	100.00
21/11/2018	154.1	-113.10	80.63	0.84	-42.65	99.99
14/04/2020	193.2	-223.85	105.56	1.25	-39.60	99.98
15/04/2020	135	-50.69	71.85	1.45	-38.95	100.00
16/04/2020	108.8	-222.15	104.70	1.30	-35.49	99.99
19/04/2020	183.9	-2341.77	284.57	0.50	-34.16	99.97
20/04/2020	295.5	-15.73	62.04	0.48	-40.08	100.00
21/04/2020	2319.7	-20530.77	828.47	0.77	-51.19	99.81
22/04/2020	3883.7	-3218.55	332.92	3.42	-69.40	99.81
23/04/2020	364.8	-1.19	57.75	0.33	-48.12	100.00
24/04/2020	**227.7**	**76.31**	**27.80**	**0.29**	**-41.12**	**99.99**
25/04/2020	**169.1**	**96.06**	**11.23**	**0.05**	**-38.53**	**99.98**
26/04/2020	**136.3**	**97.90**	**8.15**	**0.13**	**-37.14**	**100.00**
27/04/2020	**115.3**	**98.25**	**7.39**	**0.06**	**-36.86**	**100.00**
21/03/2022	108.2	NA	NA	NA	NA	NA
28/04/2020	**100.2**	**93.27**	**14.41**	**0.19**	**-35.51**	**99.98**
21/04/2022	**259.5**	**64.28**	**35.16**	**0.49**	**-36.35**	**99.96**
22/04/2022	**150.3**	**95.04**	**13.34**	**0.81**	**-22.13**	**99.99**
23/04/2022	**104**	**74.67**	**29.90**	**0.61**	**-19.69**	**99.99**

References

Acuña, V., Giorgi, A., Muñoz, I., Uehlinger, U., and Sabater, S.: Flow extremes and benthic organic matter shape the metabolism of a headwater Mediterranean stream, Freshw Biol, 49, 960–971, https://doi.org/10.1111/j.1365-2427.2004.01239.x, 2004.

Appling, A. P., Hall, R. O., Yackulic, C. B., and Arroita, M.: Overcoming Equifinality: Leveraging Long Time Series for Stream Metabolism Estimation, J Geophys Res Biogeosci, 123, 624–645, https://doi.org/10.1002/2017JG004140, 2018a.

Appling, A. P., Read, J. S., Winslow, L. A., Arroita, M., Bernhardt, E. S., Griffiths, N. A., Hall, R. O., Harvey, J. W., Heffernan, J. B., Stanley, E. H., Stets, E. G., and Yackulic, C. B.: The metabolic regimes of 356 rivers in the United States, Sci Data, 5, https://doi.org/10.1038/sdata.2018.292, 2018b.

Jin, H.-S., White, D. S., Ramsey, J. B., and Kipphut, G. W.: Mixed Tracer Injection Method to Measure Reaeration Coefficients in Small Streams, Water Air Soil Pollut, 223, 5297–5306, https://doi.org/10.1007/s11270-012-1280-8, 2012.

Raymond, P. A., Zappa, C. J., Butman, D., Bott, T. L., Potter, J., Mulholland, P., Laursen, A. E., McDowell, W. H., and Newbold, D.: Scaling the gas transfer velocity and hydraulic geometry in streams and small rivers, *Limnol Oceanogr Fluids Environ*, 2, 41–53, https://doi.org/10.1215/21573689-1597669, 2012.

Rocher-Ros, G., Sponseller, R. A., Bergström, A., Myrstener, M., and Giesler, R.: Stream metabolism controls diel patterns and evasion of CO2 in Arctic streams, Glob Change Biol, 26, 1400–1413, https://doi.org/10.1111/gcb.14895, 2019.

Odum, H. T.: Primary production in flowing waters1, Limnol Oceanogr, 1, 102–117, https://doi.org/10.4319/lo.1956.1.2.0102, 1956.

Van De Bogert, M. C., Carpenter, S. R., Cole, J. J., and Pace, M. L.: Assessing pelagic and benthic metabolism using free water measurements, Limnol Oceanogr Methods, 5, 145–155, https://doi.org/10.4319/lom.2007.5.145, 2007.