Supplemental Information: Gas exchange in large rivers influenced by multiple turbulence scales: implications for remotely sensing gas exchange via the SWOT satellite

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## Contents

This supplementary information contains 4 texts, 1 figure and 3 tables. Please consult <https://github.com/craigbrinkerhoff/RSK600> for all code to build and generate results, figures, and the manuscript.

## Test S1: Estimating how many SWOT rivers are hydraulically wide

To quantify how frequently SWOT-observable rivers are also hydraulically wide river channels (section 3 of main text), we used the dataset of field-measured river hydraulics in Brinkerhoff et al. (2019). That dataset has over 500,000 discrete measurements of river width, velocity, area, and discharge that were made by the United States Geological Survey (USGS) to calibrate streamgauge rating curves. Here, we describe how this dataset was filtered down to 171,553 measurements and how we quantified what was ‘hydraulically wide’.

First, we removed all measurements tagged by the USGS as ‘poor’, measurements with impossible values, or measurements of 0. While this would indicate a dry channel, our hydraulic geometry model necessitates within-bank flow. Likewise, because hydraulic geometry only applies to within-bank flows and not flood events, we remove all overbank flows. This was done by first filtering for sites with at least 20 measurements (to build robust estimates of bankfull hydraulics) and then calculating bankfull width and depth as the width or depth with a return period of two years. While the only true way to calculate bankfull hydraulics is manually in the field, this is obviously impractical here. A two year return period is a standard approximation for determining out-of-bank flow in single-channel meandering rivers and was the method used by Brinkerhoff et al. (2019). We then removed all measurements with a width or depth beyond their respective at-a-station 2 year values.

After joining this dataset with the hydraulics measurements provided with the 763 measurements, we classified each measurement as hydraulically wide if its hydraulic radius was within 4% of its mean flow depth. Hydraulic radius was calculated assuming a rectangular channel such that . Because these measurements were almost entirely made at streamgauges, which generally have a location bias favoring stable channels near bridges and other structures that yield lower width dynamics than those observed away from gauges (Allen & Pavelsky, 2015; Park, 1977), we used a wider threshold of 4%. In the ‘width-limited’ scenario common at streamgauges, the hydraulic radius is likely further from the mean flow depth than would occur naturally. The slightly more liberal threshold of 4% allowed for implicit accounting for this sampling bias.

## Text S2: Gas exchange model derivations

In this text we provide the full algebra to arrive at the four physically-based gas exchange models in the main text (equations 3-6). Equation 3 is derived via equations S1-S5. Equation 4 is derived via equations S6-S7. Equation 5 is derived via equations S8-S13. Equation 6 is derived via equations S14-S18. Consult Appendix A for all variable definitions. Note that and are statistical parameters obtained via least squares regression for the small-eddy and chainsaw models, respectively. Subscripts denote variants of the same parameter, depending on which model is employed.

**Small-eddy models**

*log-law-of-the-wall dissipation*

*form-drag dissipation*

**Chainsaw models**

*log-law-of-the-wall dissipation*

*form-drag dissipation*

## Text S3: BIKER hyperparameterization

In this text we explain in detail how BIKER’s hyperparameter values were set for each river.

We assign prior hyperparameters using SWOT data only. All priors are formalized within the model as truncated normal distributions of the log-transformed terms such that for , using prior hyperparameters mean (), standard deviation (), and upper () and lower bounds () for any parameter *X*.

and prior hyperparameters were assigned following an updated version of the method developed by Brinkerhoff et al. (2020). They developed a set of river channel prior hyperparameters for McFLI algorithms that are entirely RS-able and reflect differential channel hydraulics as a function of river geomorphology. They used an extensive database of field measurements and machine learning to identify patterns that associate river width with the hydraulic priors needed to run McFLIs so that prior hyperparameters may be assigned to rivers using only the existing remotely sensed data. For this study, we extracted and as the 5th and 95th percentile values rather than the absolute maximum and minimum values to avoid physically impossible bounds on .

This leaves the hyperparameters to be defined. is set by invoking the hydraulic geometry (HG) relationships developed in section 5.1.3 of the main text using the data from Brinkerhoff et al. (2019). We replaced both depth and velocity terms from our gas exchange model (equation 6 in the main text) with these HG models, resulting in equation S19 where Q is the mass-conserved streamflow for the river reach.

Obviously, we have no a priori information about Q. So, we use the Q prior that will be globally available when SWOT launches: a mean annual estimate from a water balance model. This is provided with the simulated SWOT data by both Durand et al. (2016) and Frasson et al. (2021). Again, using a temporally-invariant estimate of streamflow is the worst case scenario and BIKER’s performance will improve with a more informed prior om streamflow (and therefore ). However as noted in the main text, our primary goal with this initial validation is to benchmark BIKER’s worst case scenario for performance and so we do that here. Because BIKER treats every timestep as a different parameter, future work should investigate ways to assign temporally varying priors for .

is set to 0.30 (log-space). This corresponds to a coefficient of variation of approximately 0.30, which we took to reflect a reasonably strong agreement between the prior and the observed values. was set to log(0.001) m/day. was set to log(500) m/day. The

## Text S4: Specifiying the parameter

Here, we detail how the parameter is specified in this study, as well as how it should be specified once SWOT launches.

Recall that refers to the total uncertainty inherent in equation 8, i.e. stemming from both the chainsaw/form-drag dissipation model and the Manning’s model for . For the purposes of this study, we are validating BIKER against equation 10 in the main text and so all uncertainties associated with the parameter are ignored and we only need to reflect the Manning’s uncertainty in our specification of . Therefore, we take Hagemann et al. (2017)’s estimated uncertainty from Manning’s equation to infer streamflow from SWOT observations (0.25) and inflate it slightly to also account for the hydraulically-wide channel assumption and arrive at 0.30. This is the used in this study.

In the scenario that BIKER is run on real SWOT data, must reflect the full uncertainty implicit in equation 8 in the main text. This means we must also account for uncertainty from the parameter. Assuming perfect measurements from are made by the SWOT satellite, the relative uncertainty is expressed for some set of hydraulic observations as equation S19. We use the 166 hydraulically-wide measurements in our field-measured dataset and run 166 different Monte Carlo simulations (each 10,000 runs) to obtain 166 different terms. We then take the average of those to be a reasonable estimate of . This ultimately provided a value of 1.1 for the log-transformed that should be used once SWOT launches.

## Figure S1

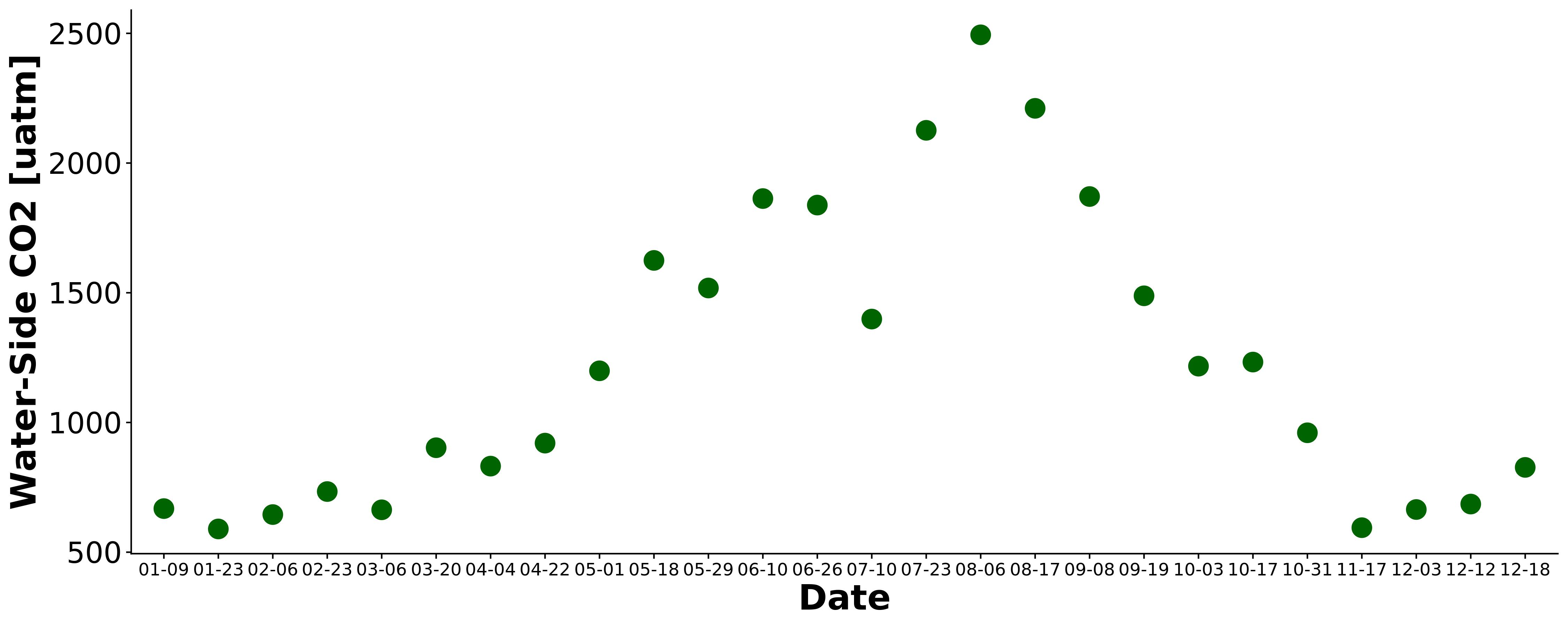


Figure S1 Timeseries of the biweekly CO2 data from Beaulieu et al. (2012). Sampling took place 2008-2009 in the Ohio River (upstream of Cincinnati, Ohio, United States). Each point here was joined to the 11-day SWOT observations used in this study (section 2.4).

## Figure S2

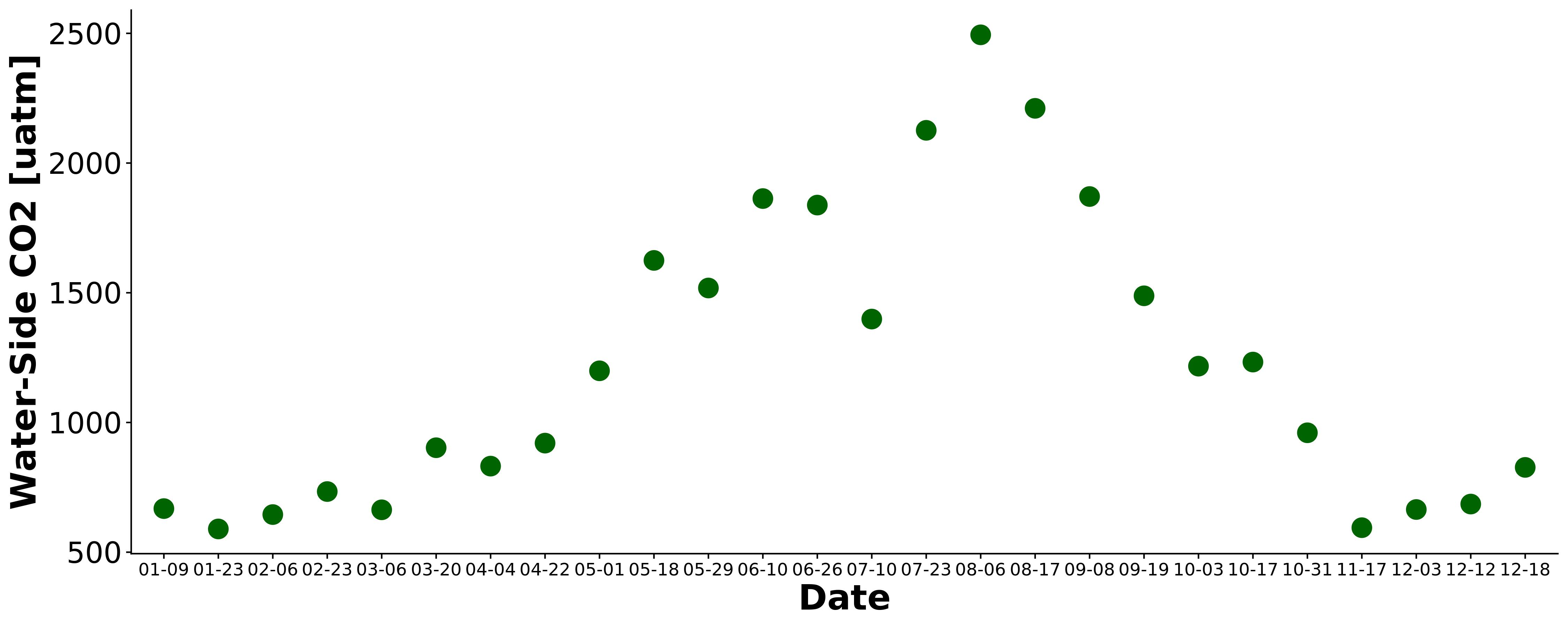


Figure S2 Conceptual river reach model used in this study following McFLI logic (Gleason et al., 2017) DOOOOOOOOO

## Table S1

*Table S1: Studies that gas exchange velocity measurements come from. ‘Study’ refers to the paper from which these measurements were taken. Any data wrangling was done by those authors. ‘Field Workers’ refers to who actually made the measurements. The Raymond et al. (2012) dataset is itself a meta-analysis. Please see that paper for how those measurements were collected. We used the set of measurements ultimately published by Ulseth et al. 2019.*

| **Study** | **Workers** | **Number of measurements** |
| --- | --- | --- |
| Ulseth et al. (2019) | Ulseth et al. (2019) |  |
| Ulseth et al. (2019) | Hall & Madinger (2018) |  |
| Ulseth et al. (2019) | Schelker et al. (2016) |  |
| Ulseth et al. (2019) | Maurice et al. (2017) |  |
| Ulseth et al. (2019) | Raymond et al. (2012) |  |
| Churchill et al. (1964) | Churchill et al. (1964) |  |
| Owens et al. (1964) | Owens et al. (1964) |  |

## Table S2

*Table S2: Validation metrics used in this study, where Nt is number of observations and i is the specific observation. σ refers to the variance of the sample and μ refers to the mean of the sample. As is standard, a carrot accent indicates the predicted value.*

| **Description** | **Acronym** | **Definition** | **Ideal Score** | **Possible Range** | **Validation Scheme** |
| --- | --- | --- | --- | --- | --- |
| Correlation Coefficient |  |  | 1 | -1 to 1 | All rivers and all timesteps |
| Root-mean-square-error | RMSE |  | 0 | 0 to ∞ | All rivers and all timesteps |
| Relative root-mean-square error | RRMSE |  | 0 | 0 to ∞ | By river |
| Normalized root-mean-square error | NRMSE |  | 0 | 0 to ∞ | By river |
| Relative bias | rBIAS |  | 0 | -∞ to ∞ | By river |

## Table S3

*Table S3: Details on the 3 depth hydraulic geometry models used to estimate FCO2 from the SWOT rivers (section 2.4).*

| **Name** | **Depth equation** | **Velocity equation** | **Description** | **Reference** |
| --- | --- | --- | --- | --- |
| Brinkerhoff 2019 |  |  | 530,945 measurements made across the United States at streamgauges | this study; Brinkerhoff et al. (2019) |
| Raymond 2012 |  |  |  | 1,026 measurements across the United States |
| Raymond 2013 |  |  | Average of the Raymond 2012 equation and one using 9,811 measurements at US streamgauges | Raymond et al. (2013) |

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