Gas exchange in large rivers controlled by largest turbulent eddies: implications for remotely sensing gas exchange via SWOT

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## Key Points

* In large rivers, there exists a local equilibrium between the production and dissipation of turbulent kinetic energy at the free surface
* Gas exchange in large rivers is equivalently parameterized across multiple turbulence scales, with the classical Kolmogorov model recovered empirically
* BIKER algorithm exploits this theory, predicting gas exchange velocity and fluxes from simulated SWOT satellite data and in situ data

## Keywords

gas exchange, open-channel flow, remote sensing, SWOT, biogeochemistry, ungauged basin

## Abstract

*AGU Advances. So 250 words here* *AGU advances is 8000 words total, the format seems to be a long letter so I've tried to right this in that style. Might be a bold organization but we'll see*

## Plain Language Summary

*Necessary for AGU advances (200 words)*

## 1 Introduction

Natural systems play a fundamental role in the budgeting and accounting of the global carbon cycle under climate change. Since the publication of Cole et al. (2007), the global river network is recognized to emit substantial amounts of carbon to the atmosphere, in addition to exporting it to the oceans. Current estimates of total carbon dioxide evasion () to the atmosphere from the global river network vary from 650-1800 Tg C/yr (Lauerwald et al., 2015; Raymond et al., 2013) **maybe add Shaoda here**, with 167 Tg-C/yr coming from mountain streams alone (Horgby et al., 2019). Despite its incredibly small percentage of the global land surface (0.47%- Raymond et al., 2013), this flux is on par with the total oceanic uptake rate (Gruber et al., 2019; Horgby et al., 2019) and the global forest carbon uptake rate (Pan et al., 2011). It is still relatively poorly constrained but is clearly a critical component of the global carbon cycle. Equation 1 represents this flux given the gas concentration gradient between the water and the air and the gas exchange velocity *k*.

The structure of equation 1 necessitates that calculations of this flux are highly sensitive to one's measurements/estimates of *k* (Hall and Ulseth, 2020). Even more broadly, fluvial *k* for various dissolved gases are of significant importance to aquatic ecologists modeling stream metabolism (e.g. Bernhardt et al., 2018) and water quality engineers modeling river responses to pollutant loadings (among other things- Chapra, 2008). Decades of work have focused on elucidating the physical mechanisms behind *k* in oceans and lakes (Wanninkhof et al., 2009) and, to a lesser extent, fluvial gas exchange (Hall and Ulseth, 2020). Given that *k* should scale with turbulence in a turbulent flow (Hall and Ulseth, 2020), a generalized model for *k* (equation 2) relies on the characteristic turbulence velocity scale , which itself is a function of the characteristic length and time scales (Katul et al., 2018). Extensive field and labratory experiments have confirmed the validity of this model when is set to the Kolmogorov velocity scale (e.g. Lamont and Scott, 1970; Lorke and Peeters, 2006; Moog and Jirka, 1999; Vachon et al., 2010; Wang et al., 2015; Zappa et al., 2007, 2003), where the idea is that turbulent kinetic energy (TKE) is produced by the largest, integral-scale turbulent eddies in the flow and then passed down the energy cascade to progressively smaller eddies until eddy motion is stable and TKE is dissipated as heat at the Kolmogorov-scale: the smallest eddies in a turbulent flow. Equation 2 via Kolmogorov-scale eddies can also be derived from both classic thin-film and surface renewal theories for gas exchange (Wang et al., 2021).

While this model works reasonably well in non-fluvial environments, there is considerable uncertainity in how it applies to fluvial systems. Specifically, the influence of the riverbed and its large roughness elements in small streams (i.e. bedforms, logjams, sediment out of suspension) complicates scaling fluvial *k* and might lead to substantially higher *k* in streams with whitewater (e.g. Hall et al., 2012; Ulseth et al., 2019). Less attention has been paid to the other side of the stream-to-river continumn, which is often conceptualized in relation to *k* as a hybrid condition of both fluvial and non-fluvial hydraulic properties. To date, the handful of existing field studies of large-river *k* have suggested that *k* begins to be notably influenced by wind dynamics, though little else is well-established (Alin et al., 2011; Beaulieu et al., 2012; Wang et al., 2021). These mechanistic uncertainties are additionally limited by a large dearth of field-measured fluvial *k*. Wang et al. (2021) attempted to address this by simulating *k* in 35 rivers using stream metabolism modeling (Appling et al., 2018) and in situ dissolved oxygen (DO) datasets, finding that equation 2 is valid in their simulated rivers and that *k*~streamflow relationships breakdown in large rivers. However, they did not directly compare against *k* data in extremely small systems (Ulseth et al., 2019) and stopped short of parsing out hydraulic explanations for why this happens.

Further, these mechanistic uncertainties are then propogated through upscaling workflows when biogeochemists predict *k* across thousands of rivers (e.g Borges et al., 2015; Horgby et al., 2019; Lauerwald et al., 2015; Raymond et al., 2013) via equation 1 coupled with hydraulic geometry (HG: the scaling relationships between streamflow and river channel hydraulics- Leopold and Maddock, 1953). It is currently not well understood how sensitive global estimates of fluvial gas evasion are to the specific HG model that is employed by the worker. Further, these approaches rely on either in situ discharge records or modeled streamflow which introduces additional uncertainities. This is all exacerbated in ungauged basins that cover large areas, especially in the carbon-rich Arctic inland waters, where little in situ information is available and fieldwork is impractical (Gleason and Durand, 2020).

A potential alternative to this upscaling approach is to directly estimate a river's hydraulic properties from remote sensing (RS) data. Remote sensing of river hydraulics is a burgeoning subfield within remote sensing of hydrology, often in service of remote sensing of river discharge (RSQ- Gleason and Durand, 2020). This is accomplished via two general approaches: 'gauged' methods which rely on in situ river data to calibrate one's method to the river(s) at hand and 'ungauged' techniques which focus on hydraulic generalizability in the service of merely improving existing knowledge in data-poor domains (Gleason and Durand, 2020). Many, but not all, of these ungauged approaches are developed in the context of the upcoming NASA/CNES/UKSA/CSA Surface Water and Ocean Topography (SWOT) satellite mission. SWOT is expected to launch in 2022 and provide the world's first global measurements of water surface extent and elevation at novel temporal resolutions. SWOT is a wide swath radar interferometer and will sample rivers every 1 to 7 days per 21 day repeat cycle and will measure rivers wider than 100m with a goal of expanding this to rivers at least 50m wide (Biancamaria et al., 2016). A decade of SWOT work has explored the multi-parameter problem of estimating the river hydraulic parameters of roughness and bathymetry from remote sensing to produce the SWOT discharge product (e.g. Andreadis et al., 2020; Brinkerhoff et al., 2020; Brisset et al., 2018; Durand et al., 2014; Garambois and Monnier, 2015; Garambois et al., 2020; Gleason et al., 2014; Hagemann et al., 2017; Larnier et al., 2020; Oubanas et al., 2018).

In this context, here we revist the fundamental mechanisms behind gas exchange and turbulence in large rivers using one of the largest available datasets of field-measured river hydraulics (Brinkerhoff et al., 2019) to answer the following question: does *k* behave fundamentally differently in large rivers than in other streams and how does this relate to the classical model of gas evasion in aquatic systems (equation 2)? We exploit the findings from this simple analysis to develop a novel methodology that predicts (*k* normalized to a Schmidt number of 600) and its explicit uncertainity solely using SWOT observations. The method requires no in situ inputs of any kind (although in situ data can be ingested and will improve results). We name the RS of algorithm BIKER, or the 'Bayesian Inference/Inversion of the Evasion Rate' and validate it for 47 SWOT-observable rivers from around the world using hydraulic models to produce SWOT-like data (as SWOT has not yet launched). We also quantify BIKER's sensitivity to the expected SWOT measurement errors on 17 of those rivers: while SWOT data represent a sea change in inland water monitoring, it is expected to have an approximately 10cm error in water surface elevation (Biancamaria et al., 2016) as well as river width errors (Frasson et al., 2021). Finally, we use previously published dissolved data to represent a hypothetical in situ sensor and compare the bulk carbon efflux from the 47 rivers as calculated using BIKER and previously published in situ techniques for predicting .

## 2 Data

Numerous datasets were used in this study. Please see Figure 1 for a map of the approximate locations for the data used in this study. We also provide a flowchart detailing the entire study as Figure S1.

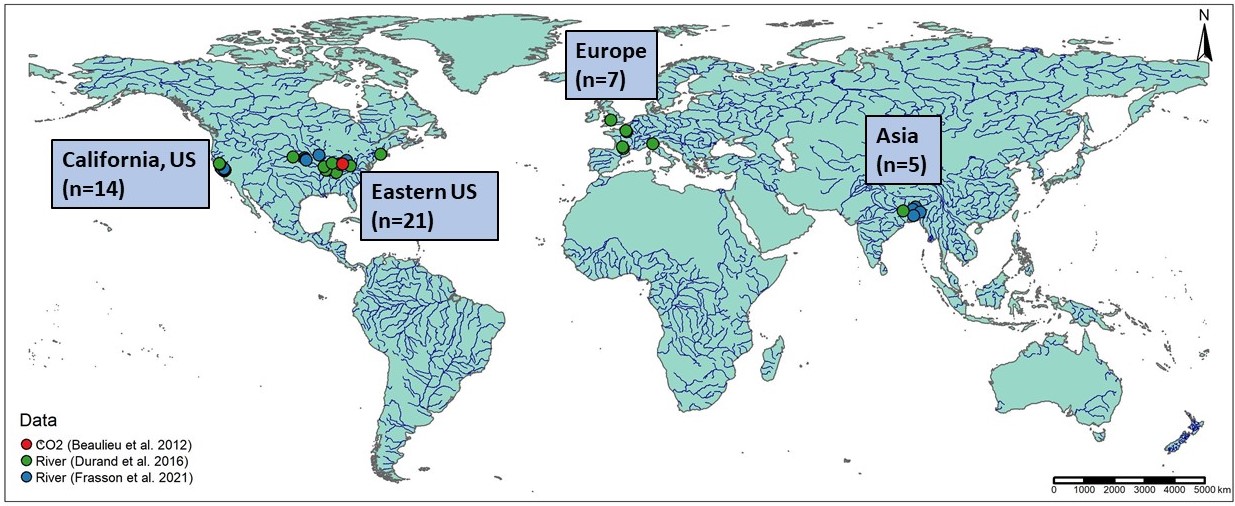


Figure 1: Map of the 47 hydraulic models and 1 timeseries of CO2 samples used in this study. Note that hydraulic model locations are approximate as some of the models are not geo-referenced. Not mapped here are over 530,000 discrete measurements of river channel hydraulics from across the continetal United States (Brinkerhoff et al. 2019) and over 700 gas exchange velocity measurements (Ulseth et al. 2019).

TKE and gas exchange theory (section 2) are explored using two datasets. First, we use a previously published compilation of field measurements that were originally made to calibrate United States Geological Survey (USGS) streamgauge rating curves and gathered by Brinkerhoff et al. (2019). That dataset contains over 530,000 unique measurements of river channel velocity, width, depth, and discharge from across the continental United States. This is to our knowledge the largest collection of field measurements of river channel hydraulics. Second, we use the dataset from Ulseth et al. (2019) who measured and/or collected from the literature over 700 measurements of stream hydraulics and and is, to our knowledge, the largest collection of field-measured river and stream . This is also the dataset used to validate our *k* scaling models.

BIKER validation (section 4) was performed on 47 SWOT-simulated rivers. Because SWOT has yet to launch, it is standard practice to benchmark SWOT-related algorithms on "SWOT-like" data. These simulated rivers are simply river-reach-averaged hydraulic model outputs where the water surface heights and widths are labelled as RS observations and are used as the sole inputs to BIKER. Here, we use 47/51 rivers collected by Frasson et al. (2021) and Durand et al. (2016). These are the two benchmarking studies that have explored RSQ algorithm performance for the SWOT mission. The approximate locations of these rivers are plotted in Figure 1, and please consult both of those papers for all of the hydraulic model specifications. Ultimately, the 47 rivers are spread across the United States, France, Italy, the United Kingdom, and Bangladesh. We omit three models from Durand et al. (2016) because they lack enough hydraulic information to calculate the shear velocity , which is necessary for algorithm validation (see Appendix A for all variable descriptions and notation used in this study). These are two models for the Saint Lawrence River and one for the Tanana River.

To assess the influence of measurement error on BIKER's performance (section 4), we use the error model developed by Durand et al. (2020) and implemented on 17/47 of the rivers by Frasson et al. (2021). Error in SWOT measurements will come from both the error tolerances intrinsic in the satellite data product as well as radar layover error. Layover error is the phenomenon when radar returns from different places arrive at the sensor at the same time, leading to taller landscape features appearing closer to the sensor than shorter landscape features that are the same horizontal distance from the sensor (Durand et al., 2020). Width errors due to poor water classification are ignored as they were in Frasson et al. (2021).

For the evasion and carbon efflux calculations (section 4), we use 26 bi-weekly dissolved samples made by Beaulieu et al. (2012) at one location in the Ohio River for one calender year from 2008-2009 (Figure S2). Note that this data is for the Ohio River only but was applied to all 47 rivers (which includes multiple sections of the Ohio River). Because we are exclusively interested in the relative differences between estimates and not the raw fluxes themselves, any data representative of SWOT-observable rivers was deemed acceptable.

## 3 The TKE budget in large rivers and implications for scaling fluvial gas exchange velocity

Turbulence is fundamental to fluvial geomorphology and open-channel flows and has been the subject of extensive research across scientific and engineering disciplines for over a century. Turbulent kinetic energy (TKE) is the energy generated and dissipated by the eddies created from the chaotic nature of turbulent flow. Nakagawa and Nexu (1993) outline the standard energy budget for TKE, at some depth *h*, for a 2-dimensional open-channel flow (equation 3). *G* is the TKE produced, is the TKE dissipated, is TKE transported from the riverbed via turbulent diffusion, and is TKE transported via viscous diffusion.

at the free surface is frequently described as where *H* is the flow depth. However in rivers, which exhibit additional depth-scale shear due to downslope flow against the channel geometry, bars, and meanders, energy dissipation occurs much more evenly over the flow depth than this parameterization allows for. It has been shown that, for rivers at least, a more appropriate dissipation model considers stream power (per unit weight water: ), which represents the energy dissipated by the total frictional resistance of the river reach's geometry (Moog and Jirka, 1999). This is often called 'energy dissipation via form-drag' in the literature, and is generally used to upscale *k* in rivers and streams (i.e. Raymond et al., 2012; Ulseth et al., 2019). Both Raymond et al. (2012) and Moog and Jirka (1999) confirmed that is far greater than in open-channel flows, therefore generating the majority of fluvial TKE dissipation.

We express *G* at the free surface in two different ways (equation 4) following Nakagawa and Nexu (1993) on the left and our derivation on the right. Text S1 details the necessary algebra to arrive at both expressions of *G*. Looking at equation 4, it is readily apparent that will cancel out if they are equal. This occurs in most large and wide rivers and is a common assumption in hydraulic modeling. In this scenario, the following three statements must be true: 1) , 2) , and 3) . More intuitively, if this "large river" condition is met then additonal TKE transported from the riverbed is functionally zero and the TKE budget at the free surface is just stream power (per unit weight water). This implies a local equilibrium between TKE produced and TKE dissipated at the free surface.

We test this hypothesis using the data from Brinkerhoff et al. (2019) and Ulseth et al. (2019) by plotting boxplots of ratios for over 531,000 different measurements of river hydraulics versus , which is equivalent to in equation 3 assuming that is neglibile away from the wall (Nakagawa and Nexu, 1993). *G* is calculated as . In order to determine when , we round all ratios to 3 significant figures and set all ratios greater than or equal to 0.995 as . If our hypothesis holds, then should be functionally zero only when the 'large river' condition is met.

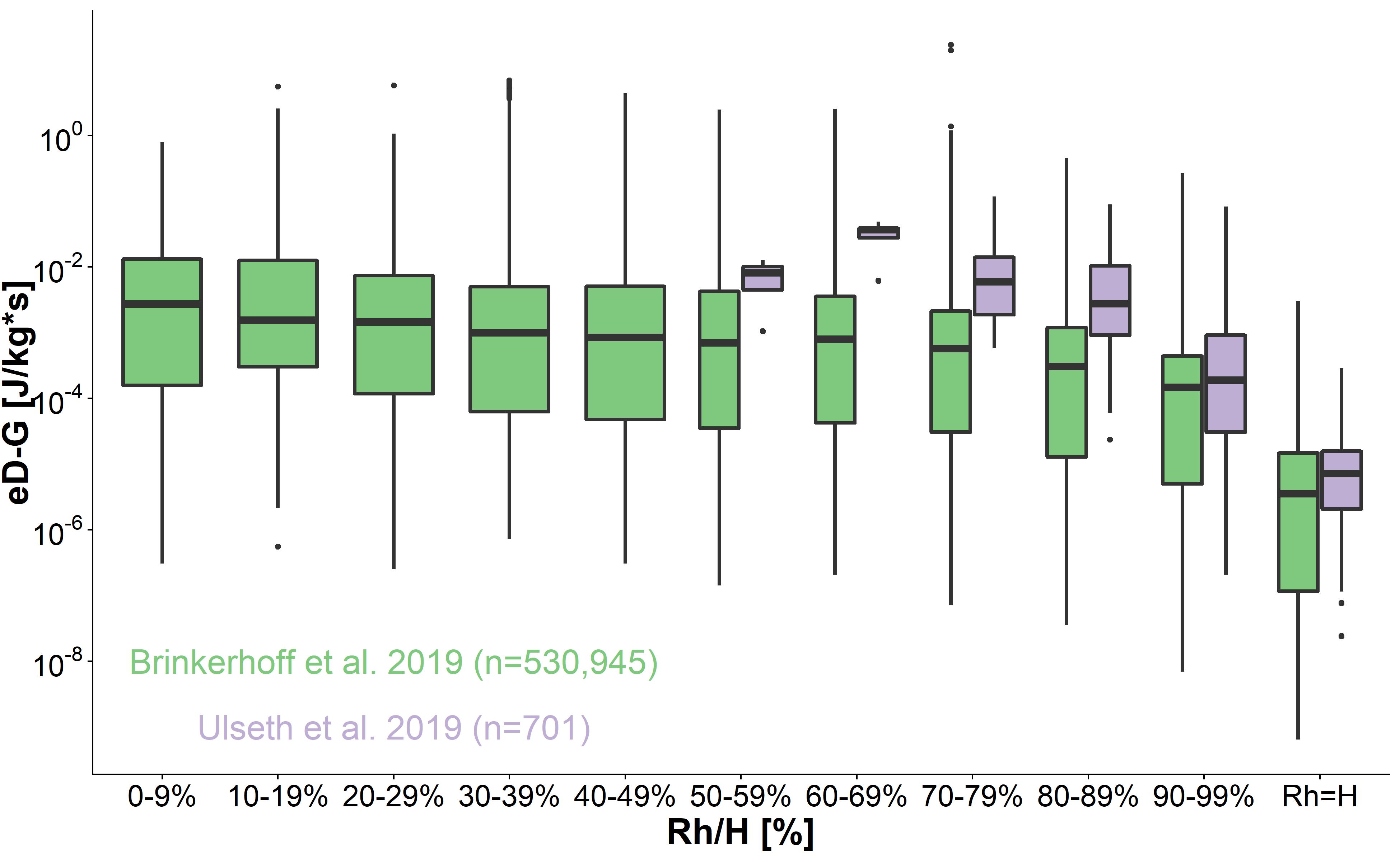


Figure 2: Rh/H versus eD-G at the free surface for our two datasets of field-measured river channel hydraulics (see Appendix A for variable descriptions). eD-G is functionally zero only when a river is sufficiently large. This indicates that a local equilibrium of TKE is acheived and energy generated by large-scale eddies is nearly equal to energy dissipated by the smallest scale eddies. In this figure, Rh/H bins contain between 573 and 138,307 measurements.

Figure 2, which plots this test, shows that is nearly two orders of magnitude less when than it is when is between 90-99% (median value across both datasets of versus , respectively). When the ratio is very small (0-9%), this rises to a median value of , or nearly three orders of magnitude larger. The values when (which are generally to ) are functionally zero. This means that a local equilibrium of free-surface TKE is achieved, where energy produced via the largest scale (turbulent) eddies is equivalent to energy dissipated via the smallest scale (Kolmorogov) eddies. This idea of a local equilibrium is certainly not new, however this is to our knowledge the first confirmation that it happens naturally in most large rivers and that is arises algebraically from the TKE budget in open-channel flows. From here on we refer to the river scenario as the 'large river' condition.

This finding has a significant impact on how we model *k* in large rivers. Because the local equilibrium acheived during the 'large river condition' necessitates that is equivalent to *G* (Figure 2), we can presumably set in equation 2 equal to the largest ('integral-scale') eddies in the system, which are much more easily remotely-sensible than the Kolmogorov velocity scale. Otherwise, *k* should continue to scale only using the Kolmogorov-scale (which is consistent across all turbulent flows by its definition).

To test this hypothesis, we fit the following three models to the Ulseth et al. (2019) dataset of *k* measurements normalized to a Schmidt number of 600: , , and under two scenarios: and . Note that because all data are normalized to a Schmidt number of 600, both the Schmidt numbers and viscosity terms are constant and are implicit in the statistical coefficients. The model structures (and the fit parameters) are detailed in Table 1. The third model tested (rows 5 and 6 of Table 1), was fit to see which slope coefficient is retrieved empirically by fitting the generalized scaling function to the data. Therfore, the for these models is reflective of the log-transformed (unlike the other two models). This was the approach used by Ulseth et al. (2019), who observed slopes steeper than 1/4 in both regimes of their breakpointed regression model.

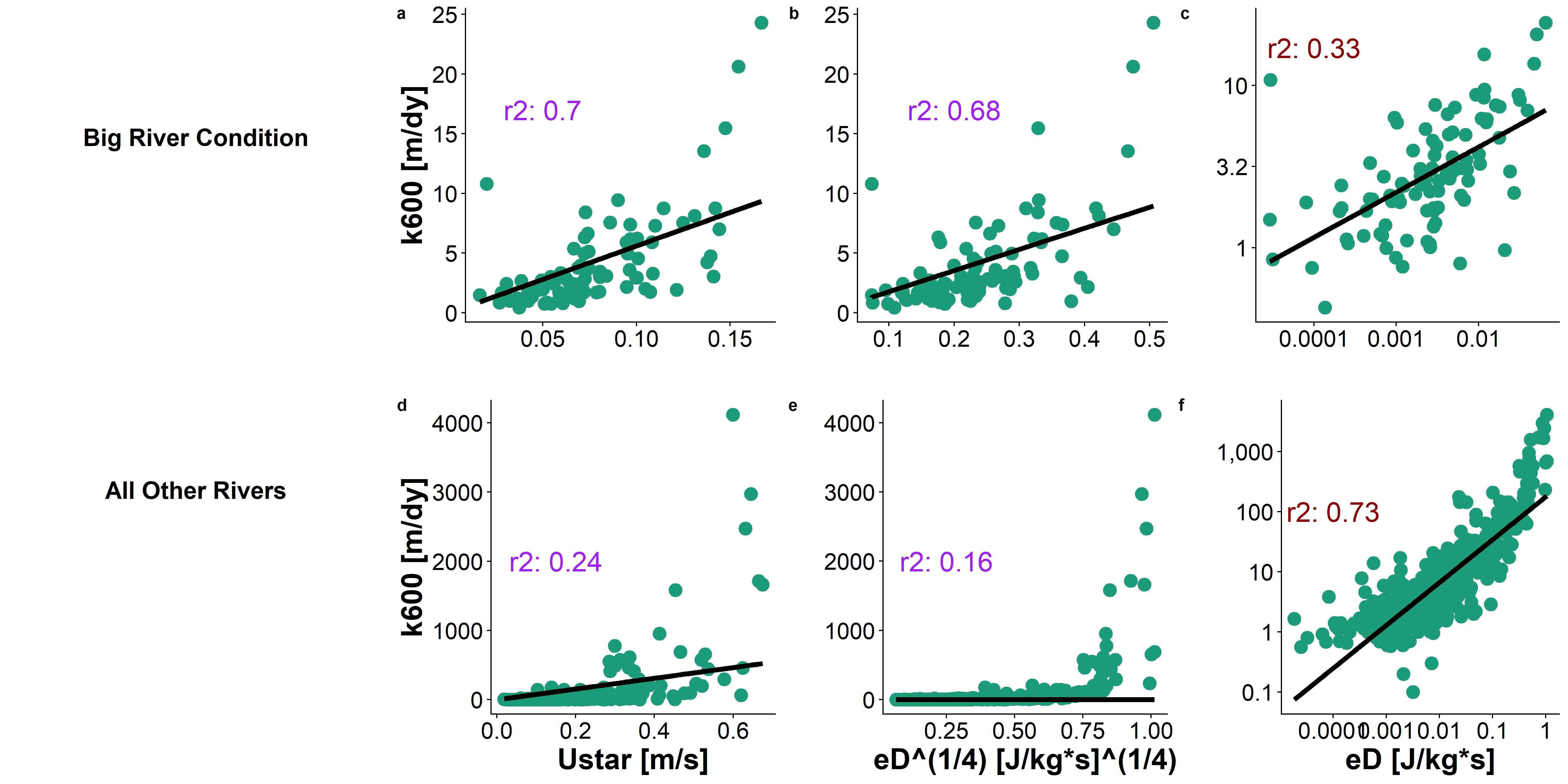


Figure 3: Six k600 predictive models tested on the dataset from Ulseth et al. (2019). a-c are fit to the 'large river condition' while d-f are not. Red coefficients of determination refer to log-tranformed quantities while blue coefficients of determination refer to the natural quantities.

The results of this test are presented as Figure 3 and Table 1, where our hypothesis is confirmed: both the and models explain ~70% of variance in *k* under the 'large river' condition while the model does not work when this condition is not met (:0.7 versus =0.24). In fact, Figures 3a and 3b are nearly visually identical in their scaling dynamics, while Figures 3d and 3e are very different, lending further evidence that these two scaling models are synonmous only when the 'large river' condition is met. This is in line with Wang et al. (2021), who found similar predictive performance and parameter values for these two models on 35 simulated riverswhich they assumed were large enough that . Further, the 1/4 slope parameter is statistically recovered in the 'large river' condition (row 3, Table 1: slope = 0.28). We note that the large residuals in Figure 3c are a byproduct of the model existing in log-space and that panels 3b and 3c are functionally identical models (see Table 1 for their nearly identical intercept and slope parameters). The top row of Figure 3 confirms that under the 'large river condition' *k* can be scaled using either integral or Kolmogorov turbulence scales and that they are synonymous. This opens the door for remotely sensing *k* using almost entirely remotely-sensed parameters. This is elaborated on in section 4.

*Table 1: Model performance and parameter values for the six models tested*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Figure 3 Panel** | **River Regime** | **Model Structure** | **r2** | **Intercept Parameter** | **Slope Parameter** |  |
| 3a |  |  | 0.7 | 56 | 1 |  |
| 3d |  |  | 0.24 | 775 | 1 |  |
| 3b |  |  | 0.68 | 17.7 | 0.25 |  |
| 3e |  |  | 0.16 | 282 | 0.25 |  |
| 3c |  |  | 0.33 | 15 | 0.28 |  |
| 3f |  |  | 0.73 | 177 | 0.71 |  |

The 1/4 exponent is clearly not valid when (Figure 3e). However, the generalized form of this model explains 73% of the variation in log-transformed *k* and was deemed a strong scaling model for fluvial *k* when rivers do not meet the 'large river' condition. That model yields a slope of 0.71 which corroborates other models with slopes steeper than 1/4 in rivers (Raymond et al., 2012; Ulseth et al., 2019; Wang et al., 2021). Further theoretical modeling is needed to parse out why fluvial *k* in systems that do not meet the 'large river condition' generally scale at a steeper rate than in non-fluvial systems, and how this relates to the breakpointed model proposed by Ulseth et al. (2019). That said, the TKE budget in equation 3 suggests that it is a function of turbulent diffusion of additional TKE from the bed to the free surface.

## 4 Exploiting the 'large river' model to remotely sense gas exchange velocity via the BIKER algorithm

We have shown that scaling by either integral or Kolmogorov turbulence scales explains ~70% of the variation in in large rivers and that their scaling dynamics are virtually identical. The integral-scale model relies solely on the shear velocity . Because of the structure of (Appendix A), we can easily reduce the 'large river' model (Figure 3a, row 1 Table 1) to an equation consisting solely of remotely-sensible river hydraulics and an intial estimate of the channel area. By scaling *k* this way, we significantly reduce potential equifinality issues by having just two unknowns: and the median channel area . Equifinality refers to an under-constrained mathematical system that has essentially infinite parameter combinations that can produce the same result: there are in essence more unknowns than equations (Garambois and Monnier, 2015). This problem is experienced by both SWOT RSQ algorithms and in situ tools that concurrently solve for *k* and stream metabolism (Appling et al., 2018; Grace et al., 2015; Holtgrieve et al., 2010). In both of these domains, the other unknown parameters are often difficult to estimate (bed roughness and stream metabolism, respectively) while for BIKER, median channel area is relatively easy to approximate from the SWOT-observable river width (Brinkerhoff et al., 2020).

That said, this all assumes that the 'large river' condition is met. Because SWOT will be limited to the widest rivers on Earth (minimum average width of 100m), the assumption is nearly always valid. First, we verified that this is true using both the Brinkerhoff et al. (2019) and Ulseth et al. (2019) datasets (Figure S3), finding that the vast majority of rivers with a width of at least 100m exhibit this behavior. Thus, our theoretical findings in sections 2 and 3 should hold in nearly all rivers that SWOT will observe and we should be able to remotely estimate via SWOT. Therefore, we develop the BIKER algorithm, which is informed by the Hagemann et al. (2017) algorithm for ungauged RSQ and further explored in more recent work by Brinkerhoff et al. (2020). These papers conceptualize discharge as a Bayesian remote sensing problem, which we largely follow here to conceptualize as a Bayesian remote sensing problem that can be solved using SWOT data.

BIKER, and Bayesian inference in general, starts from Bayes rule (equation 5), where is some set of non-remotely-sensible parameters we want to solve for (including ), *x* is the observed data, is the 'likelihood function' or sampling model conditional on the parameters, and is the joint prior distribution of the parameters. Therefore, we are interested in solving for , or the 'posterior' distribution. For BIKER, *x* is the SWOT-observables: river width *W* and water surface elevation *H* (which is used to calculate the water surface slope ). Note that is usually computationally intractable to integrate, so Bayesian inference tools require only the proportionality to be specified: . Sampling algorithms are then used to approximate the posterior distribution, as is done in BIKER.

The heart of BIKER is its reformulation of the model as a Bayesian sampling model that is conditional only on the data that SWOT will provide. To do this, is first written as a function of SWOT-observables *W* and . This algebra is carried out using the model parameter from row 1 of Table 1 and yields equation 6, where we follow our earlier assumption that where *A* is wetted channel area. *A* is further split into the SWOT-observable portion *dA* and the unobservable portion following Durand et al. (2014). *dA* is estimated assuming a rectangular river channel (usually valid when ) so that . Thus, there are no reliances on bed roughness, flow velocity, or any other terms that are difficult to infer from river width.

Next, equation 6 is written as a Bayesian sampling model, in which all of the SWOT observations are sampled from the unknown model parameters ( and ). This is equation 7 after log-transforming all of the variables. The parameter refers to the uncertainty inherent in equation 6's estimates. Equation 7 also necessitate that we specify prior distributions for the parameters and . Prior distributions, defined by their hyperparameters, formalize the a priori estimates (and uncertainties) for the non-remotely-sensed terms. More intuitively, BIKER priors represent our 'prior river knowledge' of what and probably are for some river since they cannot be remotely sensed. Hyperparameter specifications are detailed in Text S2, however the goal was to rely on absolutely no in situ information such that we could run this method on any river on Earth solely using SWOT observations.

With the sampling model (equation 7) and hyperparameters described (Text S2), a joint posterior distribution conditional on the SWOT observations is specified. To approximate this distribution, we use a Markov Chain Monte Carlo (MCMC) algorithm implemented using the Stan probabilistic programming language. Specifically, Stan uses a Hamiltonian Monte Carlo sampler which reduces computation time relative to other sampling algorithms (Hagemann et al., 2017).

We validate BIKER on 47 SWOT-simulated rivers using daily observed and observed . We also re-validate BIKER on the 17 rivers with the SWOT error model corrupting the SWOT-observables *W* and *H* (this workflow and the metrics used are detailed in Text S4 and Table S1). Regardless of the validation setup, we do not have observed data for these rivers, and to our knowledge no field dataset of exists in the type of temporal and spatial frequency that SWOT (and therefore the BIKER algorithm) provides. Therefore, we take the model outlined in row 1 of Table 1 and use that to calculate the observed that BIKER is validated against. With this setup, we are directly exploring BIKER's ability to infer observed and from *W* and *H* alone, as the *k* scaling model has already been sucessfully validated (Table 1, Figure 3).

Figure 4a plots the validation results for (with no SWOT measurement error) across all rivers and all timesteps. The points are the posterior means while the black lines are the 95% confidence intervals (CIs) for the predictions. is strongly correlated with the BIKER-predicted ( of 0.87). Using absolutely no in situ information, BIKER captures the magnitude of the predictions and most points fall on or near the 1:1 line. The regression of the estimates (solid grey line) nearly recovers the 1:1 line (dashed black), but there is an over/underestimation bias in the largest/smallest values. The RMSE for the BIKER predictions is 2.57 m/day) across all observations.

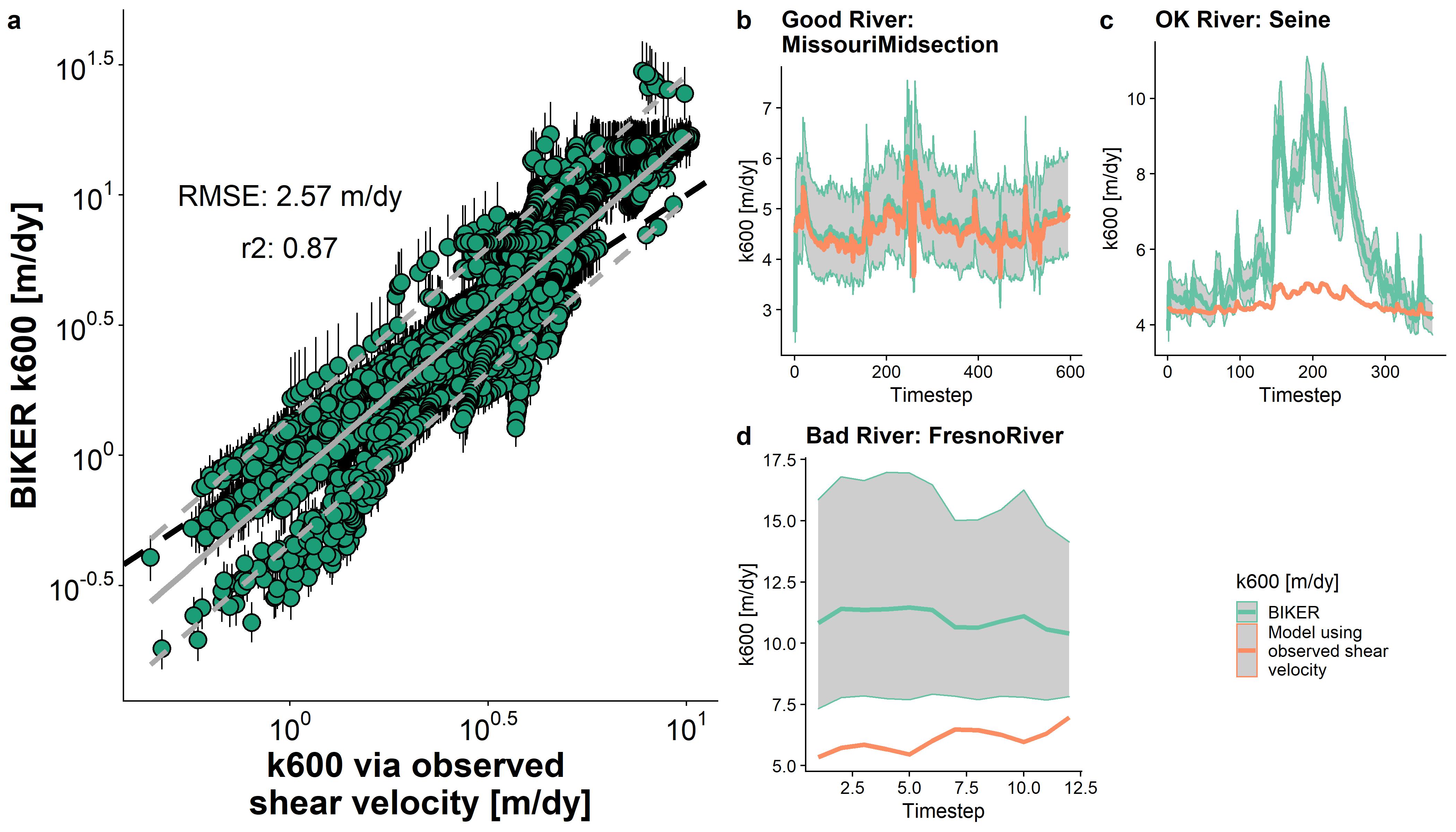


Figure 4. a: Validation of BIKER for 47 SWOT rivers. Black bars are 95% CIs for the modeled values. Grey line is linear regression (and 95% prediction intervals are dashed) and dashed black line is 1:1 line. b-d: validation timeseries for three rivers representative of good, reasonable, and poor BIKER performance. b) was randomly selected from the upper tertile of NRMSE scores, c) was randomly selected from the middle tertile, and d) from the worst tertile. See Figure S5 for all other rivers. Model results include the posterior means and 95%.

Figure 4b-d are representative timeseries plots of predicted and observed for three rivers chosen randomly from those with 'good' NRMSE scores (b), 'okay' NRMSE scores (c), and 'bad' NRMSE scores (d). See Table S1 for the definition of NRMSE, the Figure 4 caption for how this was determined, and Figure S5 for the other river timeseries plots. For the Missouri Midsection River, the entire timeseries of is nearly perfectly predicted, while in the Seine River the dynamics (peaks and valleys) are reasonably captured but they are magnified to be far larger than the observed dynamics. Generally, though, mean is reasonably recovered for the Seine, as confirmed visually. In the Fresno River, there is significant positive bias in the estimates but also massive uncertainty (per the 95% CIs) in those estimates, indicating that BIKER is highly uncertain about its output (and rightfully so). Correct temporal dynamics are also largely missing from BIKER's Fresno River predicitions.

Figure 5a plots validation metrics calculated for each river with and without SWOT measurement error (green and purple, respectively). The points making up these boxplots (47 and 17, respectively) are overlain atop the boxplots. See Table S1 for metric definitions. SWOT measurement errors neglibly influence BIKER's performance across all four error metrics (Figure 5a), though caution should be used in over-interepting boxplots with a sample size of only 17. Given Figure 5a, we deem that SWOT measurement error does not exert a significant influence on BIKER and so the results presented for the rest of the manuscript assume no measurement error in order to use all 47 rivers.

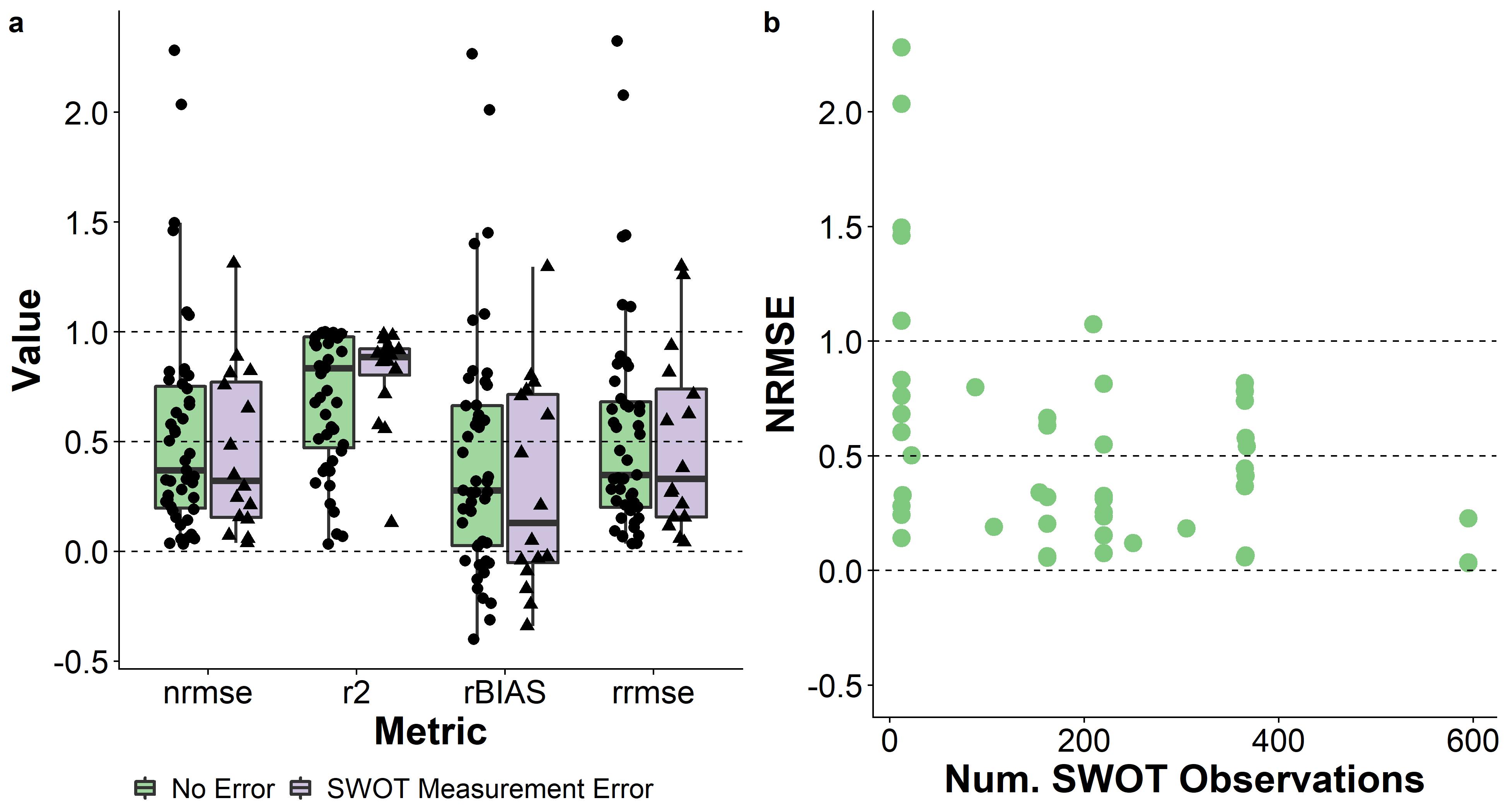


Figure 5. a: Performance metrics by river. See Table 1 for metric definitions. b: NRMSE scores (per river) versus the number of SWOT observations used in the Bayesian inversion. As expected, performance improves substantially with large amounts of data and degrades significantly with small amounts of data. Dashed lines denote scores of 0, 0.50, and 1. CIs.

Median river-specific is 0.83, which is excellent given that absolutely no in situ information is being used to predict . NRMSE and RRMSE have median scores of 0.37 and 0.35, respectively, which are again good for a completely ungauged method. These are comparable to the best NRMSE scores achieved by the SWOT RSQ algorithms (Frasson et al., 2021). Median rBIAS is 0.28, highlighting a positive bias in most rivers' predictions. This further supports the visual evidence in Figure 4 that sometimes BIKER is overestimating the magnitude of and that this might be river-specific. While median and rBIAS scores were strong, the ranges of these scores were somewhat large (standard deviation for of 0.3 and for rBIAS of 0.56).

Figure 5b highlights one benefit of using Bayesian inference to estimate : because the posterior is conditional on the SWOT observations, performance should improve with more data. Figure 5b plots by-river NRMSE scores versus the number of SWOT observations. While performance varies considerably when observations are up to ~400, the three rivers with nearly 600 observations universally show excellent BIKER performance, and the worst BIKER performance is universally in rivers with only 12 observations.

## 5 Remotely sensing carbon emissions from rivers

It is one thing to accurately predict *k*, but researchers are often most interested in the actual gas fluxes from rivers and ultimately the carbon emitted from river to atmosphere. Therefore, we also explore 1) BIKER's ability to reproduce (equation 1) from these 47 rivers, and 2) a comparison of the representative carbon efflux from BIKER with established in situ methods. The details of this workflow are in Text S4, but broadly we pair the 26 biweekly and water temperature samples (section 2, figure S2) from Beaulieu et al. (2012) with a subset of SWOT observations (as the data are not daily). We then calculate using equation 1 and assuming atmospheric is 390 uatm. Finally, we estimate a median bulk carbon efflux using BIKER's posterior means and three other in situ models for average channel depth (used to calculate ) used for upscaling: one trained on the Brinkerhoff et al. (2019) dataset, and two previously published models (Raymond et al., 2013, 2012). See Table S2 for their definitions. This allows us to assess whether BIKER's estimates (wholly ungauged) are comparable to gauged methods (all four HG models).

In Figure 6a, there is a very strong fit to the observed data, with an RMSE of 1.16 . The performance is notably better than for alone (Figure 4a) and there is no systematic bias in the predictions across all 47 rivers. This is presumably due to the structure of the equation, which reduces the relative importance of errors in *k* given that the data is measured in situ. prediction intervals are slightly narrower than those presented in Figure 4a as well.

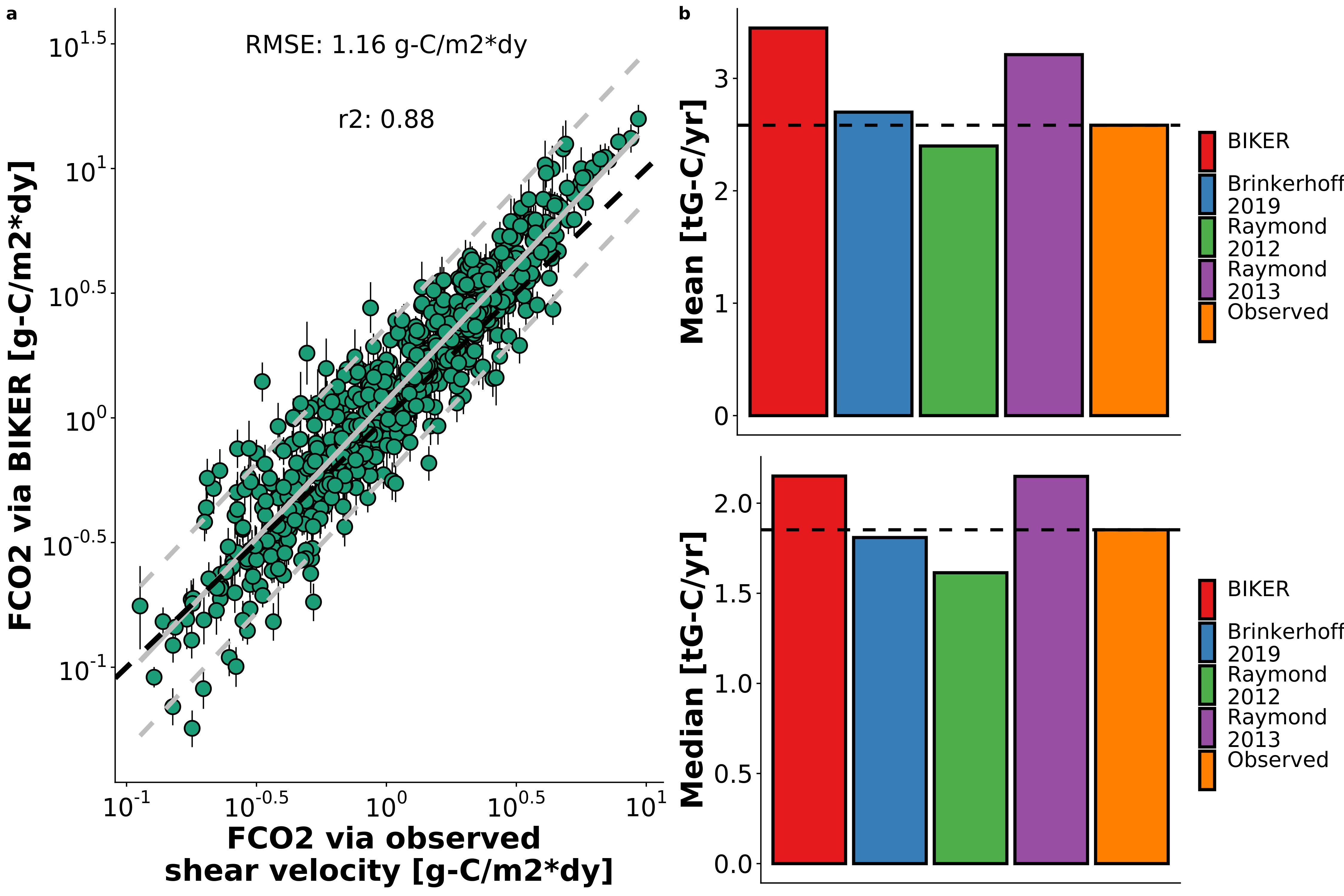


Figure 6: a: FCO2 via BIKER versus via equations 2 and 3 for every 11th timestep for the 49 rivers (grey lines are linear regression and 95% prediction intervals, while black dashed line is the 1:1 line). b-d: timeseries plots for the three example rivers from Figure 3b, 3c, and 3d.

Figure 6b compares the bulk carbon efflux (via ) from the 47 rivers using BIKER posterior means and four streamgauge-based HG models. The results are largely equivalent for both the mean and median carbon efflux. Both the BIKER estimate (2.01 gG-C/yr) and the 'Raymond 2013' estimate (2.15) are somewhat overestimated relative to the observed flux (1.85). The 'Brinkerhoff 2019' model nearly perfectly recovers the observed value (1.81). Finally, the 'Raymond 2012' model slightly underestimates this bulk efflux (1.61). Thus, despite BIKER using absolutely no streamgauge or other in situ data like the other 3 methods do, it provides a reasonable estimate of the carbon efflux (Figure 6b).

## 6 Discussion

### 6.1 Towards a mechanistic understanding of gas exchange in large rivers

Field studies of gas exchange in wide rivers have suggested that their *k* properties behave differently than in steeper and smaller rivers (Alin et al., 2011; Beaulieu et al., 2012; Ulseth et al., 2019; Wang et al., 2021). In sections 2 and 3 we have shown that this must be the case given the algebraic structure of the TKE budget in open-channel flows (Nakagawa and Nexu, 1993) and the assumptions underlying turbulent scaling with interfacial fluxes (Katul et al., 2018; Lorke and Peeters, 2006). This result significantly amends how we can scale *k* in large rivers and directly addresses a long-standing problem of upscaling fluvial *k*: that our current methods perform poorer in larger rivers than small ones.

We also statistically recovered the 1/4 scaling exponent in the classic model (Figure 3c, row 5 Table 1) for gas exchange that has been repeadely validated in non-fluvial aquatic systems. This again suggests that *k* in large rivers behaves more similarly to lakes, esturaries, and the ocean than to steeper rivers. We also suggest that the TKE budget in smaller rivers and streams is additionally complicated by diffusive transport of TKE from the bed to the free surface, and that in equation 3 might explain why fluvial does not scale to the 1/4 power in smaller rivers. The presence of an appreciable term also increases the influence of channel bed roughness. Ulseth et al. (2019) showed bed roughness loosely correlates with in steep Alpine streams. However, they coarsely estimated bed roughness from arial imagery, only studied extremely small mountain streams, and to date most similar work has focused on labratory exercises (e.g. Chanson et al., n.d.; Moog and Jirka, 1999). In this study and under the 'large river' condition, we confirm that bed roughness is exerting functionally no influence on free-surface TKE (Section 2 and figure 2) and therefore *k*. We show that free-surface TKE must be entirely produced and dissipated by form-drag and not bottom friction or roughness. However, this is only true in the largest of rivers. It is likely that the steeper slope parameter in Figure 3d and row six, Table 1 is due to the influence of bottom roughness on free-surface TKE in smaller streams.

### 6.2 Towards remote sensing of global spatiotemporal dynamics of *k* in large rivers

To date, most field-scale studies of riverine gas exchange have focused on 1) its relationship with wind speed (e.g Beaulieu et al., 2012; Borges et al., 2004; Zappa et al., 2007), 2) average flow velocity (e.g. Alin et al., 2011; Beaulieu et al., 2012; Schelker et al., 2016), or 3) discharge (Roberts et al., 2007; Uehlinger and Naegeli, 1998; e.g. Wang et al., 2021). However, the spatiotemporal dynamics of riverine gas exchange are still weakly constrained. A few studies have investigated these dynamics, but they have been limited to individual rivers and/or limited field seasons (Hall et al., 2012; Sand-Jensen and Staehr, 2012). Wallin et al. (2011) performed a preliminary analysis in northern Sweden relating cross-section specific temporal variability in gas exchange with channel slope, but they were limited to an average of only 8 measurements per river in a single watershed. This limited knowledge of large-scale *k* spatiotemporal dynamics is due both to a lack of process-level understanding (Hall and Ulseth, 2020) but also a lack of measurements.

Therefore, estimating *k* from SWOT data is an attractive option for exploring its spatiotemporal dynamics at fine temporal resolution and at the global-scale. SWOT will provide daily hydraulic measurements for a 3 month fast sampling period for calibration and validation and sampling thereafter between 1 and 7 days per 21 day repeat cycle (Biancamaria et al., 2016). BIKER's success in 1) infering using simulated SWOT data over a wide range of rivers (Figures 4 and 5) and 2) being robust to measurement errors internal to the SWOT data (Figure 5) bode well for BIKER's eventual implementation on real SWOT observations. Further, BIKER's improved performance with longer datasets (Figure 5b) bodes well for future SWOT implementation, as the three-year campaign will provide well north of 600 observations for many rivers, suggesting even better BIKER inversions than those presented here. All of this suggests that daily estimation of riverine gas exchange globally could be possible once SWOT launches.

### 6.3 Towards remotely sensing riverine carbon emissions using SWOT

Figure 6 confirms that BIKER is quite successful, without any in situ information aside from a logger, at predicting both (Figure 6a) and 2) the bulk carbon efflux (Figure 6b). This encouraging result has two main implications for future work coupling remote sensing via SWOT with in situ data. First, it confirms that we can couple BIKER and SWOT with in situ gas concentration loggers to produce estimates at novel temporal resolutions in SWOT-observable rivers. This is particualry useful given recent advances in in situ gas concentration loggers (Aho et al., 2021) but no such similar advances in modeling *k* at equivalent temporal resolutions. BIKER can likely also be ran at the field scale using arrays of pressure transducers to estimate water surface slope (rather than using satellite-based altimeters like SWOT) following recent work doing the same using the Hagemann et al. (2017) RSQ algorithm (**???**).

Secondly, it is important to stress that unlike BIKER, the HG models in Figure 6b rely on an in situ streamgauge. This means that Figure 6b represents the best performance that those models could ever have; if ran using modeled discharge their accuracy would necessarily decrease. Thus, these results suggest that BIKER will be useful in two settings: 1) upscaling in ungauged rivers as hypothesized, but also in 2) potentially improving our carbon efflux understandings at gauged sites. Future work should systematically quantify prediction error from coupling global-scope HG models with modeled discharge, as is the default workflow used in fluvial upscaling studies (Horgby et al., 2019; e.g. Lauerwald et al., 2015; Raymond et al., 2013). **I assume Shaoda's paper will still be in review and can't cite here but this is exactly what they do...**

Figure 6b also confirms that the training data used for HG models exerts a significant influence on upscaled carbon emissions from rivers. In Figure 6b there is a nearly 0.5 Tg-C range between estimates, which is significant and nearly entirely a function of the data used to fit these depth HG models. In this context, the 'Brinkerhoff 2019' model likely outperforms both 'Raymond models' because the training data is orders of magnitude larger and more geomorphically varied than those used in the 'Raymond' models (530,945 measurements versus 1,026 and 10837 measurements). Meanwhile, BIKER has no similar reliance on hydraulic parameters trained on different datasets and only assumes that *dA* can be calculated by assuming a rectangular river channel. Upon SWOT's launch, the BIKER approach to estimating *k* could be coupled with ethier existing upscaling workflows or even explicit transport models [Brinkerhoff et al. (2021); **Saccardi & Winnick in review**] to improve riverine gas flux predictions where gauges are unavailable but SWOT measurements are. This coupling could potentially be done using data assimilation techniques, which have proven very useful for similar objectives in recent RSQ work (Ishitsuka et al., 2020).

## 7 Conclusions

Gas exchange from aquatic systems has been studied for nearly a century, with a robust model (equation 2) that has been repeatedly verified across many non-fluvial environments. Despite renewed interest in fluvial gas exchange in the last decade or so, there are considerable uncertainties in how we model the gas exchange velocity in river environments and particularly in large rivers where wind increasingly influences *k*. Here, we show algebraically that TKE budgets in big rivers exist in a local equilbrium at the free surface and that we can equivalently scale *k* using any characteristic turbulence scale. We validate this using over 530,000 measurements of river channel hydraulics and over 700 discrete measurements of the normalized gas exchange velocity . We then exploit this finding to remotely sense using simulated data that will be provided by the forthcoming SWOT satellite, showing good performance and relying on absoutely no on-the-ground information. Finally, we pair this algorithm (named 'BIKER') with an in situ logger and show strong performance in reproducing evasion fluxes and carbon efflux from the rivers' surfaces.

These strong results functionally open the door for global-scale, near daily estimates of fluvial gas exchange velocity once SWOT launches in 2022. This unprecedented amount of data should allow for significant insights into both the mechanistic and temporal dynamics of fluvial gas exchange in large rivers around the world. This, in turn, should allow us to better parameterize upscaling workflows such that the global fluvial carbon flux is better constrained.

## 8 Acknowledgements

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## 9 Apendix A

*Table A1: Variable description and notation for this study. TKE refers to 'turbulent kinetic energy'*

|  |  |  |  |
| --- | --- | --- | --- |
| **Notation** | **Description** | **Calculation (if applicable)** | **Units** |
| *A* | Channel cross-sectional area | NA |  |
| *Bulk carbon efflux* | carbon mass transport rate from river to atmosphere | NA |  |
|  | Water-side concentration | NA |  |
|  | Atmospheric-side concentration | NA |  |
|  | Molecular diffusion coefficient | NA |  |
|  | TKE dissipation rate |  |  |
|  | TKE dissipation rate via form-drag |  |  |
|  | evasion flux from river to atmosphere | NA |  |
|  | gravitational acceleration | 9.8 |  |
|  | TKE production rate |  |  |
|  | Elevation above the bed | NA |  |
|  | Mean flow depth | NA |  |
|  | gas exchange velocity | NA |  |
|  | gas exchange velocity normalized to Sc=600 |  |  |
|  | Hydraulic radius |  |  |
|  | River slope | NA |  |
|  | Schmidt number |  |  |
|  | TKE turbulent diffusion rate | NA |  |
|  | Reach-averaged flow velocity | NA |  |
|  | Shear velocity |  |  |
|  | kinematic viscosity | NA |  |
|  | TKE viscous diffusion rate | NA |  |
|  | turbulence characteristic velocity scale | NA |  |
|  | Flow width | NA |  |

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