Remote sensing riverine gas exchange and carbon efflux in ungauged rivers from SWOT observations

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## Highlights

* The BIKER algorithm indirectly remotely senses riverine gas exchange velocity
* Predicted gas exchange velocities compare well with in-situ methods
* BIKER predicts fluxes when coupled with in situ gas concentration data
* Expected SWOT measurement errors exert a marginal influence on BIKER's estimates
* Errors are dominated by process-level uncertainties, not parameter inversion

## Keywords

gas exchange, SWOT, remote sensing, carbon, ungauged basin, biogeochemistry

## Abstract

Go BIKER!! *Note: this is for Remote Sensing of Environment (I think). So 400 words here. also for highlights: (3-5 points, 85 characters each w/ spaces)*

## 1 Introduction

**I don't like this opening paragraph** The Earth's carbon cycle moves carbon between the atmosphere, geosphere, hydrosphere, and biosphere via a complex set of interconnected biogeochemical processes. The primary connection between the terrestrial and oceanic biospheres is the global river network, which exports a significant amount of carbon from the continents to the oceans (Cole et al., 2007), while additionally transporting and transforming sediments, nutrients, organic matter, dissolved gases, and other constituents. Organic matter and inorganic nutrients are also produced and/or consumed within rivers via ecosystem metabolism (Odum, 1956). One net effect of all of this is the global river network is usually supersaturated with dissolved gases and evades substantial amounts of carbon from its water surface to the atmosphere (Cole et al., 2007).

Current estimates of total carbon dioxide () evasion to the atmosphere vary from 650-1800 Tg C/yr (Lauerwald et al., 2015; Raymond et al., 2013), with 167 Tg-C/yr coming from mountain streams alone (Horgby et al., 2019). Further, in-river metabolism is increasingly understood to contribute to this flux (Hotchkiss et al., 2015). Equation 1 represents this flux for any sparingly soluble gas given the gas concentration gradient between the water and the air and the gas exchange velocity *k [L/T]*. Given the structure of equation 1, calculations of this flux are very sensitive to one's measurements/estimates of *k*. Note that *k* is different for different gases and water temperatures (see Hall and Ulseth, 2020 for a thorough review of gas exchange in rivers).

*k* is also vital to understanding freshwater ecology through bulk river metabolism (more specifically, gross primary production and ecological respiration- Bernhardt et al., 2018). The general mass-balance equation for river metabolism (*M* ) is provided as equation 2, where *DO* is the dissolved oxygen concentration , *D* is river depth [L], and is *k* for oxygen at some temperature. When viewing equations 1 and 2 in aggregate, it is clear that *k* plays a critical role in two of the core, fundamental biogeochemical processes that occur in river networks. Both are reliant on accurate and high-fidelity assessments of *k*, as well as a rigorous understanding of the physical mechanisms driving *k*.

Researchers use a range of methods to measure *k*, from floating domes to eddy covariance towers to measure at a specific point in the river. They also inject tracer gases to estimate reach-scale gas exchange (Hall and Ulseth, 2020). These approaches are ideal but are infeasible when working in ungauged rivers or at the river network scale across thousands of rivers. So, predictive models are used to estimate *k* from readily available river geomorphology (e.g. O’Connor and Dobbins, 1958; Palumbo and Brown, 2014; Raymond et al., 2012). These models often, though not always, predict or *k* that has been normalized to a Schmidt number of 600 ( at 20 degrees Celsius or at 17.5 degrees).

There is a long tradition of water quality engineers and biogeochemists developing predictive models for different forms of *k*, going back to at least the 1950s (Hall and Ulseth, 2020) and extending the original work of Streeter (1935) and Phelps (1914). The goals of these models vary, from predicting oxygen reaeration coefficients to predicting gas transfer velocities. Most of these models operate under the basic assumption that river channel hydraulics govern gas exchange and so simple statisical relationships can be generated between *k* and hydraulic properties. However, many of them are not based on fundamental mass transport theory and rather are simple empirical relations. This means that those models' parameter values are sensitive to the training data used (Wang et al., 2021).

Many of these predictive models rely on the correlation between *k* both the turbulent energy dissipation rate *eD* (Raymond et al., 2012; Ulseth et al., 2019) and the water surface surface shear velocity (Katul et al., 2018; Wang et al., 2021). This is convenient because both *eD* and are calculated using easily estimated hydraulic parameters: (Tsivoglou and Neal, 1976) and , where *g* is gravitational acceleration , is water surface slope , *V* is average flow velocity and is the hydraulic radius [L] (which often approximates *D*). Because slope is readily available in any hydrographic data product, most efforts to predict *k* across thousands of rivers are thereby limited by the quality of the final parameters *V* or . Since both must be measured in the field or themselves estimated by empirical models, uncertainty in *V* or dominates errors in *k* estimates. This is exacerbated in ungauged basins that cover large areas, especially in the carbon-rich Arctic inland waters, as little in situ hydraulic information is available and fieldwork is impractical (Gleason and Durand, 2020).

To circumvent this problem in ungauged basins and across thousands of rivers, researchers have used 'global-scope' hydraulic geometry (HG) models that extend HG beyond its 'at-a-station' use. At-a-station HG models are simple power law relations between streamflow and channel width, depth, or velocity at a specific cross-section in a river (Leopold and Maddock, 1953) and a large body of geomorphology work has attempted to parse out process-based explanations for at-a-station HG parameters (e.g. Dingman, 2007; Ferguson, 1986; Parker et al., 2007; Singh, 2003). This has been extended to 'downstream HG' which relates a characteristic streamflow (i.e. mean annual or bankful discharge) to characteristic hydraulics along a specific river's course (Leopold and Maddock, 1953).

For the purposes of predicting *k* from *V* or , biogeochemists have further extended HG models by training them on large hydraulics datasets for thousands of rivers and under all streamflow conditions (e.g Borges et al., 2015; Horgby et al., 2019; Lauerwald et al., 2015; Raymond et al., 2013). However, it has long been established that HG parameters are either cross-section specific and highly variable from river to river as in at-a-station HG or they are discharge specific as in downstream HG (Gleason, 2015; Park, 1977; Rhodes, 1977). This suggests that the 'global-scope' HG models that are usually used are also sensitive to their training data and can potentially yield pretty different hydraulics for the same streamflow. It is currently not well understood how sensitive global estimates of riverine gas evasion are to the specific 'global-scope' HG model that is employed by the worker. Further, these approaches rely on ethier in situ discharge records or modeled streamflow which introduces additional uncertainity.

A potential alternative to this 'global-scope' HG 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- see Gleason and Durand (2020) for a recent review). There are many ways to perform RSQ, from calibrating RS data to local channel hydraulics (e.g. Brakenridge et al., 2007; Pavelsky, 2014; Pavelsky and Smith, 2009; Tarpanelli et al., 2013) to calibrating hydraulic/hydrologic models with both in situ and RS data (e.g. Bjerklie et al., 2005; Chandanpurkar et al., 2017; Lin et al., 2019; Neal et al., 2009) to methods that use no in situ information in their hydraulic/hydrologic models (termed 'ungauged approaches' and detailed below). Many, but not all, of these ungauged approaches were 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 Ka-band radar interferometer and will sample rivers every 1 to 7 days per 21 day repeat cycle. This yields an average sampling resolution of 11 days. It 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). A specific subset of these ungauged methods are termed McFLIs or 'Mass Conserved Flow Law Inversion' algorithms (e.g. Andreadis et al., 2020; Brinkerhoff et al., 2020; Durand et al., 2014; Hagemann et al., 2017). These use basic geomorphic theories and the concept of 'prior river knowledge' to estimate discharge from RS data where not all hydraulic terms are RS-able (Gleason et al., 2017; Gleason and Durand, 2020). McFLIs are readily implemented in any river that SWOT can observe and improve our hydrological understandings of ungauged rivers when little to no information was previously available (Brinkerhoff et al., 2020; Durand et al., 2016). Recently, McFLIs have also shown promise in providing additional and beneficial information via data assimilation of McFLIs into a traditional hydrologic model (Ishitsuka et al., 2020).

While all McFLIs to date have been developed in the context of RSQ, there is no reason their logic cannot be used to estimate *k*, particularly as McFLIs often employ Bayesian inference for equifinal inverse problems. 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), and this problem is common to both RSQ and RS of *k*. Bayesian techniques have been previously used to concurrently solve for *k* and *M* for different forms of equation 2 (Appling et al., 2018; Grace et al., 2015; Holtgrieve et al., 2010). While these studies require high-fidelity in situ data and are not applicable to *k* estimation in ungauged rivers, they suggest that Bayesian techniques could be useful for remotely sensing *k* when parameter equifinality is a problem. This matches McFLI logic (Andreadis et al., 2020).

In this context, we hypothesize that a combination of SWOT data, a Bayesian McFLI paradigm, and gas exchange theory can successfully estimate *k* using absolutely no in situ information. This would in turn improve our understanding of riverine gas fluxes in ungauged basins (equation 1), as well as potentially help in parameterizing stream metabolism models (equation 2). Therefore, this manuscript aims to answer two questions:

* Is ungauged RS of the gas exchange velocity (*k*) possible using soon-to-be-available SWOT river measurements?
* If possible, how will this RS method effect estimates of riverine carbon efflux from rivers?

To answer these questions, we developed a new McFLI algorithm that ingests SWOT data and produces estimates and their explicit Bayesian uncertainities that 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'. We validate BIKER on simulated SWOT data for 49 SWOT-observable rivers from around the world using hydraulic models to produce SWOT-like data as SWOT has not yet launched. This is standard practice in the SWOT community (Durand et al., 2016; Frasson et al., 2021). 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 hypotetical in situ sensor and compare the bulk carbon efflux from the 49 rivers as calculated using BIKER and previously published in situ techniques for predicting .

## 2 Data

Numerous datasets were used in this study to develop and validate BIKER and are detailed below. Please see Figure 1 for a map of the approximate locations for the data used in this study.

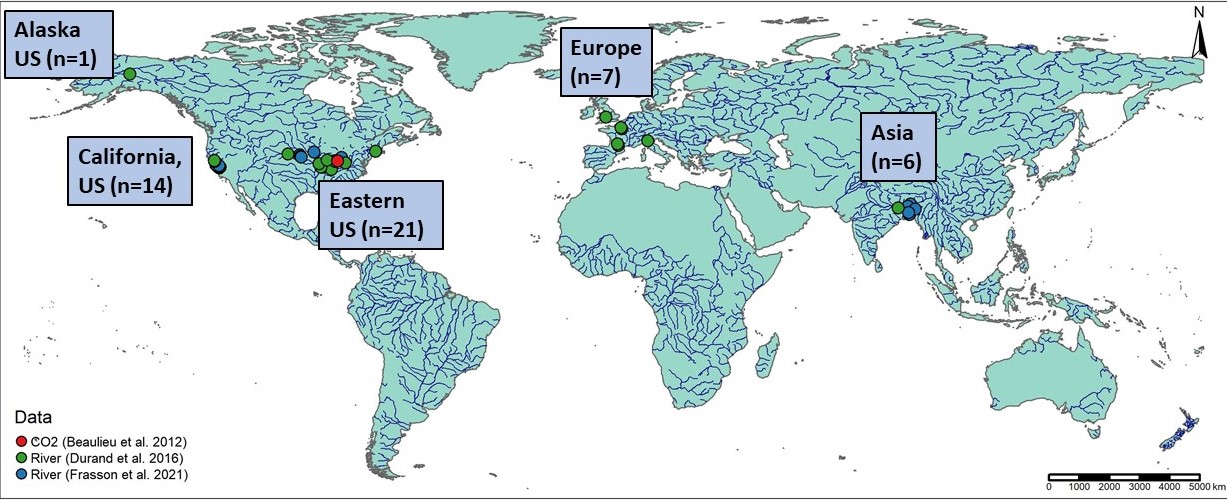


Figure 1: Map of the 49 hydraulic models and 1 timeseries of CO2 samples used in this study. Note that hydraulic model locations are approximate as most of the models are not geo-referenced. We additionally used over 530,000 discrete measurements of river channel hydraulics from across the continetal United States (Brinkerhoff et al. 2019) that are not mapped here.

BIKER validation (section 3.3) was performed on 49 SWOT-simulated rivers. Because SWOT has yet to launch, it is standard practice to benchmark SWOT-related algorithms on SWOT-like data. There are three current types of SWOT-like data: 1) AirSWOT, which is an airborne Ka-band inSAR currently limited to five rivers globally, 2) simulated rivers that mimic the type of data SWOT will provide, and 3) the SWOT simulator, which introduces measurement errors to these simulated rivers. Because we are principally interested in algorithm performance, we limit our validation setup to simulated rivers in order to benchmark across as many rivers as possible. These simulated rivers are simply 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 49/51 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 49 rivers are spread across the United States, France, Italy, the United Kingdom, and Bangladesh. We omit both models for the Saint Lawrence River, Canada from Durand et al. (2016) because they lack enough hydraulic information to calculate , which will be necessary in section 3.2.

We also assess the influence of measurement error on BIKER's performance. Error in SWOT measurements will come from both the error tolerances intrinsic in the satellite data product as well as radar layover error and width measurement 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. For river heights and slopes, we use the error model devolped by Durand et al. (2020) and implemented on 17/49 of the rivers by Frasson et al. (2021). Width errors were derived using a model built by Frasson et al. (2021) based on SWOT-simulator runs for the Sacramento river, California (Frasson et al., 2017) and the Po river, Italy (Domeneghetti et al., 2018). Those two simulations allowed for explicit characterization of width errors that were then extrapolated onto the other 15 rivers. Width errors due to poor water classification are ignored as they were in Frasson et al. (2021). Please consult Frasson et al. (2021) for the specifics of how these realistic errors were incorporated into the hydraulic models.

BIKER prior specifications (section 3.2.2) require the use of a training dataset of field-measured river hydraulics. To do this, we use a previously published compilation of field measurements that were originally made to calibrate United States Geological Survey (USGS) streamgauge rating curves (Brinkerhoff et al., 2019). That dataset contains over 530,000 unique measurements of average channel velocity, width, depth, and discharge from across the continental United States. It has been previously used to inform prior specifications for RSQ algorithms (Andreadis et al., 2020; Brinkerhoff et al., 2020). We acknowledge that our priors will therefore be biased towards the types of rivers in the continental United States and miss key hydroclimatic regions like Arctic and Tropical rivers. However, previous success in using these data in unrepresented regions (Brinkerhoff et al., 2020) bodes well for their use here. Further, 14/19 rivers are from outside of this region (Figure 1).

For the evasion and carbon efflux calculations (section 3.4), 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 S1). Note that this data is for the Ohio River only but was applied to all 49 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.

Finally, we also made extensive use of data and models developed by workers to predict gas evasion rates from river hydraulics. Specifically, we used the data measured, collected, or simulated by Raymond et al. (2012), Ulseth et al. (2019), and Wang et al. (2021). Note that much of this data was collated from many other datasets from many other authors.

## 3 Methods

To build BIKER, we join a predictive model for (section 3.1) with a McFLI framework for inverting SWOT measurements via Bayesian inference (section 3.2). Following the description of that process, we describe the validation setup (section 3.3) and the workflow for comparing estimated bulk carbon effluxes from a suite of 'global-scope' HG models (section 3.4). A flowchart detailing the entire study is provided as Figure 2.

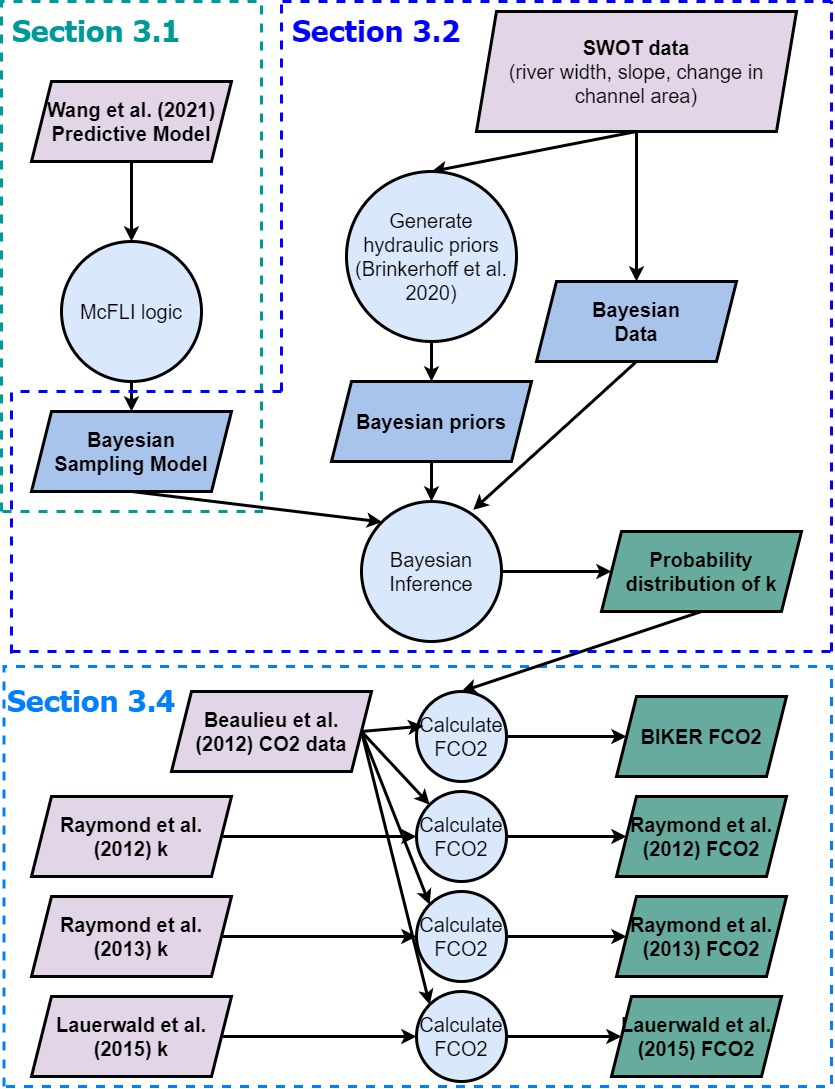


Figure 2. Flowchart of methodology used in this study. We begin by choosing a process-based model for k (section 3.1) that is a function of river hydraulics measurable by SWOT. Then, we implement this model within a McFLI ('BIKER') to estimate k solely from river width and water surface slope (section 3.2). Finally, we couple BIKER with in situ CO2 data to compare BIKER-estimated gas fluxes with established in situ methods (section 3.4). See section 3.3 for the validation setup.

### 3.1 Choosing a predictive model for *k*

To predict *k* from just the SWOT observables, a physical model for *k* is first selected. As mentioned in section 1, there are dozens of predictive models for *k* that have been devolped since the 1950s (Hall and Ulseth, 2020). Recently, many of these models were re-explored in rivers and streams by Wang et al. (2021), who significantly expanded the existing training datasets of field-measured by using the *streamMetabolizer* model to calibrate a form of equation 2 to high-fidelity in situ DO datasets (Appling et al., 2018) at 35 rivers across the United States. They showed that two models deduced from classic, process-based theories for mass transport yield approximately identical parameters when fit to ethier field measurements or this new dataset of simulated . They also showed through cross-validation that these models are more robust to overfitting on specific sets of data than many of the other models tested. While these two models still exhibit large errors, they provide the best fit of those tested and potentially suggest that there are uniform scaling realtionships between certain hydraulic properties and . Wang et al. (2021)'s better fit, and more parsimonious, of the two models is reprinted as equation 3 (with that paper's reported coefficients of determination ). is the fitted parameter in the linear regression. Equation 3-2nd line was fit to 588 field measurements of while equation 3-third line was fit to 3,919 simulated values at 35 rivers.

**I'm struggling with this paragraph, and also don't know how to write it diplomatically** We implement this model within BIKER (using 48 as a reasonable value for given both forms of equation 3) for a few reasons. First, Wang et al. (2021) suggest that an of approximately 48 is uniform across rivers and streams, regardless of the training data used. This is encouraging for use within BIKER as BIKER is specifically designed to be as river-agnostic as possible and so we sought as generalized an equation as possible. Second, it yields a simple linear relationship across all rivers, regardless of their size or steepeness. This is not necessairly true of other *k* models, for example those based on *eD* (section 1). The relationship between *eD* and *k* is not necessairly linear (Raymond et al., 2012), suggesting poorer performance for small *k* values. Further, recent work has shown that *k* does not scale with *eD* via the same statistical parameters across all river geomorphologies (Ulseth et al., 2019). We further explored the relationship presentedby (Ulseth et al., 2019) and found that the relationship fundamentally breaks down in rivers with low *eD*, which corresponds to nearly all rivers that SWOT will observe (Figure S2). Therefore, an *eD* based predictive model is less useful in SWOT rivers. Third, we sought to explicitly predict , as its use extends beyond constraining gas fluxes from rivers and into parameterizing river metabolism models (equation 2). We stress that most other predictive models for *k* could be implemented within BIKER. However, our goal of using BIKER on any river that is observable by SWOT necessitates that we pick an equation that is applicable across as many rivers as possible. Future work should look at using a river-specific *k* equation to pseudo-calibrate BIKER to a specific river.

### 3.2 Developing BIKER

With a predictive model for chosen, we now implement it within a McFLI framework. The approach used here is informed by the Hagemann et al. (2017) McFLI algorithm for ungauged RSQ, 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 4), 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 *W* and *H*. 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 and detailed below. First, we detail our likelihood specification and then our prior specifications.

#### 3.2.1 BIKER likelihood

To concieve of equation 3 as a likelihood function, first needs to be written as a function of SWOT-observables *W* and *H* (which provides water surface slope ). This algebra is carried out and results in equation 5, where we assume 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 so that .

**COLIN COMMENT from old ms: sensitivity analysis? "We investigated the sensitivity of BIKER to this rectangular assumption and found it negligible (xxx section x.x if appropriate xxx)".**

Next, equation 5 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 6. The parameter refers to the uncertainty inherent in equation 5's estimates. This will be explained in detail below. Note that in the formal model specification, equation 6 is written as a normal distribution of its log-transformed quantities. Here, it is written as a lognormal distribution for succinctness.

#### 3.2.2 Prior Specifications

Equations 4 and 6 necessitate that we specify prior distributions for the parameters and . Prior distributions formalize the a priori estimates (and uncertainties) for the non-remotely-sensed parameters. More intuitively, BIKER priors represent our 'prior river knowledge' of what and probably are for some river since they cannot be remotely sensed. 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*. In order to avoid relying on in situ information, as is the goal of BIKER and SWOT, we assign prior hyperparameters using SWOT data only. prior hyperparameters were assigned following 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. This leaves the hyperparameters to be defined. We assigned those using a simple slope regression model trained on an available subset of the Raymond et al. (2012) dataset of field-measured : equation 7 assigns while was set to equation 7's log-transformed standard error: 0.77. and were set to log(0.0001) and log(60), respectively.

Finally, we estimate using Monte Carlo (MC) methods to approximate total uncertainty in equation 5's estimates. Uncertainty in equation 5 can stem from 1) parameter uncertainty in or 2) error in the assumption that . Because total equation 5 uncertainty is a function of both uncertainity sources, we need to propogate those uncertanties through the algebra of equation 5. We use MC simulations to do this. MC simulations repeately sample from the parameter distributions to produce a distribution of model predictions from which an uncertainity term can be extracted. See Figure S3 for a flowchart of the entire methodology, but in short we run 8,000 different MC simulations on 8,000 sets of field measurements from the Brinkerhoff et al. (2019) dataset and use the median uncertainity term across those 8,000 distributions as . Each of the 8,000 simulations are themselves 10,000 runs, sampling from the normal distributions for and . We quantified the error in again using the Brinkerhoff et al. (2019) dataset.

**Still need to run this MC analysis because I don't have uncertainity terms for Wang et al (2021)'s parameters... This won't effect the paper results though b/c i don't actually use it in the validation**

With the likelihood function (equation 6), prior distributions, and the parameter described (section 3.2.2), 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, BIKER uses a Hamiltonian Monte Carlo sampler which reduces computation time relative to other sampling algorithms (Hagemann et al., 2017).

### 3.3 Validation setup

We validate BIKER on the aforementioned 49 SWOT-simulated rivers (section 2) 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*. However, regardless of the validation data or SWOT error budget used, 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. Further, we are principally interested in BIKER's ability to reproduce from SWOT observations and are less concerned with the actual accuracy of the predictive model itself, which can be validated using existing datasets as has been previously done (Raymond et al., 2012; Ulseth et al., 2019; e.g. Wang et al., 2021). Therefore, we take the model outlined in section 3.1 and use that to calculate the observed that BIKER is validated against. This is done using equation 8, where is observed river channel area divided by observed channel width. This means that relies on in situ river shear velocity, while BIKER is predicting shear velocity from *W* and alone. Therefore, we are directly exploring BIKER's ability to infer observed and from *W* and *H* alone. It also means that, for a fair validation scheme, must be set to reflect only error from our assumptions about and not the parameter uncertainity inherent in (the 48 in equation 8). Thus, is set to 0.20 for this validation as suggested in section 3.2. However once SWOT launches, it should reflect the total uncertainty calculated in section 3.2 from both sources.

Validation is performed using the BIKER posterior means. Validation metrics take two forms (and are detailed in Table 1). To validate across all rivers and timesteps, we used the coefficient of determination and the root mean square error RMSE. Four normalized metrics were used for by-river validation: RRMSE and NRMSE are normalized root mean square errors that have been normalized by the observed value and the mean observed value (respectively). rBIAS is a measure of prediction bias that is normalized by the mean observed value. KGE is a standard metric used in streamflow prediction with an intuitive basis: a value greater than 0 is often interpreted as a useful prediction in ungauged settings, and a value greater than -0.41 indicates a model outperforms a uniform prediction of the mean observed value (Knoben et al., 2019).

*Table 1: Validation metrics used in this study, where r is the correlation coefficient, 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** |
| Coefficient of determination |  |  | 1 | 0 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 |
| Kling-Gupta efficiency | KGE |  | 1 | -∞ to 1 | By river |

### 3.4 Upscaling to CO2 evasion and bulk carbon efflux

It is one thing to accurately predict , but researchers are often most interested in the actual gas fluxes from rivers and ultimately the carbon emitted from river to atmosphere. Therefore, we explore 1) the ability of BIKER to reproduce evasion fluxes ( ) from these 49 rivers, and 2) the sensitivity of the carbon efflux due to the chosen method to approximate and ultiamtely .

First, we calculate . To do this, we pair the biweekly 26 samples (section 2) with every 11th SWOT observation by date, ignoring the timesteps beyond 26 (only ~15% of the SWOT observations were ignored here and we deemed this acceptable). We chose to sample every 11 days as this is the average sampling resolution for SWOT and the data is only every 14 days. Not all of the SWOT rivers have observations for a full year, and when simulation dates were not available they were assumed to start on January 1st. We also pair the modeled values (obtained from and equation 9) with these water-side concentrations and water temperatures. In equation 9, 530 is the Schmidt number for oxygen at 20 degrees Celsius (which is the temperature at which BIKER predicts *k*) and *Sc* is the Schmidt number at one's desired temperature for some dissolved gas. Atmospheric was assumed 390 uatm. The Schmidt number, used in equation 9, was calculated following Raymond et al. (2012) and Wanninkhof (1992). validation was performed using the same metrics as validation (Table 1).

Next, we estimate bulk carbon efflux using five models for average channel depth (used to calculate ): BIKER's posterior means and four gauge-based HG models previously used for upscaling (Horgby et al., 2019; Lauerwald et al., 2015; Raymond et al., 2013, 2012). See for their definitions. It is worth stressing that the Lauerwald et al. (2015) model is actually one of two components of the Raymond et al. (2013) model, and so was developed by the latter's authors. The names used here refer to the specific implementation used in each study. The Horgby et al. (2019) was developed explicitly for steep mountain streams, of which SWOT will not sample. We include it here to explore just how sensitive efflux estimates are to the HG model that is employed, noting that it will likely perform poorly. For this study, all HG methods use the in-situ discharge record while BIKER does not. This allows us to assess whether BIKER's estimates (wholly ungauged) are comparable to gauged methods (all four HG models). Finally, we express the bulk carbon efflux as the average mass flow rate of carbon (via evasion) per year from the 49 rivers after accounting for total river surface area.

## 4 Results

First, we present the results from the BIKER validation on 49 SWOT rivers and on 17 SWOT rivers with measurement errors (section 4.1). Next, we compare BIKER inversion errors to the errors inherent in equations 2 and 3, as well as the rivers' hydraulic properties (section 4.2). Finally, we use five different models for to compare and bulk carbon efflux estimates made using gauged and ungauged methods (section 4.3).

### 4.1 Validating the BIKER algorithm

Figure 3a plots the validation results for (with no SWOT measurement error) across all 49 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 . Using absolutely no in situ information, BIKER captures the magnitude of the predictions and most points fall on or near the 1:1 line. However, the 95% prediction intervals (dashed grey lines) highlight a slight underestimation bias for many predictions and a small number of predictions that are significantly underestimated. The RMSE for the BIKER predictions is only 1.86 m/day) across all predictions.

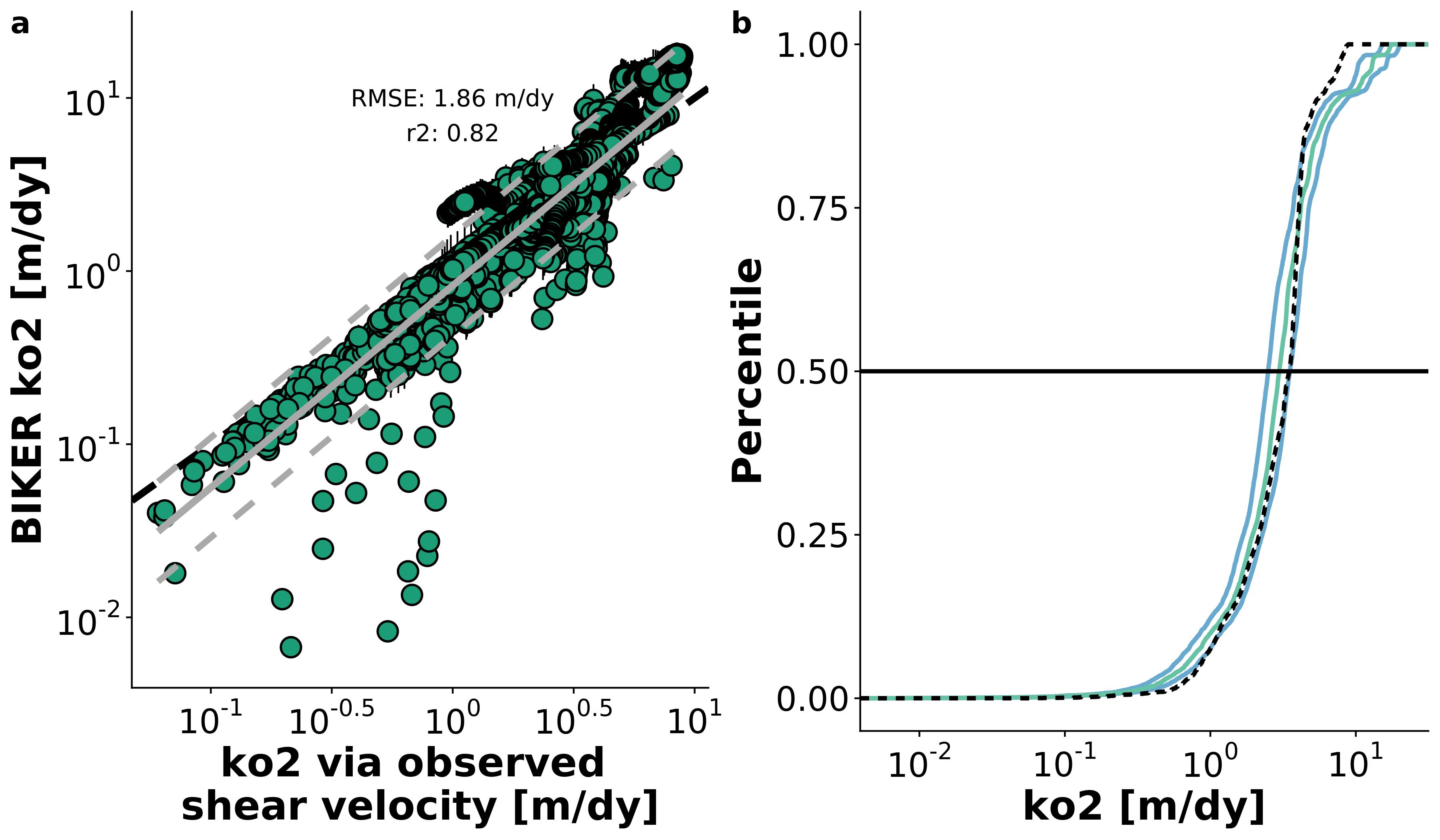


Figure 3. a: Validation of BIKER for 22 SWOT rivers. Black bars are 95% CIs for the modeled values. Grey line is linear regression (and 95% prediction intervals are dashed) and dashed black line is 1:1 line. b: Cumulative density functions (CDFs) of the same results: dashed black line are observed values, green line are BIKER posterior means, and blue lines are BIKER 95% CIs.

Figure 3a highlights a small number of values that are grossly underestimated by BIKER, which is confirmed in Figure 3b. Figure 3b plots the cumulative density functions (CDFs) of observed and predicted where the green line is the CDF of the BIKER posterior means, the blue lines are the CDFs of the BIKER posterior 95% CIs, and the dashed black line is the CDF of observed . We see, more clearly than in Figure 3a, that BIKER captures very well: most of the observed CDF falls between the 95% CIs or on the posterior mean (Figure 3b). Most of the values poorly captured by BIKER are extremes: the uppermost quartile is systematically overestimated by BIKER, and a handful of the smallest in this data are underestimated (also visible in Figure 3a). In summary, Figure 3 confirms that we improve upon our baseline understanding of in these rivers: we accurately capture with no in situ information about the river while simultaneously and explicitly accounting for the uncertainties inherent in our estimates.

Figure 4a plots validation metrics calculated for each river with and without SWOT measurement error (green and purple, respectively). The boxplots are composed of validation scores for either the 49 or 17 rivers- see Table 1 for metric definitions. SWOT measurement uncertainties slightly degrade performance across all four error metrics (Figure 4a), though caution should be used in over-interepting boxplots with a sample size of only 17. 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 49 rivers.

Median KGE is 0.45, which is excellent given that absolutely no in situ information is being used to predict . 34/49 rivers score a KGE > -0.41 and 30/49 are greater than 0, indicating that BIKER provides additional meaningful information in an ungauged setting. Median rBIAS is 0.04, suggesting nearly no bias in most rivers' predictions. However, some rivers are substantially biased in both directions (particuarly positive bias, where 3 rivers have scores > 1). This further supports the visual evidence in Figure 3 that sometimes BIKER is substantially under/overestimating the magnitude of and that this is river-specific. NRMSE and RMSE have median scores of 0.26 and 0.28, respectively. While median KGE and rBIAS scores were strong, the ranges of these scores were somewhat large (standard deviation for KGE of 1.25 and for rBIAS of 0.39).

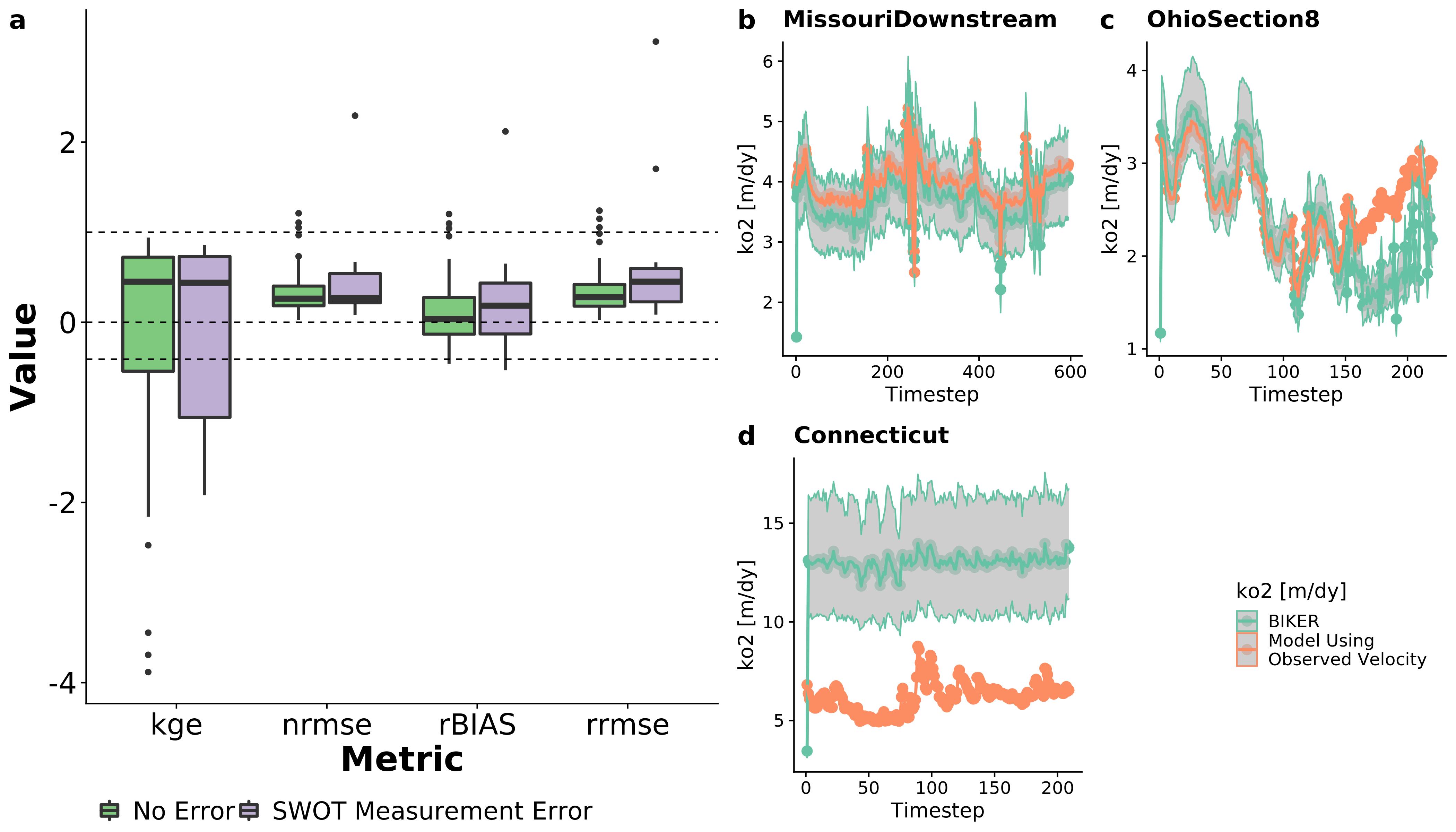


Figure 4. a: Performance metrics by river. See Table 1 for metric definitions. Dashed lines denote scores of 1, 0, and -0.41 for KGE (section 3.2). b-d: validation timeseries for three rivers representative of good, reasonable, and poor BIKER performance. b) was randomly selected from the upper tertile of KGE scores, c) was randomly selected from the middle tertile, and d) from the worst tertile. Model results include the posterior means and 95% CIs.

Figure 4b-d are representative timeseries plots of predicted and observed for three rivers chosen randomly from those with 'good' KGE scores (b), 'okay' KGE scores (c), and 'bad' KGE scores (d). See the Figure 3 caption for how this was determined. For the Missouri Downstream River, the entire timeseries of is correctly predicted, while in the Ohio Section 8 River there is a positive bias in the later estimates. Interestingly, there is near perfect recovery of for the first approximately 150 days. In the Connecticut River, there is significant positive bias in the estimates but also massive uncertainty (per the 95% CIs) in those estimates. Temporal dynamics are also largely missing from BIKER's Connecticut River predicitions.

### 4.2 BIKER performance versus *k* model performance

The MC simulations described in section 3.2.2 yielded an overall BIKER uncertainity of **must update alpha uncertainty** (Figure S4). While this will be useful for running BIKER on actual SWOT data, recall that the validation presented here (section 4.1) accounts for parameter error for a fair comparison against the 'observed' values (section 3.3). In that context, figure 5 compares BIKER inversion error per river and via NRMSE to the error generated by process-level uncertainities. This is the dashed black line in Figure 5 and is the reported cross-validated model performance for equation 3 (Wang et al., 2021). This is approximately 57%. Note that Wang et al. (2021) calculate the NRMSE but refer to it as 'relative error'. 43/49 rivers have lower inversion errors than the cross-validated model error for equation 3 (~57%), with most rivers' scores far less than 57% (Figure 5). The median relative error in BIKER inversion is 0.26 which is less than 1/2 of the reported error for . For the six rivers with inversion errors greater than the parameter error, 4/6 are approaching or over 100% error. This means that BIKER inversion errors are nearly always far less than the parameter error, however occasionally the inversion is very poor and introduces significantly more error than equation 3 does. It should also be stressed that NRMSE is one of the worst perfoming metrics for BIKER (figure 3a) and so a similar comparison using KGE or rBIAS would likely yield even stronger results. In summary, BIKER introduces a small amount of additional error into the predictive model for and any errors in the final estimates are dominated by process-level uncertainity in predicting via equation 3 rather than uncertainity in inverting SWOT observations to solve equation 3.

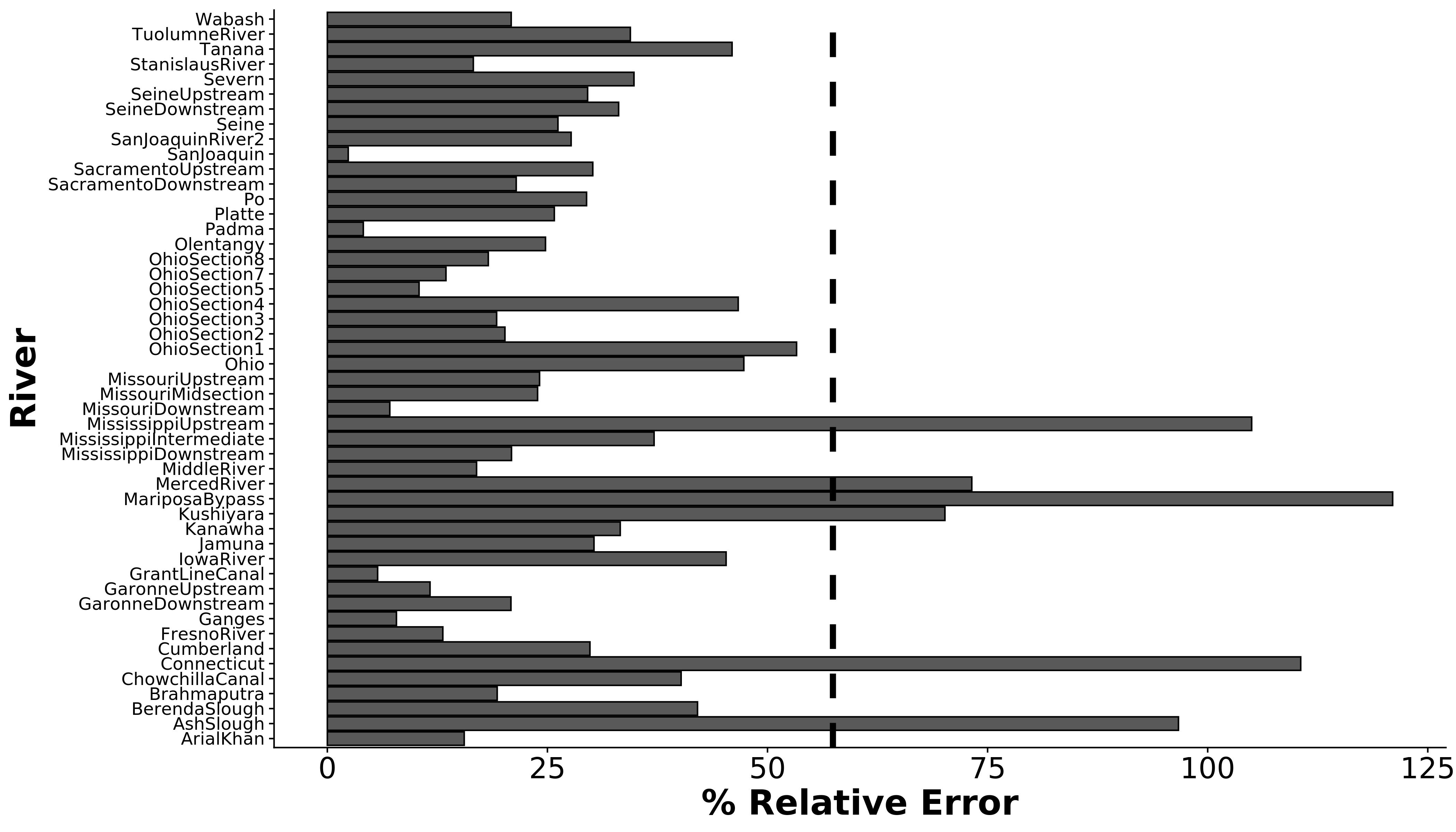


Figure 5: NRMSE, referred to as relative error by Wang et al. (2021), for all 49 rivers. Dashed line is the cross-validation relative error for the ko2 model used in this study (~57%), reprinted from Wang et al. (2021). We see that errors introduced by BIKER are nearly always much less than prediction uncertainity stemming from the ko2 model itself. NRMSE is also one of the worst perfoming metrics for BIKER (figure 3a).

**This paragraph needs some work** Figures 4 and 5 show that BIKER performs extremely poorly on 6/49 rivers. To explore this, and more broadly why some rivers perform well and others do not, we also compared BIKER performance against the following river hydraulic properties: mean observed , *W*, and . We found two patterns that emerged from this analysis. First, rBIAS (figure 6) exhibited no dataset-wide correlations with hydraulic properties, however we did find a uniform, positive bias in BIKER's predictions in the narrowest and steepest rivers. For the 49 rivers used in this study, these are rivers with slopes approximately > 0.0005 (Figure 5c) and widths < 100m (Figure 6b). Following basic gas exchange theory, these are also the rivers with the greatest values (Figure 6a). Second, KGE, NRMSE, and RRMSE (Figures S5, S6, and S7, respectively) similarly showed no dataset-wide correlations with the hydraulic properties. However for the seven widest rivers tested (> 1000m wide), not a single river performed extremely poorly, as subjectively interpreted from Figures S5, S6, and S7. Taken in aggregate, this means that a river's hydraulic properties alone cannot predict how BIKER will perform, however narrow/steep rivers will likely have positive bias in their predictions and the widest rivers will likely perform adequately (not not necessiarly great).

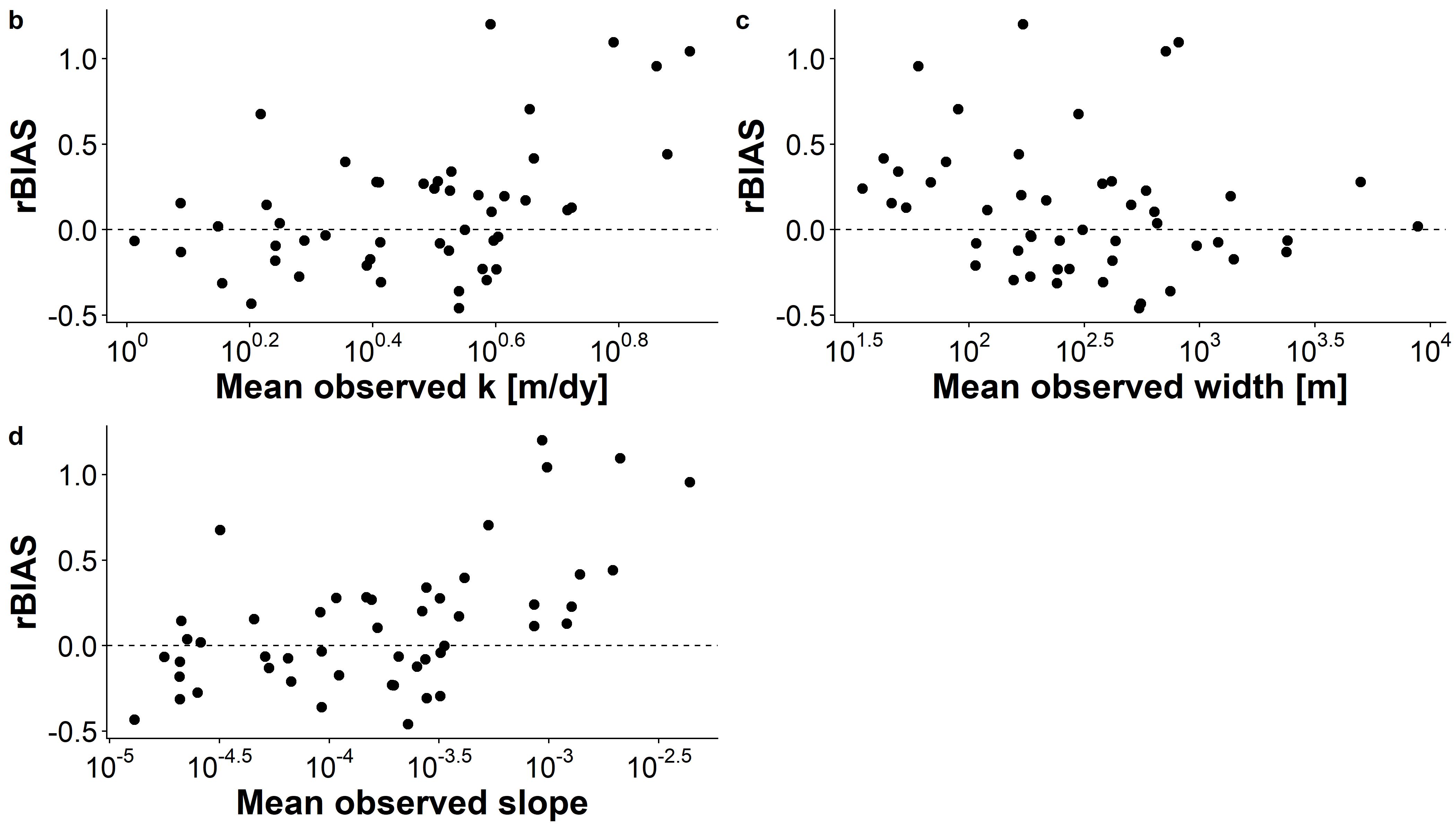


Figure 6: BIKER performance (defined by rBIAS- Table 1) versus (a) mean river ko2, (b) mean river width, and (c) mean river slope. An rBIAS of zero (dashed black line) indicates no bias in the predictions.

### 4.3 Predicting carbon efflux from large rivers

Finally, we explore our ability to 1) use BIKER-produced to estimate and 2) estimate bulk carbon efflux from evasion (section 3.4).

In Figure 7a, there is a very strong fit to the observed data, with an RMSE of 3.34 . The is just slightly lower than (Figure 6a). Overall, there is less systematic bias in the predicitons across all 49 rivers than in the predictions (Figure 3a). 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 wider than those presented in Figure 3a. Figure 7b-d includes subplots for the same rivers as Figure 3b-d, however with plotted instead of . There is near perfect recovery of in the Missouri Downstream River and very good recovery in the Ohio Section 8 river (Figures 7b and 7c, respectively). Both the magnitude and temporal dynamics are modeled very well, with the Ohio Section 8 River experiencing a small amount of bias in some later predictions. The Connecticut river is systematically over estimated aside from the last four points (Figure 7d), though BIKER's CIs do reflect quite uncertain estimates and the temporal dynamics are not far from the observed dynamics. This suggests that BIKER can easily estimate the changing dynamics of gas exchange but is at the mercy of the prior on to accurately estimate the magnitude of the evasion.

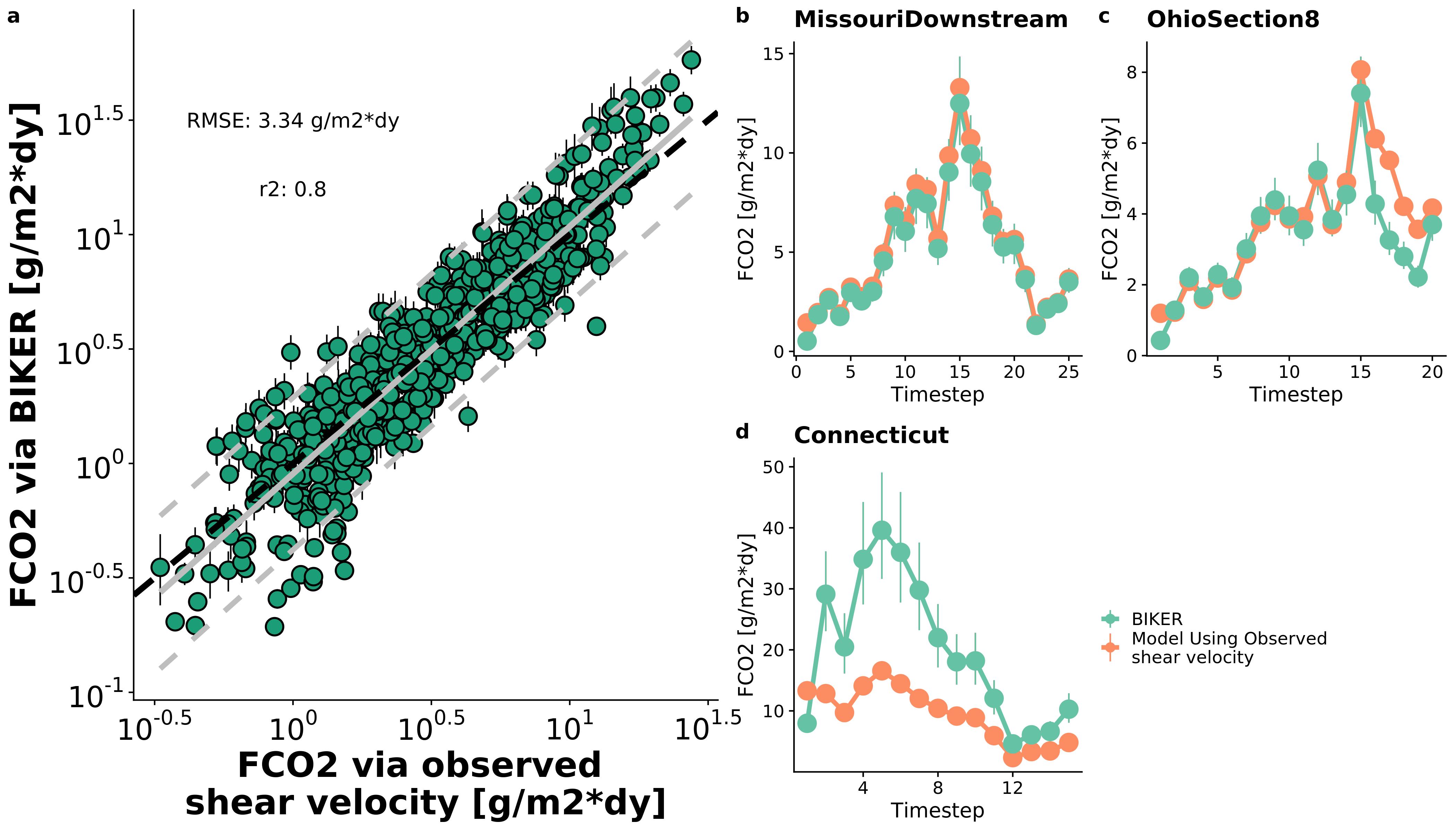


Figure 7: a: FCO2 via BIKER versus via equations 2 and 3 for every 11th timestep for the 49 rivers (grey lines are linear regression and 95% prediction intervals, while black dashed line is the 1:1 line). b-d: timeseries plots for the three example rivers from Figure 3b, 3c, and 3d.

Finally, we compare and bulk carbon efflux (via evasion) from the 49 rivers using BIKER posterior means and four gauge-based HG models (Figure 8). Figure 8a are barplots of the bulk carbon efflux (via evasion) across the 49 rivers in gigagrams of carbon per year. Both the BIKER bulk carbon efflux (2406 gG-C/yr) and the 'Raymond 2012' estimate (1949) are quite close to the observed flux (2098), though the former is overestimated and the latter is underestimated. The 'raymond 2013' model is slightly more overestimated (2609), while the 'Lauerwald 2015' model grossly overestimates this bulk efflux (3070). As expected, the 'Horgby 2019' model is ill-suited for rivers this large and produces signifiantly wrong estimates (1305). Thus, despite BIKER using absolutely no in situ data, it provides similar estimates of the carbon efflux to one of the in-situ approaches and the observed efflux itself (Figure 8a).

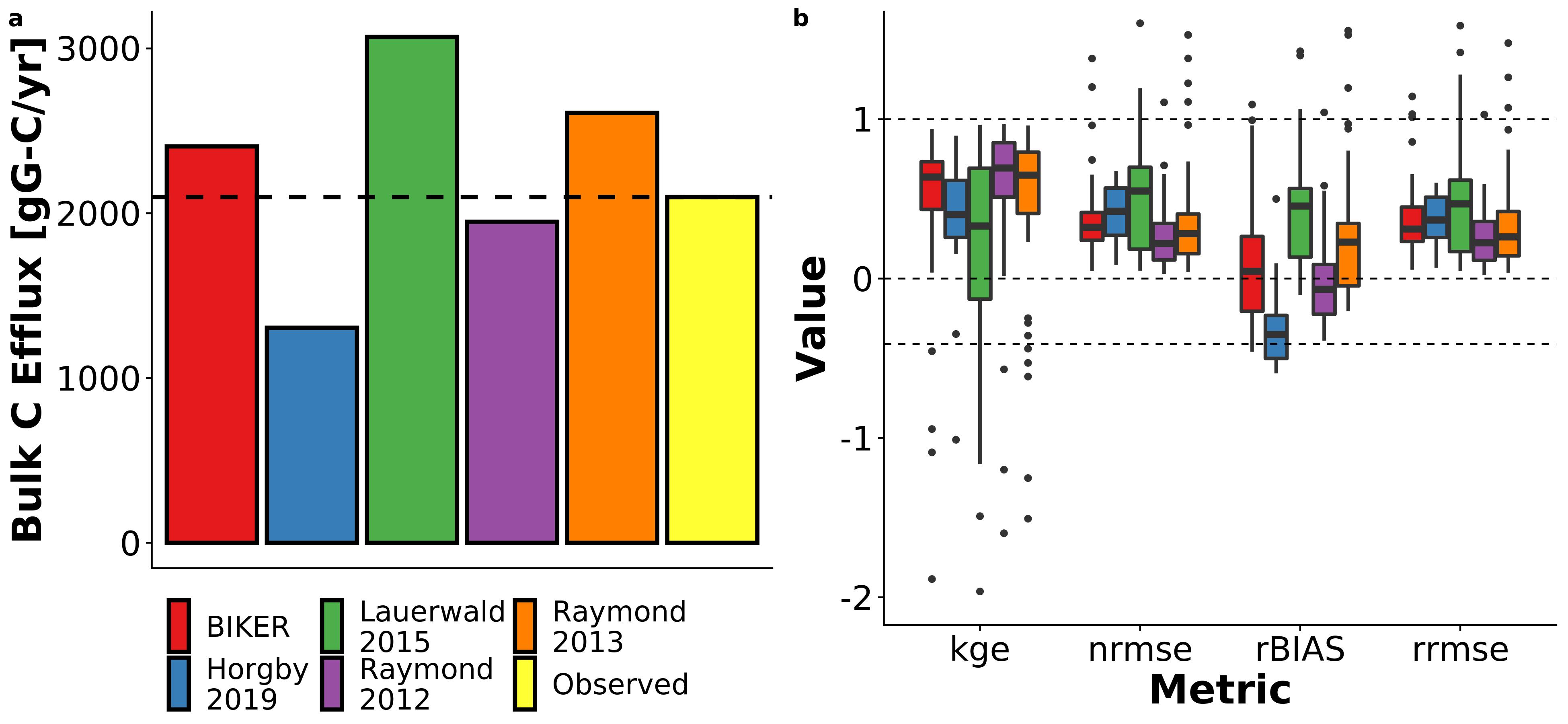


Figure 8. a: Bulk carbon efflux, per year, from the 22 SWOT rivers as calculated using four different average flow velocity estimates: 1) BIKER, 2) through 4) average flow velocity as calculated using HG models from the literature. b: Boxplots of by-river performance in estimating FCO2 across all timesteps and rivers for the same five velocity models. Dashed lines are identical to Figure 6a.

Figure 8b plots the by-river performance scores for . In line with the Figure 7a results, 'Lauerwald 2015' and 'Horgby 2019' are the worst performing (median KGEs, respectively: 0.33 and 0.4) while BIKER (median KGE: 0.64) is on par with the other two in-situ methods (median KGEs: 0.65 and 0.69 for 'Raymond 2013' and 'Raymond 2012', respectively). For rBIAS, both BIKER and 'Raymond 2012' indicate the least bias in some rivers and similar bias to the other models in other rivers. For BIKER, this is indicated by the scores' inter-quartile range (0.47) and median (0.05). Meanwhile, both 'Lauerwald 2015' and 'Horgby 2019' produce significant bias in their estimates: 'Lauerwald 2015' has a median rBIAS of 0.46, while 'Horgby 2019' had -0.35 . Similar patterns play out for NRMSE and RRMSE. In summary, BIKER performance across all four metrics is either similar or slightly worse than one of the in-situ approaches tested here and better than the the other three in situ approaches. This is despite relying on absolutely no streamgauge data like all three other models do.

## 5 Discussion

### 5.1 Towards remote sensing of global spatiotemporal dynamics of *k*

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. Authors have argued that the key to explaining the large residual variation in upscaling models is to explore at-a-station temporal variability in *k* (Hall and Ulseth, 2020).

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 3 and 4) and 2) being robust to measurement errors internal to the SWOT data (Figure 3) bode well for BIKER's eventual implementation on real SWOT observations. The results presented here suggest that daily estimation of riverine gas exchange globally could be possible once SWOT launches.

### 5.2 Estimating bulk carbon efflux using SWOT

Section 4.3 confirms that BIKER is successful, without any in situ information, at predicting 1) (Figure 7) and 2) the bulk carbon efflux (Figure 8). This encouraging result has two main implications for future work coupling remote sensing via SWOT and in situ data. First, section 4.3 confirms that we can couple BIKER and SWOT with in situ gas concentration loggers to produce estimates at novel temporal resolution in SWOT-observable rivers. This is particualry useful given recent advances in high temporal resolution in situ gas concentration measurements (Aho et al., 2021). BIKER can likely also be ran at the field scale using arrays of pressure transducers to estimate water surface slope (rather than using RS techniques) following recent work doing the same using the Hagemann et al. (2017) RSQ algorithm (Harlan et al., n.d.).

Secondly, it is important to stress that unlike BIKER, the HG models in Figure 8 rely on an in situ streamgauge. This means that Figure 8 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 recent upscaling studies (Horgby et al., 2019; e.g. Lauerwald et al., 2015). **I assume Shaoda's paper will still be in review and can't cite here but this is exactly what they do...**

Figure 8 also confirms that the training data used for HG models exerts a significant influence on upscaled carbon emissions from rivers. The 'Lauerwald 2015' model, which was trained on larger rivers than the data used in either the 'Raymond 2013' or 'Raymond 2012' models, should perform best on SWOT-observable rivers (which are greater than 50m wide). Figure 8 confirms this. Meanwhile, BIKER has no similar reliance on hydraulic parameters trained on different river sizes and only assumes that the channel's hydraulic radius can be approximated by mean flow depth (which is generally the case in rivers large enough to be SWOT-observable- **text Sx**). 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).

### 5.2 Sources of BIKER uncertainty: process-level or remote sensing?

Throughout the BIKER validation, we have assumed no parameter uncertainity in the upscaling parameters . We have shown that BIKER estimate uncertainty is almost always less than uncertainity, and usually far less (Figure 5). Implicit measurement errors in SWOT data also exert a trivial influence on BIKER accuracy (Figure 4a). Therefore, most of the total BIKER uncertainity stems from the predictive model itself. We argue that BIKER's total uncertainity is therefore limited by current process-level understanding of riverine *k* and not by SWOT measurement errors or the BIKER inversion process. This suggests that BIKER's predictive performance can only improve as we continue advancing our understandings of the physical processes governing gas exchange from SWOT-observable rivers.

We speculate that for BIKER to be useful on actual SWOT data post-launch, we will need to begin 'closing the gap' on process-level uncertainitites in predicting *k* from river hydraulics. Future work should focus on two areas. First, we must expand theoretical work on predicting *k* from hydraulics in large, SWOT-observable rivers where wind exerts a non-trivial influence on *k* (Beaulieu et al., 2012). While the predictive models for *k* that have been discussed in this manuscript are useful, they are limited by their inability to account for wind-induced turbulence that is common in large rivers and the primary controller of *k* in lakes and estuaries. Second, future work must compare BIKER-generated *k* values to field measured values to explicitly validate the algorithm. This will be possible once SWOT launches and those data are available.

## 6 Conclusions

Efforts to predict gas exchange velocities from river networks generally do so using river channel hydraulics. Therefore, gas evasion estimates are sensitive to available in situ hydraulics data. In ungauged basins, this poses a problem because hydraulics~discharge relationships can not be built. To circumvent this problem, we propose using established techniques from the ungauged remote sensing of river discharge literature and applying them to gas exchange velocity in ungauged rivers. This is formalized as the BIKER algorithm, which uses data from the upcoming SWOT satellite to remotely sense gas exchange velocity (for dissolved oxygen) solely from river width and water surface height. We validate BIKER on 49 'rivers' of simulated SWOT data (Durand et al., 2016; Frasson et al., 2021), obtaining an RMSE of 72.44/day after accounting for upscaling parameter uncertainity. When generalized to estimate bulk carbon efflux (via evasion) from these 49 rivers, BIKER reasonably captures the observed efflux (2406 gG-C/yr versus gG-C/yr, respectively). Further, BIKER's estimates across the 49 rivers are only modestly worse than those made using a streamgauge and the hydraulic geometry models frequently used in the literature. This suggests that BIKER will be useful not only for upscaling in ungauged rivers, but also in potentially improving our understandings in gauged rivers too. As drainage network models of GHG evasion gain in sophistication and continue to ingest higher and higher temporal resolution data, BIKER and SWOT should prove useful in providing such information.

## 7 Acknowledgements

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