AOS DESIGN OPTIMIZATION: REAERATION

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1 RELATED DOCUMENTS AND ACRONYMS

1.1 Reference Documents

RD [01]	NEON.DOC.000693	AOS Protocol ad Procedure: REA – Reaeration in streams

1.2 Acronyms

Acronym	Explanation
C_o	Concentration of SF6 at the upstream station (units mg/L)
C_x	Concentration of SF6 at downstream distance x (units mg/L)
K_d	Longitudinal gas loss rate of SF6 (units m-1)
k_{600}	Gas transfer velocity normalized to Schmidt number of 600 (units m/d)
k_{SF6}	Gas transfer velocity for SF6 (units m/d)
Q	Discharge (units L/s)
SF_6	Sulfur Hexafluoride
TWG	Technical Working Group
v	Stream velocity (units m/d)
x	Downstream distance (units m)
z	Stream mean depth (units m)

2 BACKGROUND AND GOALS

2.1 Description of sampling design and available data

The NEON Reaeration data product (DP1.20190.001) contains measurements that can be used to calculate the rate at which dissolved gases exchange between the water and the atmosphere. Accurate estimation of abiotic gas exchange is critical for calculating rates of aquatic metabolism (Mulholland et al., 2001; Appling et al., 2018) and fluxes of CO_2 (Conroy et al., 2023) and other ecologically important gases (Aho et al., 2023).

As part of the NEON Reaeration protocol (RD[01]), sulfur hexafluoride (SF_6) gas was continuously injected at a constant rate to measure gas exchange along with a conservative tracer (either NaCl or NaBr), which is used to correct for lateral inflows, such as tributaries and groundwater. Samples were collected at four downstream locations along a ~500m study reach. For more information on the experimental procedure, see RD [01]. The observed longitudinal decline in SF_6 concentration (C_o; mg/L) from the injection point to the downstream concentration (C_x; mg/L) at some distance (x, m^{-1}) can be fit with a first-order exponential decay function to estimate the longitudinal rate of gas loss (Kd; m^{-1}).

$$C_x = C_o e^{-K_d x} \quad (1)$$

The ratio of SF_6 concentrations to the conservative salt concentrations can be used in place of C_x and C_0 in Equation 1 to correct for possible dilution by lateral inflows. The longitudinal rate of gas loss can then be converted to the gas exchange velocity (k_{SF6}; m/d) by multiplying by the velocity (v; m/d) and the mean depth (z; m).

$$k_{SF6} = zvK_d \quad (2)$$

The SF_6 specific gas exchange velocity (k_{SF6}) is typically reported as k_{600} by normalizing to a Schmidt number of 600, making the gas exchange velocity more comparable across other gases of interest, such as CO_2 or O_2.

NEON conducted reaeration experiments in 22 of 24 wadeable stream sites (the exceptions were BLUE, which is too large to successfully conduct a tracer experiment, and ARIK, where the velocity is too slow). These experiments were conducted up to 10 times per year during site characterization, starting in 2014, and up to 6 times per year during initial operations, starting in 2019.

2.2 Analytical Goals

During the spring of 2021, NEON convened a Technical Working Group (TWG) of external experts to assess whether sufficient data had been collected to justify discontinuing SF_6 release, which would save resources and reduce the environmental impacts of collecting this data. While SF_6 is inert and detectable down to minute concentrations, making it ideal for reaeration experiments, it is also an extremely potent greenhouse gas. Thus, NEON's intent was to discontinue SF_6 releases once site-specific k_{600} versus Q relationships could be developed using the Reaeration data product (DP1.20190.001).

Gas exchange is primarily driven by turbulence and rates are often, but not always, positively correlated with stream discharge (Q) in steep streams (Maurice et al., 2017; McDowell and Johnson 2018; Ulseth et al., 2019). Alternatively, in low gradient streams where turbulence does not increase with Q, reaeration rates may remain relatively constant across a range of Q values (Ulseth et al., 2019). Once gas exchange has been measured across a range of Q values at a site, a site-specific rating curve can be developed, relating k_{600} to Q. The goal of this optimization analysis was to determine whether the existing relationships are sufficient to discontinue the release of SF_6 as part of reaeration experiments.

3 METHODS AND RESULTS

3.1 Methods

The analysis was performed on all reaeration experiments included in RELEASE-2023, plus additional experiments which were provisional at the time (Fall 2024). All experiments were first reviewed to verify their suitability for inclusion in the analysis. Because NEON has performed almost 700 SF_6 release experiments, we could be selective about which experiments to include. The most common reasons for omitting experiments were missing or contaminated samples, incomplete mixing of the SF_6, and missing or corrupted conductivity time-series files used to estimate the velocity. For more details on the screening process, see Aho et al., 2024a.

Instead of solving equations 1 and 2 for each of the individual experiments independently, a multi-level Bayesian modeling approach was used, which pools across all experiments performed at a site, reducing uncertainty. The model was coded in the Stan probabilistic modeling space and included in the reaRate R package (Cawley et al., 2024), which is available on GitHub and Zenodo. Using a power law function relating k_{600} to Q, the model estimated the exponent b from the posterior distribution of 1000 iterations over 4 Markov chains. For more information on how the model was implemented, see Aho et al., 2024a.

$$k_{600} = aQ^b \tag{3}$$

The discharge dependency of k_{600} was defined using the coefficient of variation (CV; standard deviation divided by mean) of the posterior distribution of the exponent b in equation 3. Sites with a CV >0.3 were assessed to have high discharge dependency, while sites with a CV <0.3 were determined to have a low discharge dependency.

We also compared the estimated values of k_{600} to the rate of energy dissipation (eD), calculated from the streambed slope (S) and velocity (v), where g is the acceleration due to gravity (9.8 m/s^2).

$$eD = Svg \tag{4}$$

3.2 Results

The model outputs are available from the Environmental Data Initiative (Aho et al., 2024b), and analysis of the results summarized below can be found in Aho et al., 2025. The range of k_{600}, Q, and eD varied significantly by site (**Figure 1)**. Boxes represent the median and interquartile range (IQR), points denote outliers more extreme than 1.5xIQR. Color indicates if k_{600} had low (blue) or high (red) Q dependency.

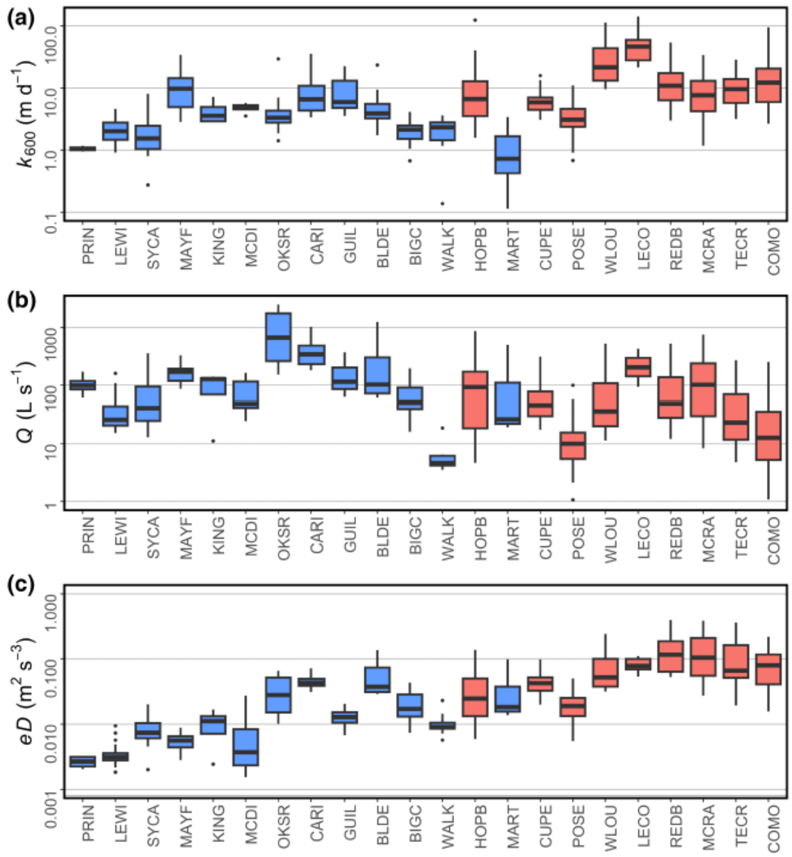

Figure 1. k600, Q and eD. Taken from Aho et al., 2025. Sites are arranged by increasing slope from left to right. Blue indicates sites where k_{600} had low discharge dependence, and red indicates sites where k_{600} had high discharge dependence.

Sites with shallow streambed slopes generally had lower and less variable ranges of k_{600}, rarely greater than about 10 m/d and spanning less than an order of magnitude (Figure 1, panel a). These sites also exhibited low discharge dependency (Figure 2). In contrast, sites with steep streambed slopes had higher and more variable ranges of k600 and exhibited high discharge dependency (Figure 2). The mean and standard deviation of b from the relationship $k_{600}=aQ^b$ is indicated on each panel, with values in blue indicating low discharge dependence and values in red indicating high discharge dependence (Figure 2).

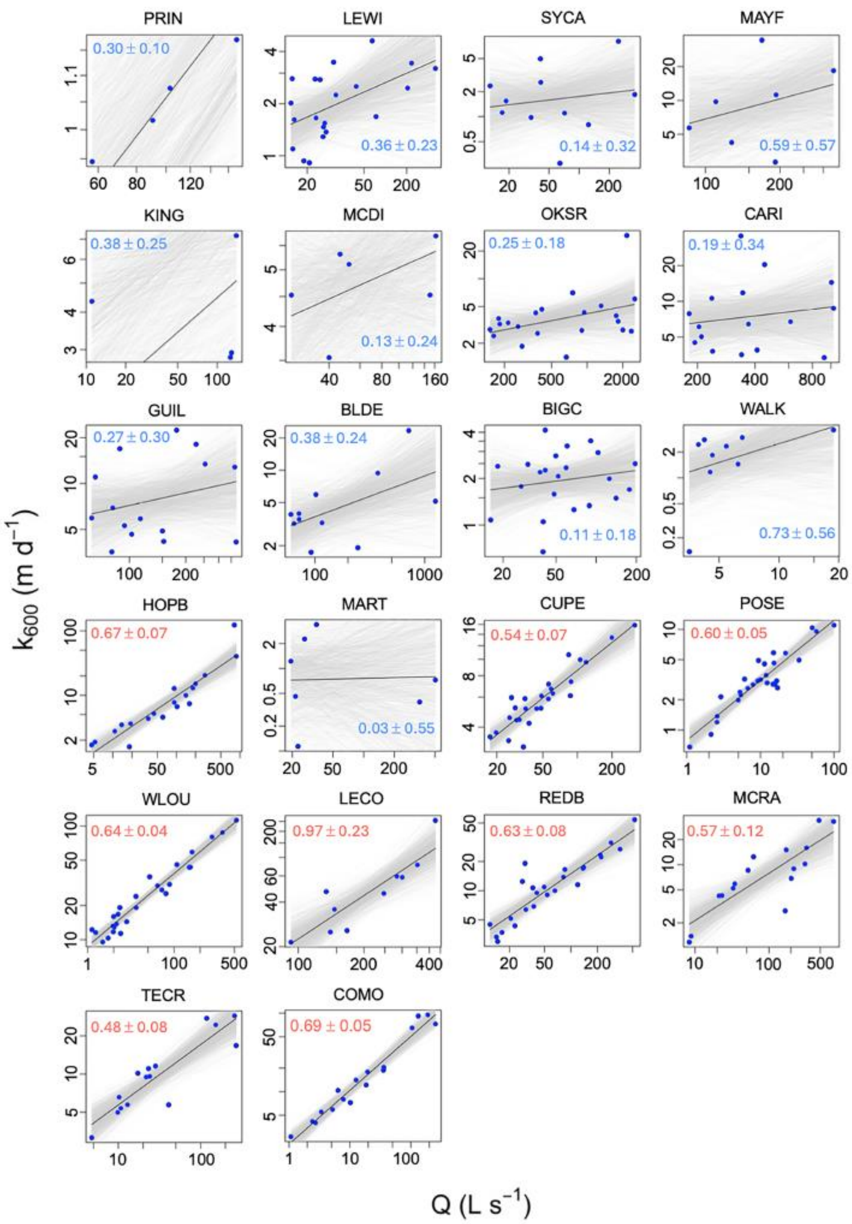

Figure 2. k600 vs Q. Taken from Aho et al., 2025. Sites are arranged by increasing slope from left to right, top to bottom. The mean and standard deviation of b from the relationship $k_{600}=aQ^b$ is indicated on each panel. Note the different scales for the y-axis depending on site.

Similarly, k_{600} appeared correlated with eD for streams with high values of k_{600} and eD, while less correlated in streams with lower values of k_{600} and eD (**Figure 1**). These relationships strongly matched those previously found in the literature (Ulseth et al., 2019).

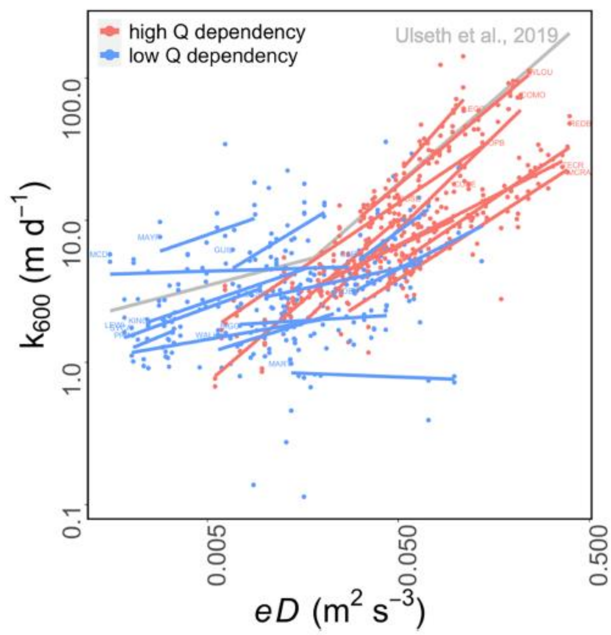

Figure 3. k600 vs eD. Taken from Aho et al., 2025.

4 DISCUSSION

Estimated rates of gas exchange can strongly influence inferred rates of stream metabolism (Aristegi et al., 2009). Recently, models have been developed that can simultaneously estimate k_{600} along with metabolism (gross primary production and ecosystem respiration) from diel dissolved oxygen signals, the most common of which is streamMetabolizer (Appling et al., 2018b). The accuracy of these models depends on the strength of the dissolved oxygen signal, which is optimized when primary production is high and k_{600} is low (Appling et al., 2018a). In small headwater streams (i.e., most of the NEON wadeable stream sites) where riparian shading limits primary production and dampens the dissolved oxygen signal, it becomes essential to constrain k_{600} to get accurate metabolism estimates.

Here, in steep gradient streams where k_{600} was high and likely to exert a strong effect on the dissolved oxygen signal, we observed strong discharge dependence, indicating that the relationship with discharge can be used to constrain k_{600} in the streamMetabolizer model. In sites with shallow streambed slopes, while k_{600} was not strongly dependent on discharge, the magnitude of k_{600} was also lower and less variable, indicating that gas exchange exerts less influence on the dissolved oxygen signals. The distribution of k_{600} observed in these low-slope sites can still be used to constrain the streamMetabolizer model, even if there is not a strong relationship with discharge.

There were a few sites (KING, MCDI, PRIN, SYCA) where we were only able to perform a handful of successful SF_6 experiments. These sites tend to experience low flows and seasonal drying. When higher flows do occur at these sites, they are extremely flashy and difficult to predict in advance, making it hard to capture gas exchange rates at those higher flows. Moreover, the sites often cannot be accessed safely in these conditions. Therefore, it is unlikely that experiments could ever be conducted in these higher flow ranges. However, these sites do not show a strong k_{600} dependence on discharge, at least over the range of flows that were able to be sampled. Moreover, primary production is typically inhibited during high flow events, reducing the need for reaeration estimates to calculate metabolism.

5 RECOMMENDATIONS

As a result of these analyses, in February 2025 NEON Science staff, in collaboration with the Reaeration TWG members, deemed the site-specific relationships developed between k_{600} and stream hydraulics to be sufficient to constrain k_{600} and recommended discontinuing SF_6 gas releases at all NEON sites. NEON will continue to perform the NaCl salt slug portion of the reaeration experiments four times per year at each site across a range of discharges. These salt releases are relatively easy to perform, require less equipment, do not include manual sampling with the expense of laboratory analysis, and do not use a greenhouse gas tracer. They provide valuable information about stream hydraulics, such as estimates of travel time, mean depth, and discharge.

If the salt slug experiments indicate that the hydraulic properties controlling gas exchange rates have significantly changed, NEON could potentially resume gas release experiments. However, resuming gas injections would involve switching to an alternative, non-greenhouse gas such as Argon, which has similar solubility and diffusivity as O_2 (Hall and Madinger, 2018). Switching to an alternative gas would require several significant changes to the sampling and analysis procedures. The NEON streams have historically been stable, and a massive change in stream geomorphology would have to occur to require new gas exchange curves. Major storm events, such as past hurricanes at NEON sites in D04, have not altered the channels enough to change the gas exchange and hydraulic relationships.

6 ACKNOWLEDGEMENTS

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7 REFERENCES

Aho, Kelly, Taylor Maavara, Kaelin Cawley, and Peter Raymond. 2023. “Inland waters can act as nitrous oxide sinks: Observation and modeling reveal that nitrous oxide undersaturation may partially offset emissions.” Geophysical Research Letters, 50, e2023GL104987. https://doi.org/10.1029/2023GL104987

Aho, K. S., Cawley, K., Hensley, R., Hall Jr, R. O., Dodds, W., & Goodman, K. (2024a). Gas exchange velocities (k600), gas exchange rates (K600), and hydraulic geometries for streams and rivers derived from the NEON Reaeration field and lab collection data product (DP1. 20190.001). Earth System Science Data Discussions, 2024, 1-24. https://doi.org/10.5194/essd-2024-330.

Aho, K.S., K. Cawley, R. Hensley, R.O. Hall, W. Dodds, and K. Goodman. 2024b. Gas exchange velocities (k600), gas exchange rates (K600), and hydraulic geometries for streams and rivers derived from the NEON Reaeration field and lab collection data product (DP1.20190.001) ver 2. Environmental Data Initiative. https://doi.org/10.6073/pasta/18dcc1871ee71cf0b69f2ee4082839d0.

Aho, K. S., Cawley, K. M., Hall Jr, R. O., Hensley, R. T., Dodds, W. K., Harrison, N., & Goodman, K. J. (2025). Gas transfer velocity (k600) increases with discharge in steep streams but not in low-slope streams. Limnology and Oceanography Letters. https://doi.org/10.1002/lol2.70003

Appling, A.P., Read, J.S., Winslow, L.A., Arroita, M., Bernhardt, E.S., Griffiths, N.A., Hall, R.O., Harvey, J.W., Heffernan, J.B., Stanley, E.H. and Stets, E.G., 2018. The metabolic regimes of 356 rivers in the United States. Scientific data, 5(1), pp.1-14. https://doi.org/10.1038/sdata.2018.292

Aristegi, L., Izagirre, O., & Elosegi, A. (2009). Comparison of several methods to calculate reaeration in streams, and their effects on estimation of metabolism. Hydrobiologia, 635, 113-124. https://doi.org/10.1007/s10750-009-9904-8

Cawley, K., K. S. Aho, and R. O. Hall. 2024. reaRates R Package,NEONScience/NEON-reaeration: v0.0.2. Zenodo. https://doi.org/10.5281/zenodo.12786089.

Conroy, H. D., Hotchkiss, E. R., Cawley, K. M., Goodman, K., Hall, R. O., Jr., Jones, J. B., et al. (2023). Seasonality drives carbon emissions along a stream network. Journal of Geophysical Research: Biogeosciences, 128, e2023JG007439. https://doi.org/10.1029/2023JG007439

Hall Jr., R. O. and Madinger, H. L. (2018). Use of argon to measure gas exchange in turbulent mountain streams. Biogeosciences, 15, 3085–3092. https://doi.org/10.5194/bg-15-3085-2018

Maurice, L., Rawlins, B. G., Farr, G., Bell, R., & Gooddy, D. C. (2017). The influence of flow and bed slope on gas transfer in steep streams and their implications for evasion of CO2. Journal of Geophysical Research: Biogeosciences, 122(11), 2862-2875. https://doi.org/10.1002/2017JG004045.

Mulholland, P.J., Fellows, C.S., Tank, J.L., Grimm, N.B., Webster, J.R., Hamilton, S.K., Martí, E., Ashkenas, L., Bowden, W.B., Dodds, W.K. and McDowell, W.H., 2001. Inter-biome comparison of factors controlling stream metabolism. Freshwater biology, 46(11), pp.1503-1517. https://doi.org/10.1046/j.1365-2427.2001.00773.x

McDowell, M. J., & Johnson, M. S. (2018). Gas transfer velocities evaluated using carbon dioxide as a tracer show high streamflow to be a major driver of total CO2 evasion flux for a headwater stream. Journal of Geophysical Research: Biogeosciences, 123(7), 2183-2197. https://doi.org/10.1029/2018JG004388.

Ulseth, A. J., Hall Jr, R. O., Boix Canadell, M., Madinger, H. L., Niayifar, A., & Battin, T. J. (2019). Distinct air–water gas exchange regimes in low-and high-energy streams. Nature Geoscience, 12(4), 259-263. https://doi.org/10.1038/s41561-019-0324-8.