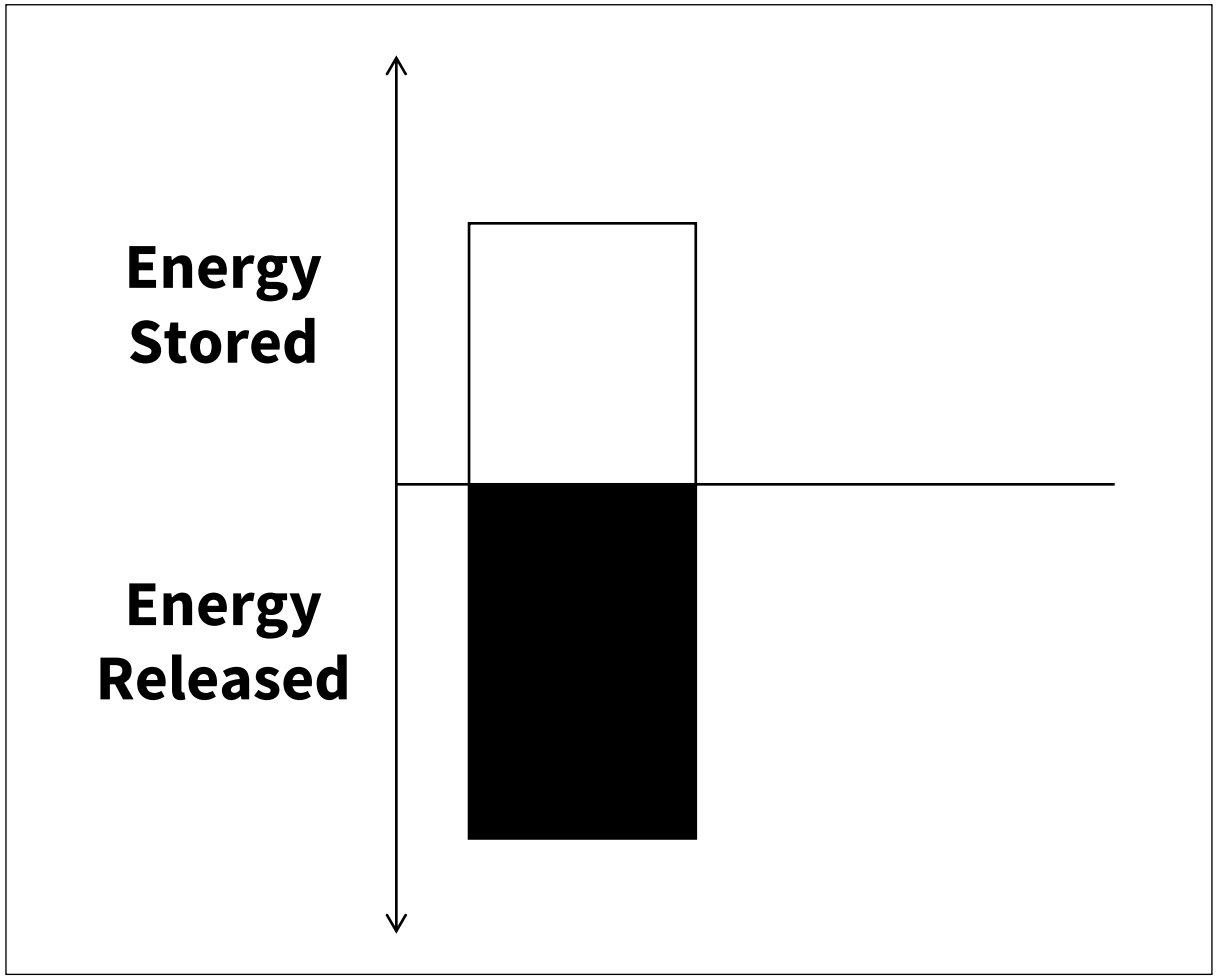
Are anaerobic energy-generation pathways significant contributors to stream energy budgets?

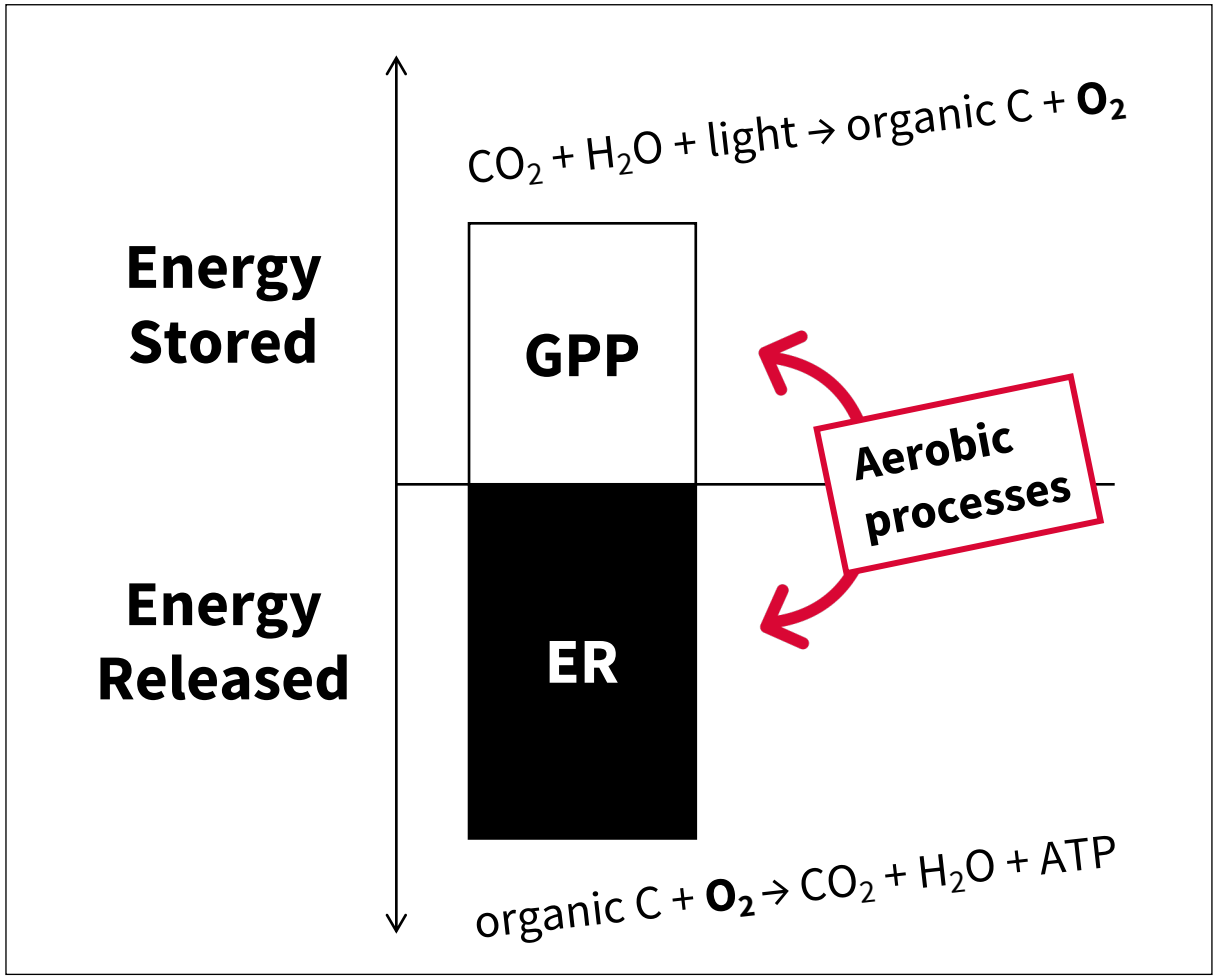
Michelle Catherine Kelly[1,2], Erin K. Eberhard[1], Kevin Nevorski[1], Amy M. Marcarelli[1]
[1]Department of Biological Sciences, [2]Data Science Graduate Program
Michigan Technological University, Houghton, MI, USA

Scan for a link to the HTML version of this talk and all source code

Stream metabolism =
Energy stored – energy released



Stream metabolism =
Energy stored – energy released



What about anaerobic processes?

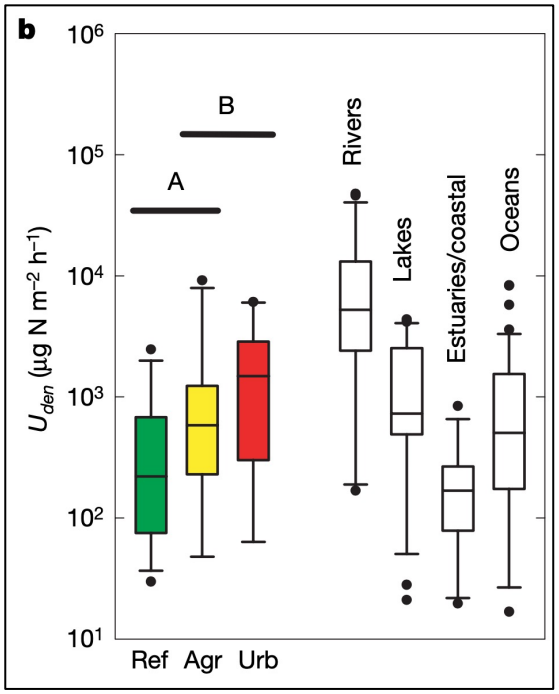
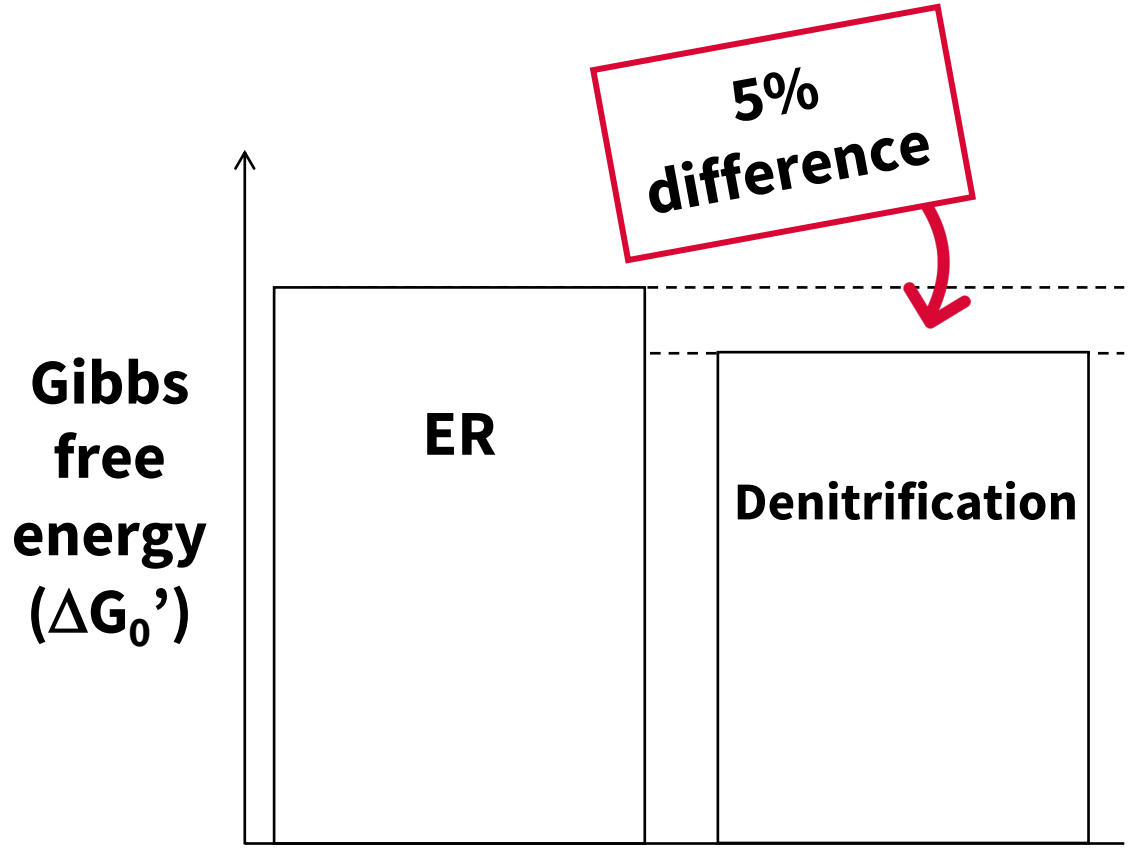
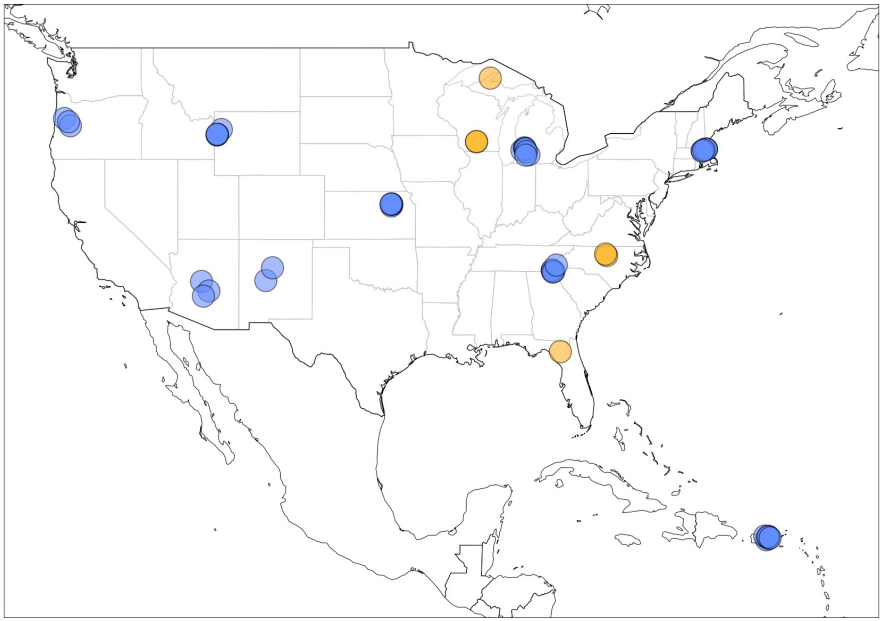


Figure from Mulholland et al. 2008



Are anaerobic processes significant contributors to stream energy budgets?

Sites and Data



LINX II Project
(n = 48)

Whole-stream **denitrification** measured using **15-N tracer**, data obtained from Mulholland et al. 2009 Supplemental, https://www.doi.org/10.4319/lo.2009.54.3.0666

Modeled **metabolism** data obtained from Bernot et al. 2010 Supplemental, https://www.doi.org/10.1111/j.1365-2427.2010.02422.x

Marcarelli Nationwide Denitrification and N Fixation
(here n = 7, 31 streams total in survey)

Denitrification measured on individual stream substrates using **amended acetylene inhibition** assays, see Amy Marcarelli's Wednesday AM talk.

Modeled **metabolism** obtained from StreamPULSE repository, https://data.streamPULSE.org

Energy Budget Calculation

Aerobic respiration, reduction half-reaction: $O_2 + 4\ H^+ + 4\ e^- \rightarrow 2\ H_2O$

Energy released from ER, kCal per m² hr

= ER rate × Gibbs free energy (at pH = 7) × e^- in full reaction

= ER rate in g-O_2 per m^2 day × 29.9 kCal per e^- × 4 e^- per reaction
÷ 32 g-O_2 per mol O_2 × 2 mol-O per mol O_2 ÷ 1 mol-O_2 per reaction ÷ 24 hours per day

Denitrification, reduction half-reaction: $2\ NO_3^- + 12.5\ H^+ + 10\ e^- = N_2 + 6\ H_2O$

Energy released from denitrification, kCal per m² hr

= Denitrification rate × Gibbs free energy (at pH = 7, kCal per e^-) × e^- in full reaction

= Denitrification rate in mg-N per m^2 hr × 28.4 kCal per e^- × 10 e^- per reaction
÷ 1000 mg-N per g-N ÷ 14 g-N per mol ÷ 2 mol-N per reaction

Scan for a link to the HTML version of this talk and all source code

Energy Budget Calculation

Total energy released, kCal per m^2 hr

= Energy released from ER + Energy released from denitrification

Energy released from denitrification as a proportion of total energy budget

= Energy released from denitrification ÷ Total energy released × 100%

Energy released from aerobic respiration as a proportion of total energy budget

= Energy released from ER ÷ Total energy released × 100%

Scan for a link to the HTML version of this talk and all source code

Predictive Modeling

Pre-processing

- **Dummy variables** for categorical predictors
- Removed **near zero variance** predictors, cutoff ratio = 95/5
- **Centered, scaled**

Splitting and resampling

- Data **randomly split** into training and testing sets, **80% training** and **20% testing**
- **10-fold cross-validation** for resampling, repeated **10 times**

Evaluating model performance

- **Best fit model = Lowest** root mean squared error **(RMSE)** on testing set

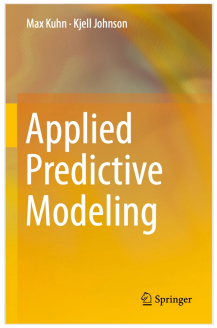
Pre-processed **Marcarelli Nationwide dataset:**

- **17 observations, 24 predictors**

Pre-processed **LINX II dataset:**

- **28 observations, 28 predictors**
  - 8 categorical (ex. state, land use, biome)
  - 20 continuous (ex. discharge, reach width, DOC, NO3, SRP, GPP, ER)
- **Response:** Energy released from denitrification as a proportion of total energy (%)

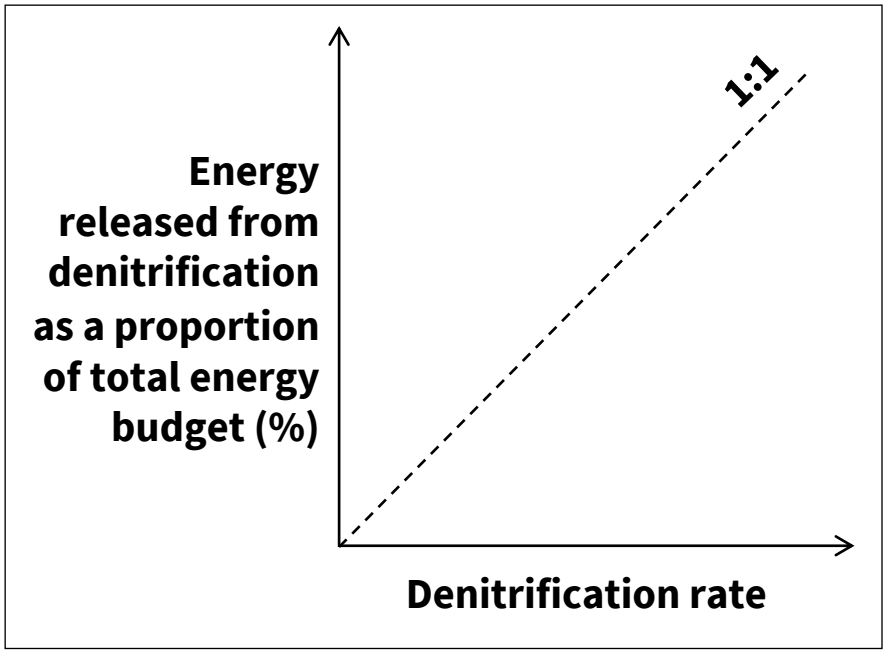
Resources



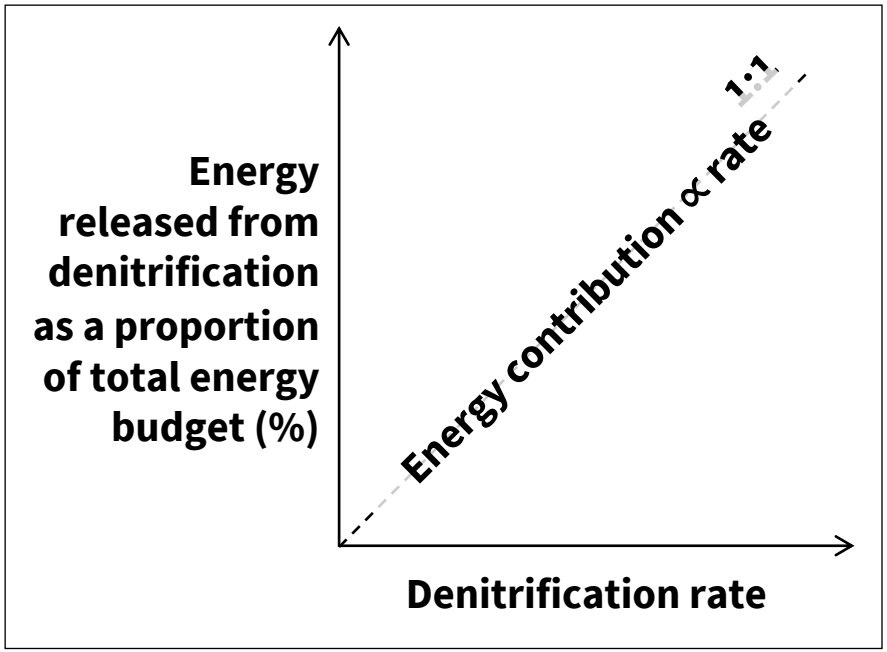
Kuhn et al. 2019. *caret: Classification and Regression Training* R package. https://topepo.github.io/caret/

Kuhn and Johnson. 2013. *Applied Predictive Modeling.* https://appliedpredictivemodeling.com/

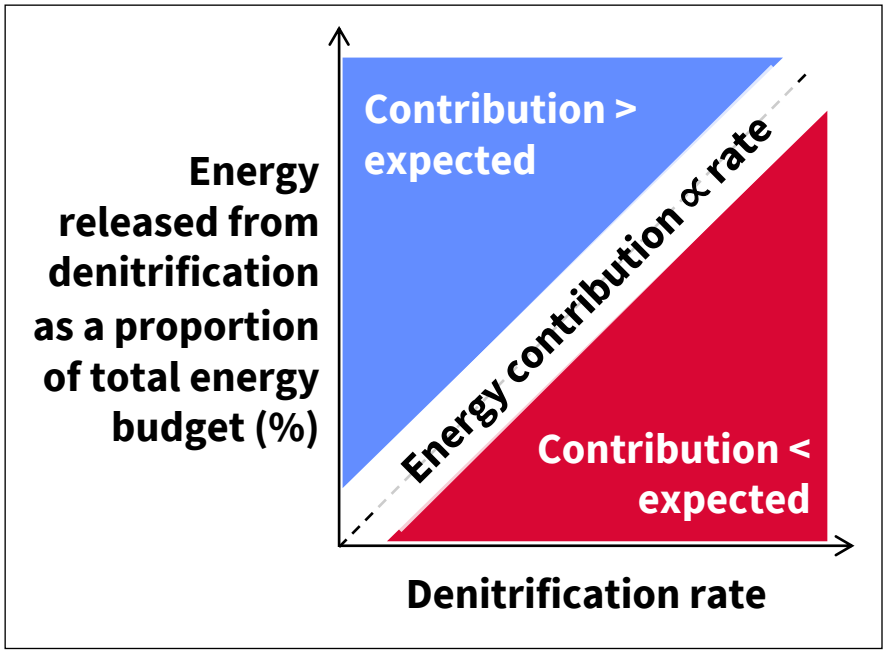
Denitrification as a proportion of total energy



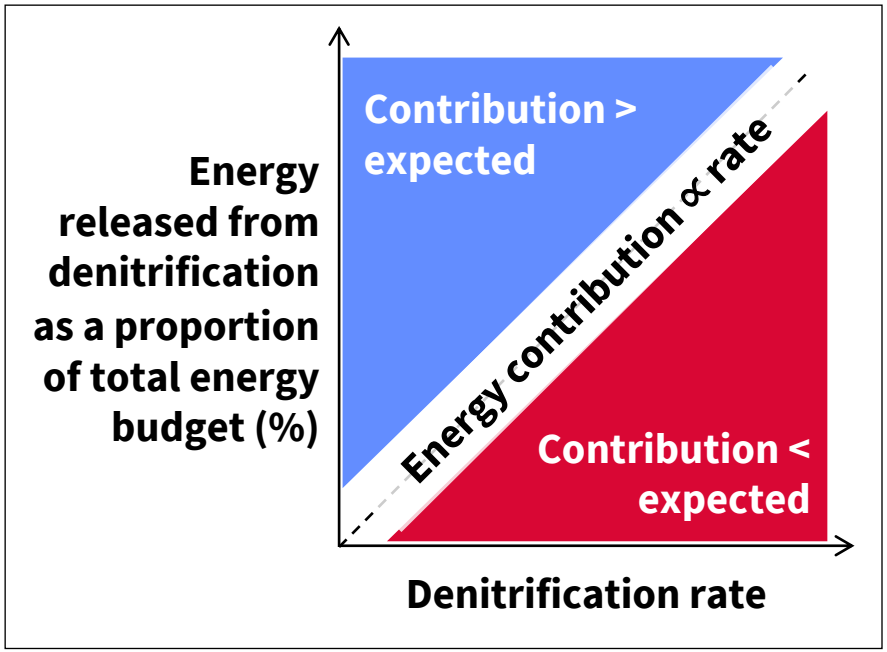
Denitrification as a proportion of total energy

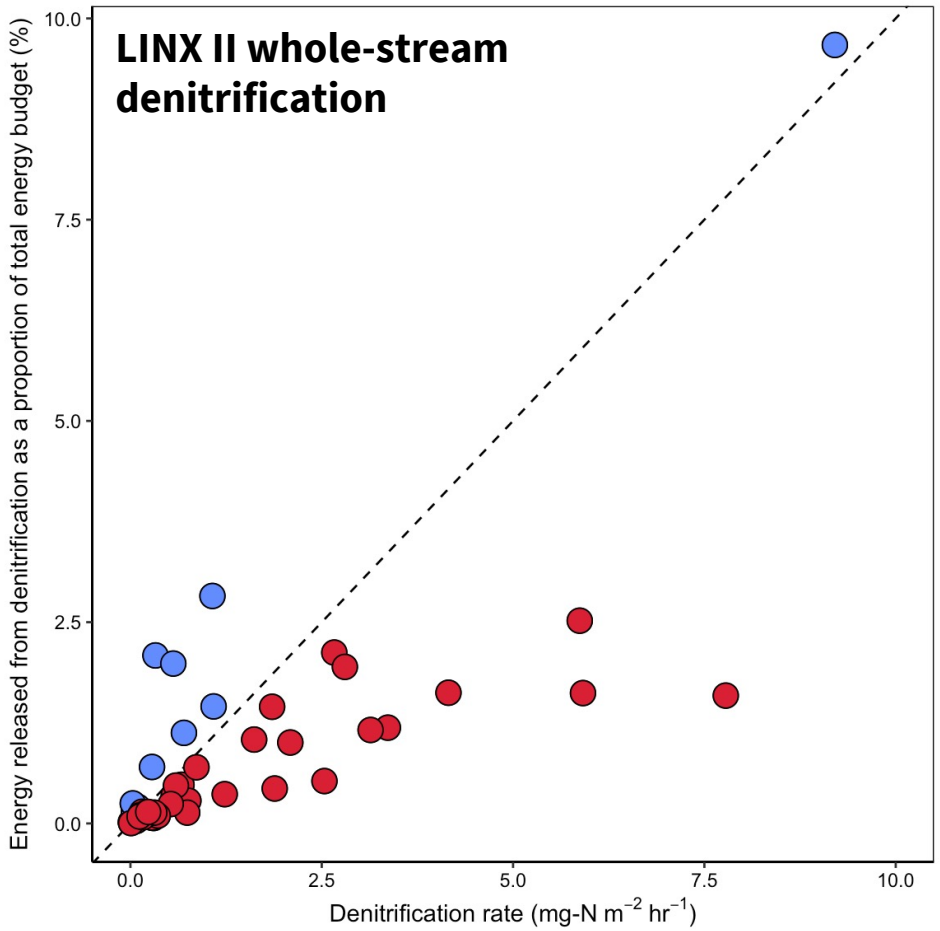


Denitrification as a proportion of total energy

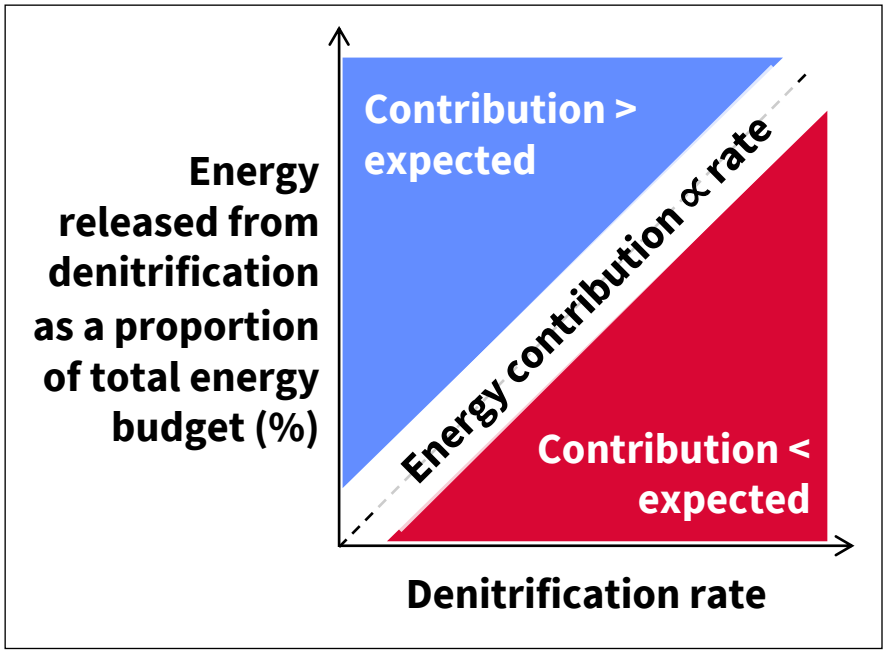


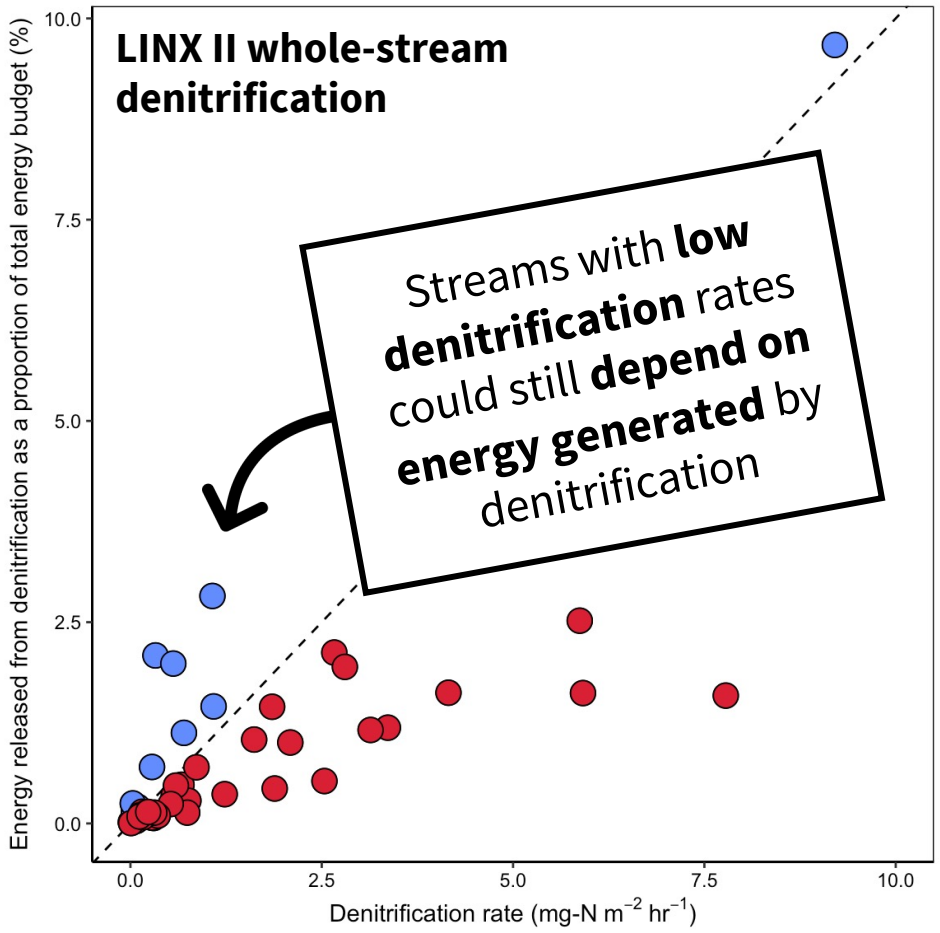
Denitrification as a proportion of total energy





Denitrification as a proportion of total energy



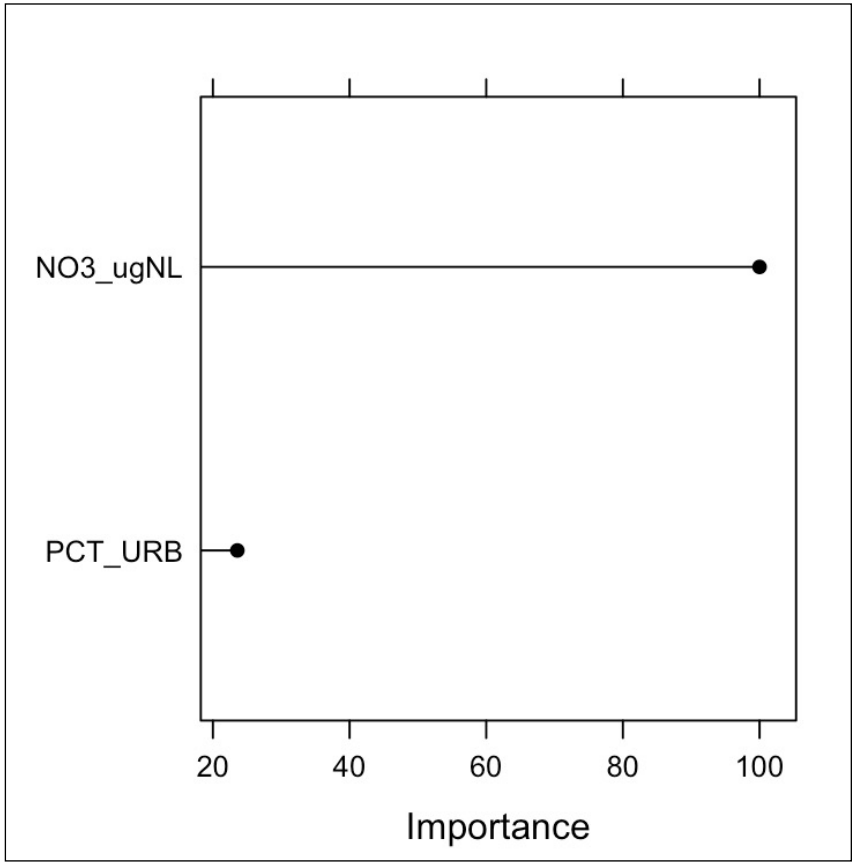


Predictive modeling results

LINX II dataset

Response: energy released from denitrification as a proportion of total energy (%)

Model	RMSE on testing set
Partial least squares (PLS)	0.548
Elastic net	0.423
Neural net	0.526
MARS	**0.394**
SVM	0.5347
KNN	0.5304
Random forest	0.4799
Boosted tree	0.54749



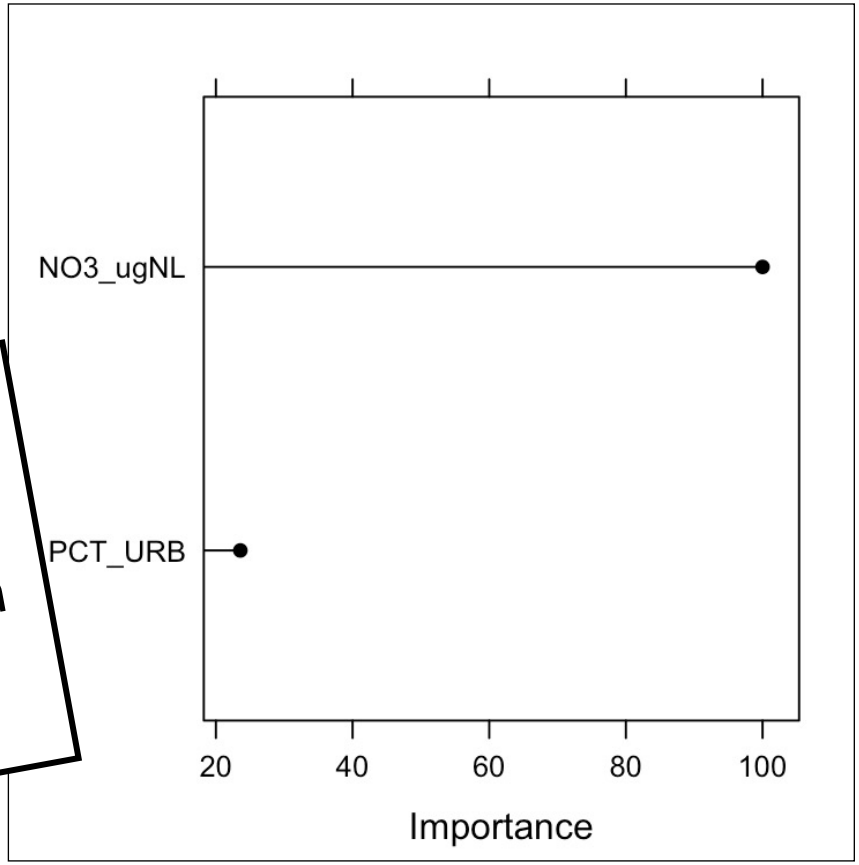
Predictive modeling results

LINX II dataset

Response: energy released from denitrification as a proportion of total energy (%)

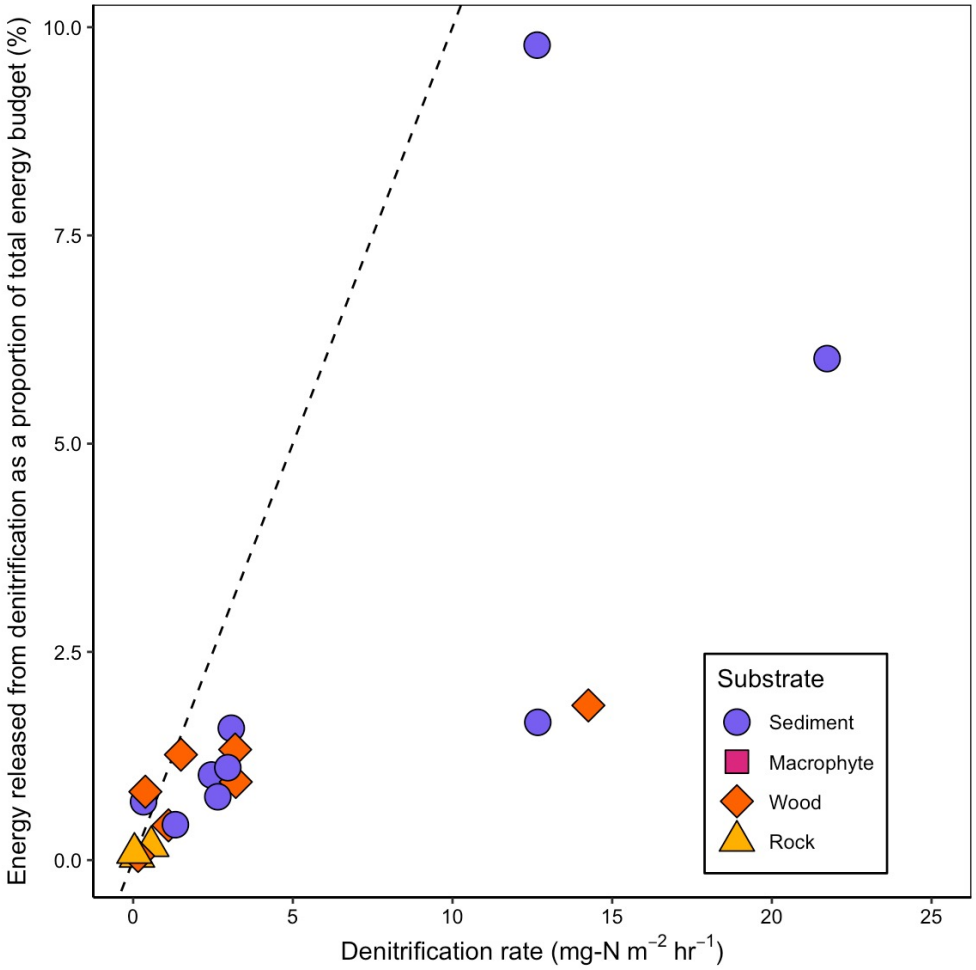
Model	RMSE on testing set
Partial least squares (PLS)	0.548
Elastic net	0.423
Neural net	0.526
MARS	**0.394**
SVM	0.5347
KNN	
Random fo	
Boosted tre	

[Nitrate] important factor in **controlling energy** production from **denitrification**



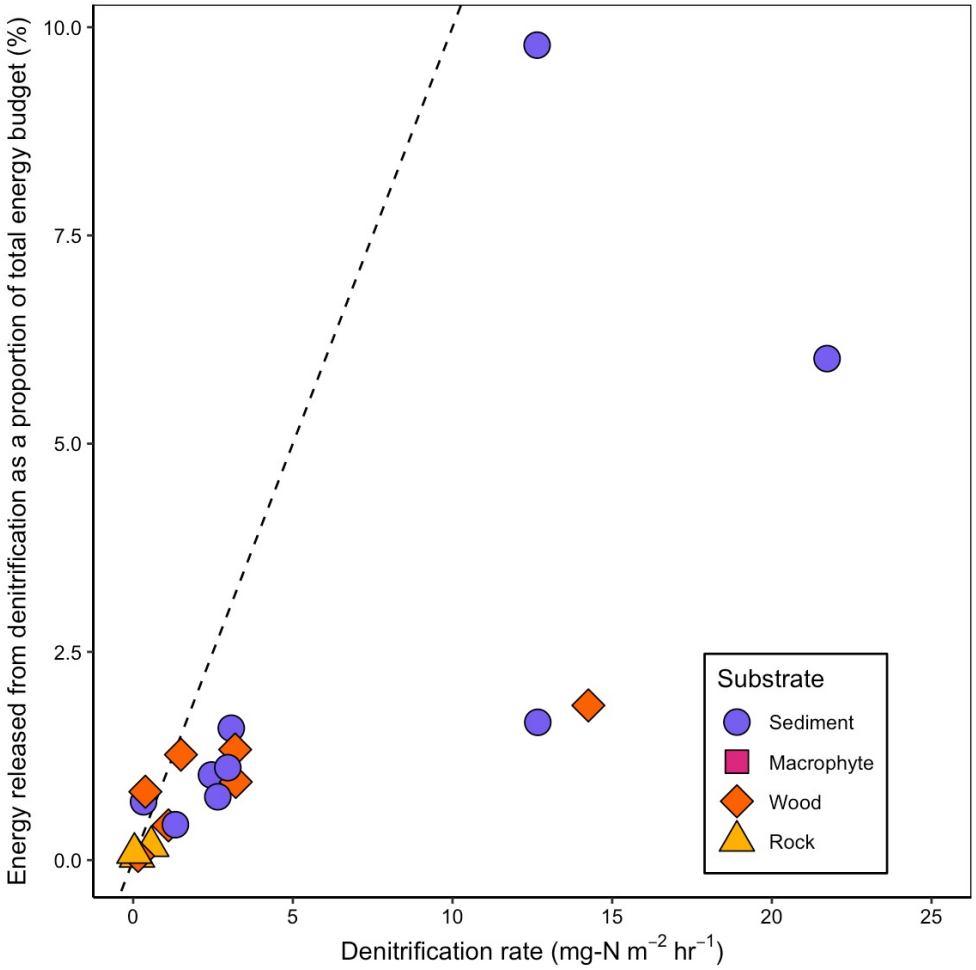
Denitrification as a proportion of total energy: Substrate breakdown

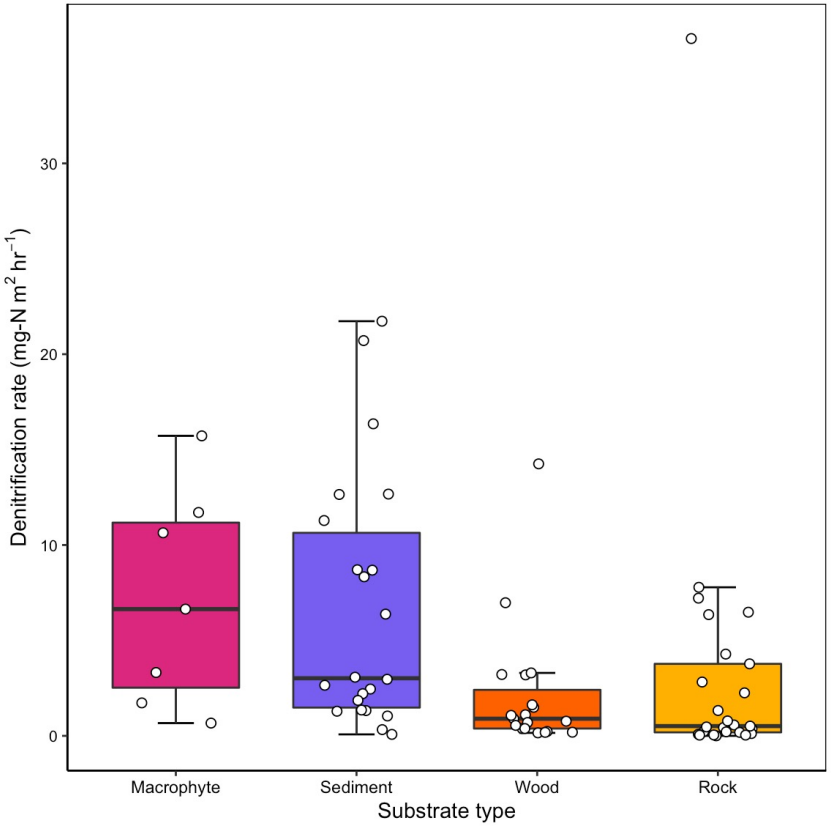
Marcarelli Nationwide chamber denitrification



Denitrification as a proportion of total energy: Substrate breakdown

Marcarelli Nationwide chamber denitrification

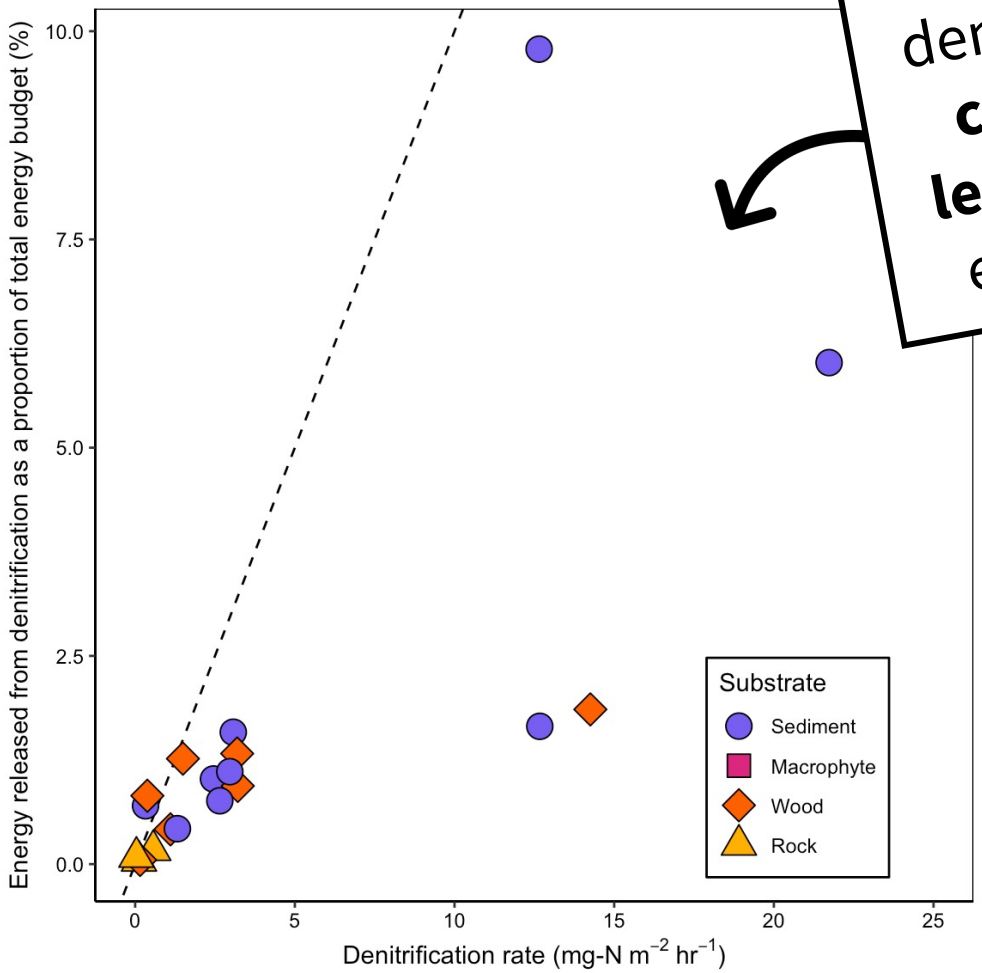


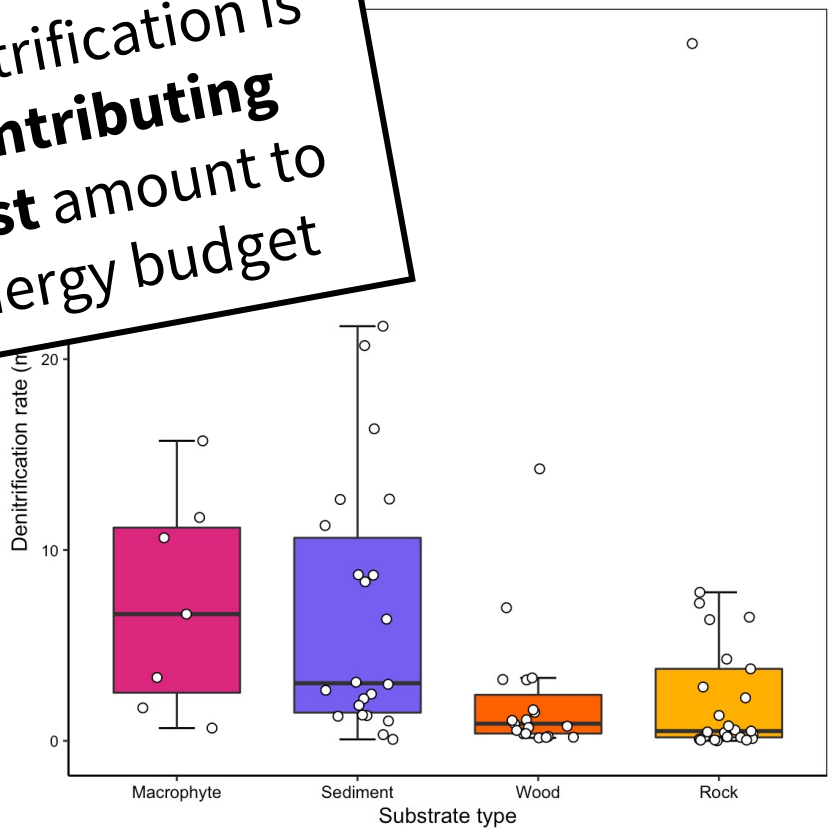


Denitrification as a proportion of total energy: Substrate br

Substrate with highest rates of denitrification is **contributing least** amount to energy budget

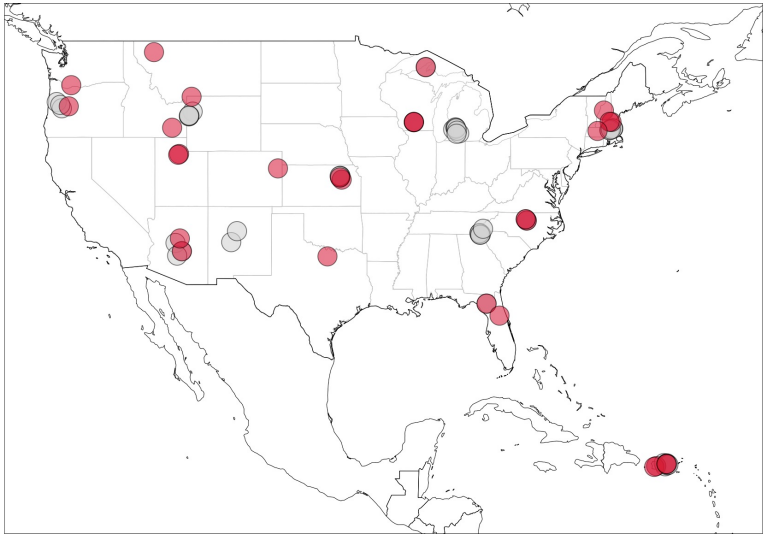
Marcarelli Nationwide chamber denitrificat





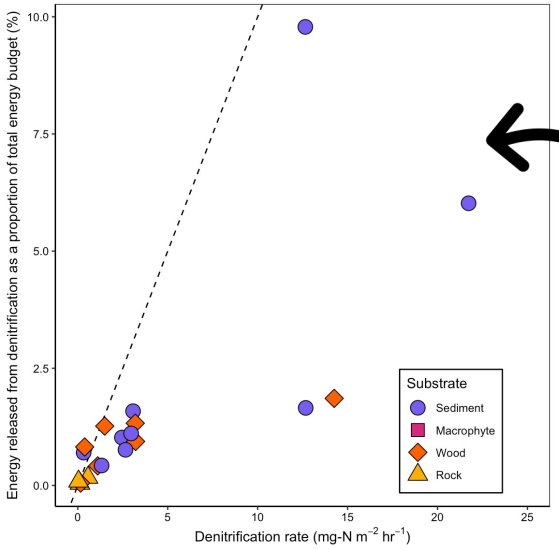
Further directions

1. **Remaining metabolism modeling** for Marcarelli Nationwide Survey **(n = 24)**



2. **Scaling** chamber rates to **whole-stream estimates** at NEON sites (n = 14) using **NEON stream morphology data products**

3. **Exploring** factors that impact the **energy production from denitrification** in each **substrate**



What's happening here?

Acknowledgements

Marcarelli Nationwide Denitrification and N_2 Fixation Survey

We thank C. Allison, A. Copley, J. Cornell, E. Coscarelli, A. Eckersell, H. Harris, D. Larson, J. Ortiz, J. Paris, H. Roose, R. Schipper, and R. Van Goethem for field and laboratory assistance. This research was funded by the National Science Foundation Grant DEB 14-51919 to Amy M. Marcarelli.

Lotic Intersite Nitrogen eXperiment II (LINX-II)

Funding for the LINX-II project was provided by the National Science Foundation Division of Environmental Biology (NSF Grant DEB-0111410).

StreamPULSE Network

Data sets were provided by the StreamPULSE Network, with funding provided by the National Science Foundation Macrosystems program (NSF Grant EF-1442439).

National Ecological Observatory Network (NEON)

We especially thank Kaelin Cawley, Keli Goodman, and Bobby Hensley for their assistance with metabolism modeling efforts. NEON is sponsored by the National Science Foundation and operated under cooperative agreement by Battelle Memorial Institute. This material is based in part upon work supported by the National Science Foundation through the NEON Program.

@michelleckelly_

mckelly1@mtu.edu

https://github.com/michelleckelly

mimsy R package:
Calculate MIMS dissolved gas concentrations without getting a headache.