

Relating biomolecular data to denitrification rates in infiltrating river water

Insights from enzyme-based reactive transport modelling

Anna Störiko¹ ✉, Holger Pagel², Adrian Mellage¹, Olaf A. Cirpka¹

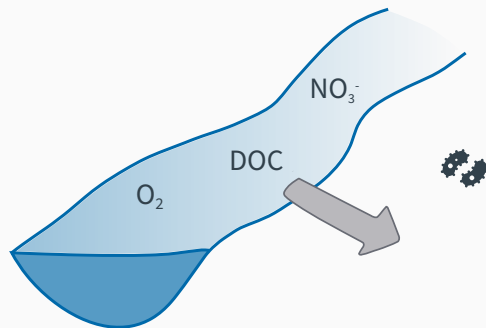
¹Center for Applied Geoscience, University of Tübingen, Germany ²Institute of Soil Science and Land Evaluation, University of Hohenheim, Germany



Motivation



Research
questions



transcripts

enzymes

denitrification rates

Implications for
measurements



Relationship between
transcripts or enzymes
and rates



Simulation scenario



$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} = r$$

Model set-up



Spatio-temporal patterns



Click for details



Nitrogen cycling by microbial processes modulates the water quality in rivers and groundwater.



Quantitative biomolecular data (abundances of functional genes, transcripts and enzymes) have been suggested to provide information about nitrogen cycling processes.

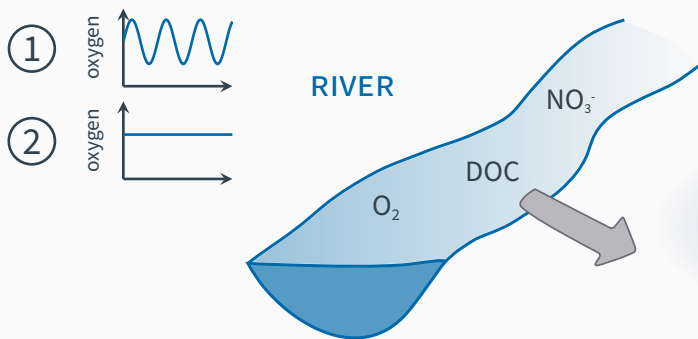


The quantitative interpretation of these novel data types and their relationship with reaction rates need further validation.

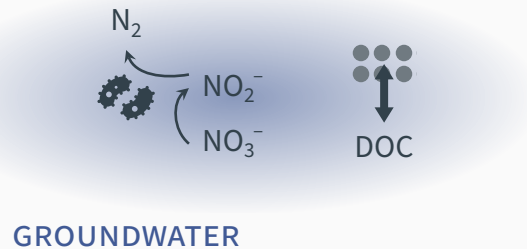
- How do biomolecular quantities respond to dynamic redox conditions in groundwater?
- How do these quantities relate to reaction rates?
- What should be considered when measuring biomolecular variables to obtain information about reaction rates?

APPROACH We use a transcript- and enzyme-explicit reactive transport model to address these questions at the example of the river-groundwater-interface.

Oxygen concentrations in the river water are subject to diurnal fluctuations (scenario 1) or constant (scenario 2).



Oxygen and nitrate serve as electron acceptors for the oxidation of organic carbon from the river water and aquifer matrix.



Oxic river water with high nitrate concentrations infiltrates groundwater.

- Denitrification is described by an enzyme-explicit model formulation.
- Simulated functional enzyme concentrations directly influence denitrification rates.
- Reactions are coupled to the 1-D advection-dispersion equation with a finite volume approach.

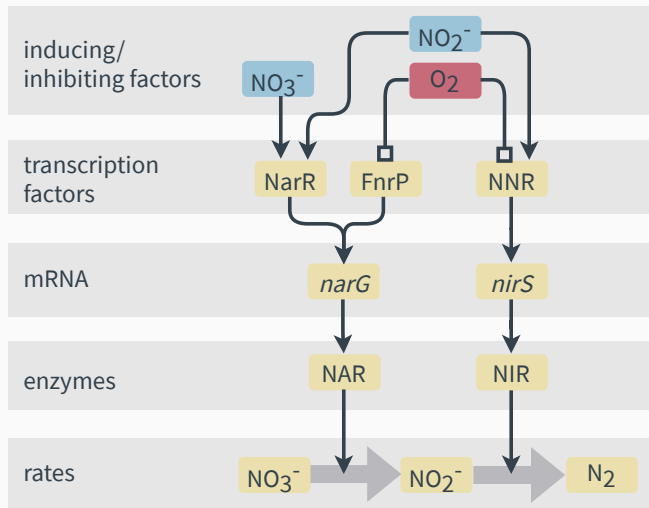


Figure 1: Scheme of the enzyme-explicit reaction model (Störiko et al., in press).

- Periodic oxygen fluctuations propagate into the domain.
→ Zone of active denitrification shifts back and forth (panel A and D).
- Strong daily fluctuations in functional-gene transcript concentrations (panel B).
- Functional-enzyme and biomass concentrations are stable over time (panel C and E).

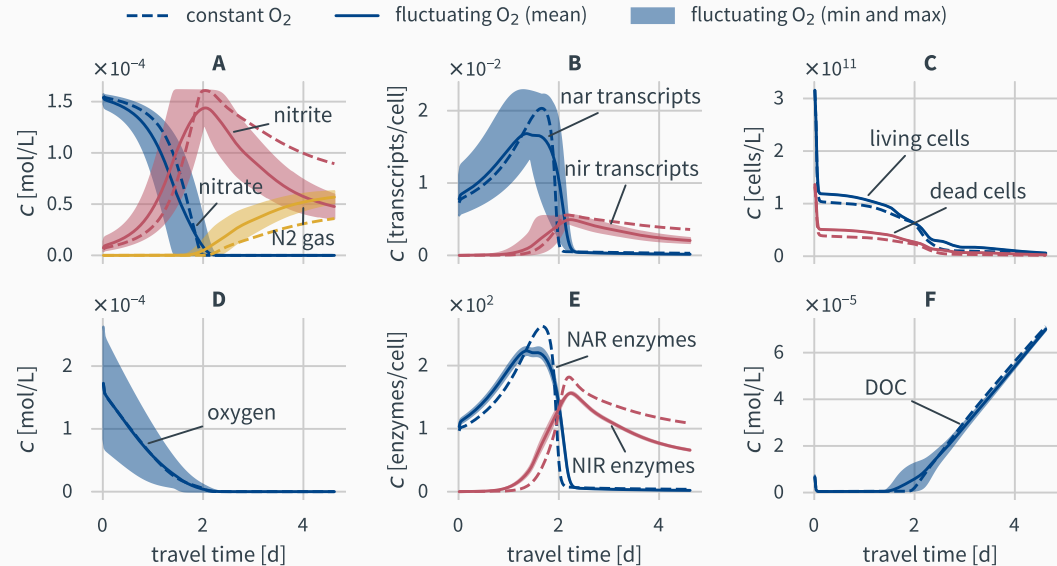


Figure 2: Spatial concentration distributions in the two scenarios, aggregated over time in the fluctuating case.

- Diurnal fluctuations of the denitrification rates and transcript concentrations are hysteretic.
- A single measurement of functional-gene transcripts at one time point poorly predicts reaction rates.

Often, we are more interested in average reaction rates—how do they relate to transcript and enzyme concentrations?

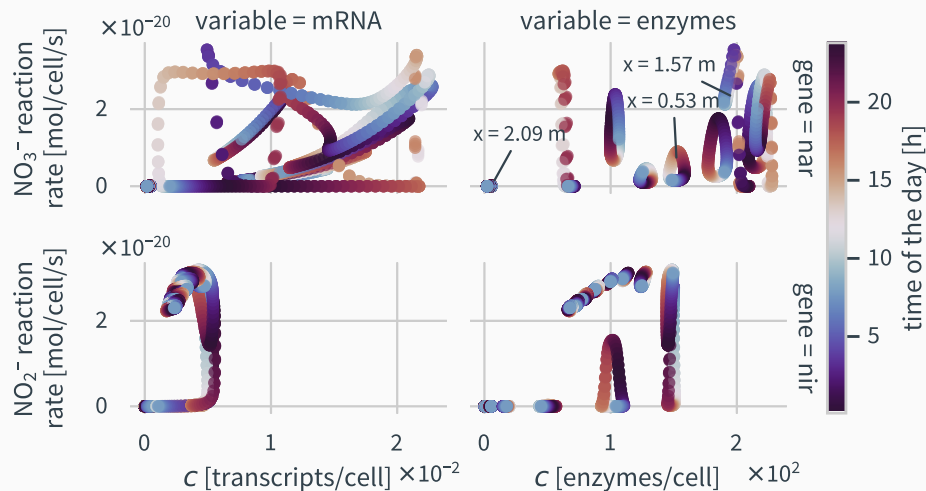


Figure 3: Relationship of concentrations and rates over time (indicated by color) and space (several loops).

- Daily averages of transcript or enzyme concentrations and denitrification rates show a clear relationship that is similar for transcripts and enzymes.
- However, the relationship is highly non-linear and non-unique because denitrification rates are not only limited by gene expression (enzyme concentrations) but also by substrate availability and oxygen inhibition.

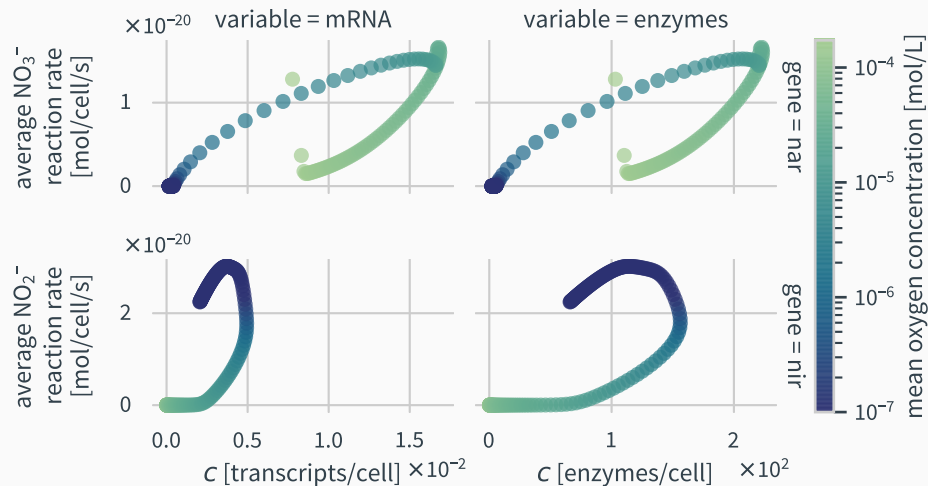


Figure 4: Relationship of average concentrations and average reaction rates over space (several dots).



- ⌚ Different time scales of production and decay cause daily fluctuations of transcript, but not enzyme concentrations.
- UU To get a picture of the transcriptome regardless, measurements at several time points (averages, time series) are necessary.
- ⊗ Functional-gene transcripts and enzymes cannot uniquely predict reaction rates—even when the system is at steady state. → A linear correlation approach is too simple.

- ✎ Störiko, A., Pagel, H., Mellage, A., & Cirpka, O. A. (2021, March 19). *Nitrogene: Modelling code and data of an enzyme-based denitrification model* (Version 0.0.2).
<https://doi.org/10.5281/zenodo.4620167>
- 📄 Störiko, A., Pagel, H., Mellage, A., & Cirpka, O. A. (in press). Does it pay off to explicitly link functional gene expression to denitrification rates in reaction models? *Frontiers in Microbiology*, 12. <https://doi.org/10.3389/fmicb.2021.684146>



 Anna Störiko, M.Sc. 

 Center for Applied Geoscience,
University of Tübingen, Germany

 anna.stoeriko@uni-tuebingen.de

 Comments are also welcome *here*.



EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



CRC 1253

CATCHMENTS AS REACTORS

CAMPOS

DFG

This work was funded by the German Research Foundation (DFG) within the Research Training Group RTG 1829 “Integrated Hydrosystem Modelling” (DFG grant agreement GRK 1829) and the Collaborative Research Center CRC 1253 “CAMPOS – Catchments as Reactors”, project P7 (DFG grant agreement SFB 1253/1).

 This work © 2021 by Anna Störiko and co-authors is licensed under CC BY 4.0 (except institutional logos).