



Unraveling biogeochemical transformation of organic carbon and nitrogen turnover in groundwater along the hillslope transect

¹Thanh Quynh Duong, ^{2, 4}Anke Hildebrandt, ^{1, 3}Martin Thullner

OSPP voting



- (1) Department of Applied Microbial Ecology, UFZ,
- (2) Department of Computational Hydrosystems, UFZ, Leipzig, Germany
- (3) Federal Institute of Geosciences and Natural Resources (BGR), Hanover, Germany
- (4) Institute of Geoscience, Friedrich Schiller University Jena, Germany

Introduction:

The Earth's Critical Zone: where all of life happens



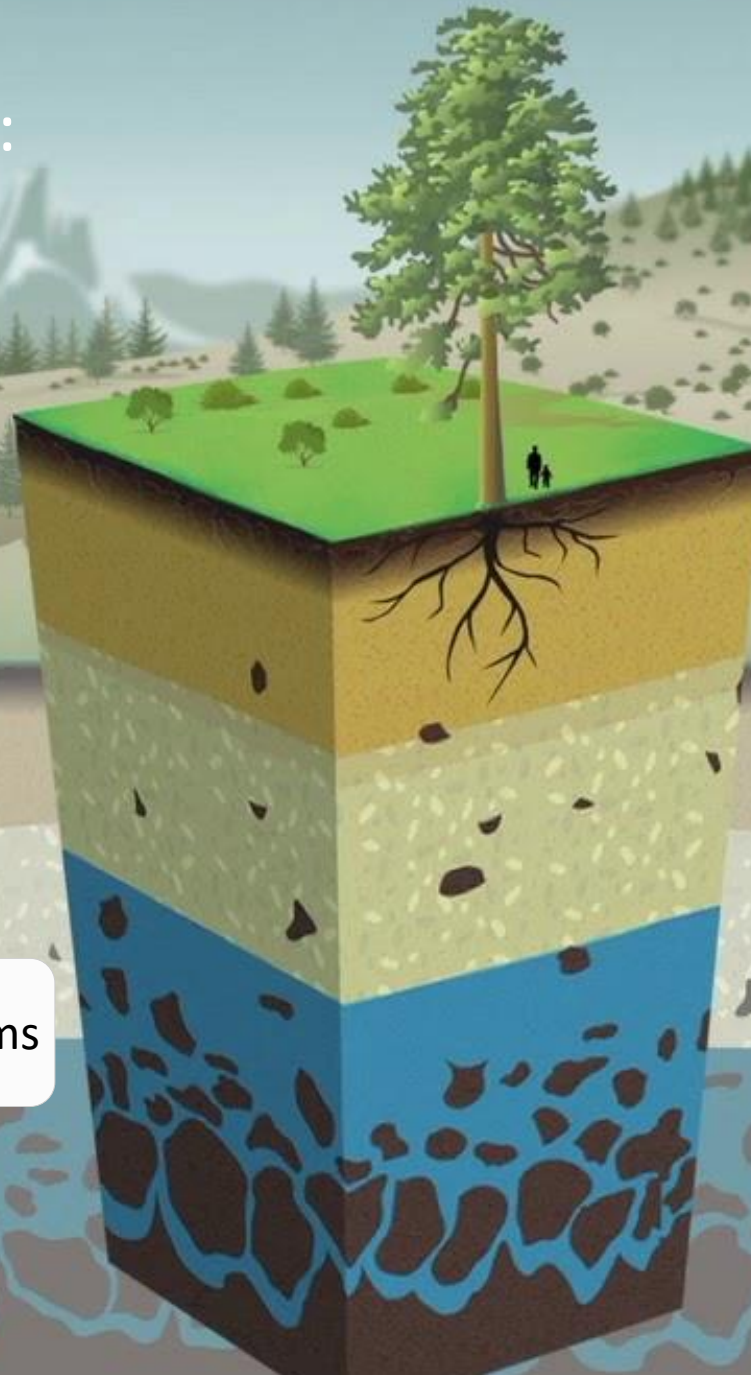
Collaborative research Centre AquaDiva
Understanding the links between Surface and Subsurface Biogeosphere

The Earth's Critical Zone =
earth's thin, heterogeneous,
living, permeable layer

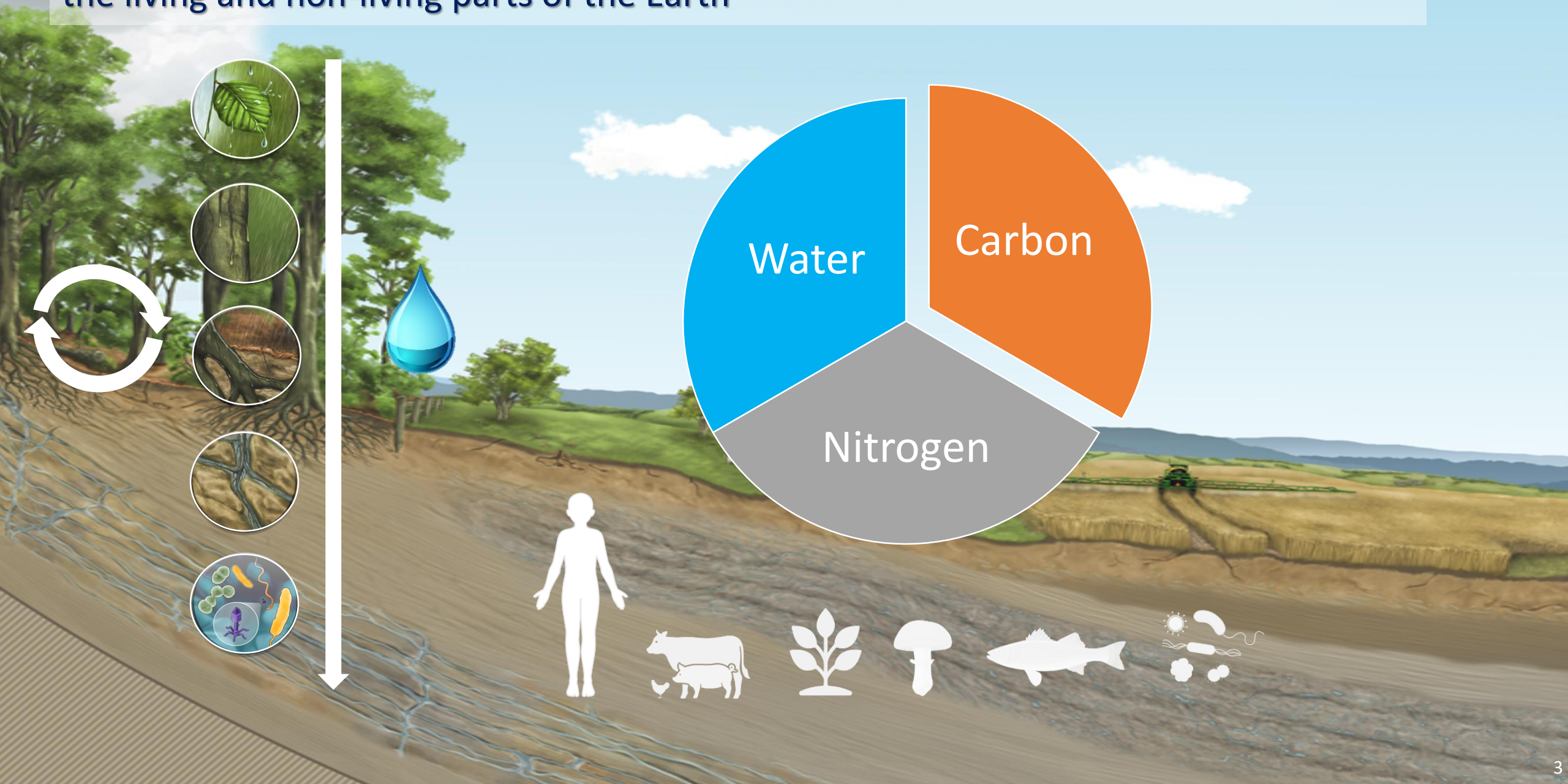
“biogeochemical reactor” transforms water,
gases, and other materials

require a large transdisciplinary team

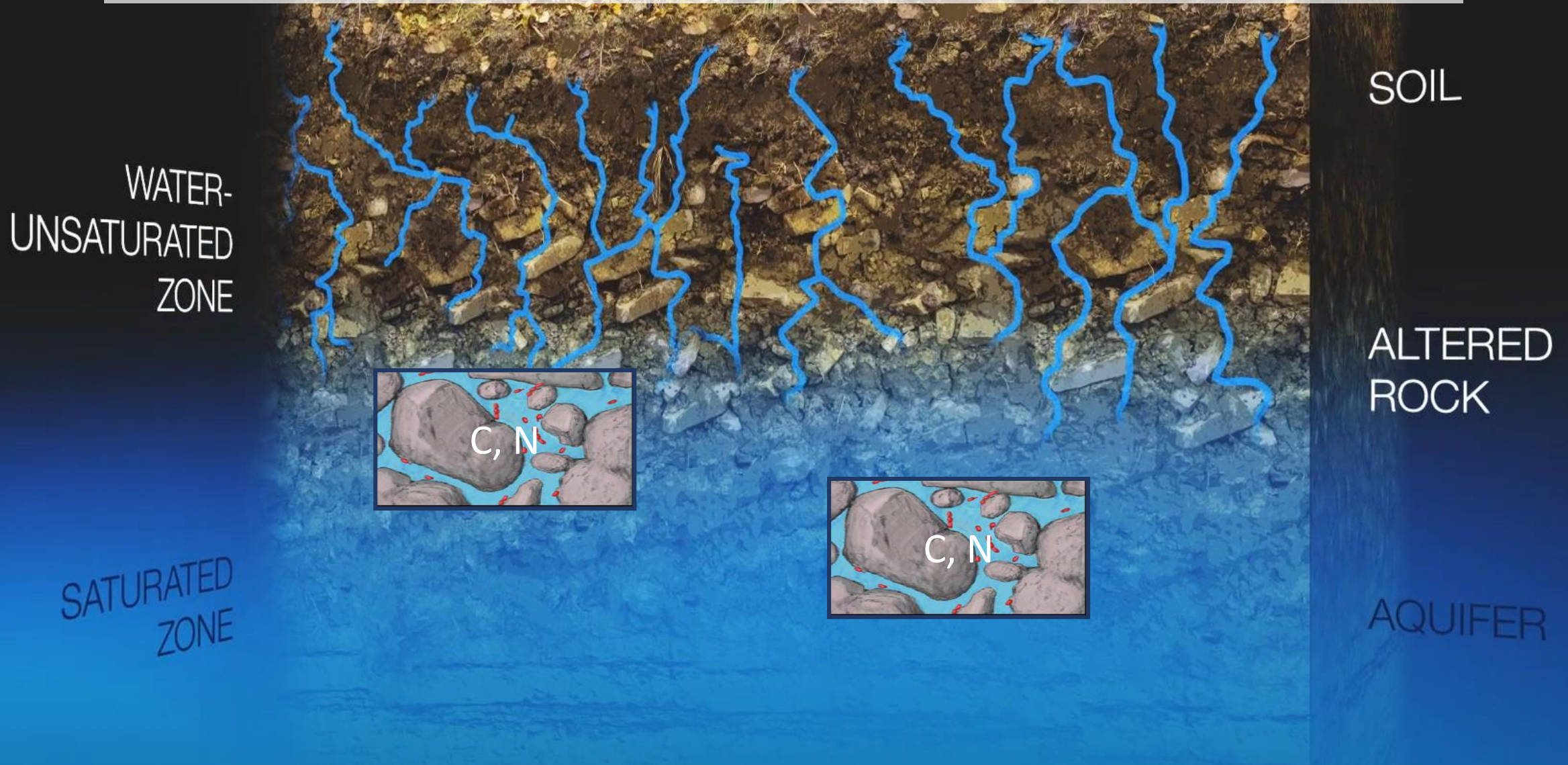
rock, soil, water, air, and living organisms



BIOGEOCHEMICAL CYCLES: cycles of chemical elements and compounds between the living and non-living parts of the Earth

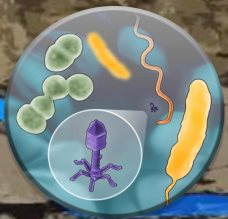
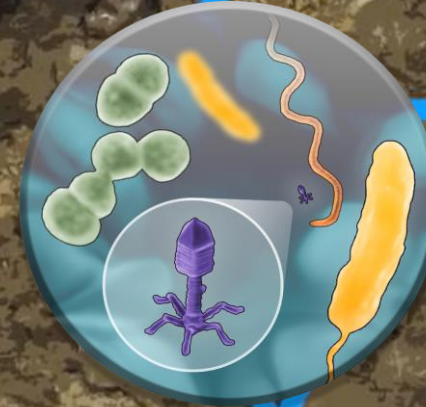


SUBSURFACE IS A BIG STORE OF C & N

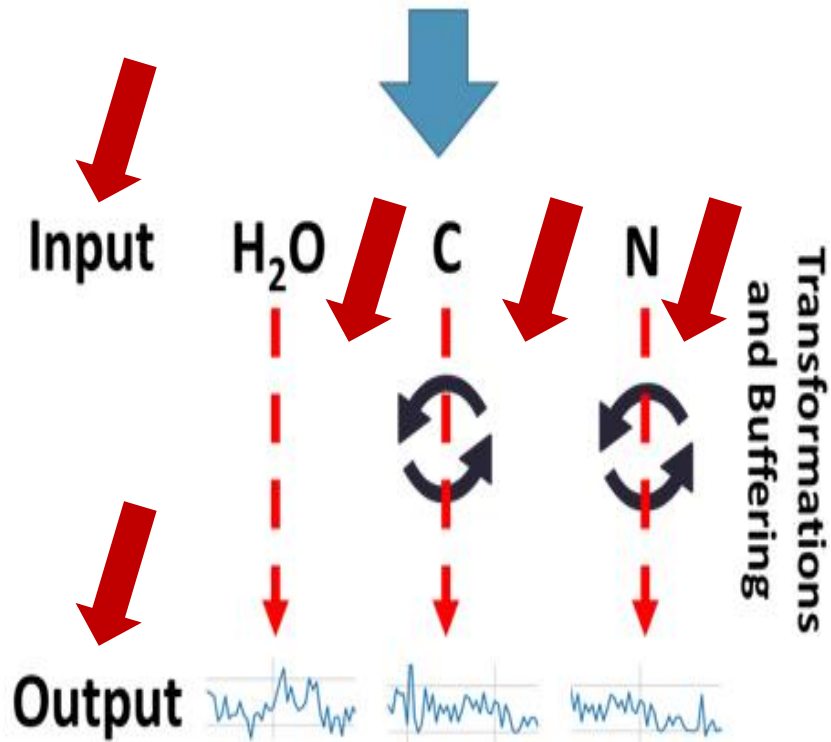
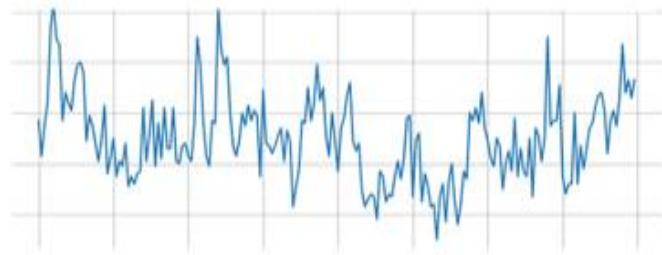
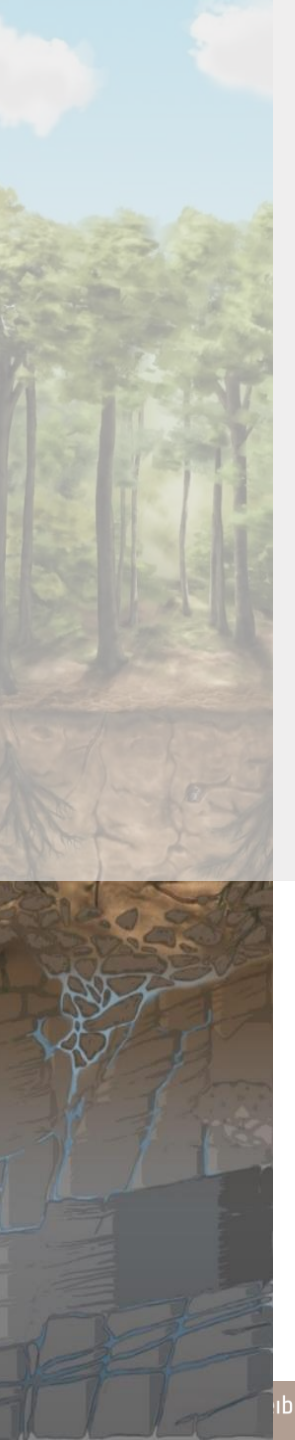


MAIN CHALLENGE: SPATIAL HETEROGENEITY OF THE SUBSURFACE

Transformation of C, N mediated by microbes



C, N, and microbes distribute heterogeneously

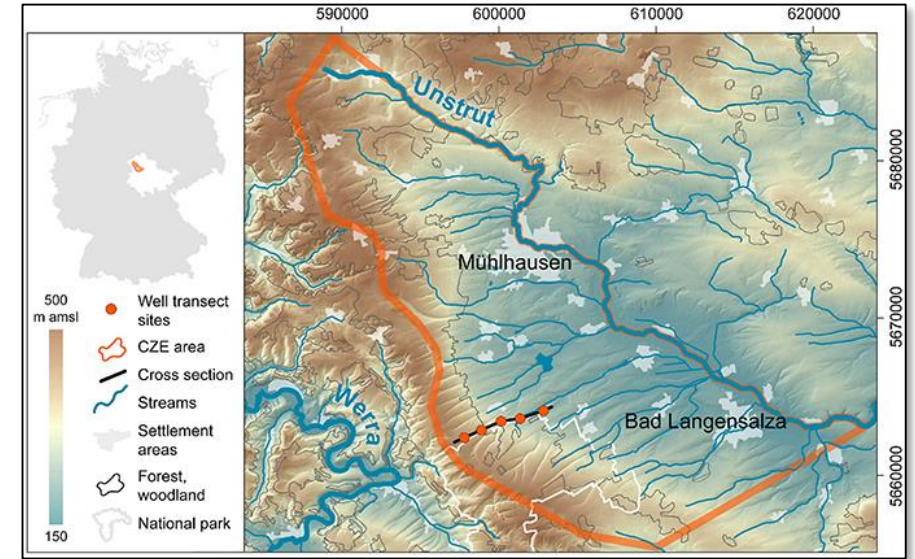


The overarching aim of the modeling

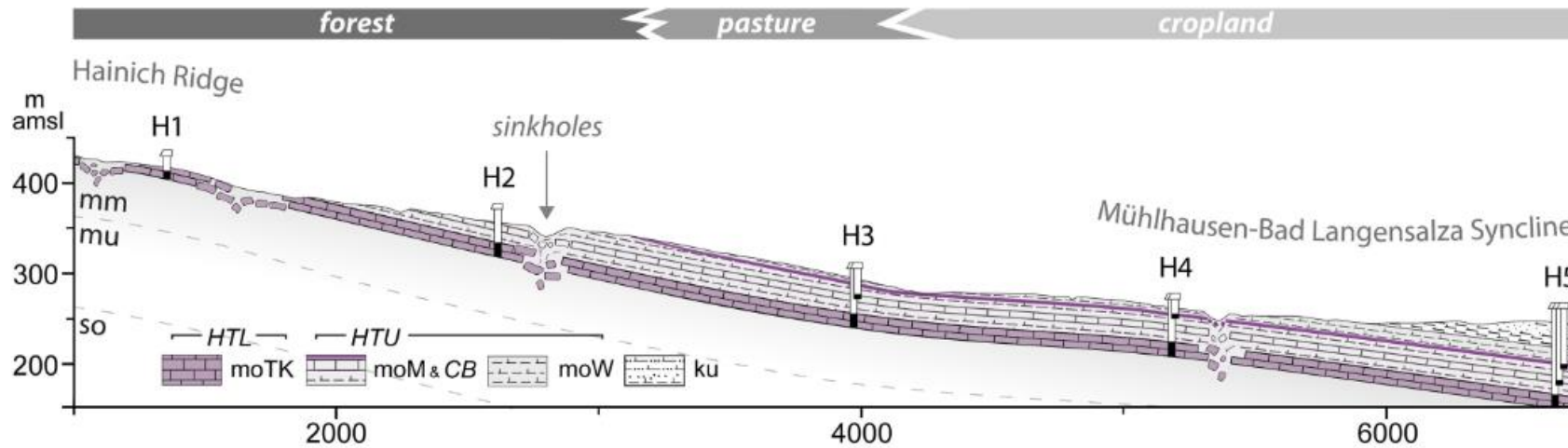
- How deep penetrate signals from the surface?
- What are the long-term effects due to climate and land use change?

STUDY SITE: HAINICH TRANSECT

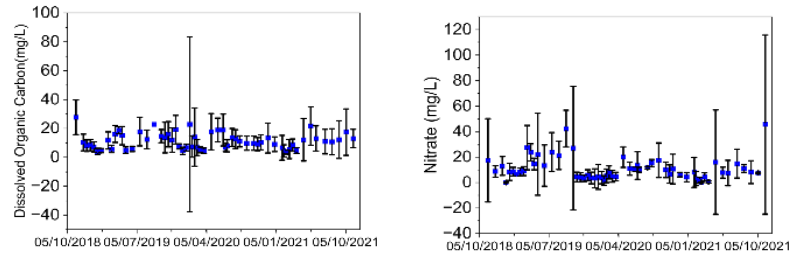
- Located northwest of Thuringia (central Germany) in a hillslope sub-catchment Nängelstedt of river Unstrut (850 km²)
- Hainich CZE: 5.4km long hillslope transect.
- Intensively monitoring of surface and subsurface



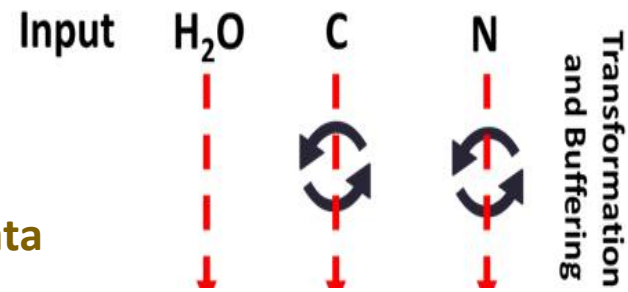
(Kuesel et al., 2016)



DATA MEASUREMENTS

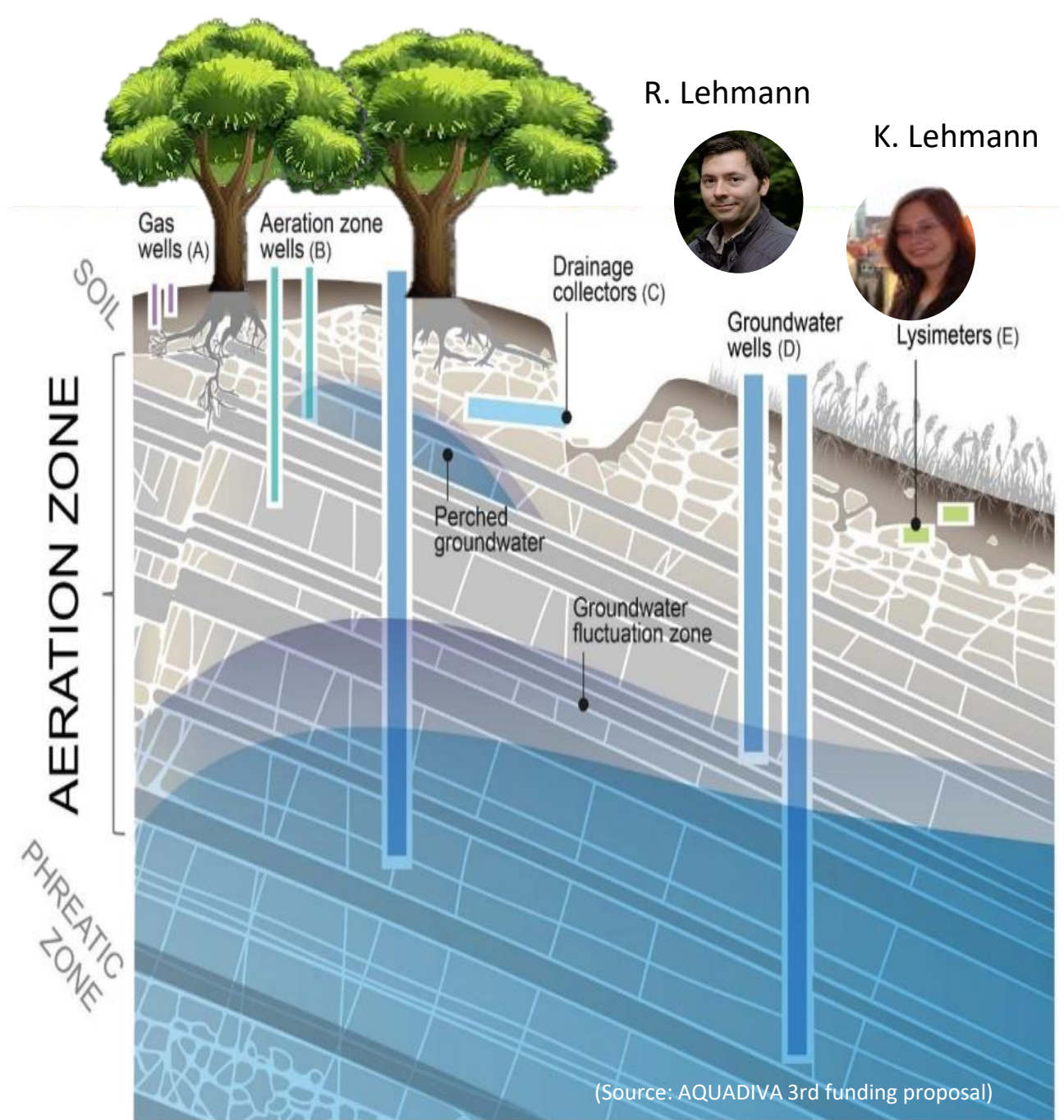
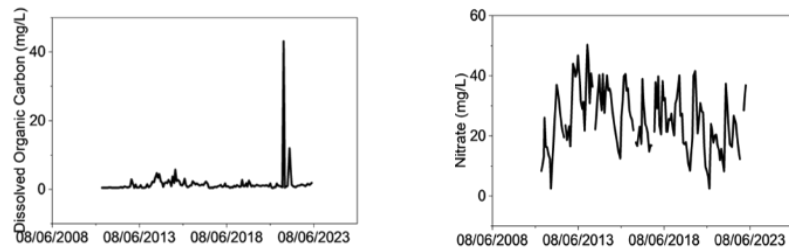


Lysimeter data



Groundwater data

Output



R. Lehmann



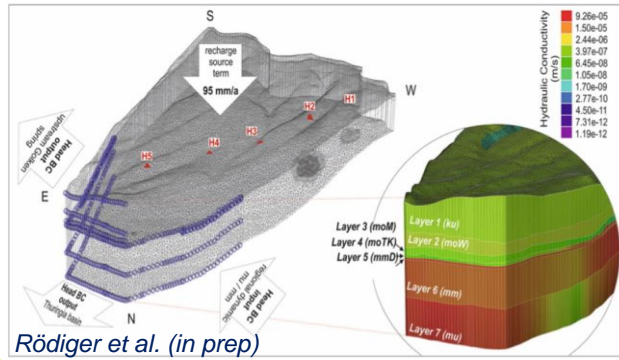
K. Lehmann



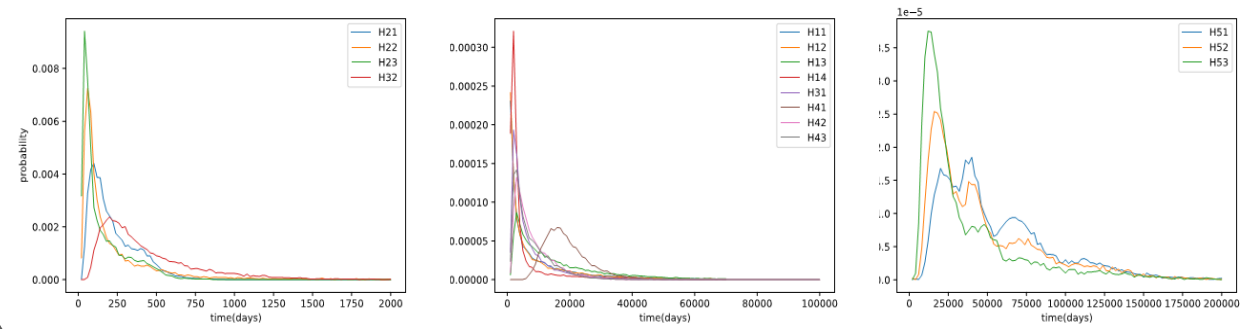
(Source: AQUADIVA 3rd funding proposal)

TRAVEL TIME-BASED MODEL APPROACH

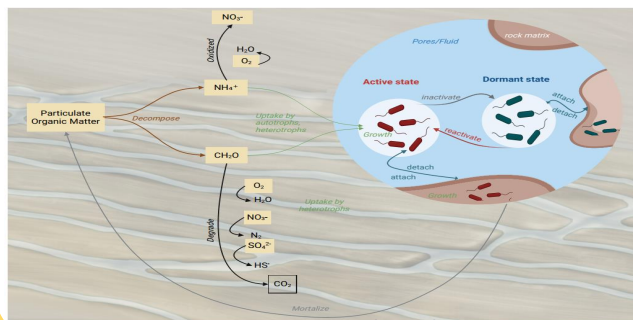
1. Flow model of Hainich CZE



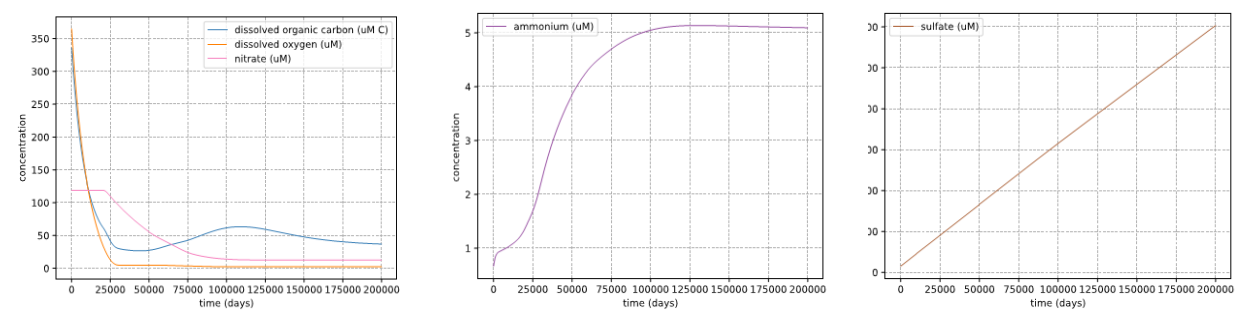
Travel time distribution $p_i(t)$ for well i



2. Schematic of simulated biochemical reaction networks



Simulated concentration $c_j(t)$ of reactive species j along a flow path

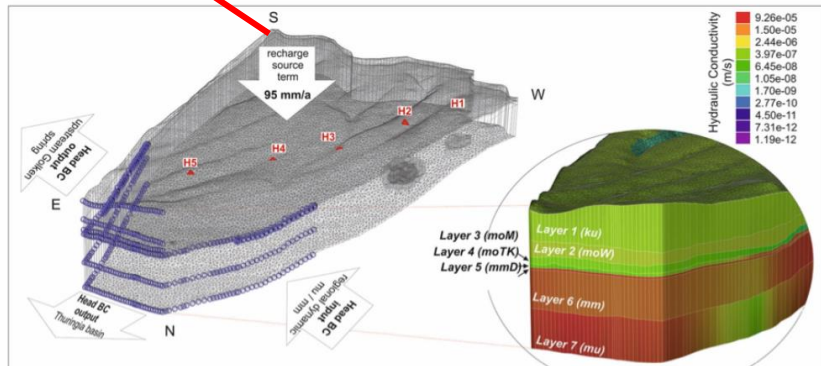
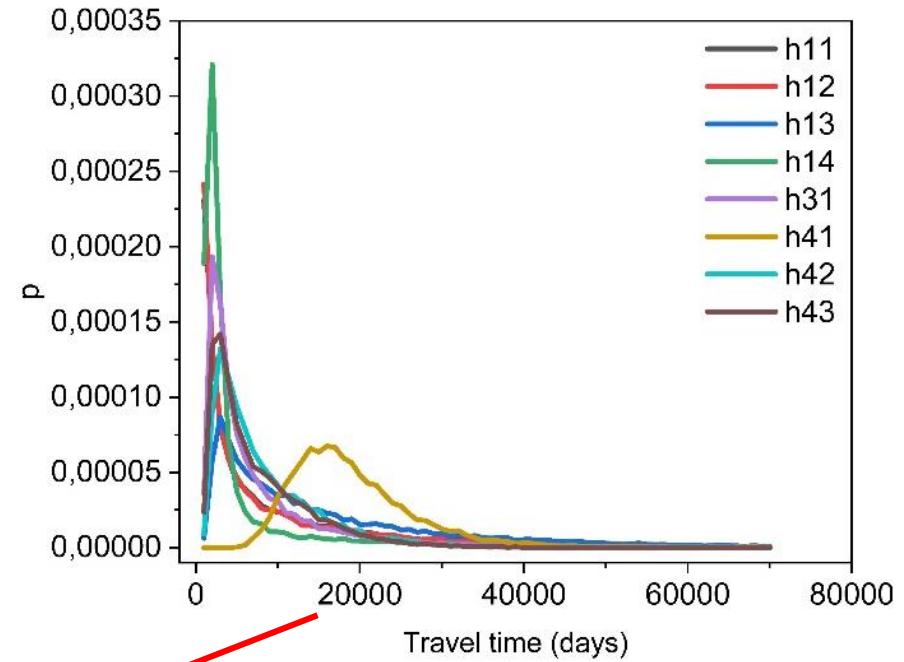
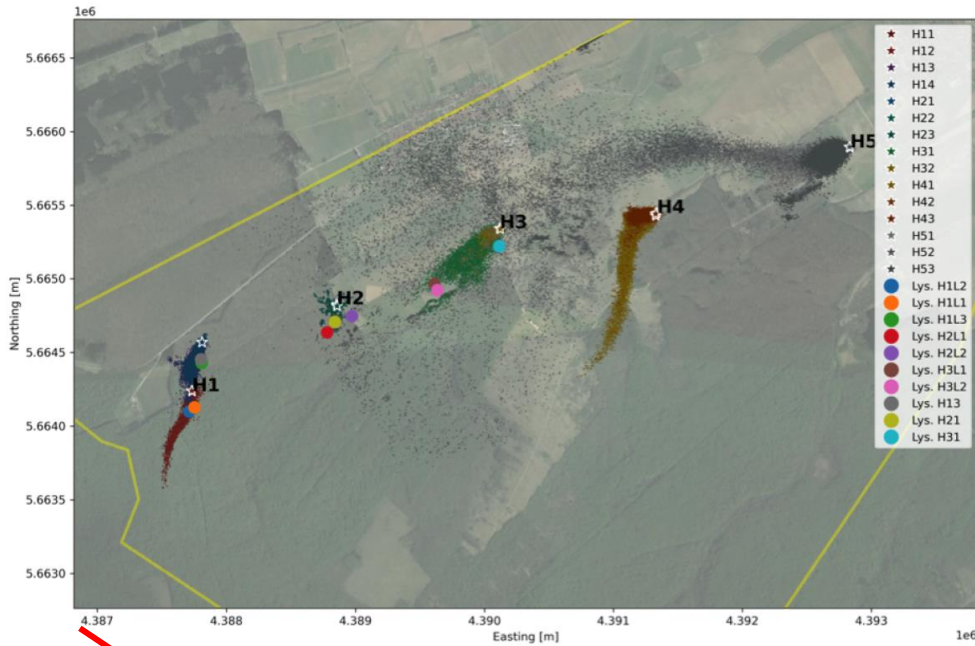


Combine 1st and 2nd components, we have:
3. Simulated concentration of species j at well i

$$c_{i,j} = \int p_i(t) \cdot c_j(t) dt$$

Flow model of Hainich CZE transect

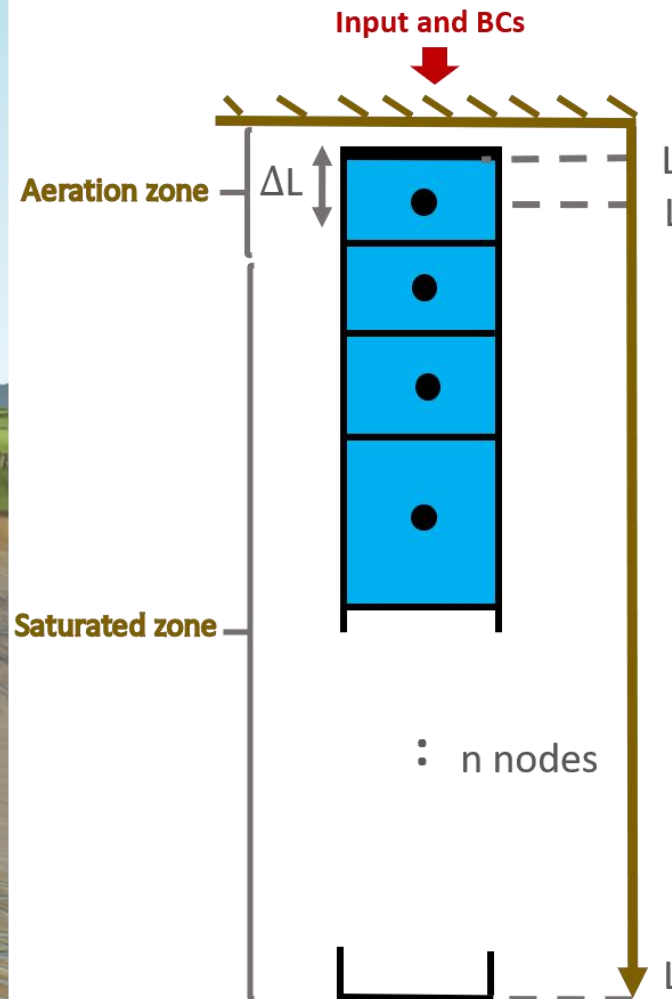
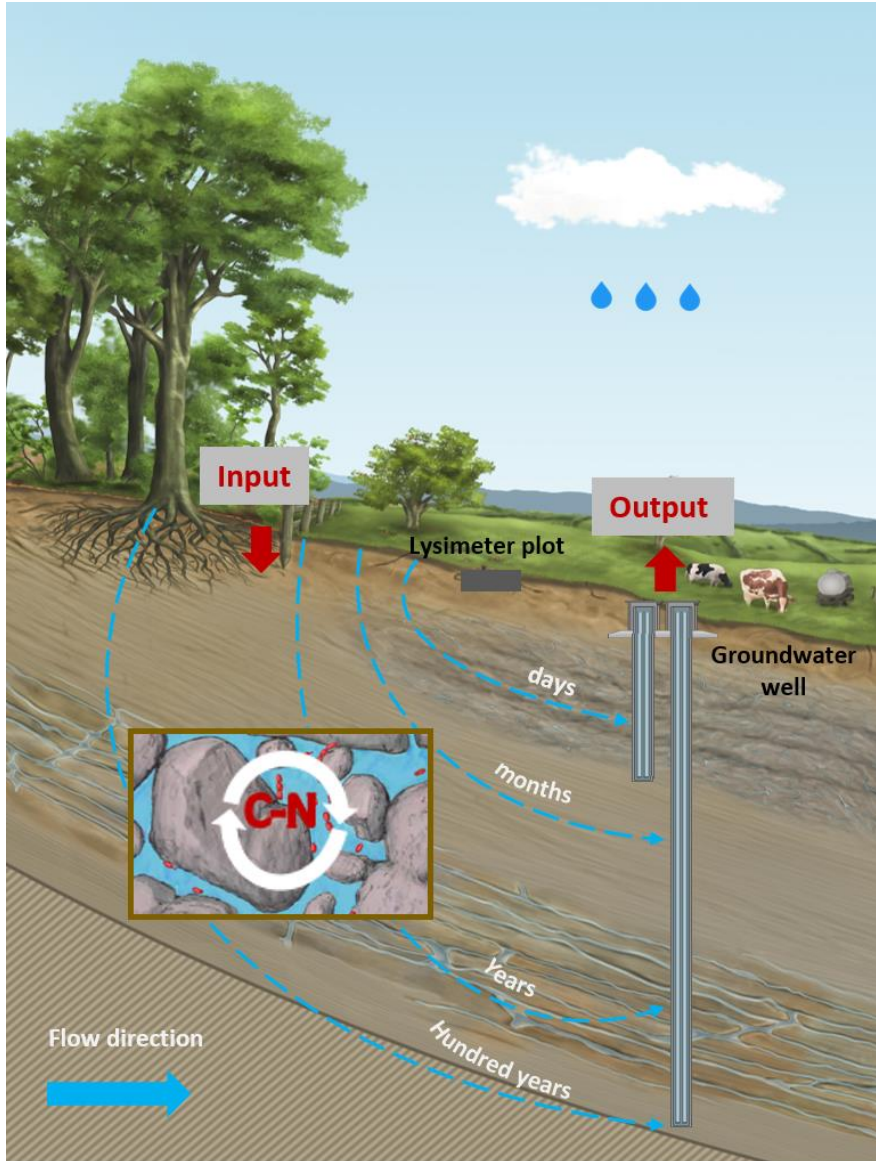
FLOW PATHS AND TRAVEL TIMES TO THE OBSERVATION WELLS



Groundwater flow model

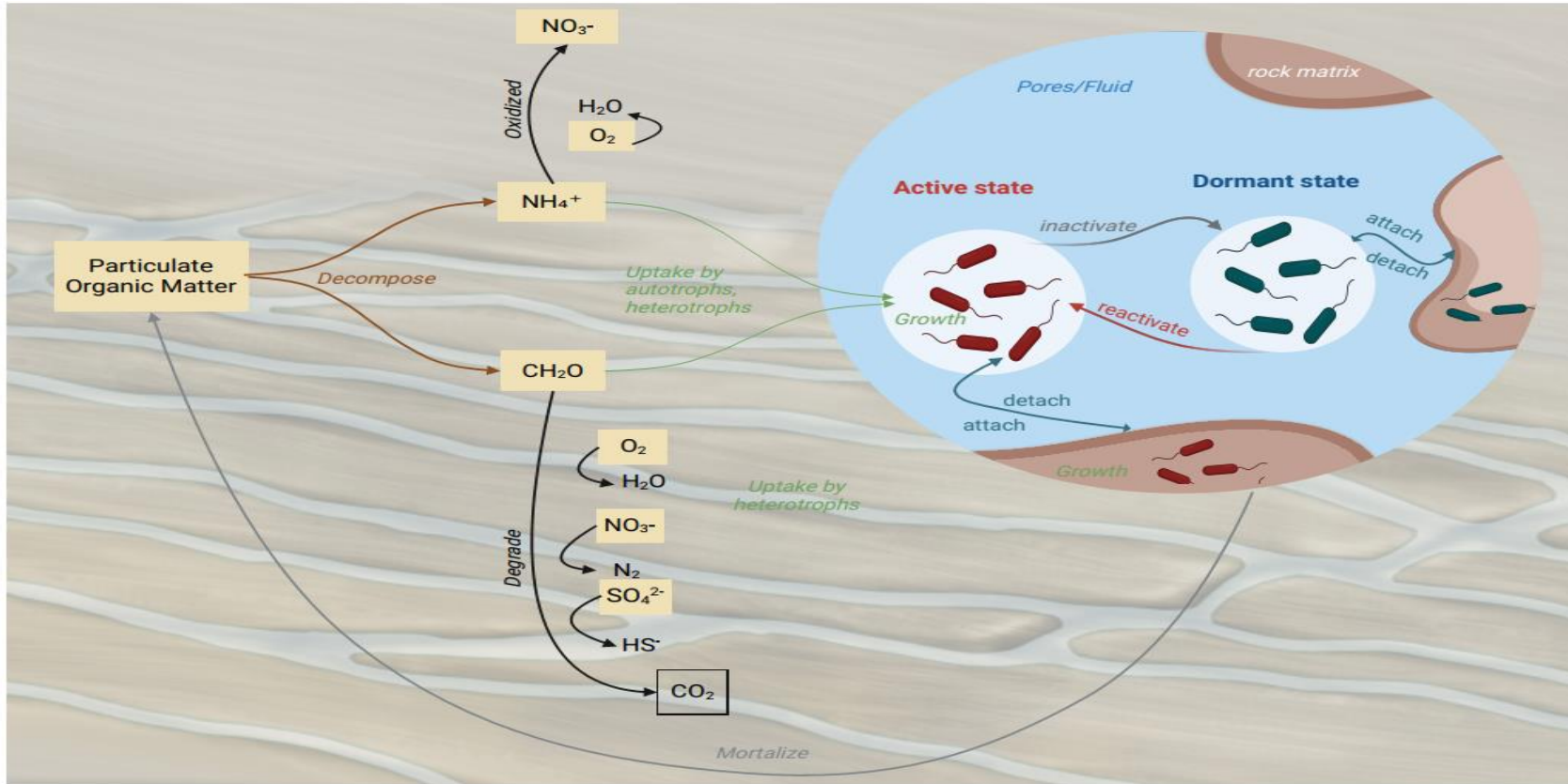
Rödiger, Houben et al. (in prep.)

BIOGEOCHEMICAL PROCESSES ALONG 1D FLOW PATHS



- 1D advective-dispersive-reactive transport
- Upper 50m of profile: aerobic conditions, abundant supply of oxygen
- Numerical mesh grid: non-uniform, with grid sizes ranging from fine to coarse.
- Total length (L) = 20000m
- Total time (t) = 200000 days

BIOCHEMICAL REACTION NETWORK



Chemical compounds:

1. dissolved organic carbon (DOC)
2. Particulate organic carbon (POC)
3. Oxygen (O₂)
4. Nitrate (NO₃)
5. Sulfate (SO₄)
6. Ammonium (NH₄)

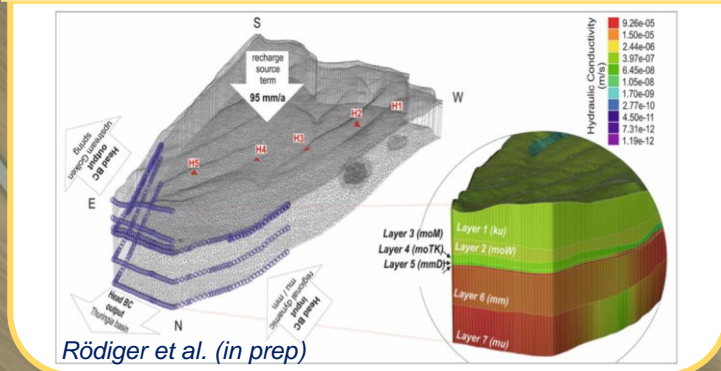
Microbial species:

1. Aerobic DOC degraders (BO2)
2. Nitrate reducers (BNO3)
3. Sulfate reducers (BSO4)
4. Ammonia oxidizers (BNH4)

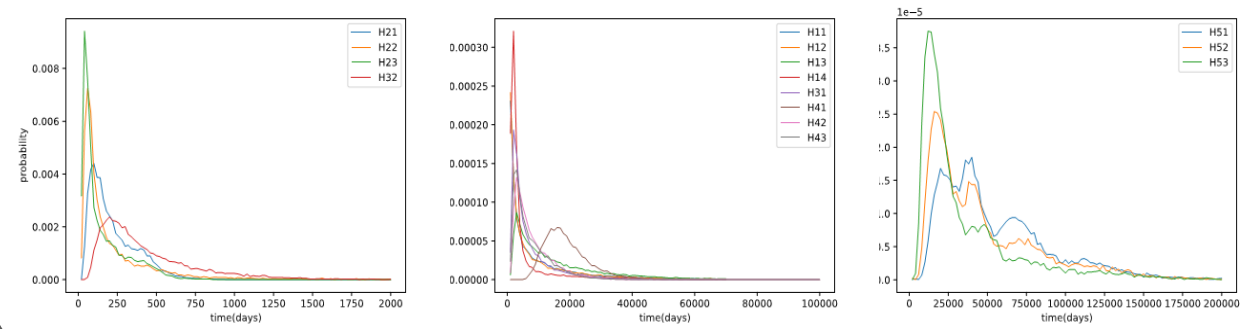
- 23 concentration variables
- 68 microbially driven reactions expressed by modified Monod-type expressions

TRAVEL TIME-BASED MODEL APPROACH

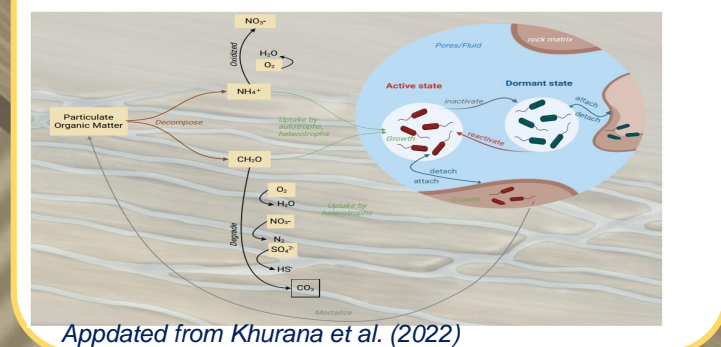
1. Flow model of Hainich CZE



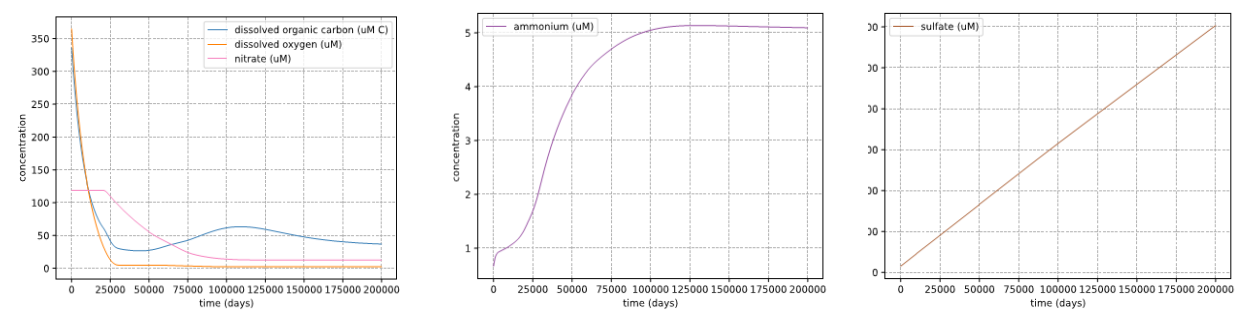
Travel time distribution $p_i(t)$ for well i



2. Schematic of simulated biochemical reaction networks



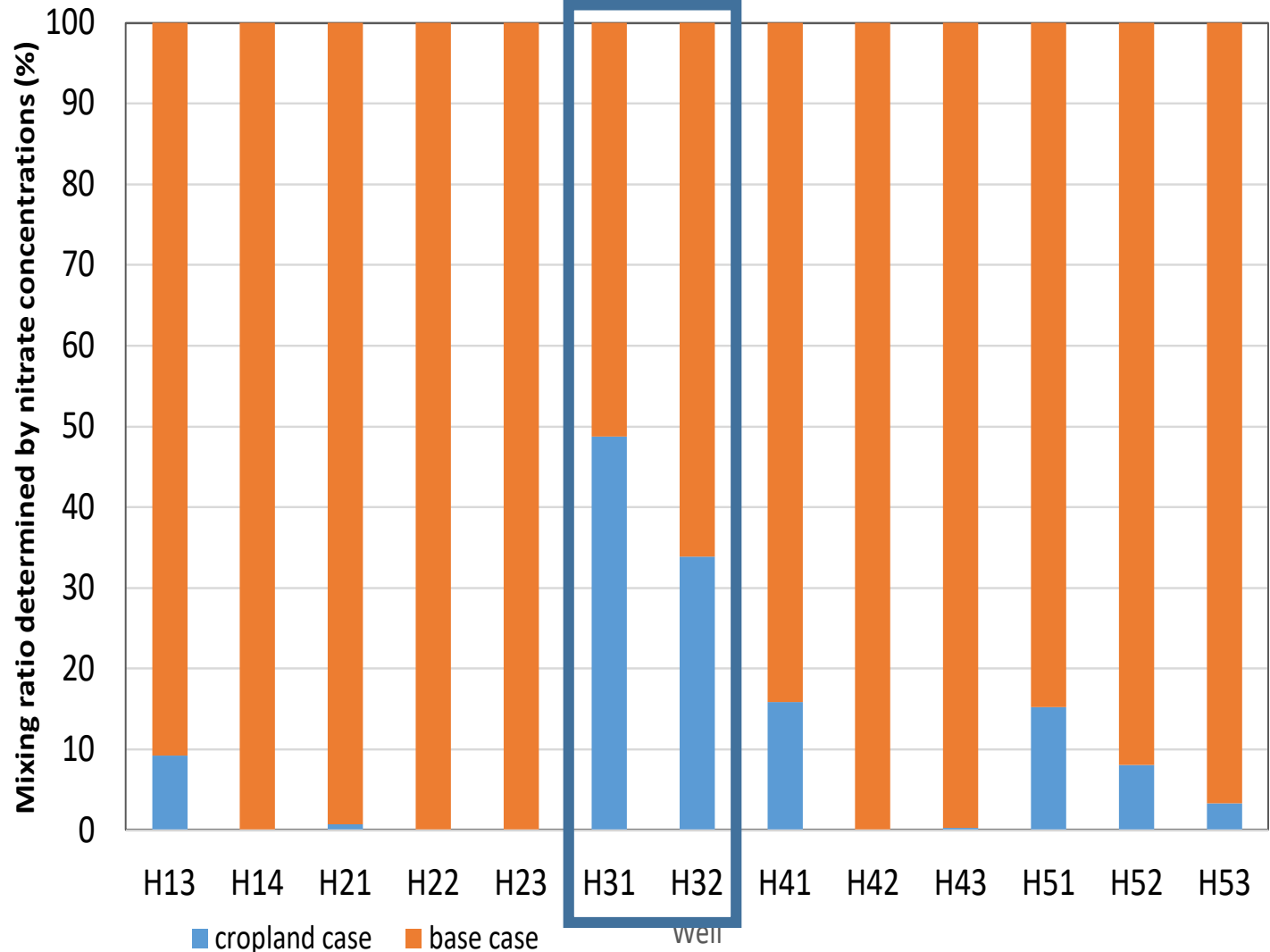
Simulated concentration $c_j(t)$ of reactive species j along a flow path



Combine 1st and 2nd components, we have:
3. Simulated concentration of species j at well i

$$c_{i,j} = \int p_i(t) \cdot c_j(t) dt$$

THE MIXING RATIO DETERMINED BY NITRATE CONCENTRATIONS BETWEEN THE BASE AND CROPLAND CASES

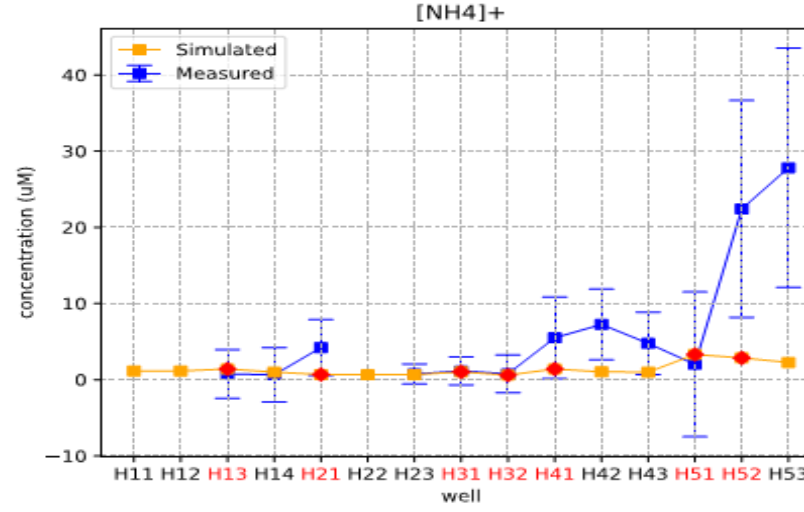
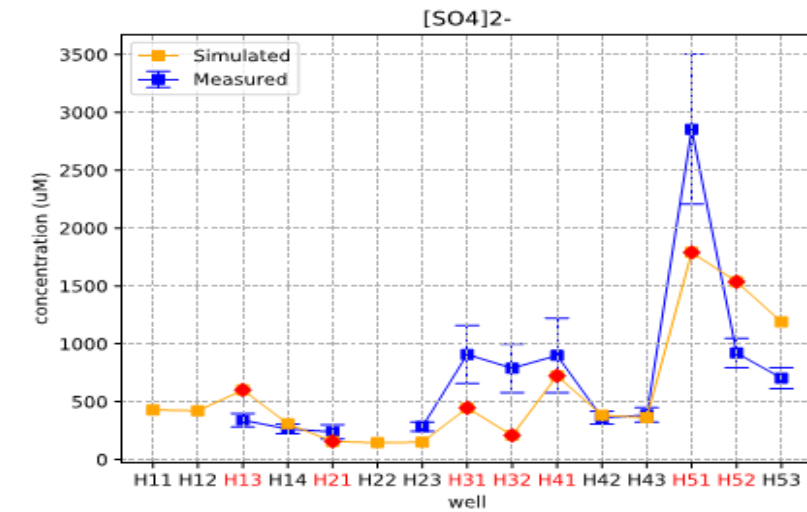
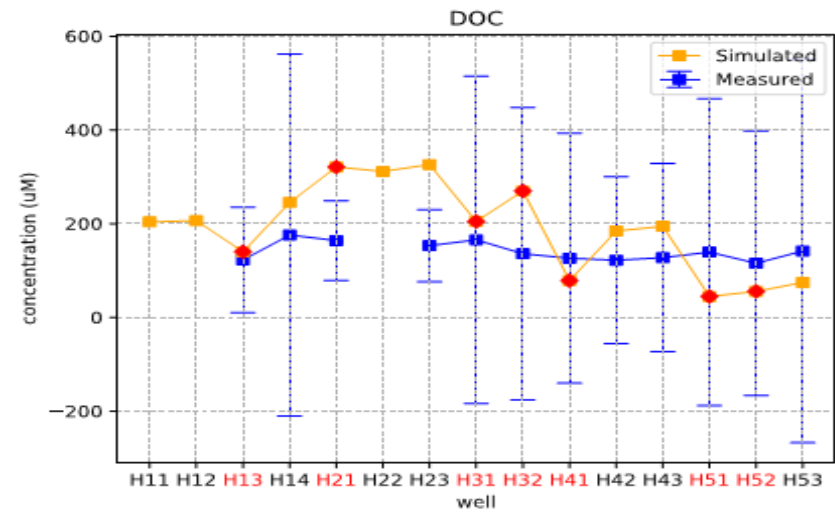
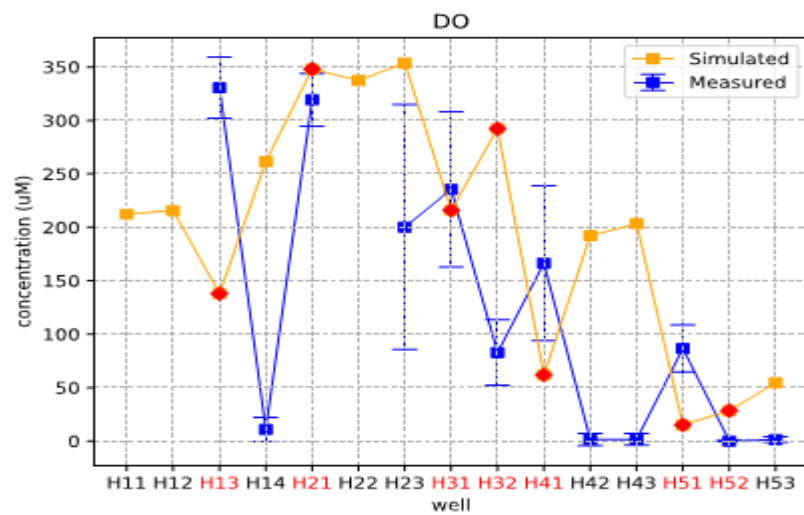
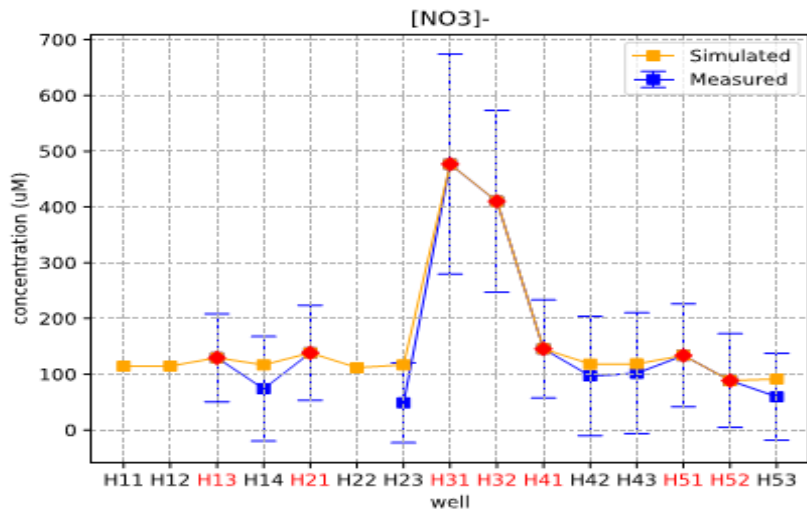


Confirmed spatial variations of land use-dependent input.

- H31 and H32 receive 30% to 50 % water from the cropland areas (which generally agrees with the origin of flow paths predicted by the flow model)



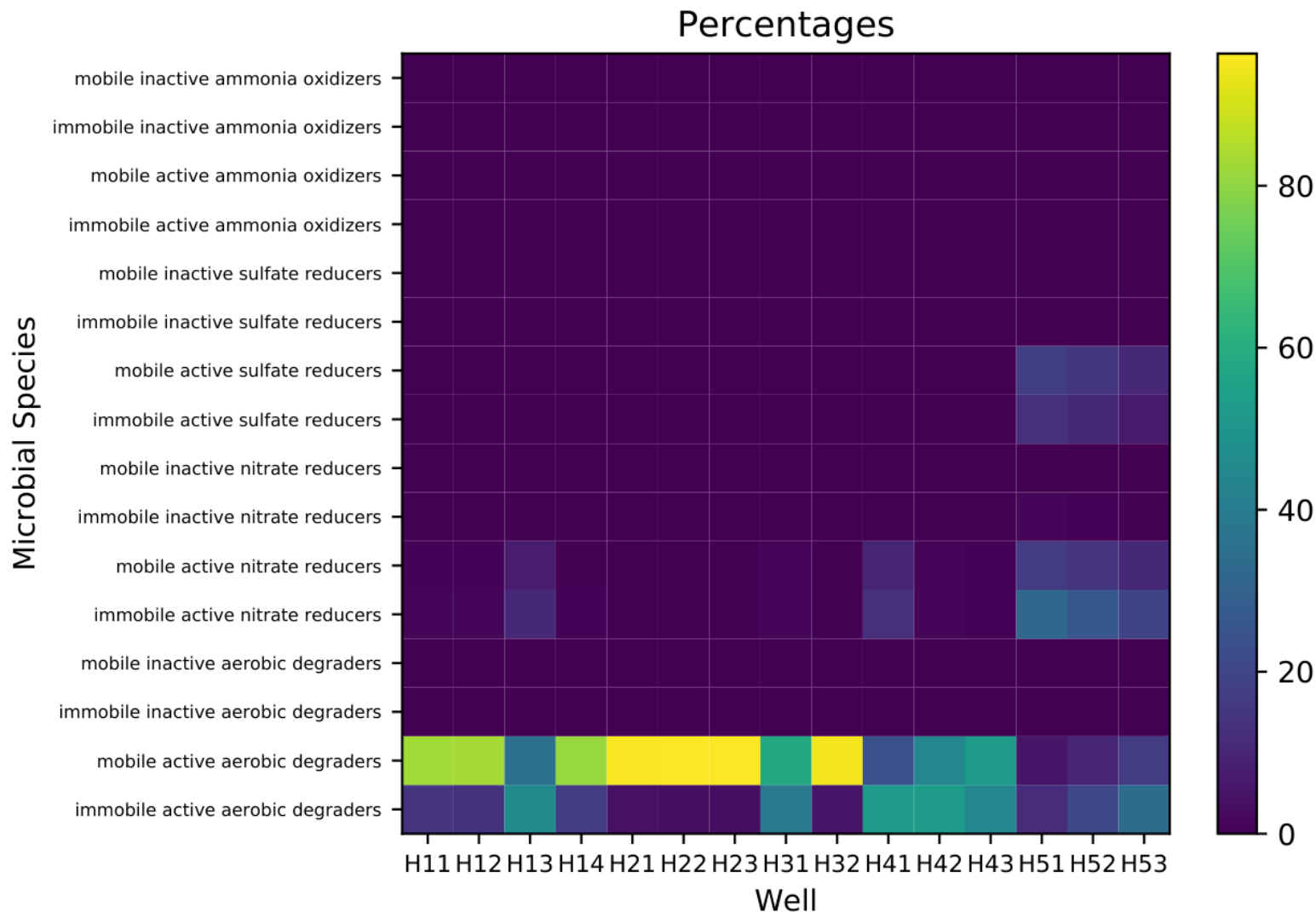
Suggesting a strong link with the surface signals.



Simulated concentrations calibrated with nitrate concentrations are shown in two categories: non-mixing and mixing wells (red code).

SIMULATED CONCENTRATION OF REACTIVE SPECIES AT GROUNDWATER WELLS

MICROBIAL DISTRIBUTIONS AT GROUNDWATER WELLS



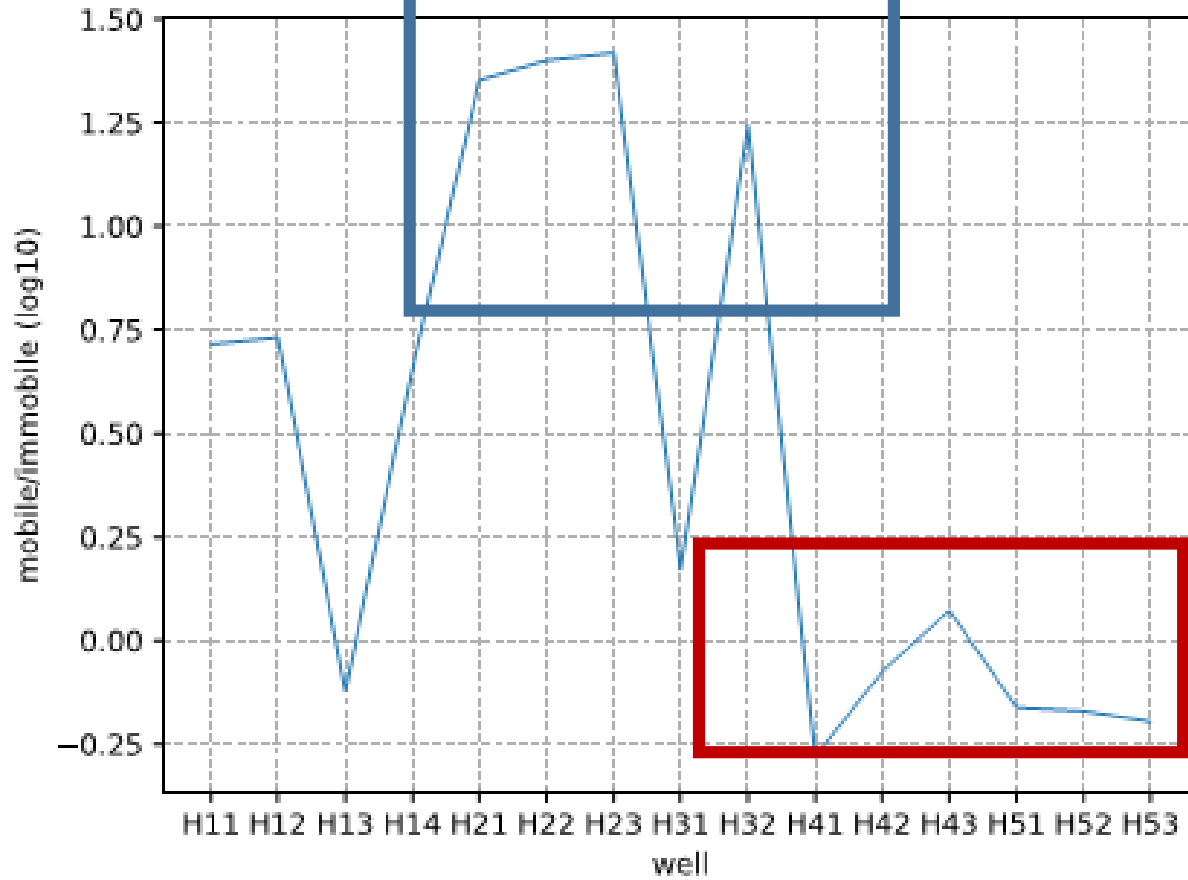
- **Aerobic degraders** dominate communities at most wells.
- **Mobile active aerobic** degraders contributed the most to microbial biomass at wells with short travel times (H21, H22, H23, H32)



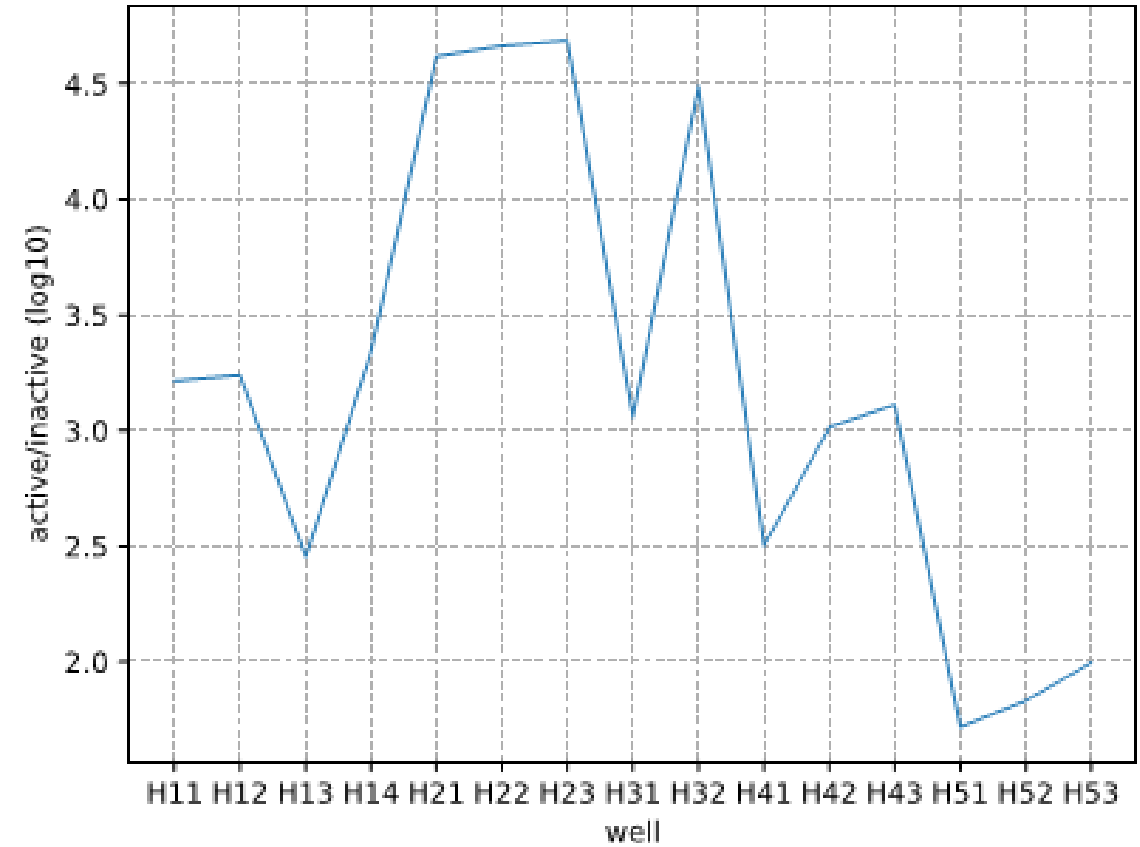
RATIOS BETWEEN MOBILE/IMMOBILE AND ACTIVE /INACTIVE BACTERIA

Mobile bacteria

Short travel time



Active

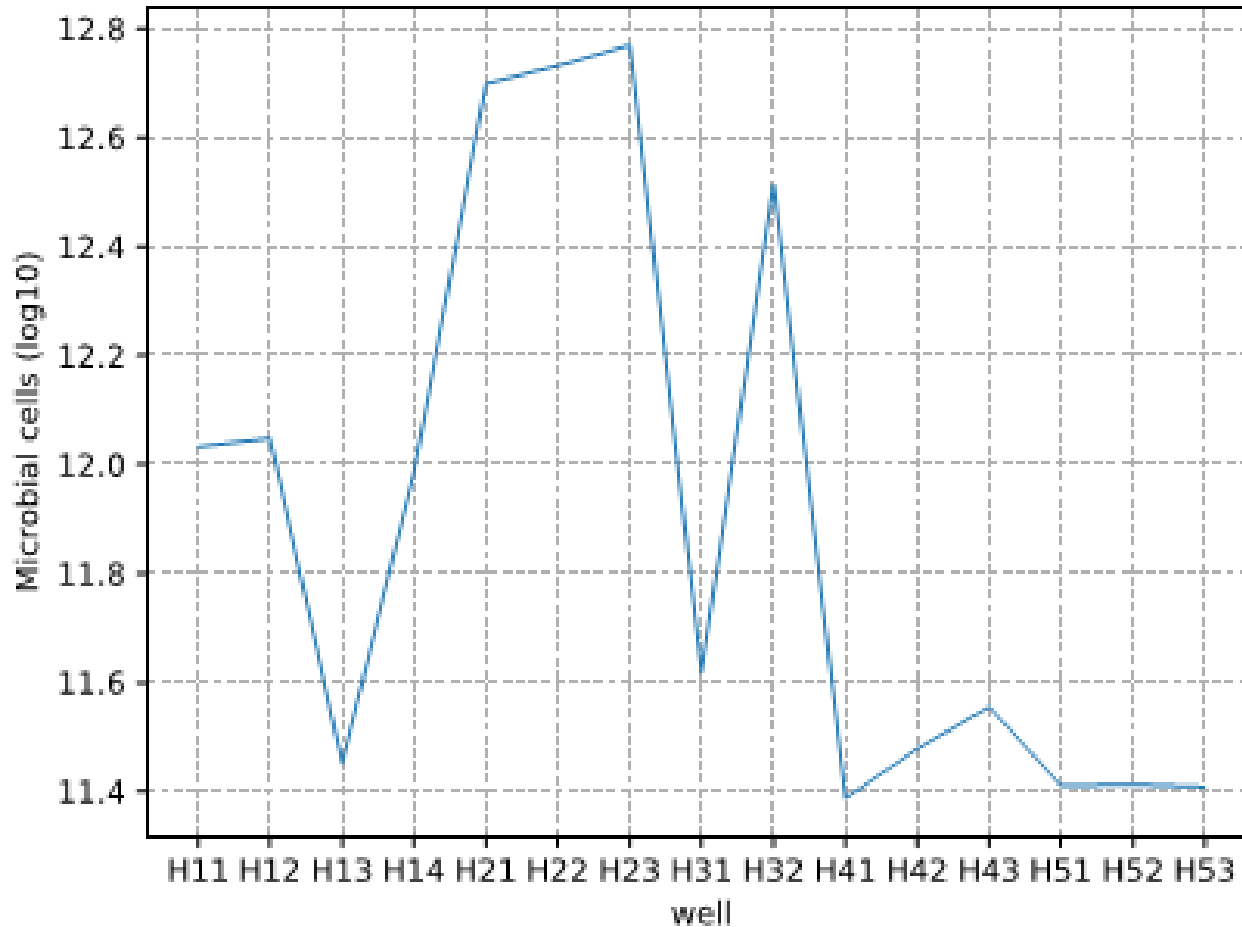


Immobile bacteria

Travel time is XXX years



MICROBIAL ABUNDANCE: total biomass varies from 10^{11} to 10^{12} cells



- Highly abundant in groundwater wells strongly linked to surface inputs
- Relatively stable at deep wells with long travel times (H51, H52, H53)

TAKE-HOME MESSAGES

- **Travel time-based approach** untangles **field-scale reaction transport processes**.
- The results confirmed the **spatial variations of land use-dependent input**.
- **The majority of microbes are mobile**, which agrees with the observation at the Hainich site.
- Aeration zone is crucial for surface DOC degradation.
- Groundwater organic carbon mainly originates from subsurface release rather than surface sources.



OUTLOOK

- Analysis of main factors controlling concentrations at the Hainich CZE

Relevance of surface signals for observations in the subsurface.

- Extrapolation to the catchment scale

Assessment of the applicability of the used travel time-based approach

Analysis of carbon and nitrogen turnover for different climatic projections





CONTACT: thanh-quynh.duong@ufz.de

Hall A | A.105
OSPP voting



EGU General Assembly #EGU24 14-19 April 2024

AquaDiva

Unraveling biochemical transformation of organic carbon and nitrogen compounds in groundwater along a hill slope transect

Thanh Quynh Duong¹, Anke Hildebrandt^{2,3}, Martin Thullner^{1,4}

¹ Helmholtz Center for Environmental Research - UFZ, Department of Applied Microbial Ecology, Leipzig, Germany; ² Department of Computational Hydrogeology, Leipzig, Germany; ³ Friedrich Schiller University Jena, Institute of Geosciences, Jena, Germany; ⁴ Federal Institute of Geosciences and Natural Resources (BGR), Hannover, Germany

BACKGROUND

- The origin and fate of organic carbon and nitrogen compounds in groundwater plays a crucial role in the global biogeochemical cycles of carbon and nutrients, thereby impacting drinking water quality.
- Land use strongly influences the input of these compounds, while their transport and transformation through the subsurface are governed by a complex interplay between hydrological and biogeochemical processes occurring on various spatial and temporal scales that control the variable diversity of microbial communities in the subsurface.
- We eventually want to address the question: To what extent can surface input variations influence subsurface conditions? For this purpose, we use a travel time-based approach to account for heterogeneous subsurface conditions, which can simplify reactive transport modeling in a heterogeneous medium and reduce computational efforts.

TRAVEL TIME-BASED MODEL APPROACH

1. Flow model of Hainich CZE

2. Schematic of simulated biochemical reaction networks

3. Simulated concentrations of species j at well i

$$c_{ij} = \int p_i(t) \cdot c_j(t) dt$$

Combine 1st and 2nd components, we have:
3. Simulated concentrations of species j at well i

For each observation well of the Hainich CZE, groundwater travel time distributions (TTDs) are derived from the three-dimensional hydrogeological model, showing a large variability in mean travel times. These TTDs are combined with reactive transport simulations along flow paths based on the reaction networks. The resulting steady-state concentration profiles are converted into concentrations at observation wells using TTDs.

RESULTS: SIMULATED CONCENTRATION OF REACTIVE SPECIES AND COMPOSITION OF MICROBIAL COMMUNITIES AT THE OBSERVATION WELLS

1. Nitrate concentrations determined the mixing ratio between the base and cropland cases

2. Microbial distributions: percentage contribution of each subpopulation of each microbial functional group

3. Ratio between mobile and immobilized bacteria along the flow paths

BIOGEOCHEMICAL PROCESSES ALONG 1D FLOW PATHS

1D advective dispersive-reactive transport

- Upper 50m of profile: aerobic conditions, abundant supply of oxygen
- Numerical mesh grid: non-uniform, with grid sizes ranging from 1m to 200m
- Total length (L) = 20000m
- Total time (t) = 200000 days

We performed numerical reactive transport simulations of species conversion along individual flow paths. We consider varying microbial functional groups, such as aerobes and anaerobes, as well as key microbial life processes under different redox conditions, including aerobic, nitrate-reducing, ammonia-oxidizing, and sulfate-reducing conditions that eventually influence the turnover of organic carbon and nitrogen compounds.

KEY MESSAGES

- The travel time-based approach can disentangle the field-scale reaction transport processes.
- The results confirmed the spatial variations of land use-dependent input.
- The majority of microbes are mobile, which agrees with the observation at the Hainich site.
- The aeration zone is considered highly important for the degradation of surface DOC.
- Organic carbon in groundwater mainly originates from subsurface release rather than surface sources

OUTLOOKS

- Explore how temporal surface variations influence microbial activity and carbon and nitrogen transformations and identify hot spots and hot moments within the groundwater system.
- Extrapolate the reactive transport model at the hill slope transect to the catchment scale to assess their responses to warming scenarios and associated surface condition variations.

ACKNOWLEDGMENTS:

This study is part of the Collaborative Research Centre AquaDiva of the Friedrich Schiller University Jena, funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - SFB 1076 - Project Number 21827072.

REFERENCES

Philz, K., Totsche, K.U., Trumbore, S.E., Lehmann, R., Steinhilber, C., Herrmann, M. (2016). How deep can surface signals be traced in the critical zone? Merging biodiversity with biogeochemistry research in a central German Muschelkalk landscape. *Front. Earth Sci.* 4, 32.

Lehmann, K., Lehmann, R., Totsche, K.U. (2021). Event-driven dynamics of the total mobile inventory in undisturbed soil account for significant fluxes of particulate organic carbon. *Science of The Total Environment* 796.

Chauras, S., F. Hilde, A. Hildebrandt, M. Thullner (2022). Predicting the impact of spatial heterogeneity on microbially mediated nutrient cycling in the subsurface. *Biogeochemistry* 19, 605-618.

Rösiger, T., Houben, T., Schwab, V., Schroeter, S. A., Lehmann, R., Totsche, K.U., Altinger, S., Helle, F. Using molecular biomarkers, isotopic data and travel time analyses to improve numerical sub-catchment groundwater flow modeling in Triassic limestone: *hydrostone alterations*.

AUTHOR CONTACT
thanh-quynh.duong@ufz.de

UFZ HELMHOLTZ Centre for Environmental Research

EGU

Interesting?

X YES



Thank you!



UFZ HELMHOLTZ
Centre for Environmental Research

DFG Deutsche
Forschungsgemeinschaft