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Spatio-temporal heterogeneity affects redox microbial dynamics in the subsurface

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AquaDiva

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Outline

Context

- Background
- Research objective

Approach

- Investigated scenarios
- Process Network

Results I

- Velocity distribution patterns due to **spatial heterogeneity**
- Impact on travel time of conservative tracers in the domain
- Select single scenario examples of biomass and dissolved species concentrations in the domain: 2-D and 1-D profile
- Impact on groundwater sampling and analysis
- Aggregated impact on mass removal and biomass in the domain with heterogeneity

Results II

- Investigated scenario for **temporal heterogeneity** and single scenario example
- Aggregated results on the sensitivity of mass removal and biomass

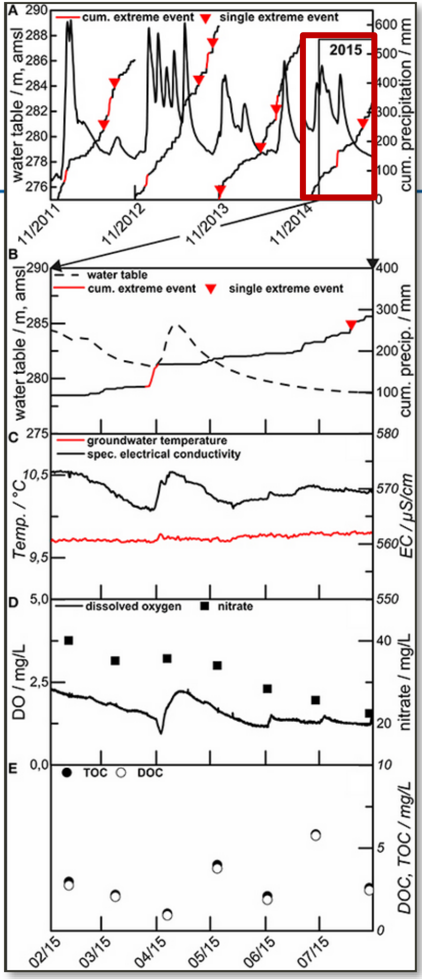
Summary

- Summary of spatio-temporal heterogeneity effects on mass removal and biomass

Context

Background

Study links between surface and subsurface	AquaDiva
Complex non-linear system and temporally dynamic	Critical Zone
Spatially heterogenous and limited observational opportunities	Subsurface / Surface
Resolve biogeochemical dynamics at the small scale focusing on spatio-temporal heterogeneities	Numerical modeling of biogeochemical dynamics / Research objective



(Küsel et al., 2016)

Context

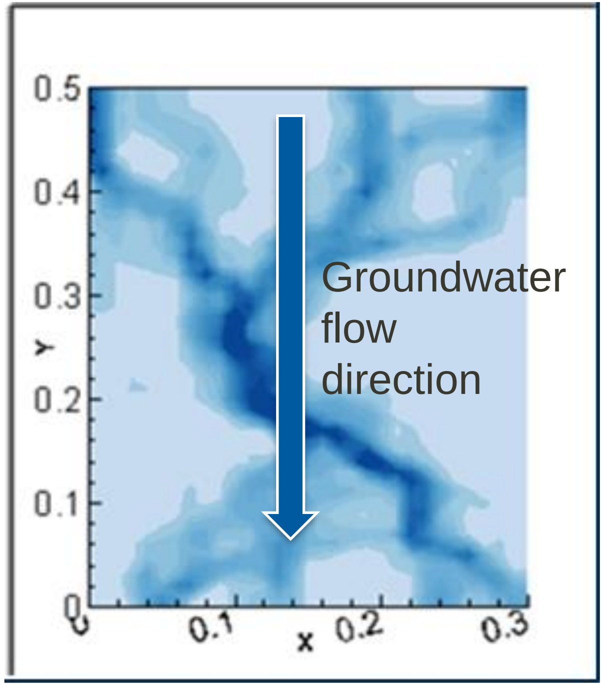
Research objective

Resolve biogeochemical dynamics in the earth‘s critical zone using a numerical modeling approach

Identification of environmental factors governing biogeochemical processes at the small scale with respect to physicochemical changes and biological activity with a focus on spatial heterogeneity and time variable flow rates

Domain:

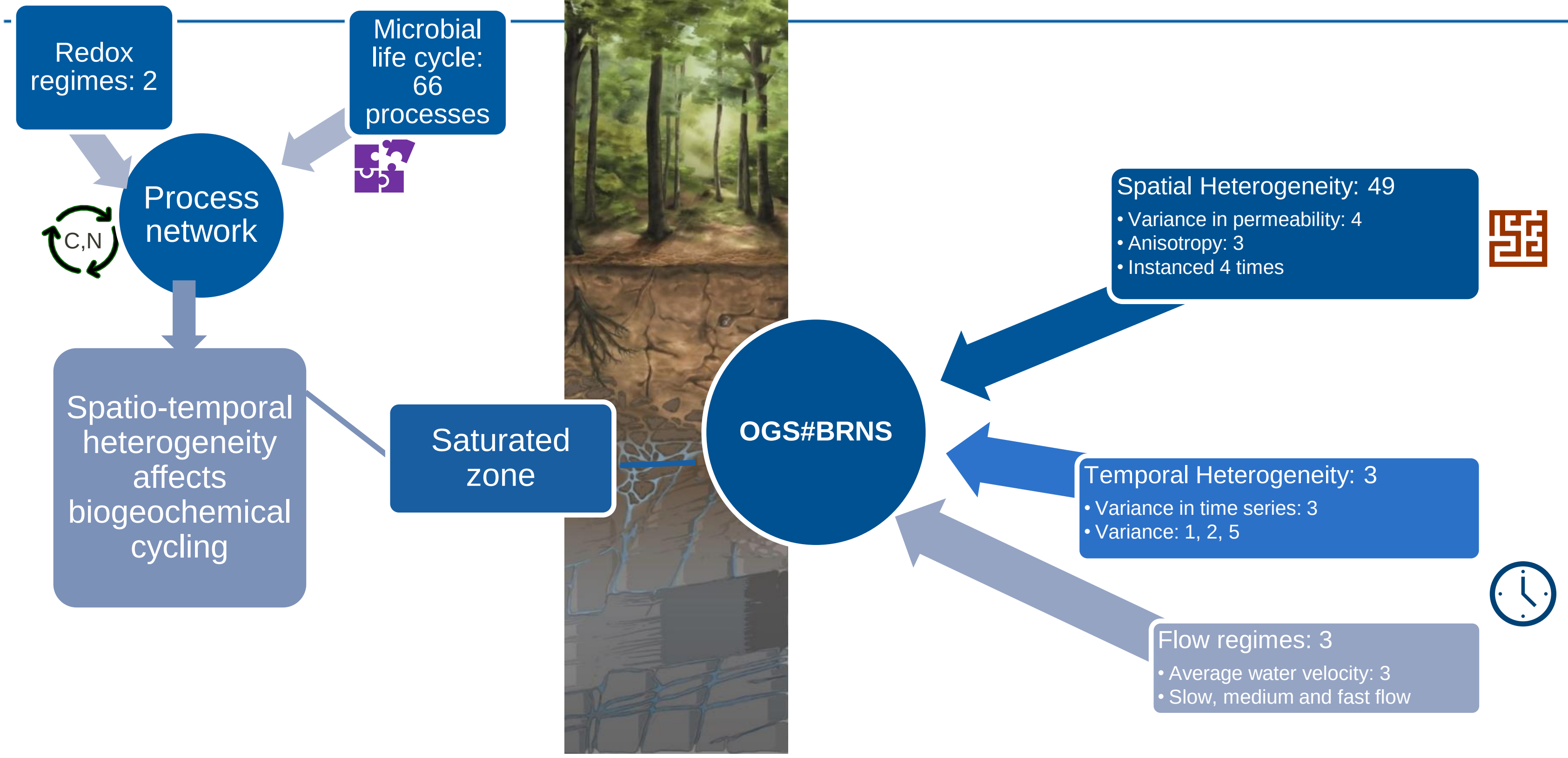
- 0.5m x 0.3m
- Mass influx – top boundary
- Mass outflux – bottom boundary



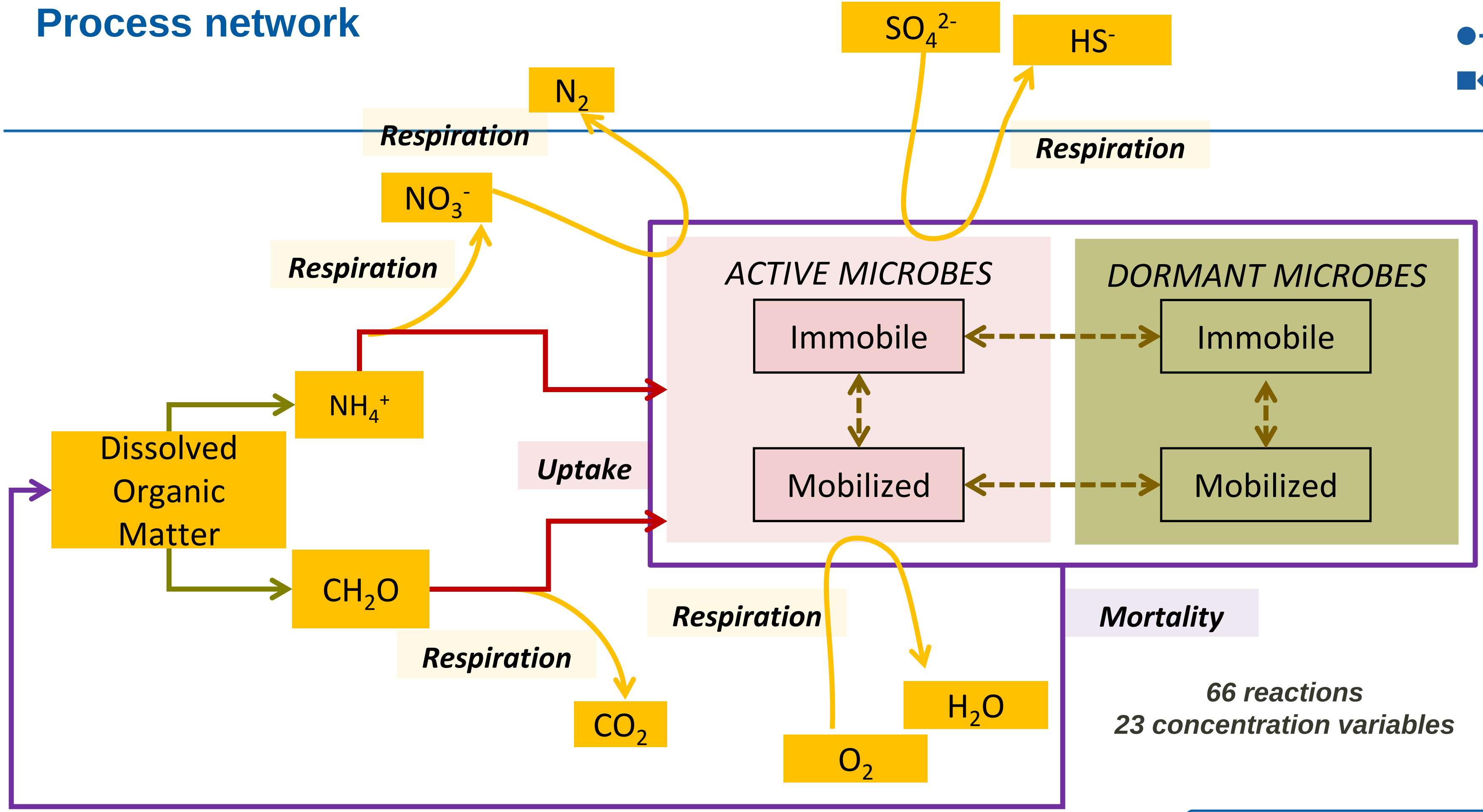
Example of a heterogeneous domain with a preferential flow path

Approach

Investigated scenarios



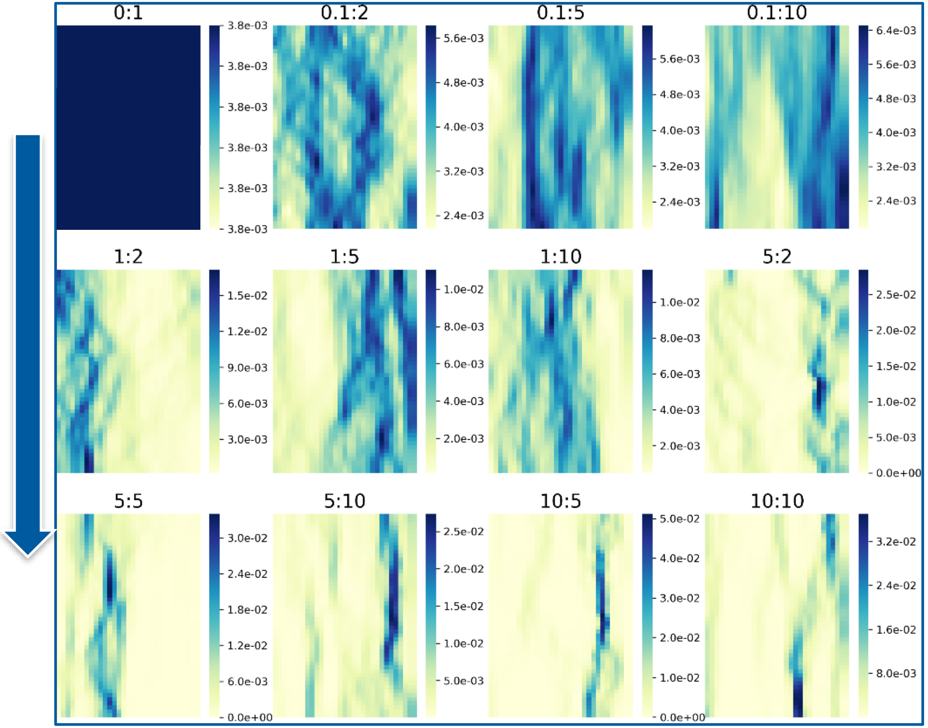
Process network



66 reactions
23 concentration variables

Results I: Spatial heterogeneity

Impact on velocity distribution patterns: Same across all flow regimes

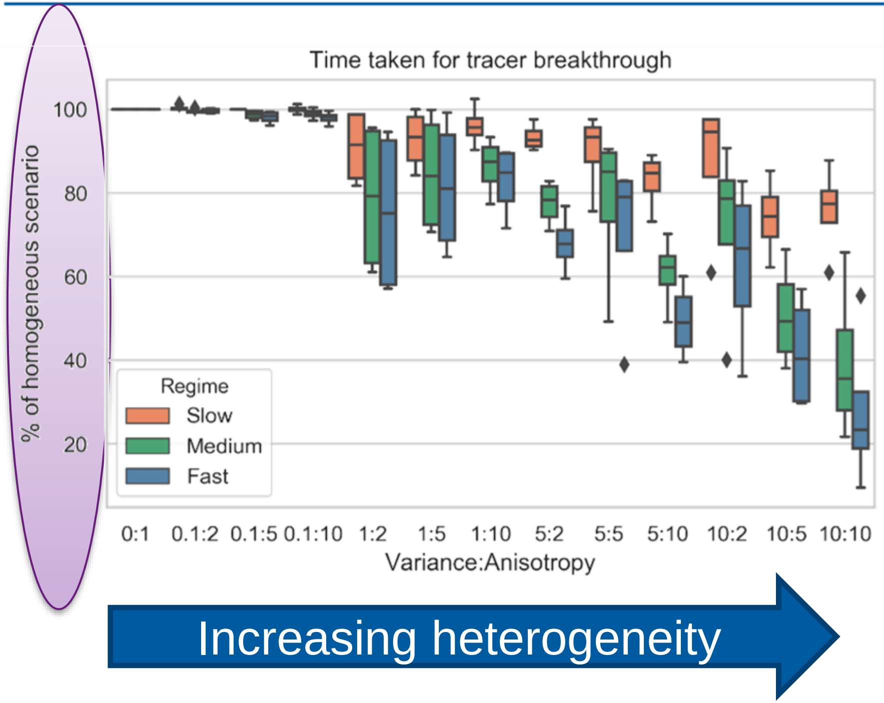


Velocity distribution (m/d) in heterogeneous scenarios (Variance:Anisotropy) in medium flow regime

- Heterogeneity results in corresponding velocity distribution patterns in the domain, but
- ➢ **Average water flux is the same for a given flow regime**
- Absolute values of velocity depends on the flow regime, but
- ➢ **Distribution pattern is same across all flow regimes**

Results I: Spatial heterogeneity

Velocity distribution: Impact on breakthrough time: Varies with flow regime



- Shorter breakthrough times in heterogeneous domains
- Indicates relative importance of flow processes (diffusion v/s dispersion v/s advection)

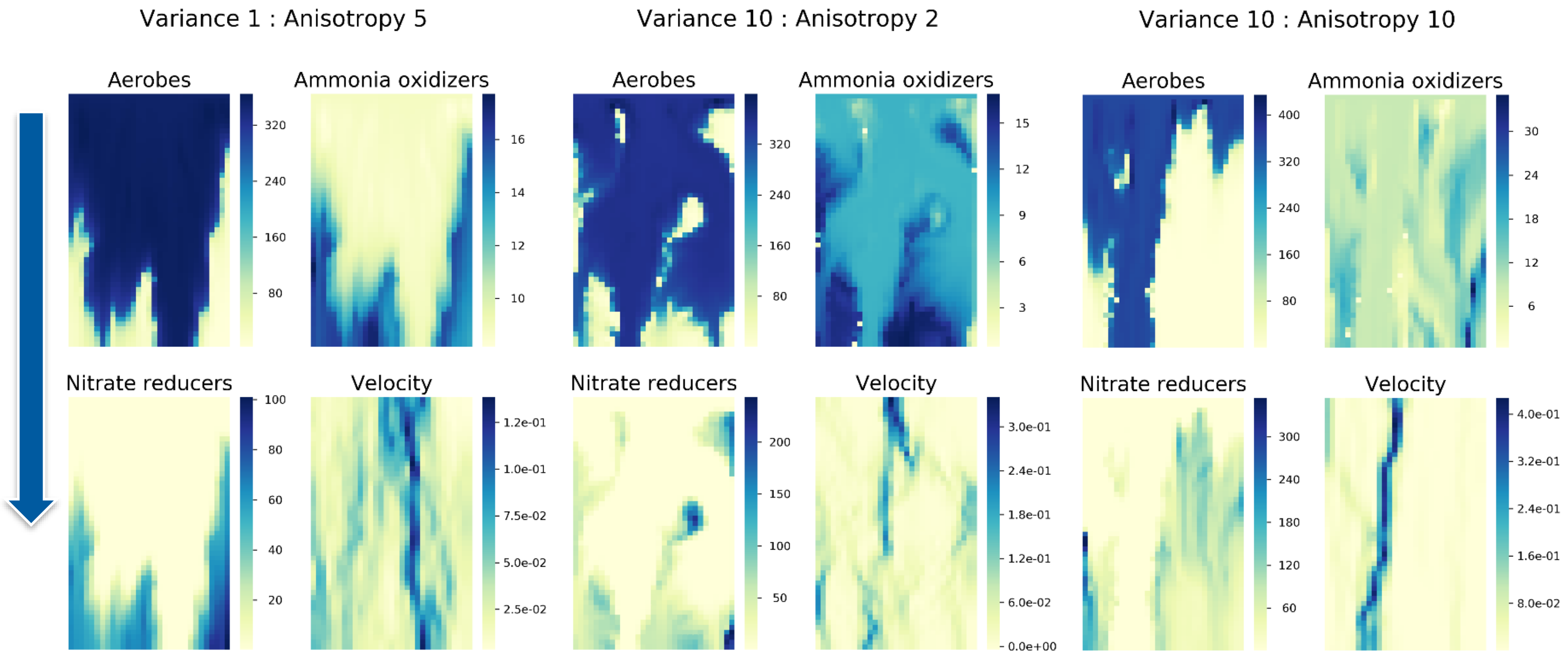
➢ **Peclet # is important to describe impact of spatial heterogeneity on velocity distributions**

$$Pe = \frac{advection}{diffusion + dispersion}$$

➢ **Impact on breakthrough time shall be used to indicate heterogeneity**

Results I: Spatial heterogeneity

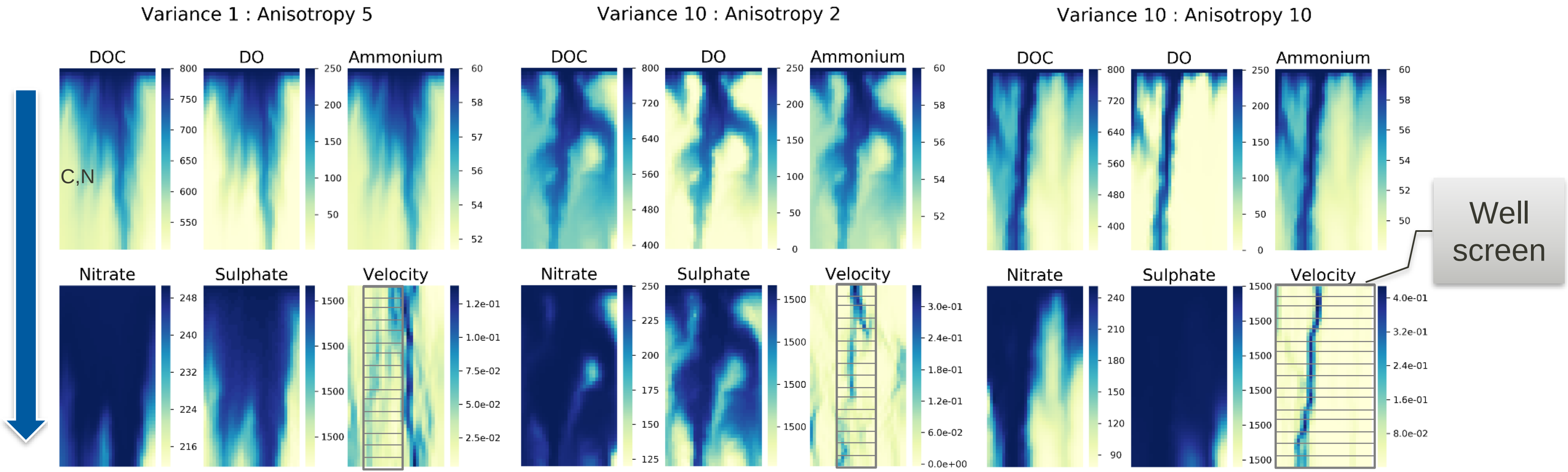
Single scenario examples: Biomass: 2D



Concentrations in µM and velocity in m/d.

- Microbial biomass distribution is not uniform.
- Linked with the heterogeneity structure and associated velocity distribution.

Results I: Spatial heterogeneity
Single scenario examples: Dissolved chemical species: 2D



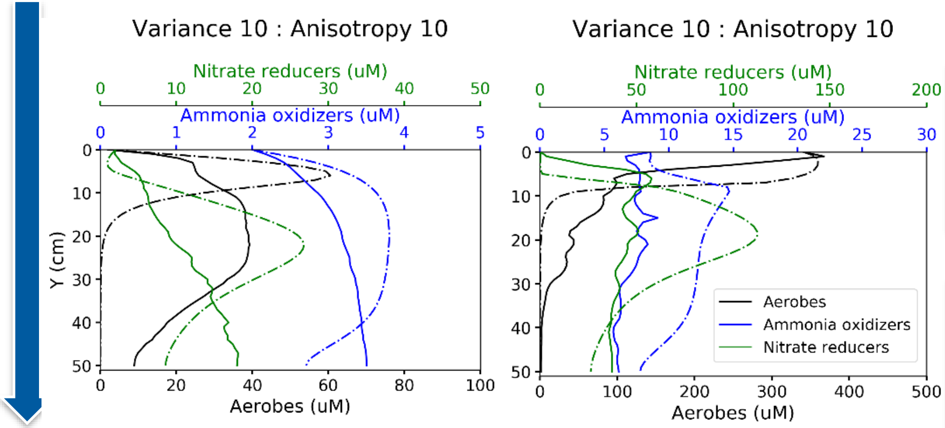
Concentrations in µM and velocity in m/d.

- Dissolved species concentration is also distributed and linked with heterogeneity and associated velocity distribution.
- Groundwater sampling aggregates the solutes resulting in loss of information.

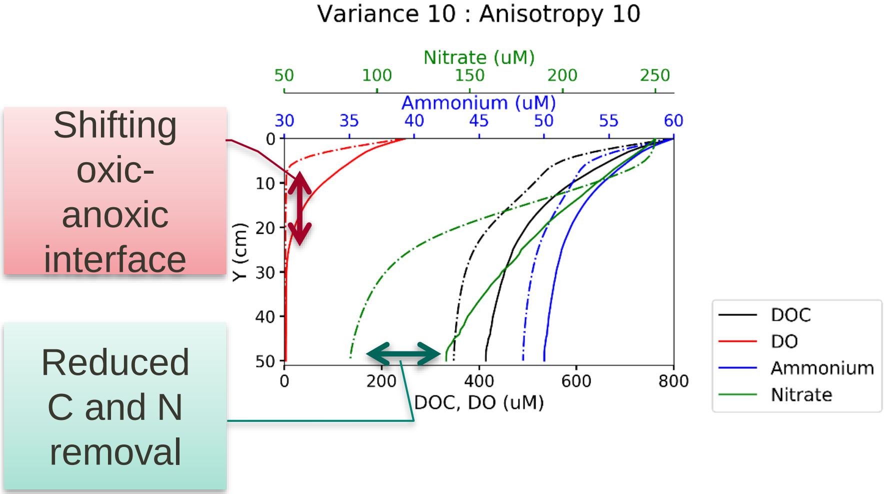
Results I: Spatial heterogeneity
Mobile and immobile biomass, dissolved species concentration: 1D

Since scenario: biomass distribution

Mobile | **Immobile**



Single scenario: dissolved species



➢ **Apparent "co-occurrence" of microbial species in heterogeneous domains.**

Flux and spatially averaged concentrations of active mobile and immobile microbial species along the dominant flow direction in heterogeneous domains displayed against the base homogeneous case (dashed lines)

➢ **The removal of carbon and nitrogen is lower in heterogeneous scenarios compared to the homogeneous base case.**

Flux averaged concentrations of dissolved species along the dominant flow direction in heterogeneous domains displayed against the base homogeneous case (dashed lines)

Results I: Spatial heterogeneity
Implications for sampling and analysis: Summary

Nutrient cycling

- Nutrient distribution governed by the heterogeneity structure: longer persistence in high flow zones.

Biomass distribution

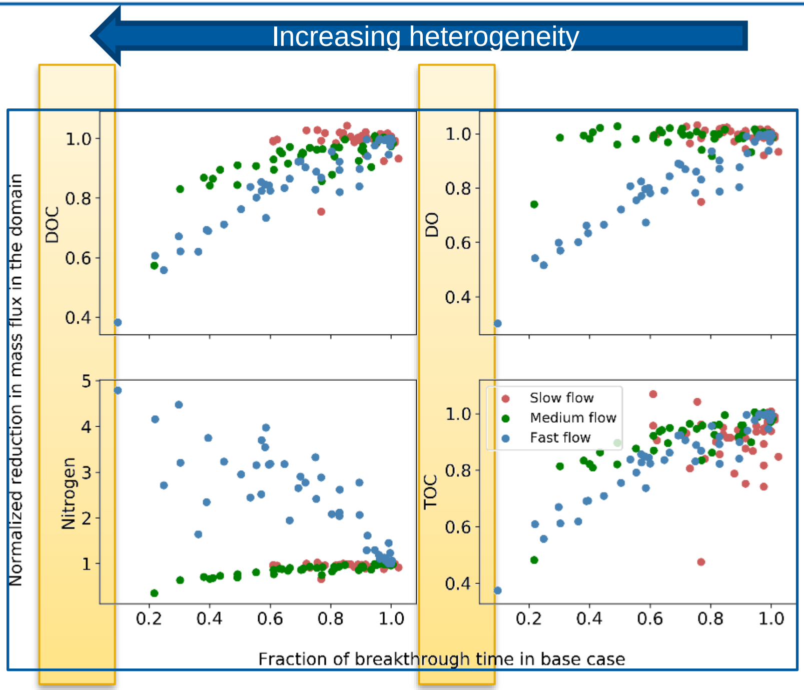
- Biomass distribution governed by nutrient and electron acceptor availability:
    - Aerobes are dominant in DO rich zones
    - Anaerobes are active at the interface of high flow and low flow zones

Caution for sampling and analysis

- Groundwater sampling techniques:
    - Collect flux averaged/volume averaged mobile matter in the subsurface
        - ➢ **Does not reflect the heterogeneity in mobile matter distribution**
    - Capture a fraction of the microbial population present in the subsurface
        - ➢ **Does not reflect the dominant species that cycle the nutrients in the subsurface**
- Core sampling must be part of the drilling program for monitoring wells

Results I: Spatial Heterogeneity

Aggregated results: Nutrient cycling: Summary



Aggregated impact on carbon and nitrogen removal against decreasing breakthrough time resulting from spatial heterogeneity

$$\textit{Impact on nutrient cycling} = \frac{\textit{Species removal in heterogeneous scenario}}{\textit{Species removal in homogeneous scenario}}$$

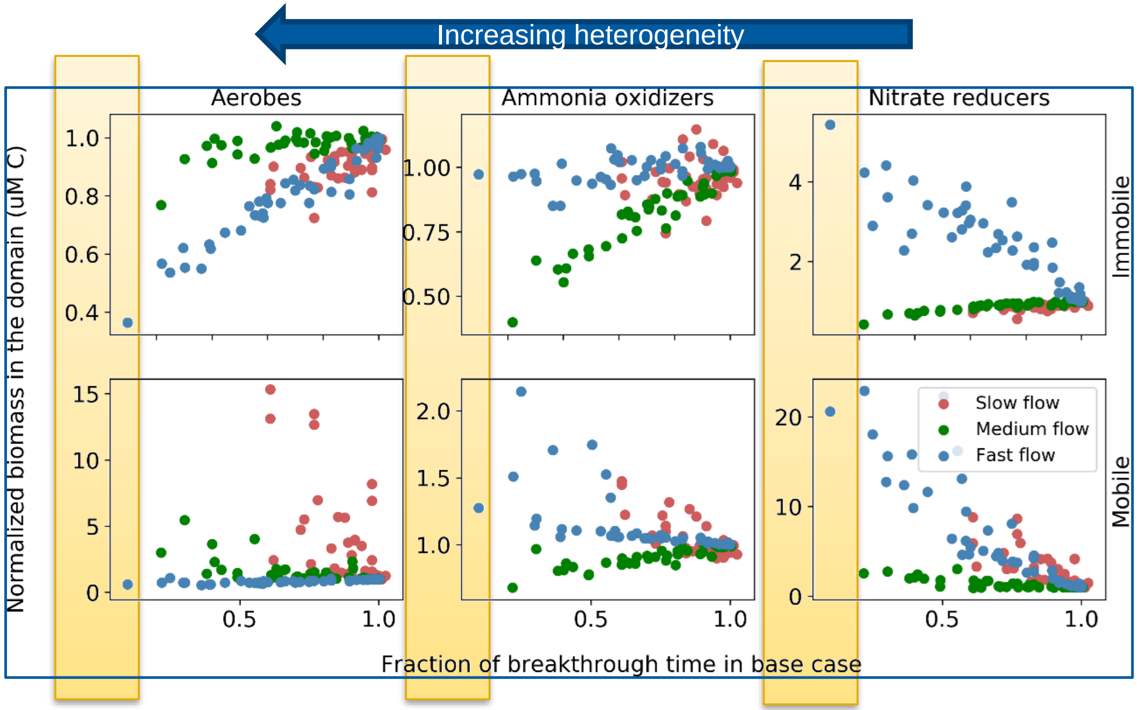
- Impact depends on:
  - **Flow regime (Pe#)**
  - **Relative time scale of reaction and transport (Da#) in the domain**

$$Da = \frac{\textit{reaction time scale}}{\textit{transport time scale}}$$

- Linear relationship between impact and reduction in breakthrough time

Results I: Spatial Heterogeneity

Aggregated results: Active biomass: Summary



$$\text{Impact on biomass} = \frac{\text{Biomass in heterogeneous scenario}}{\text{Biomass in homogeneous scenario}}$$

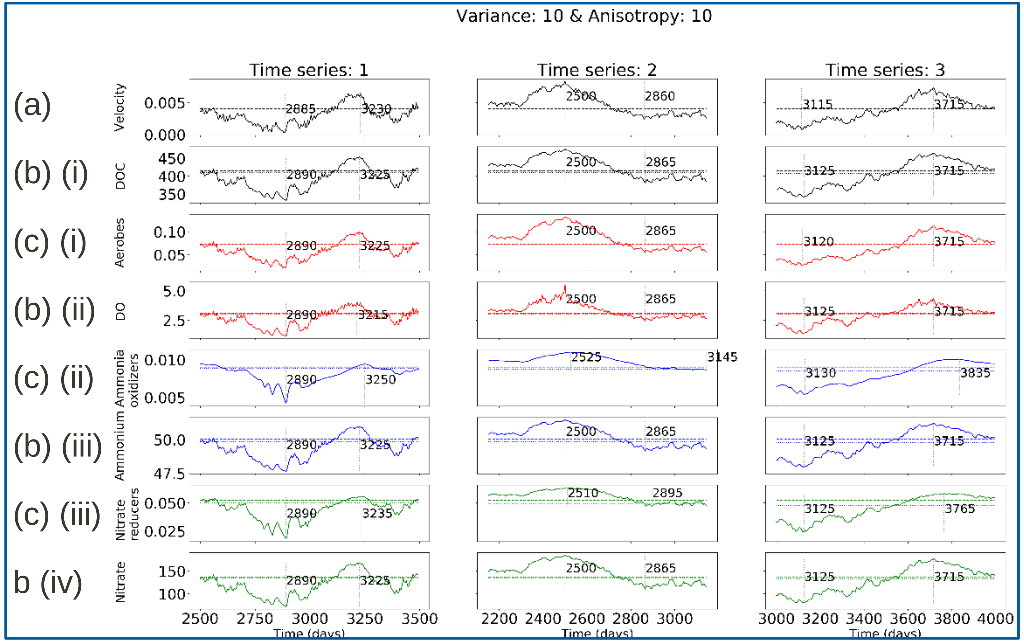
- **Note that mobile fraction is sampled and measured in groundwater sampling**
- **Impact on mobile biomass is not commensurate with the impact on nutrient cycling**

Aggregated impact on biomass (%) of each species against decreasing breakthrough time resulting from spatial heterogeneity

Results II: Temporal heterogeneity and spatial heterogeneity

Time series: Scenario setup

- Generated time series for average groundwater flux through the domain for a period of 15 years
- Common observation that is recorded in groundwater monitoring wells at reasonably high frequency
- Attributable to diurnal fluctuations in temperature, seasonality or super-annual cycles in weather



Example time series data for:

(a) groundwater velocity in the domain

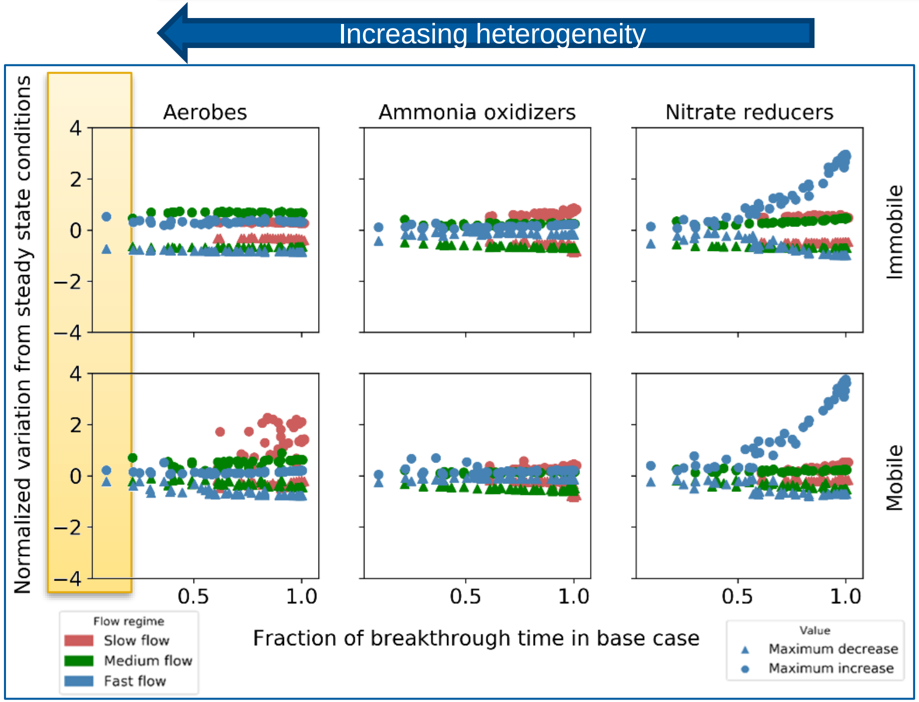
(b) (i) – (iv) flux averaged concentration of chemical species in the domain

(c) (i) – (iii) biomass in the domain

Results II: Temporal heterogeneity and spatial heterogeneity

Aggregated results: Active biomass: Sensitivity

$$Senstivity = \frac{Variation\ in\ biomass\ of\ domain\ from\ steady\ state\ conditions}{Value\ in\ steady\ state\ conditions}$$



Maximum variation induced in biomass from steady state conditions

- Slow and medium flow regimes: Low sensitivity
- Fast flow regime: Increased presence of nitrate reducers with temporal heterogeneity, influenced by spatial heterogeneity

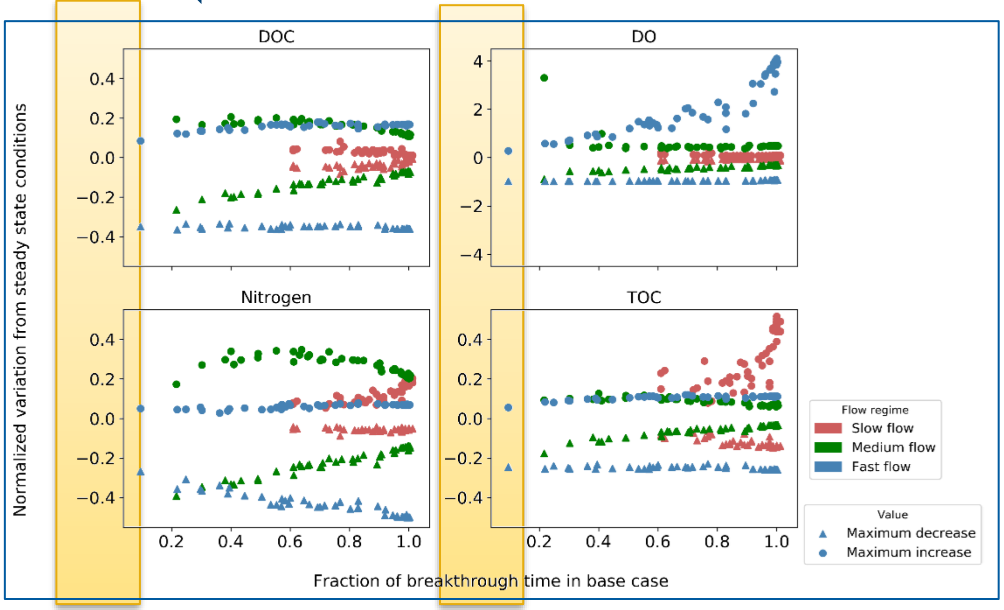
➢**The Da# associated with the growth dynamics of the microbial species is a governing factor to evaluate impact of temporal dynamics**

Results II: Temporal heterogeneity and spatial heterogeneity

Aggregated results: Nutrient cycling: Sensitivity

$$Senstivity = \frac{Variation\ in\ flux\ averaged\ concentration\ at\ outlet\ of\ domain\ from\ steady\ state\ conditions}{Value\ in\ steady\ state\ conditions}$$

Increasing heterogeneity



Maximum variation induced in flux averaged concentrations from steady state conditions at the outlet of the domain

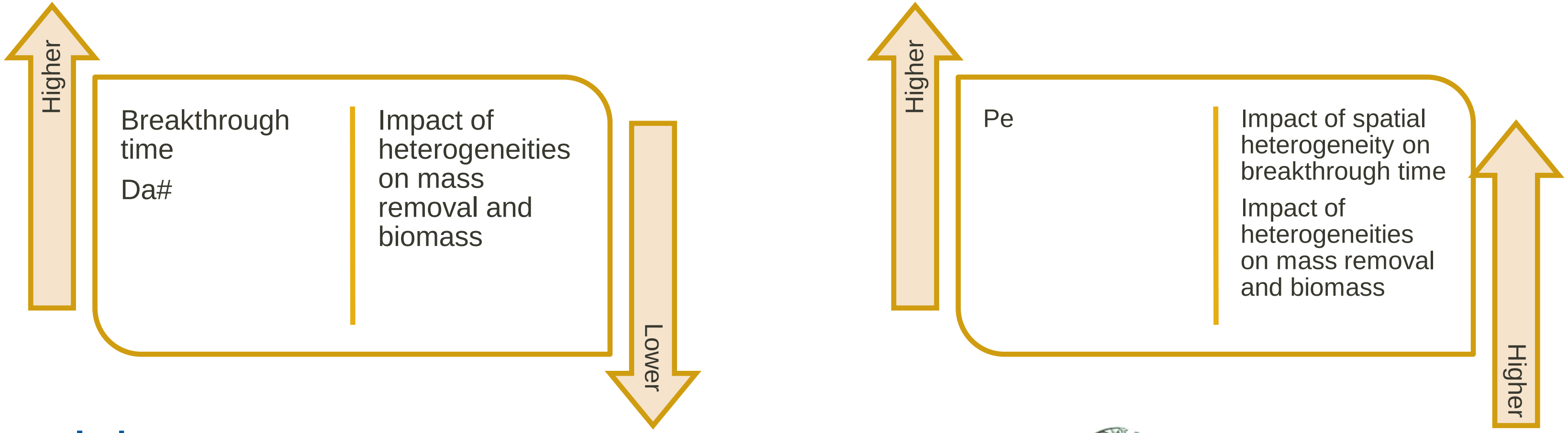
- Slow flow regime: low sensitivity
- Medium flow regime: changing capability to remove nitrogen with spatio-temporal heterogeneities
- Fast flow regime: increased capability to remove nitrogen with temporal heterogeneity

➢ **Spatio-temporal heterogeneity impacts sensitivity depending on the chemical species (Da#) and the flow regime (Pe#)**

Summary

- Spatial heterogeneity impacts microbial biomass distribution and nutrient cycling in the subsurface and must be accounted for while conducting groundwater sampling and analysis.

- Impact of temporal heterogeneity depends on the relative time scale of disturbances with respect to reaction time scales.



Acknowledgements

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