Redox interpretation and important groundwater chemical results

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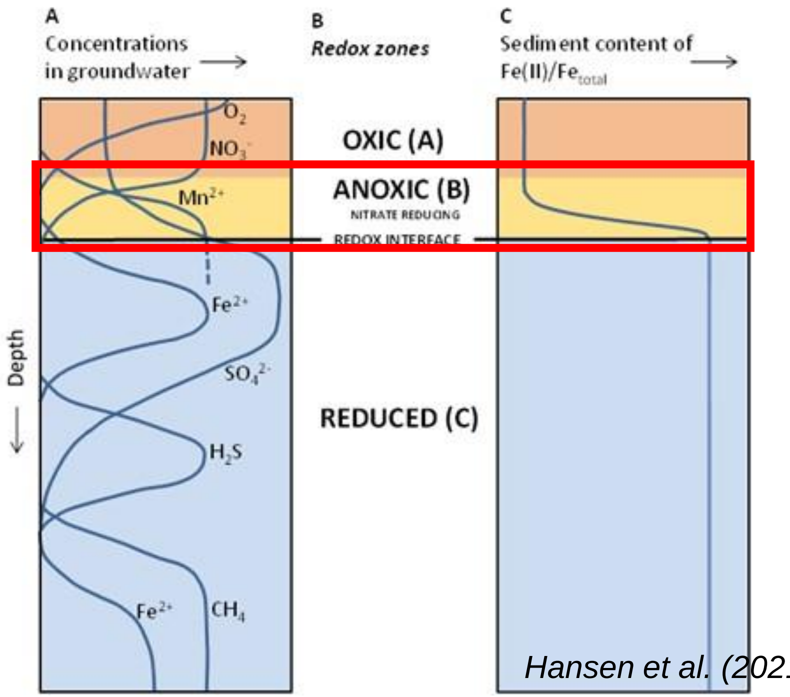
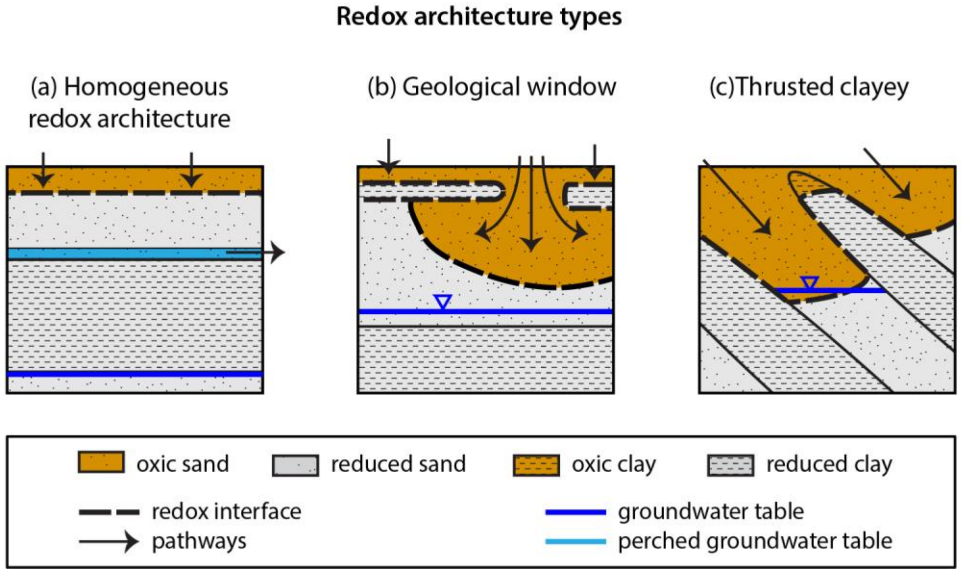
Redox architecture and N fate

- Redox conditions control the fate of N in water
  - No reduction in oxic conditions
  - N reduction in N-reducing conditions
  - Complete N reduction in reduced conditions
- Input data for N retention simulations
  - **Subsurface redox architecture**
  - **N reduction rates**
- Complexity of the redox architecture and challenges
  - Upscaling of field measurements
  - Parameterization of N reduction rates



Hansen et al. (2021)

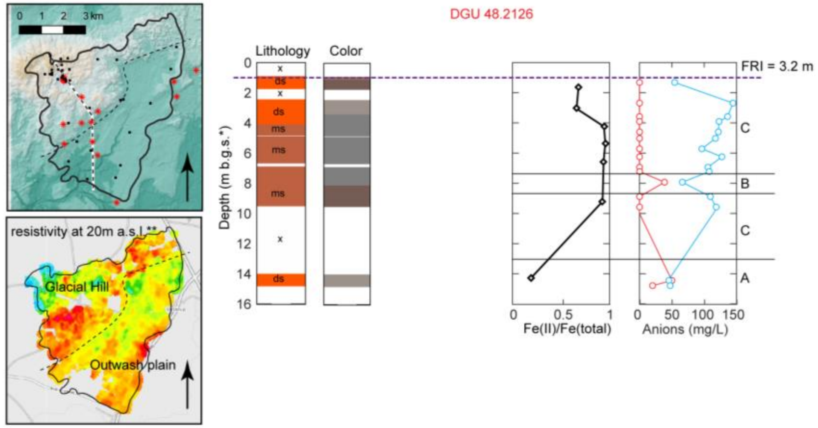


Kim et al. (2019)

Challenges I: Upscaling

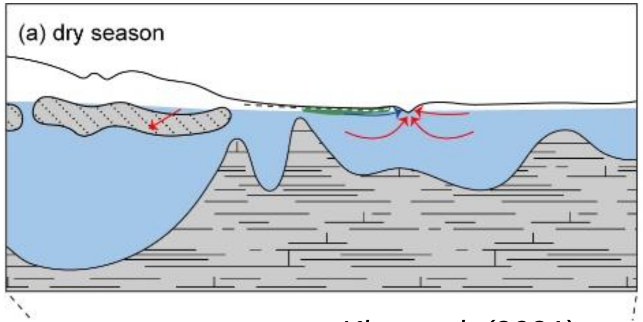
- Upscaling of point measurements to 3D scale

1D scale → 2D scale → 3D scale



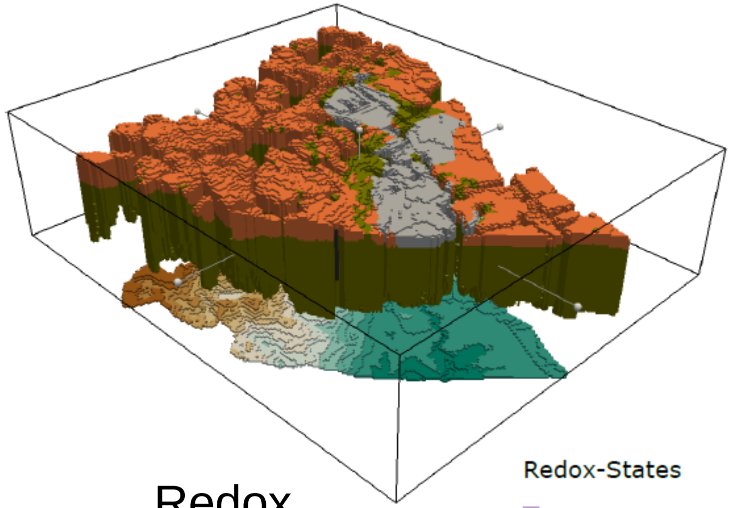
Hansen et al. (2021)

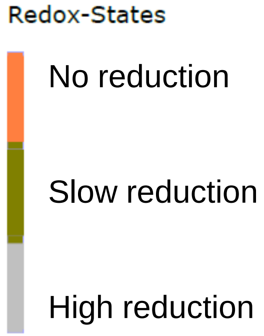
Hydrogeochemical data



Kim et al. (2021)

Conceptual model of water and nitrate transport





Redox training image

Challenges II: Parameterization

- **Parameterization of N reduction rates**

- N retention map:

$$N_{reduction} = \sum_{i=1}^{n}\left[\tau_i \frac{\partial c}{\partial t_i}\right]$$

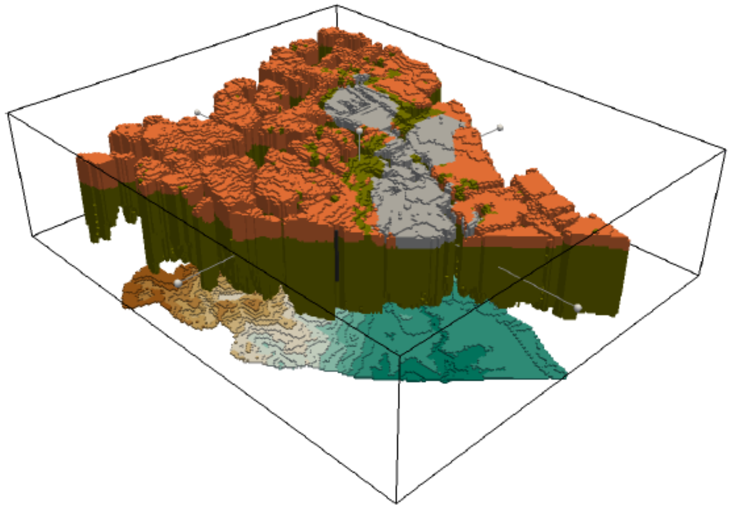
τ_i transit time in redox zone *i*

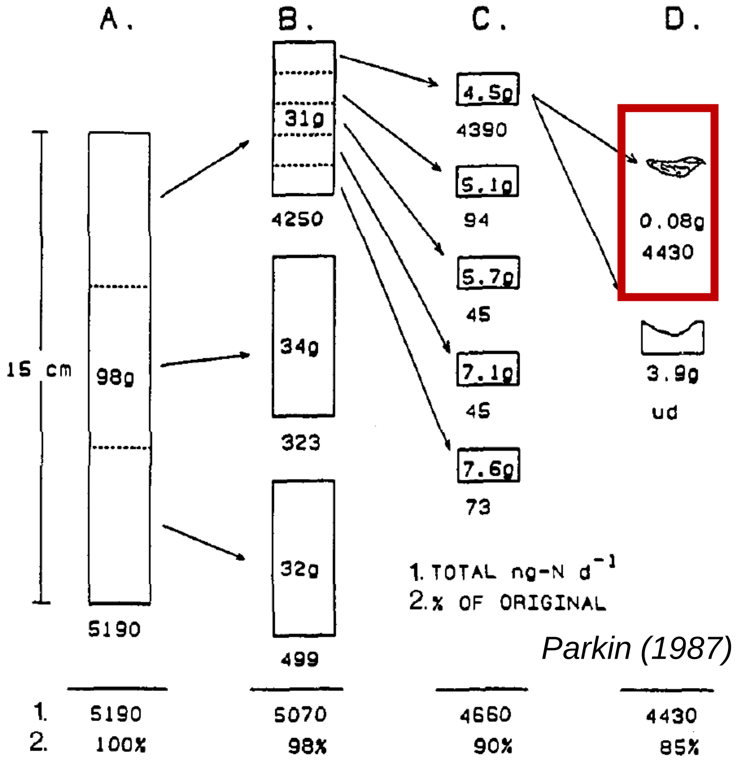
$\frac{\partial c}{\partial t_i}$ N reduction rate of redox zone *i*

- How to get a representative $\frac{\partial c}{\partial t_i}$ for each redox zone ?

= Extremely heterogenous N reduction rates at various scales

= e.g., <0.1 % of mass of soil responsible for 85% of N reduction capacity (Parkin, 1987)

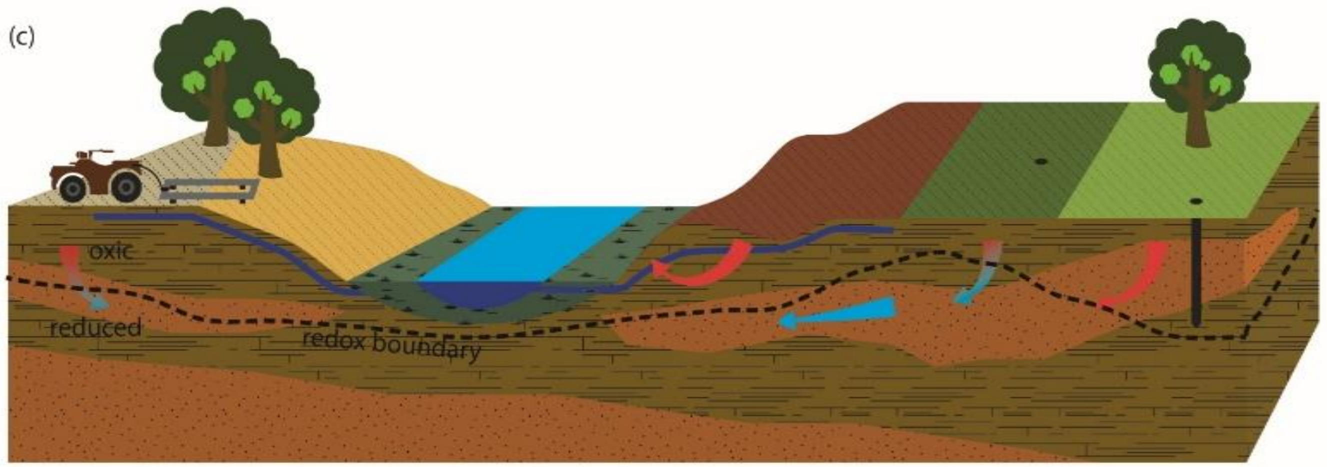




Parkin (1987)

Redox architecture in glacial landscapes

- **Primary controls on the redox architecture development**
  - Oxygen influx since the Holocene (~ 11 kyr)
  - Nitrate influx since the Anthropocene
  - Amount and reactivity of the reduced compounds (e.g., organic matter, pyrite)
  - Flow pathways



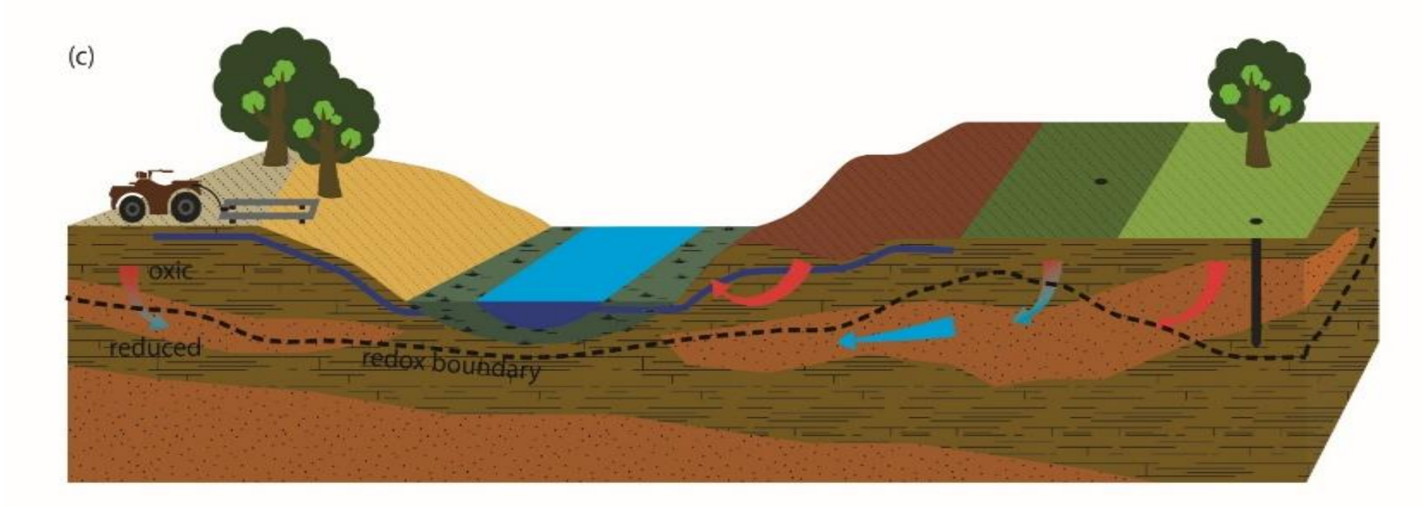
Challenge I: Upscaling

- **Primary controls on the redox architecture development**
  - Oxygen influx since the Holocene (~ 11 kyr)
  - Nitrate influx since the Anthropocene
  - Amount and reactivity of the reduced compounds (e.g., organic matter, pyrite)
  - Flow pathways

Weathering time

Geology

Geochemistry



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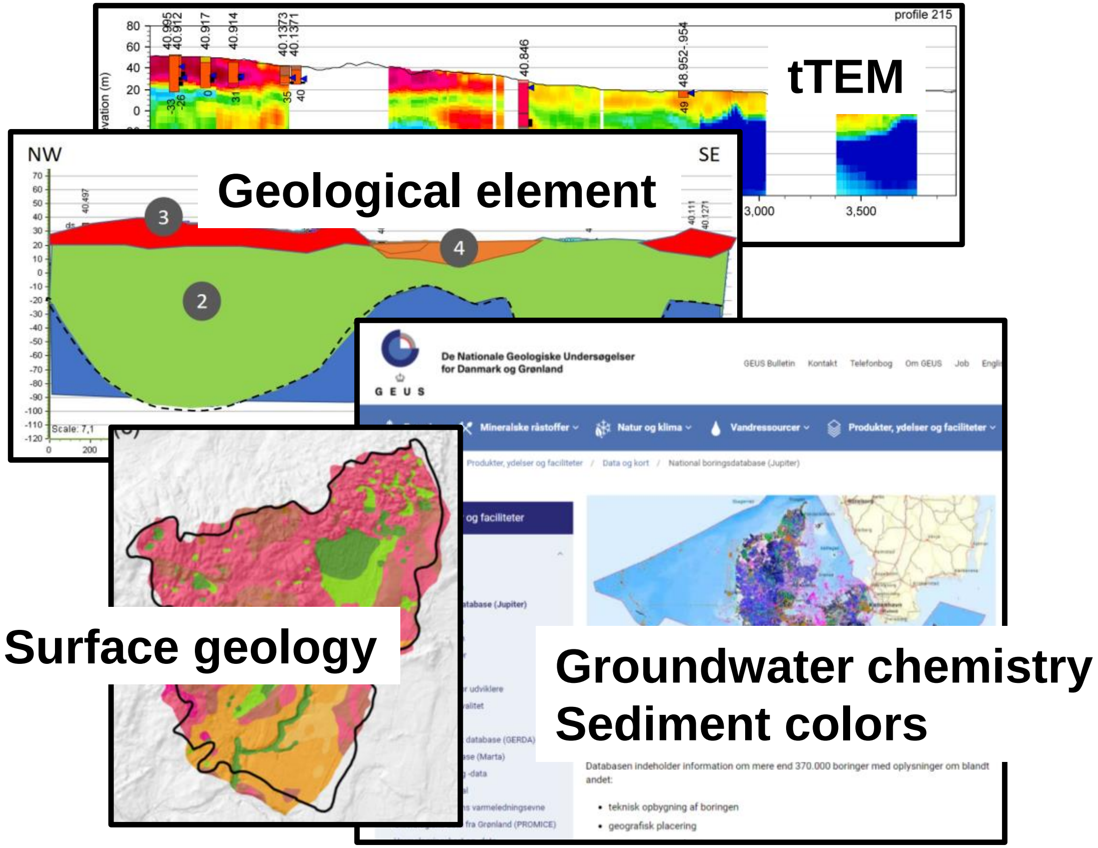
Challenge I: Upscaling

- Starts from planning…

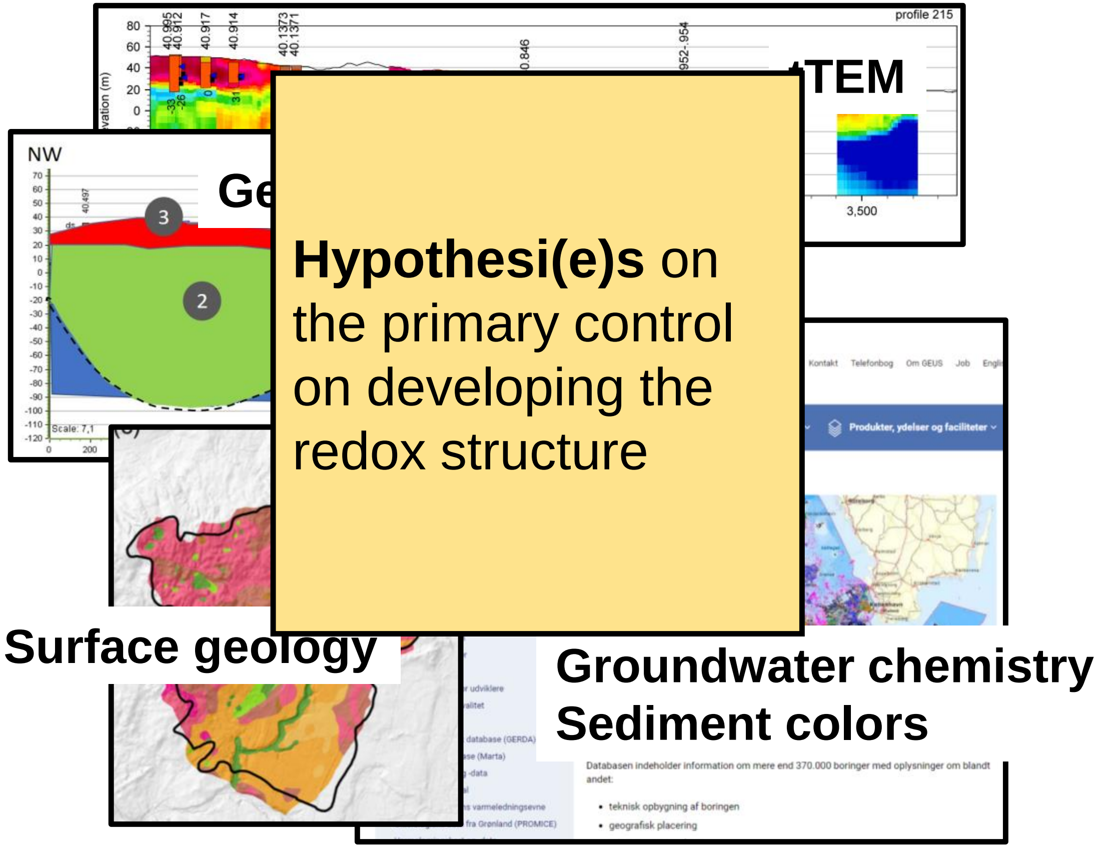
Selecting **representative** sampling point



Challenge I: Upscaling

- Starts from planning…

Selecting **representative** sampling point

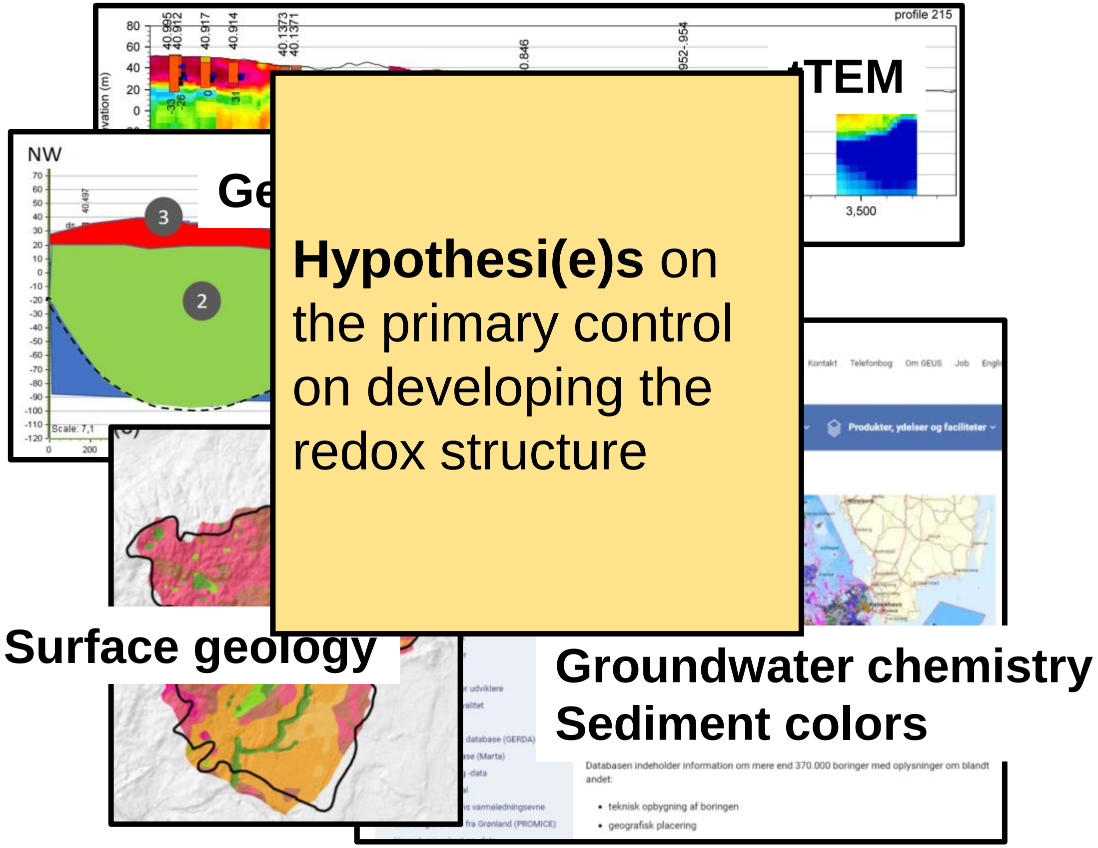


Hypothesi(e)s on the primary control on developing the redox structure

Challenge I: Upscaling

- Starts from planning…

Selecting **representative** sampling point → Field sampling → Laboratory analysis

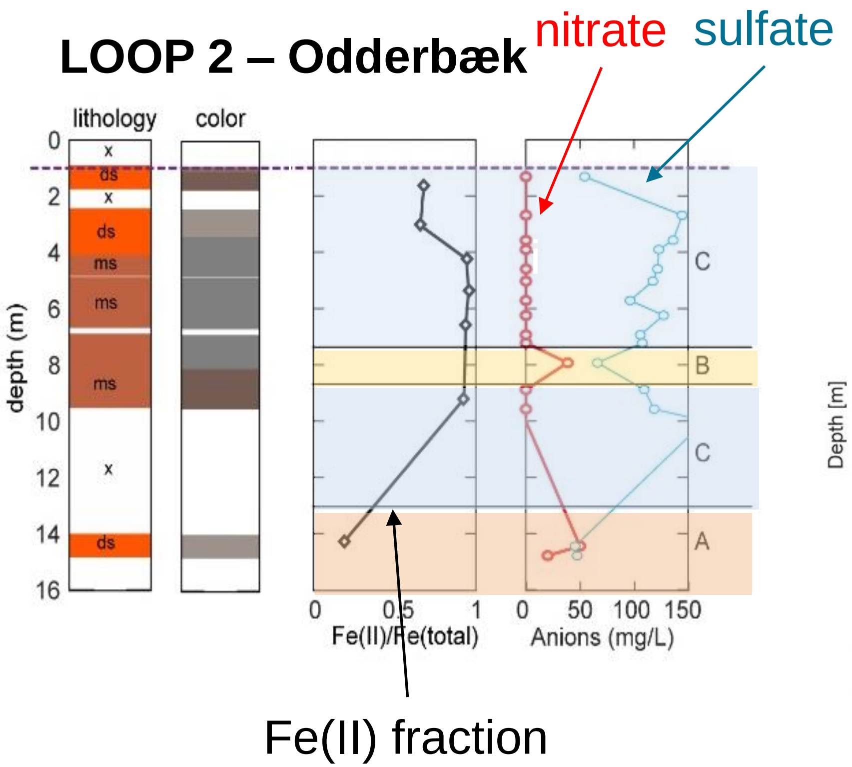


Hypothesi(e)s on the primary control on developing the redox structure

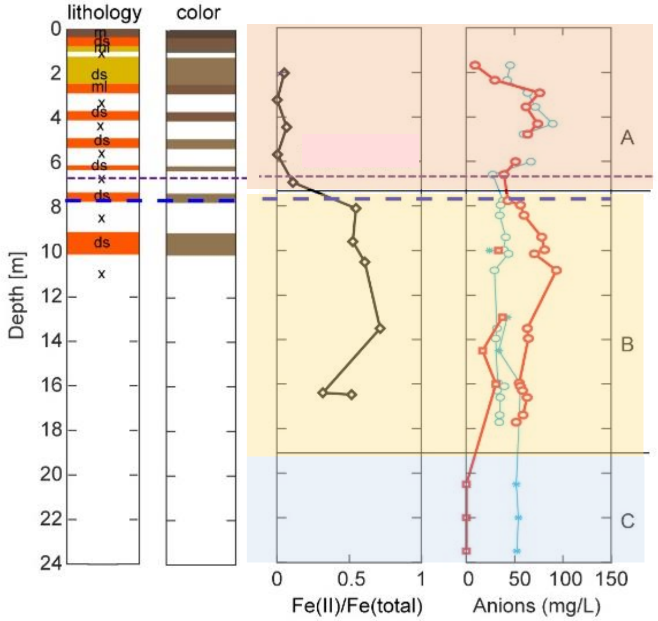
Challenge I: Upscaling

- Redox interpretations
  - Multiple redox conditions shifts in many cases

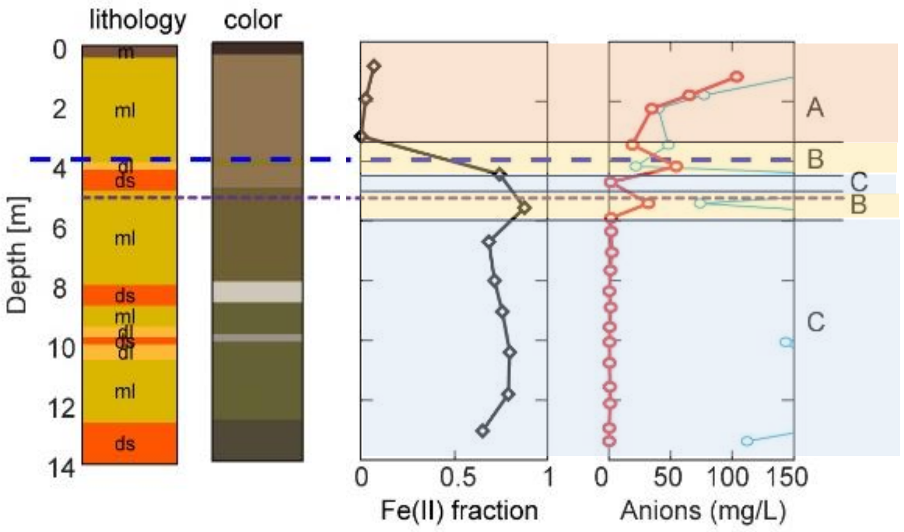
LOOP 2 – Odderbæk



Javngyde



Sillerup



Hansen et al. (2021)

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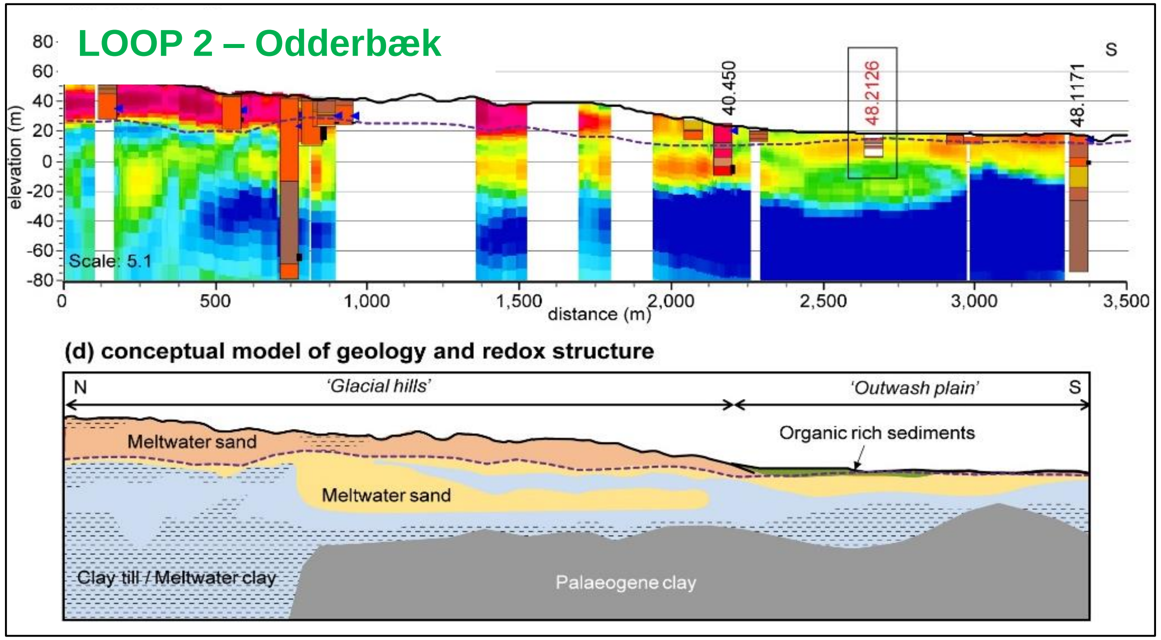
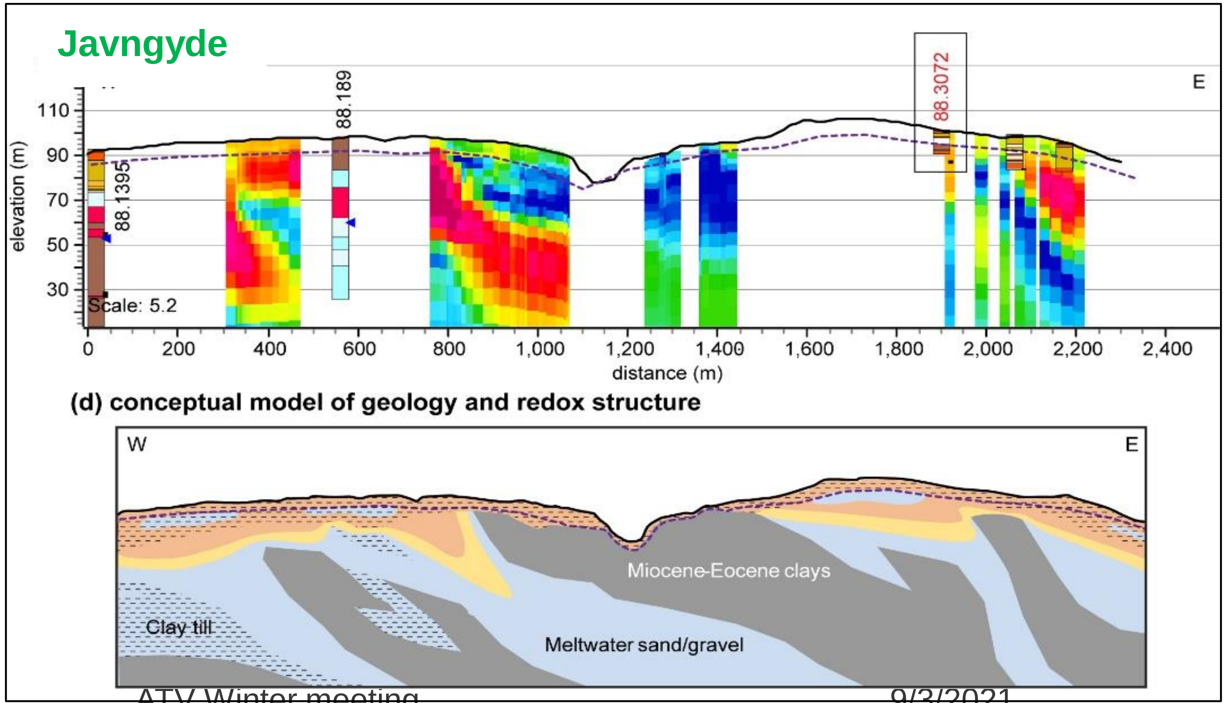
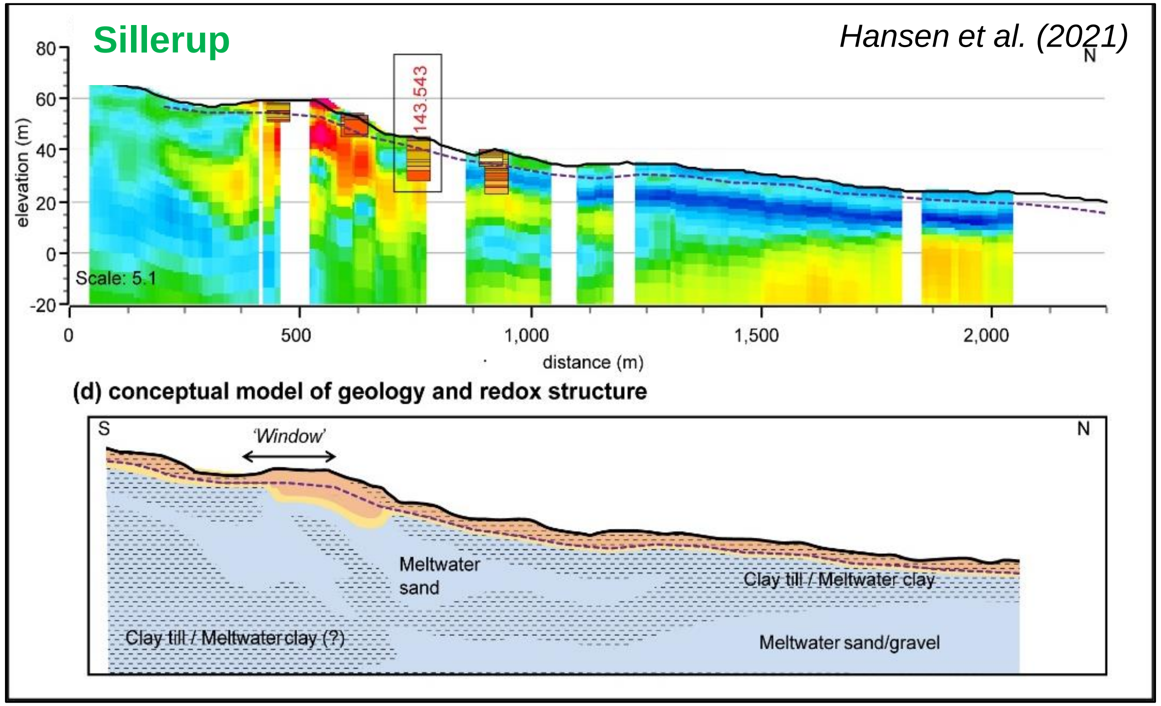
Challenge I: Upscaling

- Redox interpretations and upscaling

  - Conceptual interpretation of the redox architecture



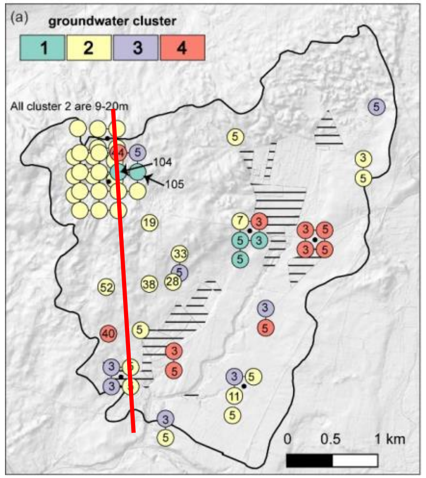


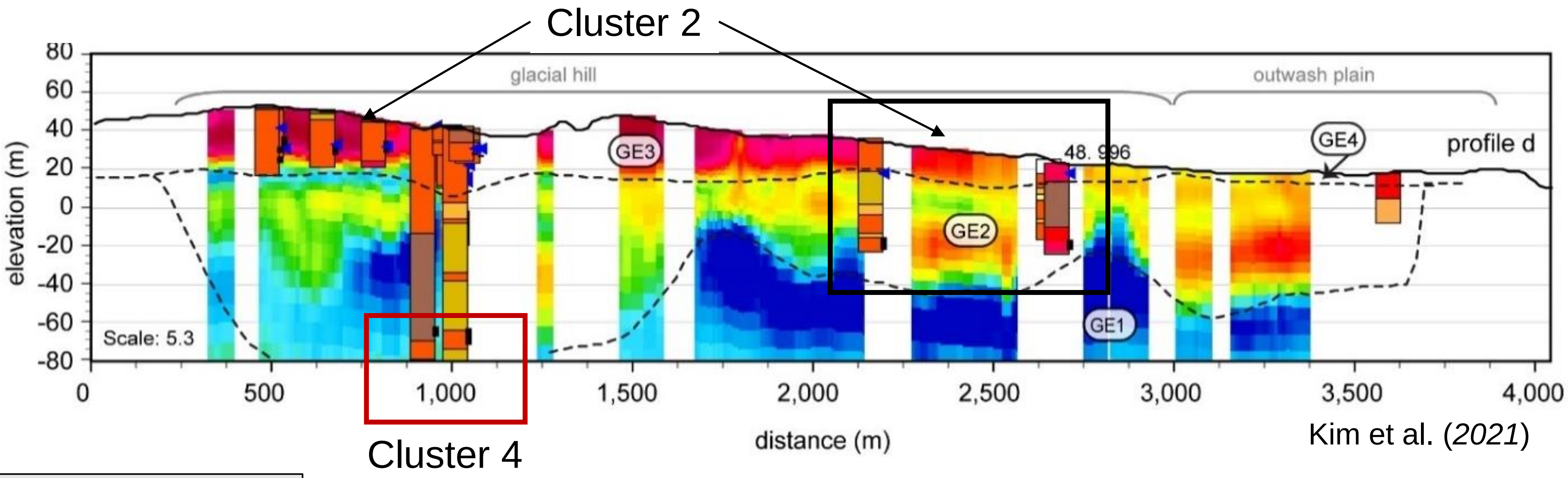


Hansen et al. (2021)

Challenge I: Upscaling

- Redox interpretation and upscaling
    - Statistical analysis of the groundwater heterogeneity





Kim et al. (*2021*)

Cluster 1 = **(N reduction)** organic carbon oxidation – nitrate reduction
Cluster 2 = **(Oxic)** weathering with CO_2 or nitric acid
Cluster 3 = **(Oxic)** weathering with nitric acid
Cluster 4 = **(N reduction)** pyrite oxidation –nitrate reduction

GE1: Paleogene Clay
GE2: Quaternary Sequence of clay and sand
GE3: Glacial Hill
GE4: Outwash plain

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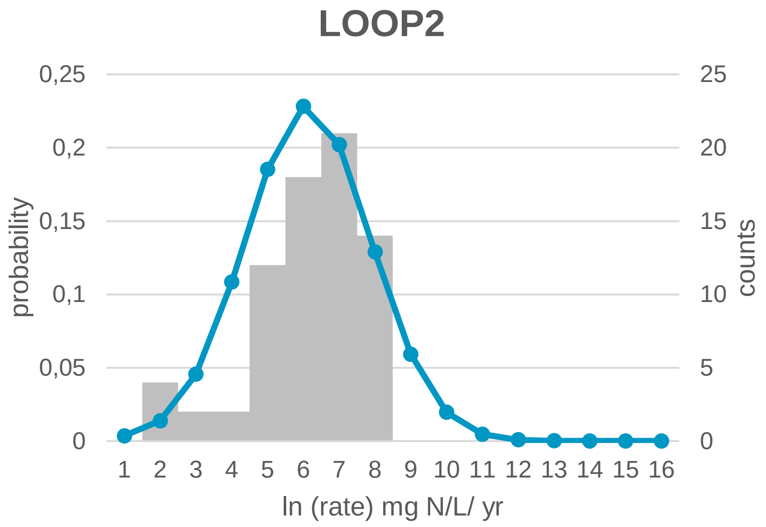
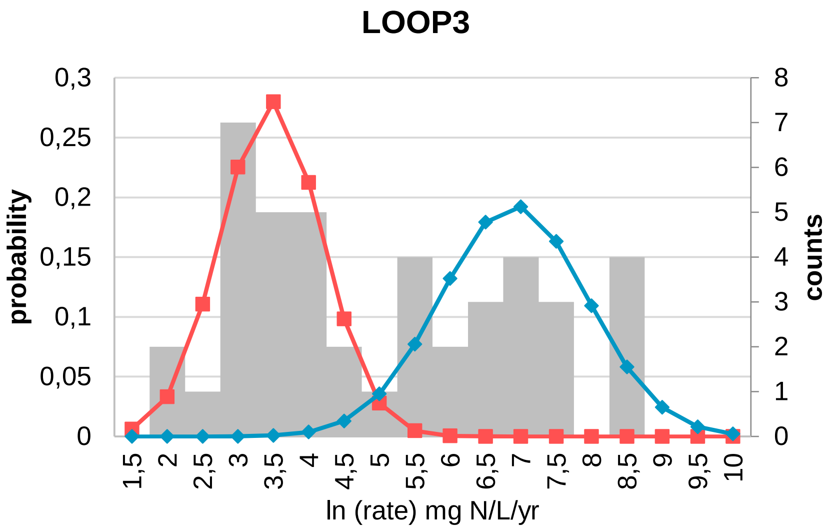
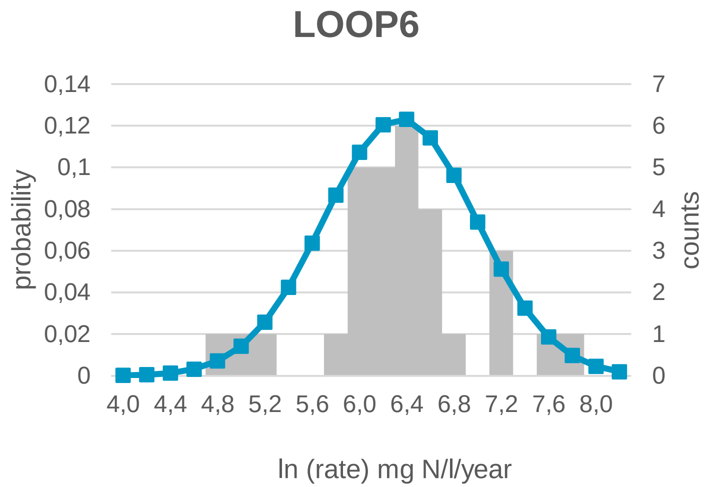
Challenge II: Parameterization

- **Representative N reduction rates?**







- sampling sites were carefully selected based on the structural information but the N reduction rates vary over a few orders of magnitude.

- In general, N reduction rate measurements of each site show a log-normal distribution.

= multiplicative effects may show a log normal distribution

= **reduced compounds x microbial density x oxygen free condition**

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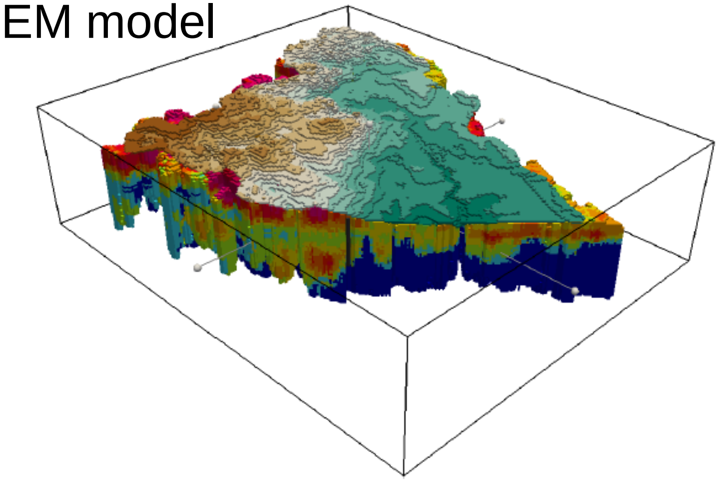
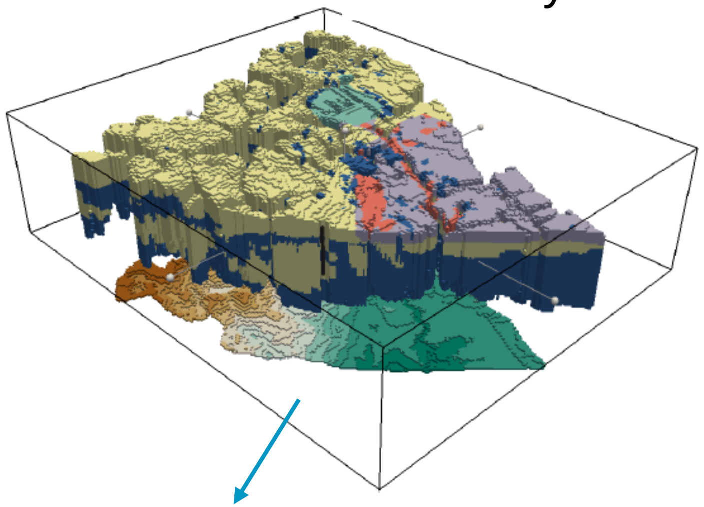
Summary: upscaling and parameterization

tTEM model



Geological structure
Hydrogeological information

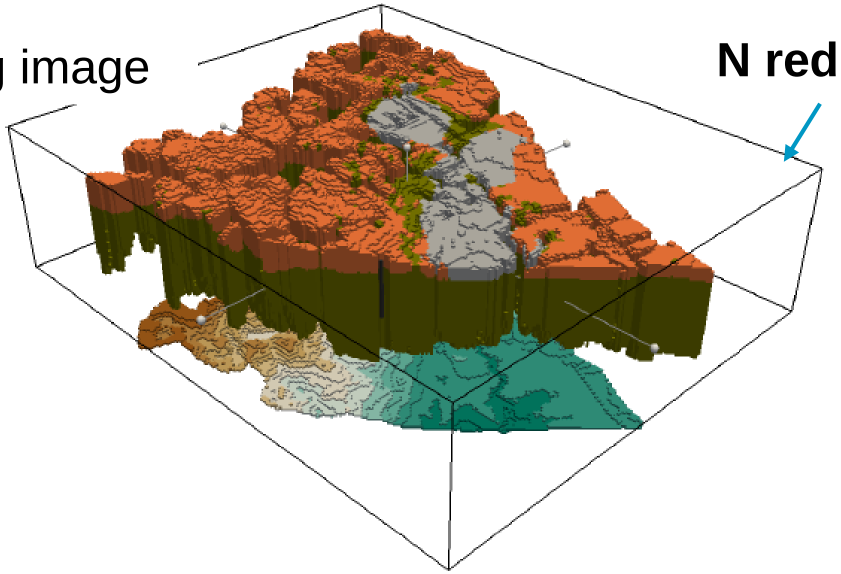
Groundwater chemistry model



Field campaign planning

N reduction rate determination

Redox training image



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Summary: upscaling and parameterization

Groundwater chemistry model

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Lessons learned…

- Geological structure plays a primary role in shaping the redox structure.
- Field measurements are required to locate the denitrifying zones.
- A reduced condition does not necessarily indicate a high N reduction capacity (or rate).
- Denitrification rates vary significantly site to site. Underlying controls on this variability requires further research.
- Solid understandings of the geological structure and the hydrogeochemical dynamics of the catchment is critical to interpret the geophysical information into the redox information.