Using tTEM to Upscale Geochemical Knowledge

Geofysik Forum

7th June 2023

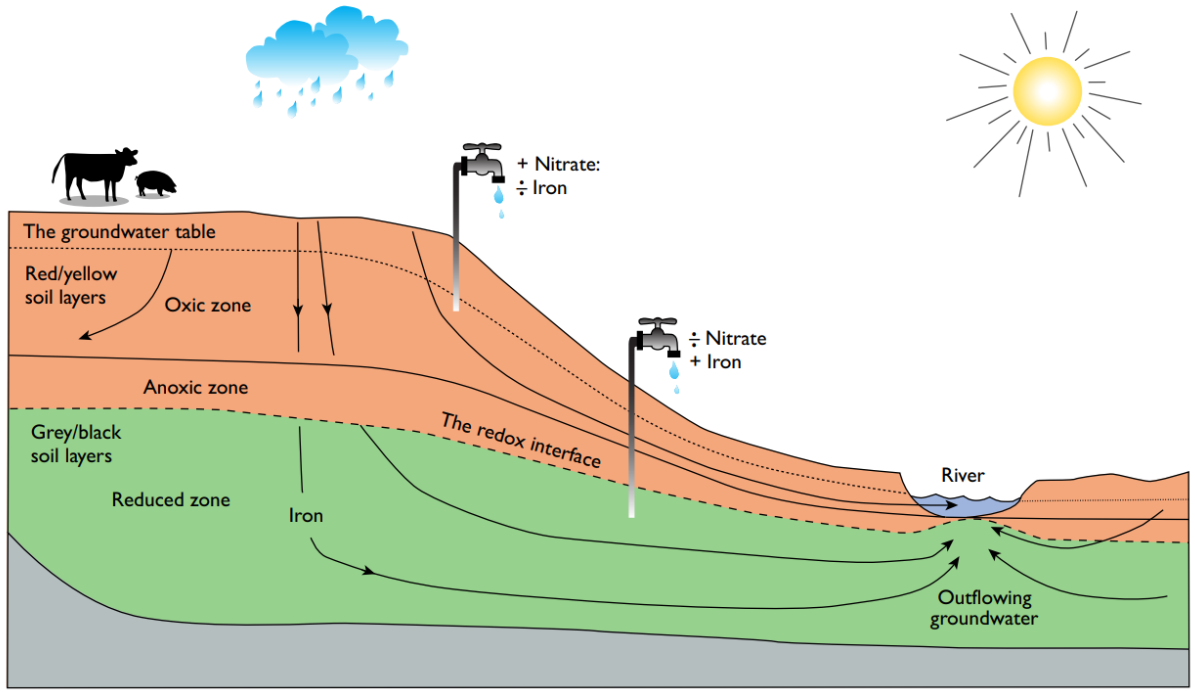
Hyojin Kim
Rasmus Jakobsen, Jens Aamand, and Birgitte Hansen

Innovationsfonden MapField

GEUS

What we already know about the nitrate reduction in the subsurface

- Nitrate is reduced only after oxygen is depleted.



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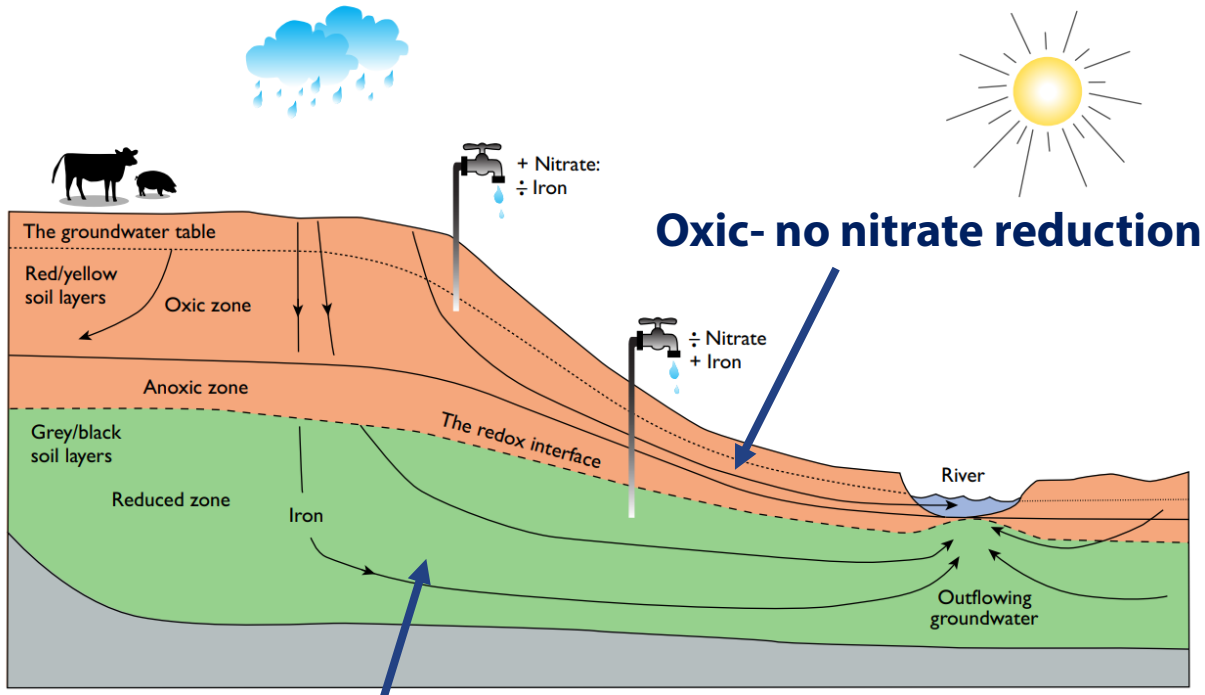

Oxic- no nitrate reduction

Reduced- nitrate reduction

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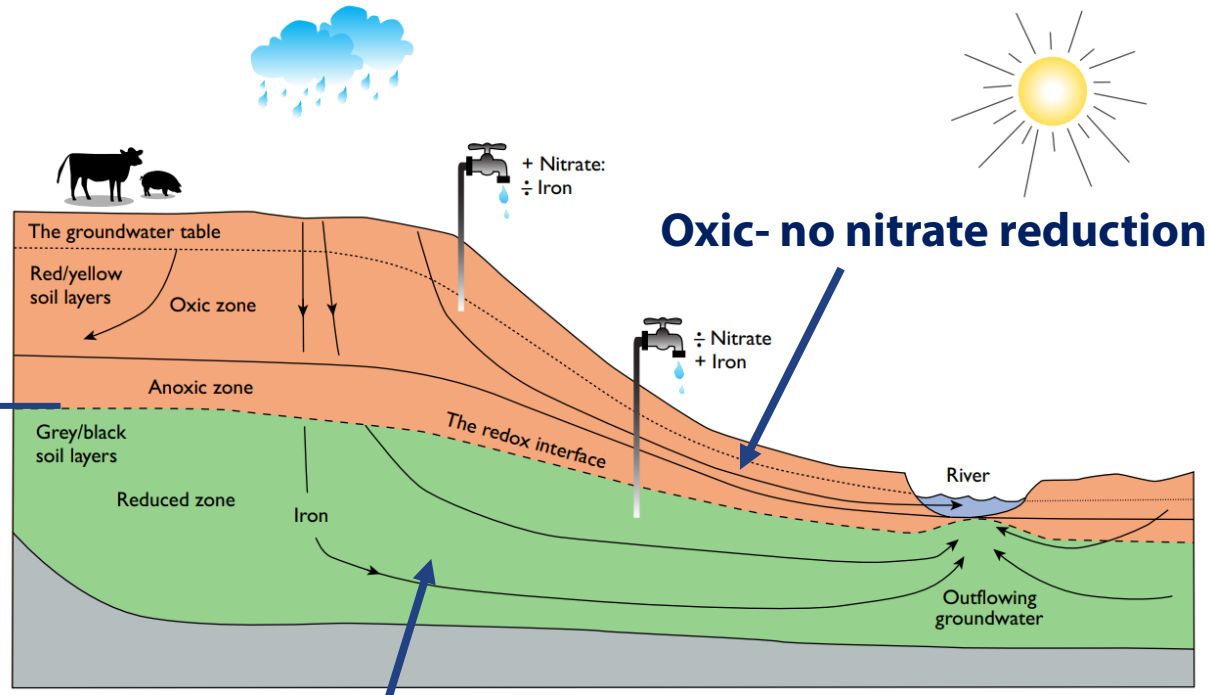
Redox boundary



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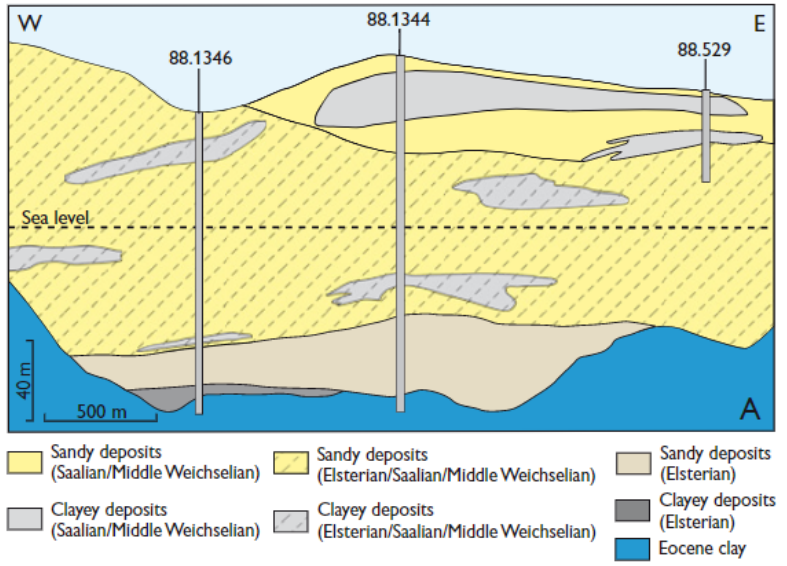

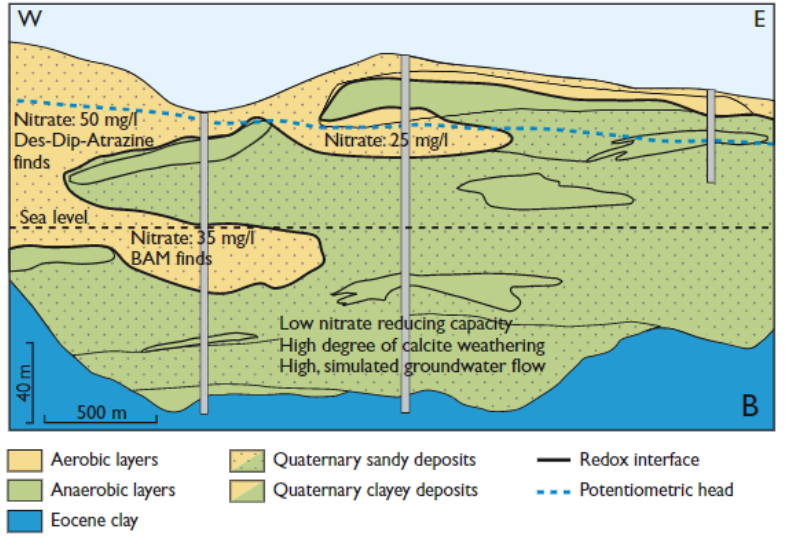

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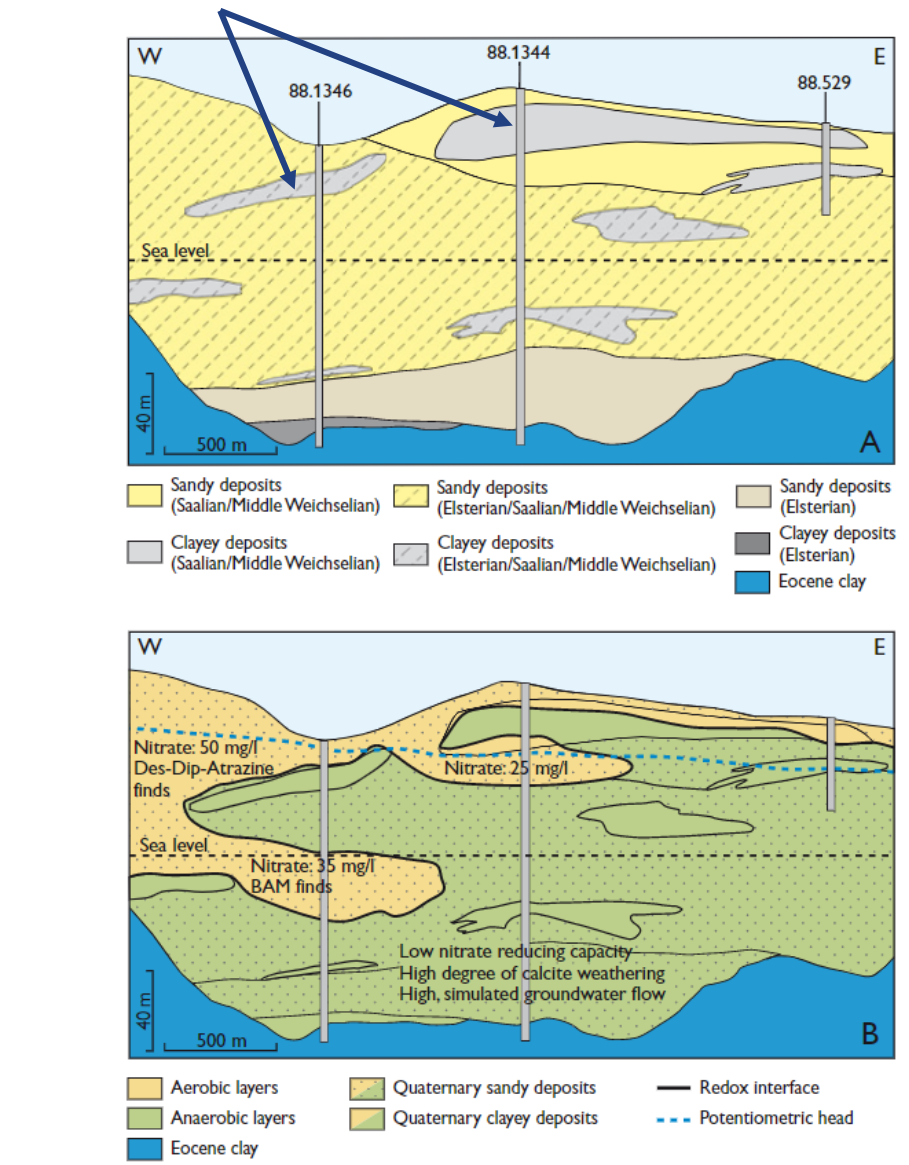

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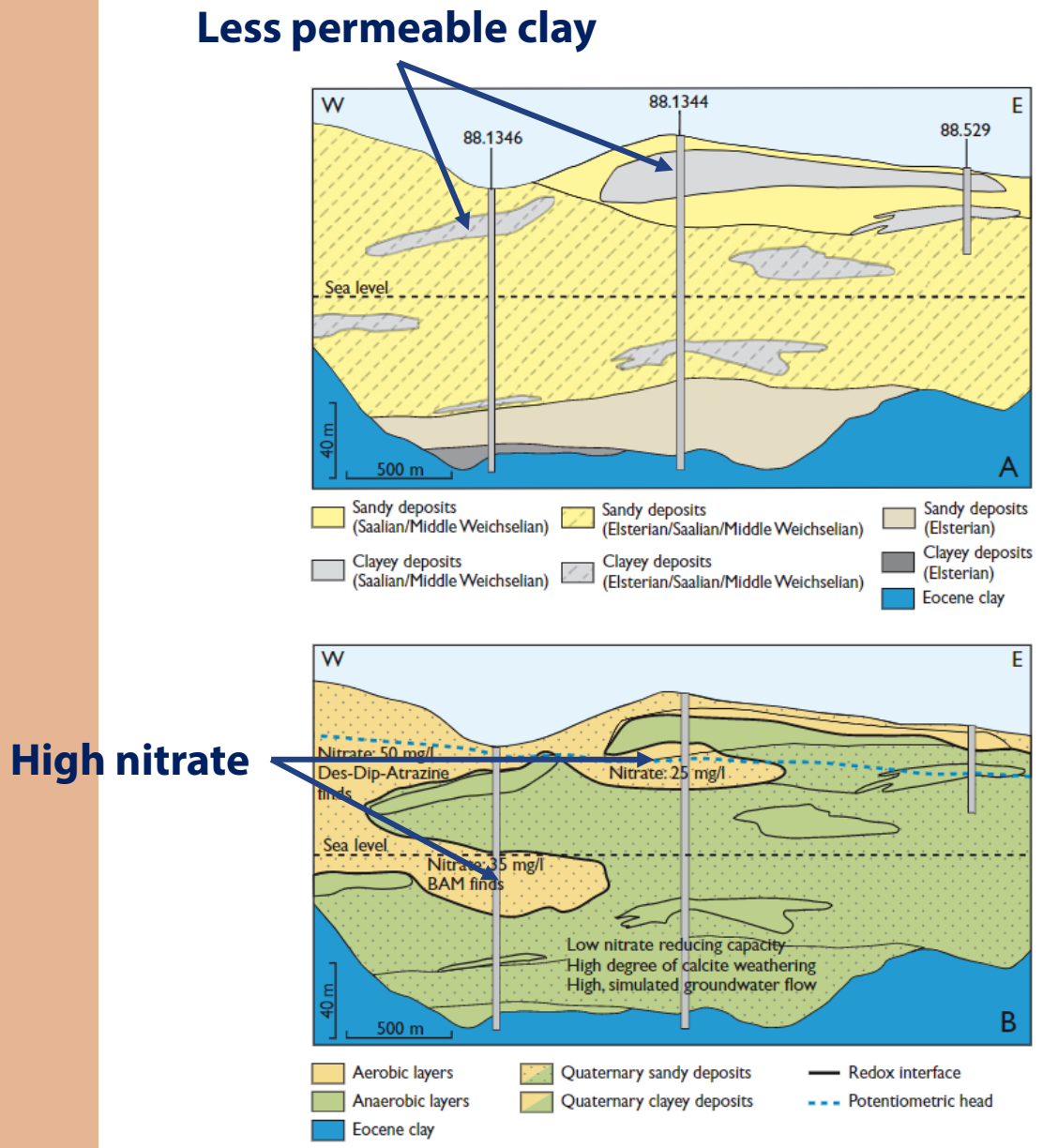

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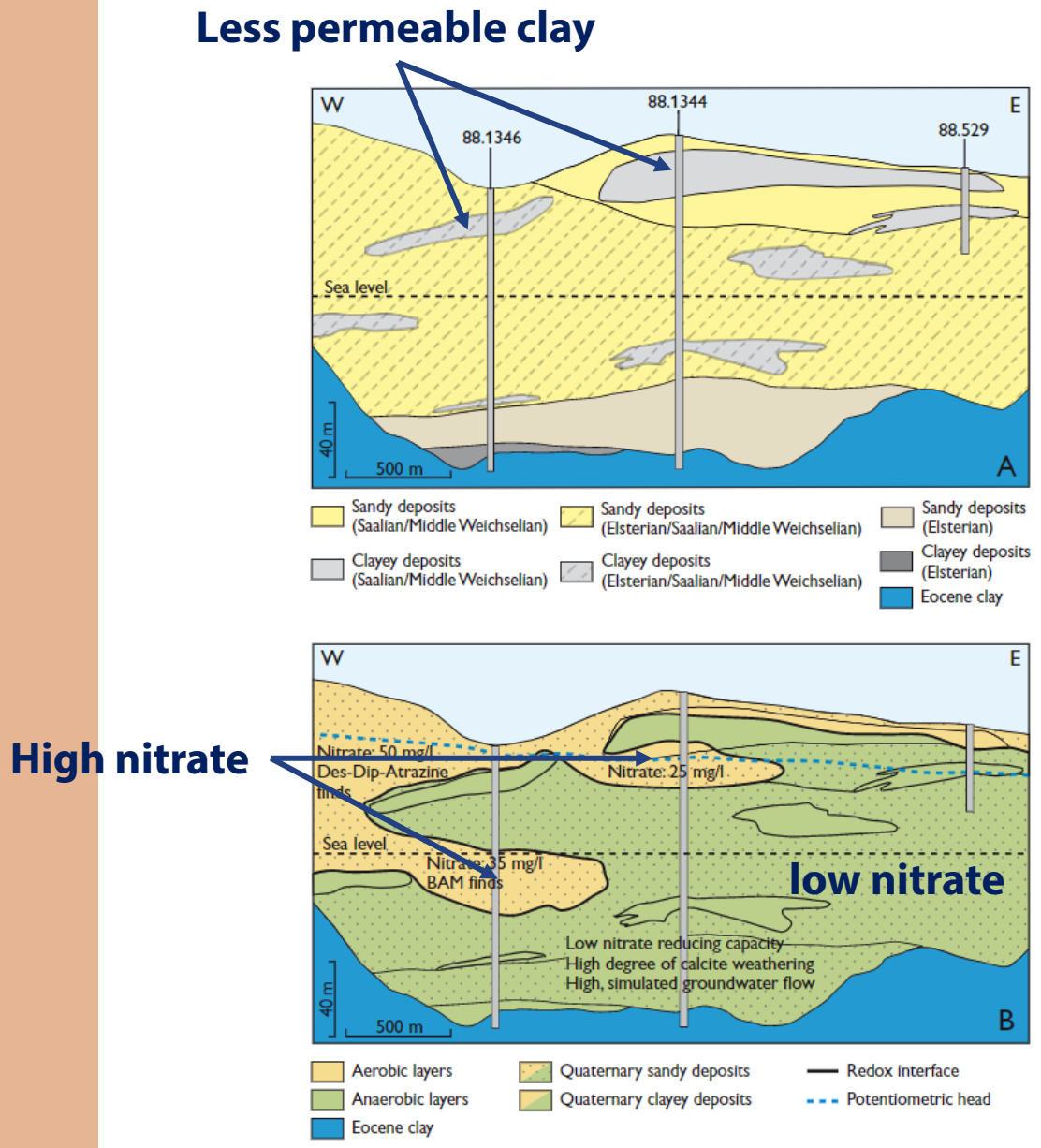

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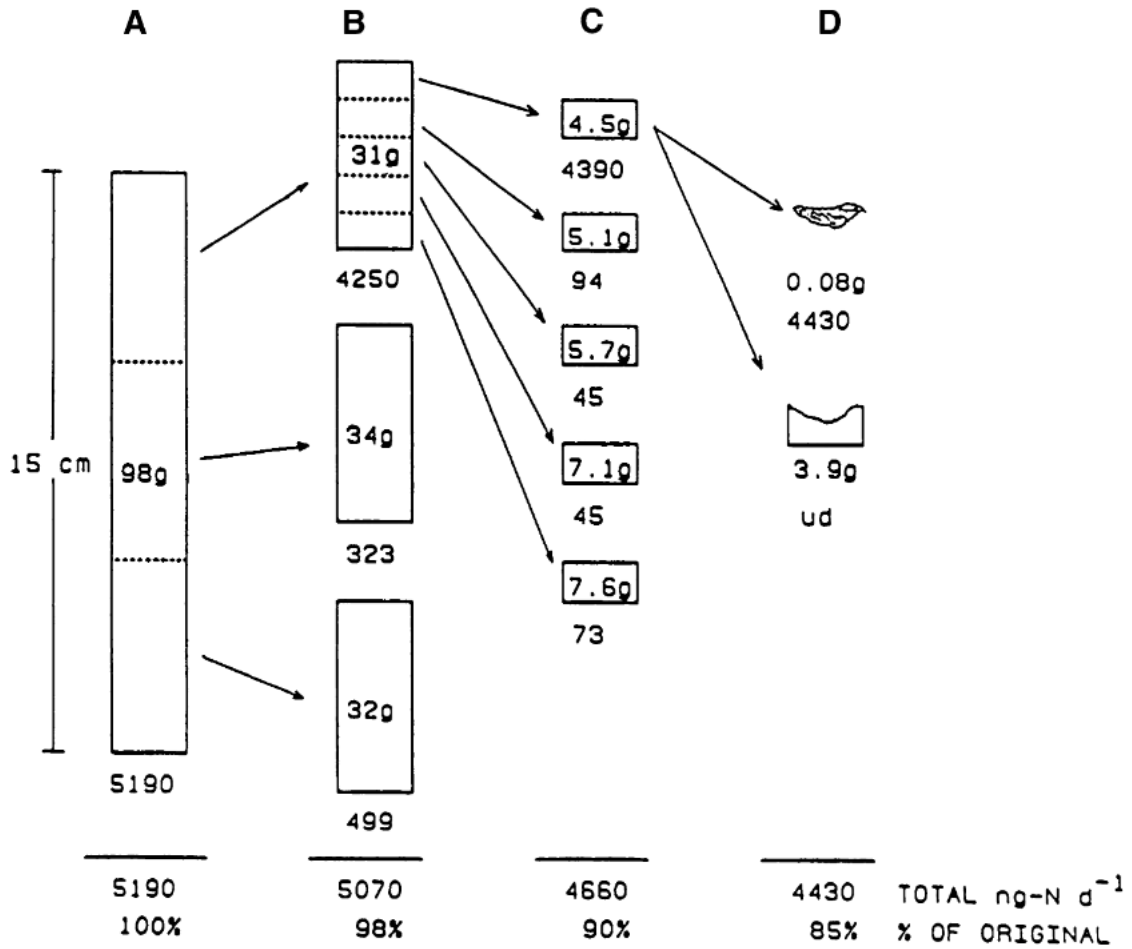
- Hotspots of denitrification result in the high variability of denitrification



Parkin (1987)

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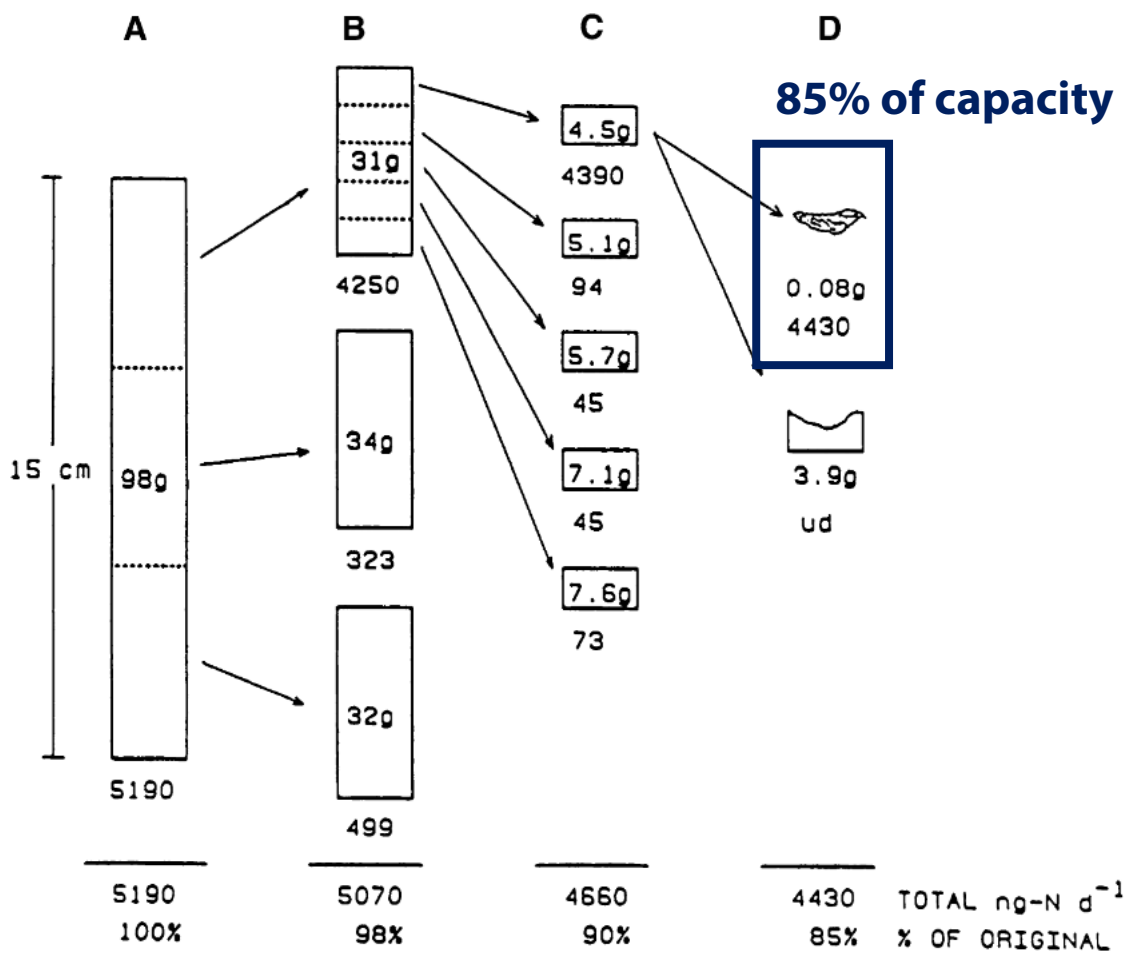

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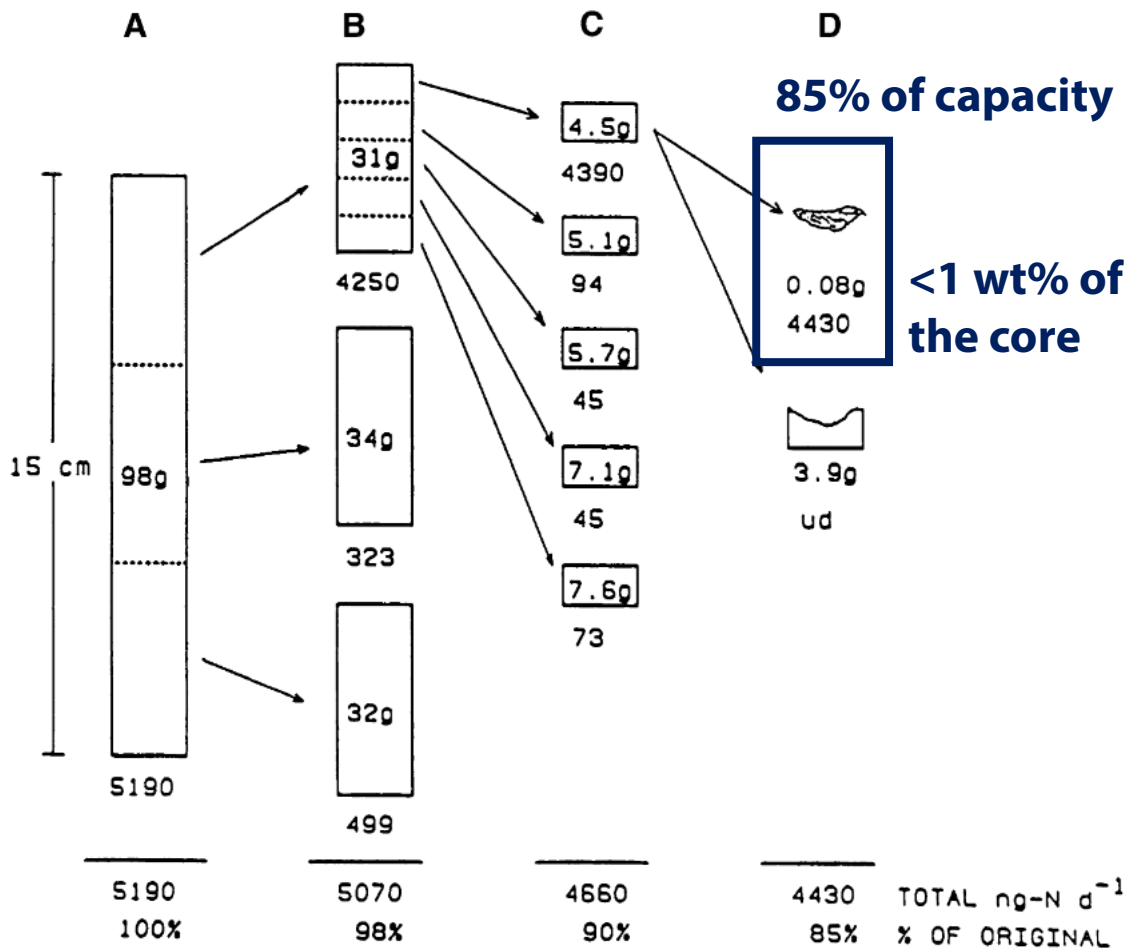

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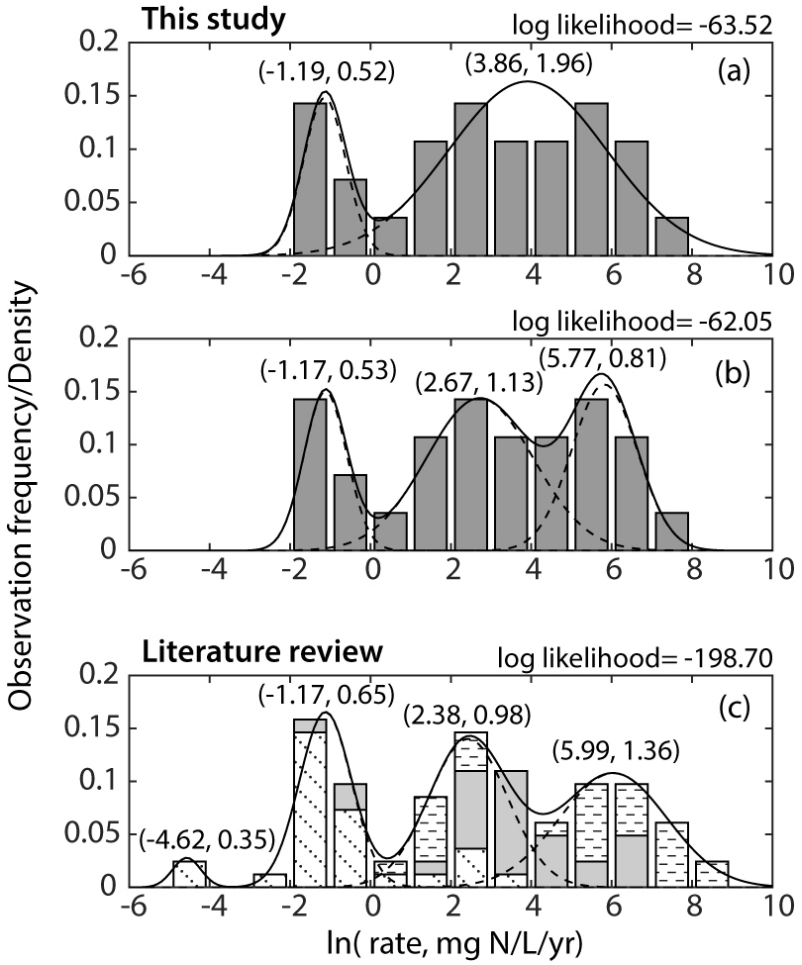

Kim et al. (2021b)

What we already know about the nitrate reduction in the subsurface

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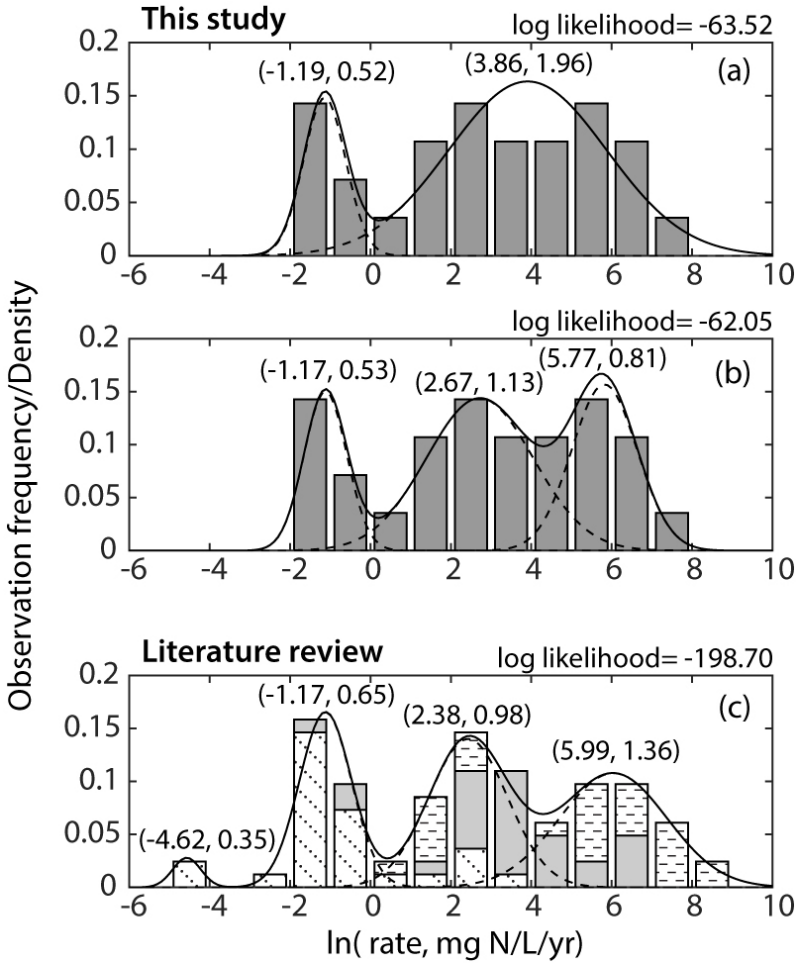
How could we upscale point-scale geochemical information to the catchment or larger scale?



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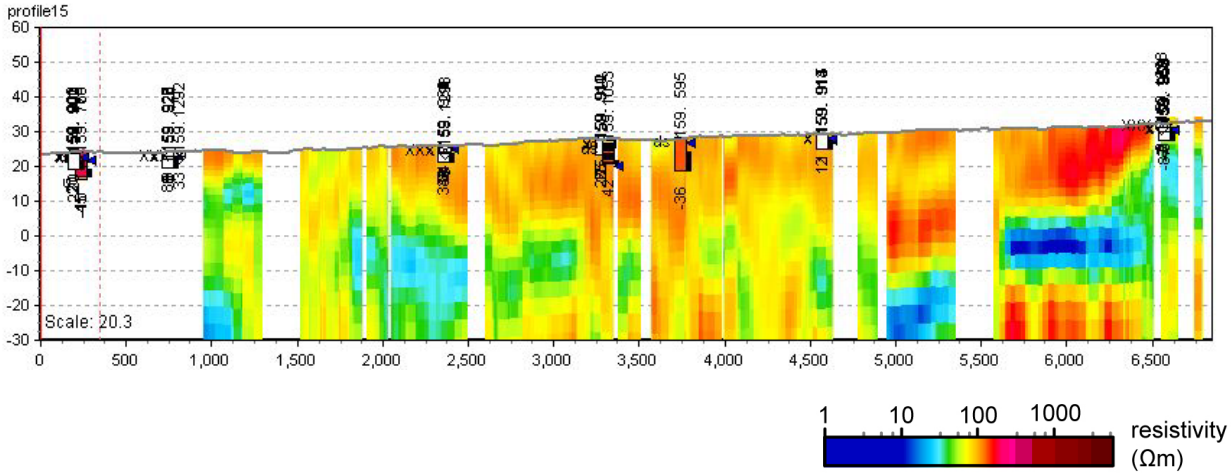
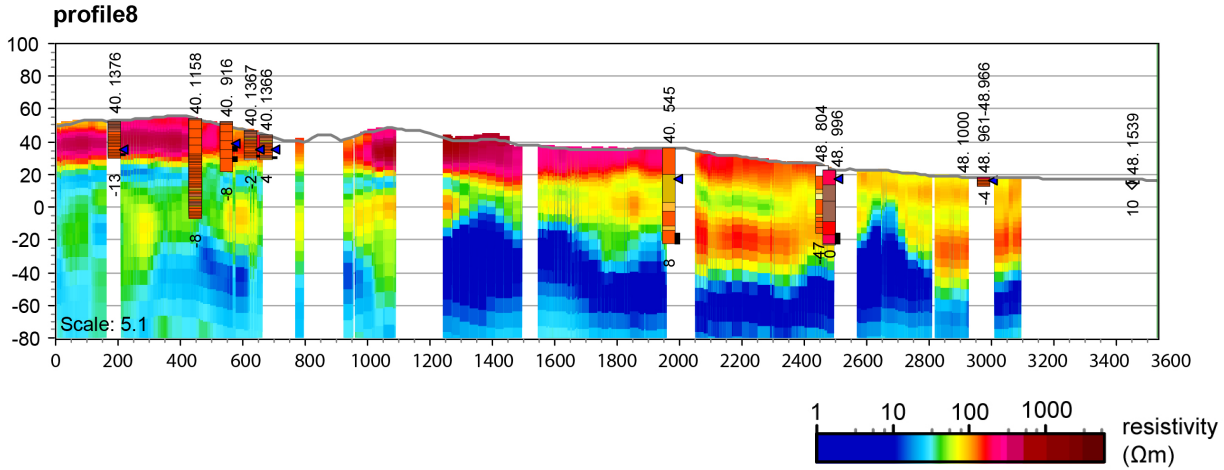
How could we upscale point-scale geochemical information to the catchment or larger scale?
: Using geophysical information





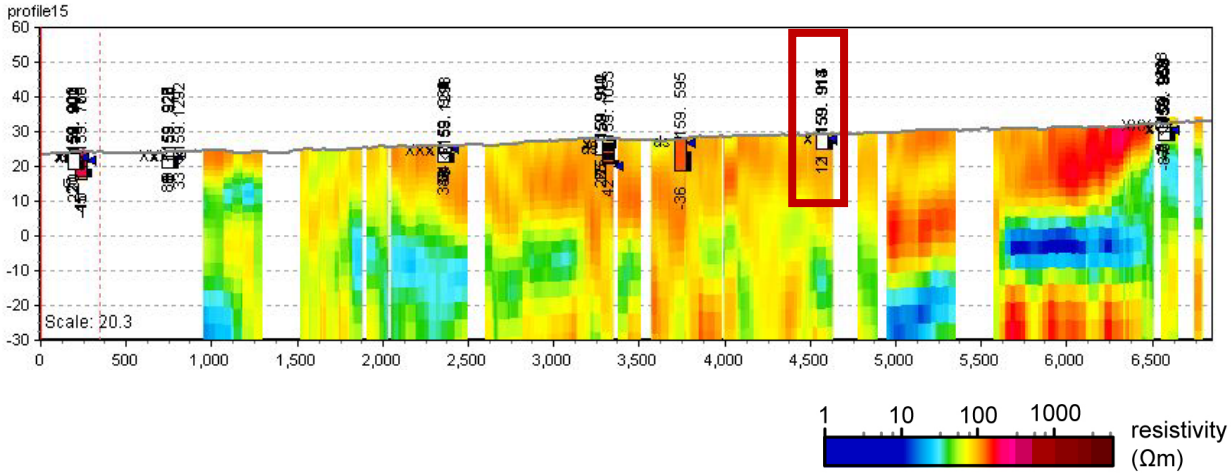
Innovationsfonden MapField

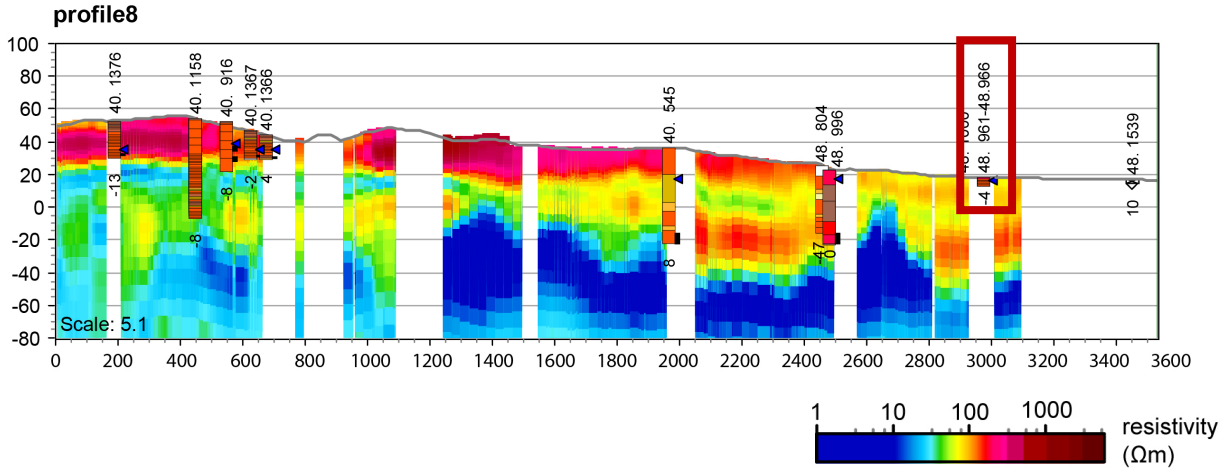
What we already know about the nitrate reduction in the subsurface

- Nitrate is reduced only after oxygen is depleted.

How could we upscale point-scale geochemical information to the catchment or larger scale?
: Using geophysical information. But cannot be directly translated into geochemical information.

: more comprehensive understanding of both geochemical and hydrogeological information is needed.





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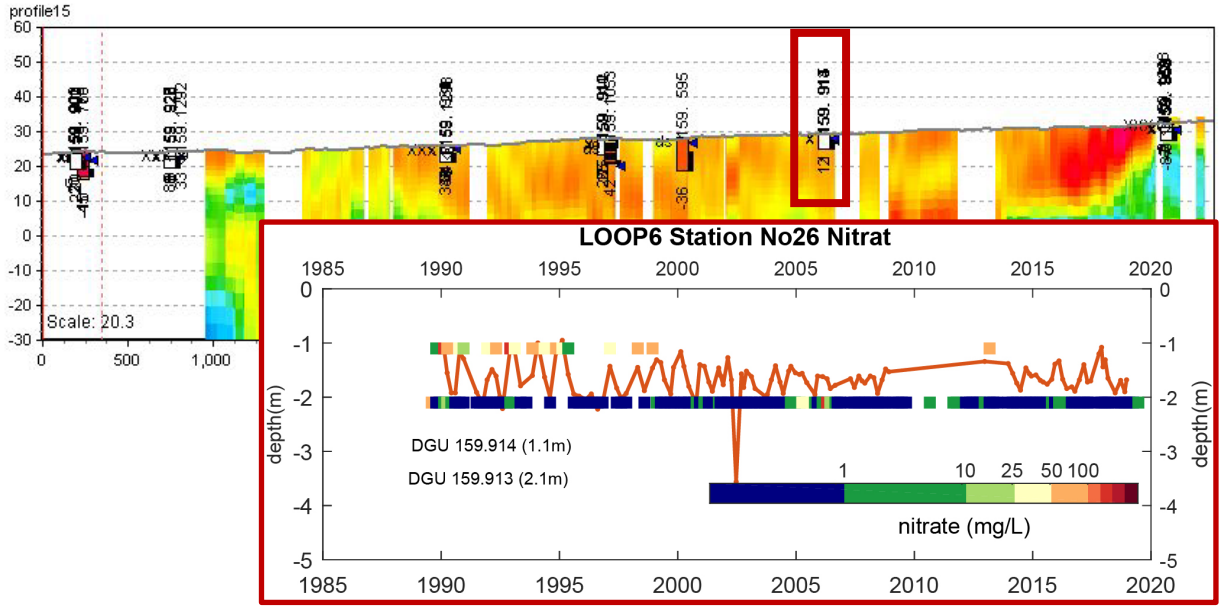

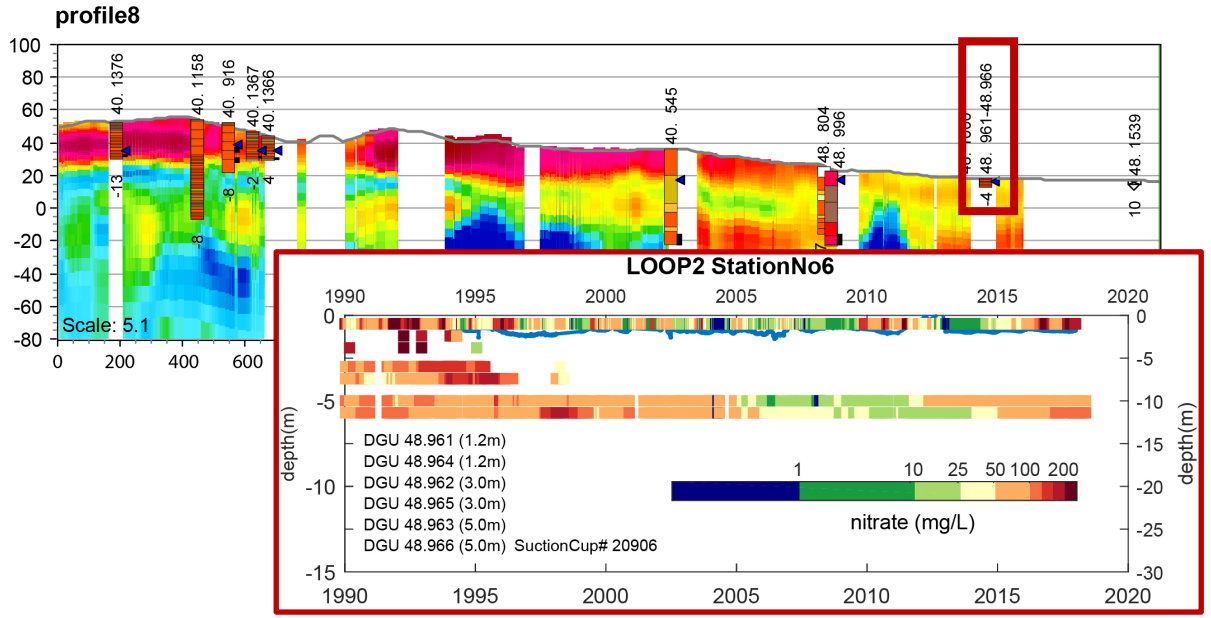

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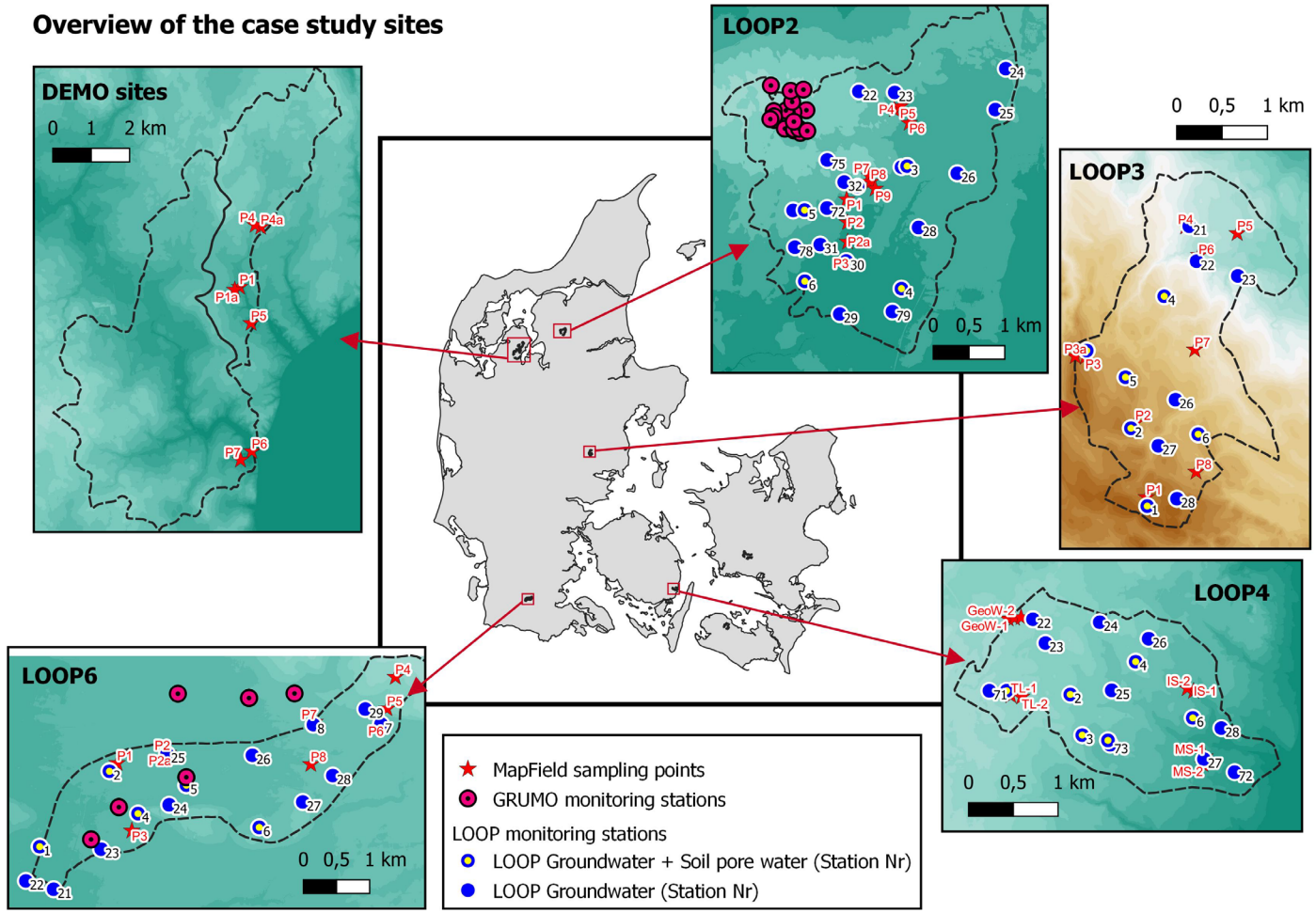
MapField case sites

- Long-term monitoring data of groundwater and stream chemistry
- Subsurface structural information from geophysical and geological investigations
- Sediment color data
- High resolution surface geology map



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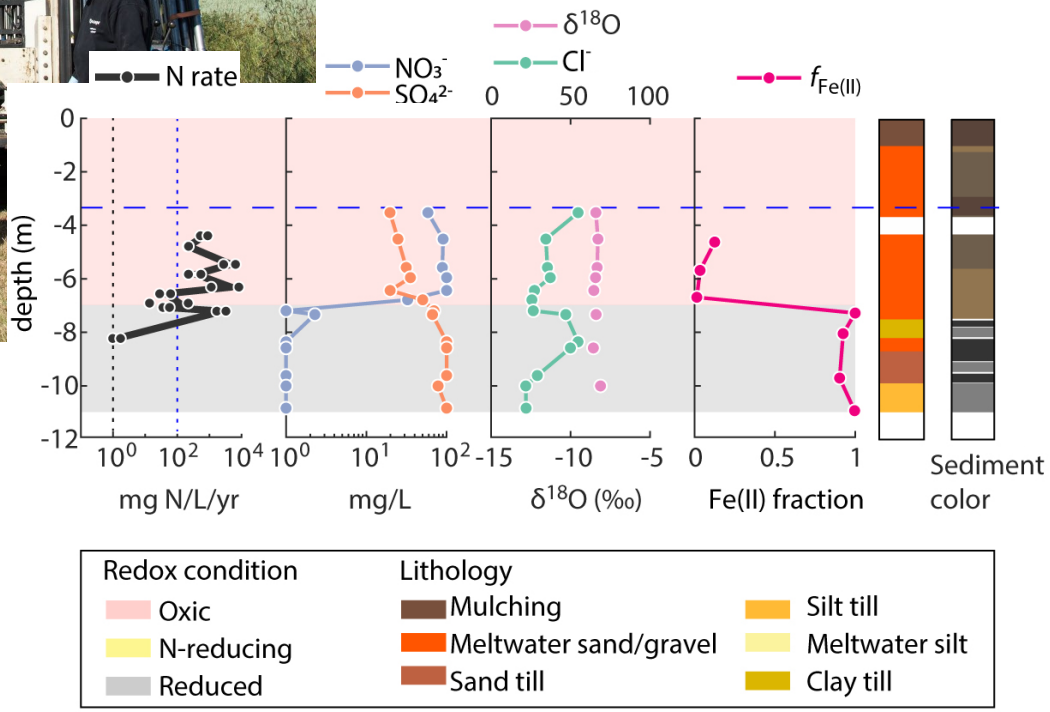

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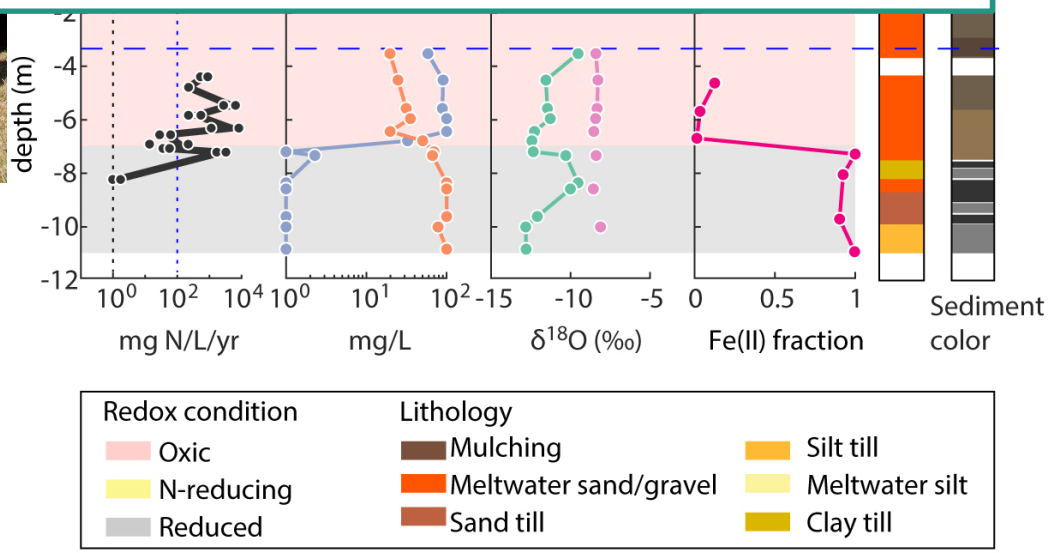
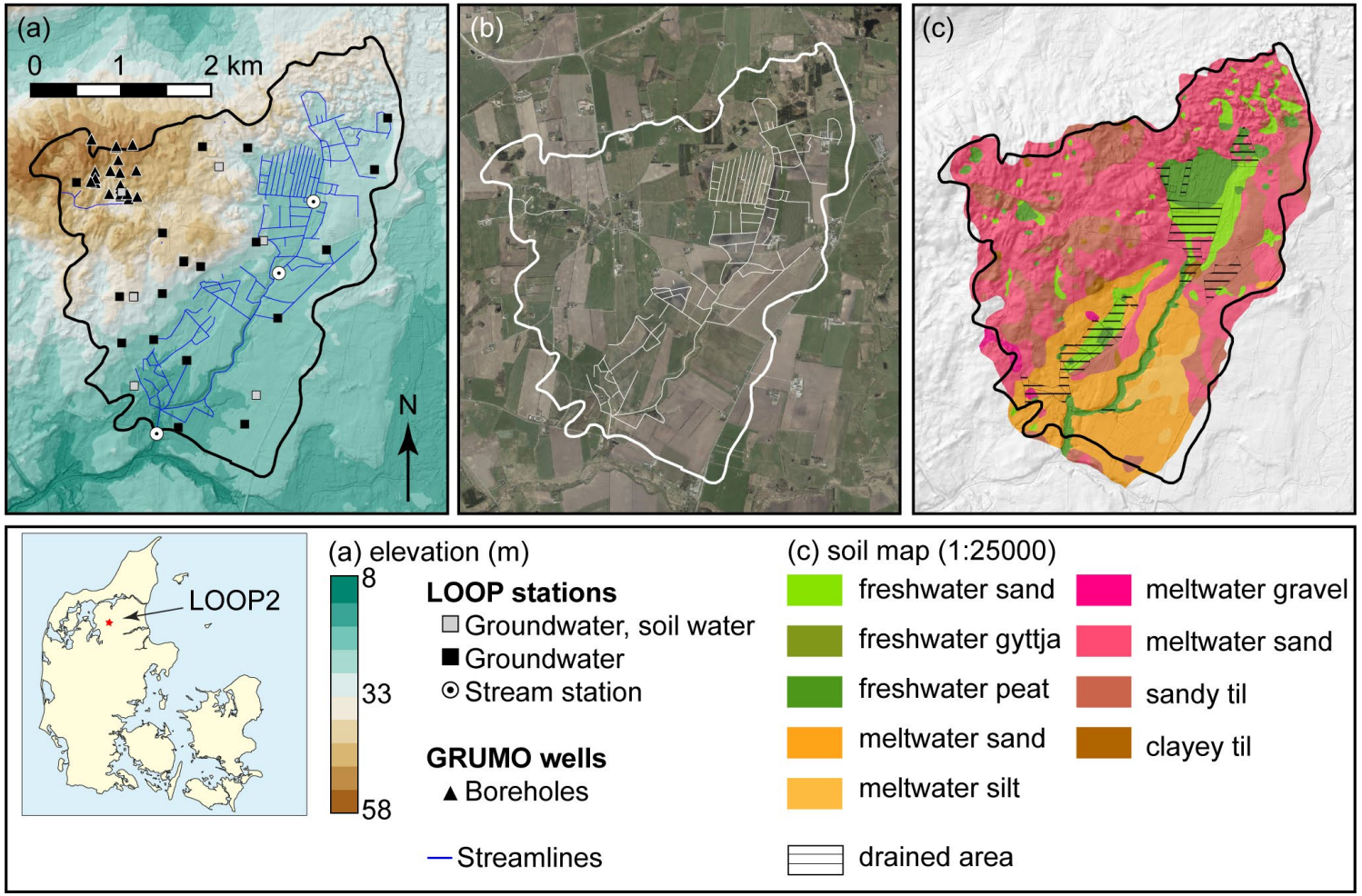
Objective: Building training images (TI) of geochemical properties for geostatistical and hydrological modelling



Case I: Where does denitrification occur in the subsurface at the catchment scale?

LOOP2 case study site

- Intensively-managed agricultural catchment
- Meltwater sand/gravel dominated surface geology
- Part of the National monitoring program

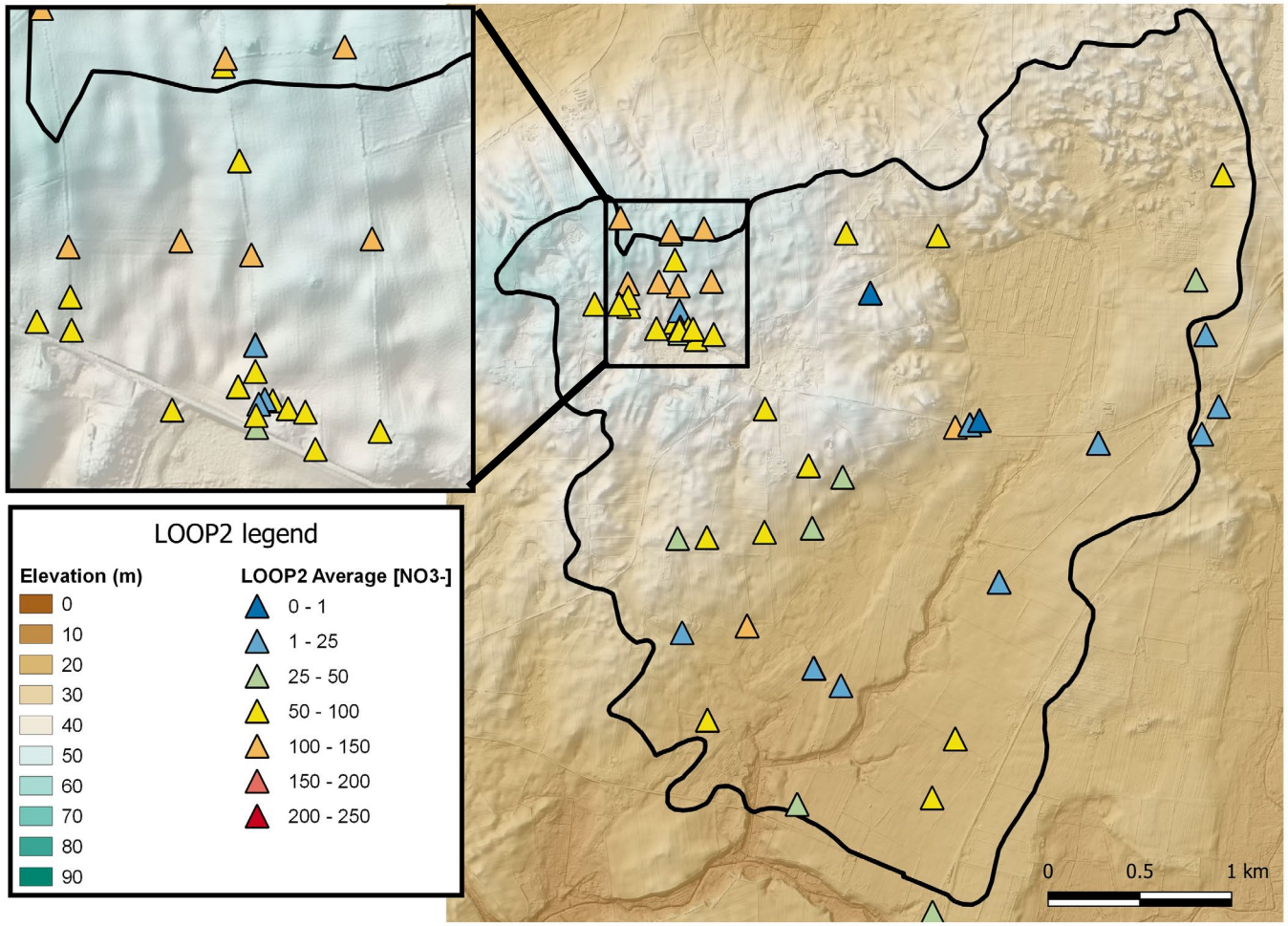


Kim et al. (2021b)

Case I: Where does denitrification occur in the subsurface at the catchment scale?

LOOP2 case study site

- Overall, high nitrate in high elevation vs. low nitrate in low elevation
- But still, high nitrate cases in low elevation

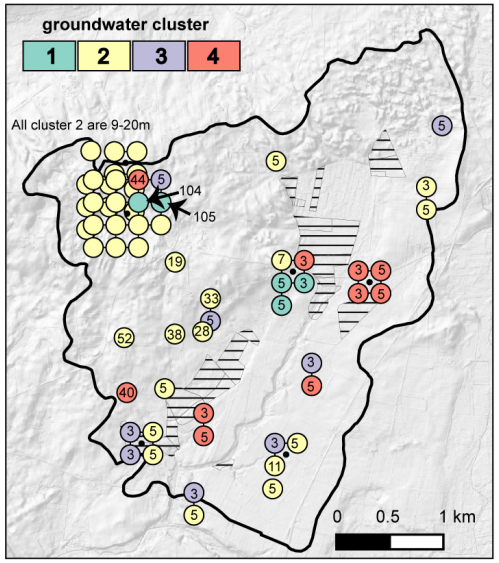


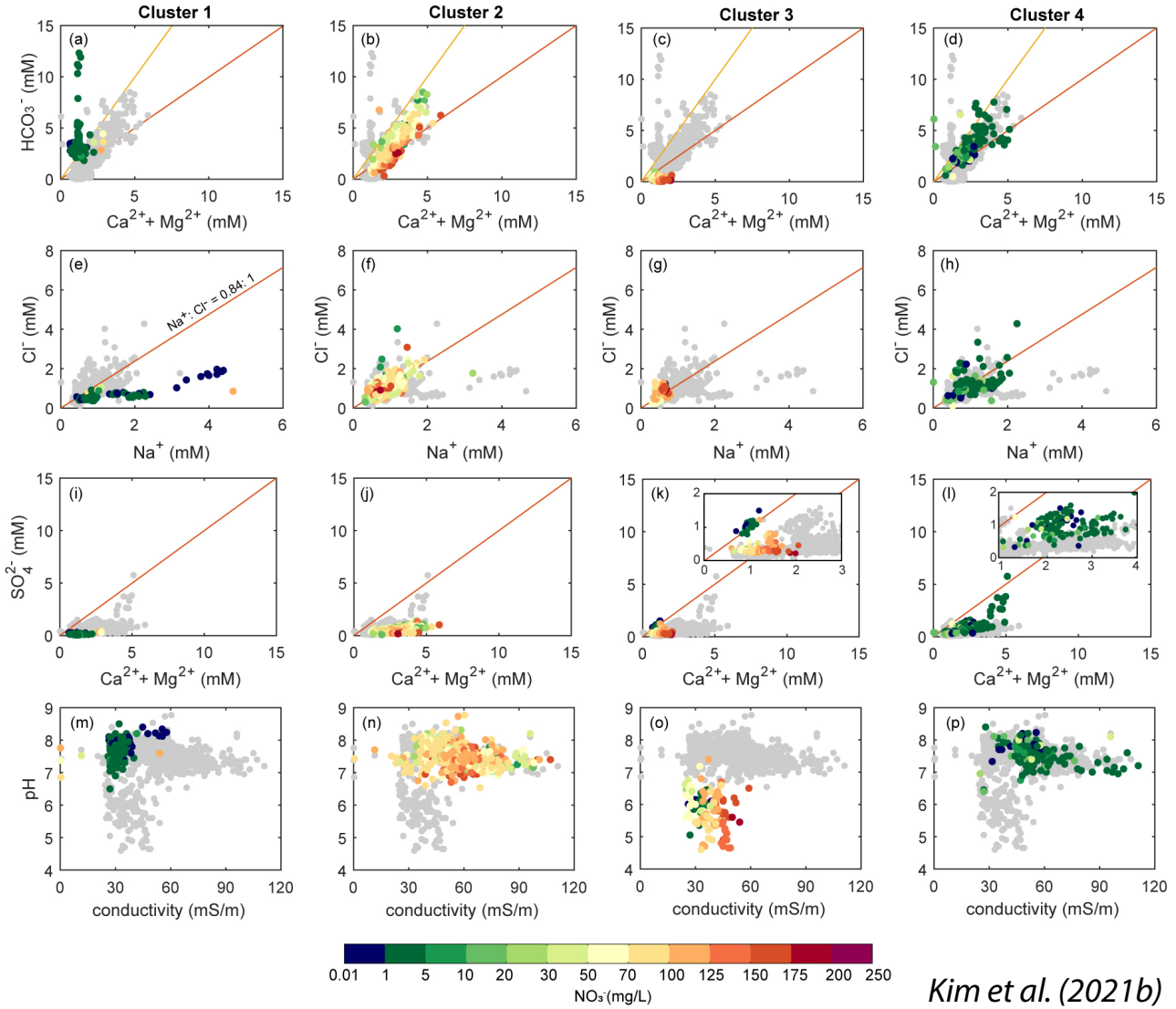
Kim et al. (2021b)

Case I: Where does denitrification occur in the subsurface at the catchment scale?

K-means clustering analysis of groundwater chemistry

- Cluster 1
- Cluster 2
- Cluster 3
- Cluster 4





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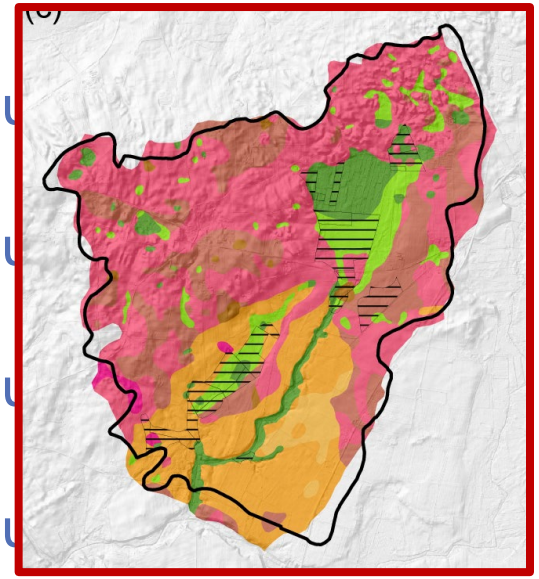
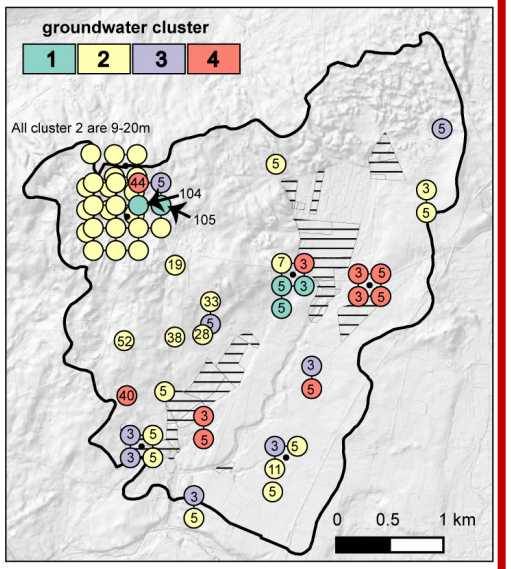
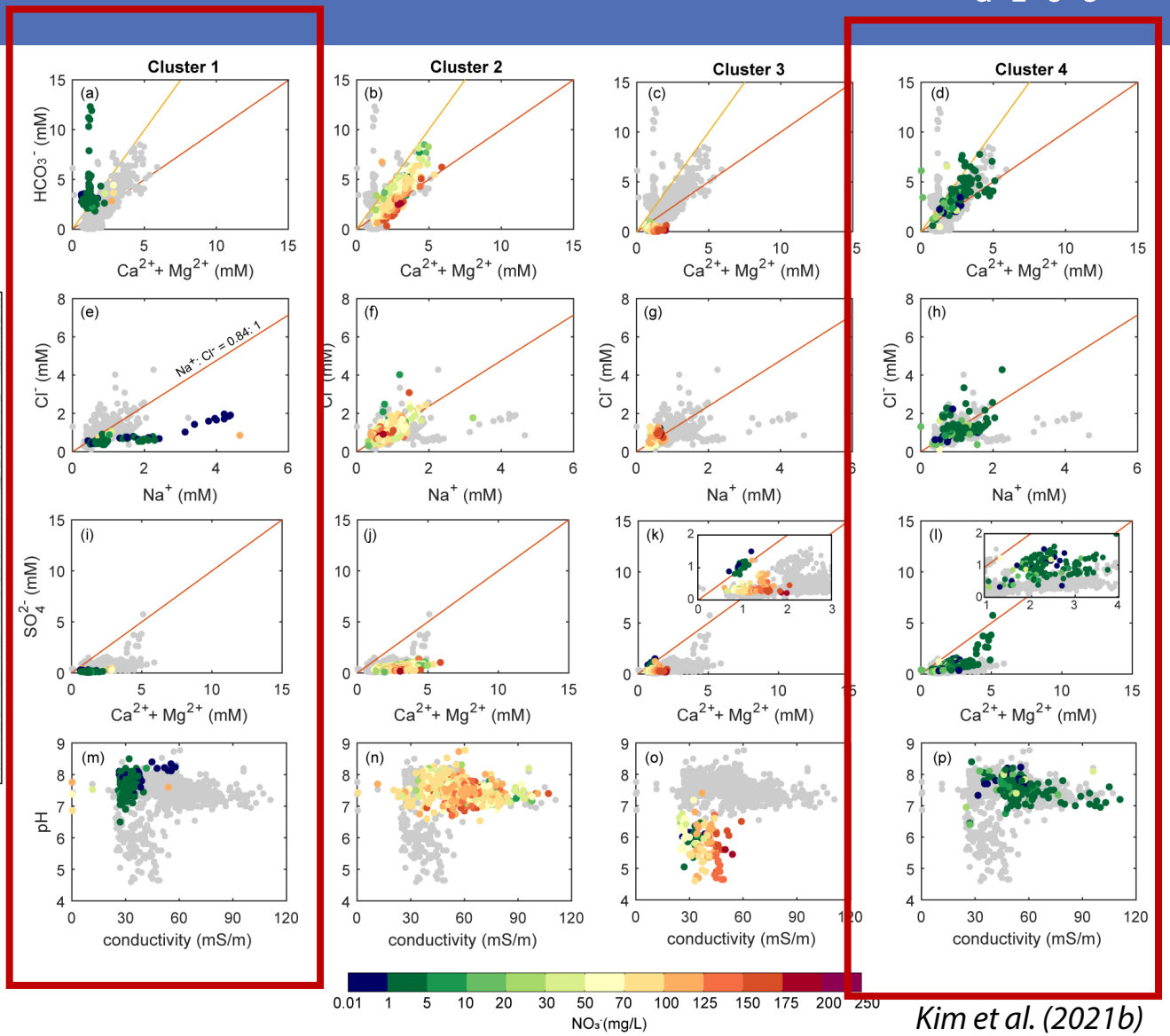




Organic-rich postglacial sediments



Kim et al. (2021b)

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K-means clustering analysis of groundwater chemistry

- Cluster 1
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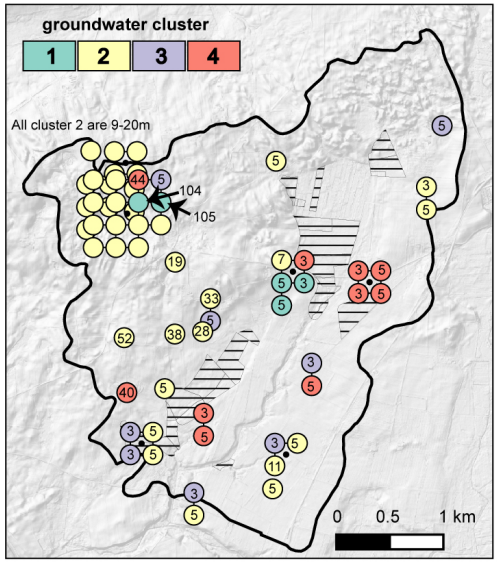
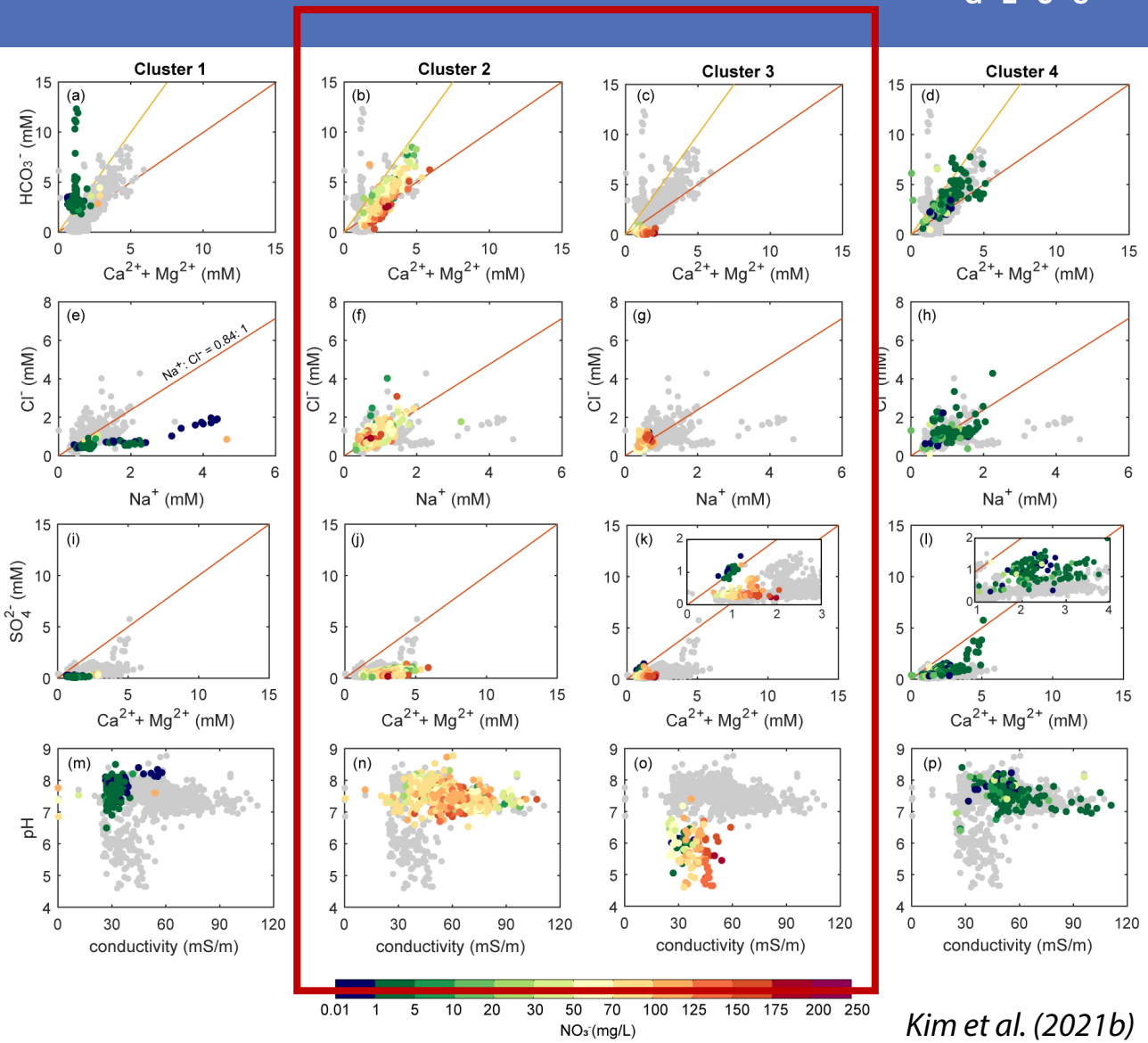
- Cluster 4





Kim et al. (2021b)

Case I: Where does denitrification occur in the subsurface at the catchment scale?

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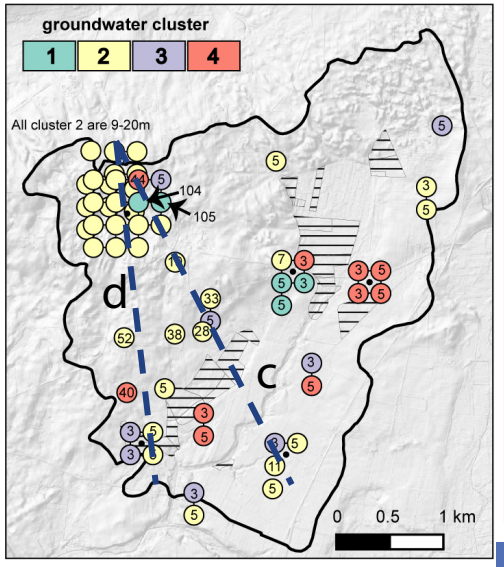
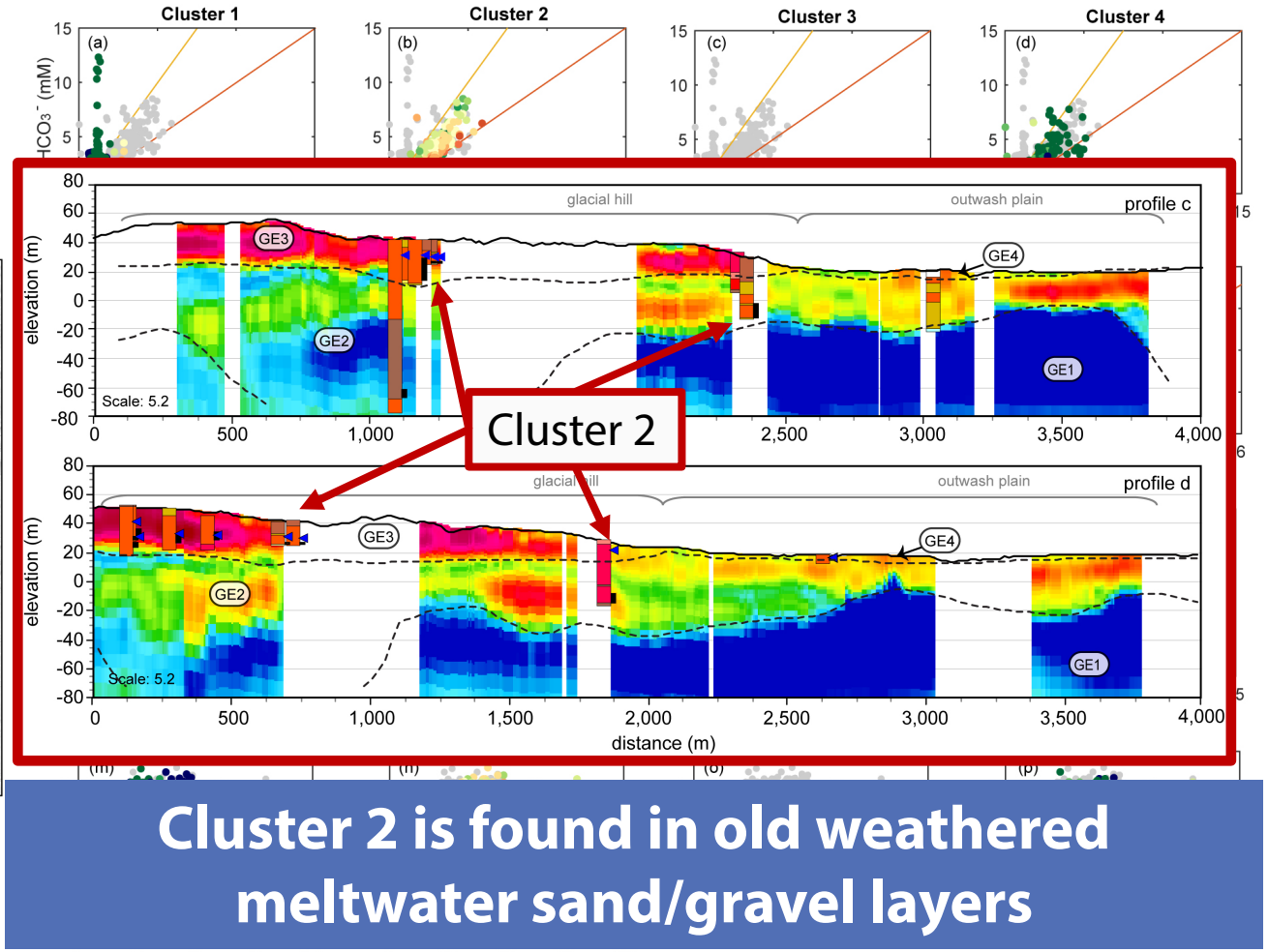
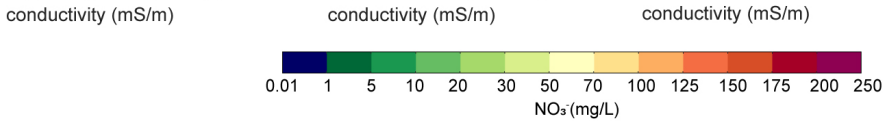
- Cluster 2 (oxic)
- Cluster 3 (oxic)
- Cluster 4 (reduced)





Cluster 2 is found in old weathered meltwater sand/gravel layers

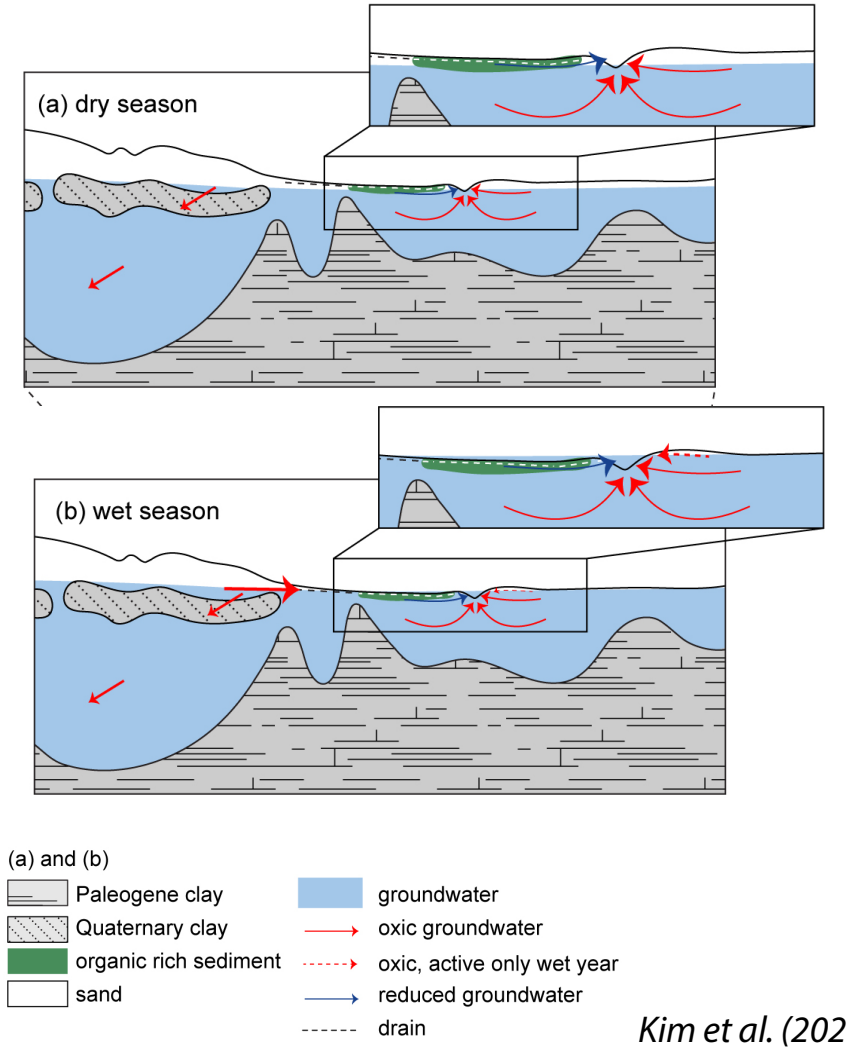


Kim et al. (2021b)

Case I: Where does denitrification occur in the subsurface at the catchment scale?

Conceptual model of the distribution of denitrification zone in LOOP2

- Denitrification occurs near the organic-carbon rich postglacial sediments at shallow depth by oxidation of either organic carbon or pyrite.
- Meltwater sand/gravel in LOOP2 is weathered, thus, is depleted with N-reducing material. Thus, denitrification may be extremely slow or does not occur.



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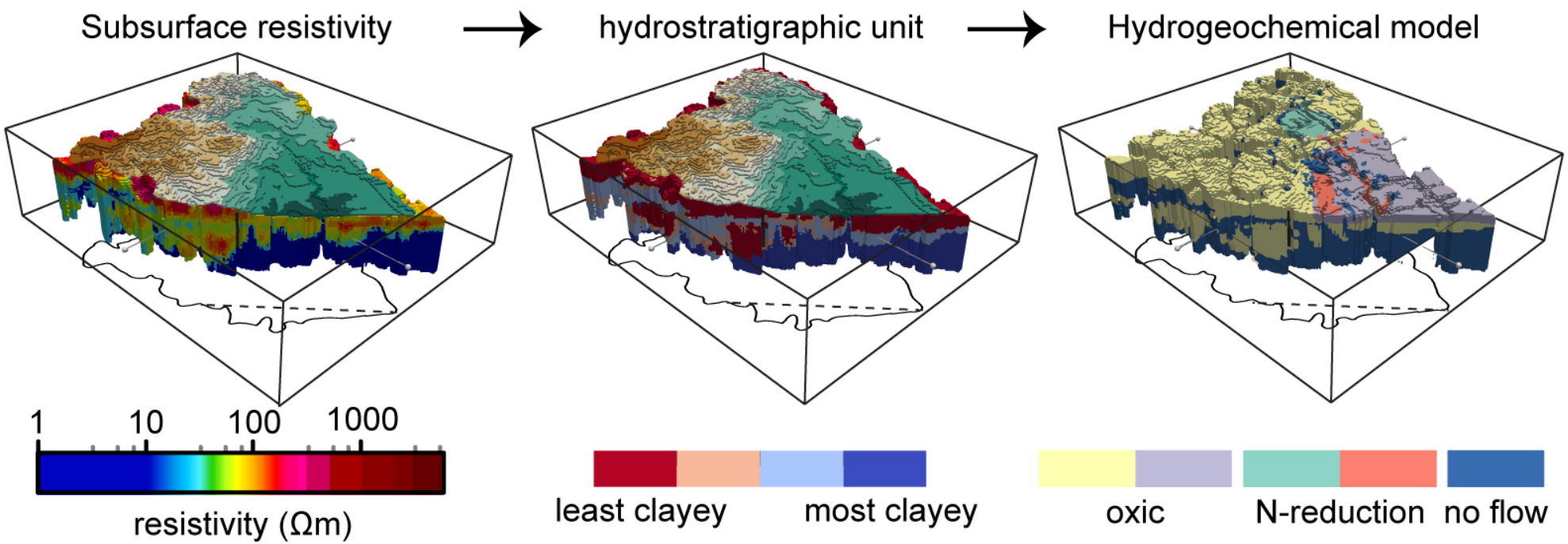

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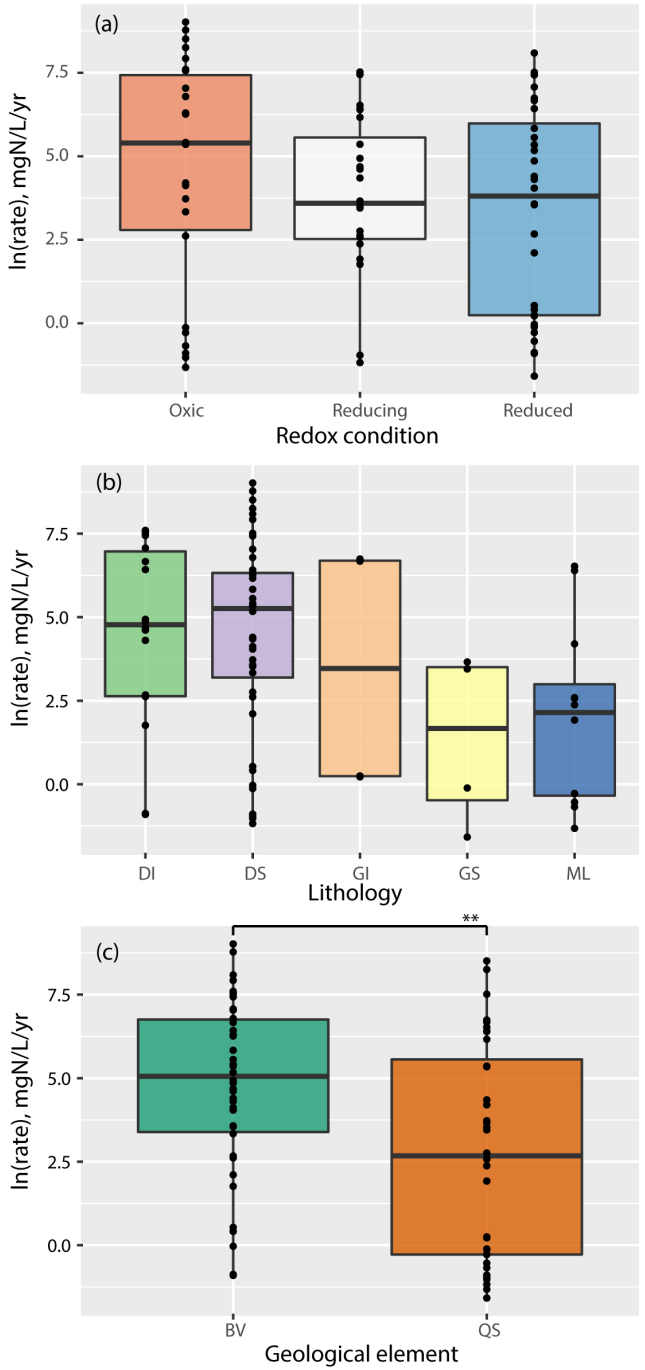

Case II: Where are the denitrification hotspots?

Kim et al. (2021a)

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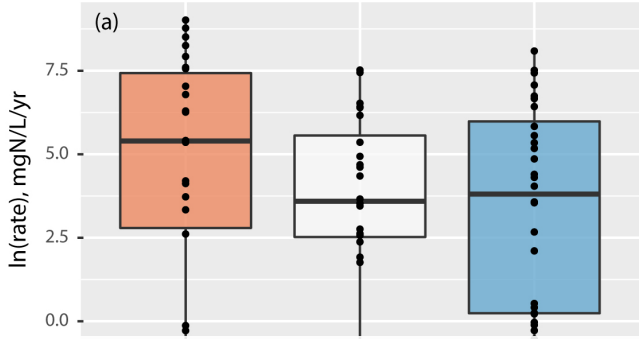
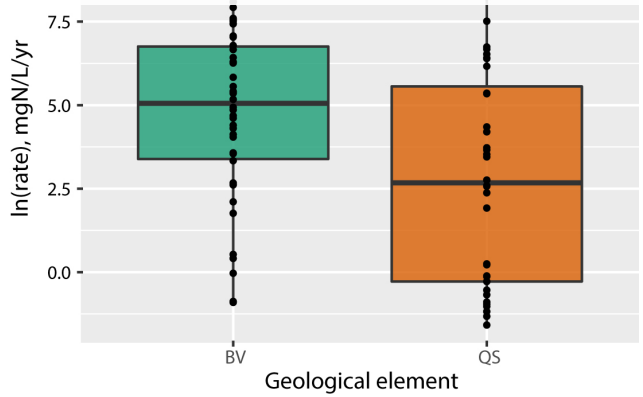


No statistically significant difference among different categories of redox types and lithology.

But the difference is statistically significant between geological elements.



Kim et al. (2021a)

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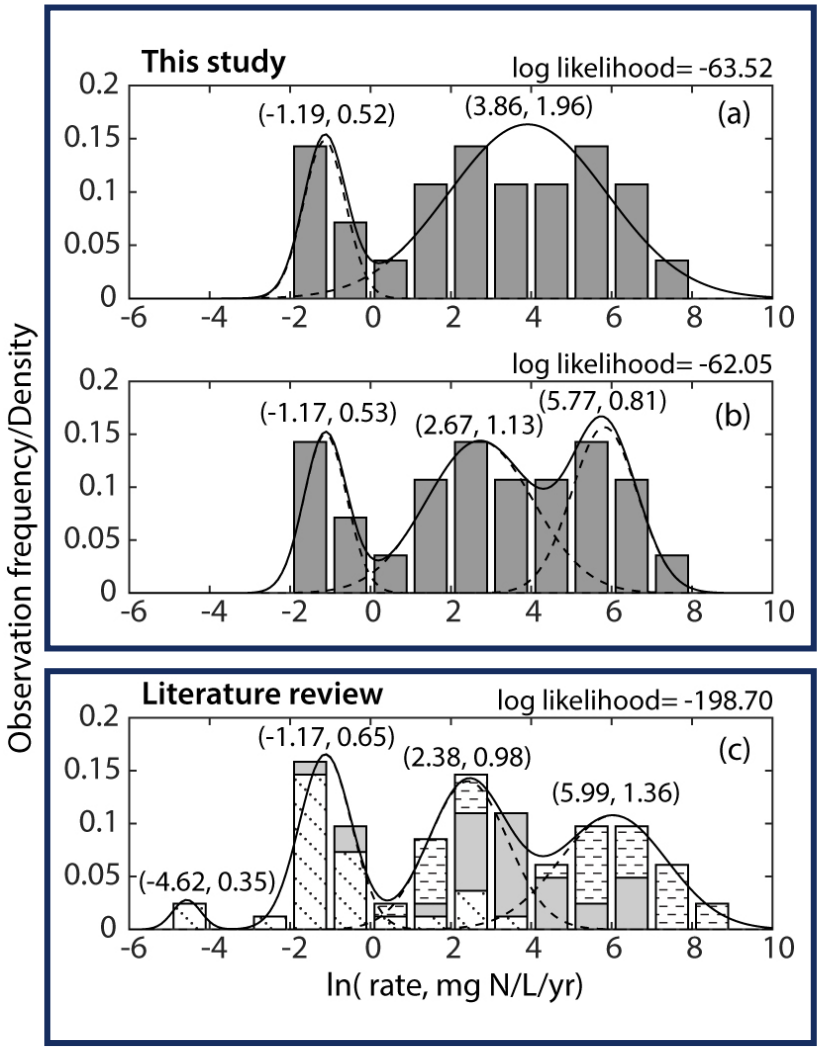
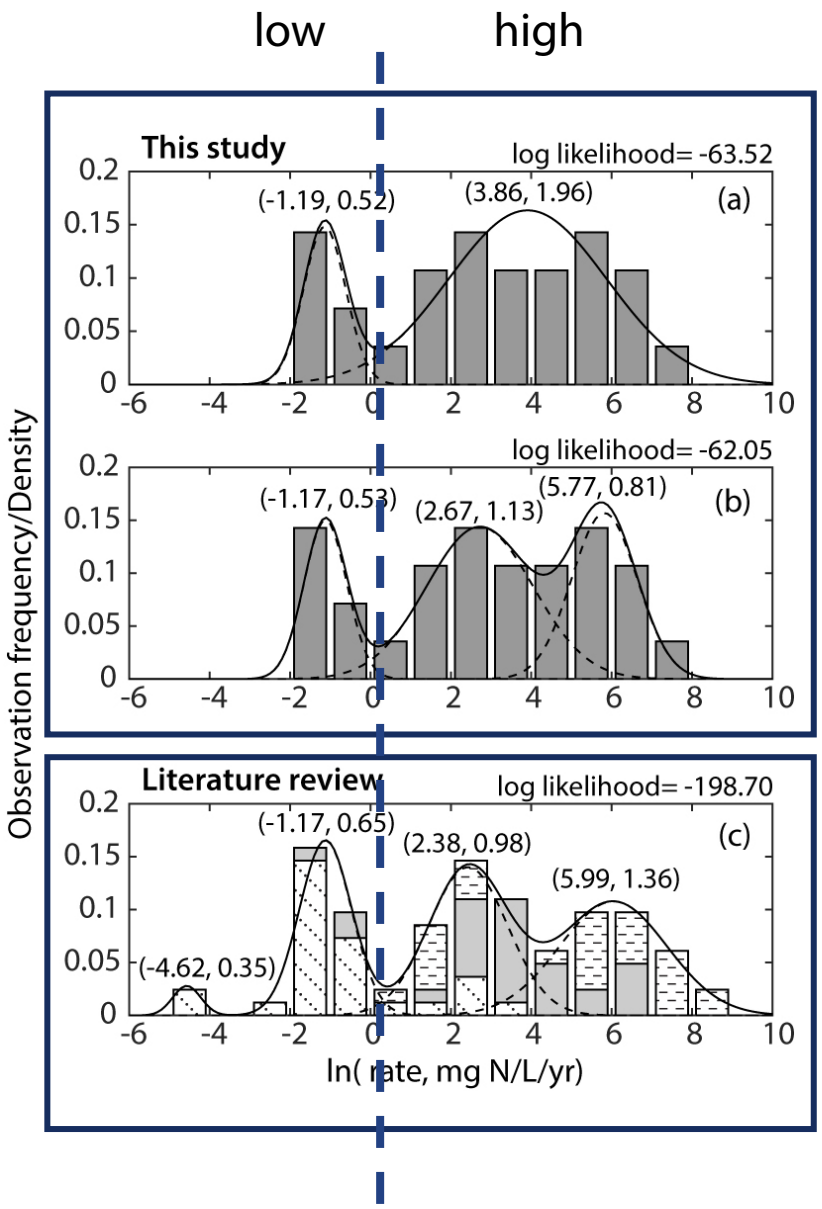


Kim et al. (2021a)

Case II: Where are the denitrification hotspots?

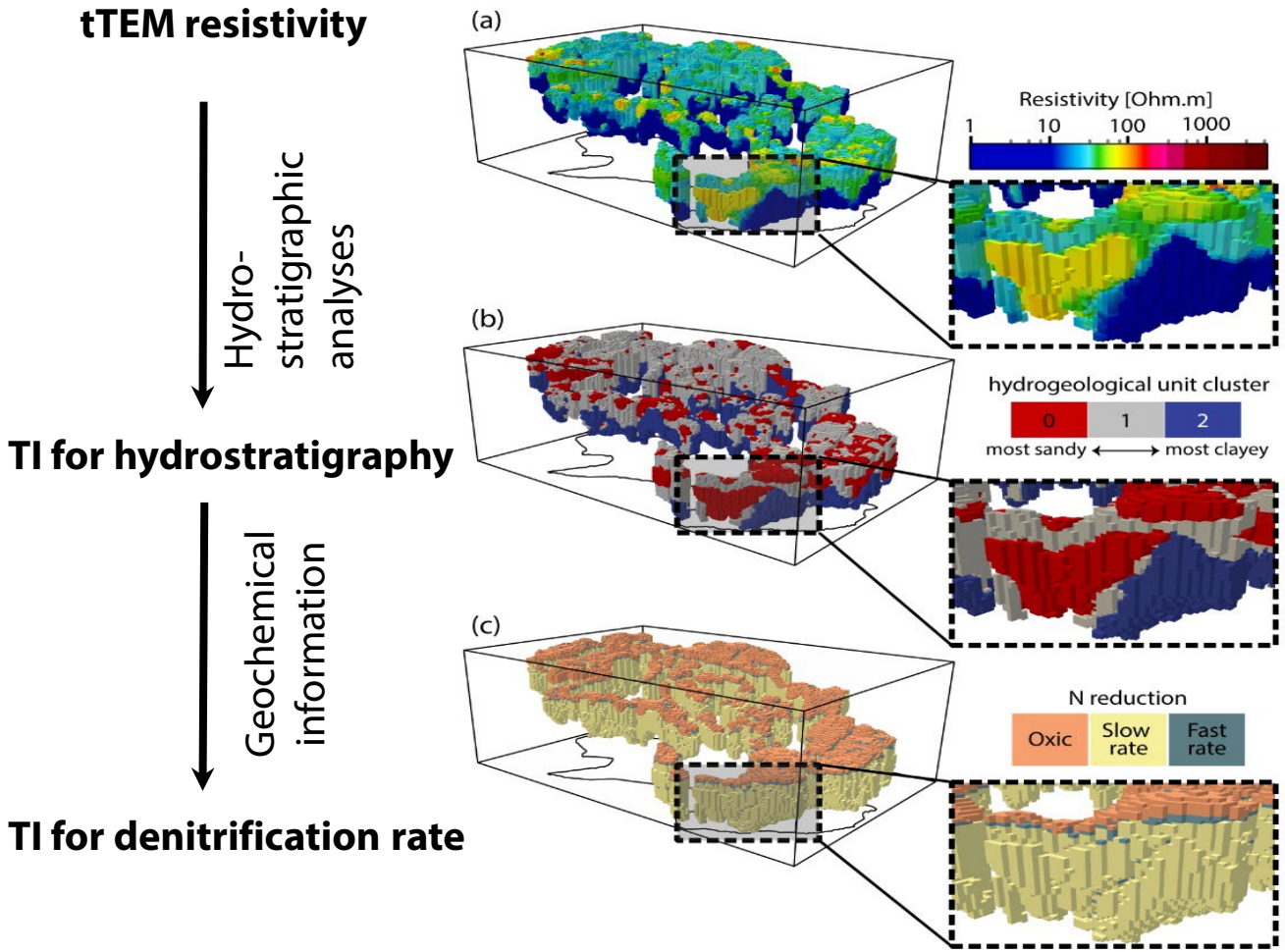
- Multi-modal log-normal distribution
- Literature shows the similar pattern



Kim et al. (2021a)

Case II: Where are the denitrification hotspots?

- Low-rate zones: geological window in the recharging area and reduced clay
- High-rate zones: flow boundary and postglacial sediments



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Summary

- Point-scale geochemical information provides process-based understanding of nitrate transport and fate (where, how, and why).

- Process-based understanding identifies the key controls of the spatial distribution of denitrification zone, and then can be upscaled to the catchment scale by synthesizing geophysical, geological and geochemical information.

- Direct geochemical measurements and process-based understanding of nitrate fate and transport are as important as the high-resolution structure information to obtain the spatial knowledge of denitrification in the subsurface.

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References

- Hansen, B.; Voutchkova, D. D.; Sandersen, P. B. E.; Kallesøe, A.; Thorling, L.; Møller, I.; Madsen, R. B.; Jakobsen, R.; Aamand, J.; Maurya, P.; Kim, H. Assessment of Complex Subsurface Redox Structures for Sustainable Development of Agriculture and the Environment. Environmental Research Letters 2021, 16 (2), 025007.
- Hansen, B., & Thorling, L. (2008). Use of geochemistry in groundwater vulnerability mapping in Denmark. Geological Survey of Denmark and Greenland Bulletin, 15, 45–48.
- Kim, H.; Jakobsen, R.; Aamand, J.; Claes, N.; Erlandsen, M.; Hansen, B. Upscaling of Denitrification Rates from Point to Catchment Scales for Modeling of Nitrate Transport and Retention. Environ Sci Technol 2021a, 55 (23), 15821–15830.https://doi.org/10.1021/acs.est.1c04593.
- Kim, H.; Sandersen, P. B. E.; Jakobsen, R.; Kallesøe, A. J.; Claes, N.; Blicher-Mathiesen, G.; Foged, N.; Aamand, J.; Hansen, B. A 3D Hydrogeochemistry Model of Nitrate Transport and Fate in a Glacial Sediment Catchment: A First Step toward a Numerical Model. Science of The Total Environment 2021b, 776, 146041. https://doi.org/10.1016/j.scitotenv.2021.146041.
- Parkin, T. B. (1987). Soil Microsites as a Source of Denitrification Variability. Soil Science Society of America Journal, 51(5), 1194–1199. https://doi.org/10.2136/sssaj1987.03615995005100050019x

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