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Combining geostatistics and physically-based simulations to characterize contaminated soils

Context

- How to **characterize contamination in soils or groundwater** when dealing with a polluted site needing remediation and with **a small amount of available observations**?

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Geostatistical estimation (kriging)

- + Observations honored
- Physical information not taken into account
- Performances limited if few data available

Direct flow-and-transport simulations

- + Physically-based model
- Uncertainties in modeling parameters
- Observations not honored

Outline

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 1. The Kriging with Numerical Variograms (KNV) method
 2. A synthetic reference test case
 3. Comparison of KNV to classical krigings

Kriging with Numerical Variograms (KNV)

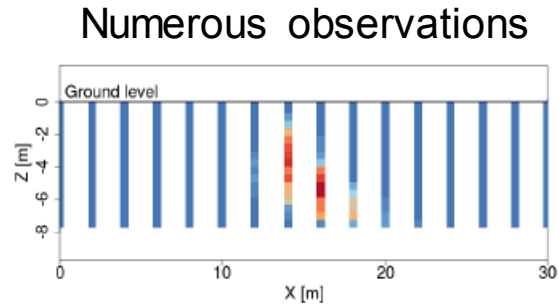
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- 2. A synthetic reference test case**

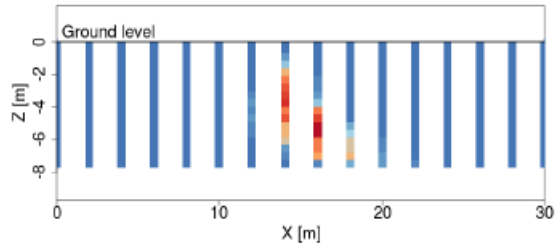
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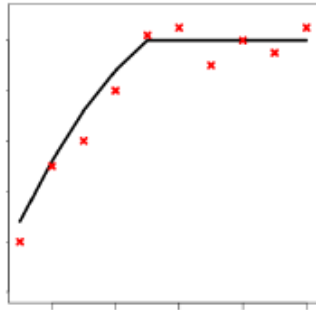


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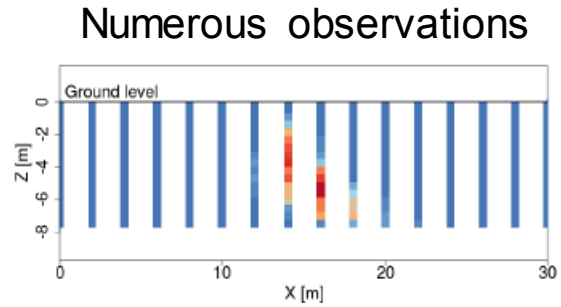
Numerous observations



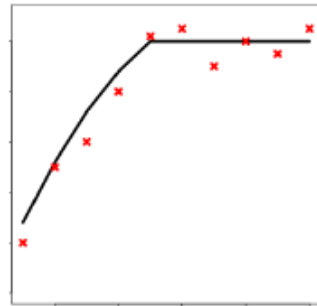
↓ Variogram fitting



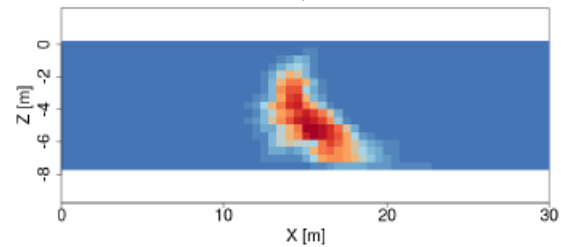
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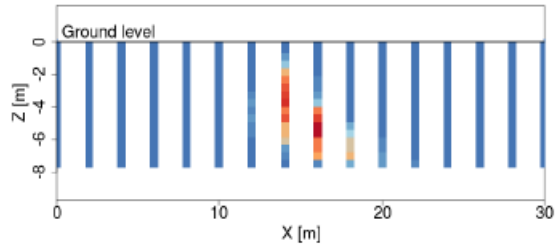


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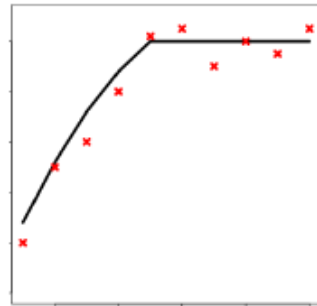


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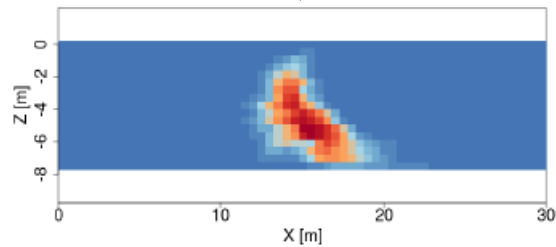
Numerous observations



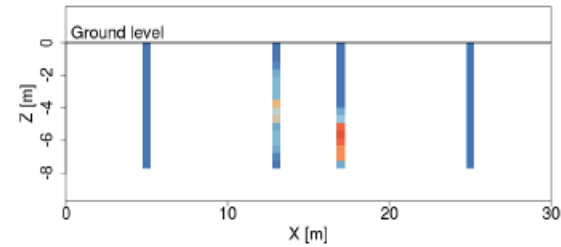
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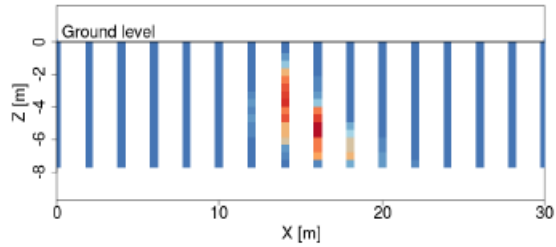


Small amount of observations

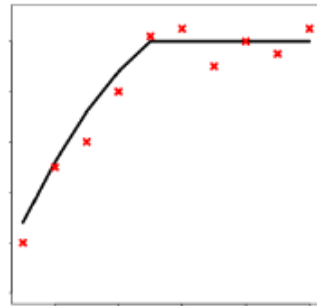


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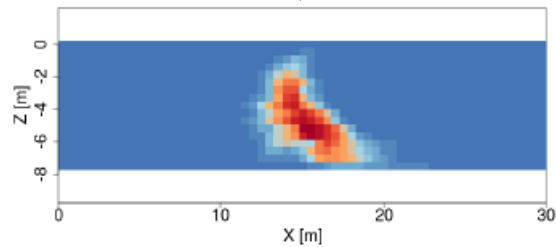
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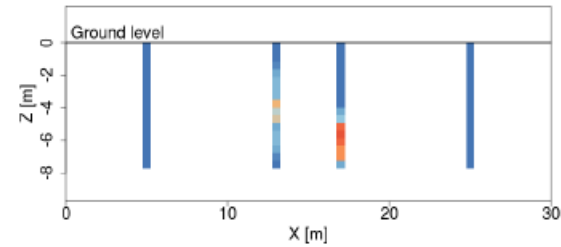
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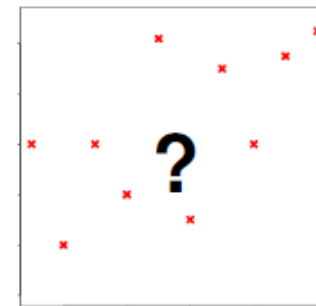
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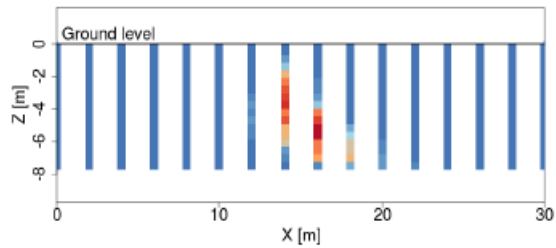


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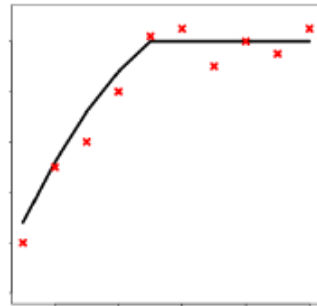


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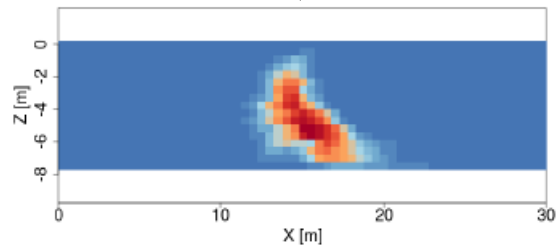
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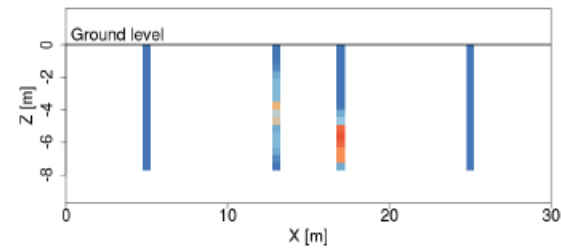
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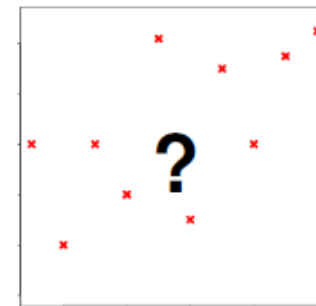
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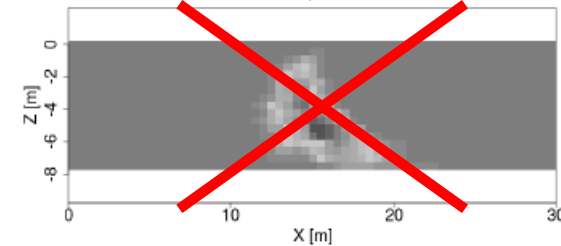
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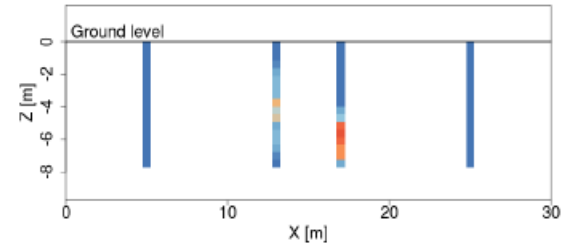


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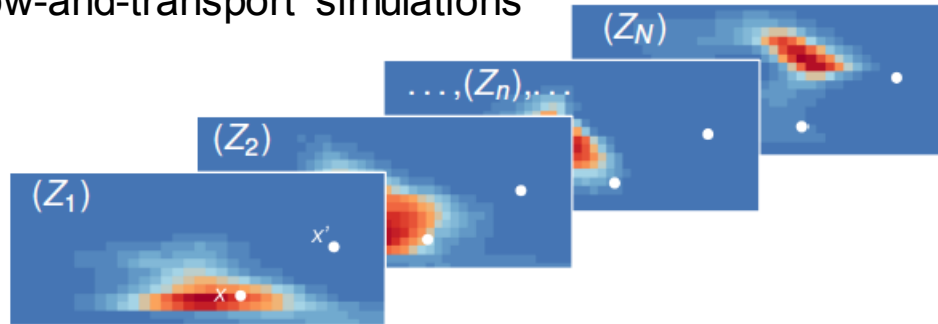
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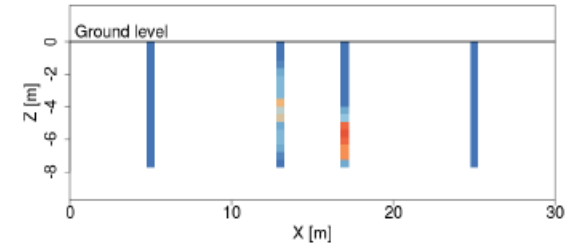


Kriging with Numerical Variograms (KNV)

Flow-and-transport simulations

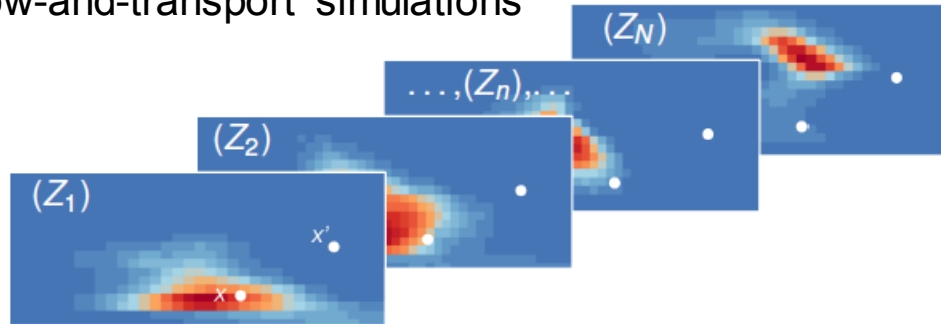


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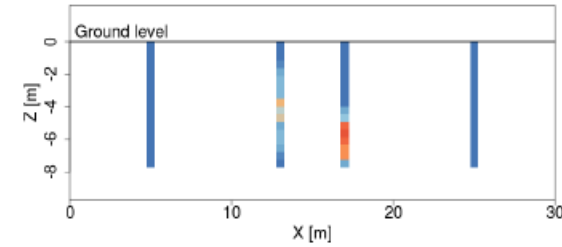
Flow-and-transport simulations



↓ Numerical variograms

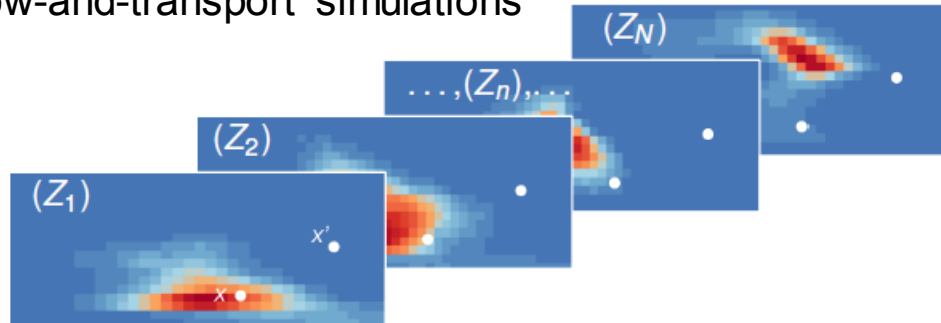
$$\gamma(x, x') = \frac{1}{N} \sum_{n=1}^N \frac{1}{2} [Z_n(x) - Z_n(x')]^2$$

Small amount of observations



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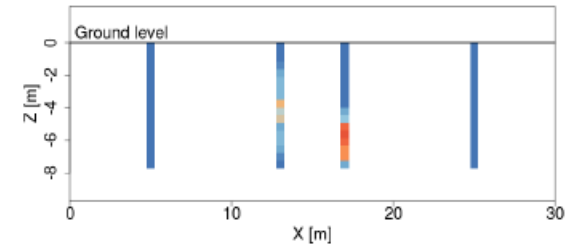
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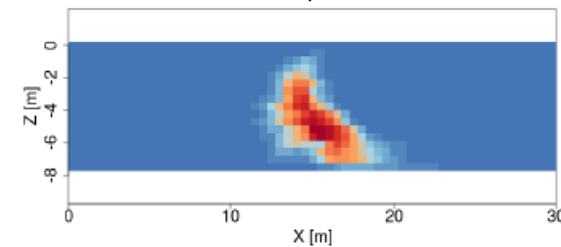
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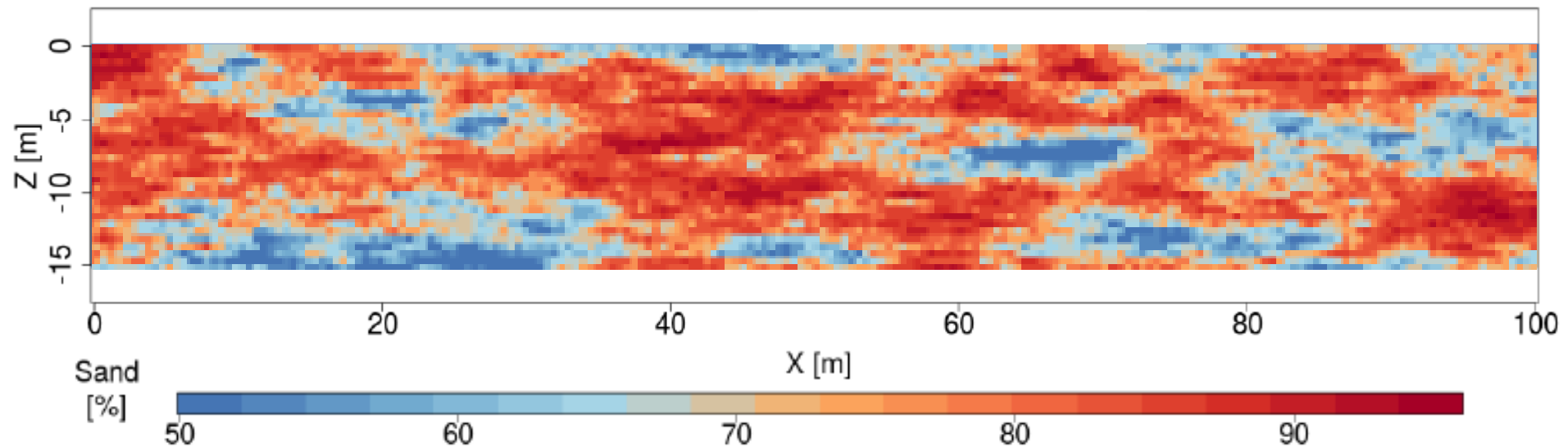


Synthetic reference test case

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Synthetic reference test case

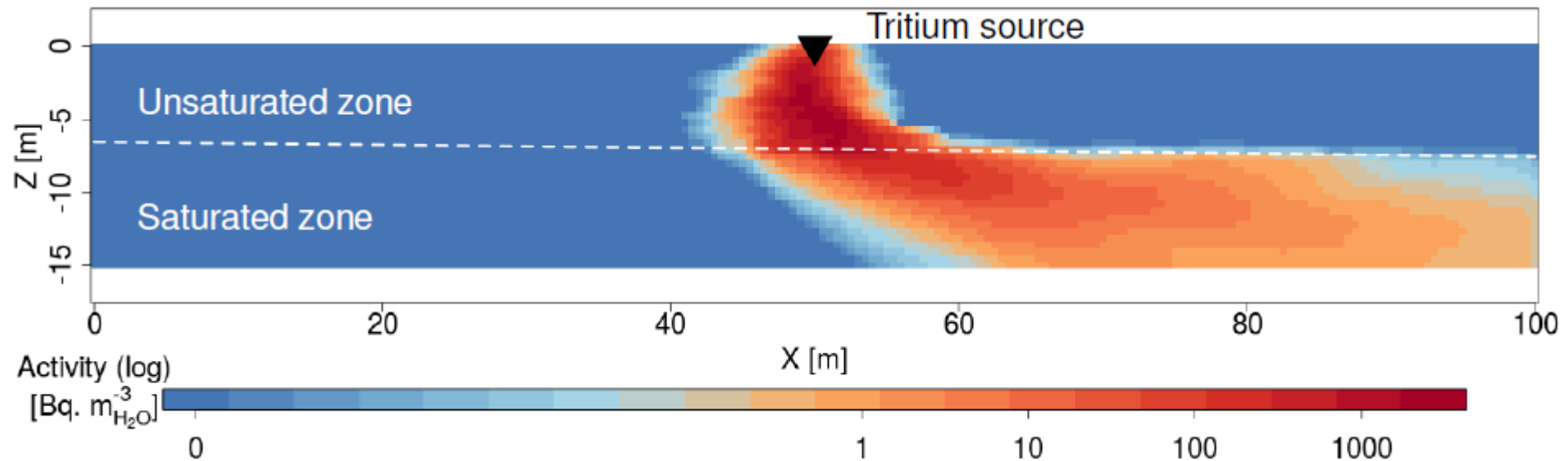
- Model settings (2D vertical section)
 - Sandy loam facies with heterogeneous textural properties (i.e., sand, silt, clay contents);



Synthetic reference test case

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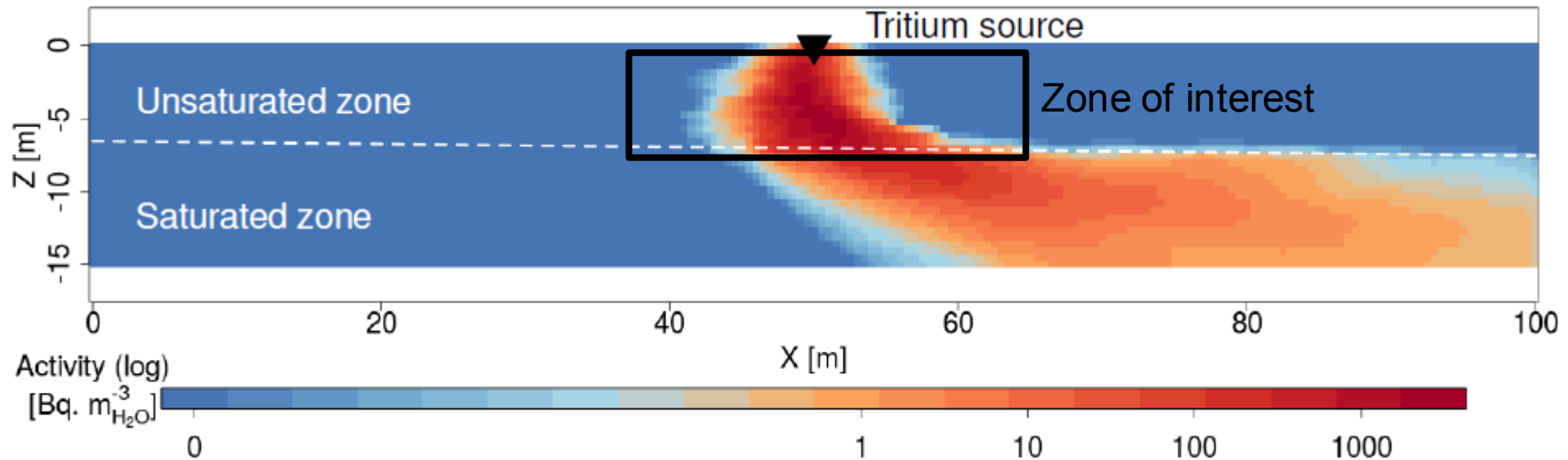
- Sandy loam facies with heterogeneous textural properties (i.e., sand, silt, clay contents);
- Fixed upstream-downstream head: unsaturated zone ~7 m deep;
- Contamination due to a point source of tritium: 4 years simulation with the code MELODIE.



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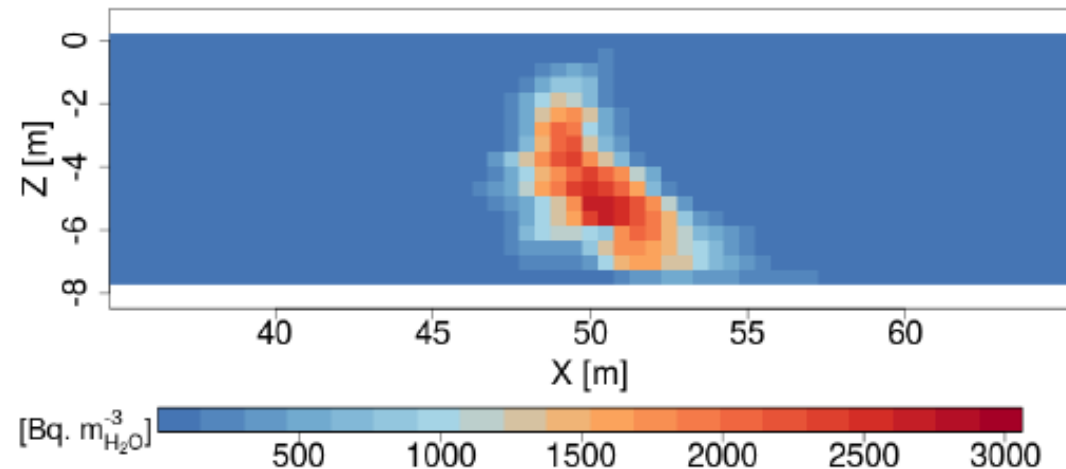
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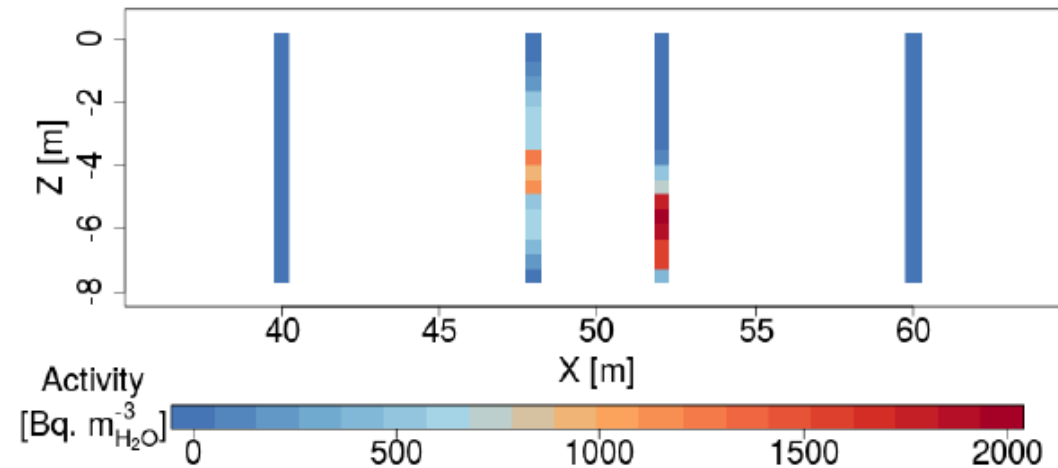
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- Sampling scenario

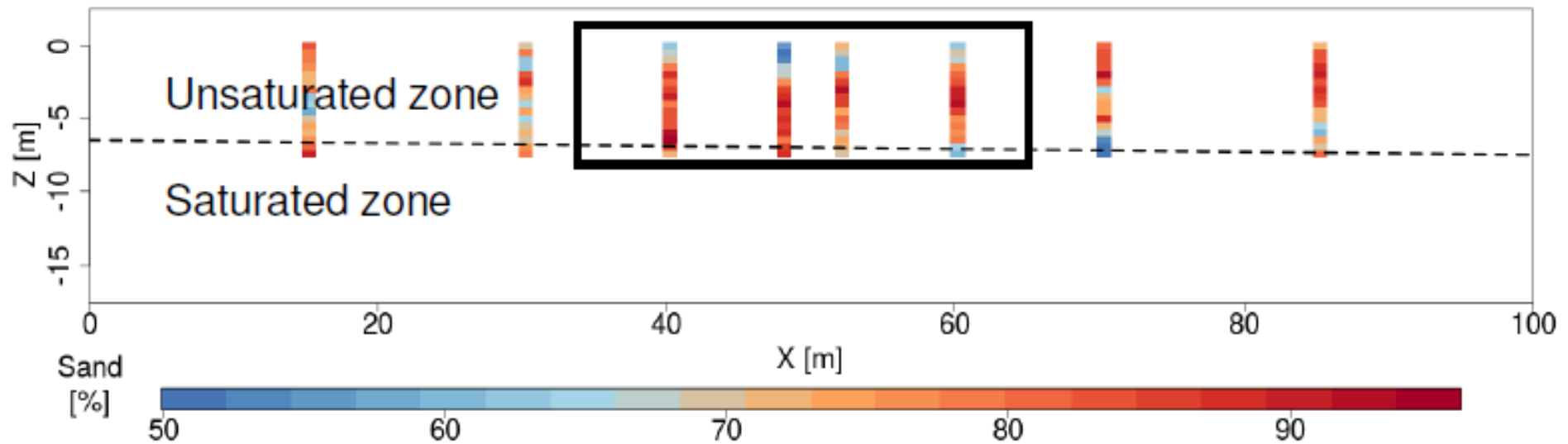
- 4 boreholes with activity;



Synthetic reference test case

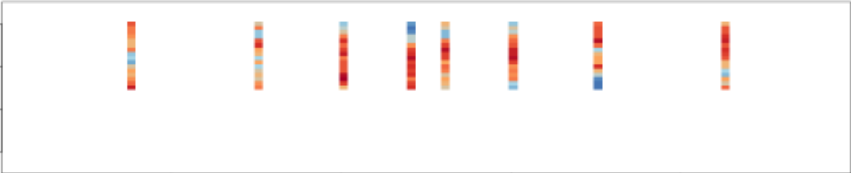
- Sampling scenario

- 4 boreholes with activity;
- 8 boreholes with soil texture.



Synthetic reference test case

Observations of texture



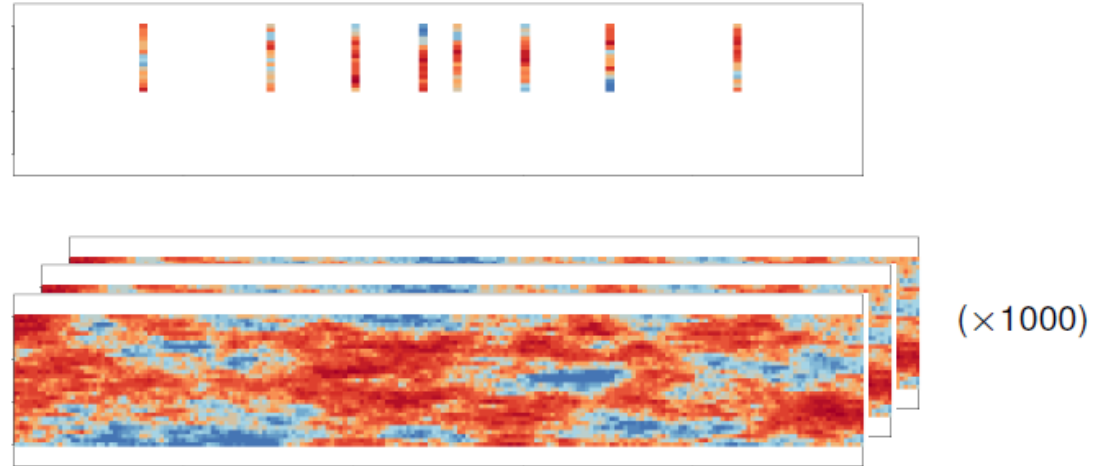
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Observations of texture

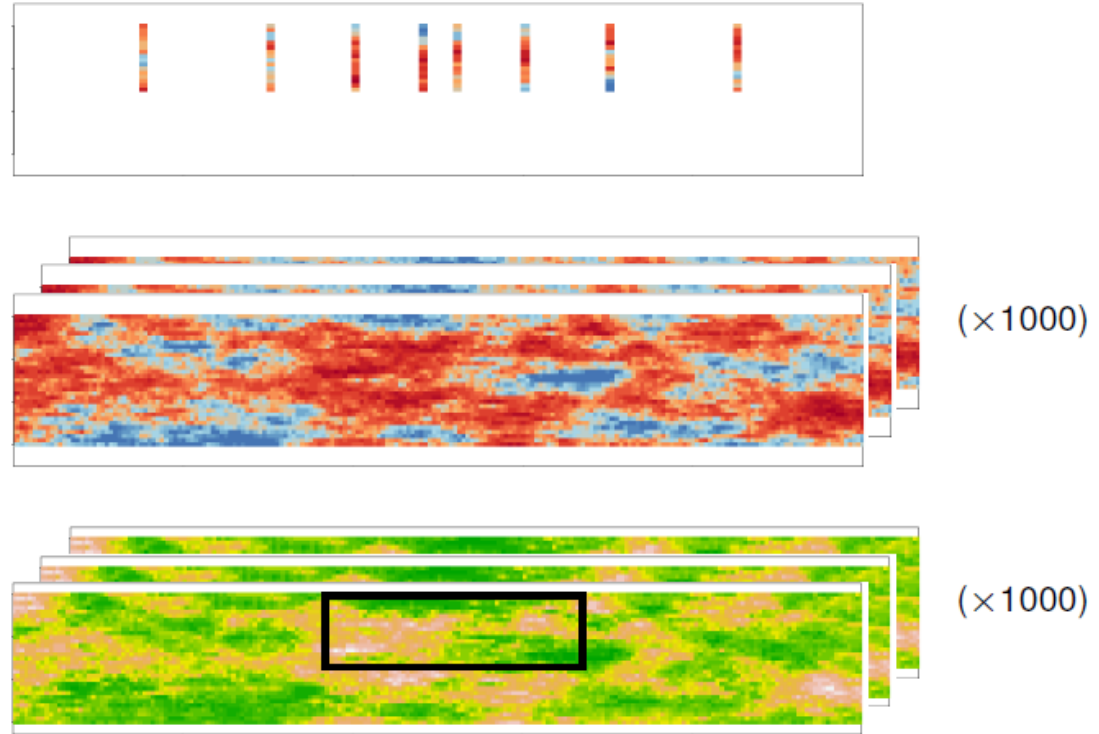
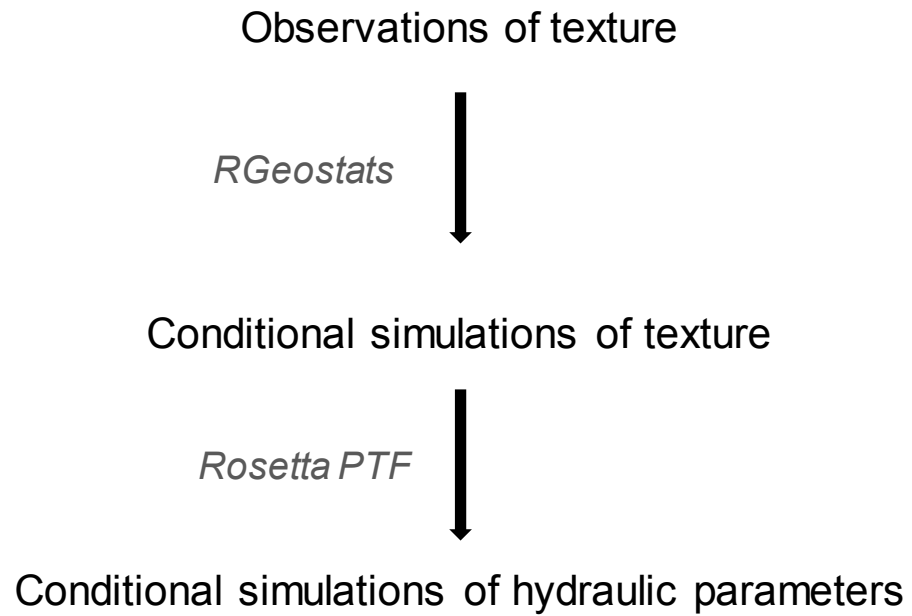
RGeostats



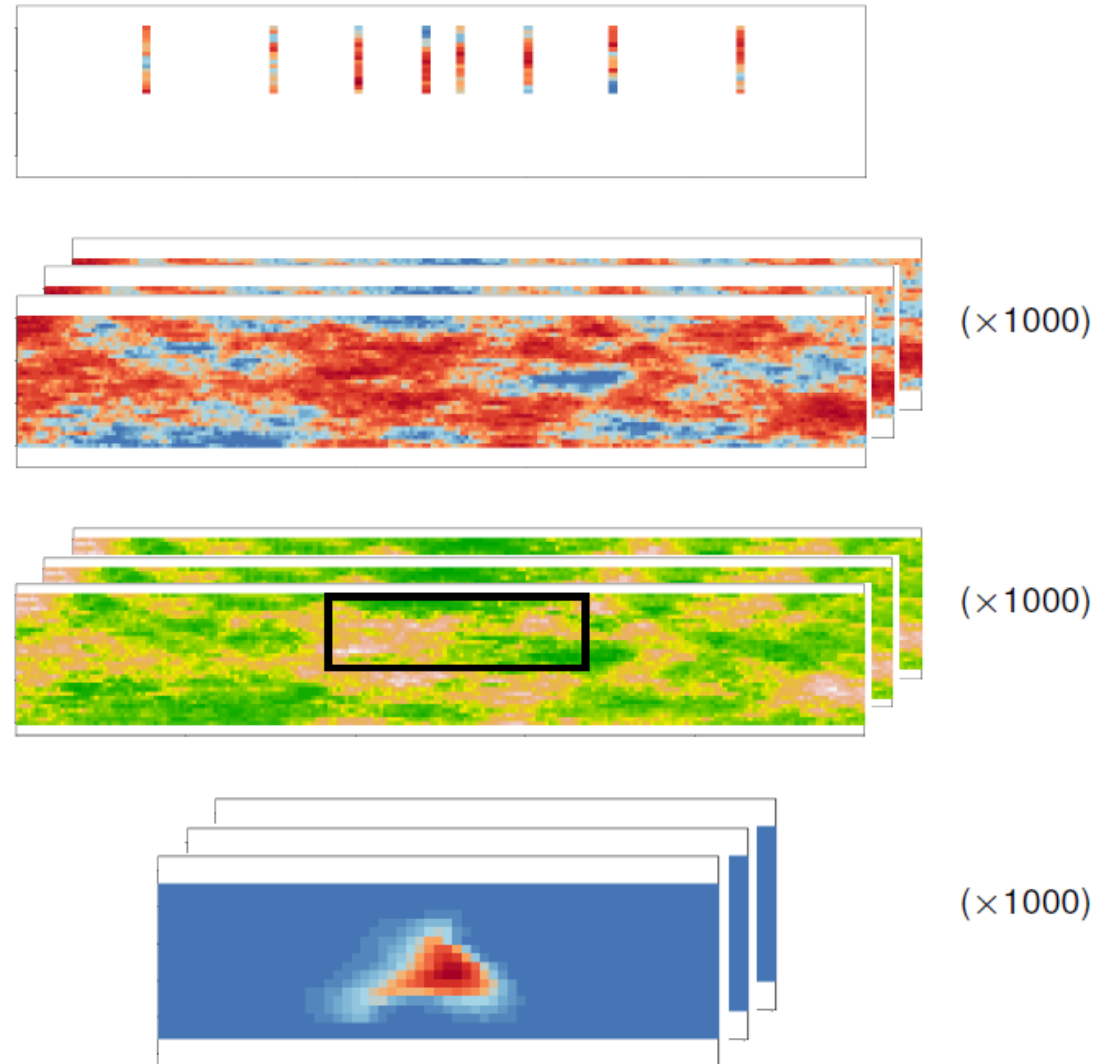
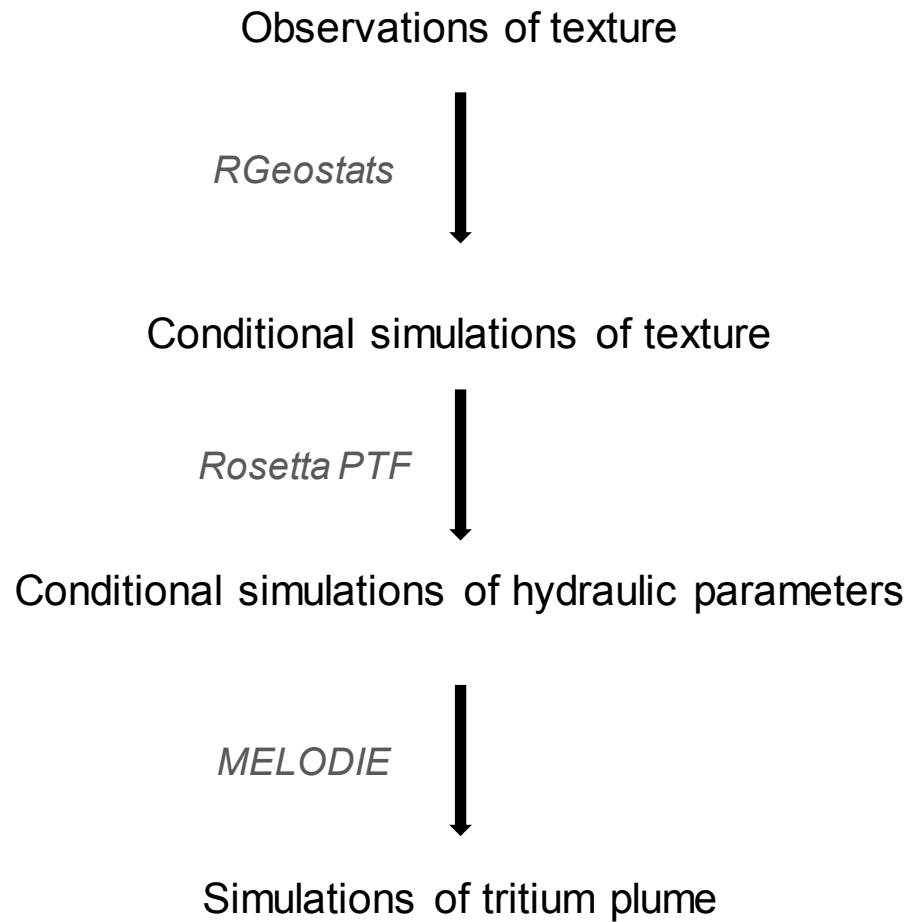
Conditional simulations of texture



Synthetic reference test case

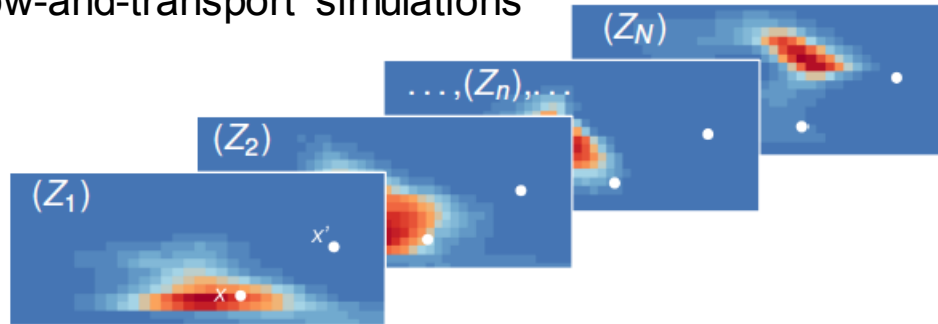


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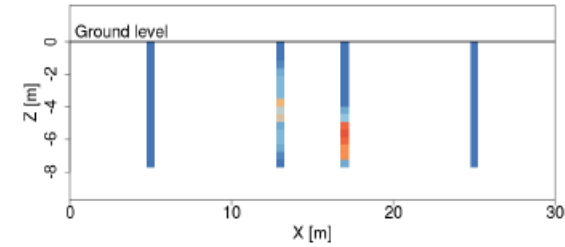
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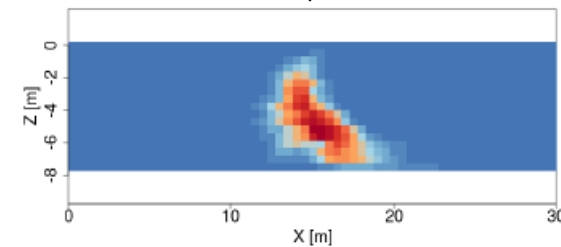
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KNV vs. classical krigings

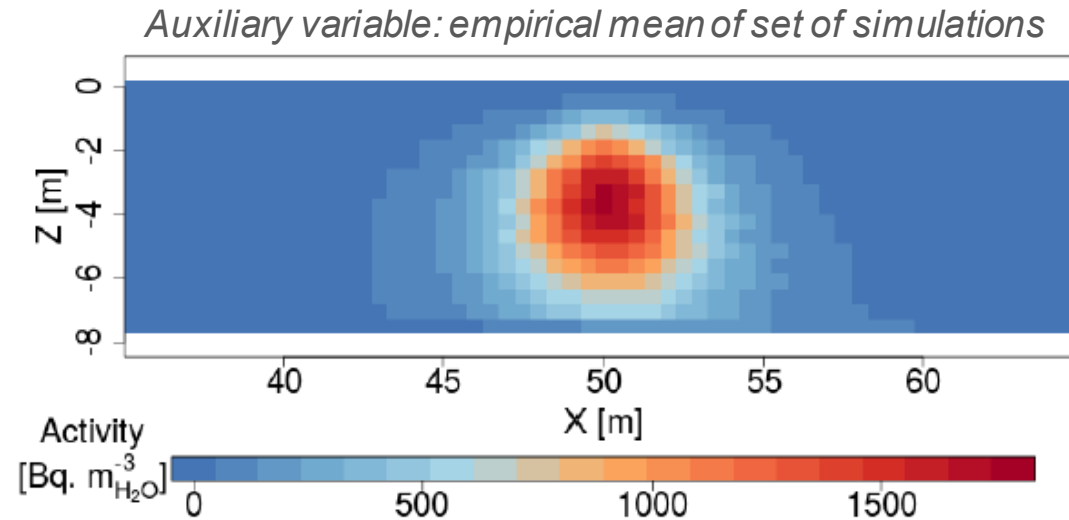
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KNV vs. classical krigings

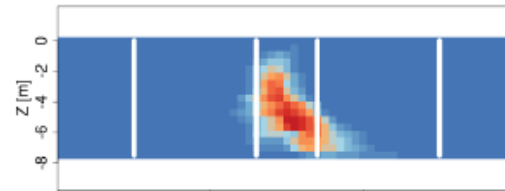
- **Ordinary kriging (OK)**, which is widely used but known to perform poorly when the number of data is too small or when the phenomenon under study is complex;
- **Kriging with external drift (KED)**, which enables the incorporation of auxiliary variables to take non-stationarity into account.

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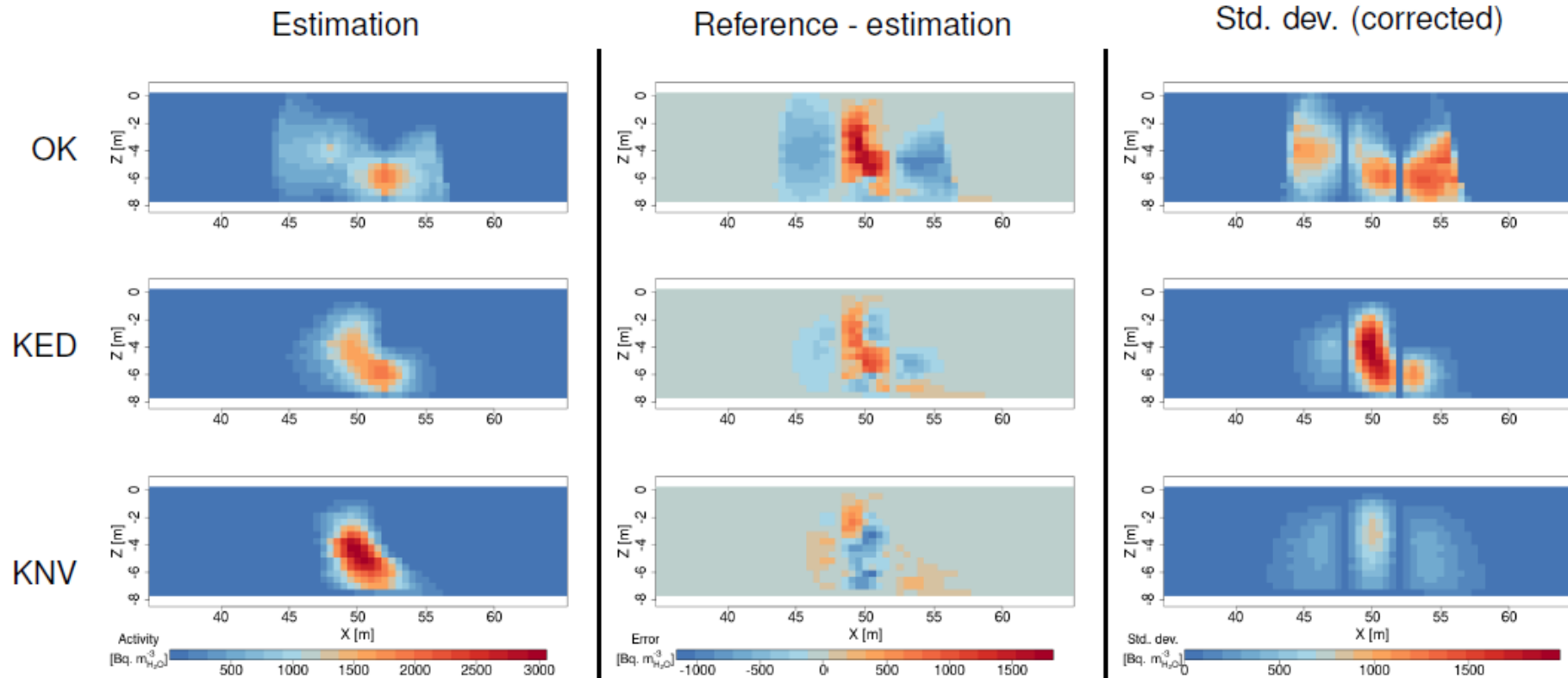
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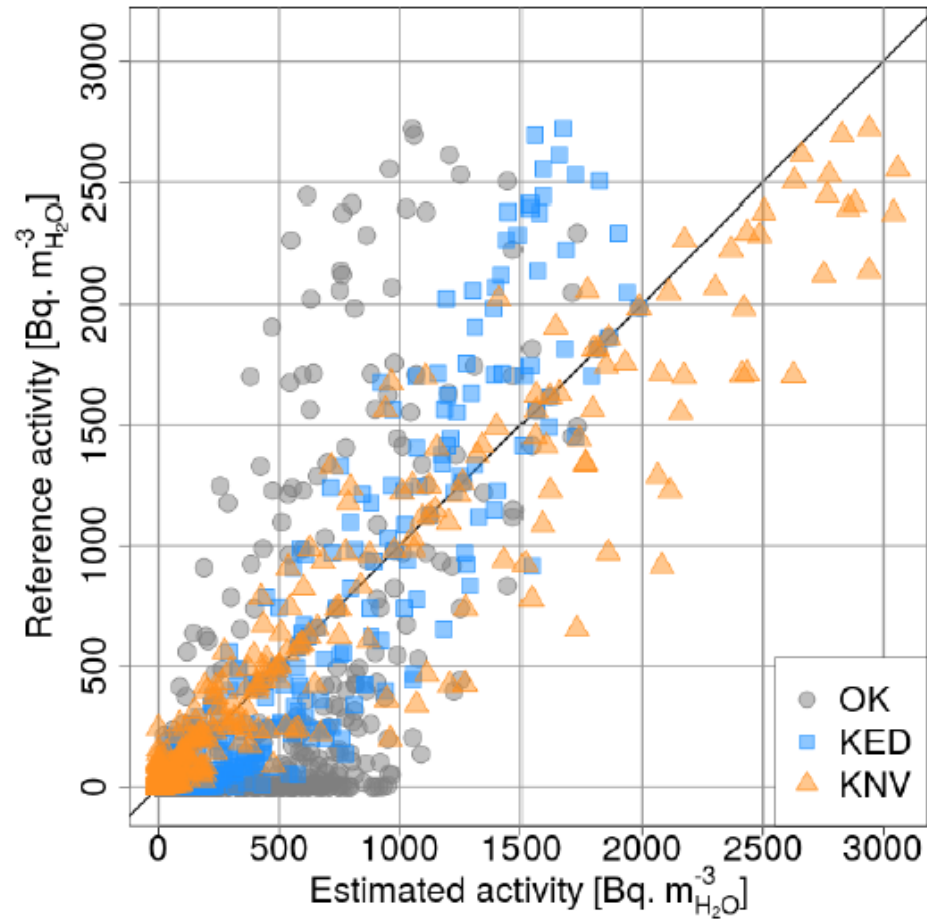
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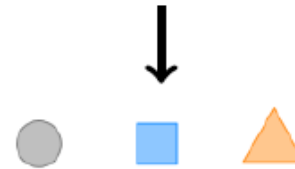
Reference tritium plume



KNV vs. classical krigings



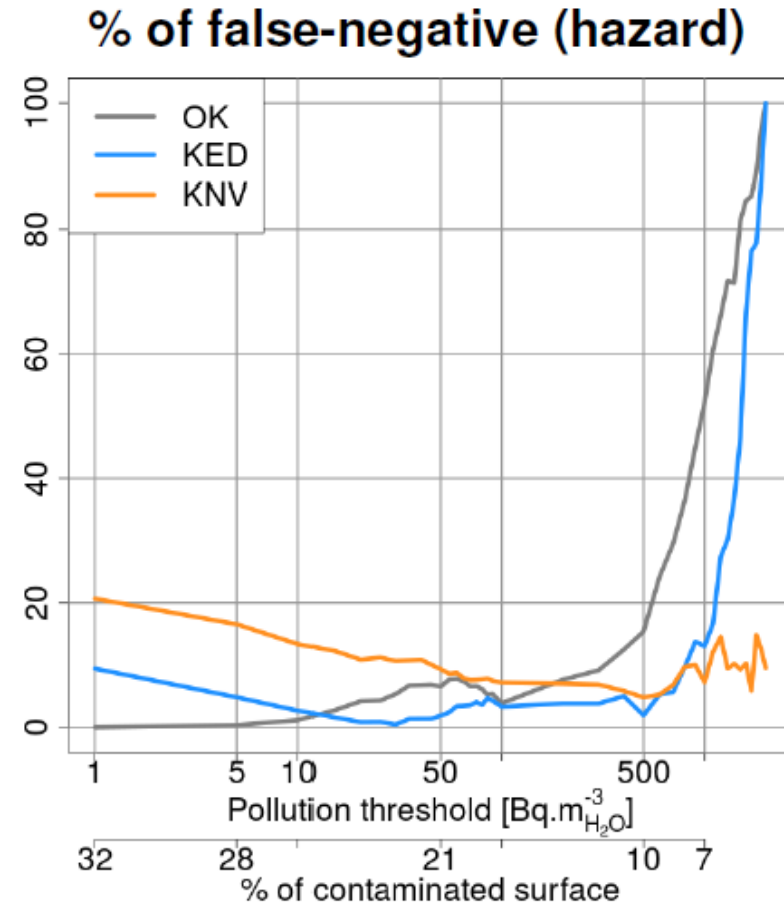
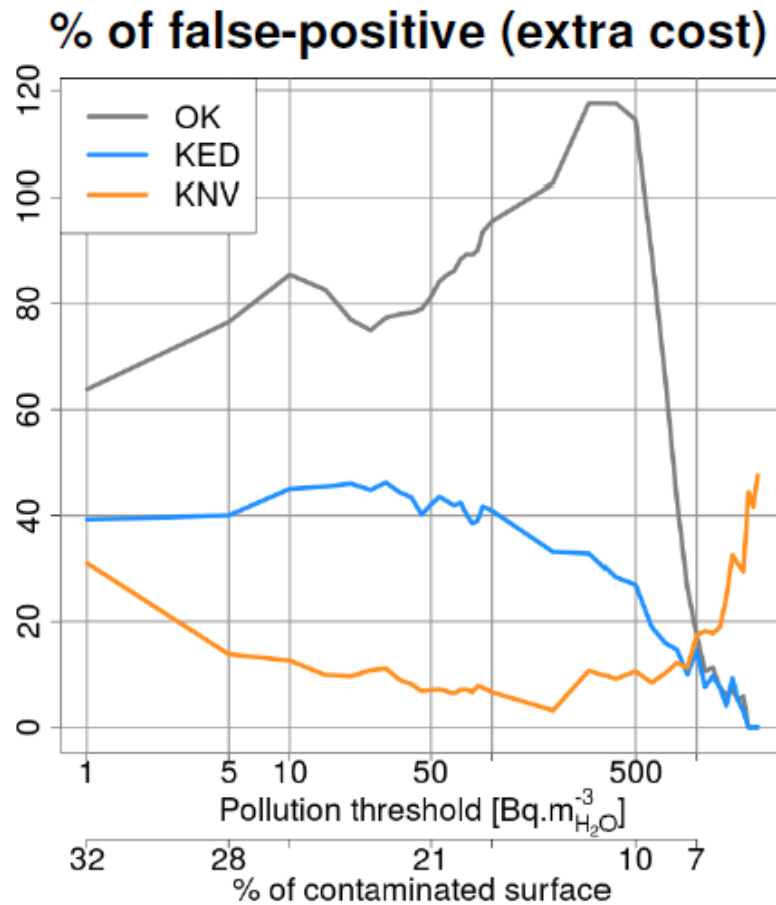
1 point of the domain



Global statistics

	OK	KED	KNV
MAE [Bq.m ⁻³ _{H₂O}]	173	71	47
RMSE [Bq.m ⁻³ _{H₂O}]	348	174	147
MRE [-]	-47	-6.8	-0.8

KNV vs. classical krigings



Conclusion

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- Ongoing work: implementation on a real 3D study-case...

Thank you for your attention

This study is a part of Kri-Terres project, supported by the French National Radioactive Waste Management Agency (ANDRA) under the French “Investments for the Future” Program.