

*Mathieu Le Coz (IRSN) / Léa Pannecoucke (Mines ParisTech) / Xavier Freulon (Mines ParisTech) / Charlotte Cazala (IRSN) / Chantal de Fouquet (Mines ParisTech)*

# 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)

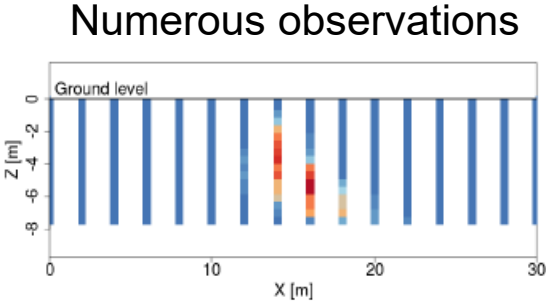
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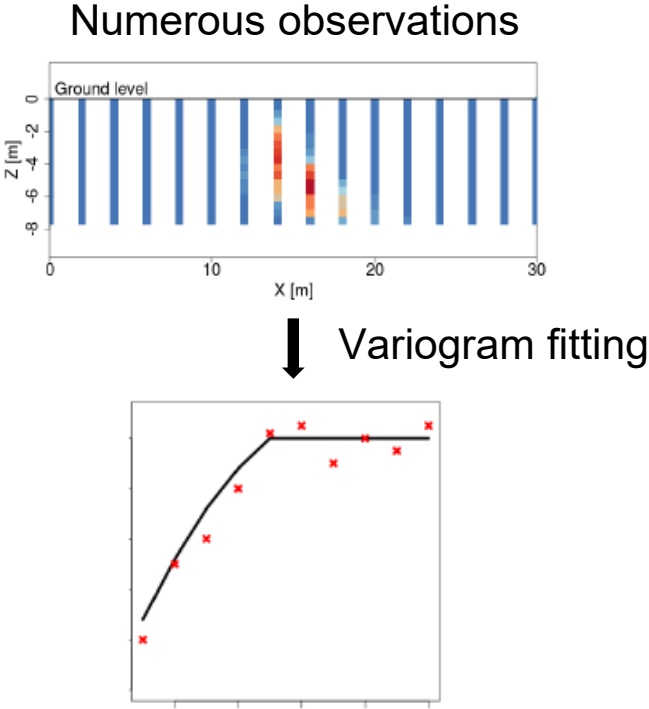
2. A synthetic reference test case

3. Comparison of KNV to classical krigings

# Kriging with Numerical Variograms (KNV)



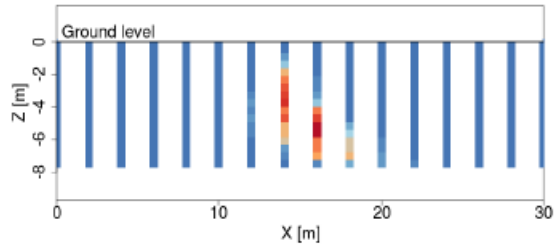
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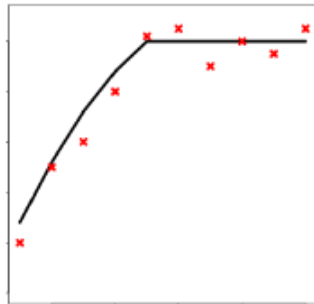


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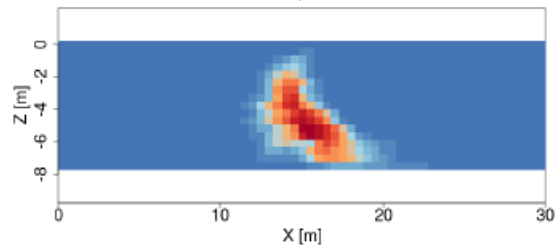
Numerous observations



↓ Variogram fitting

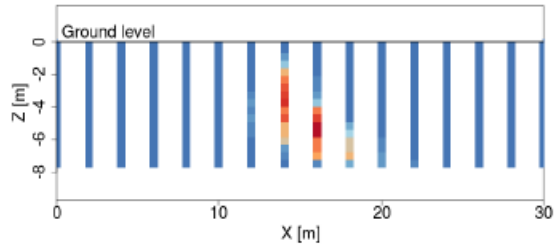


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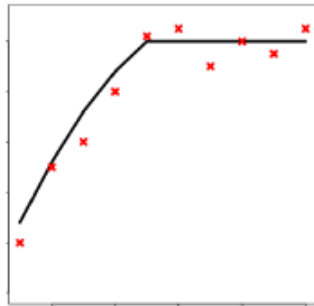


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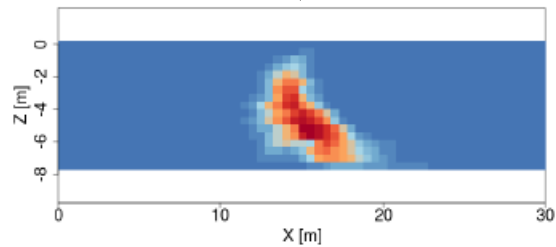
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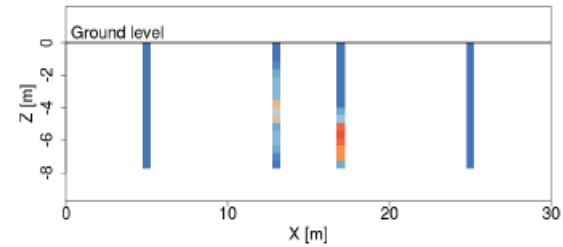
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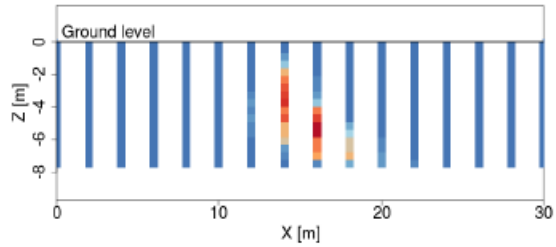


Small amount of observations

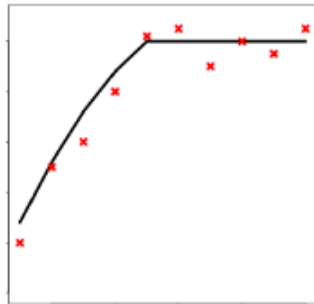


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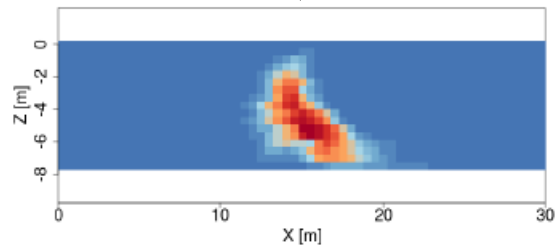
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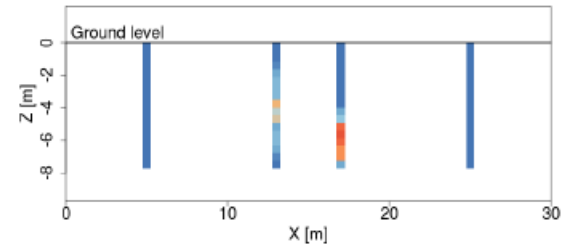
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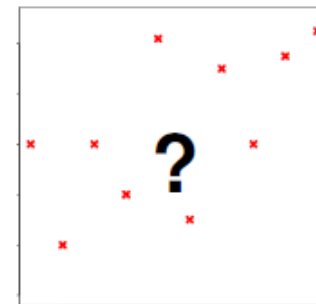
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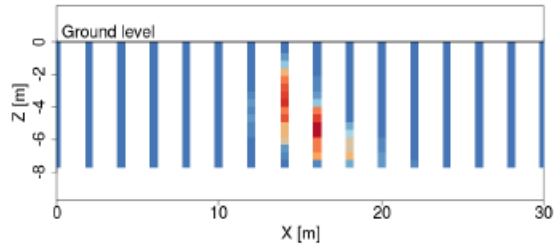


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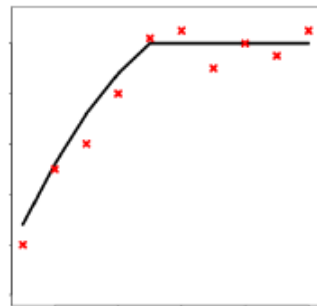


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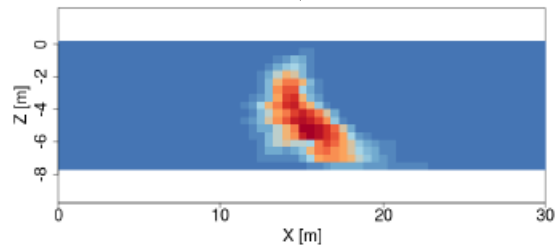
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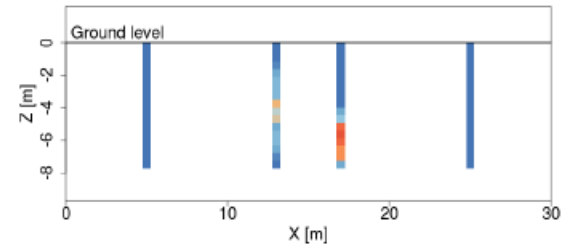
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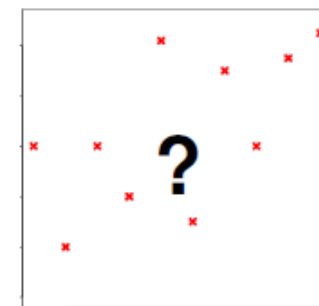
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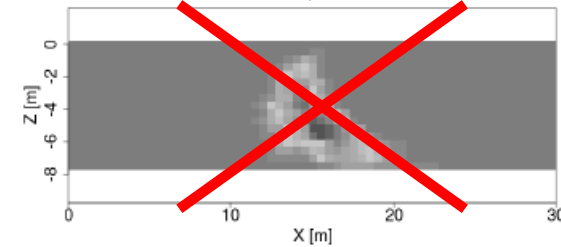
Small amount of observations



↓ Variogram fitting

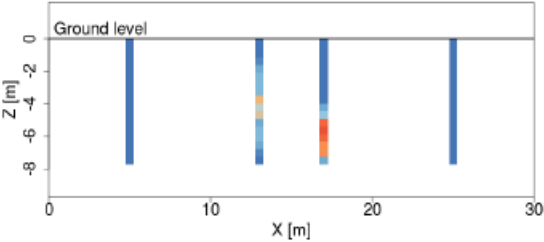


↓ Kriging?



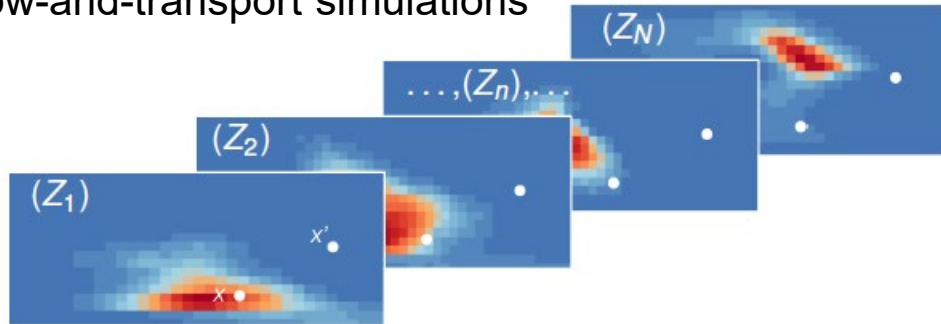
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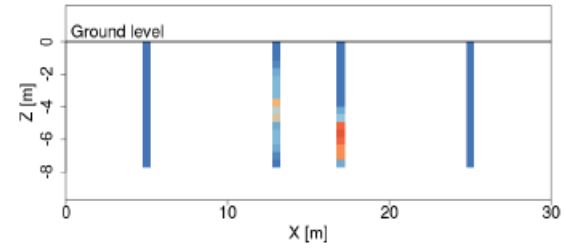


# Kriging with Numerical Variograms (KNV)

Flow-and-transport simulations

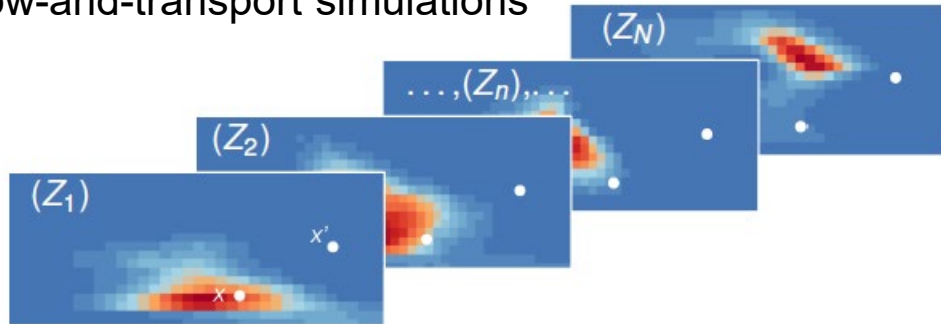


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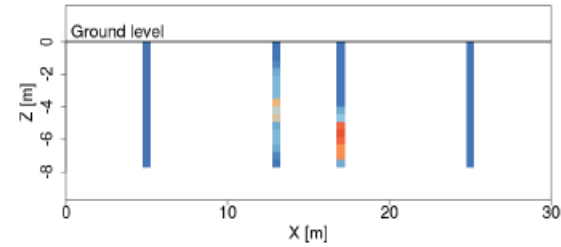
Flow-and-transport simulations



↓ Numerical variograms

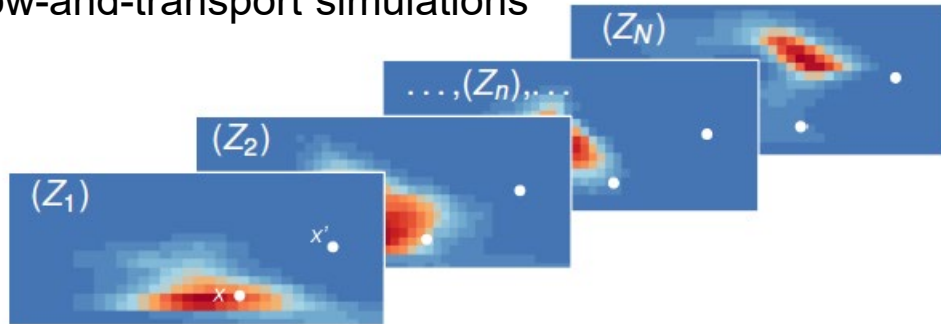
$$\gamma(x, x') = \frac{1}{N} \sum_{n=1}^N \frac{1}{2} [Z_n(x) - Z_n(x')]^2$$

Small amount of observations



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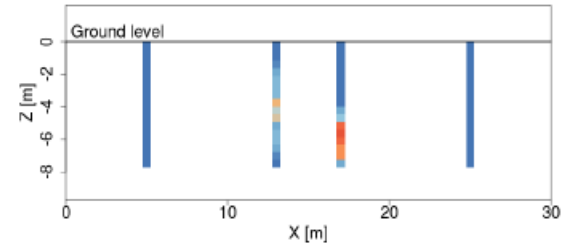
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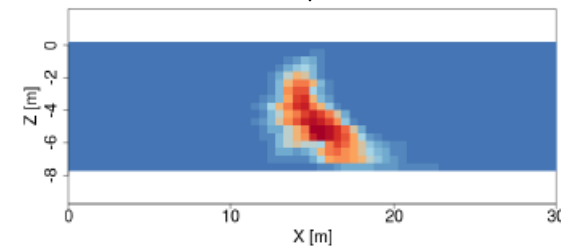
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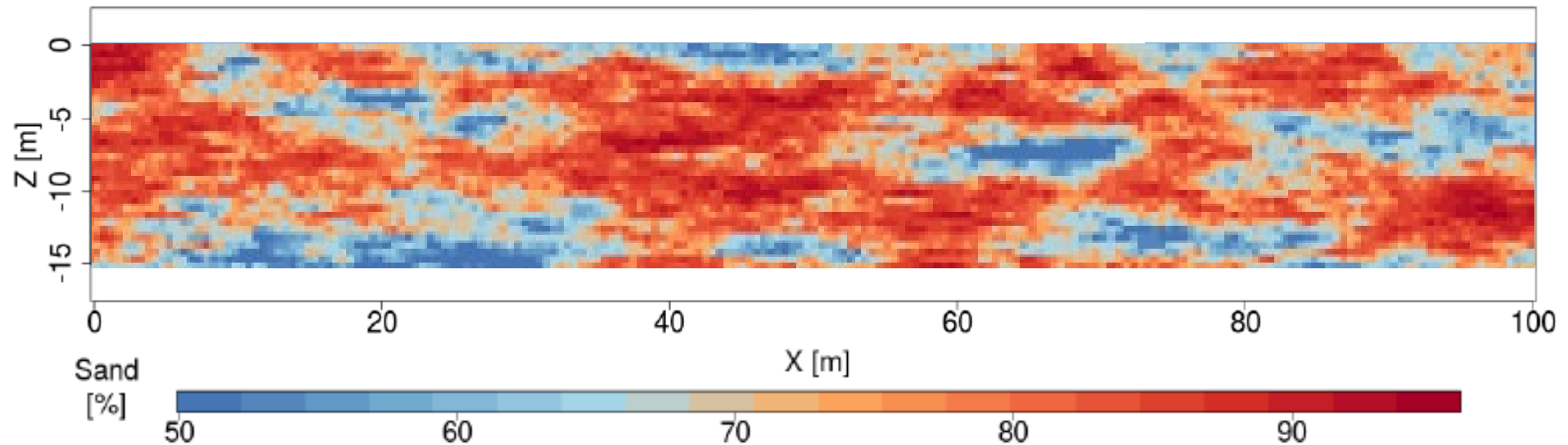
## Synthetic reference test case

- Development of a method using physical information given by physically-based simulations into a geostatistical framework:
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## Synthetic reference test case

- Model settings (2D vertical section)

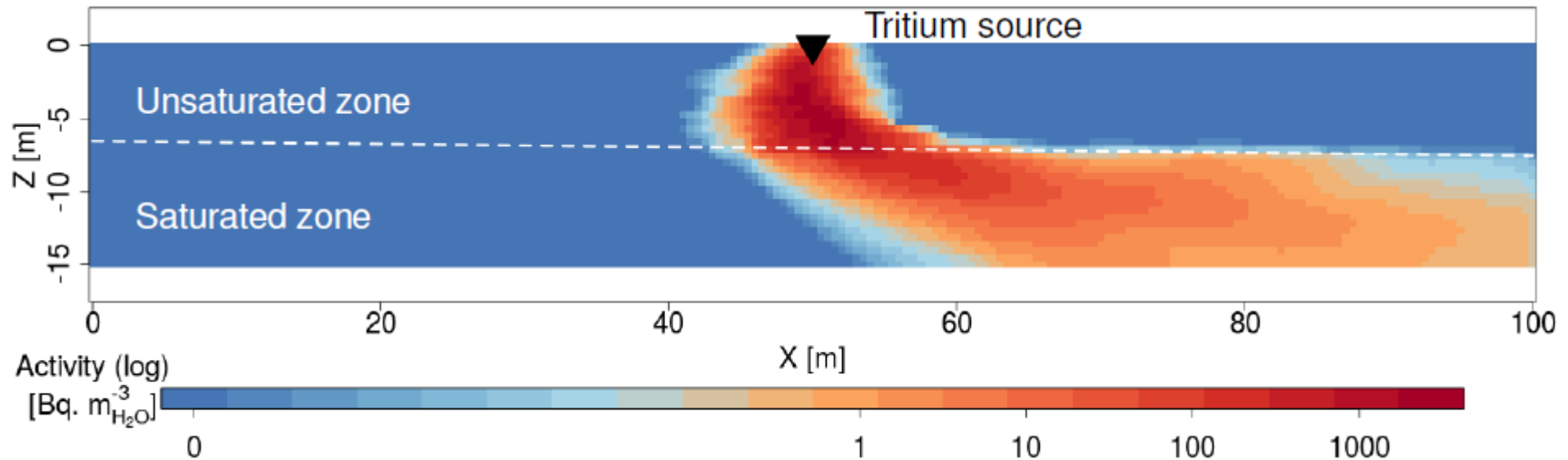
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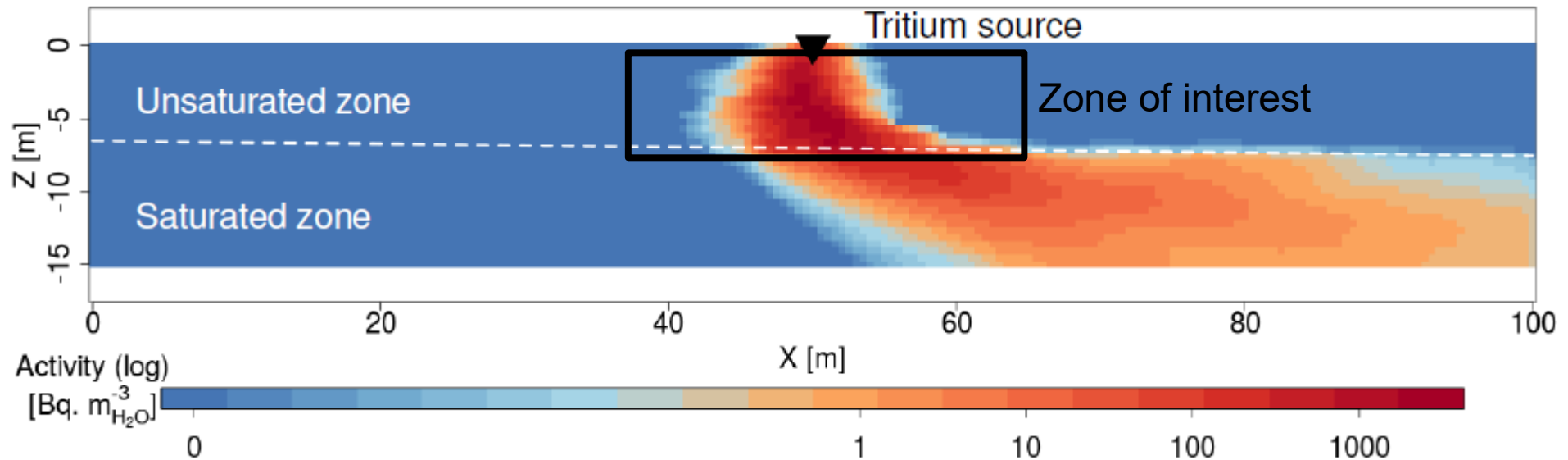
- Sandy loam facies with heterogeneous textural properties (i.e., sand, silt, clay contents);
- Fixed upstream-downstream head: unsaturated zone ~7 m deep;
- Contamination due to a point source of tritium: 4 years simulation with the code MELODIE.



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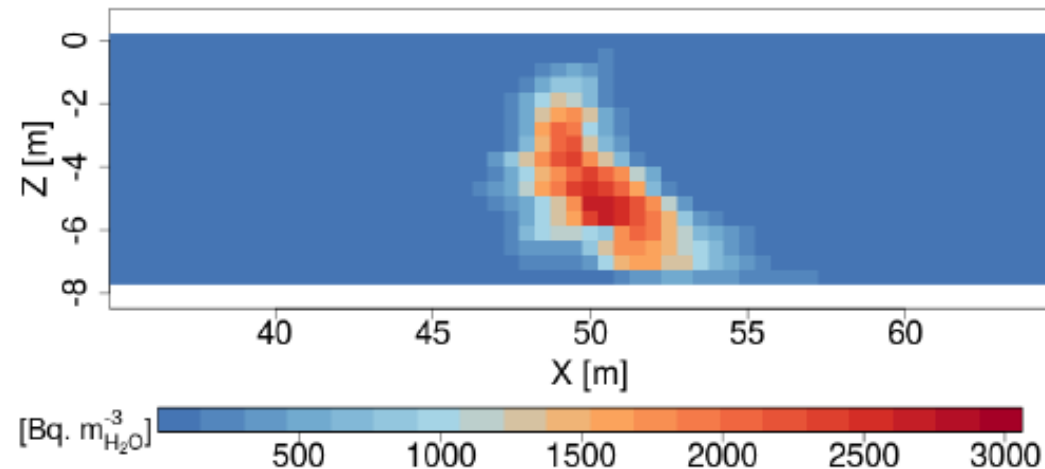
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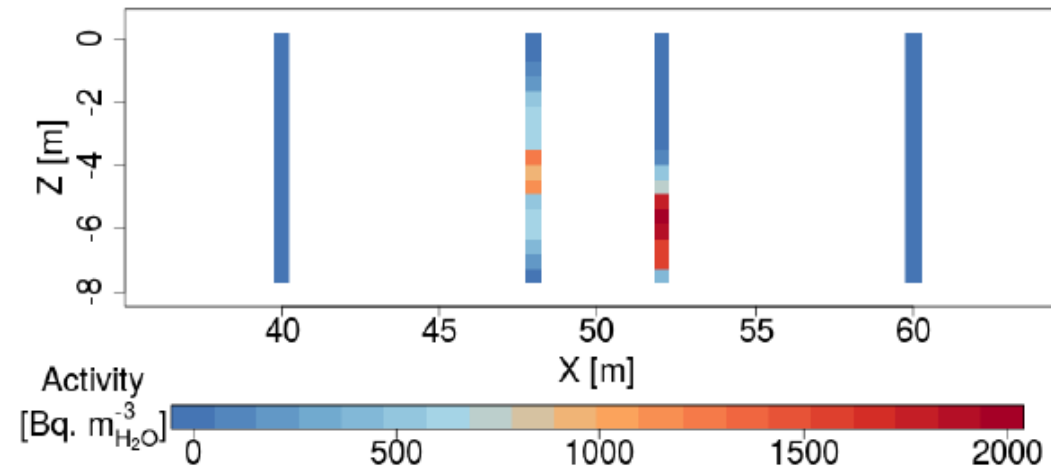
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## Synthetic reference test case

- Sampling scenario

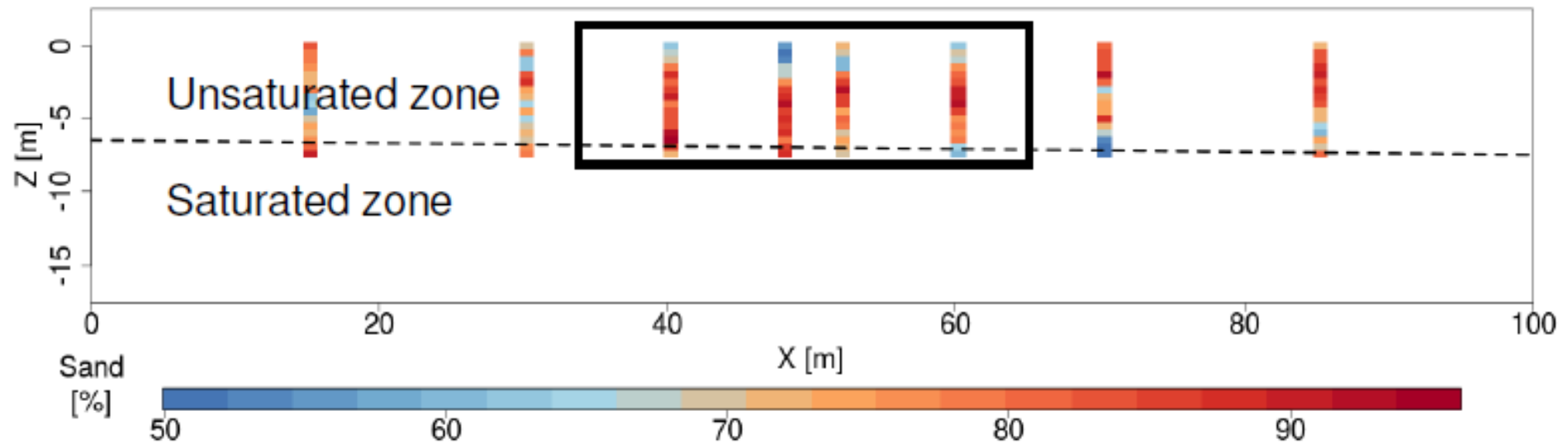
- 4 boreholes with activity;



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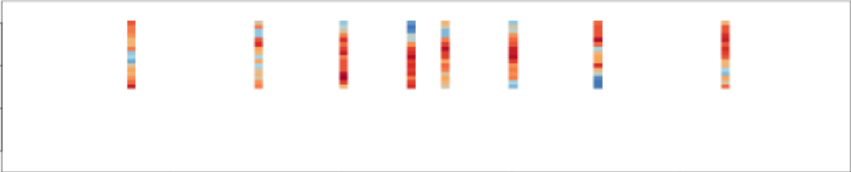
- Sampling scenario

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



# Synthetic reference test case

Observations of texture





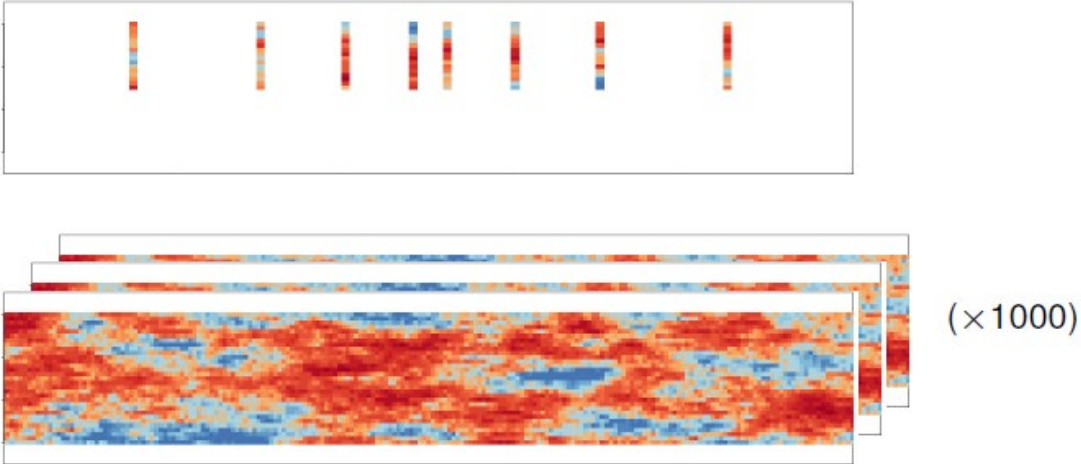
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Observations of texture

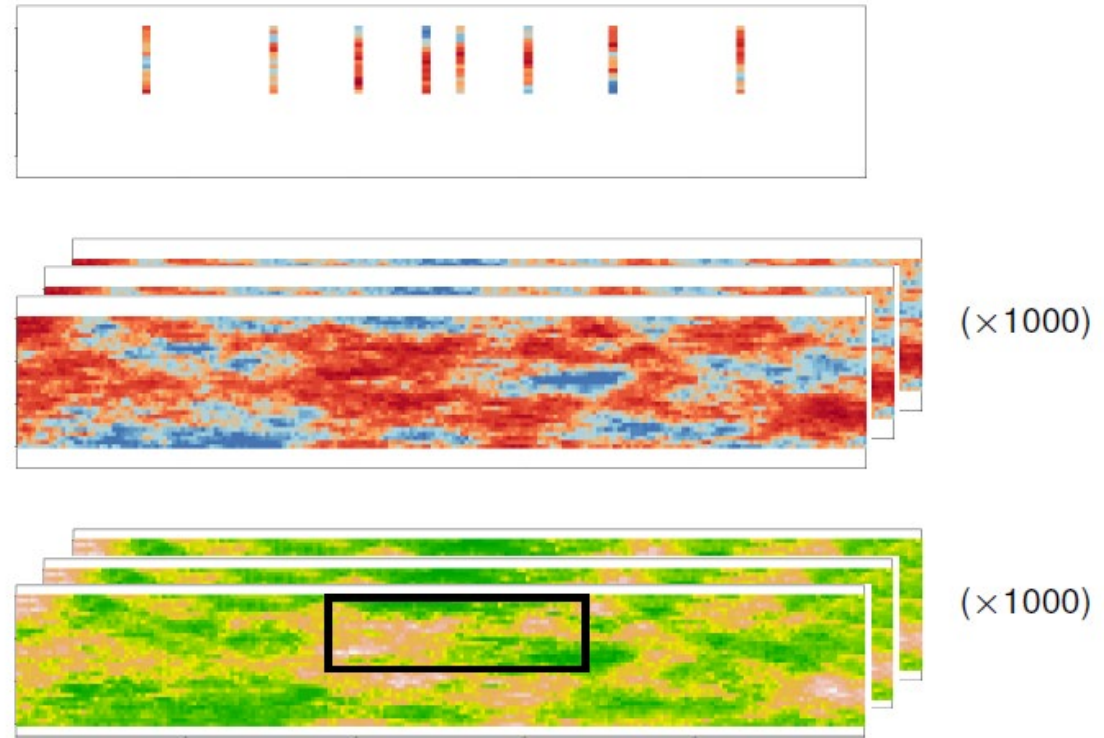
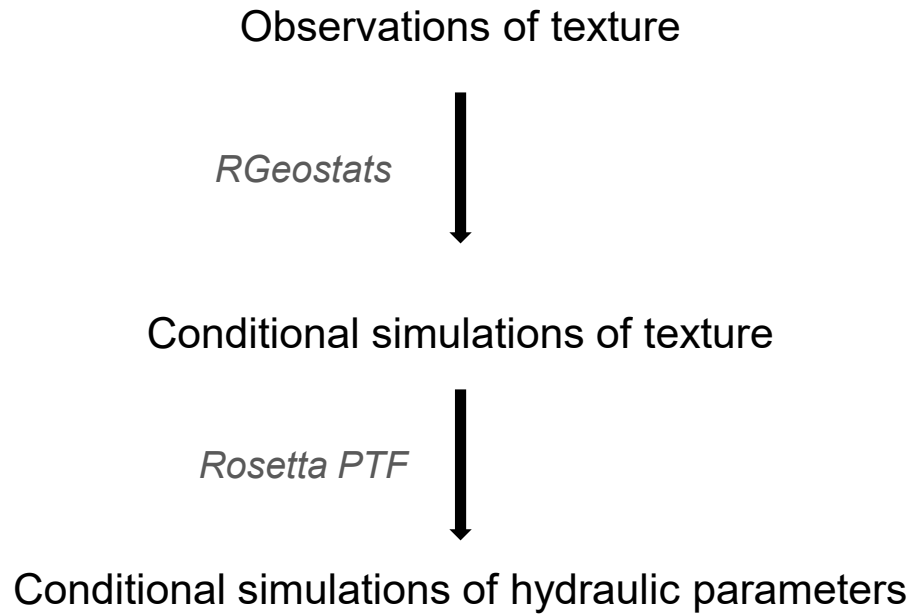
*RGeostats*



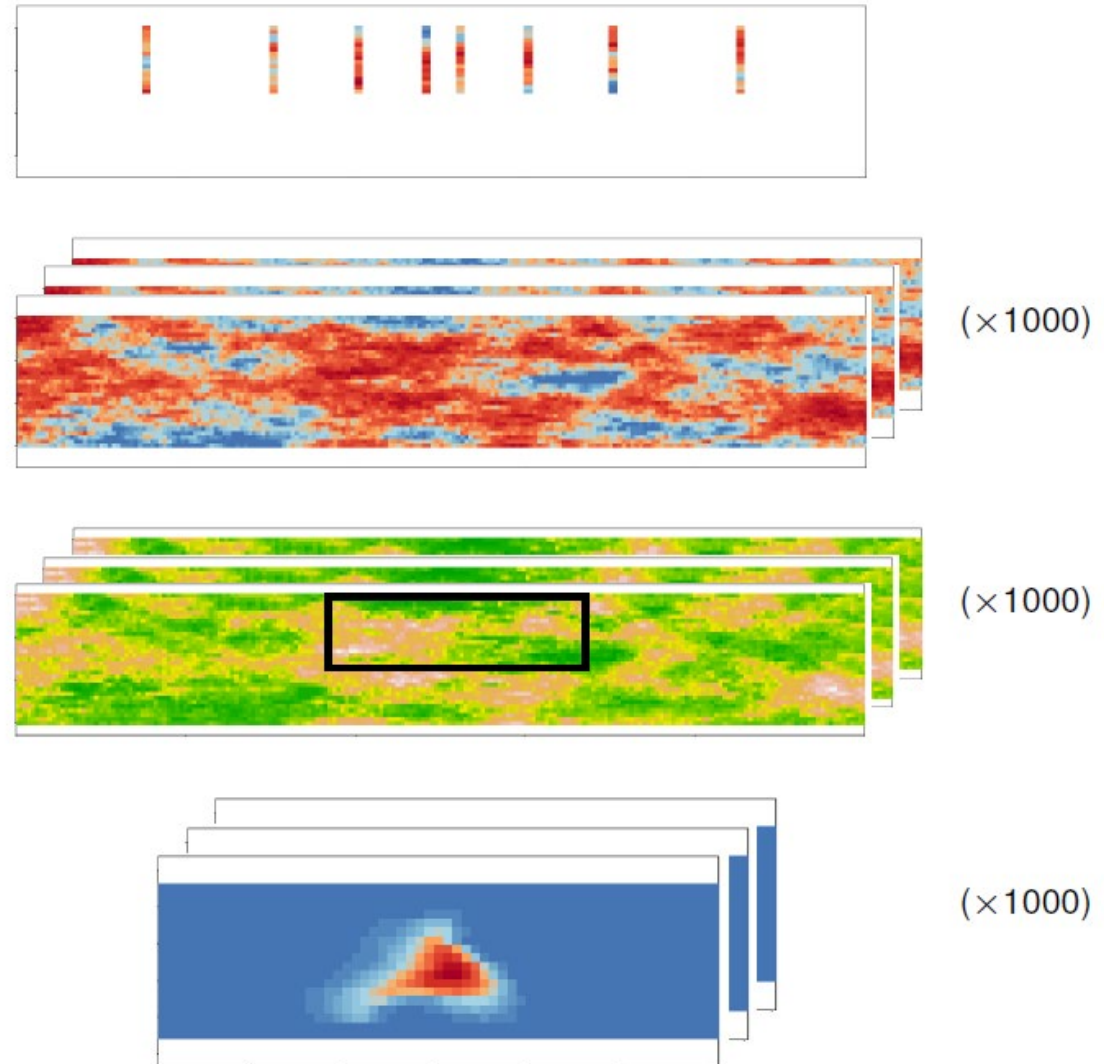
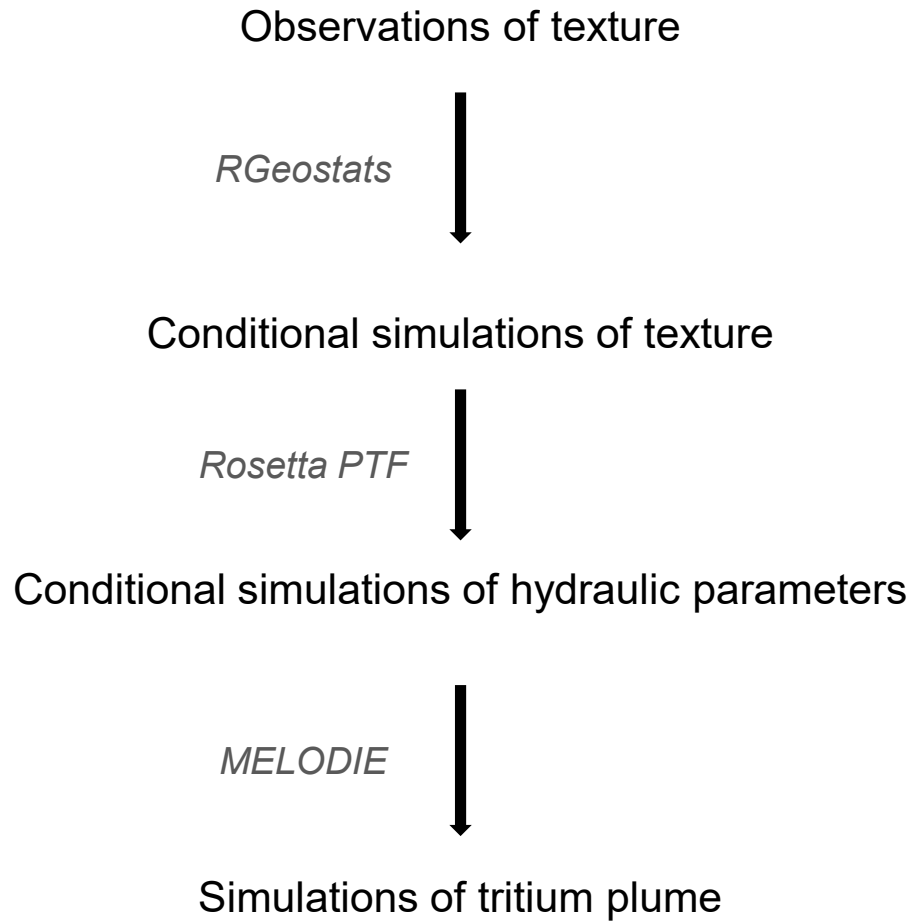
Conditional simulations of texture



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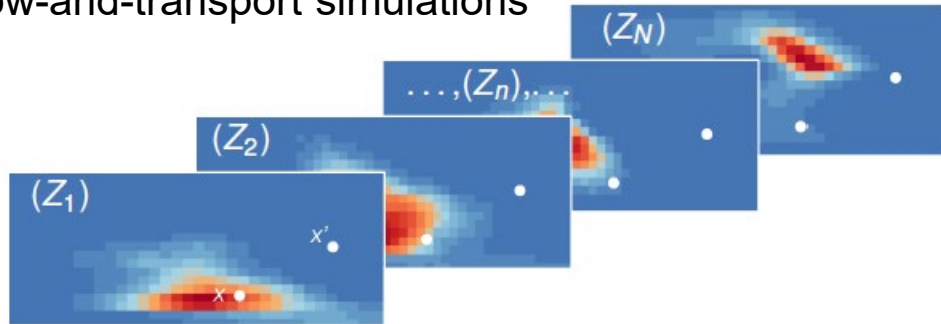


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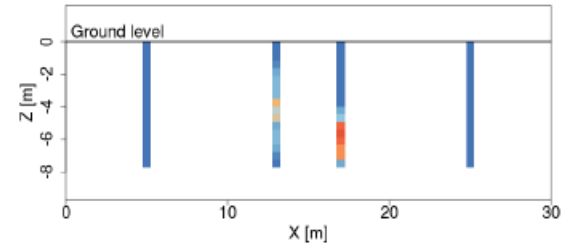
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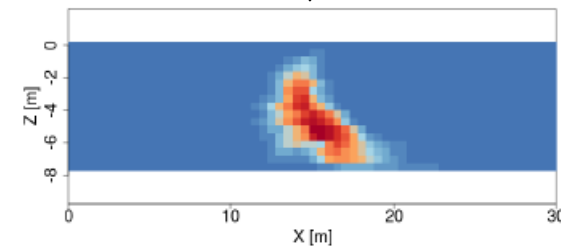
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## KNV vs. classical krigings

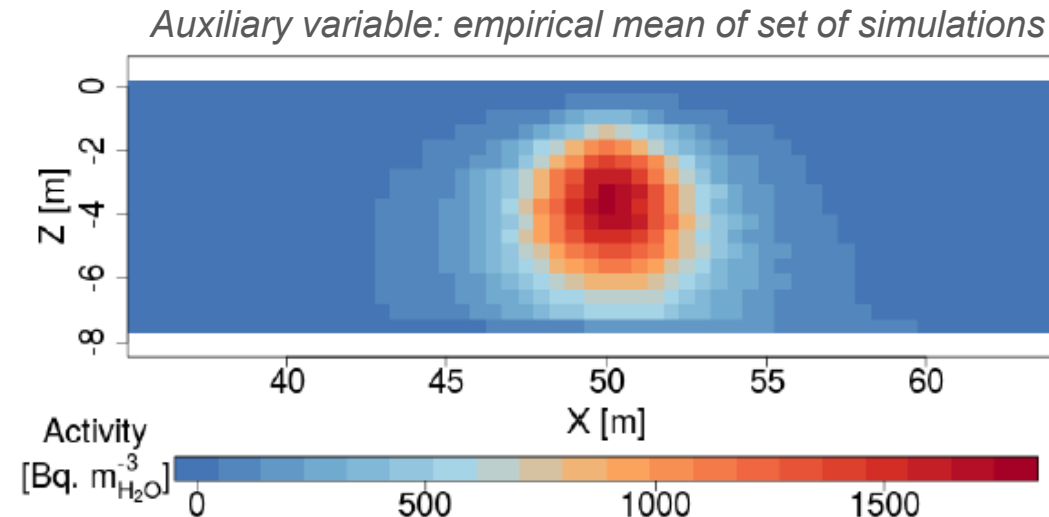
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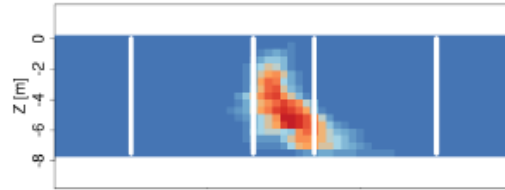
- **Ordinary kriging (OK)**, which is widely used but known to perform poorly when the number of data is too small or when the phenomenon under study is complex;
- **Kriging with external drift (KED)**, which enables the incorporation of auxiliary variables to take non-stationarity into account.

## KNV vs. classical krigings

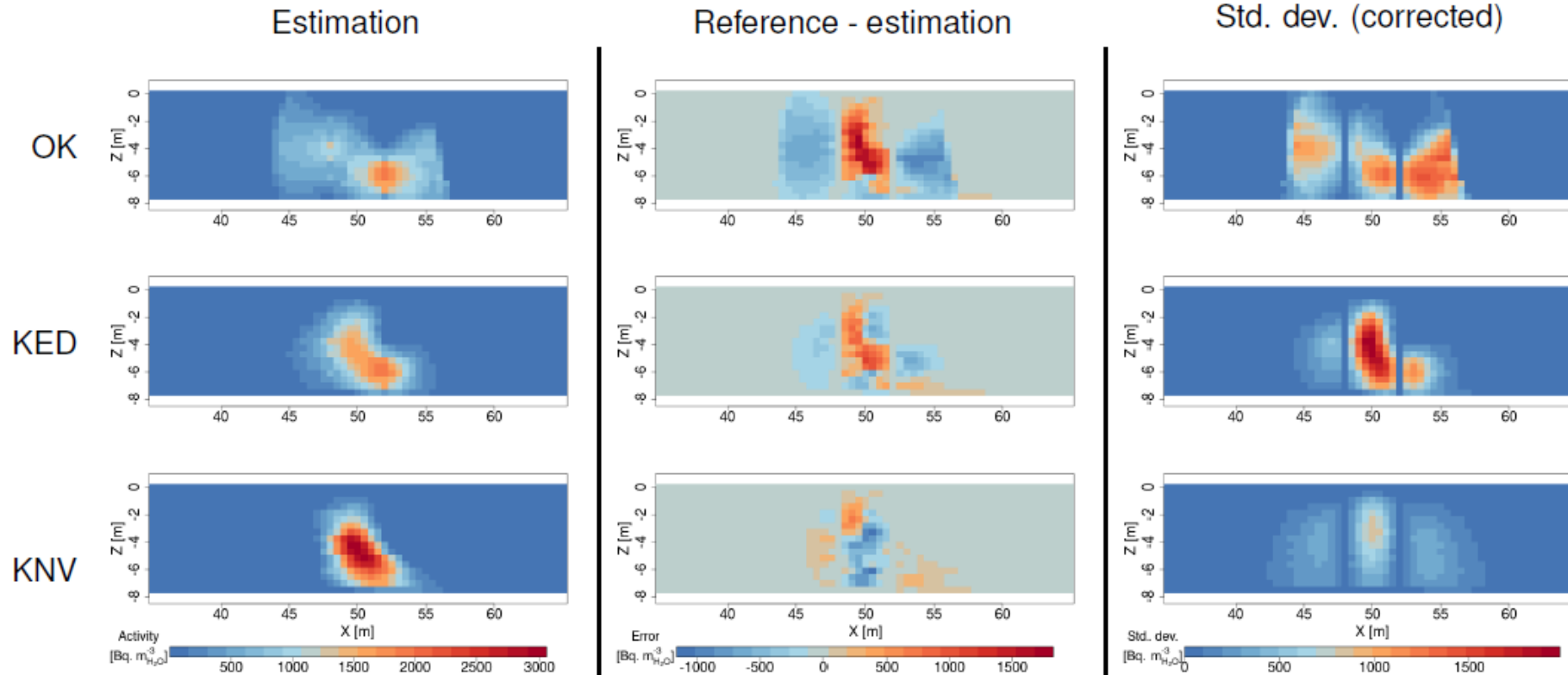
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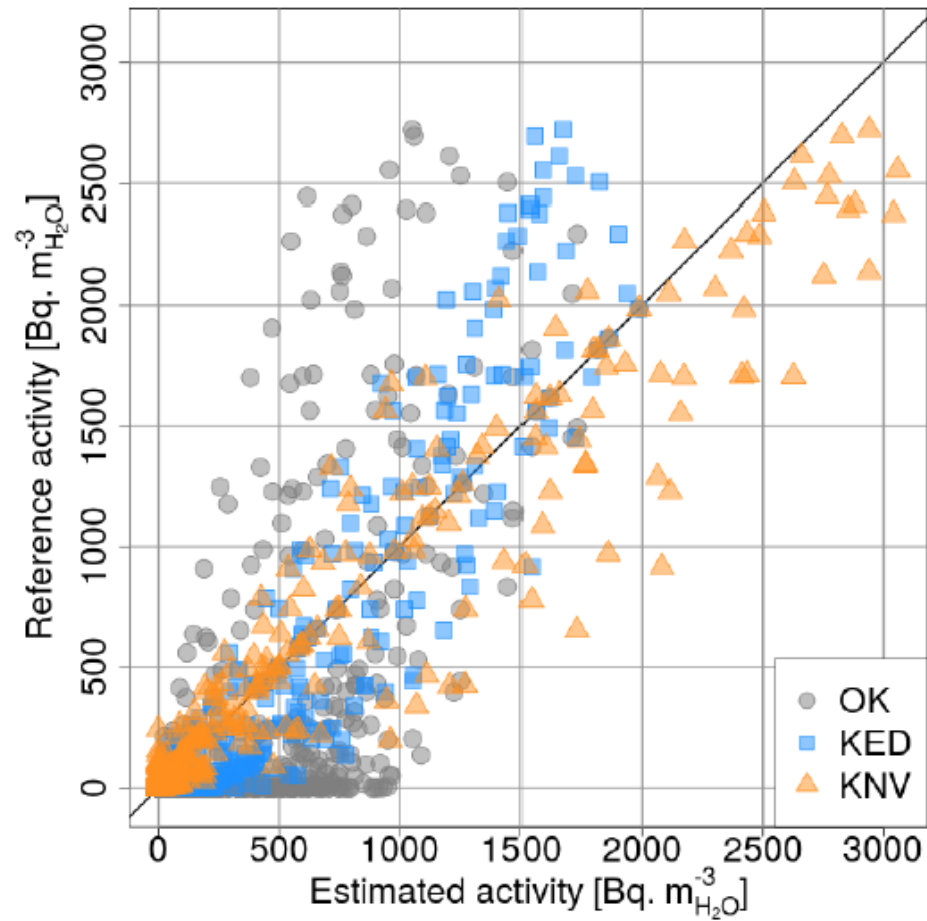


Reference tritium plume

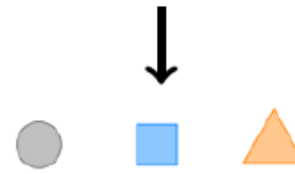




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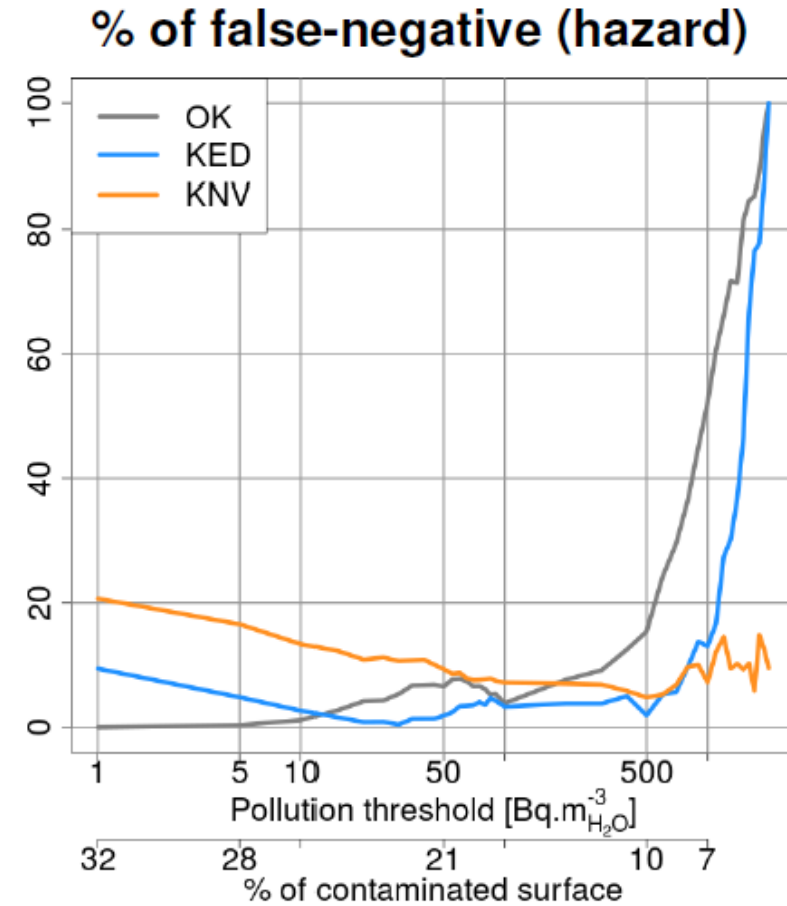
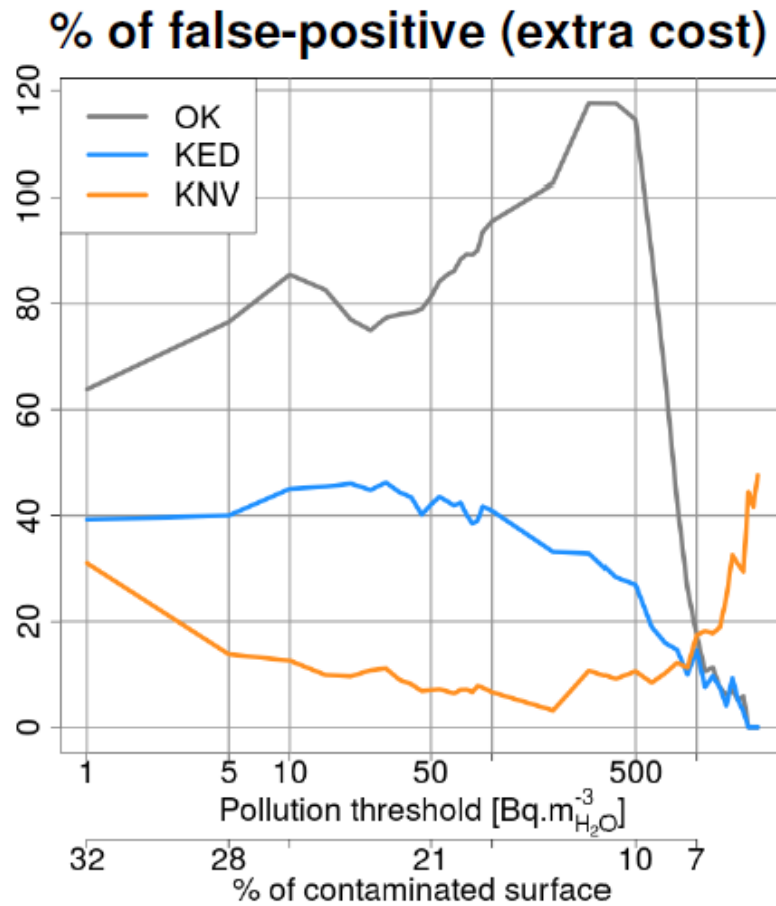
1 point of the domain



## Global statistics

	OK	KED	KNV
MAE [ $\text{Bq. m}^{-3}_{\text{H}_2\text{O}}$ ]	173	71	<b>47</b>
RMSE [ $\text{Bq. m}^{-3}_{\text{H}_2\text{O}}$ ]	348	174	<b>147</b>
MRE [-]	-47	-6.8	<b>-0.8</b>

# KNV vs. classical krigings



## Conclusion

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- KNV is even more interesting **when the number of observations of pollutant is reduced**. It also works when the boreholes are located around the zone of high values of activities.
- 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.*