

Combining geostatistics and physically-based simulations to characterize contaminated soils



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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**?

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

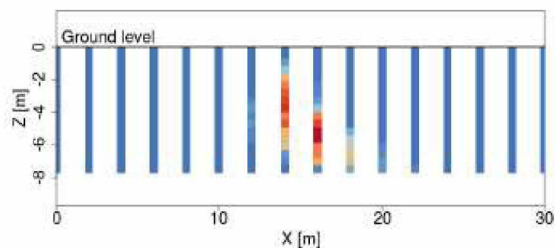
Outline

Development of a method using physical information given by physically-based simulations into a geostatistical framework:

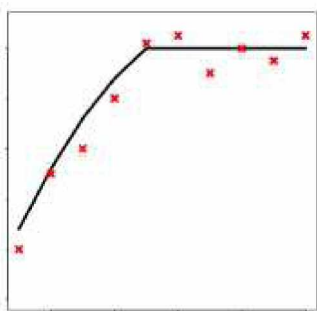
- 1. The Kriging with Numerical Variograms (KNV) method**
2. A synthetic reference test case
3. Comparison of KNV to classical krigings

Limitation of classical geostatistical approaches

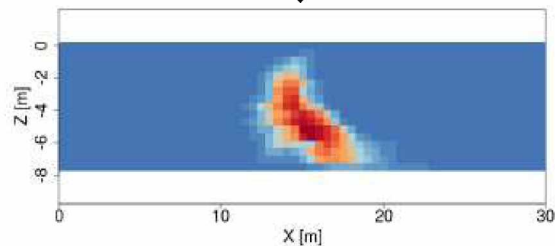
Numerous observations



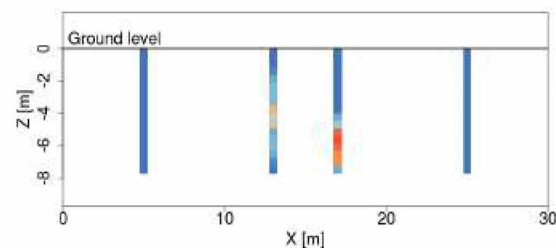
↓ Variogram fitting



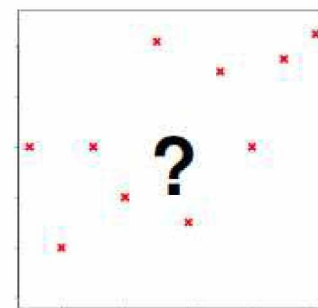
↓ Kriging



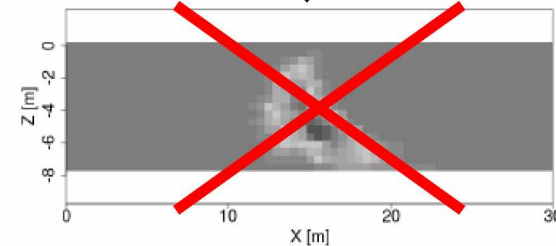
Small amount of observations



↓ Variogram fitting

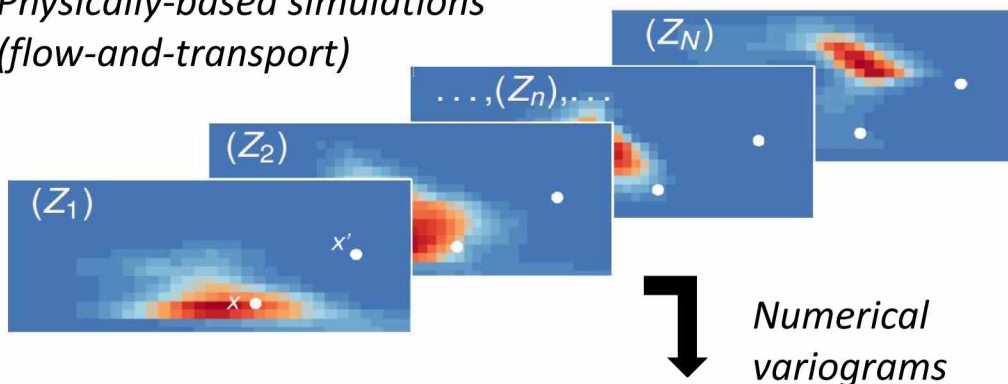


↓ Kriging?



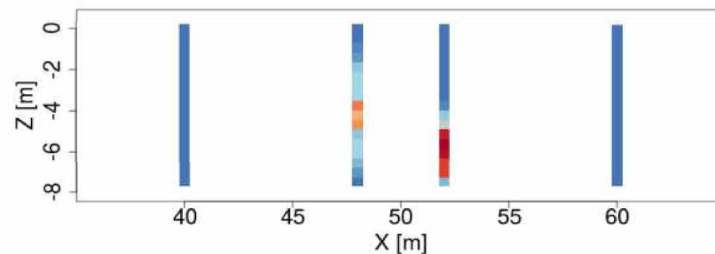
The KNV principle

Physically-based simulations
(flow-and-transport)

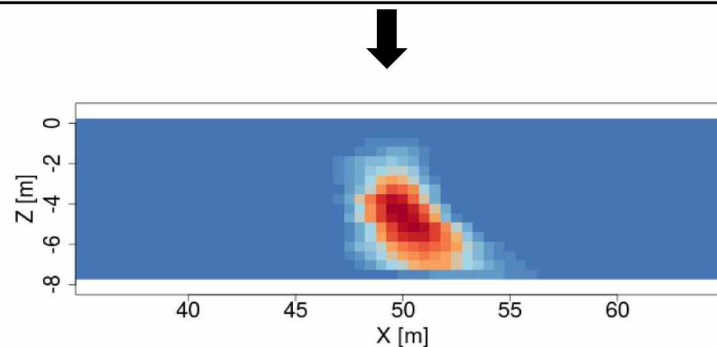


$$\gamma(x, x') = \frac{1}{N} \sum_{n=1}^N \frac{1}{2} [Z_n(x) - Z_n(x')]^2$$

Small amount of observations



Kriging with numerical variograms

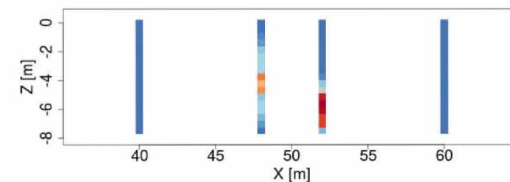
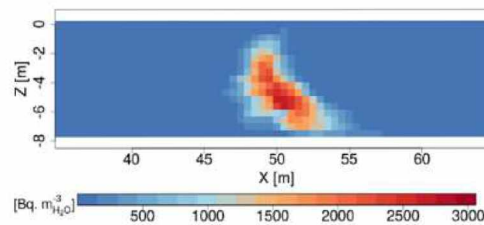
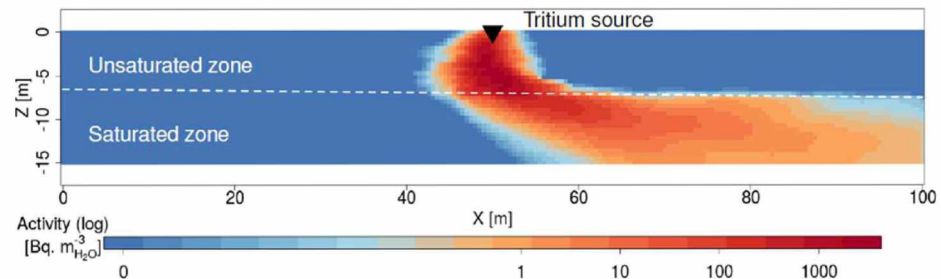
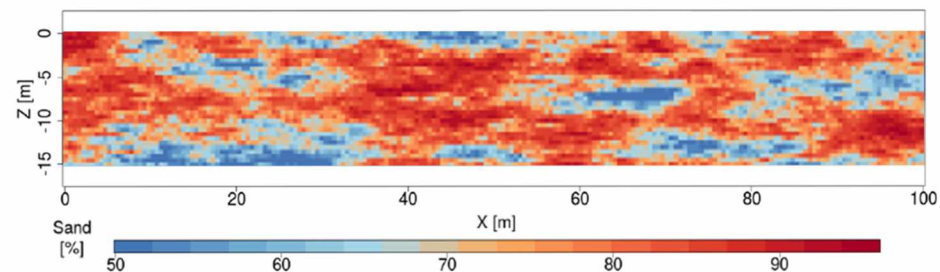
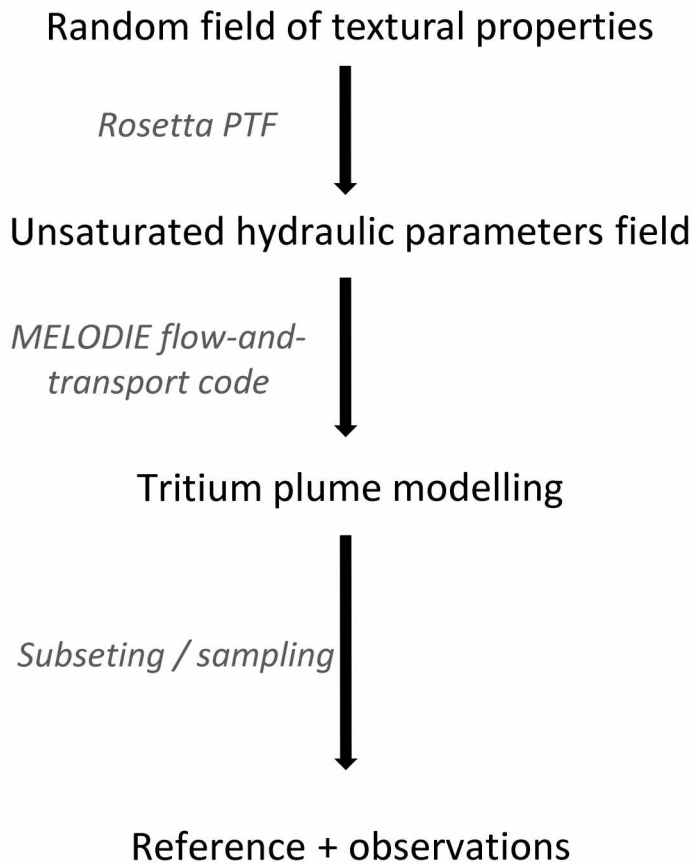


Outline

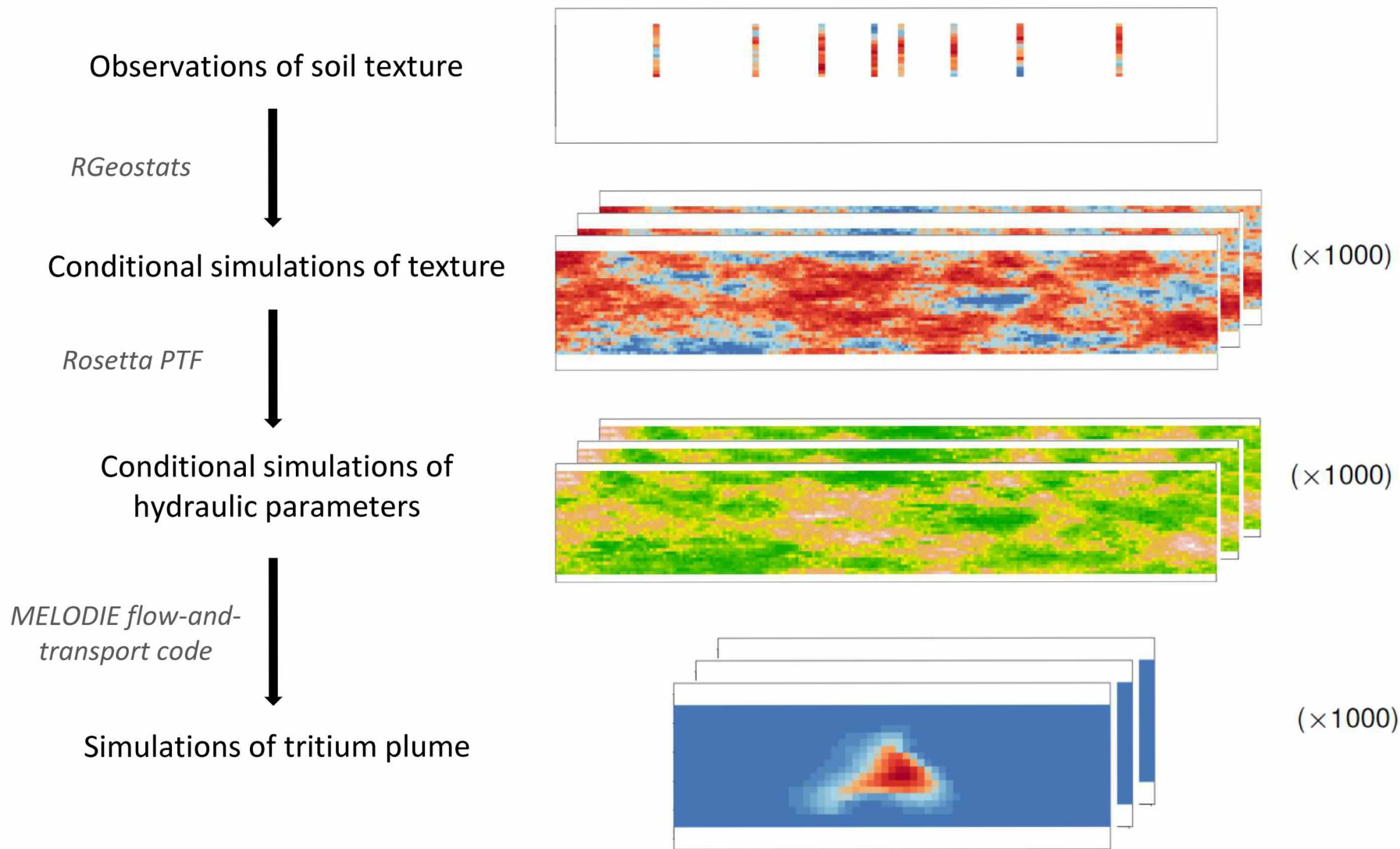
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Small amount of observations

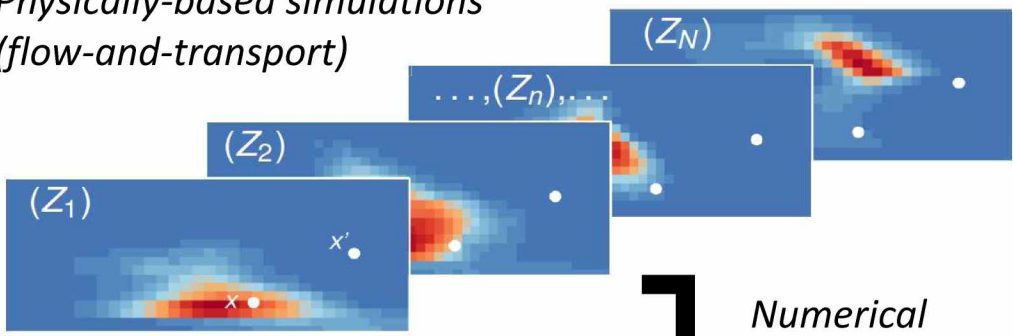


Flow-and-transport simulations



Kriging with Numerical Variograms

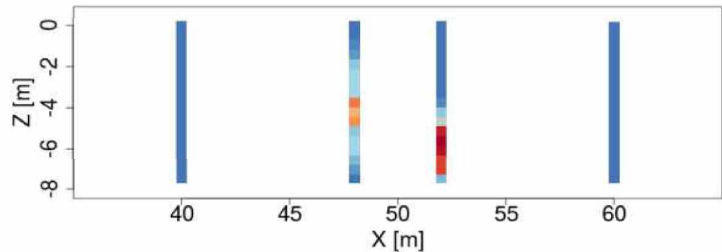
Physically-based simulations
(flow-and-transport)



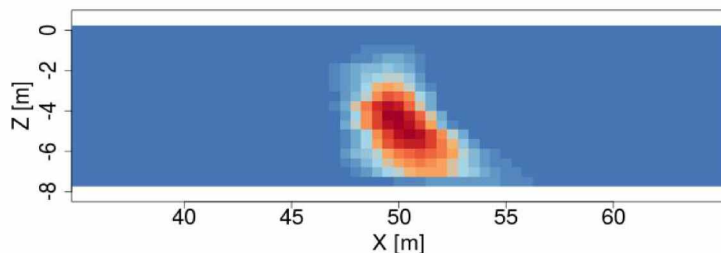
↓
Numerical
variograms

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

Small amount of observations



Kriging with numerical variograms



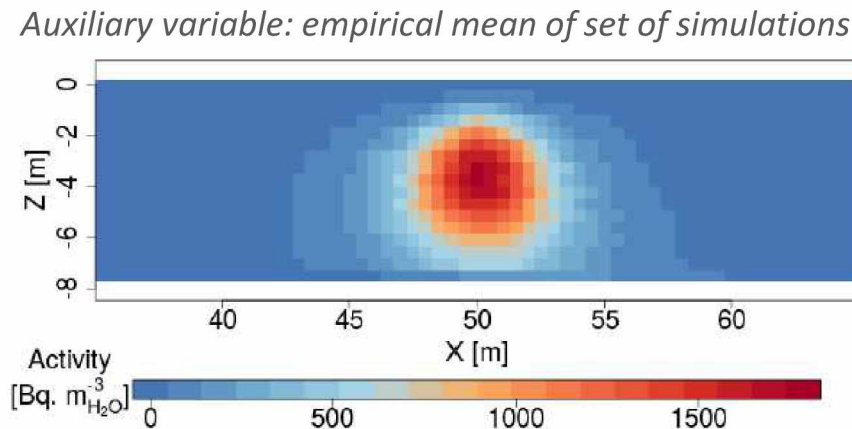
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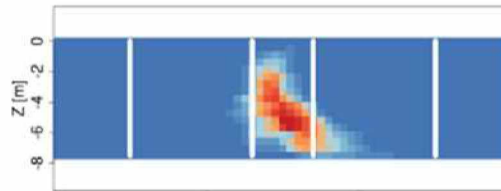
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Classical methods

- **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.



Results (1)



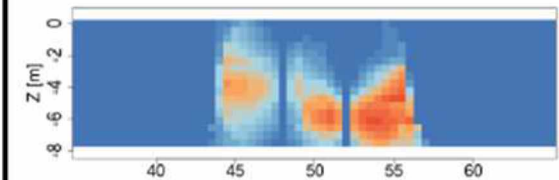
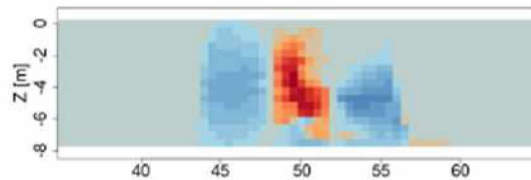
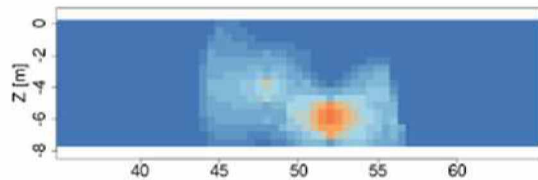
Reference tritium plume

Estimation

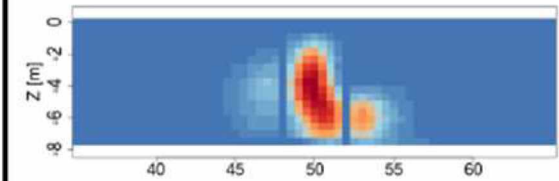
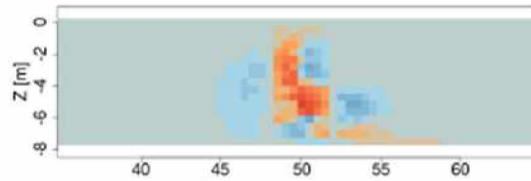
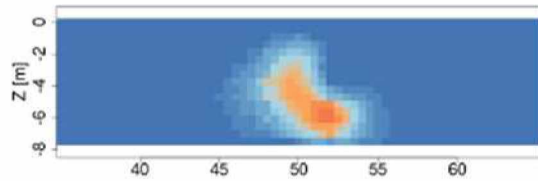
Reference - estimation

Std. dev. (corrected)

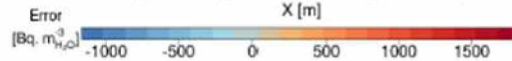
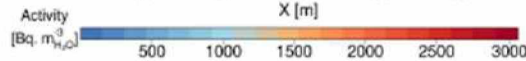
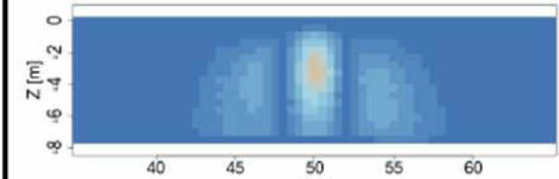
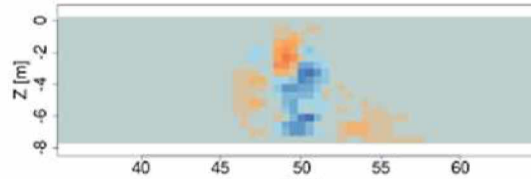
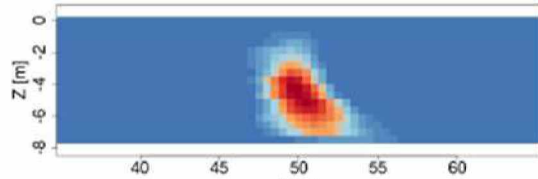
OK



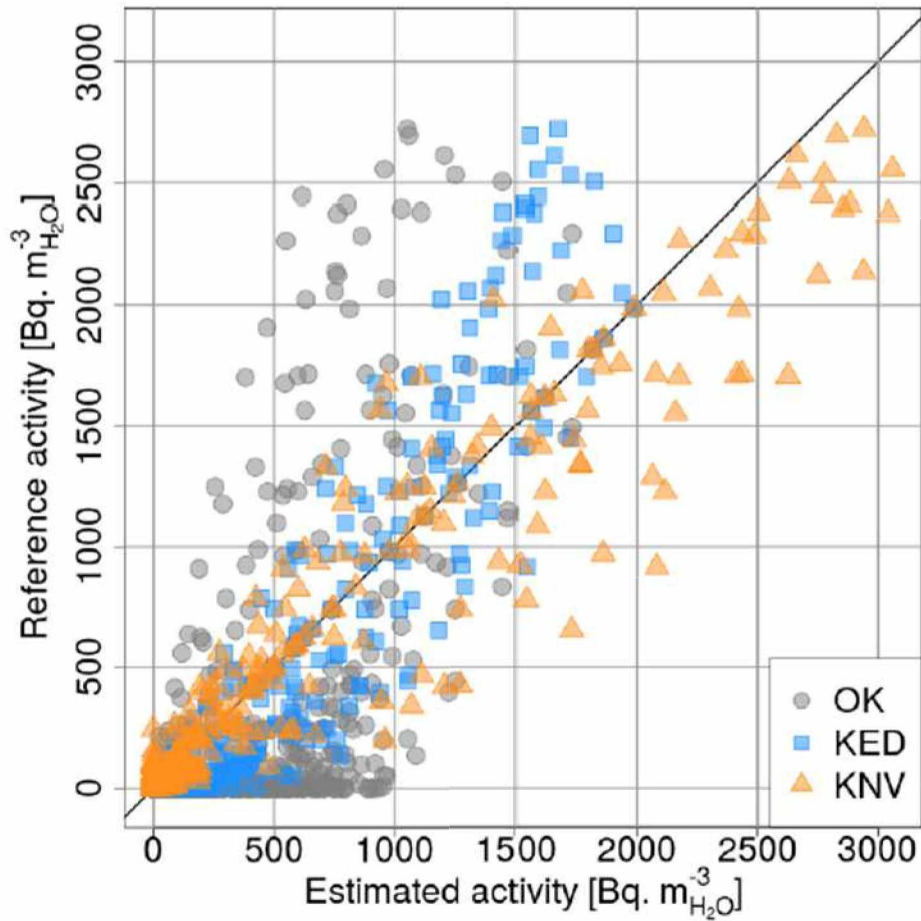
KED



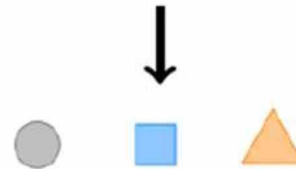
KNV



Results (2)



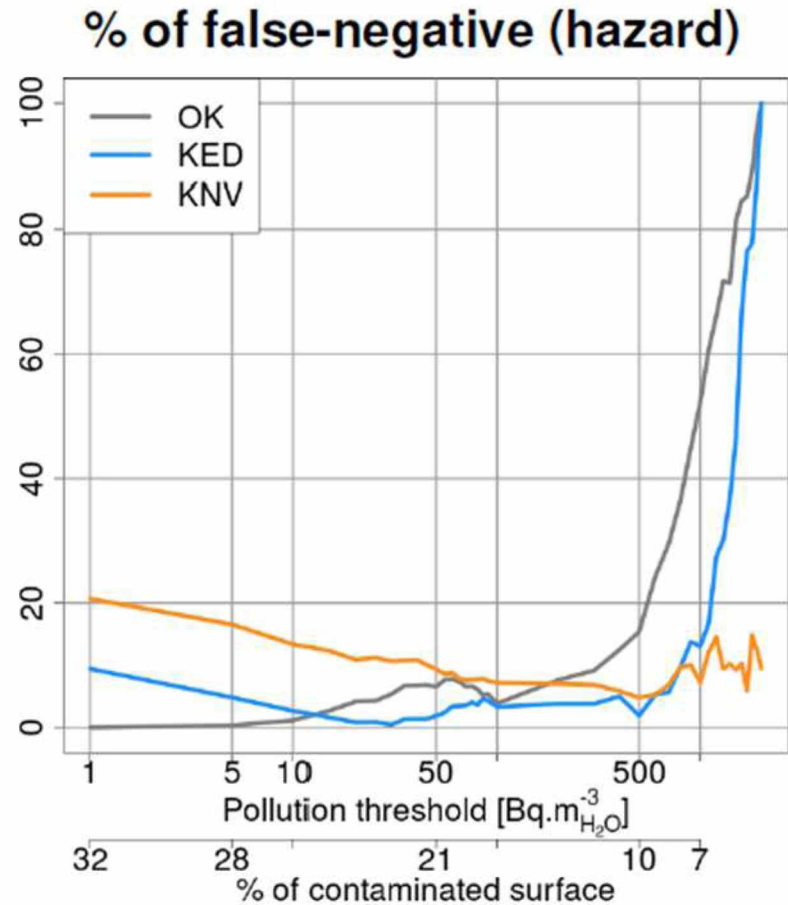
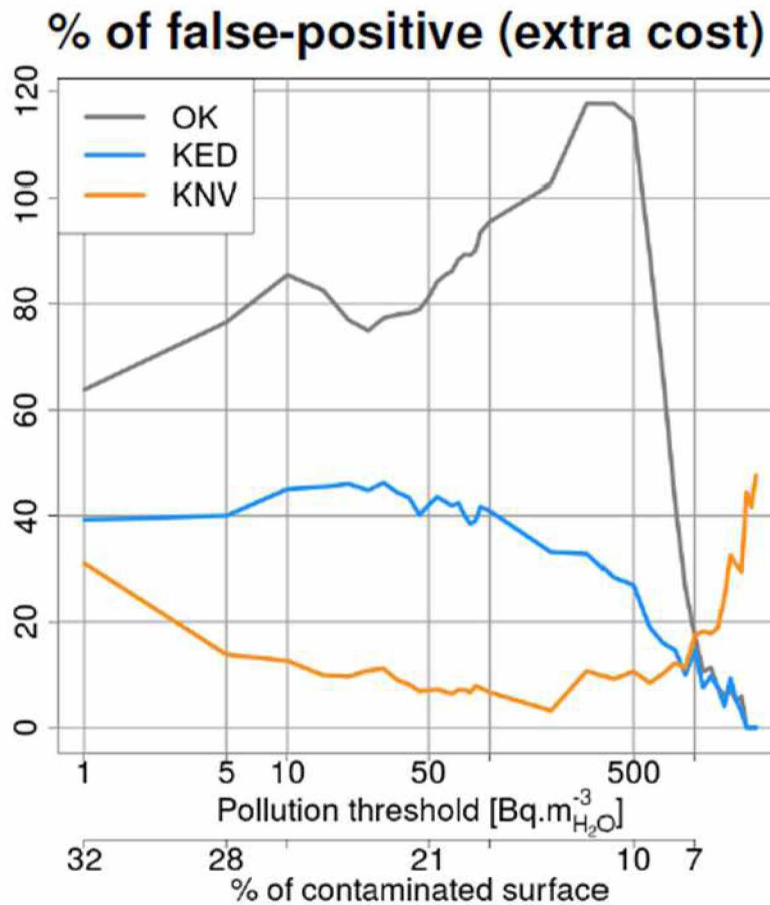
1 point of the domain



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

Results (3)



Conclusion

The characterization of the tritium plume within the unsaturated zone is not accurate, **due to the uncertainties related to hydraulic parameters**, even if the initial boundary conditions of the flow-and-transport model are fixed.

KNV improves the estimates of the tritium plume in the unsaturated zone compared to OK and KED: estimation errors and standard deviation errors are reduced.

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.

For more information:

Pannecoucke, L., Le Coz, M., Freulon, X., de Fouquet, C. 2019. Combining geostatistics and simulations of flow and transport to characterize contamination within the unsaturated zone. Science of The Total Environment 699.