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)	Direct flow-and-transport simulations
+ Observations honored	+ Physically-based model
- Physical information not taken into account	- Uncertainties in modeling parameters
- Performances limited if few data available	- Observations not honored

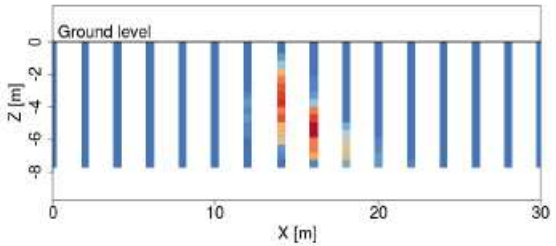
Outline

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

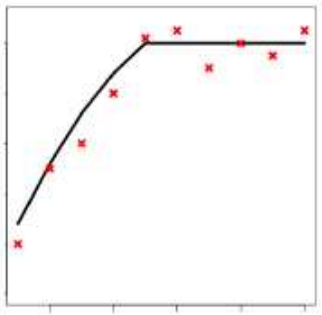
1. **The Kriging with Numerical Variograms (KNV) method**
2. A synthetic reference test case
3. Comparison of KNV to classical krigings

Limitation of classical geostatistical approaches

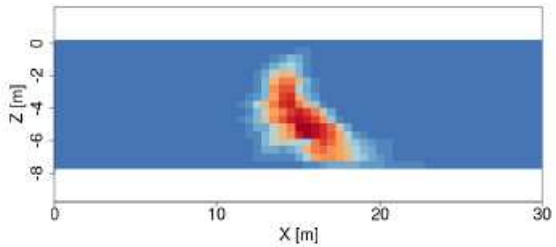
Numerous observations



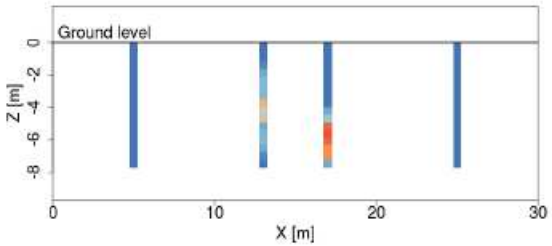
Variogram fitting



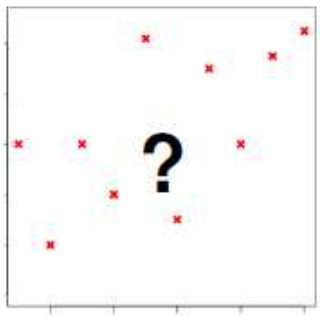
Kriging



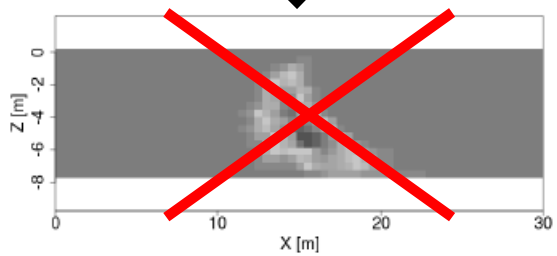
Small amount of observations



Variogram fitting

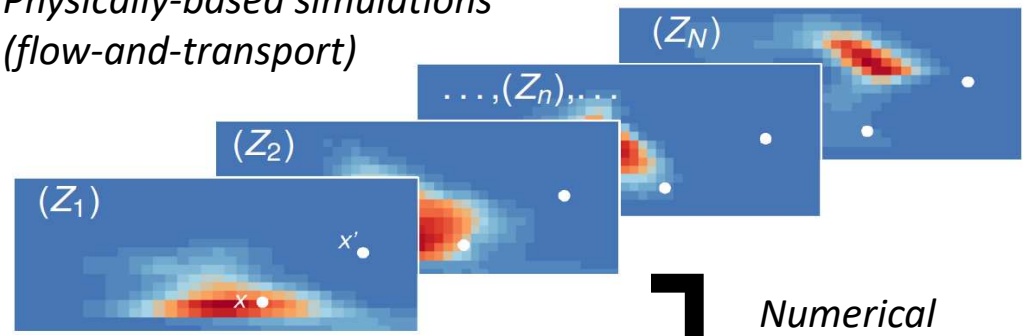


Kriging?



The KNV principle

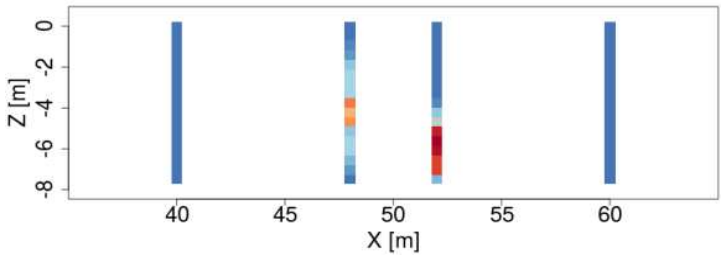
Physically-based simulations (flow-and-transport)



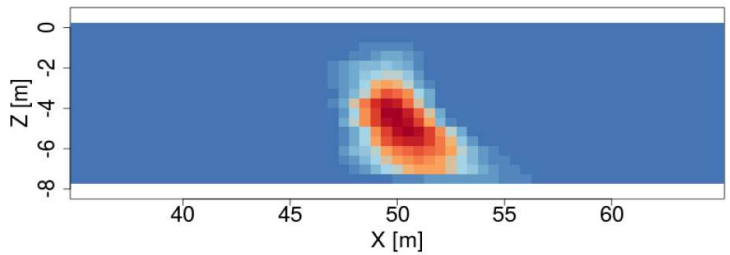
Numerical variograms

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

Small amount of observations



Kriging with numerical variograms



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Small amount of observations

Random field of textural properties

Rosetta PTF

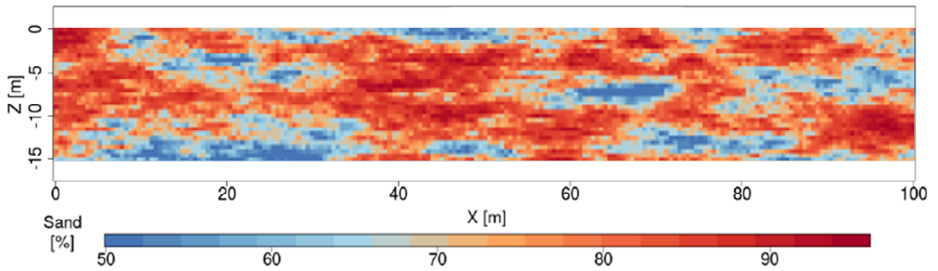
Unsaturated hydraulic parameters field

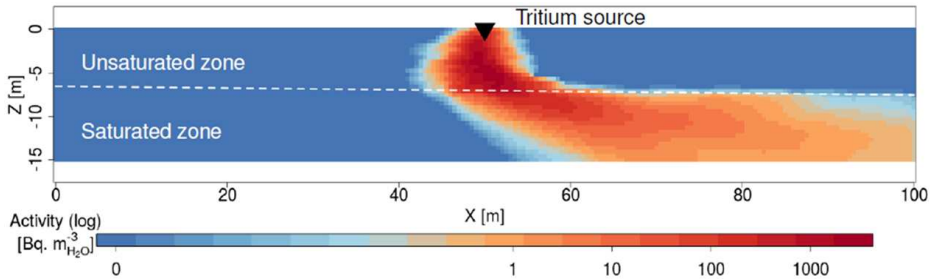
MELODIE flow-and-transport code

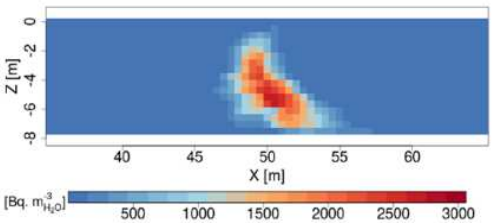
Tritium plume modelling

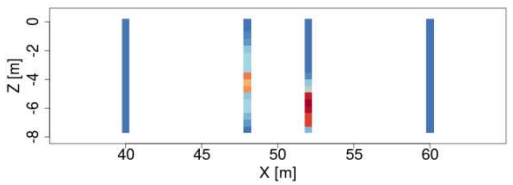
Subseting / sampling

Reference + observations









Flow-and-transport simulations

Observations of soil texture

RGeostats

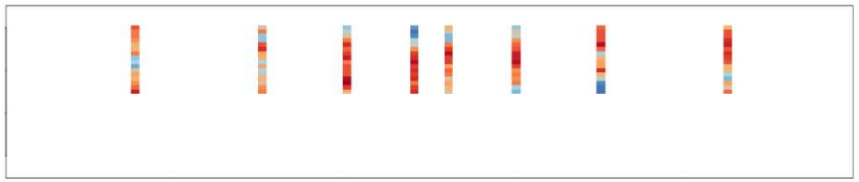
Conditional simulations of texture

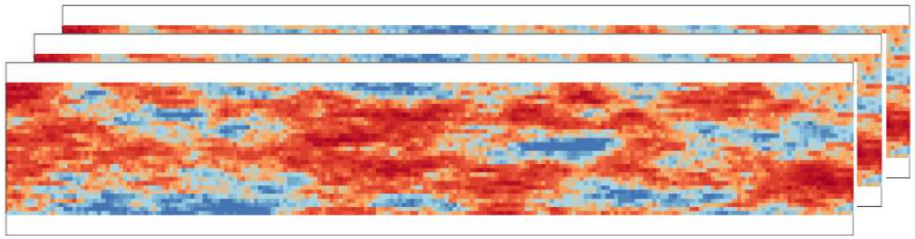
Rosetta PTF

Conditional simulations of hydraulic parameters

MELODIE flow-and-transport code

Simulations of tritium plume





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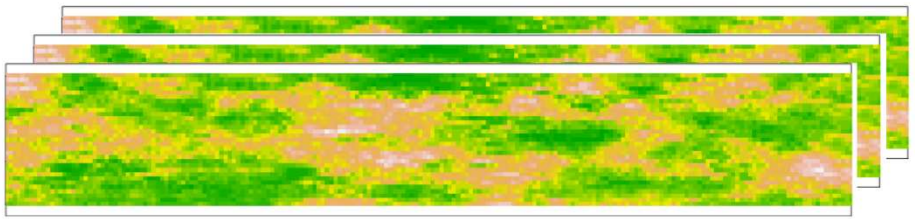

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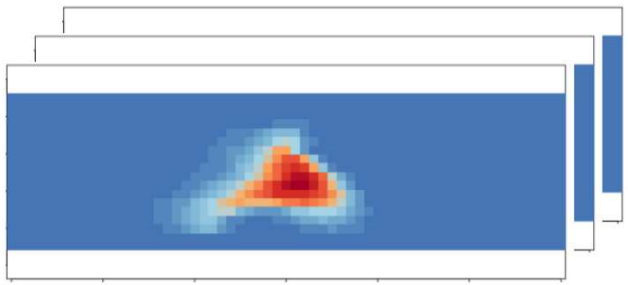

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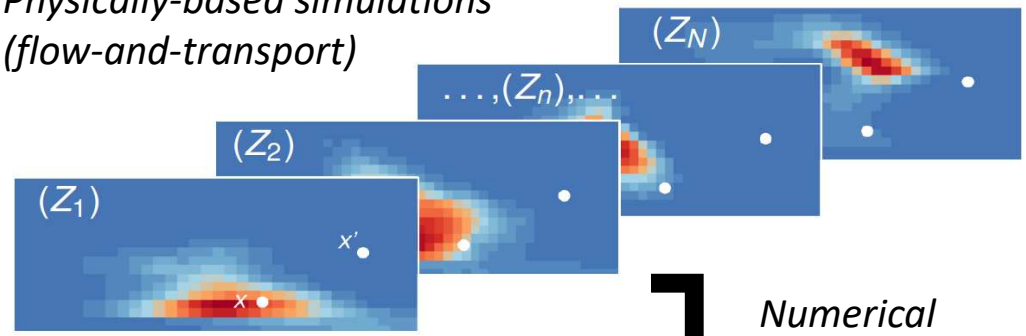
Kriging with Numerical Variograms

Physically-based simulations (flow-and-transport)



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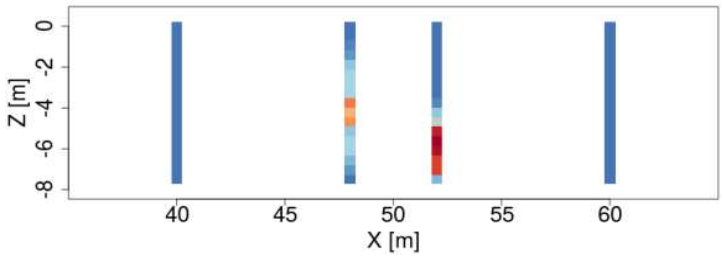

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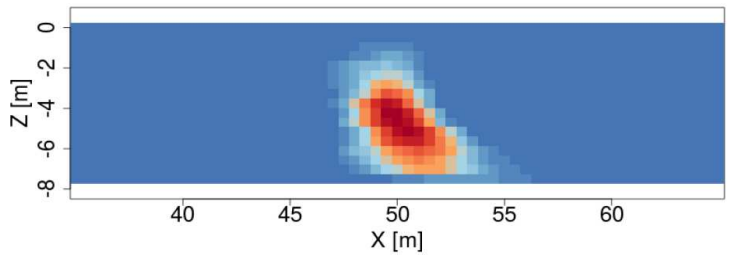

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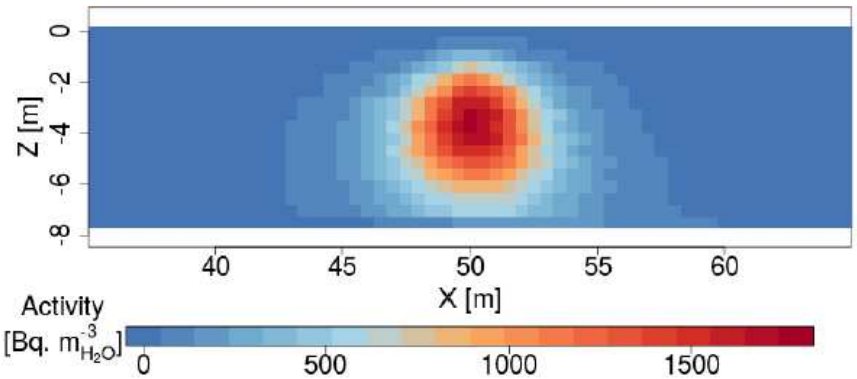
Classical methods

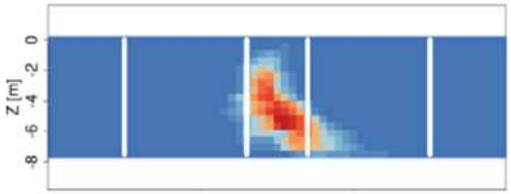
- Ordinary kriging (OK), which is widely used but known to perform poorly when the number of data is too small or when the phenomenon under study is complex;

- Kriging with external drift (KED), which enables the incorporation of auxiliary variables to take non-stationarity into account.

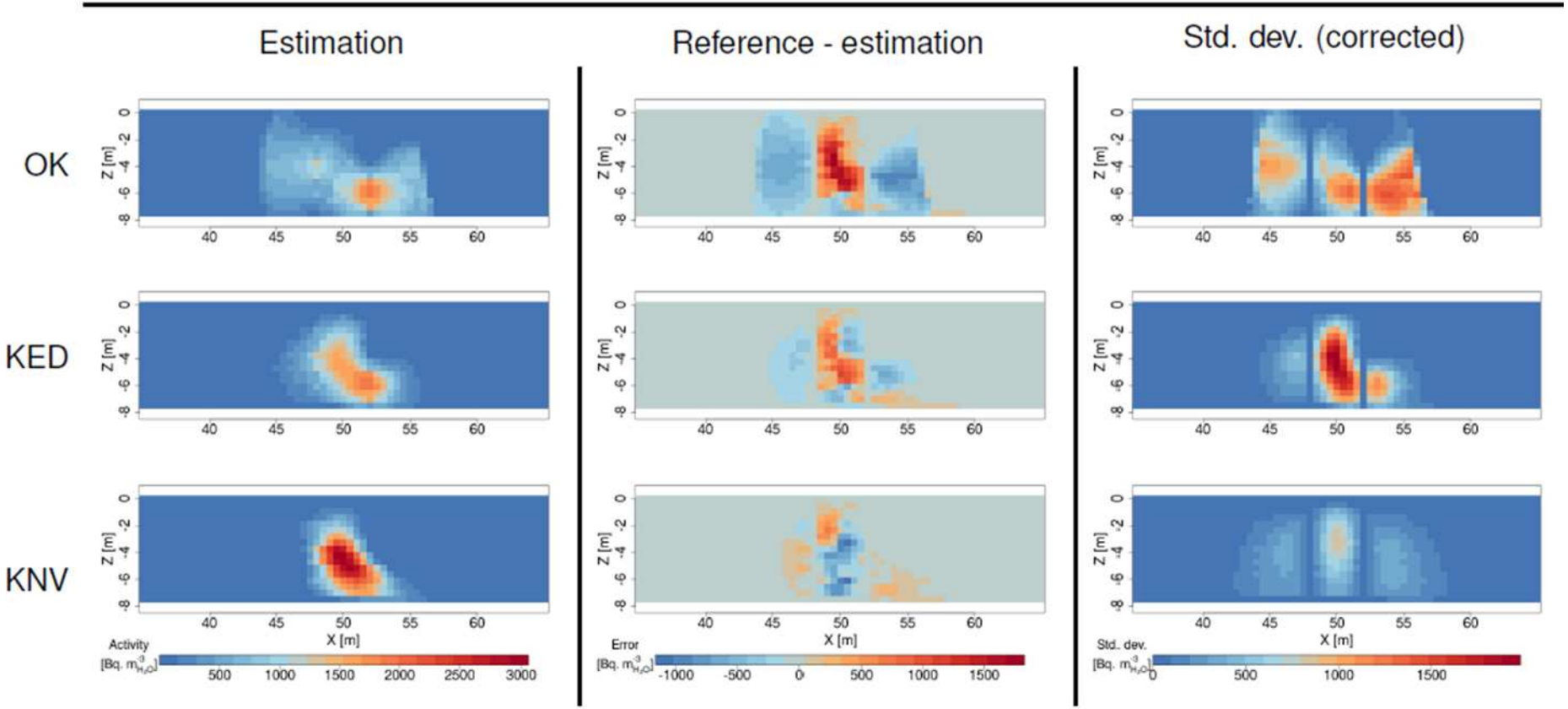
Auxiliary variable: empirical mean of set of simulations



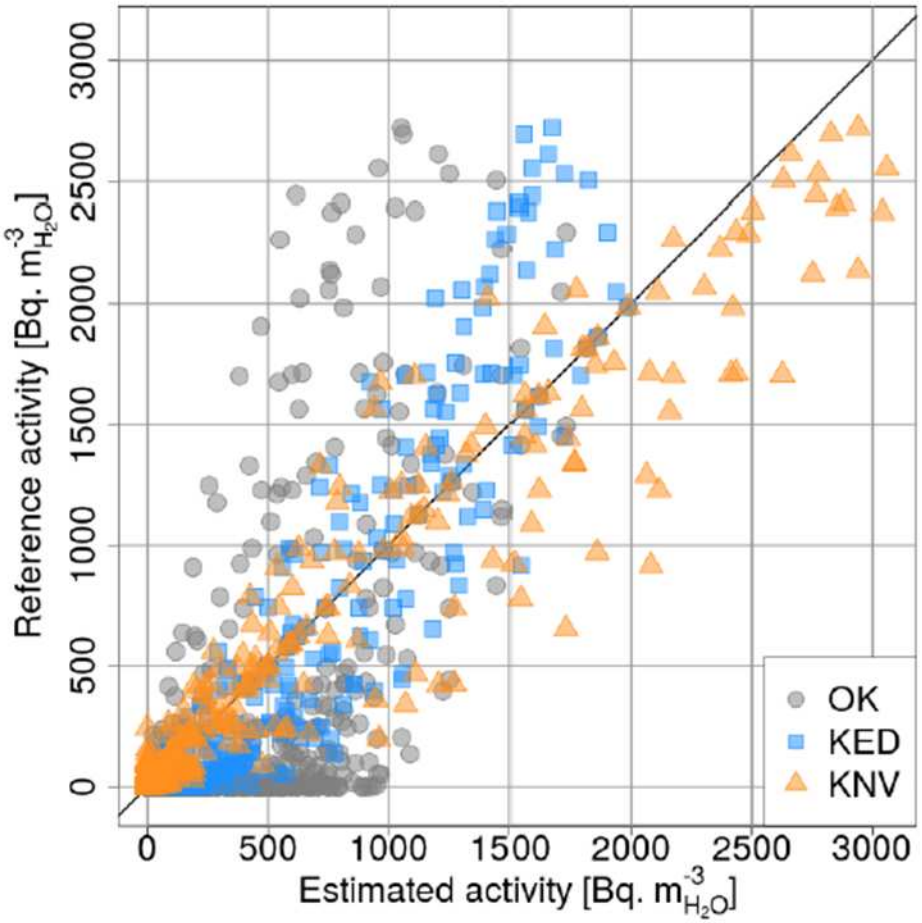
Results (1)

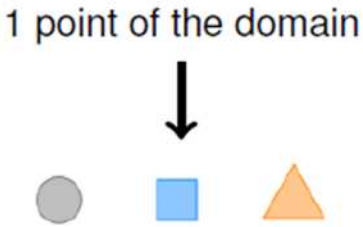


Reference tritium plume



Results (2)

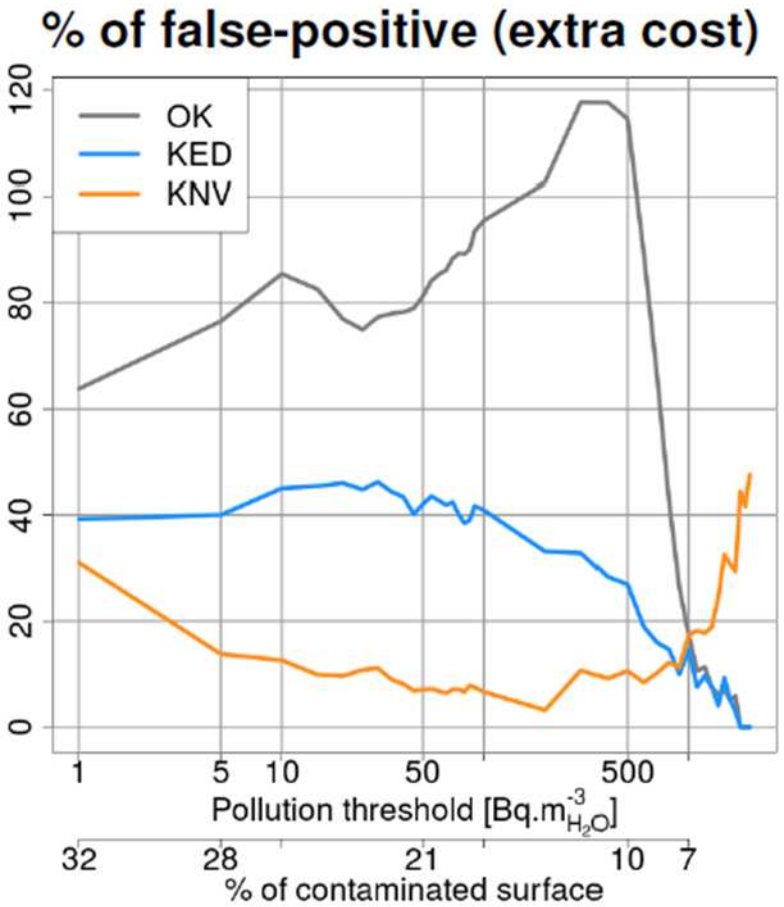


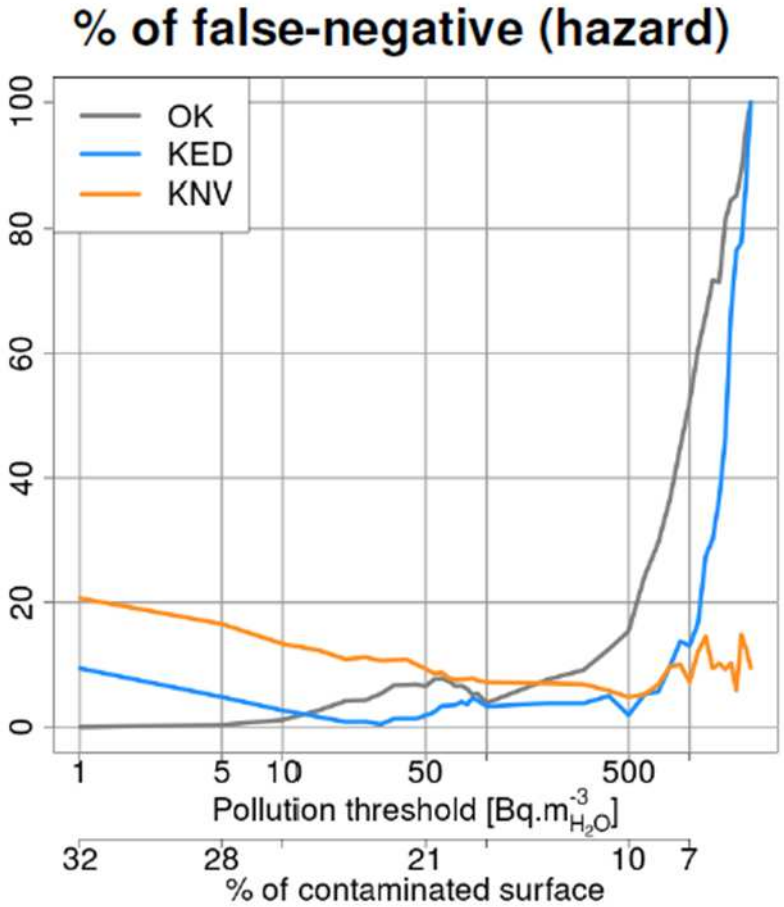


Global statistics

	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)


% of false-positive (extra cost)
OK
KED
KNV
0
20
40
60
80
100
120
1
5
10
50
500
Pollution threshold [Bq.m-3H2O]
32
28
21
10
7
% of contaminated surface


% of false-negative (hazard)
OK
KED
KNV
0
20
40
60
80
100
1
5
10
50
500
Pollution threshold [Bq.m-3H2O]
32
28
21
10
7
% of contaminated surface

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.