Combining geostatistics and numerical simulations to improve estimations of pollution plumes in groundwater.

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Abstract:

Characterization of contaminated soil and groundwater around industrial plants is a major challenge for site remediation. A classical approach consists in providing an estimation of the polluted zone extent thanks to observations (data of pollutant concentration) and geostatistical tools (*e.g.* kriging). However, this estimation might turn out to be of low precision if only few data are available. Besides, flow and contaminant transport simulation is widely used to assess potential migration paths of pollutants through the subsurface. It is efficient even if information from sampling is not available, as long as input parameters are consistent with the site under study.

Thus, the approach developed in this work combines classical geostatistical tools and results of simulations of flow and contaminant transport. It aims at improving the quality of the estimation of the polluted zone extent and reducing the associated uncertainties.

The proposed method is adapted from the work of C. Roth [1]. It consists in building an *a-priori* model of the subsurface of the site under study and simulating the migration of a pollutant plume on several realisations of that model, thus obtaining several unconditionnal realisations of pollutant plume migration. Then, hundreds of these realisations are used to compute empirical covariances accounting for the spatial variability of the regionalized variable ($\mathcal{Z}$) representing the pollution under study :

$$\mathcal{C}(x,x') = \frac{1}{N}\sum_{k=1}^{N}(\mathcal{Z}_k(x) - \overline{\mathcal{Z}(x)})(\mathcal{Z}_k(x') - \overline{\mathcal{Z}(x')}) \tag{1}$$

where $\mathcal{C}(x,x')$ is the covariance value for the couple of points (x,x'), N is the number of realisations, $\mathcal{Z}_k(x)$ is the value of $\mathcal{Z}$ at x for the k-th realisation and $\overline{\mathcal{Z}(x)}$ is the average of $\mathcal{Z}(x)$ over N realisations. Hence, we are able to compute non-stationary covariances that reproduce the spatial variability of $\mathcal{Z}$ better than a model based on observations only. Finally, a kriging estimate using these non-stationnary covariances is performed. The same approach can also be applied if the spatio-temporal aspect of $\mathcal{Z}$ is considered, by computing empirical spatio-temporal covariances.

The performances of this method are assessed on a two-dimensionnal synthetic model of subsurface with a scenario of pollution due to a tritium source. The model includes an unsaturated zone of a few meters deep in which the flow and contaminant transport is simulated. Only few observations are extracted from the reference simulation (*e.g.* Figure 1) so as to evaluate the extent of the polluted zone. Then, hundreds of flow and contaminant transport simulations are run with input parameters differing from the reference simulation, in order to take into account the uncertainties on the input parameters of the modeling.

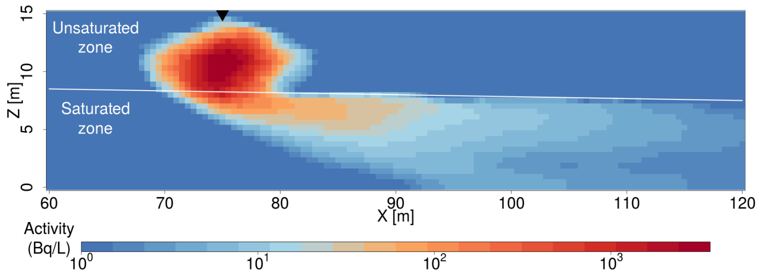

Figure 1: Example of tritium plume used as reference. The triangle highligths the pollution source point.

The extent of the reference polluted zone is then estimated using (i) a classical geostatistical method considered here as a benchmark and (ii) the above-mentioned method combining geostatistical tools and data from simulations. The results show that the estimations are improved when using data from simulations in a geostatistical modeling framework, even if few observations are available, which underlines the interest of this method.

Finally, the proposed approach could help better estimate volumes of soils to be decontaminated in the context of remediation of industrial sites. It is presented here in the context of a radiological pollution but it could be transposed to other types of pollution.

References

[1] Christopher Roth. *Contribution de la géostatistique à la résolution du problème inverse en hydrogéologie*. Thèse. École Nationale Supérieure des Mines de Paris, 1995.

Short biography – After an engineer degree at MINES ParisTech, I started a PhD thesis in applied geostatistics in november 2017. This PhD thesis is part of a project supported by Andra through the "Investments for the Future" Program. This project aims at improving the characterization of polluted soils around nuclear facilities, prior to their dismantlement. Both MINES ParisTech, IRSN and GEOPS (Paris Sud University) collaborate on this project.