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A Bayesian geostatistical approach for evaluating the uncertainty of contaminant mass discharges from point sources

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Abstract

Estimates of mass discharge (mass/time) are increasingly being used when assessing risks of groundwater contamination and designing remedial systems at contaminated sites. Mass discharge estimates are, however, prone to rather large uncertainties as they integrate uncertain spatial distributions of both concentration and groundwater flow. For risk assessments or any other decisions that are being based on mass discharge estimates, it is essential to address these uncertainties.

We present a novel Bayesian geostatistical approach for quantifying the uncertainty of the mass discharge across a multilevel control plane. The method decouples the flow and transport simulation and has the advantage of avoiding the heavy computational burden of three-dimensional numerical flow and transport simulation coupled with geostatistical inversion. It may therefore be of practical relevance to practitioners compared to existing methods that are either too simple or computationally demanding.

The method is based on conditional geostatistical simulation and accounts for i) heterogeneity of both the flow field and the concentration distribution through Bayesian geostatistics, ii) measurement uncertainty, and iii) uncertain source zone and transport parameters. The method generates multiple equally likely realisations of the spatial flow and concentration distribution, which all honour the measured data at the control plane. The flow realisations are generated by co-simulating the hydraulic conductivity and the hydraulic gradient across the control plane and are consistent with measurements of both hydraulic conductivity and head at the site. An analytical macro-dispersive transport solution is employed to simulate the mean concentration distribution across the control plane, and a geostatistical model of the Box-Cox transformed concentration data is used to simulate observed deviations from this mean solution. By combining the flow and concentration realizations, a mass discharge probability distribution is obtained. Tests show that the decoupled approach is both efficient and able to provide accurate uncertainty estimates.

The method is demonstrated on a Danish field site contaminated with chlorinated ethenes. For this site, we show that including a physically meaningful concentration trend and the co-simulation of hydraulic conductivity and hydraulic gradient across the transect helps constrain the mass discharge uncertainty. The number of sampling points required for accurate mass discharge estimation and the relative influence of different data types on mass discharge uncertainty is discussed.

Key words mass discharge; groundwater contamination; risk assessment; uncertainty; geostatistics; Bayesian statistics