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Sensitivity and Uncertainty Assessment of a Model for Pathogen Transport across a River Bank Filtration set-up

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We present a workflow to diagnose the response of a model designed to assess pathogen transport across river bank filtration set-ups in the presence of uncertain model parameters. We rest on a combined use of local and global sensitivity analyses to enucleate the most relevant model parameters which are then employed to quantify uncertainty associated with model predictions. The study is motivated by the documented presence of pathogens (bacteria and viruses) in surface waters, as a result of inflow of wastewater and surface run-off from agricultural activities. These organisms can migrate to groundwater and potentially reach humans through river bank filtration. The latter is an important source for drinking water production but is also at risk of pathogenic contamination due to a combination of (possibly high) pathogen concentrations in surface water and short subsurface travel times between the river and the production wells. We developed a two-dimensional reactive transport model to simulate pathogen transport for the bank filtration at the waterworks Flehe in Düsseldorf (Germany). The model takes advantage of a long-term data set of hydraulic, thermal, and chemical data (including concentration of E. coli and coliforms) sampled in the river Rhine, within observation wells and an active production well.

The reactive transport model simulates advective-dispersive transport mechanisms, also including particle-driven transport using the colloid-filtration-theory coupled with the Maxwell approach to predict collision efficiency based on the DLVO interaction energy. The model also includes the ability to mimic attachment and detachment of pathogens to and from the sediment, inactivation, straining and blocking of pathogens.

A drawback of the model is its high parametrization, resulting in 19 hydraulic and conservative transport parameters (e.g., permeability, porosity and dispersivity), and 29 pathogen transport parameters (e.g., pathogen size, inactivation coefficients, and zeta potentials). A sensitivity analysis is performed for a zoned subsurface heterogeneity and for a single pathogen species. We start by evaluating local sensitivity metrics via the Morris Indices. These are used for a preliminary screening of the parameter set, identifying parameters with limited influence on the target model outputs. The remaining 30 parameters are then subject to a Global Sensitivity Analysis and stochastic model calibration. We do so through Quasi-Monte-Carlo sampling of the parameter space and ensuing construction of a surrogate model. The latter is based on a Polynomial Chaos Expansion (PCE) approach, which has the additional benefit of yielding variance-based sensitivity indices (i.e. ‚Sobol' indices). The latter are employed to quantify the expected contribution of relevant model parameters to the variance of the target model output. Finally, stochastic model calibration is performed taking advantage of the PCE approximation to provide posterior distributions (conditional on observations) of model parameters. Our results suggest that pathogen size and inactivation coefficients are highly influential to model outcomes. Additional influential parameters include for example dispersivity or zeta potentials. While pathogen size and inactivation coefficients can be characterized through stochastic calibration, the presence of different pathogen species, each associated with a given set of characteristics, can hamper the efficiency of a (stochastic) calibration approach.