Global sensitivity analysis and Bayesian parameter inference for transport in a dual flowing continuum

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Abstract

In this work, Global Sensitivity Analysis (GSA) and Bayesian parameter estimation are employed to interpret conservative mass transfer in a porous medium colonized by a biofilm. The GSA investigates how the model behaves with respect to its parameters as the Bayesian parameter estimation assesses the identifiability of model parameters from a set of noisy data.

GSA is useful to distinguish between influential (that contribute the most to the variability of model outputs) and non-influential parameters and hence to understand the behavior of the modeled system. In this work, GSA is performed using variance-based sensitivity indices (Sobol', 1993; Homma and Saltelli, 1996; Sobol', 2001) because they do not require any assumption regarding the linearity or the monotonicity of the model responses. These indices measure the contribution of an input (alone or via interactions with other inputs) to the output variance (Sobol', 2001). The sensitivity indices are estimated by way of a Polynomial Chaos Expansion (PCE) from a probabilistic collocation sample as in Sudret (2008) and Fajraoui et al. (2011).

Bayesian parameter estimation is performed using $DREAM_{(ZS)}$ software (Laloy and Vrugt, 2012) based on the Markov Chain Monte Carlo process (MCMC). The MCMC inversion provides not only the best estimates of the parameters but also allows for exploring a large portion of parameter space in agreement with a targeted posterior distribution of the parameters. MCMC also provides the pairwise parameter correlations and the uncertainty associated with model predictions.

In the studied problem, solute transport through the porous medium colonized by biofilms is ruled by two transport equations that consider solute mass transfer in two flowing phases (porous medium and biofilm) with different velocities and dispersion coefficients (Delay et al., 2013). In a macroscopic system which cannot distinguish between the porous and the biofilm phases, the results of GSA indicate that, for weak mass transfer between phases, the output concentrations are mainly controlled by the velocity in the porous medium and by the porosity of both phases. In the case of high exchange between phases, the output concentrations are also controlled by the kinetic rate of mass transfer. The results of MCMC inversion show that transport with large mass exchange between phases is more likely subject to equifinality (i.e. lack of parameter identification) than transport with weak exchange. The Bayesian inversion also indicates that weakly sensitive parameters, such as the dispersion in each phase, can be accurately identified. However, removing these from the calibration procedures is not recommended because this model reduction might result in biased estimations of the highly sensitive parameters.

References

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