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Numerical methods for improving sensitivity analysis and parameter estimation of virus transport simulated using sorptive–reactive processes

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Abstract

Using one- and two-dimensional homogeneous simulations, this paper addresses challenges associated with sensitivity analysis and parameter estimation for virus transport simulated using sorptive–reactive processes. Head, flow, and conservative- and virus-transport observations are considered. The paper examines the use of (1) observed-value weighting, (2) breakthrough-curve temporal moment observations, and (3) the significance of changes in the transport time-step size. The results suggest that (1) sensitivities using observed-value weighting are more susceptible to numerical solution variability, (2) temporal moments of the breakthrough curve are a more robust measure of sensitivity than individual conservative-transport observations, and (3) the transport-simulation time step size is more important than the inactivation rate in solution and about as important as at least two other parameters, reflecting the ease with which results can be influenced by numerical issues. The approach presented allows more accurate evaluation of the information provided by observations for estimation of parameters and generally improves the potential for reasonable parameter-estimation results.

Keywords: Regression analysis; Sensitivity analysis; Solute transport; Viruses; Sorption; Reaction

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1. Introduction

Using numerical methods to assess the potential for virus contamination of groundwater drinking-water supplies is challenging for many reasons including: (1) virus contamination typically occurs when the rate of transport from the virus source is relatively fast, which reflects advection-dominated flow, (2) viruses remain a health threat at concentrations that typically can be more than eight orders of magnitude less than the source concentration, and (3) accurate parameter values can be difficult to determine. Variability of site conditions suggests that a site-specific assessment of the parameter values controlling virus transport is necessary to produce accurate transport predictions (Bales et al., 1997). Sensitivity analysis can be used to determine the relative importance of each parameter so that characterization efforts focus on reducing uncertainty of the most important parameters, providing the most efficient improvement in prediction accuracy. However, modeling the sorptive–reactive processes characteristic of virus transport under the typically advective-transport conditions and over many orders of magnitude of observed concentrations can be problematic, complicating sensitivity analysis and parameter estimation.

Sensitivity analysis and parameter estimation are already complicated by parameter insensitivity and correlation (Poeter and Hill, 1997), and the potential for introducing a bias through the choice of weighting (Anderman and Hill, 1999). In fact, the considerable potential for misuse and misinterpretation has led to publications focused entirely on developing a systematic approach to guide the calculation and interpretation of parameter sensitivities and estimates (e.g., Hill, 1998). The objective of this paper is to address issues specific to sensitivity analysis and parameter estimation of sorptive–reactive transport, improving the potential for accurate calculation of virus-transport parameter sensitivities and parameter estimates. Although presented in the context of the approach suggested by Hill (1998), the analysis and suggestions presented in this work are broadly applicable to typical field site investigations.

The best method for calculating parameter sensitivities depends on the application. For example, Yeh (1986) notes that the adjoint-state method requires less execution time for situations where the number of parameters is greater than the number of observations while the perturbation method and the more accurate sensitivity-equation method, which are often equivalent in terms of execution time, require less execution time if the number of observations is greater than the number of parameters. The relative execution time of each method can also depend on the simulation. Of the methods mentioned perturbation methods are most versatile because they do not require changes to the code. They can, however, be more susceptible to some types of numerical difficulties. In this work, perturbation methods are used, providing a versatile approach, and the associated numerical difficulties are addressed.

Assessment of potential virus contamination typically includes many observations of several types including heads, flows, and conservative and non-conservative transport observations. The information from the various types of observations aids understanding of the physico-chemical system and the processes controlling virus transport. Previous virus-transport sensitivity analysis has focused on more limited types of observations related to virus transport. For example, Yates (1990) used analytical methods to assess