Reactive-Transport Prediction Uncertainty and Simulation Accuracy, Observation Errors, and Sensitivity Analysis

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1. Introduction

Prediction uncertainty is the likely discrepancy between model predictions and the actual, unrealized system responses. Contributions to uncertainty include solution error and limited capabilities of numerical models, error and deficiency of data, and errors in system conceptual models. Uncertainty can be reduced by improving numerical models and using numerical models, data, and conceptual models together. For example, using conceptual models to build simulations forces ideas about system behavior that are often vague and possibly wrong to be clarified and tested thoroughly against data. Problems with the numerical methods or constitutive relations, however, can obscure results. This article considers three issues important to this process: (1) a common numerical-methods issue for ground-water transport simulations; (2) the problem of matching data too closely; and (3) using a model to evaluate the importance of observations to parameters, parameters to predictions, and observations to predictions.

2. A common numerical-methods issue for ground-water transport simulations

A common numerical issue in transport models is numerical dispersion. Mehl and Hill (2001) investigated the effects of numerical dispersion in the simulation of conservative transport on parameter estimation. The investigation used results from a two-dimensional laboratory experiment constructed of discrete, randomly distributed, homogeneous blocks of five sands. Measured hydraulic conductivities varied over more than two orders of magnitude; measured dispersivities varied over more than one order of magnitude. The five dispersivity values were not estimated due to insensitivity. The small amounts of numerical dispersion evident in Figure 1A resulted in significantly different optimized values of hydraulic conductivity and the different breakthrough curves shown in Figure 1B. Slightly better fits were achieved for the methods with more numerical dispersion, suggesting that the measured dispersivities are consistently too small. Basically, the estimated hydraulic conductivities are making up for the bias in the measured dispersivities, and methods with larger numerical dispersion require less adaptation. If the measured dispersivities were more accurate, the methods with less numerical dispersion would produce the more accurate results. In general, the bias is unknown, and it is advantageous to estimate dispersivity. In Mehl and Hill (2001), the insensitivity is addressed by lumping the five dispersivities and estimating a single value.

3 The problem of matching data too closely

Closer correspondence between the simulation and measurements often indicates the model more accurately represents a system. However, when models are calibrated, predictive capability can be degraded by fitting measurements too closely, as shown in Figure **2**. This can occur when the model is overparameterized and close model fit is achieved by fitting the errors in the data. Thorough evaluation of data errors and the possibility of overfitting are critical. This is especially true for methods in which many parameters are defined. In these situations generally overfitting can be controlled using prior information and smoothness constraints, but the consequences of these methods may not be well understood by the modeler.

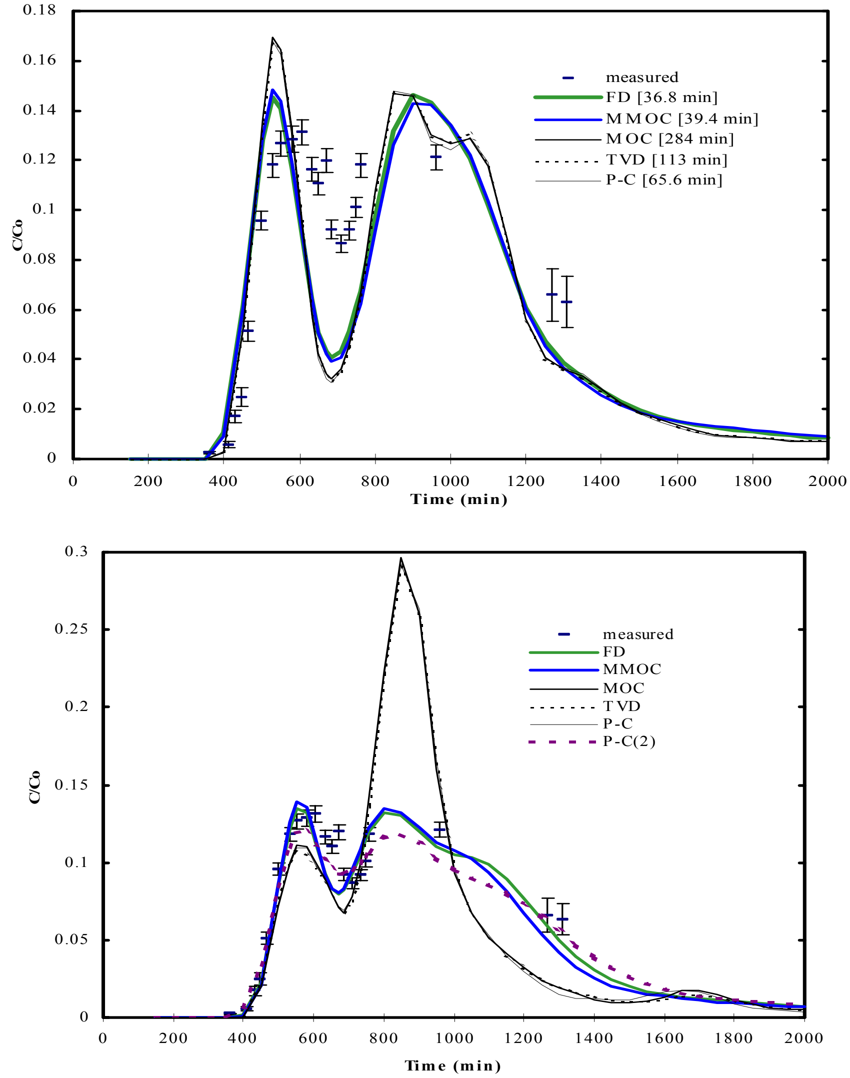

Figure 1. Results from Mehl and Hill (2001). For the measured concentration values, 95% confidence intervals are shown and reflect expected measurement error. Simulations used the finite-difference (FD), modified method of characteristics (MMOC), method of characteristics (MOC), and Total Variation Diminishing (TVD) numerical methods as coded in MT3DMS (Zheng and Wang, 1998), and a predictor-corrector (P-C) method coded for Mehl and Hill (2001). MOC, TVD, and P-C have the least numerical dispersion. (A) BTC's using measured hydraulic conductivities and dispersivities match measured concentrations poorly. Computation times are listed in brackets and are from a Linux workstation, Pentium II - 333, 64Mb Ram. (B) BTC's using optimized hydraulic conductivities and measured dispersivities. The solution labeled P-C(2) uses dispersivity values increased to approximate the numerical dispersion common to the FD and MMOC methods of MT3DMS.

4 Using a model to evaluate the importance of observations to parameters, parameters to predictions, and observations to predictions

Once a reasonably accurate simulation of a system has been achieved through careful model development, calibration, and error evaluation, the simulation itself becomes a valuable tool for sensitivity analysis, data assessment, and uncertainty evaluation. Sensitivity and data assessment methods can be categorized as identifying (1) observations that dominate model calibration (observations important to parameter values); (2) parameter values that dominate the predictions; and (3) observations that dominate the predictions. For instance, gradient-based methods such as dimensionless and composite scaled sensitivities, and parameter correlation coefficients (dss, css, and pcc); prediction scaled sensitivities, the value of improved information, and parameter correlation coefficients (pss, voii, and pcc); and the observation-prediction statistic (opr) can be used to address the three categories, respectively (Hill, 1998; Hill and others, 2001; Tiedeman and others, 2003). These local-sensitivity methods are often useful for nonlinear models, but can become useless if the nonlinearity is too extreme (Poeter and Hill, 1997; Hill, 1998). More computationally intensive methods that do not depend on model linearity include variance-based global sensitivity analysis methods for identifying parameters important to predictions, which address category 2 above (Saltelli and others, 2000), and jackknife and bootstrap methods for identifying observations that dominate parameter estimates or predictions, which address categories 1 and 3 (Davison and Hinckley, 1997)).

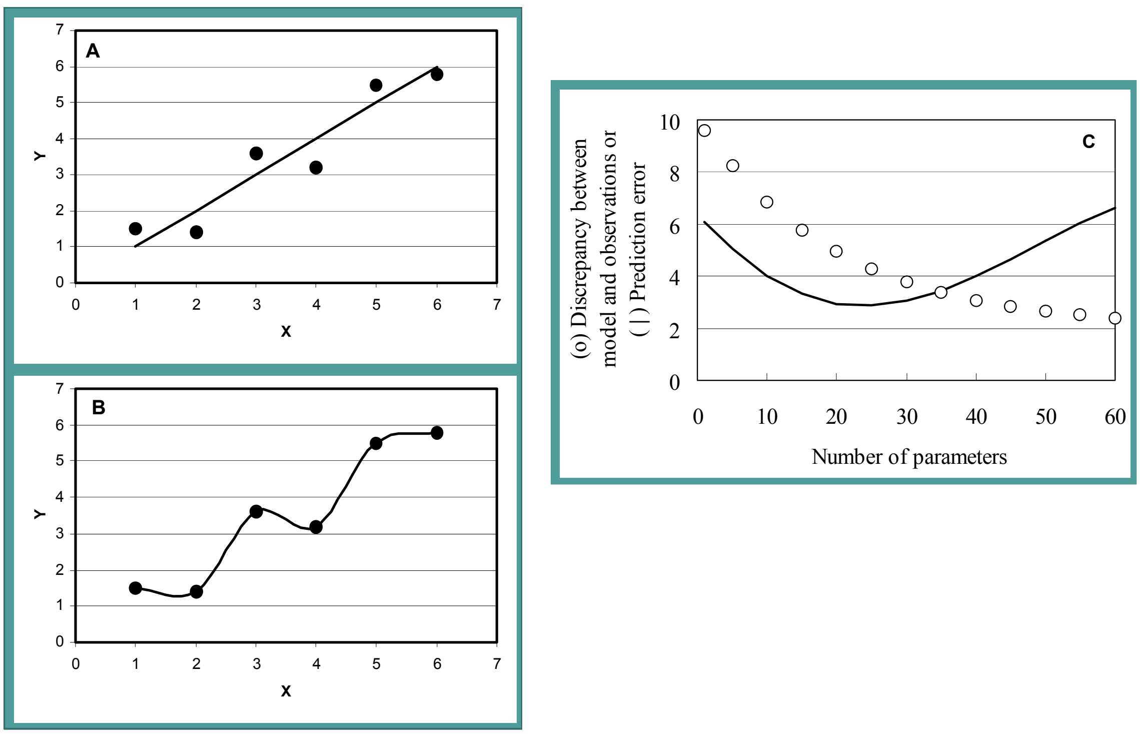

Figure 2. (A) Data with a true linear model. (B) The same data with an overly complex model with little predictive capability. (C) Schematic diagram showing the tradeoff between model fit to observations and prediction accuracy with an increasing number of parameters.

Figure **3** shows css values investigated by Barth and Hill (in review-b). The simulation mimics conditions of field experiments conducted by Schijven et al. [1999], and includes observations of hydraulic head (which have no sensitivity because the system is homogeneous and constant-head boundaries are imposed), flow through the system, normalized first temporal moments of conservative-transport concentrations, and virus concentrations. The observations provide the most information for the two hydraulic parameters, K and θ. Including TSS in Figure **3** allows evaluation of whether the information provided by the observations is sufficient to overcome typical numerical inaccuracies [*Barth and* Hill, in review-a]. Even with virus concentration observations, the css for λ1 is smaller than for TSS, suggesting that estimation of λ1 is likely to be affected by numerical inaccuracies.

5 Conclusions

Model development and evaluation are complex endeavors and predictions are always uncertain. To make wise societal decisions based on model predictions, it is important (1) for numerical methods to be as accurate as possible, and for any weaknesses to be sufficiently understood and accounted for; (2) to judge model fit in the context of a thorough evaluation of observation error; and (3) to use solid methods for evaluating the importance of observations to parameters, parameters to predictions, and observations to predictions.

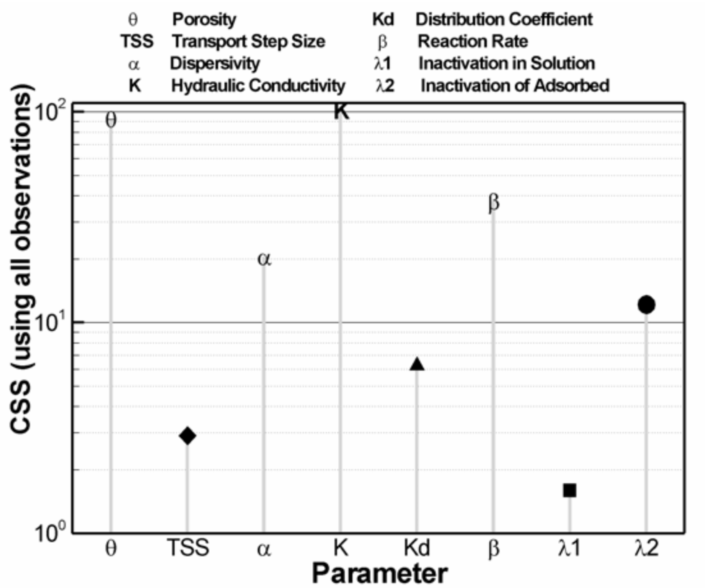

Figure 3. Composite-scaled sensitivities of seven system parameters and the simulation transport step size, TSS, evaluated using parameter set A. Observations include hydraulic heads, moments of conservative transport, and reactive transport concentrations. Composite-scaled sensitivities indicate the amount of information that the observations provide. K and θ are the most important parameters; TSS is more important than λ1. (from Barth and Hill, in review-b)

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