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Using models to manage systems subject to sustainability indicators

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Abstract Mathematical and numerical models can provide insight into sustainability indicators using relevant simulated quantities, which are referred to here as predictions. To be useful, many concerns need to be considered. Four are discussed here: (a) mathematical and numerical accuracy of the model; (b) the accuracy of the data used in model development, (c) the information observations provide to aspects of the model important to predictions of interest as measured using sensitivity analysis; and (d) the existence of plausible alternative models for a given system. The four issues are illustrated using examples from conservative and transport modelling, and using conceptual arguments. Results suggest that ignoring these issues can produce misleading conclusions.

Key words analytical; data analysis; flow; groundwater; models; numerical; sensitivity analysis; sustainability; transport; uncertainty

INTRODUCTION

Mathematical and numerical models are often used to determine how to manage important water resources of natural systems. When sustainability indicators are defined, they generally can be represented in these models as predictions, and the models can be used to answer useful questions such as: (a) what field measurements are most likely to improve the accuracy of predictions? and (b) how uncertain are the predictions? Contributions to prediction accuracy and uncertainty include solution error and the 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 behaviour 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 test results. This paper present four issues important to this process that affect the utility of models in managing resources subject to sustainability indicators: (a) a common numerical-methods issue important to indicators of solute concentrations; (b) the problem of matching data too closely; (c) using a model to evaluate the importance of observations to parameters, parameters to predictions, and observations to predictions; and (d) evaluating alternative conceptual models.

COMMON NUMERICAL-METHODS ISSUE FOR GROUNDWATER TRANSPORT SIMULATIONS

A common numerical issue in transport models is numerical dispersion. Mehl & 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 (2-D) 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 Fig. 1(a) resulted in significantly different optimized values of hydraulic conductivity and the different breakthrough curves shown in Fig. 1(b). 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 & Hill (2001), the insensitivity was addressed by lumping the five dispersivities and estimating a single value.

THE PROBLEM OF MATCHING DATA TOO CLOSELY

Closer correspondence between simulated and measured values often indicates that 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 Fig. 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 overfitting generally can be controlled using prior information and smoothness constraints, but the consequences of these methods may not be well understood by the modeller.

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 can be a valuable tool for sensitivity analysis, data assessment, and uncertainty evaluation. Sensitivity and data assessment methods can be categorized as identifying: (a) observations that dominate model calibration (observations important to parameter values); (b) parameter

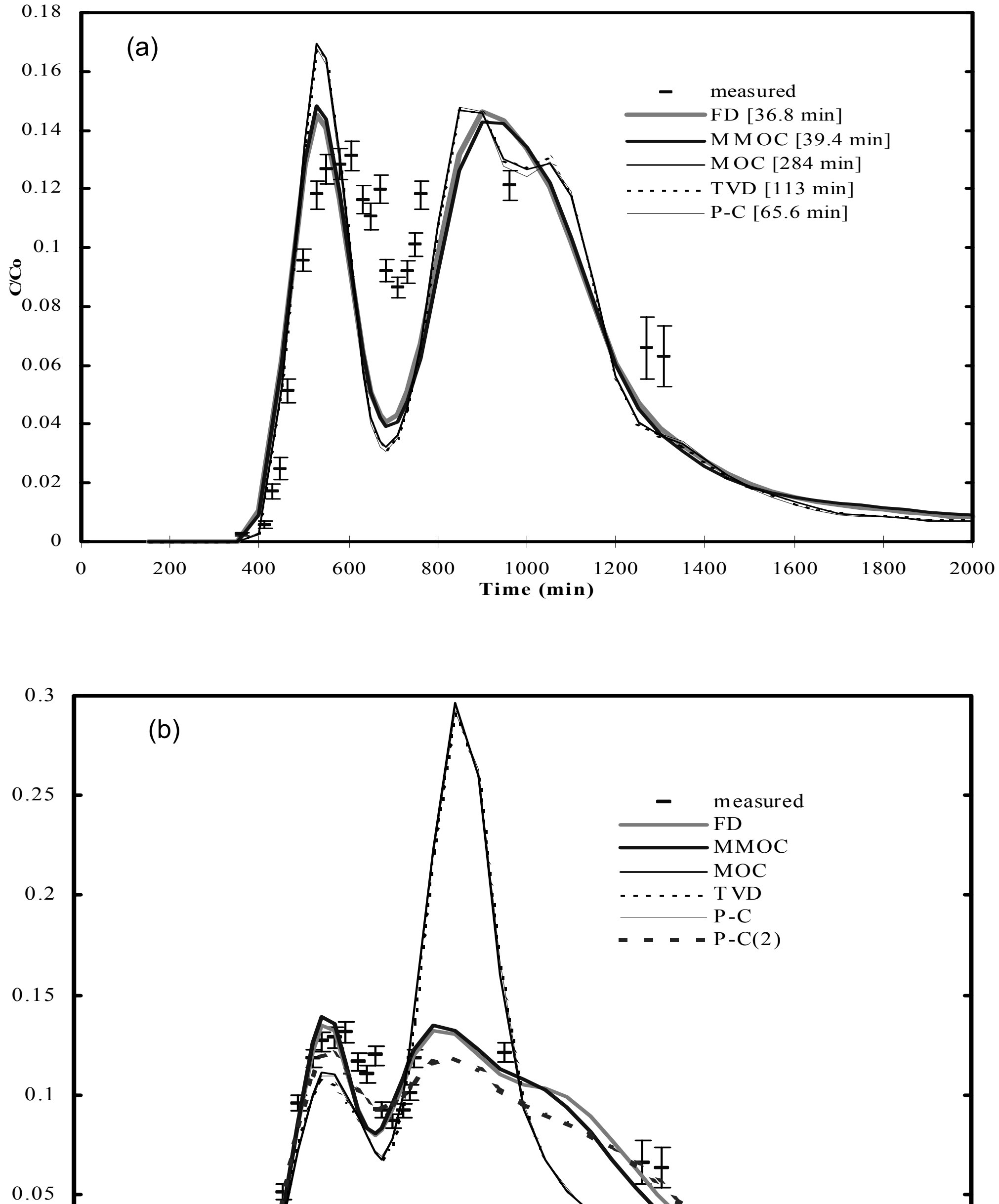

Fig. 1 Results from Mehl & Hill (2001). For the measured concentration values, 95% confidence intervals are shown to reflect expected measurement error. Simulations used the finite-difference (FD), modified method of characteristics (MMOC), method of characteristics (MOC), and Total Variation Diminishing (TVD) numerical methods as coded in MT3DMS (Zheng & Wang, 1998), and a predictor-corrector (P-C) method coded for Mehl & Hill (2001). MOC, TVD, and P-C have the least numerical dispersion. (a) BTCs 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) BTCs using optimized hydraulic conductivities and measured dispersivities. The solution labelled P-C(2) uses dispersivity values increased to approximate the numerical dispersion common to the FD and MMOC methods of MT3DMS.

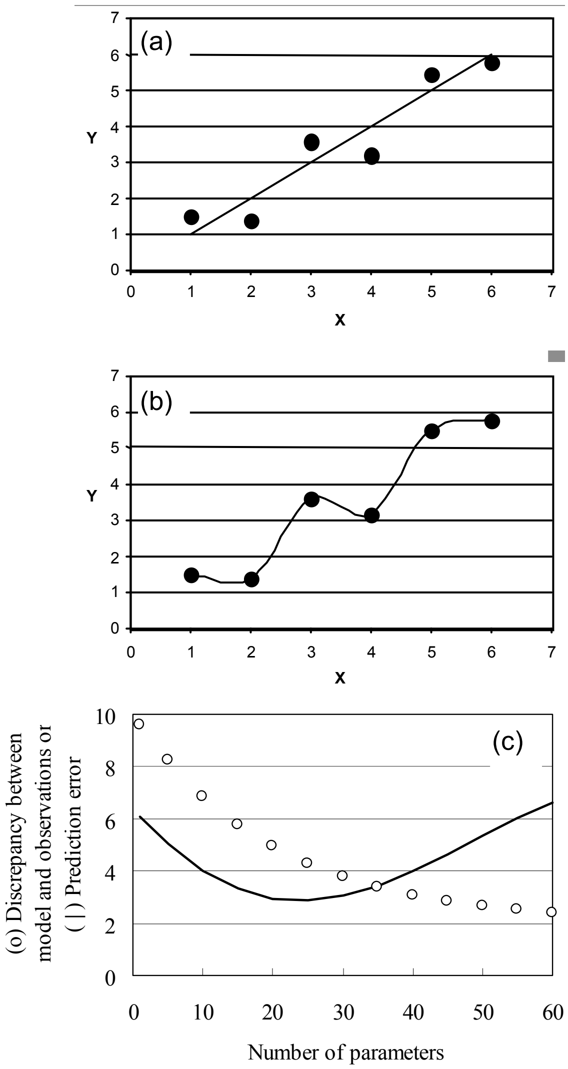

Fig. 2 (a) Data with a true linear model. (b) The same data with an overly complex model with little predictive capability. (c) Schematic diagram showing the tradeoff between model fit to observations and prediction accuracy with an increasing number of parameters.

values that dominate the predictions; and (c) observations that dominate the predicttions. For instance, gradient-based methods such as dimensionless and composite scaled sensitivities, and parameter correlation coefficients (dss, css, and pcc); predicttion 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 *et al.*, 2001; Tiedeman *et al.*, 2003, 2004). These local-sensitivity methods are often useful for nonlinear models, but can become useless if the nonlinearity is too extreme (Poeter & Hill, 1997; Hill, 1998). More computationally intensive methods that do not depend on model linearity include variance-based global sensitivity analysis methods, which address category (b) above (Saltelli *et al.*, 2000), and jackknife, bootstrap, and cross-validation methods, which address categories (a), (b) and (c) (Davison & Hinckley, 1997).

Figure 3 shows css values investigated by Barth & Hill (2005b). The simulation mimics conditions of field experiments conducted by Schijven *et al.* (1999), and includes observations of hydraulic head (which have little sensitivity because the system is homogeneous and constant-head boundaries are imposed, as indicated by dimensionless scaled sensitivities), 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 Fig. 3 allows evaluation of whether the information provided by the observations is sufficient to overcome typical numerical inaccuracies (Barth & Hill, 2005a). 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.

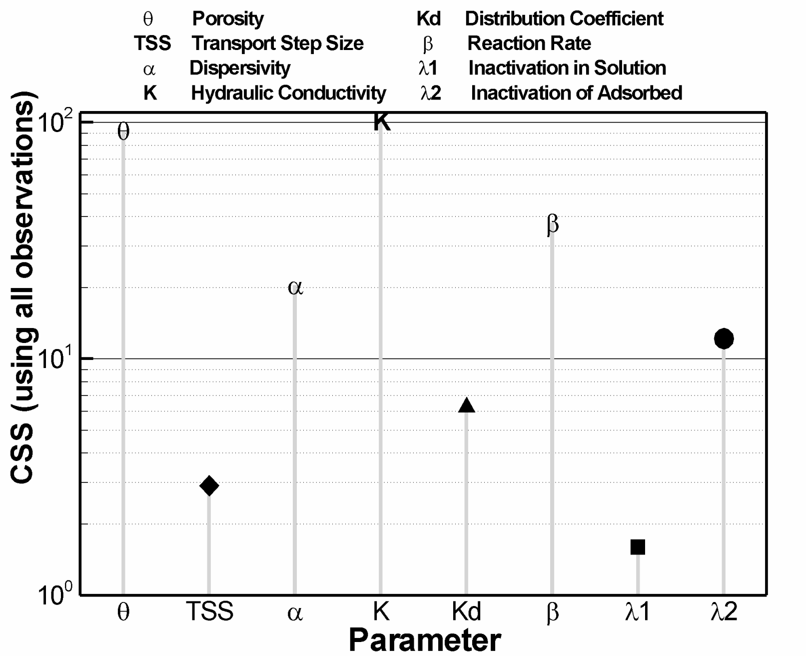

Fig. 3 Composite-scaled sensitivities of seven system parameters and the simulation transport step size, TSS, evaluated using parameter set A. Observations include hydraulic heads, moments of conservative transport, and reactive transport concentrations. Composite-scaled sensitivities indicate the amount of information that the observations provide. *K* and θ are the most important parameters; TSS is more important than λ1. (from Barth & Hill, 2005b).

EVALUATING ALTERNATIVE CONCEPTUAL MODELS

Most naturals systems are not clearly defined by available data. It therefore becomes important to consider alternative models that may produce different predictions related to the sustainability indicators. The different predictions can be used to quantify prediction uncertainty using the methods suggested by a number of authors, including Poeter & Anderson (2005). New software called J_MMRI (Multi-Model Ranking and Influence) supports such analyses (Poeter *et al.*, 2005).

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 (a) for numerical methods to be as accurate as possible, and for any weaknesses to be sufficiently understood and accounted for; (b) to judge model fit in the context of a thorough evaluation of observation error; and (c) to use solid methods for evaluating the importance of observations to parameters, parameters to predictions, and observations to predictions.

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