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A comparison of solute-transport solution techniques based on inverse modelling results

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Abstract Five common numerical techniques (finite difference, predictor-corrector, total-variation-diminishing, method-of-characteristics, and modified-method-of-characteristics) were tested using simulations of a controlled conservative tracer-test experiment through a heterogeneous, two-dimensional sand tank. The experimental facility was constructed using randomly distributed homogeneous blocks of five sand types. This experimental model provides an outstanding opportunity to compare the solution techniques because of the heterogeneous hydraulic conductivity distribution of known structure, and the availability of detailed measurements with which to compare simulated concentrations. The present work uses this opportunity to investigate how three common types of results—simulated breakthrough curves, sensitivity analysis, and calibrated parameter values—change in this heterogeneous situation, given the different methods of simulating solute transport. The results show that simulated peak concentrations, even at very fine grid spacings, varied because of different amounts of numerical dispersion. Sensitivity analysis results were robust in that they were independent of the solution technique. They revealed extreme correlation between hydraulic conductivity and porosity, and that the breakthrough curve data did not provide enough information about the dispersivities to estimate individual values for the five sands. However, estimated hydraulic conductivity values are significantly influenced by both the large possible variations in model dispersion and the amount of numerical dispersion present in the solution technique.

INTRODUCTION

Many contemporary groundwater problems include investigations of flow and transport of contaminants. Concentration data are being used to calibrate models (e.g. Wagner & Gorelick, 1987; Sun & Yeh, 1990; Anderman *et al.*, 1996; Barlebo *et al.*, 1998) and transport simulations are being used to investigate the effects of subsurface heterogeneity (e.g. Poeter & Gaylord, 1990; Scheibe & Cole, 1994; Webb & Anderson, 1996). Various techniques are available to solve the advection–dispersion equation, but all have shortcomings. Numerical techniques are plagued by oscillations, numerical dispersion, and (or) long execution times, while analytical methods only apply to elementary cases. With the increase of computing capabilities, heterogeneities can be represented more explicitly (using finer spatial structure) than ever before, but an inaccurate transport solution can undermine this advantage. Selection of the best technique for a given problem can be difficult.

This article addresses this issue by comparing simulated breakthrough curves (BTCs) from five common numerical techniques—finite difference (FD), predictor-corrector (P-C), total-variation-diminishing (TVD), method-of-characteristics (MOC), and modified-method-of-characteristics, (MMOC)—to one another, and to experimental data. The significance of the differences between the five solution techniques was evaluated based on: (a) breakthrough curves simulated using measured values of hydraulic conductivity, porosity, and dispersivity, (b) sensitivity analysis results, and (c) discrepancies between the measured hydraulic conductivities and values produced through fitting measured concentrations using nonlinear regression. MT3DMS (Zheng & Wang, 1998), modified to include the predictor-corrector (MacCormack) technique (Chapra, 1997, p. 229), incorporates these techniques with an identical solution to the flow field. All the techniques employ the explicit solution approach with a Courant number of 0.5. Thus, all differences between the techniques can be attributed solely to the method used to solve the advection–dispersion equation.

Most comparisons of numerical procedures are limited in two ways: (a) comparisons to analytical solutions are rigorous but restricted to simple systems, which results in limited insight into how the technique will perform in more realistic conditions; (b) comparisons to real data from more realistic systems are less rigorous because unknowns, such as the hydraulic conductivity distribution, and source geometry and concentration, can affect results of the simulation (Wagner, 1992). These limitations are minimized in this study by using results from a heterogeneous, intermediate-scale experiment to evaluate the numerical techniques. The distribution of the five sands comprising the porous media and the source geometry and concentration are accurately known. The only unknowns are the *in situ* values of hydraulic conductivity, porosity, and dispersivity.

In practice, all models of subsurface transport need to be calibrated to determine *in situ* values of hydrogeological parameters. Inverse modelling using nonlinear regression provides a formal mechanism for determining parameter values that fit the measured data optimally, as reflected by a weighted least squares objective function (Hill, 1998). Evaluation of how the different solution techniques affect inverse modelling for the problem being considered here is used to infer how the different techniques are likely to affect model calibration in general.

The first part of this work presents forward simulations to show the numerical grid resolution required to adequately model flow and transport so that grid resolution problems do not dominate the results. Also, the simulated and measured concentrations are compared to determine how well laboratory-measured hydraulic conductivities, porosities, and dispersivities are able to reproduce the measured BTC. Second, a sensitivity analysis, designed as suggested by Hill (1998), was conducted with UCODE (Poeter & Hill, 1998) to evaluate the relative importance of the hydraulic conductivity, porosity, and dispersivity of the five sands to simulation of the BTC. Third, UCODE was used to estimate the three most important hydraulic conductivity values, employing each of the five solution techniques. Finally, the resulting optimized parameter values are compared to one another and to the laboratory measurements.

DESCRIPTION OF EXPERIMENT

The flow and transport experiments considered in this work were conducted using an intermediate-scale sand tank, and are described by Mapa *et al.* (1994) and Garcia, (1995). The two-dimensional, horizontal sand tank was 244 cm long and 122 cm wide. The tank was packed with five different sieve size sands: Grade ID #8, #16, #30, #70, #110. The tank was divided into 200 cells with dimensions of 12.2 × 2.2 cm and an average sample depth of 6.22 cm; the packing was configured to represent a lognormal hydraulic conductivity distribution. Laboratory measured properties of the sands are listed in Table 1. The tank had constant-head boundaries at two ends and no-flow boundaries on the top, bottom, and sides. The hydraulic heads at the inflow and outflow constant head boundaries were 56.91 and 55.56 cm, respectively. The conservative tracer experiment consisted of a line-source injection for 110 min of 1.2 g l^{-1} of bromide at the inflow constant-head boundary. Concentration of the outflow from the tank was measured 21 times during the experiment.

Table 1 Measured flow and transport parameters used in the forward simulations. Values are derived from other works as noted by Mehl (1998).

	Sand type:				
	#8	#16	#30	#70	#110
*Permeameter hydraulic conductivity (cm h^{-1})	4320	1550	418	48.6	15.3
†Column hydraulic conductivity (cm h^{-1})	5936	2132	686	75.1	23
*Porosity	0.472	0.389	0.438	0.483	0.347
‡Dispersivity, α_L (cm)	0.550	0.285	0.07	0.0565	0.03
Number of cells in the sand tank	19	51	70	43	17

*Garcia (1995); †Barth (1996), University of Colorado, Boulder, written communication. ‡Dispersivity values measured in a 64.7 × 38.1 × 5.1 cm homogeneously packed sand tank.

FLOW AND TRANSPORT MODELLING

Preliminary modelling of flow through the tank was accomplished using MODFLOW-96 (Harbaugh & McDonald, 1996) with numerical block dimensions of 6.1 × 6.1 cm (1/4 of a 12.2 × 12.2 cm physical block; referred to as 1/4 resolution). It was determined that this resolution was sufficient for modelling hydraulic heads and flow through the tank by halving the numerical block size in each direction (to achieve a 1/16 resolution) and comparing the results from the 1/4 and 1/16 resolutions. The results were close enough not to warrant further discretization. This same procedure of comparing doubled resolutions was used to evaluate solute transport and it was found that finer resolutions were required. Results from 1/64 and 1/256 resolutions are shown in Fig. 1 and the run time for each technique is shown in brackets.

Figure 1 shows that all techniques reproduce the dual peak of the BTC, but values of the peak concentrations vary up to 20%. MOC, TVD, and P-C simulate sharper peaks, and the BTCs are similar at both resolutions. The FD and MMOC BTCs match measured concentrations better based on the sum of squared weighted residuals, but for these techniques there is still a noticeable difference in the concentrations of the peaks and troughs between the two resolutions. Thus, even at this very fine grid resolution, some numerical dispersion plagues the FD and MMOC solutions.

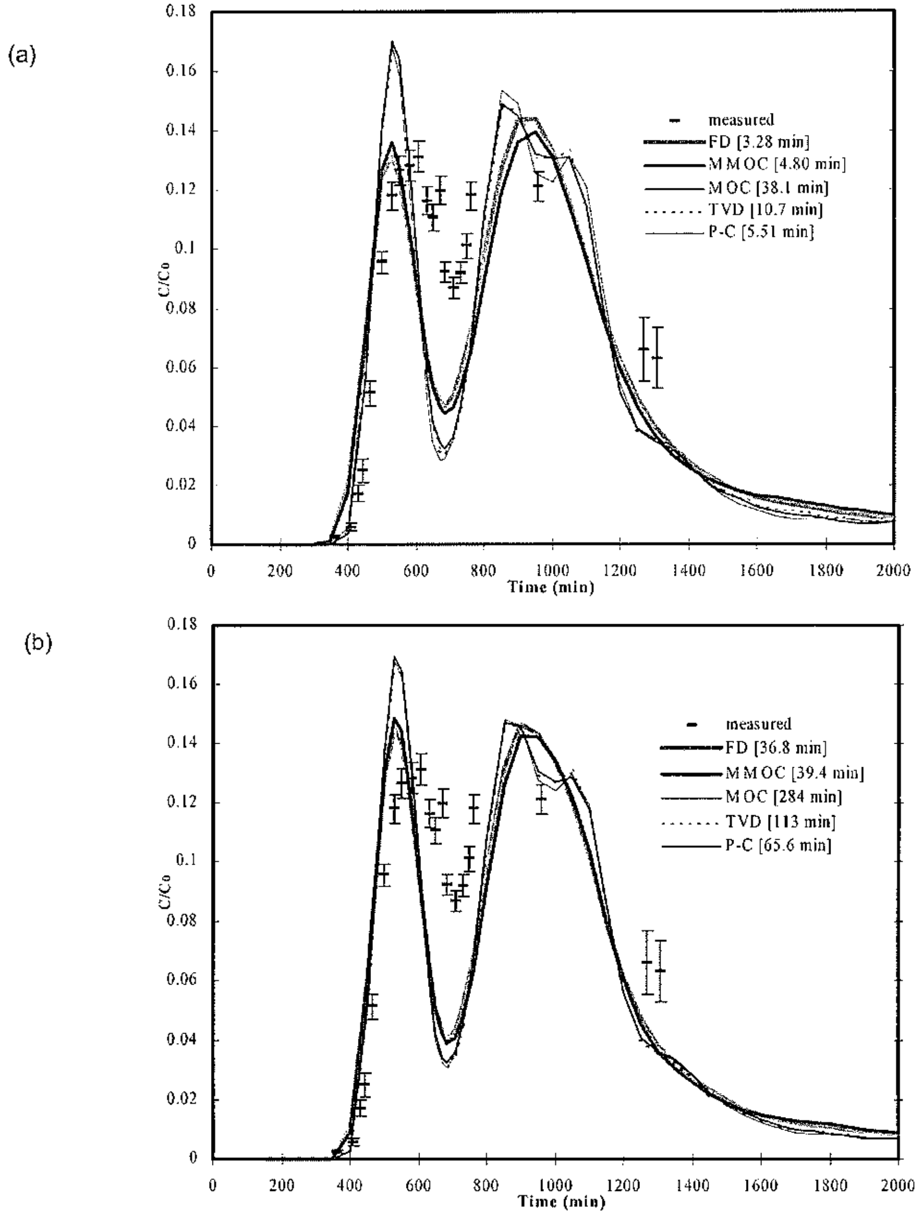

Fig. 1 Forward simulations using the parameter values of Table 1 and (a) 64, and (b) 256 numerical blocks for each sand cell. The 95% confidence intervals shown for the measured values reflect expected measurement error; coefficients of variation ranged between 4% and 20%. (Computation times using a Linux workstation, Pentium II - 333, 64 Mb Ram).

SENSITIVITY ANALYSIS

Before inverse modelling is conducted, the information provided by the data is evaluated and used to choose which parameters to estimate. UCODE was used to calculate composite scaled sensitivities (Hill, 1998, p. 15) for the observations (21 concentrations and one flow) to the hydraulic conductivity, porosity, and dispersivity of each sand. Composite scaled sensitivities calculated using the FD technique are shown in Fig. 2; the outcome was similar for the other techniques. The results show that the BTC was most sensitive to hydraulic conductivity and porosity values, and to the parameters of the #8, #16, and #30 sands. Parameter correlation coefficients calculated as part of the sensitivity analysis revealed a high correlation between porosity and hydraulic conductivity. Based on the composite scaled sensitivities, and avoiding correlated parameters, the hydraulic conductivities for the #8, #16, and #30 sands were estimated by the regression, while all other parameters were fixed at the values presented in Table 1 (permeameter values were used for hydraulic conductivity). Additional data, such as hydraulic heads, could allow for estimation of other parameters, but such data were not available. Determining dispersivity values can be difficult because measured dispersivity can vary widely with the scale of the plume and the measurement procedure (Chao, 1999), and model values may be less than measured values to make up for numerical dispersion. The values from Table 1, which were measured using bromide tracer tests in a homogeneously packed sand tank, were expected to be closely applicable to the experiment.

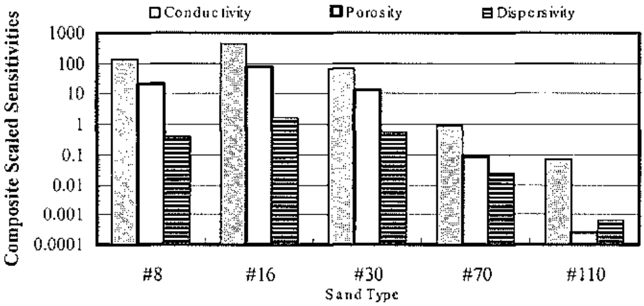

Fig. 2 Composite scaled sensitivities calculated for each sand using the parameter values of Table 1 and the finite-difference (FD) technique.

INVERSE MODELLING

Inverse simulations were conducted using all five solution techniques. Optimized parameter values are compared to one another and to the permeameter and column values of Table 1. A numerical grid resolution of 1/64 was used because of its shorter execution time and the small differences between this and the 1/256 resolution (Fig. 1). Figures 3(a–c) show that the hydraulic-conductivity values estimated using the MOC, TVD, and P-C are similar to one another, but are distinctly, and, for the #8 sand, dramatically different than the values estimated using FD and MMOC. Linear confidence intervals on the estimates indicate that the differences are significant for the #8 sand (in that the confidence intervals do not overlap), and become progressively less significant for the finer #16 and #30 sands despite proportionately smaller confidence intervals on the estimates.

It was hypothesized that the numerical dispersion detected in analysing Fig. 1 was causing the difference between the two groups of estimates. To determine if this was so, the P-C technique was used with the values of dispersivity for the #8, #16, and #30 sands increased to 1.875, 1.450, and 1.037 cm, respectively. The P-C method was used because the "corrector" effectively centres the finite difference approximations for the spatial and temporal derivatives, which eliminates second-order numerical dispersion, and execution times were smaller than similarly accurate MOC and TVD techniques. The results, labelled as P-C(2) in Fig. 3, are similar to the FD and MMOC solutions, which inherently have more numerical dispersion. This suggests that the numerical dispersion present in FD and MMOC, which this analysis indicates is much greater than the measured values of dispersivity, significantly affects the optimized parameter values. This is consistent with the sensitivity analysis because the relative changes in dispersivity are so large. Despite the small resolution (spatial discretization) used in this work, these results are expected to be indicative of the difficulties that can arise in less idealized situations because numerical dispersion is common to both cases.

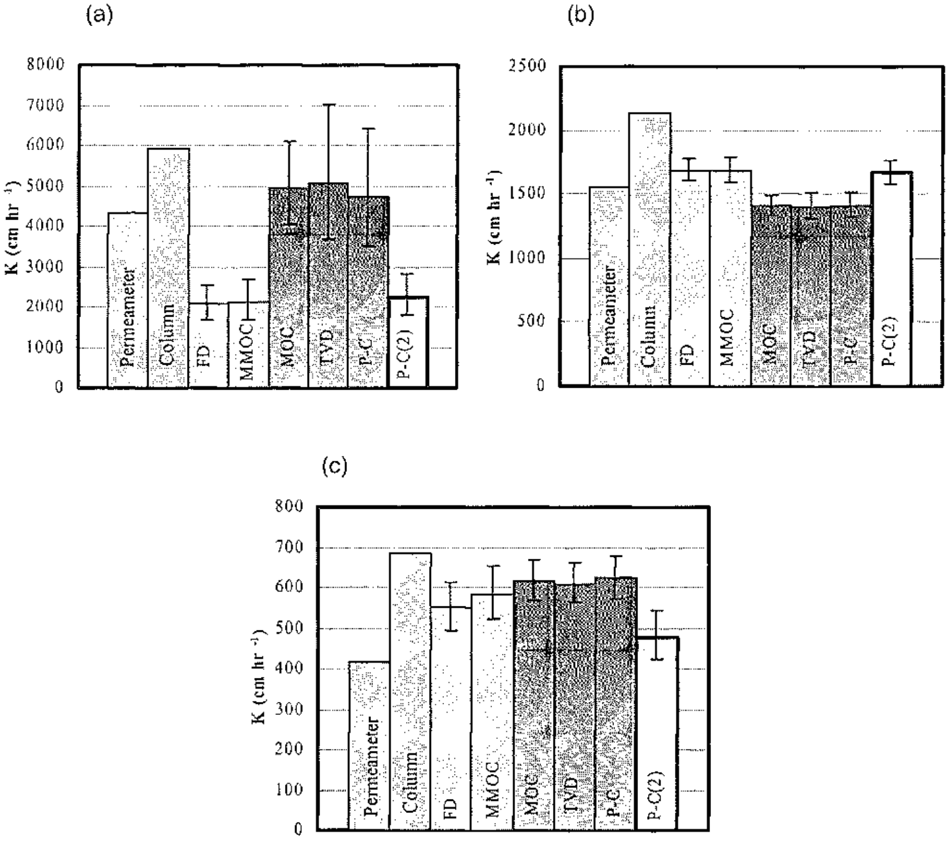

Fig. 3 Comparison of measured and optimized hydraulic-conductivity values for (a) #8, (b) #16, and (c) #30 sand. 95% linear confidence intervals are shown for the optimized values.

CONCLUSIONS

This investigation shows that despite differences in forward simulations at very fine grid resolutions, the same relationships for the sensitivity analysis were produced for all five numerical techniques evaluated. This is a promising result, indicating that the sensitivity analysis suggested is relatively robust in the presence of numerical dispersion.

Optimized values of hydraulic conductivity differed significantly because of the amount of numerical dispersion present in the solution techniques. However, similar BTCs were obtained with larger values of model dispersivity while using a technique with little numerical dispersion. There is always a question of what values of dispersivity are appropriate for a given model because of scale dependencies, and this analysis indicates the importance of the values chosen. Attempts to simultaneously calibrate both hydraulic conductivity and dispersivity were not possible in this investigation, as is commonly the case, because of insensitivity.

This investigation demonstrates that when using solute-transport data to calibrate model values of hydraulic conductivity, the dispersivity values used are important. Imposition of measured values of dispersivity can be problematic because: (a) dispersivity values can extend over a large range, and measured values for the same media can be very different depending how it was measured, (b) the deficiencies of some numerical techniques can mimic the effects of dispersivity, which is not the case for hydraulic conductivity or porosity, and (c) available data are often insufficient to estimate dispersivity directly. The results of this work indicate that, depending on the solution technique employed and the choice of model dispersivity, model calibration can produce significantly different results for hydraulic conductivity, resulting in different simulated flow fields, and potentially very different predictions.

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