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TESTING A METHOD-OF-CHARACTERISTICS MODEL OF THREE-DIMENSIONAL SOLUTE TRANSPORT IN GROUND WATER

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ABSTRACT

A new three-dimensional model of solute transport in ground water that is based on a widely-used two-dimensional method-of-characteristics model, and that is coupled to a modular finite-difference flow model is under development. The model's accuracy for ideal aquifers having homogeneous properties, uniform boundary conditions, and steady flow along a grid direction is demonstrated by comparison with conventional analytical solutions. The effect of spatially and temporally variable flow velocities is investigated by comparison with special analytical solutions. To test the performance of the model for typical hydrogeologic conditions, we compare results with those from other models as well as to results from the same model using smaller grid spacings and time steps. This model generally provides accurate results for realistic simulations, and is particularly efficient for advection-dominated transport.

INTRODUCTION

Konikow and Bredehoeft (1978) developed a general numerical model of ground-water flow and solute transport in two dimensions that has been widely applied throughout the international hydrogeologic community. The method-of-characteristics used to solve the advection-dispersion equation minimizes numerical dispersion and oscillation associated with finite-difference and finite-element solutions. Practical experience using the model indicates that it provides accurate solutions for a wide range of aquifer conditions and is particularly efficient when advection is the dominant transport process.

This paper highlights tests of a new model (MOC3D hereinafter for brevity) under development that extends the method-of-characteristics approach of Konikow and Bredehoeft (1978) to three-dimensions. It is linked to the finite-difference model of McDonald and Harbaugh (1988) that simulates three-dimensional saturated flow. The general capabilities and characteristics of MOC3D include: steady-state or transient flow; confined, unconfined, or confined/unconfined conditions; heterogeneous hydraulic conductivity, storativity, and porosity; anisotropic hydraulic conductivity; specified head, specified flux, and leaky flow boundaries; solute-transport boundary conditions as specified concentration in fluid inflows;

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linear reversible equilibrium sorption; first-order decay; and distinct horizontal and vertical transverse dispersivities. Because MOC3D employs the method-of-characteristics, it is capable of solving the transport equation for the case of dispersion coefficients equal to zero.

The three-dimensional flow and transport equations, and problems associated with their numerical solution are described by several authors (e.g., Burnett and Frind, 1987). Model test cases presented here highlight these problems, including grid orientation effects, artificial or numerical dispersion, transient flow conditions, nonuniform flow conditions, and transport in heterogeneous media.

POINT INITIAL CONDITION IN UNIFORM FLOW

A common analytical test problem for transport models is the spread of a point or Dirac initial condition in a uniform flow field. Figure 1 shows analytical and numerical solutions for advection and three-dimensional dispersion for the cases of flow in the x-direction and flow at 45 degrees to x and y. In both cases, the z-component of flow is zero, but dispersion occurs in all three directions. The x-component of velocity is the same for each case, so the resultant magnitude of velocity is higher for the case of flow at 45 degrees to x and y. For purposes of comparison, the same contouring program (Harbaugh, 1990) is used for all cases and the resolution (grid spacing) of the analytical solution is the same as the numerical model grid spacing. Some of the minor differences in the contours for the analytical solutions are artifacts of the contouring algorithm. The longitudinal dispersivity is one-tenth of the equilateral grid spacing and the transverse dispersivity is one-hundredth the grid spacing.

MOC3D yields good results for flow in the x-direction (Fig. 1a and 1c) with minor numerical dispersion, primarily in the transverse direction. However, a significant grid orientation effect is exhibited for flow at 45 degrees to x and y (Figs. 1b and 1d). When flow is oriented with the grid, or when the longitudinal and transverse dispersivities are equal, the cross-product terms of the dispersion tensor are zero. In other cases, the cross-product components are nonzero and at a maximum when flow is at 45 degrees to the grid. In the model, the cross-product concentration gradients are estimated less accurately than the gradients associated with the diagonal components of the dispersion tensor. Increasing the size of the initial condition to 3 by 3 by 3 cells does not significantly improve results. Further analysis of the numerical errors for this problem are underway, including reexamination of the explicit method's stability (Konikow and Bredehoeft, 1978).

CONSTANT SOURCE IN NONUNIFORM FLOW

Numerical models are used for practical simulation because real aquifers do not meet the simplifying assumptions of uniform flow. Hence, it is important to test models for cases of nonuniform flow. Burnett and Frind (1987) tested a three-dimensional transport model for a hypothetical case having homogeneous properties, but nonuniform boundary conditions that result in nonuniform flow. For the two-dimensional case considered here, the rectangular domain is bounded by no-flow boundaries on the aquifer bottom and on one of the rectangle's ends (x=0). At the other (x=200) end, heads are fixed at zero, and heads are specified as a one-quarter cosine from 1 m to 0 m on the top to simulate a water table. Because of the nonuniform flow field, the transport problem has no analytical solution.

MOC3D results (Fig. 2a) agree well with the two-dimensional results of Burnett and Frind (1987, their Fig. 8a). Because the longitudinal dispersivity is relatively large compared to the grid spacing, the transport time step is limited by the explicit dispersion stability criterion. Even for coarse grids, which require much less computation, solutions using MOC3D retain the same overall features, although some resolution is lost (Figs. 2b and 2c).

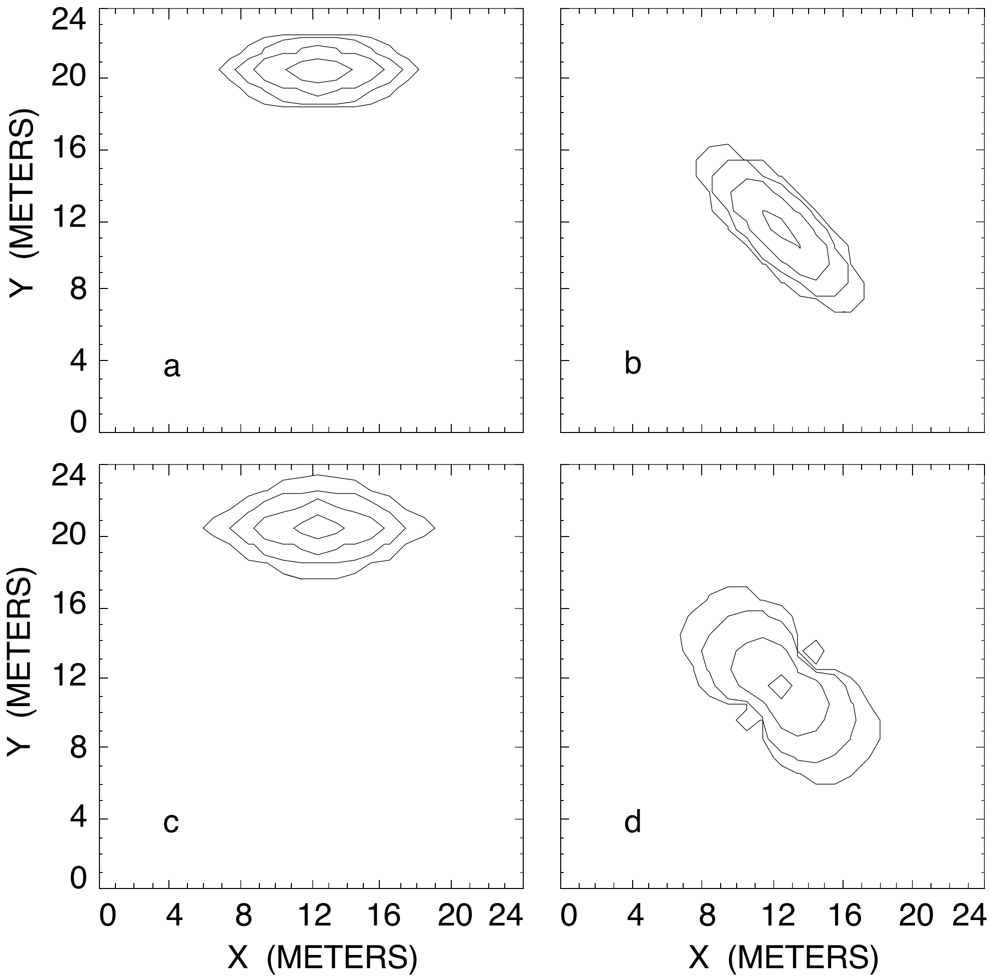

Fig. 1.— Concentration contours for dispersion of a Dirac initial condition in uniform flow: (a) analytical solution for flow in the x-direction; (b) analytical solution for flow at 45 degrees to x and y; (c) numerical solution for flow in the x-direction; (d) numerical solution for flow at 45 degrees to x and y. Contour levels are 0.1, 1, 10, and 100 arbitrary units.

CONSTANT SOURCE IN A HETEROGENEOUS LAYERED AQUIFER SYSTEM

Realistic test cases exhibit nonuniform flow due to nonuniform boundary conditions, as well as due to heterogeneous properties, particularly hydraulic conductivity. Sanford and others (1990) used the finite-difference model HST3D (Kipp, 1987) to investigate flow and solute transport around an active volcano with a brine lake in the crater. The model aquifer was composed of alternating layers having significant contrasts in hydraulic conductivity and porosity; hydraulic conductivity also decreased with depth. We resimulated two-dimensional solute transport in one of the cross-sections presented by Sanford and others (1990) using HST3D without density effects to compare with MOC3D results.

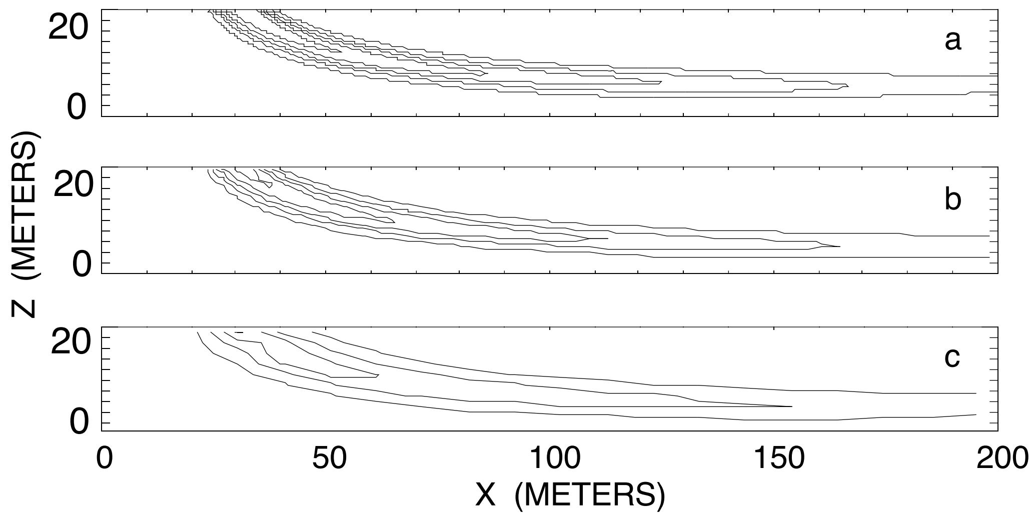

Fig. 2.— Simulation of example problem of Burnett and Frind (1987): (a) 180 (x) by 90 (z) grid; (b) 60 by 30 grid; (c) 20 by 10 grid. Contour levels are 0.1, 0.3, 0.5, 0.7, and 0.9 times the source concentration.

Despite the differences in the numerical approaches for this very complex hydrogeologic system, the results of the models agree well (Figs. 3a and 3b). This is somewhat surprising, given that the distinct property layers within the system were discretized by only a single layer of finite-difference blocks in both models. MOC3D uses a linear velocity interpolation method (Goode, 1990b) that preserves velocity discontinuities in layered systems. Flow and dispersion computations use block-centered finite-differences where aquifer properties are defined over blocks centered on the nodes. In contrast, HST3D employs grid-centered finite-differences where aquifer properties are defined over blocks with nodes at the block corners. Thus, there are minor differences in the head solutions as well as in the simulation of advection and dispersion. Again, the dispersivities for this example are relatively large compared to the block size. Because HST3D uses the finite-difference method to simulate both advection and dispersion, smaller dispersivities result in numerical dispersion.

Certain features of transport in hydrogeologic systems may become evident only when dispersion is not included in the simulation. MOC3D can simulate transport even if dispersivities are small relative to the block size, or if no dispersion is considered. As shown in Figure 3c, for advection alone, the solute front reaches the bottom of the simulated area well before the disperse front. Essentially all of the solute mass remains within a single sloping high-permeability layer.

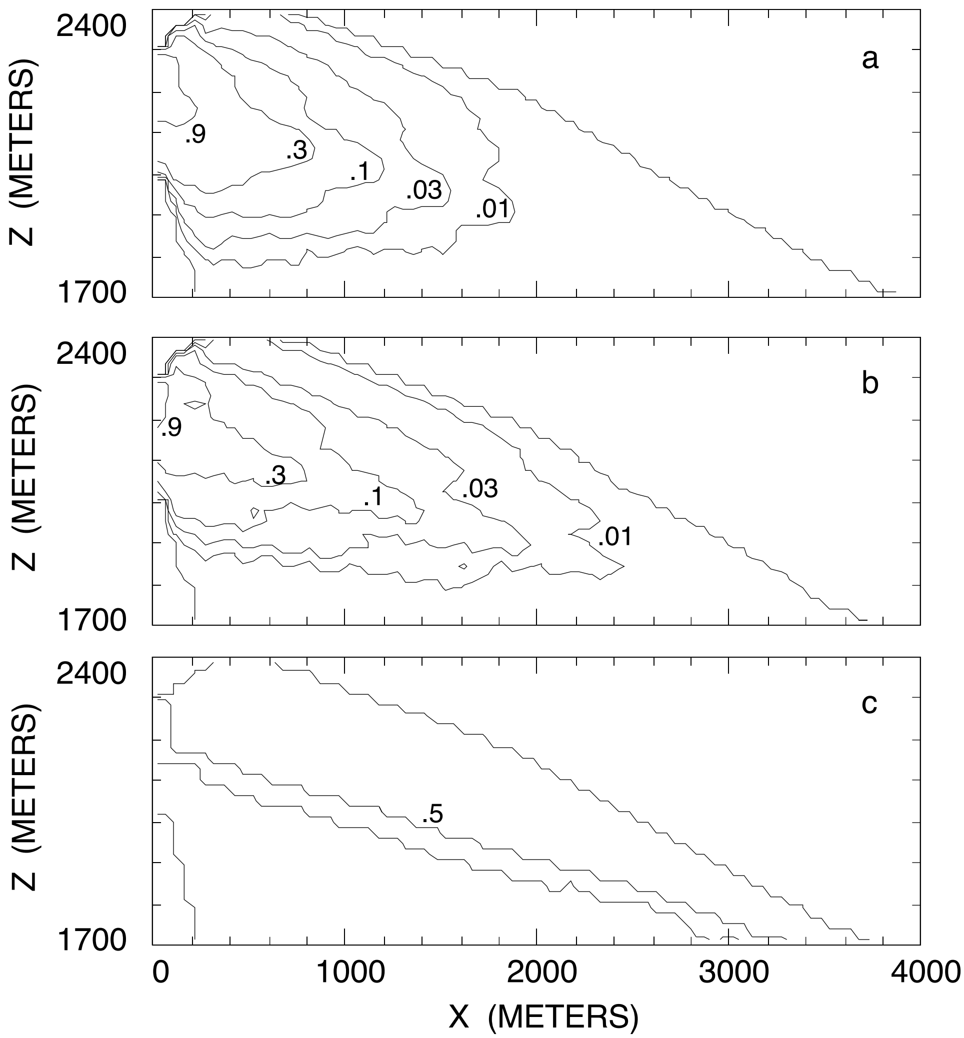

Fig. 3.— Constant density simulation of volcano cross section of Sanford and others (1990): (a) using HST3D (Kipp, 1987); (b) using MOC3D; (c) using MOC3D with no dispersion. Top and bottom-left lines designate boundary of aquifer.

FRONT ADVECTION IN TRANSIENT FLOW

In addition to steady-state flow cases, general transport models should be tested under transient flow conditions. Gelbard (1989) and Goode and Konikow (1990) derive analytical solutions for transport under quasi-steady flow conditions where velocity changes in time but the aquifer system has no fluid storage capacity (storativity=0). Tests using these types of solutions are underway. Unfortunately, no closed form analytical solutions are known for the general case of advection and dispersion in transient (storativity≠0) flow. Some of the model's abilities can be investigated by simulating advection in transient flow.

An expression for the rate of advective front movement can be derived from an analytical solution for potentiometric head in a one-dimensional semi-infinite confined aquifer where the head is initially at zero and is instantly raised to a higher level at x=0 (Marsily, 1986). This solution can be differentiated with respect to x to yield transport velocity as a function of x and t, accounting for changes in porosity and thickness due to increasing head and nonzero storativity (Goode, 1990a). The resulting ordinary differential equation can be integrated numerically to yield advective movement of a front in a transient flow field.

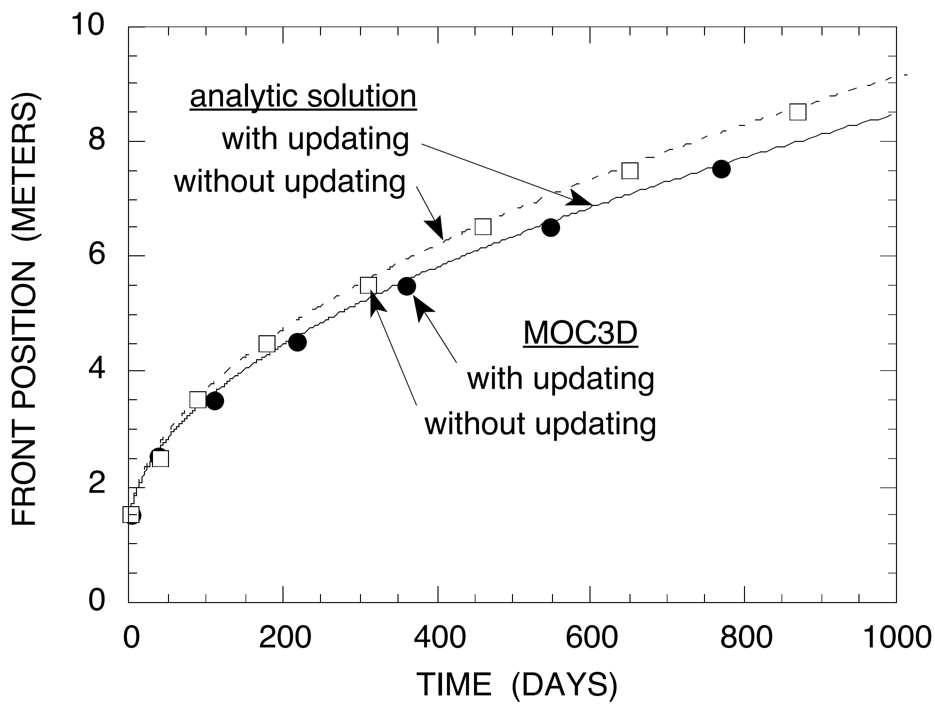

Fig. 4.— Comparison of analytical and numerical solution for front advection in transient flow showing effect of updating fluid-storage terms in transport equation

MOC3D yields an accurate solution for this advection only problem (Figure 4). In addition to comparing the analytical and numerical results, this figure also shows the minor effect of ignoring changes in fluid-storage changes during transient flow. For this case, ignoring the effect of increasing head on fluid-storage in the aquifer leads to slightly increased front velocity (see also Goode, 1990a). Future tests will include solute dispersion under transient flow conditions.

SUMMARY

Although certainly not an exhaustive collection, these examples demonstrate some of the strengths and weaknesses of a three-dimensional method-of-characteristics model of solute transport in ground water. In general, the model yields acceptable results for many problems. The model is particularly efficient for the advection-only case or when dispersivities are small. The explicit dispersion method used is adversely affected by grid orientation when the cross-product dispersion coefficients are large; future work in this area is suggested.

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