GROUND WATER

Computer Notes

Modeling Transport in Transient Ground-Water Flow: An Unacknowledged Approximation

by Daniel J. Goode[a]

Abstract. During unsteady or transient ground-water flow, the fluid mass per unit volume of aquifer changes as the potentiometric head changes, and solute transport is affected by this change in fluid storage. Three widely applied numerical models of two-dimensional transport partially account for the effects of transient flow by removing terms corresponding to the fluid continuity equation from the transport equation, resulting in a simpler governing equation. However, fluid-storage terms remaining in the transport equation that change during transient flow are, in certain cases, held constant in time in these models. For the case of increasing heads, this approximation, which is unacknowledged in these models' documentation, leads to transport velocities that are too high, and increased concentration at fluid and solute sources. If heads are dropping in time, computed transport velocities are too low. Using parameters that somewhat exaggerate the effects of this approximation, an example numerical simulation indicates solute travel time error of about 14 percent but only minor errors due to incorrect dilution volume. For horizontal flow and transport models that assume fluid density is constant, the product of porosity and aquifer thickness changes in time: initial porosity times initial thickness plus the change in head times the storage coefficient. This formula reduces to the saturated thickness in unconfined aquifers if porosity is assumed to be constant and equal to specific yield. The computational cost of this more accurate representation is insignificant and is easily incorporated in numerical models of solute transport.

Introduction

The ground-water flow and solute transport model of Konikow and Bredehoeft (1978) has been applied to a wide range of hydrogeologic conditions over the past 20 years. Recently, I examined the model results for a simulation in which a large volume of contaminated water was injected into a thin aquifer. Despite repeated adjustment of various simulation parameters such as grid spacing and time steps for the flow and transport solutions, the transport solution exhibited unacceptably high mass balance errors, on the order of 30 percent. The fluid injection resulted in large increases in the potentiometric head, and there were numerous concerns about whether the physical scenario was consistent with the assumptions of the two-dimensional horizontal model. However, even if these assumptions were not appropriate from a physical basis, the model itself should still conserve solute mass, mathematically and numerically.

Detailed examination of these simulations and the model algorithms showed that the lack of solute mass conservation resulted from an unnecessary and unacknowledged approximation in the transport solution for the case of unsteady or transient flow. The solute-transport model did not fully account for changes in fluid storage (the volume of water per unit area of aquifer) that occurred during transient flow. As a result, the ground-water velocities, dispersion coefficients, and dilution volumes (fluid volume per model cell) used in the transport solution were incorrect. Subsequent examination of other models indicated that the models of Prickett and others (1981) and of Voss (1984) contain analogous unacknowledged approximations that can cause mass balance errors and incorrect solutions of the solute transport equation for some cases of transient flow. These three computer programs are probably the most widely used simulators in the world for solute transport in two dimensions. These errors exist in the codes, in part, because typical test cases for transport models do not include transient flow conditions. Other models (e.g., Reddell and Sunada, 1970) properly account for the effects of temporal changes in fluid-storage terms on solute transport.

More recently, Illangasekare and Doll (1989) present a new transport model and report 4 percent solute mass balance error for a transport simulation under transient flow conditions. It is not clearly stated whether fluid-storage changes are accounted for in their transport solution when

[a]U.S. Geological Survey, 345 Middlefield Road, MS 496, Menlo Park, California 94025.

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transmissivity is constant. However, in comparing their model to the confined-flow model of Konikow and Bredehoeft (1978), "the mass balance errors . . . were found to be approximately the same for both models" (Illangasekare and Doll, 1989, p. 865), suggesting that temporal fluid-storage changes are not maintained in the transport equation. The ambiguous treatment of fluid-storage terms appearing in the two-dimensional transport equation suggests that a reminder is needed.

This note briefly reviews the two-dimensional solute-transport equation as simulated by the models of Konikow and Bredehoeft (1978) and Prickett and others (1981). A numerical example is presented to illustrate errors induced in the solute-transport solution by ignoring fluid-storage changes during transient flow. A simple updating procedure is suggested to correctly account for changing fluid storage in the numerical algorithm.

Review of Governing Equation

The governing equation for two-dimensional horizontal solute transport in transient incompressible-fluid flow can be written as (Konikow and Grove, 1977, p. 21; cf. Bear, 1979, p. 258):

$$\frac{\partial(\epsilon bC)}{\partial t} + \frac{\partial}{\partial x_i}(\epsilon bCV_i) - \frac{\partial}{\partial x_i}\left(\epsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + C'W = 0 \tag{1}$$

where $i, j = 1, 2$ are indices for Cartesian coordinates ($x_1 = x$; $x_2 = y$); ϵ is porosity; b is saturated thickness; C is volumetric concentration (solute mass per unit volume of fluid); V_i is the linear fluid velocity; D_{ij} is the dispersion coefficient tensor; W is the fluid sink rate (negative for fluid sources); and C' is the concentration in the sink or source fluid. For sinks ($W > 0$), it is often (Konikow and Grove, 1977, p. 13), though not necessarily, assumed that the concentration in fluid leaving the aquifer is equal to the concentration in the aquifer at that point, i.e., $C' = C$. This boundary condition is adequate for most field-scale modeling studies, but may not be appropriate for detailed examination of, for example, the concentration immediately adjacent to a pumping well, particularly at relatively early times. The assumptions embodied in this governing equation are described by numerous authors (e.g., Konikow and Grove, 1977; Bear, 1979).

Expanding the accumulation and advection derivatives in (1), adding ($CW - CW = 0$), and rearranging yields (after Konikow and Grove, 1977, p. 22):

$$\epsilon b\frac{\partial C}{\partial t} + \epsilon bV_i\frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\epsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + (C' - C)W + C\left[\frac{\partial(\epsilon b)}{\partial t} + \frac{\partial}{\partial x_i}(\epsilon bV_i) + W\right] = 0 \tag{2}$$

The last bracketed term in (2) is the sum of the fluid accumulation rate, flux divergence, and sources, and must be zero to satisfy fluid mass balance or continuity, leaving (cf. Bear, 1979, p. 242):

$$\epsilon b\frac{\partial C}{\partial t} + \epsilon bV_i\frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\epsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + (C' - C)W = 0 \tag{3}$$

or, dividing by ϵb (Konikow and Bredehoeft, 1978; cf. Prickett et al., 1981, p. 2; cf. Illangasekare and Doll, 1989, p. 860),

$$\frac{\partial C}{\partial t} + V_i\frac{\partial C}{\partial x_i} - \frac{1}{\epsilon b}\frac{\partial}{\partial x_i}\left(\epsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + \frac{(C' - C)W}{\epsilon b} = 0 \tag{4}$$

This simpler form of the solute-transport equation may reduce errors in numerical models because some of the numerical errors in the flow equation solution are not propagated into the solute-transport equation, as in (1) (Voss, 1984). Using finite-difference or finite-element techniques for the flow equation, the numerical errors in the spatial gradient of velocity and the temporal gradient of head, needed in (1), are larger than the numerical errors in the point value of velocity and head needed in (4). Based on the mathematical mechanics of its derivation, equation (4) can be thought of as a "flow-equation-removed" form; Voss (1984, p. 60) designates an analogous form for the case of compressible-fluid flow as "fluid-mass-conservative." Equation (4) may also be somewhat advantageous for Lagrangian-type models of solute transport because the advective term has only C within the derivative, and not V or other terms, although that is not a general requirement for Lagrangian models. In addition, fluid sinks are naturally handled: if it occurs or is assumed that $C' = C$ at sinks ($W > 0$), the last term drops out. Regardless of the possible motivations for using (3) or (4), for the purposes of this note, it is sufficient to state that these forms are used in at least three numerical models that purport to simulate solute transport in transient flow. Equations (3) and (4) are only appropriate for transient flow cases if the temporal variability in the product ϵb is maintained.

Contrary to the assumptions embodied in the computer program of Konikow and Bredehoeft (1978), the product ϵb in (3) and (4) is not constant in time during transient flow. The first term in the bracket in equation (2) is the time rate of change of fluid volume per unit area of aquifer, and is commonly related to potentiometric head (h) by:

$$\frac{\partial(\epsilon b)}{\partial t} = S\frac{\partial h}{\partial t} \tag{5}$$

where the storage coefficient, S, accounts for changes in fluid volume per unit area due to changes in head. Here we follow Fried (1975, p. 283) and Bear (1979) and consider that equation (5) is an operational definition of S, "without analyzing [its] internal relationship to the compressibilities of water and solid matrix" (Bear, 1979, p. 86), or whether the aquifer is unconfined or not.

The conceptualization of fluid-storage changes depends on whether the aquifer is confined or not. For unconfined or water-table aquifers, the storage change due to fluid and aquifer matrix compressibility is small compared to the storage change due to vertical movement of the top of the saturated zone (the water table). In this case, a common assumption is $S = \epsilon$ = specific yield, and (5) equates changes in saturated thickness with potentiometric head changes. It has been observed that specific yield can be significantly less than porosity. However, this difference is ignored here to be consistent with the models of Konikow and Bredehoeft (1978) and Prickett and others (1981). On the other hand, thickness (b) is often assumed to be constant in confined aquifers (e.g. de Marsily, 1986, p. 131), in which case (5) tracks the change in porosity due to head change. Here, no assumptions are made about how either porosity or thickness changes individually, only that their product is represented by (5). If both porosity and thickness are assumed to be constant, then $S = 0$ and aquifer heads are in steady-state equilibrium with imposed boundary conditions.

Prickett and others (1981) account for transient changes in saturated thickness in unconfined aquifers, but incorrectly use constant porosity and saturated thickness for confined systems, in which transmissivity is constant, even if $S \neq 0$. Voss (1984) holds porosity, thickness, and fluid density constant in an analogous solute-transport equation in transient compressible-fluid flow (see Goode, 1990). The removal of the flow-continuity equation from (1) removes the time derivative of the product ϵb, but does not imply that the product is constant in time, even for confined aquifers.

Changes in fluid storage in the aquifer (if $S \neq 0$) correspond to changes in porosity and thickness, and the product ϵb is a function of head [from (5)]:

$$\epsilon b = (\epsilon b)_0 + \int_0^t S \frac{\partial h}{\partial t} dt \tag{6}$$

or, for constant S,

$$\epsilon b = (\epsilon b)_0 + S[h - h_0] \tag{7}$$

where subscript 0 indicates the initial condition. Thus, for constant S, the product of porosity and thickness is a simple linear function of head. If porosity is assumed to be constant in time and equal to the storage coefficient, equation (7) equates changes in saturated thickness with head changes, a common model of fluid storage in water-table aquifers (Prickett et al., 1981).

Models that do not account for changes in fluid storage during transient flow will yield inaccurate solutions to the transport equation. In addition to using the incorrect volume for dilution, velocities and dispersion coefficients will be incorrect. Using Darcy's law, velocity is given by the flux per unit width of aquifer divided by the product of porosity and saturated thickness:

$$V_i = -\frac{1}{\epsilon b} T_{ij} \frac{\partial h}{\partial x_j} \tag{8}$$

where ϵb is given by (7). Equation (8) applies for confined or unconfined flow, regardless of whether transmissivity is a function of head or not. Likewise, the term $1/\epsilon b$ modifying the dispersion term also changes in time during transient flow. In an aquifer in which heads are increasing in time and $S \neq 0$, the use of the initial value $(\epsilon b)_0$ will result in exaggerated velocities. This occurs because the ground-water flux or specific discharge, which is independent of changes in ϵb associated with fluid storage and depends only on the head gradient and transmissivity, is divided by a constant $(\epsilon b)_0$ that is smaller than the actual transient value (7). Goode (1990) quantifies these errors for two simple transient flow cases having analytical solutions. Analogous errors occur in models of transport in transient compressible-fluid flow (e.g. Voss, 1984) that hold fluid density constant in the flow-equation-removed transport equation (Goode, 1990). In the next section, the impact of ignoring fluid-storage changes during solute transport in transient flow are illustrated by a numerical example.

Illustration of Approximation Errors

The combined effects of dilution volume, velocity, and dispersion errors can be illustrated by numerical simulation of transient flow and transport using the model of Konikow and Bredehoeft (1978). This model solves the transient linear flow equation using finite-difference techniques, and solves the flow-equation-removed solute-transport equation (4) using finite differences and the method of characteristics. The method of characteristics introduces minimal numerical dispersion when the dispersion coefficients are small relative to velocity, as assumed here. The computer program was recently updated (D. J. Goode and L. F. Konikow, written communication, 1988) to account for temporal changes in the product of porosity and thickness in the transport equation during transient flow. These modifications do not affect the flow-equation solution.

The previous model version, which ignored temporal changes in ϵb, and the updated version are applied to a 185 m long aquifer discretized by 37 finite-difference blocks (5 m each) in x and 15 blocks (1 m each) in y (Figure 1). Potentiometric head at the nodes at one end of the aquifer ($x = 180$ m) is held constant at $h = 100$ m, which is also the initial condition throughout the aquifer. Water is injected at a constant rate of $W = -129.6$ m^3/day per meter of boundary at the other end of the aquifer (blocks centered at $x = 2.5$ m). The model y boundaries are zero flux for both water and solute. Initial concentrations are zero everywhere and in the injected fluid except for the block centered at $x = 2.5$ m, $y = 0.5$ m, where the concentration in the injected fluid is $C' = 5000$ (arbitrary units). Aquifer hydraulic conductivity is $K = 8.64$ m/day, initial saturated thickness is $b_0 = 100$ m, and initial porosity is $\epsilon_0 = 0.1$. The storage coefficient is also $S = 0.1$. This storage coefficient corresponds to either an unconfined aquifer, or to a confined aquifer with a porous matrix compressibility of about 10^{-7} m^2/N, the upper limit for sand reported by Freeze and Cherry (1979, p. 55). The "rough" range of storage coefficients for confined aquifers is considered to be 0.05 to 10^{-5} by de Marsily (1986, p. 111). Use here of this large value ($S = 0.1$) for a confined aquifer results in larger errors than would be expected for most confined aquifers given similar head changes. This example is for illustrative purposes only.

For comparison, the model is also applied under the assumption of steady-state confined flow, using constant porosity and thickness equivalent to the initial condition of

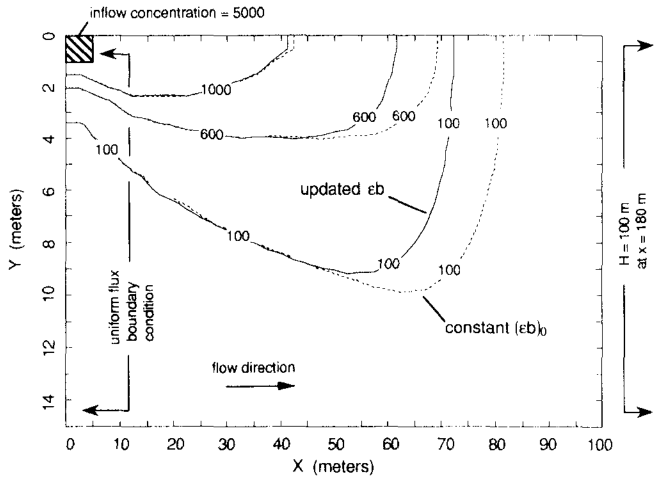

Fig. 1. Concentration contours at six days using different numerical model formulations: transient confined flow using ϵb updated in time (solid curves); transient confined flow using constant $\epsilon b = (\epsilon b)_0$ (dashed curves). Simulation boundary conditions and the resulting flow direction are also indicated.

the transient simulations. Furthermore, a modified version of the flow and transport model, in which transmissivity is a linear function of head (T = Kh), is applied to show the effect of ignoring transmissivity changes in an unconfined aquifer for this transient flow problem.

Figure 1 shows the spatial distribution of solute mass at six days assuming constant transmissivity and either constant $(\epsilon b)_0$ (dashed curves) or changing ϵb due to changing heads (solid curves). The plume front advances too rapidly if the increase in ϵb is ignored, whereas behind and ahead of the front the differences between the solutions are minor. For this transient flow problem, the product of porosity and thickness increases because heads increase and the storage coefficient is nonzero.

Potentiometric heads in the aquifer, which are uniform in y because of the one-dimensional boundary conditions, are essentially at steady-state after about seven days (Figure 2; these results are for the confined case, T = constant in time). At steady-state, heads vary linearly from one end of the aquifer to the other for constant T. Because the storage coefficient is not zero, and heads increase in time, the volume of water stored in the aquifer also increases in time following (7). The maximum increase in storage occurs in the injection block (in this model, fluid and solute sources are assumed to be distributed uniformly over the finite-difference grid block) where the relative increase in storage (change in storage divided by initial storage) is 27 percent:

$$\frac{S(h - h_0)}{(\epsilon b)_0} = \frac{0.1(127 - 100)}{0.1(100)} = 0.27 \qquad (9)$$

The error in velocity is clearly illustrated by concentration breakthroughs at several distances from the injection block on the plume centerline (Figure 3) using either constant $\epsilon b = (\epsilon b)_0$ (dashed curves) or updating ϵb in time following (7) to account for fluid-storage changes (solid curves). Figure 3 also shows the breakthrough at 75 m for steady-state confined flow simulation using $\epsilon b = (\epsilon b)_0$ (dots), and for transient unconfined flow conditions (triangles) in which transmissivity is a linear function of head. The minor fluctuations in the concentrations are due to the discrete nature of the method of characteristics (Konikow and Bredehoeft, 1978). The differences between the solid and dashed curves at the injection block (x = 0 m) indicate that the dilution volume using constant ϵb (dashed curve) is too low, resulting in slightly elevated concentrations (Figure 4).

The error in the advection term is most significant for this problem—constant ϵb (dashed curves in Figure 3) yields a travel time about 14 percent too short at 75 m. This error would be larger if the boundary flux was larger or if the initial thickness was smaller. Breakthrough under transient-

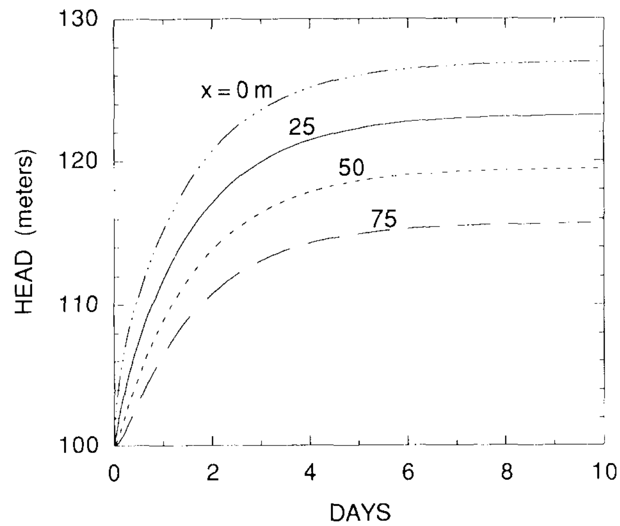

Fig. 2. Hydrographs of potentiometric head at several distances from injection blocks for transient confined (constant T) flow.

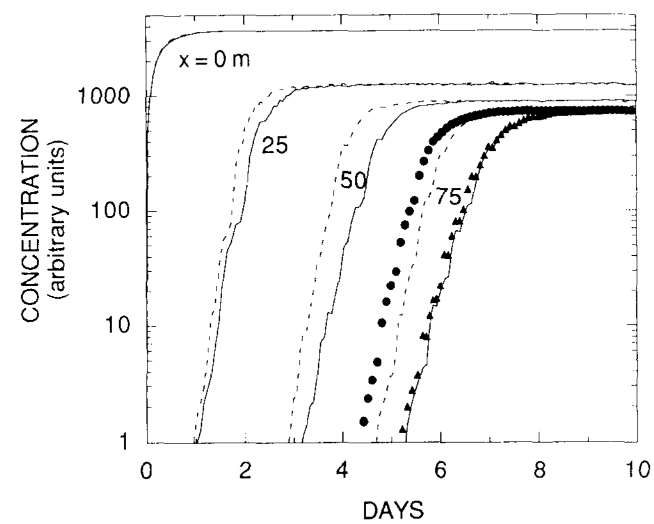

Fig. 3. Centerline concentration breakthrough at several distances from the injection block using different numerical model formulations: transient confined flow using ϵb updated in time (solid curves); transient confined flow using constant $\epsilon b = (\epsilon b)_0$ (dashed curves); steady-state confined flow using $\epsilon b = (\epsilon b)_0$ (dots); and transient unconfined flow (triangles).

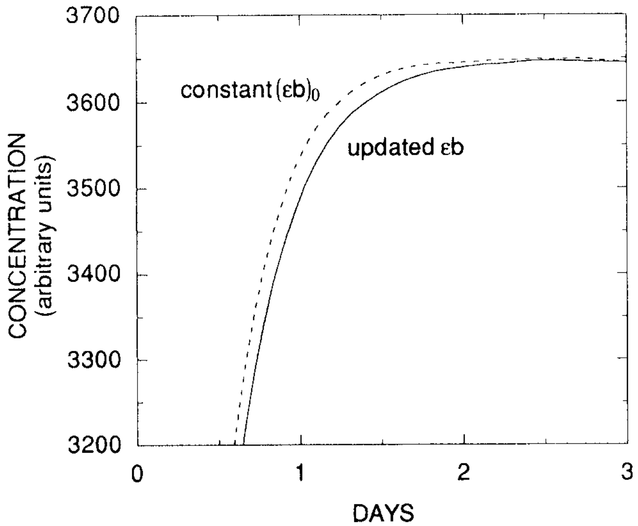

Fig. 4. Detail of Figure 3 showing concentrations in the injection block using different numerical model formulations: transient confined flow using ϵb updated in time (solid curves); transient confined flow using constant $\epsilon b = (\epsilon b)_0$ (dashed curves).

flow conditions using constant $(\epsilon b)_0$ is very similar to breakthrough under steady-flow conditions using the same $(\epsilon b)_0$ (dots). For this problem, the primary impact of the transient flow conditions is the resulting change in fluid storage in time, and not the temporal variability in velocity caused by changing gradients.

Because this flow problem is one-dimensional, and a flux boundary condition is used, accounting for changes in transmissivity due to water-table movement only slightly changes the solute-transport solution (Figure 3, triangles). The ultimate steady-state heads for unconfined conditions are somewhat lower due to the increase in transmissivity. However, the solute-transport solution for this case is very similar to that for the case of constant transmissivity (Figure 3). The major effect of increasing saturated thickness on transport for this case is the change in fluid storage, not transmissivity, and the effect of changing fluid storage is accounted for simply by updating ϵb in time in the transport model.

As mentioned in the introduction, this problem first came to light because of mass balance errors. For this case of confined (constant T) transient flow, using constant $(\epsilon b)_0$ yielded mass balance errors on the order of 5 percent, while updating ϵb in time yielded mass balance errors on the order of 1 percent. The simulation mentioned in the introduction exhibited larger mass balance errors because the relative change in fluid storage [equation (9)] was over 100 percent.

Summary and Conclusions

Removing the time derivative of fluid storage and flow divergence terms from the solute-transport equation does not imply that fluid-storage terms—porosity, saturated thickness, and fluid density—remaining in the transport equation are constant in time during transient flow. Nevertheless, this has been assumed in three widely applied numerical models. For the numerical simulation presented using the model of Konikow and Bredehoeft (1978), ignoring temporal changes in fluid storage, the product of porosity and saturated thickness, results in about 14 percent error in solute travel time. From a practical perspective, of course, this error is small relative to the uncertainty and variability inherent in model parameters for field-scale simulation. However, eliminating the dilution, velocity, and dispersion errors associated with fluid-storage transients is straightforward and computationally inexpensive. Any transport model that purports to simulate the effects of transient ($S \neq 0$) flow should maintain temporal changes in fluid-storage terms appearing in the transport equation.

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Since 1987, Dan Goode has been with the USGS Water Resources Division's National Research Program where his interests include simulation methods for ground-water flow and solute transport. He received his Bachelor's (1980) and Master's Degrees (1982) in Civil Engineering/Water Resources from the Massachusetts Institute of Technology. He has worked as a consultant to EPA and private industry, and from 1983 through 1986 he was the lead hydrogeologist for low-level radioactive waste disposal programs with the U.S. Nuclear Regulatory Commission.