GOVERNING EQUATIONS AND MODEL APPROXIMATION ERRORS ASSOCIATED WITH THE EFFECTS OF FLUID-STORAGE TRANSIENTS ON SOLUTE TRANSPORT IN AQUIFERS

By Daniel J. Goode

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PREFACE

This report evaluates a common and often unacknowledged assumption used in numerical models of solute transport in transient ground-water flow. This work was conducted as part of the Research Project on Transport Modeling in Saturated Zone and the improved numerical procedures described herein have been incorporated into the general solute-transport model of Konikow and Bredehoeft (Techniques of Water-Resources Investigations, Book 7, Chapter C2, 1978). Correspondence on this report and on the computer program of Konikow and Bredehoeft should be addressed to:

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Copies of the computer program for the model of Konikow and Bredehoeft are available at cost of processing from:

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Multiply	by	To Obtain
meter (m)	3.281	foot (ft)
meter squared per second (m^2/s)	10.76	foot squared per second (ft^2/s)

GOVERNING EQUATIONS AND MODEL APPROXIMATION ERRORS ASSOCIATED WITH THE EFFECTS OF FLUID-STORAGE TRANSIENTS ON SOLUTE TRANSPORT IN AQUIFERS

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ABSTRACT

During 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 incorporate the effects of transient flow on solute transport by removing redundant flow-equation terms from the transport equation. However, in certain circumstances fluid-storage terms remaining in the transport equation are erroneously held constant in these models. For the case of increasing heads, this approximation leads to velocities that are too high and reduced dilution at fluid and solute sources. These errors are quantified by means of two simple analytical examples and a numerical simulation. In some cases, the errors induced in transport simulations by ignoring temporal changes in fluid-storage terms are comparable to the errors from assuming steady-state flow. Errors in source calculations are generally smaller than errors in flux terms. During transient flow in water-table aquifers, solute transport may be affected more by changing fluid storage than by changes in transmissivity due to saturated thickness changes. For conceptual models that are based on the assumption of constant fluid density, the product of porosity and aquifer thickness changes in time: initial porosity times thickness plus the change in head times the storage coefficient. This formula reduces to the saturated thickness in water-table aquifers if porosity is assumed to be equal to the storage coefficient.

INTRODUCTION

For quantitative simulation, ground-water flow and solute transport in aquifers are represented by a system of equations, with attendant boundary and initial conditions, and parameters, that hopefully capture all significant features of the real processes. The features that are significant may vary from case to case. Although practical model accuracy is limited primarily by the lack of detailed information on spatially variable aquifer properties, and usually not by numerical errors, it is nonetheless important that the models themselves do not induce unnecessary approximation errors. This report examines the error introduced by a common approximation used in solute-transport simulation that is associated with changes in fluid storage during transient flow.

Useful approximations for aquifer simulation include: ignoring vertical variability by averaging or integrating over the vertical dimension, thus yielding two-dimensional equations; assuming transmissivity is constant in time and independent of potentiometric head, thus yielding a linear flow equation; and, representing fluid-storage changes through a storage coefficient that can include the effects of fluid compressibility as well as compressibility of the aquifer and movement of the water table. Three widely applied numerical models of transient two-dimensional flow and solute transport (Konikow and Bredehoeft, 1978; Prickett and others, 1981; Voss, 1984) use these approximations and a "flow-equation-removed" form of the solute-transport equation. In this form, the divergence of flux and temporal derivative of fluid-storage terms are removed from the governing solute-transport equation. This form of the equation can reduce numerical errors because this manipulation occurs prior to numerical approximation of the derivative terms. Furthermore, this form is advantageous for Lagrangian-type models, such as those of Konikow and Bredehoeft (1978) and Prickett and others (1981), because only velocity, and not its derivative, appears in the solute-transport equation. However, in each of these numerical models the changes over time in fluid-storage terms remaining in the solute-transport equation are not considered. The inclusion of these changes in numerical models is not difficult because the derivatives of the fluid-storage terms do not occur in the flow-equation-removed transport equation; consequently there is little reason to make this approximation.

This report evaluates approximation errors in solute-transport models associated with fluid-storage changes during transient ground-water flow. The two-dimensional flow equation for constant fluid density and a consistent flow-equation-removed formulation of the solute-transport equation are briefly reviewed. Errors induced in the solute-transport solution by ignoring fluid-storage changes during transient flow are examined using two simple analytical models and an example numerical simulation. The appendix presents an analogous flow-equation-removed form of the solute-transport equation for aquifers where fluid density is a function of pressure alone.

GOVERNING EQUATIONS

For an incompressible fluid flowing in a two-dimensional aquifer, continuity requires (Konikow and Grove, 1977, p. 22):

$$\frac{\partial(\varepsilon b)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon b V_i) + W = 0 \quad , \tag{1}$$

where i = 1, 2 is an index for Cartesian coordinates ($x_1 = x$, $x_2 = y$) with implied summation, ε is porosity, b is saturated thickness, V_i are velocity components, and W is the withdrawal rate from the aquifer ($W<0$ for sources). The first term in (1) is the time rate of change of fluid volume per unit area, which is commonly related to potentiometric head, h, changes by:

$$\frac{\partial(\varepsilon b)}{\partial t} = S\frac{\partial h}{\partial t} \quad , \tag{2}$$

where the storage coefficient, S, accounts for changes in fluid volume per unit area from changes in aquifer saturated thickness and changes in porosity. For phreatic or water-table aquifers, a common assumption is $S=\varepsilon=$constant (specific yield), and (2) equates changes in saturated thickness with potentiometric head changes. For confined aquifers, thickness may be assumed to be constant, in which case (2) tracks the change in porosity due to head change. Here, no assumptions are made on changes in porosity or thickness except that their product is represented by (2). If both porosity and thickness are assumed to be constant, then $S=0$ and the aquifer is in steady-state equilibrium with imposed boundary conditions. The appendix considers the case of compressible flow.

The second term in (1) is the divergence of volumetric flux and is related to head using Darcy's law:

$$\varepsilon b V_i = -T_{ij}\frac{\partial h}{\partial x_j} \quad , \tag{3}$$

where j = 1,2, and T_{ij} is the transmissivity tensor. Substituting (2) and (3) into (1) yields a common form of the two-dimensional flow equation (Bear, 1979; Konikow and Bredehoeft, 1978, p. 2; Prickett and others, 1981, p. 5):

$$S\frac{\partial h}{\partial t} - \frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) + W = 0 \quad . \qquad (4)$$

For water-table aquifers, transmissivity is often assumed to be a linear function of head in that the saturated thickness changes proportionally to head: T = Kb = K (h - (elevation of aquifer bottom)), where K is hydraulic conductivity. For this study, this assumption is considered conceptually distinct from the assumptions on aquifer storage and thickness and porosity changes.

The governing equation for two-dimensional solute transport in incompressible flow can be written (Konikow and Grove, 1977, p. 21):

$$\frac{\partial(\varepsilon bC)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon bCV_i) - \frac{\partial}{\partial x_i}\left(\varepsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + C'W = 0 \quad , \qquad (5)$$

where C is volumetric concentration (solute mass per unit volume of fluid), C' is the concentration in the sink or source fluid, and D_{ij} is the dispersion coefficient tensor. For sinks (W>0), it is often assumed that C'=C. The accumulation term in (5) can be expanded:

$$\frac{\partial(\varepsilon bC)}{\partial t} = \varepsilon b\frac{\partial C}{\partial t} + C\frac{\partial(\varepsilon b)}{\partial t} \quad . \qquad (6)$$

Substituting (6) into (5), similarly expanding the advective term, adding (CW-CW), and rearranging yields (after Konikow and Grove, 1977, p. 22):

$$\varepsilon b\frac{\partial C}{\partial t} + \varepsilon bV_i\frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\varepsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + (C'-C)W$$
$$+ C\left[\frac{\partial(\varepsilon b)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon bV_i) + W\right] = 0 \quad . \qquad (7)$$

But, from the fluid continuity equation (1), the last bracketed term in (7) is zero, leaving:

$$\varepsilon b\frac{\partial C}{\partial t} + \varepsilon bV_i\frac{\partial C}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\varepsilon bD_{ij}\frac{\partial C}{\partial x_j}\right) + (C'-C)W = 0 \quad , \qquad (8)$$

or, dividing by εb (Konikow and Grove, 1977),

$$\frac{\partial C}{\partial t} + V_i \frac{\partial C}{\partial x_i} - \frac{1}{\varepsilon b}\frac{\partial}{\partial x_i}\left(\varepsilon b D_{ij}\frac{\partial C}{\partial x_j}\right) + \frac{(C'-C)W}{\varepsilon b} = 0 \quad . \qquad (9)$$

This form may reduce errors in numerical models because numerical errors in the flow equation solution are not propagated into the solute-transport equation, as in (5) (Voss, 1984). This form can be thought of as a "flow-equation-removed" form; Voss (1984, p. 60) designates this form as "fluid-mass-conservative". This form is also advantageous for Lagrangian-type models of solute transport because the advective term has only C within the derivative, and not V or other terms. In addition, sinks are naturally handled: if C'=C, the last term drops out.

The product εb in (9) is not necessarily constant in time, as assumed in the numerical model of Konikow and Bredehoeft (1978). Prickett and others (1981) account for changing b in water-table aquifers, but use constant εb 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 compressible-flow (see the appendix). The removal of the flow equation terms from (5) removes the time derivative of the product εb, but does not imply that the product is constant, even for confined aquifers. If εb is assumed to be constant, then by (2) $S=0$ and flow is at steady-state and in equilibrium with imposed boundary conditions.

Changes in fluid storage in the aquifer (if $S \neq 0$) are due to changes in porosity and thickness, and the product εb is a function of head (from (2)):

$$\varepsilon b = (\varepsilon b)_0 + \int_0^t S \frac{\partial h}{\partial t} dt \quad , \qquad (10)$$

or, for constant S,

$$\varepsilon b = (\varepsilon b)_0 + S\,[h - h_0] \quad , \qquad (11)$$

where subscript 0 represents the initial condition. For constant S, the product of porosity and thickness is a simple linear function of head. For water-table aquifers, porosity change often can be ignored and from (2), $\varepsilon = S$. In this case, (11) equates changes in saturated thickness with head changes.

The εb within the dispersion spatial derivative in (9) is a notational result of writing the dispersion coefficient as a function of velocity. The dispersion coefficient as a function of velocity is, for example (after Konikow and Grove, 1977):

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} \quad . \qquad (12)$$

In two-dimensional transport εbD may be written, using Darcy's law:

$$\varepsilon b D_{xx} = -\alpha_L \left[T_{xx}\frac{\partial h}{\partial x} + T_{xy}\frac{\partial h}{\partial y} \right] \frac{V_x}{|V|} - \alpha_T \left[T_{yy}\frac{\partial h}{\partial y} + T_{yx}\frac{\partial h}{\partial x} \right] \frac{V_y}{|V|} \quad , \qquad (13)$$

and similarly for other components. The product εb cancels out of the velocity ratios in (13). Thus, the term $\varepsilon b D_{ij}$ within the derivative in (9) is determined from (13) and similar equations for other components and is independent of temporal changes in εb due to fluid storage. The velocity term in (9) is determined by (3) using εb from (11).

Models that do not account for changes in εb during transient flow will yield inaccurate solutions to the transport equation. In an aquifer undergoing transient flow with increasing heads, the use of a constant εb will result in exaggerated velocities. In addition, the contribution of sources is in error because the source mass is diluted by a storage term that is too small. These errors are quantified in the next section.

MODEL APPROXIMATION ERRORS

Two simple analytical examples and a numerical simulation illustrate the error induced by ignoring temporal changes in aquifer fluid storage during two-dimensional solute transport. Fluid density is assumed to be constant so that changes in fluid storage are due to changes in porosity and saturated thickness. Analogous errors occur in models of aquifers having compressible flow that hold fluid density constant in the flow-equation-removed transport equation (see the appendix).

Errors in Source Terms

Errors associated with the source term in the transport equation may be illustrated using a single-cell or lumped-parameter model of an aquifer within which solutes are completely mixed. The aquifer state is characterized by spatially averaged values of head and volumetric concentration. The flow equation reduces to:

$$S\frac{\partial h}{\partial t} + W = 0 \quad , \tag{14}$$

which for constant W and S has the solution:

$$h = h_0 - \frac{W}{S}(t-t_0) \quad . \tag{15}$$

From (11), the product of porosity and thickness is given by:

$$\varepsilon b = (\varepsilon b)_0 - W(t - t_0) \quad . \tag{16}$$

For a single-cell model, the governing flow-equation-removed solute-transport equation (9) becomes:

$$\frac{\partial C}{\partial t} + \frac{(C'-C)W}{\varepsilon b} = 0 \quad , \tag{17}$$

where εb is given by (16). The solution for this case (for constant C') is:

$$C = C' - \frac{(C' - C_0)(\varepsilon b)_0}{(\varepsilon b)_0 - W(t - t_0)} \quad . \qquad (18)$$

Equation (17) can also be solved under the assumption that εb is constant at its initial value, $(\varepsilon b)_0$. The solution for this approximate governing equation is:

$$C_1 = C' - (C' - C_0)\exp\left[\frac{W}{(\varepsilon b)_0}(t - t_0)\right] \quad . \qquad (19)$$

The relative error using this approximation of constant εb can be compared to a solution that assumes steady-state flow. Instead of using the flow-equation-removed form (9), the single-cell model can be developed from the complete transport equation (5). Assuming that εb is constant, again at its initial value, $(\varepsilon b)_0$, the governing equation is (from (5)):

$$\frac{\partial C}{\partial t} + \frac{C'W}{(\varepsilon b)_0} = 0 \quad . \qquad (20)$$

By integration the solution to this approximation is:

$$C_2 = C_0 - \frac{C'W}{(\varepsilon b)_0}(t - t_0) \quad . \qquad (21)$$

A dimensionless error for the two approximations can be compared. For the first approximation, C_1, this error is:

$$1 - \frac{(C_1 - C')}{(C - C')} = 1 - \left[1 - \frac{W}{(\varepsilon b)_0}(t - t_0)\right]\exp\left[\frac{W}{(\varepsilon b)_0}(t - t_0)\right] \quad . \qquad (22)$$

For the second approximation, C_2, this error is:

$$1 - \frac{(C_2 - C')}{(C - C')} = \frac{W}{(\varepsilon b)_0}(t - t_0) + \frac{C'}{C_0 - C'}\left[\frac{W}{(\varepsilon b)_0}(t - t_0)\right]\left[1 - \frac{W}{(\varepsilon b)_0}(t - t_0)\right] \quad . \qquad (23)$$

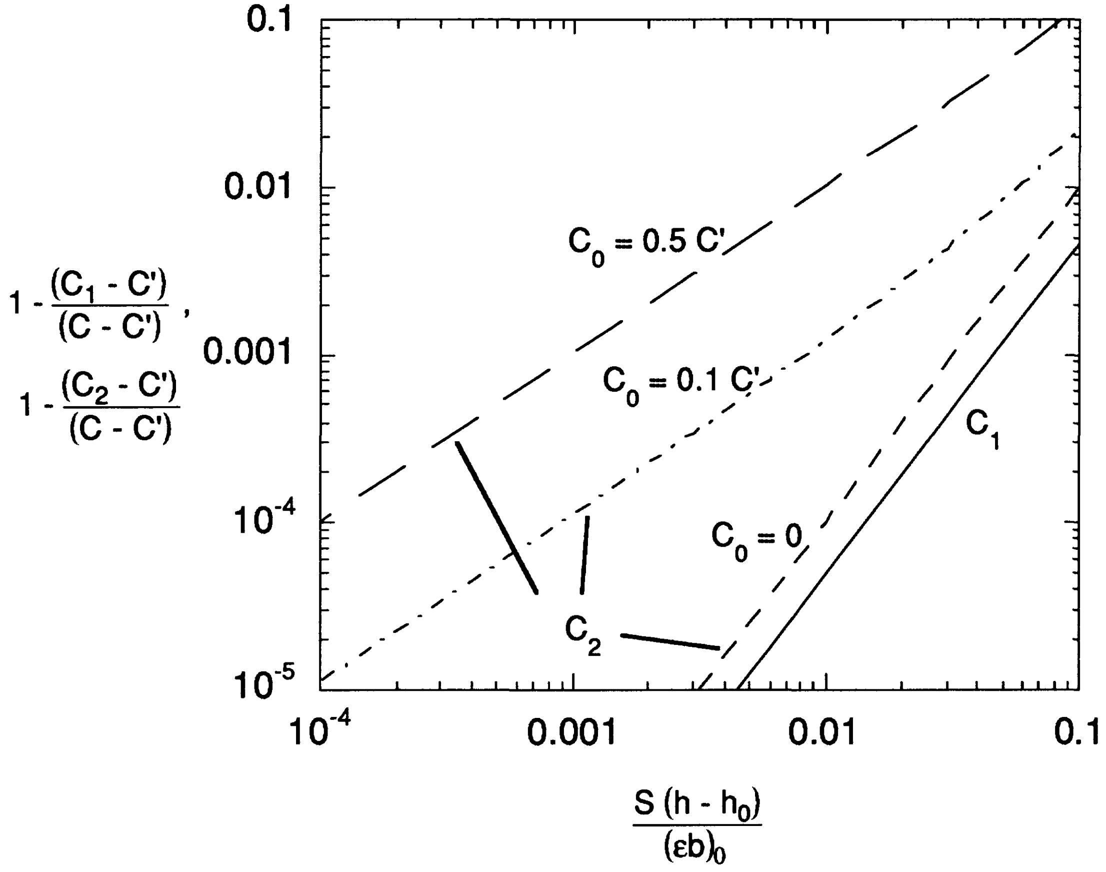

Figure 1. Graph showing relative error for approximate single-cell models: approximation C_1 assumes constant εb (equation (22)); approximation C_2 assumes steady-state flow (constant head) and is shown for different values of C_0 (equation (23)).

The relative errors are illustrated in Figure 1 as functions of the ratio (from (15))

$$\frac{S(h - h_0)}{(\varepsilon b)_0} = \frac{-W}{(\varepsilon b)_0}(t - t_0) \quad , \qquad (24)$$

which is the change in fluid volume divided by the initial fluid volume. The error of the steady-flow approximation C_2 is shown for several values of C_0 relative to C'. For an initial concentration of zero, the error induced by ignoring changes in εb in the flow-equation-removed solute-transport equation is about one-half the error induced by assuming that the flow system is at steady state and head is constant. If transients in the flow system are considered important and a transient flow model is used, then changes in εb in the flow-equation-removed transport equation may also be important, and the effect of these changes of a similar order-of-magnitude. For higher initial concentrations, the relative error is much greater for the steady-state flow approximation, although relative changes in C are smaller.

Errors in Velocity

In addition to the errors induced in source terms, dispersive and advective fluxes are also in error when changes in εb are ignored during transient flow. The relative error for advective fluxes can be compared to errors induced by ignoring transients completely. For an advancing front, the error in the dispersive flux should be of comparable magnitude and in the same direction, because both the advective and dispersive flux terms are divided by the changing product εb in the governing equation (9). For this examination, consider transient radial flow from a fully-penetrating well in a confined (T=constant) aquifer. The transient head solution for constant Q_w is given by (e.g., Bear, 1979):

$$h = h_0 - \frac{Q_w}{4\pi T} W(u) \quad , \qquad (25)$$

where Q_w is the pumping rate ($Q_w>0$ is withdrawal), $W(u)$ is the well function, and u, the well function parameter is:

$$u = \frac{Sr^2}{4Tt} \quad , \qquad (26)$$

where r is the radial coordinate. From the definition of the well function (e.g., Bear, 1979), the velocity is:

$$V = -\frac{Q_w}{2\pi \varepsilon b r} e^{-u} \quad . \qquad (27)$$

The product εb changes in time if fluid density is assumed to be constant, and is given by (11). An approximate velocity, V_1, is obtained by assuming that εb is constant at its initial value $(\varepsilon b)_0$ in (27). The relative velocity error of this approximation is:

$$1 - \frac{V_1}{V} = \frac{-S}{(\varepsilon b)_0}(h - h_0) \quad . \tag{28}$$

As with source-term errors, the relative error in velocity is dependent on the ratio of the change in fluid storage to the initial fluid storage.

From geometric considerations, the steady-state velocity is:

$$V_2 = \frac{-Q_w}{2\pi\varepsilon br} \quad . \tag{29}$$

If the initial value of εb is used in this steady-state flow approximation, then the error is:

$$1 - \frac{V_2}{V} = 1 - \left[1 + \frac{S}{(\varepsilon b)_0}(h - h_0)\right] e^u \quad . \tag{30}$$

The relative errors in velocity using the approximations V_1 and V_2 are shown in Figure 2 for the case of injection ($Q_w<0$).

The steady-state approximation has errors from two sources: (1) the initial εb is used instead of the changing value; and (2) all fluid volume comes from (or goes to) the boundary (at infinity) whereas in the transient solution a portion of the fluid volume comes from (or goes into) storage in the aquifer. The first source of error yields low velocities for pumping and high velocities for injection wells. The second error always results in velocities that are too high. The second error is most important at early times, when the well function parameter u is large. At large times, and for large changes in the product εb the errors of the steady-state approximation approach the error of the transient solution using εb fixed at its initial value, $(\varepsilon b)_0$. When the relative change in storage (see abscissa in Figure 2) is greater than u, the two approximations result in errors of the same order of magnitude.

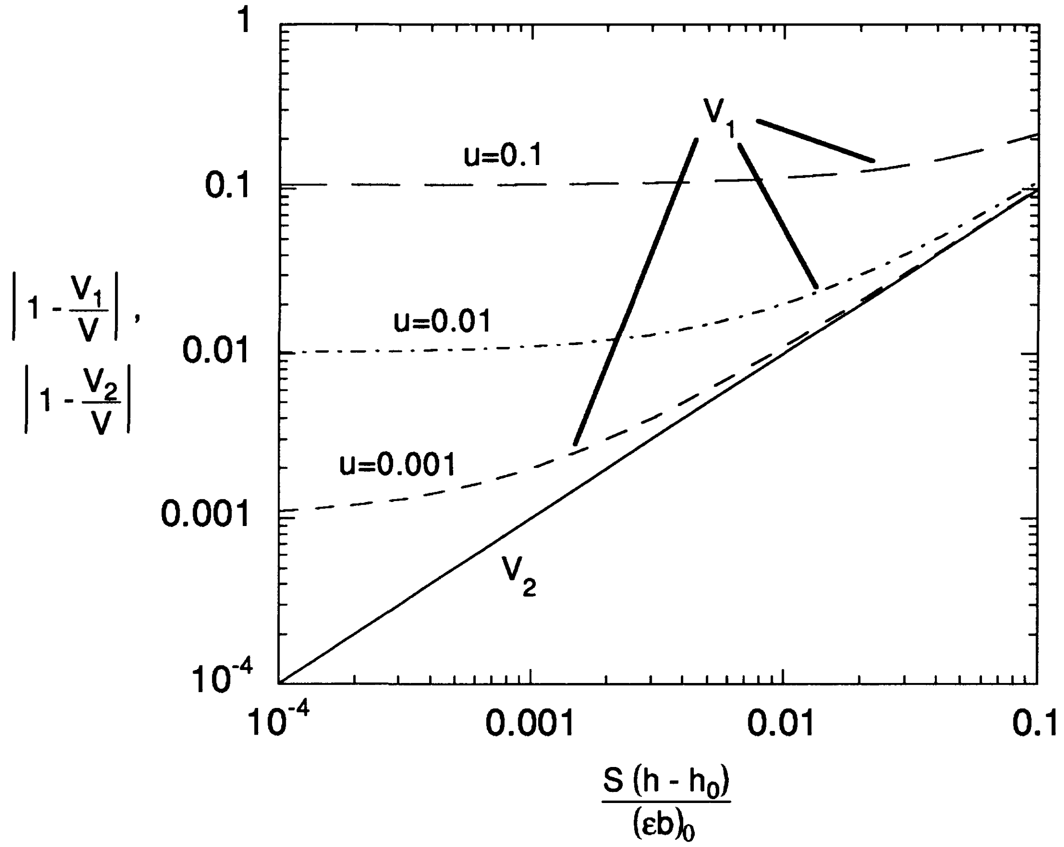

Figure 2. Graph showing relative error for approximate radial velocity during injection: approximation V_1 is transient velocity using constant εb (equation (28)); approximation V_2 is steady-state velocity (equation (30)) and is shown for several values of the well function parameter $u=(Sr^2)/(4Tt)$.

Errors during Numerical Simulation of Advective Transport

The combined effects of source-term and velocity errors can be examined through numerical simulation of transient flow and advection-only transport in one dimension. The model of Konikow and Bredehoeft (1978) solves the transient flow equation using finite-difference techniques, and solves the volumetric-concentration form of the flow-equation-removed solute-transport equation (9) using finite-differences and the method of characteristics. The method of characteristics introduces no numerical dispersion when the dispersion coefficients are zero, as assumed here. Fluid density and aquifer transmissivity are assumed to be constant. The computer program was recently updated by the writer to account for changes in the product of porosity and thickness in the transport equation during transient flow. 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). Potentiometric head at one end of the aquifer is held constant at 100 m, which is also the initial condition throughout the aquifer. Water containing solute at concentration 1.0 is injected at a constant rate of 0.0005 m^2/s at the other end of the aquifer. Initial concentrations are zero everywhere. Aquifer hydraulic conductivity is 0.0001 m/s, initial saturated thickness is 100 m, and initial porosity is 0.1. The storage coefficient is also 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). For comparison, the model is also applied under the assumption of steady-state flow, using constant porosity and thickness equivalent to the initial condition of the transient simulations. In addition, a modified version of the model, in which transmissivity is a linear function of head, is applied to show the effect of ignoring transmissivity changes in a water-table aquifer for this one-dimensional problem.

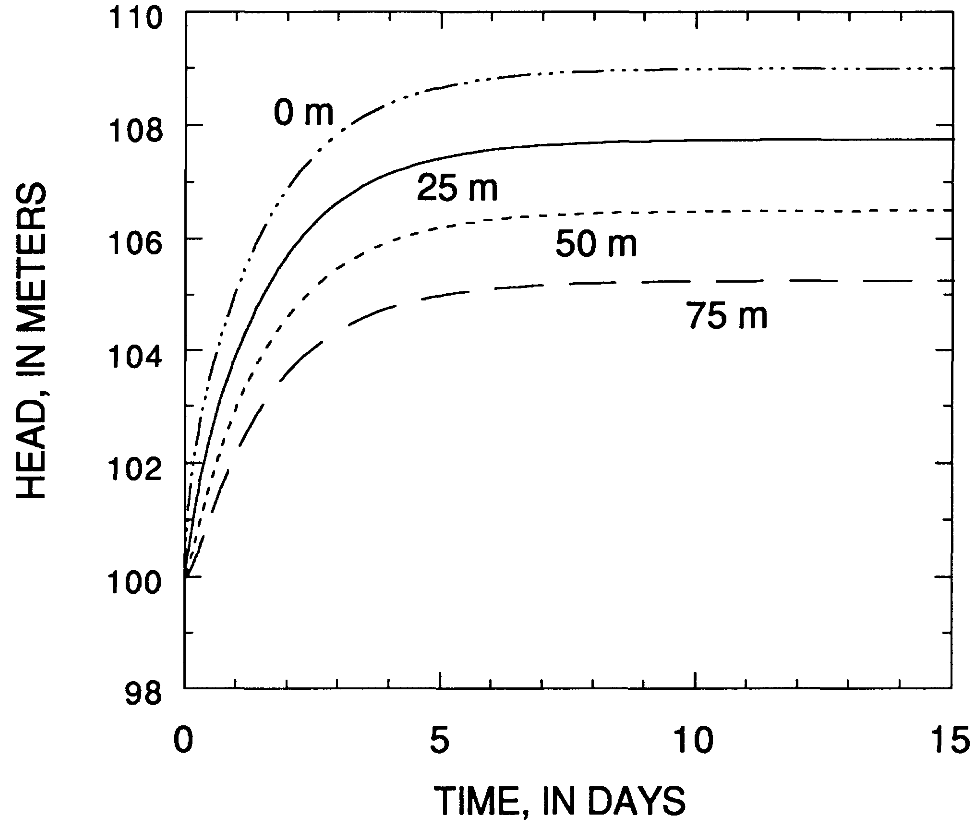

Figure 3. Hydrographs of potentiometric head at several distances from injection block.

Potentiometric heads in the aquifer (Figure 3) are essentially at steady-state after about 7 days. Using constant transmissivity, at steady-state heads vary linearly from one end of the aquifer to the other. Because the storage coefficient is not zero, and heads have increased, the amount of water stored in the aquifer has increased. The maximum increase in storage occurs in the injection block (in this model, 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 approximately

$$\frac{S(h-h_0)}{(\varepsilon b)_0} = \frac{0.1(109-100)}{0.1(100)} = 0.09 \quad . \qquad (31)$$

Concentration breakthrough is shown in Figure 4 for several distances from the injection block using constant $\varepsilon b = (\varepsilon b)_0$ (dashed curves) and updating εb in time following

(11) to account for fluid-storage changes (solid curves). In addition, the breakthrough at 75 m is shown for a steady-state flow simulation using $\varepsilon b=(\varepsilon b)_0$ (dots), and for transient water-table conditions (squares). Concentrations in the injection block do not immediately go to 1.0 because of the mixing of the injected water with the resident water in the block. This is an artifact of the model's representation of sources as areally distributed over the entire block. The differences between the solid and dashed curves at this point indicate that the dilution volume using constant εb (dashed curve) is too low, resulting in slightly increased concentrations.

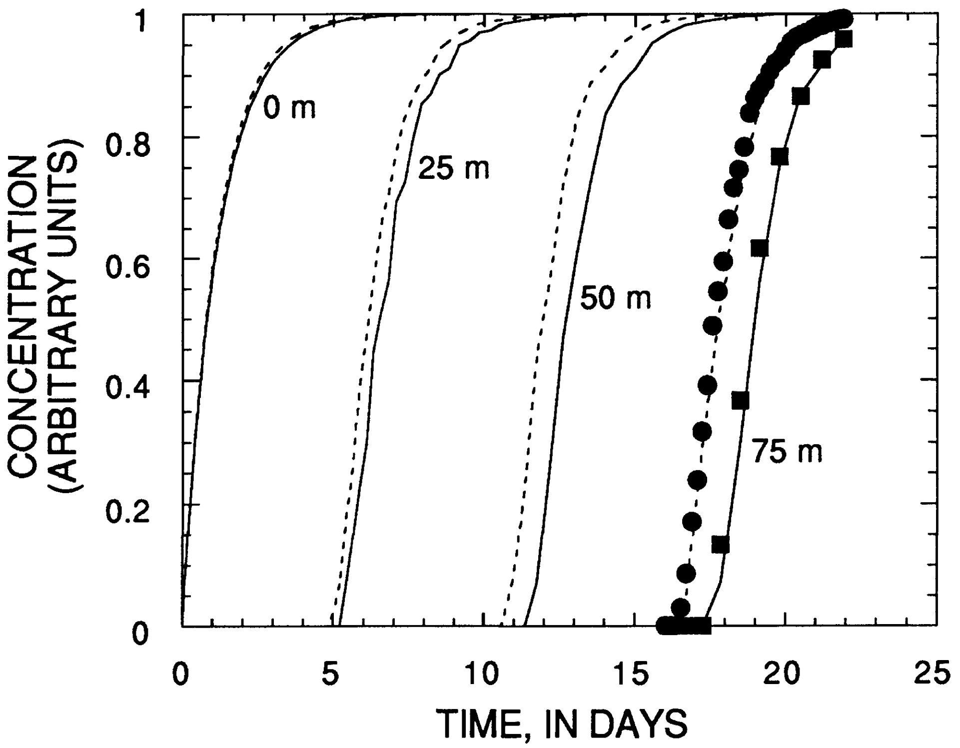

Figure 4. Graph showing concentration breakthrough at several distances from the injection block using different numerical model formulations: transient flow using εb updated in time (solid curves); transient flow using constant $\varepsilon b=(\varepsilon b)_0$ (dashed curves); steady-state flow using $\varepsilon b=(\varepsilon b)_0$ (dots); and transient flow under water-table conditions (squares).

The error in the velocity term is more significant for this problem--constant εb (dashed curve in Figure 4) yields a travel time about 7 percent too short at 75 m. At 75 m, breakthrough under transient-flow conditions using constant εb is essentially the same as breakthrough under steady-flow conditions using the same εb (dots). For this problem, if εb is not updated in time, the transport simulation is essentially unaffected by flow transients. Because this problem is one-dimensional, and a flux boundary condition is used, incorporating changes in transmissivity due to water-table movement does not significantly affect the solute transport solution (squares). The major effect of increasing saturated thickness on transport for this case is the change in fluid storage, not transmissivity, and this effect can be accounted for simply by updating εb in time.

SUMMARY AND CONCLUSIONS

Fluid divergence terms may be removed from the solute-transport equation to reduce numerical errors, to automatically handle sink boundary conditions, and to remove velocity spatial derivatives. This removes the time derivative of fluid storage from the transport equation, however, it does not imply that fluid-storage terms--porosity, saturated thickness, and fluid density--remaining in the transport equation are constant during transient flow, as assumed in three widely applied numerical models.

When fluid-storage terms are held constant in the transport equation during transient flow, errors in both source and velocity calculations increase with increasing relative change in fluid storage. The source or dilution error is probably smaller than the velocity error for most cases. In water-table aquifers, changing fluid storage may have more impact on transport than changing transmissivity. For the one-dimensional numerical simulation presented, in which a fluid-flux boundary condition was used, solute transport in transient flow was essentially unaffected by incorporation of the dependence of transmissivity on head. However, ignoring changes in fluid storage resulted in about 7 percent error in solute travel time.

Fluid-storage terms in the flow-equation-removed form of the solute-transport equation must be updated in time to be consistent with the transient flow equation. This updating is quite simple, for constant storage coefficients, and should add insignificant computational burden to practical flow and transport models.

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APPENDIX

GOVERNING EQUATIONS FOR TRANSPORT IN COMPRESSIBLE-FLUID FLOW

This appendix presents a flow-equation-removed form of the solute-transport equation for the case of compressible fluid. Mass continuity for two-dimensional flow when fluid density is considered a function of pressure alone, $\rho = \rho(p)$, may be written (after Bear, 1979, p. 92):

$$\frac{\partial(\varepsilon\rho b)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon\rho b V_i) + \rho' W = 0 \quad , \qquad \text{(A.1)}$$

where $i = 1, 2$ is an index for Cartesian coordinates ($x_1 = x$, $x_2 = y$) with implied summation, ε is porosity, b is saturated thickness, V_i are velocity components, ρ' is the sink or source fluid density, and W is the withdrawal rate from the aquifer ($W<0$ for sources). The first term in (A.1) is the time rate of change of fluid mass per unit area of aquifer. If density, porosity, and thickness are all assumed to be constant, then flow in the aquifer is in steady-state equilibrium with imposed boundary conditions.

A mass-concentration form of the solute-transport equation, useful for aquifers having variable fluid density, can be written (after Bear, 1979, p. 241):

$$\frac{\partial(\varepsilon\rho bc)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon\rho bcV_i) - \frac{\partial}{\partial x_i}\left(\varepsilon\rho bD_{ij}\frac{\partial c}{\partial x_j}\right) + \rho' c' W = 0 \quad , \qquad \text{(A.2)}$$

where $j = 1, 2$, c is the mass of solute per unit mass of fluid, c' is the concentration of the sink or source, and ρ' is the fluid density of the sink or source. For sinks it is often assumed that $c'=c$ and $\rho'=\rho$. The accumulation term in (A.2) can be expanded:

$$\frac{\partial(\varepsilon\rho bc)}{\partial t} = \varepsilon\rho b\frac{\partial c}{\partial t} + c\frac{\partial(\varepsilon\rho b)}{\partial t} \quad . \qquad \text{(A.3)}$$

Substituting (A.3) into (A.2), similarly expanding the advective term, adding ($\rho' cW-\rho' cW$), and rearranging yields:

$$\varepsilon\rho b\frac{\partial c}{\partial t} + \varepsilon\rho b V_i\frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\varepsilon\rho b D_{ij}\frac{\partial c}{\partial x_j}\right) + \rho'(c'-c)W$$
$$+ c\left[\frac{\partial(\varepsilon\rho b)}{\partial t} + \frac{\partial}{\partial x_i}(\varepsilon\rho b V_i) + \rho' W\right] = 0 \quad . \qquad \text{(A.4)}$$

But, from flow continuity, (A.1), the last bracketed term is zero, leaving:

$$\varepsilon\rho b\frac{\partial c}{\partial t} + \varepsilon\rho b V_i\frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\varepsilon\rho b D_{ij}\frac{\partial c}{\partial x_j}\right) + \rho'(c'-c)W = 0 \quad . \qquad \text{(A.5)}$$

The product of porosity, fluid density, and saturated thickness in (A.5) is not constant in time unless the aquifer is considered to have no fluid storage capacity such that the flow field responds instantly to changing boundary conditions.

For the case of constant and uniform saturated thickness, (A.5) becomes (Voss, 1984, p. 59):

$$\varepsilon\rho\frac{\partial c}{\partial t} + \varepsilon\rho V_i\frac{\partial c}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\varepsilon\rho D_{ij}\frac{\partial c}{\partial x_j}\right) + \frac{\rho'(c'-c)W}{b} = 0 \quad . \qquad \text{(A.6)}$$

In the model of Voss (1984, p. 24), fluid mass storage is related to pressure by:

$$\frac{\partial(\varepsilon\rho)}{\partial t} = \rho_0 S_{op}\frac{\partial p}{\partial t} \quad , \qquad \text{(A.7)}$$

where S_{op} is the specific pressure storativity and ρ_0 is the initial fluid density. However, the product $\varepsilon\rho$ is held constant in the solute-transport equation (A.6) in the model. Because both S_{op} and ρ_0 are constant, the product of porosity and fluid density is given, as a function of pressure, by a simple linear relation:

$$\varepsilon\rho = (\varepsilon\rho)_0 + \rho_0 S_{op}[p - p_0] \quad , \qquad \text{(A.8)}$$

where subscript 0 designates the initial condition.

As shown in the body of this paper for the analogous case of constant density but changing thickness, holding fluid-storage terms constant in the solute-transport equation (A.6), as in the model of Voss (1984), leads to errors in velocity and source-term calculations. The magnitudes of these errors depend on the relative change in fluid mass storage.