DENSITY-INDUCED DOWNWARD MOVEMENT OF SOLUTES DURING A NATURAL-GRADIENT TRACER TEST, CAPE COD, MASSACHUSETTS

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ABSTRACT

Density contrasts can cause a plume of contaminated ground water to sink within an ambient flow field. Earlier studies had hypothesized that the downward movement of a bromide tracer cloud during the early part of a natural-gradient tracer test on Cape Cod, Massachusetts, was caused by density-induced sinking. Two analytical models of density-dependent flow were applied to the Cape Cod test to show that the density contrast between the ambient ground water and the tracer solution was sufficient to cause at least part of the observed sinking. The analytical models also illustrate that the amount of sinking depends on the anisotropy of hydraulic conductivity. A comparison of two- and three-dimensional analytical models for density-induced sinking indicates that downward movement predicted by the two-dimensional model is less than the downward movement predicted by the three-dimensional model of this fundamentally three-dimensional process. A numerical solute-transport model was used to show that downward movement increases with decreasing dispersion and increasing source size because both conditions serve to enhance the persistence of high concentrations in the solute cloud. The sensitivity to dispersion and the need to represent the system in three dimensions present computational difficulties for numerical simulations of density-dependent flow and solute transport.

INTRODUCTION

Vertical movement of contaminants in ground water can occur even in shallow, unconfined aquifers in which most ground water flows laterally. The movement of contaminant plumes downward because of areal recharge has been reported in several studies (Kimmel and Braids, 1980; MacFarlane and others, 1983; LeBlanc, 1984; Ryan and Kipp, 1985). The density of a contaminant plume also may cause its downward movement, even in cases where solute concentrations are well below those associated with the widely studied saltwater-intrusion problem. Kimmel and Braids (1980) suggested that dense leachate from landfills on Long Island was moving downward through ambient, uncontaminated ground water. Freyberg (1986) reported that a tracer cloud moved downward during the first part of a natural-gradient tracer test at Base Borden, Ontario, and attributed the movement to the greater density of the injected tracer solution. Van Walsun (1987) attempted to simulate the density effect observed by Freyberg (1986) with a two-dimensional numerical model, but the model predicted less sinking than had been observed during the tracer test.

This paper describes the density-induced downward movement of tracers observed during a natural-gradient tracer test that was conducted on Cape Cod, Mass. (fig. 1), in 1985-88 (LeBlanc and others, 1991) and examines the factors that affect this process by using analytical and numerical simulations. This examination is still underway, so only preliminary results are reported here.

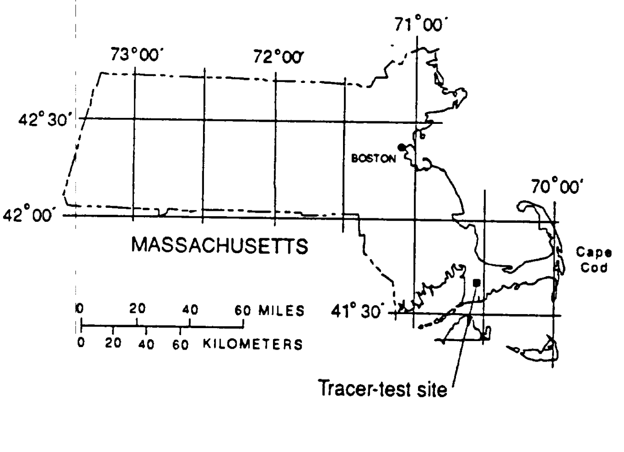

Figure 1. Location of the Cape Cod natural-gradient tracer-test site.

CAPE COD TRACER TEST

The Cape Cod natural-gradient tracer test began with the injection of 7.6 cubic meters of tracer solution into an unconfined, sand and gravel aquifer (LeBlanc and others, 1991). The solution, which was injected in three wells over a 16-hour period to approximate a pulse input, contained a nonreactive tracer, bromide, and two reactive tracers, lithium and molybdate. Movement of the tracer cloud under a natural hydraulic gradient was observed by periodic collection of water samples from a three-dimensional array of 9,840 sampling points.

The location of the center of mass of the bromide cloud was computed for each of 16 sampling rounds by the method of spatial moments (Garabedian and others, 1991). The vertical position of the center of mass (one component of the first moment) clearly showed an initial period during which the tracer cloud moved downward (fig. 2). The angle of downward movement was initially as great as 3° below the horizontal. The downward movement during the first 237 days of the test was 3.2 m (meters), which is about 70 percent of the total downward movement observed during the entire 511-day experiment.

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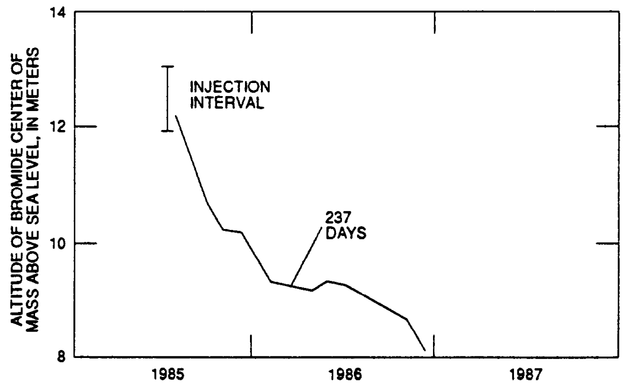

Figure 2. Vertical position of the center of mass of the bromide tracer cloud during the Cape Cod natural-gradient tracer test, 1985-87. Altitude was determined from first spatial moment in vertical direction (Garabedian and others, 1991, fig. 9).

LeBlanc and others (1991) note that vertical flow caused by accretion of areal recharge accounts for only part of the initial downward movement of the tracer cloud. Ground-water flow is nearly horizontal in the aquifer, and the estimated recharge during the first 237 days after injection was insufficient to cause all the observed drop. They hypothesized that the additional downward movement was caused by the difference in density between the ambient ground water and the tracer solution.

The densities of the tracer solution and ambient ground water could not be determined by direct measurement because too little tracer solution was saved to allow an accurate measurement of the density contrast. Therefore, LeBlanc and others (1991) used the concentrations of dissolved solids to estimate that the density of the tracer solution was 1.00089 g/cm^3 (grams per cubic centimeter), whereas the density of the ambient ground water was 1.00004 to 1.00015 g/cm^3.

MODELING DENSITY-INDUCED VERTICAL MOVEMENT

The hypothesis that density caused the tracer cloud to sink during the Cape Cod test is being examined by use of analytical and numerical mathematical models. The ultimate objective is to simulate the observed downward movement. Work thus far has focused on determination of the sensitivity of density-induced sinking to hydrologic factors affecting solute transport.

Analytical Models

Two analytical models (Hubbert, 1953; Yih, 1965) were used to evaluate the likelihood that density was a factor in causing the observed downward movement of the tracer cloud. In the method of Hubbert (1953), the hydraulic potential of the tracer fluid is calculated in terms of the hydraulic potential of the ambient, or dominant, fluid. The direction of force acting on the tracer solution can then be determined from the gradient of its potential field. Hubbert's method, originally developed to explain the migration and entrapment of petroleum in reservoir rocks, assumes that both fluids can occupy any point in the aquifer and that the fluids do not mix. The predicted angle of downward movement for the Cape Cod tracer test, if the hydraulic conductivity is assumed to be isotropic, is 28 to 31° below the horizontal (table 1). An anisotropic conductivity tensor changes the predicted angle. For a ratio of vertical to horizontal hydraulic conductivity of 0.5 (approximately that observed at the test site), the angle reduces to 14 to 16°. Anisotropy of hydraulic conductivity affects the amount of downward movement because the direction of movement in an anisotropic aquifer is biased toward the principal direction of the hydraulic-conductivity tensor.

Table 1. *Angles of downward movement of the Cape Cod bromide tracer cloud below the horizontal as predicted by the analytical models of Hubbert (1953) and Yih (1965)*

[Tracer-solution density equals 1.00089 grams per cubic centimeter; ambient horizontal ground-water velocity is 0.42 meters per day]

	Angle of downward movement (degrees below horizontal)	
Analytical model	ρ_a[1] = 1.00004	ρ_a[1] = 1.00015
Hubbert (1953)		
K_V/K_H[2]=1.0	31.3	27.9
K_V/K_H = 0.5	15.6	13.9
K_V/K_H = 0.2	3.1	2.8
Yih (1965)		
3-D sphere	9.0	7.9
2-D infinite cylinder	6.8	5.9

[1] Ambient ground-water density, in grams per cubic centimeter.
[2] Ratio of vertical to horizontal hydraulic conductivity.

The method of Yih (1965) computes the components of velocity of a three-dimensional solute body in an ambient flow field by solving the Laplace equation with appropriate continuity and pressure conditions at the boundary between the two fluids. The method assumes that the hydraulic conductivity is isotropic and that the body, although it displaces fluid as it sinks, does not deform or become diluted by dispersion. The results do not depend on the size of the solute body. For the Cape Cod tracer test, the predicted angle of downward movement of a spherical body is 8 to 9° below the horizontal. This angle is smaller than that predicted by the Hubbert (1953) method because the method of Yih (1965) accounts for energy losses associated with the displacement of ambient ground water by the sinking tracer cloud.

Reduction of the Yih (1965) solution to two dimensions (an infinitely long circular cylinder, or a circle in the two-dimensional plane) results in a predicted downward angle about 25 percent smaller than that obtained from the three-dimensional analysis (table 1). In the two-dimensional model, all displacement of water must occur parallel to the section, whereas displacement occurs in all directions in the real, three-dimensional system. Therefore, a two-dimensional model constrains movement of water to a two-dimensional plane, and the solute body cannot sink as rapidly as it would if the ambient ground water were free to move in any direction. This limitation would also apply to two-dimensional numerical models and may help explain why Van Walsun (1987) was unable to reproduce the observed downward movement of tracers during the Borden experiment with a two-dimensional model without using a large density contrast and a large ambient vertical hydraulic gradient.

During the Cape Cod tracer test, the density contrast between the ambient ground water and the tracer cloud decreased as the tracer cloud was diluted by dispersion (LeBlanc and others, 1991, table 3). The decreasing density would be expected to cause a gradual decrease of the angle of downward movement, which, in turn, would result in a parabolic trajectory of the center of mass similar to that observed during the test (fig. 2). Because this gradual decrease in density is not accounted for in the models of Hubbert (1953) and Yih (1965), these models tend to predict a greater rate of sinking than would be predicted in models that include the effect of dispersion.

Numerical Model

The results obtained from the analytical models were extended by using numerical simulations to examine density-induced sinking when solute concentrations and density are allowed to decrease because of dispersion. SUTRA (Voss, 1984), a two-dimensional finite-element model that simulates solute tranport and dispersion in a density-dependent flow field, was used for these simulations. The numerical simulations described below used a rectangular grid and assumed that solute concentration and density were linearly related. Also, the dispersivity components were assumed to be independent of the direction of flow (Voss, 1984, p. 48-50).

Description of Simulations

For the simulations reported here, SUTRA was used to simulate a transport problem similar to the Cape Cod tracer test. This simplification was acceptable because the purpose of these preliminary simulations was to examine the factors that affect density-induced sinking, not to match the sinking observed during the Cape Cod test. Accurate simulations of the field test are the goal of the next phase of work.

The grid, a two-dimensional vertical section, encompassed an area 2.5 m high and 15 m long. This area was subdivided into 3,750 elements. Because longitudinal and transverse dispersivities as small as 0.05 and 0.005 m, respectively, were used in the models, each element was only 0.2 m long and 0.05 m high. With this fine grid spacing, the Peclet number was less than 4 and the transverse spacing was less than 10 times the transverse dispersivity (Voss, 1984, p. 232-233).

Aquifer characteristics were similar to those reported for the Cape Cod tracer-test site (LeBlanc and others, 1991). An ambient, steady, horizontal velocity of 0.45 m/d (meters per day) was established by specifying a hydraulic conductivity of 120 m/d, a porosity of 0.39, and appropriate pressures along the left and right boundaries of the model. Hydraulic conductivity was assumed to be isotropic, although planned work will include simulations in which it will be anisotropic. The top and bottom of the model were specified as zero-flux boundaries.

Most simulations began with the instantaneous release of a solute cloud that covered an area 0.5 m high and 2.0 m long (fig. 3). The solute cloud was simulated for 10 days (40 time steps). A small time step of 0.25 days was needed to minimize numerical dispersion (Voss, 1984, p. 234). Each simulation took about 3 hours of CPU time on a PR1ME[3] 9955 computer.

The movement of the simulated tracer cloud was displayed by means of contoured plots of calculated concentrations generated using a plotting program developed by Souza (1987). Spatial moments of the simulated concentration distributions were calculated by numerical integration of concentrations using bilinear interpolation across the model elements.

Simulated Movement of the Tracer Cloud

The simulated tracer cloud moved downward because of the density difference between the ambient ground water and the tracer solution. A series of simulations confirmed that the downward component of movement is sensitive to the initial density difference. This downward movement is evident in the results of a typical simulation shown in figure 3. For this simulation, a large initial source concentration was used to increase the density-induced sinking; the initial tracer-cloud density was about four times greater than that in the actual tracer test. The tracer cloud develops a saddle shape as the cloud disperses while being tranported (fig. 3). This shape develops because the center of the cloud, where concentrations are highest and the downward forces caused by density are strongest, moves downward more rapidly than do the edges of the cloud, where concentrations are diluted by dispersion and the downward forces are weaker.

The downward movement also affects directions of flow in the ambient fluid as it is displaced by the sinking tracer cloud. Although the largest downward component of flow coincided with the highest concentration and greatest density in the tracer cloud, the largest upward component of flow was immediately behind and above the cloud where ambient water moves to fill the area left by the downward moving cloud. As the initial density contrast is increased, the disturbance of the velocity field increases and the saddle shape of the cloud becomes more pronounced.

The downward component is also very sensitive to the rate at which concentrations in the cloud are diluted by dispersion. Even a small amount of dispersion can quickly decrease maximum concentrations and limit the amount of vertical movement. This effect is shown in figure 4 for a set of simulations in which source size and initial densities of the ambient fluid and tracer solution (equal to those of the Cape Cod test) were held constant, but the longitudinal

[3]The use of brand names in this paper is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

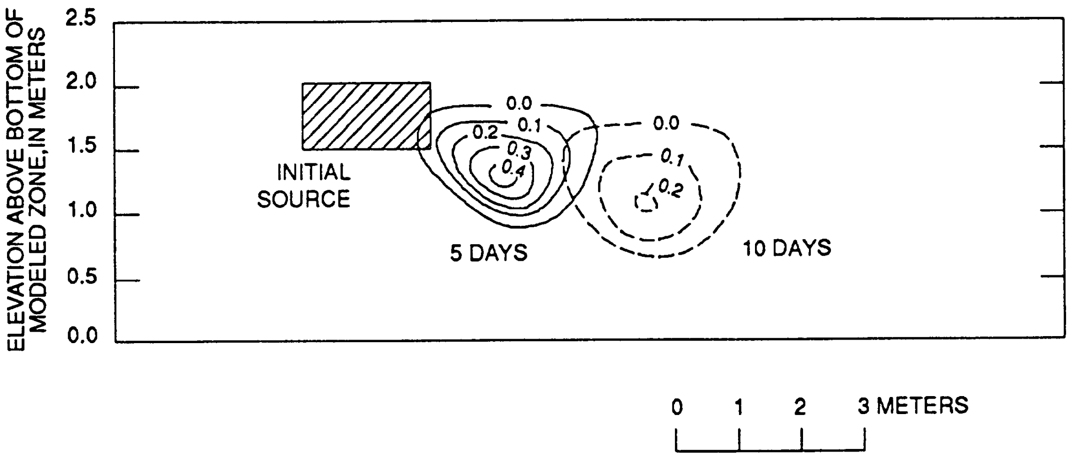

Figure 3. Vertical section showing simulated position of tracer cloud at 5 and 10 days after start of simulation. Contour interval 0.1 relative concentration (ratio of simulated to initial concentration). Longtitudinal and transverse dispersivities are 0.11 and 0.005 meters, respectively.

dispersivity was varied from 0.11 to 1.01 m. The effects of dispersion are also related to source size. High concentrations persist longer in large clouds than in small clouds, so the centers of mass of large clouds tend to sink more than those of small clouds of the same initial density.

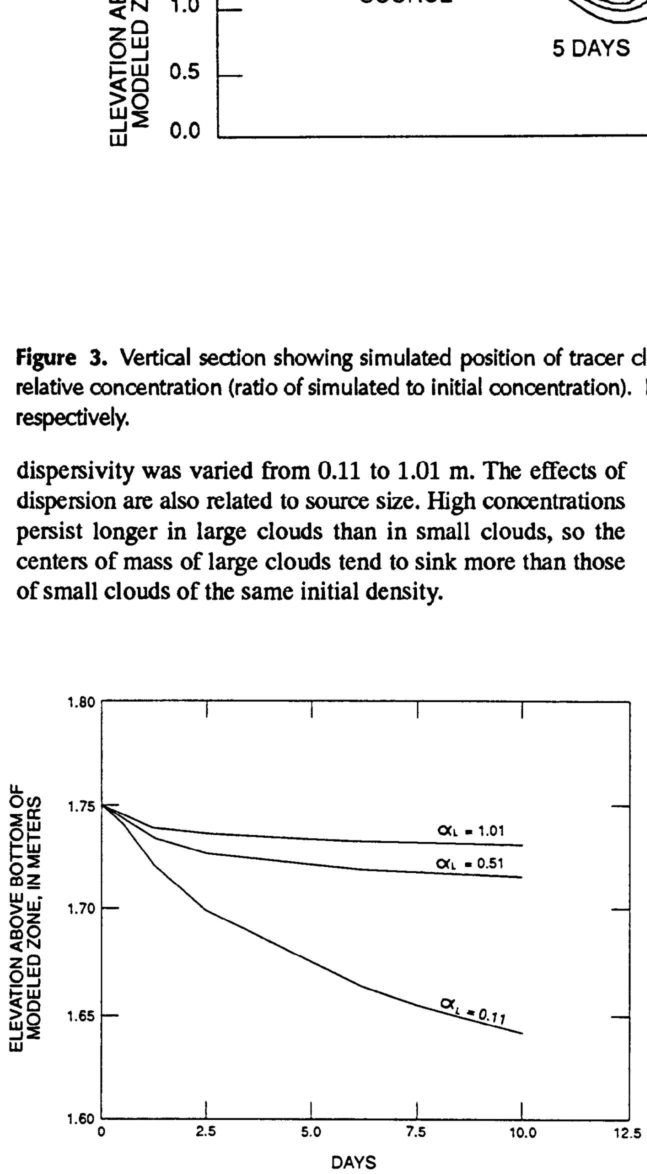

Figure 4. Vertical position of the center of mass of the simulated tracer cloud during a 10-day-long period for longitudinal dispersivities of 0.11, 0.51, and 1.01 meters. Transverse dispersivity was 0.005 meters.

DISCUSSION

The analytical models of Hubbert (1953) and Yih (1965) were used to show that the density difference between the ambient ground water and the tracer solution for the Cape Cod test was sufficient to cause part of the observed downward movement of the tracer cloud. However, their usefulness in predicting the amount of sinking is limited because neither approach accounts for the critical effect of dispersion.

The numerical modeling clearly indicates that dispersion and source size greatly affect density-induced sinking. Field experiments (Freyberg, 1986; Garabedian and others, 1991) and stochastic transport theory (Dagan, 1984) indicate that field-scale dispersion is initially very small but increases to an asymptotic limit as the solute cloud travels through the heterogeneous aquifer. The numerical simulations suggest that this initially small dispersivity limits dilution that would otherwise rapidly diminish the density-induced downward movement. The consequence is that numerical models must use very small initial dispersivities to simulate density-induced sinking accurately. Van Walsun (1987) reported that the trajectory of the Borden tracer cloud was best simulated in a two-dimensional model when a very small initial dispersivity was used that increased with time. This requirement greatly increases the number of grid cells needed near the source. Accurate modeling may also require simulation of three-dimensional flow. Both requirements add significantly to the computational effort.

SUMMARY

Downward movement of the center of mass of the solute cloud was observed during the first 237 days of the Cape Cod tracer test. Earlier studies had hypothesized that this sinking was caused in part by the density difference between the ambient ground water and the injected tracer solution.

Two analytical models of density-dependent flow were used to demonstrate that the density contrast during the Cape Cod test was sufficient to cause part of the observed sinking. Application of the Hubbert model showed that the extent of sinking depends on the anisotropy of hydraulic conductivity, whereas application of the Yih model showed that the tendency to move downward is balanced, in part, by the displacement of water around the sinking tracer cloud. The Yih model also suggested that less sinking is predicted in two-dimensional models than in three-dimensional models of this fundamentally three-dimensional process.

The SUTRA numerical model was used to illustrate that the amount of downward movement is related to dispersion and source size because both factors affect the persistence of high concentrations in the center of the solute cloud. The sensitivity to dispersion and the need to represent the system three-dimensionally present computational challenges when simulating this type of process with numerical models.

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