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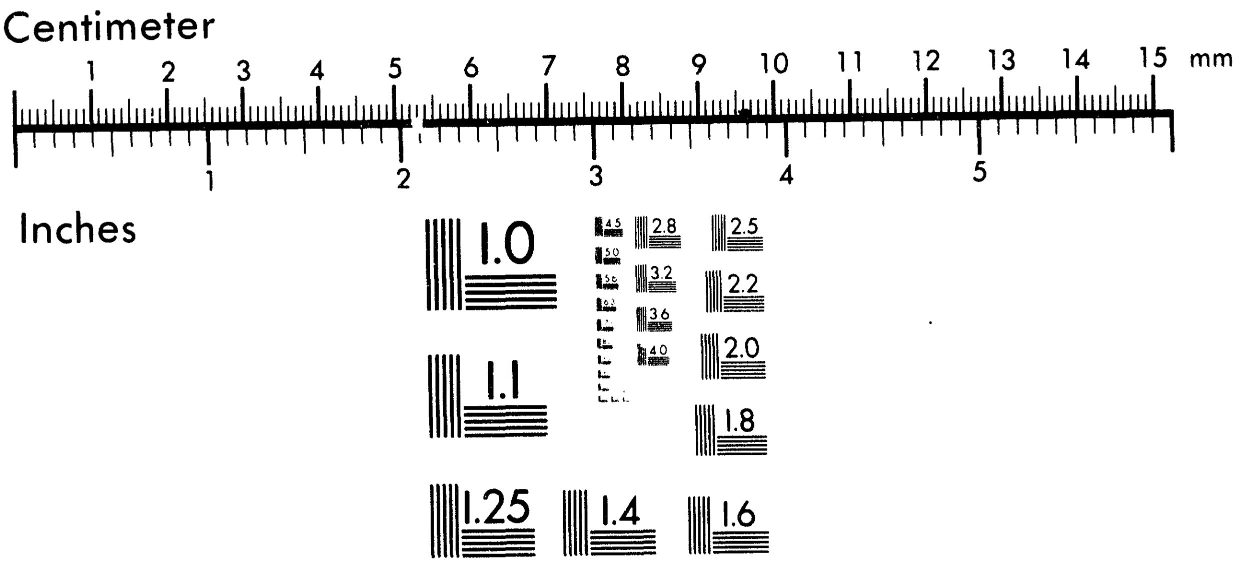

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Simulation of Two- and Three-Dimensional Dense Solute Plume Behavior with the METROPOL-3 Code

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ABSTRACT

Contaminant plumes emanating from waste disposal facilities are often denser than the ambient groundwater. These so-called dense plumes sink deeper into phreatic aquifers and may, under certain conditions, become unstable. The behavior of variable density, aqueous-phase contaminant plumes in saturated, homogeneous 2-D and 3-D intermediate-scale aquifer models was investigated with the finite element code METROPOL-3. The numerical results compare, in a quantitative sense, to previously reported laboratory-scale transport experiments. The simulations show that dense plumes are more likely to penetrate deeper into aquifers and eventually become unstable with increasing density differences between the leachate solution and the ambient groundwater, and other important parameters as the saturated hydraulic conductivity of the porous medium, leakage rate of the contaminant solution, and source width. The significance of unstable behavior decreases with increasing dispersivity values. It was observed that 3-D flow patterns have a stabilizing effect on dense contaminant plume behavior.

INTRODUCTION

Many contaminant plumes originating from waste disposal facilities are denser than the ambient groundwater in natural aquifers (Freeze and Cherry, 1979). When density differences are significant, solute transport is not only a result of forced (hydraulically driven) advection and dispersion/diffusion but also of free convection. Studies reviewed by Gebhart et al. (1988) showed that, when a dense liquid overlies a less dense liquid, density gradients can introduce gravitational instabilities, giving rise to free convective transport. Such instabilities lead to enhanced mixing and dilution of contaminants. As a result of instabilities, dense contaminant plumes tend to contaminate larger areas of aquifers. Behavior of dense contaminant plumes has not been studied in great detail, and knowledge of variable density plume behavior remains incomplete. Published results of field studies are scarce (Kimmel and Braids, 1980), while only a few related laboratory studies have been reported (List, 1965; Paschke and Hoopes, 1984; Schincariol and Schwartz, 1990; Oostrom et al., 1992a,b; Hayworth, 1993). Oostrom et al. (1992a,b) studied dense plume behavior in relatively narrow flow containers by means of flow visualization and detailed salt

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concentration measurements with a dual-energy gamma radiation technique. They found that, for a given porous medium, dense plumes were either stable or unstable depending on magnitude of the horizontal flow velocity, the contaminant leakage rate, and the difference between the contaminant solution and the ambient groundwater. Hayworth (1993) performed similar experiments in wider flow containers and observed the source configuration also has a distinct effect on plume behavior. He noted that the likelihood of the occurrence of instabilities increased when the contaminant solution entered the flow container from a line source instead of a point source.

The objective of this paper is to present initial attempts to simulate dense plume behavior in both 2-D and 3-D flow domains similar to the experimental intermediate-scale laboratory flow containers used by Oostrom et al. (1992a,b) and Hayworth (1993). The METROPOL-3 results and experimental data can only be compared in a qualitative sense since the experiments were conducted in partly saturated porous media and METROPOL-3 allows saturated conditions only. Due to the strong coupling of flow and transport equations, simulations of dense contaminant plumes are not trivial. So far, only Frind (1982) and Koch and Zhang (1992) have published simulations of 2-D variable density plumes. The density effects in the plumes generated by Frind's finite element model (1982) were masked by the relatively high values of the dispersivity values used. Koch and Zhang (1992), using the code MOCDENSE, showed that, on a regional scale, 2-D dense plumes tend to sink deeper into aquifers. Instabilities were observed when the dense leachate concentrations were larger than 9000 ppm in combination with relatively small longitudinal dispersivities.

NUMERICAL METHOD

The simulations reported in this paper were conducted with the finite element code METROPOL-3 (Sauter et al., 1993). The coupled nonlinear partial differential equations for either the 2-D or 3-D flow and transport equations are solved simultaneously for liquid pressure and salt mass fraction using an approximate finite element solution. The mass balance equations for the liquid and the dissolved solute are, respectively,

$$\frac{\partial(n\rho)}{\partial t} + \nabla\cdot(\rho q) = 0 \tag{1}$$

$$\frac{\partial(n\rho\omega)}{\partial t} + \nabla\cdot(\rho q\omega) + \nabla\cdot J = 0 \tag{2}$$

where n is the porosity, ρ is the liquid density (ML^{-3}), q is the Darcy velocity (LT^{-1}), ω is the salt mass fraction, and J is the hydrodynamic dispersive flux ($MT^{-1}L^{-2}$). The Darcy velocity is written as

$$q = -\frac{k}{\mu}\cdot(\nabla p - \rho g) \tag{3}$$

where k is the intrinsic permeability tensor (L^2), μ is the fluid viscosity ($ML^{-1}T^{-1}$), p is the fluid pressure ($MT^{-1}L^{-2}$), and g is the gravitational acceleration (LT^{-2}). The dispersive flux is written as

$$J = -n\rho D\cdot\nabla\omega \tag{4}$$

where D is the hydrodynamic dispersion tensor. Equations (1) and (2) are nonlinear because of the dependency of the liquid properties μ and ρ on ω. The equations are coupled through q and ρ. The equations of state for the fluid properties ρ and μ are, respectively,

$$\rho = \rho_0 \exp^{\gamma\omega + \beta(p - p_r)} \quad (5)$$

$$\mu = \mu_0 (1 + 1.85\omega - 4.1\omega^2 + 44.5\omega^3) \quad (6)$$

where ρ_0 is the reference density, p_r the reference pressure, γ is a constant (0.69), and μ_0 the reference viscosity. The system of ordinary differential equations and the resulting algebraic equations are obtained after application of the Galerkin weighted residual method. The time derivatives are approximated by first-order finite differences and a fully implicit or Euler backward timestepping scheme is used. This method has the advantage that the time step size is not restricted by stability requirements. However, since the algebraic equations are non-linear, convergence requirements limit the time step size that can be used. In the solution procedure, the time derivatives are not reduced, but rather a lumped formulation has been adopted. The sets of algebraic mass balance equations can be conveniently written in matrix form as follows

$$A_p p = b_p \quad (7)$$

$$A_\omega \omega = b_\omega \quad (8)$$

where p and ω are the vector of unknowns. The matrix A_p and vector b_p are only mildly dependent on the pressure p. When the darcy velocity q and the boundary mass fluxes do not change significantly, the matrix A_ω and vector b_ω are also only slightly affected by changes in the pressure p. However, both matrices and both vectors in Eqs. (7) and (8) are strongly dependent on the salt mass fraction. Based on these considerations, a two-step iteration scheme was developed (Leijnse, 1992). First, the salt mass fraction equation is solved with a Picard iteration scheme using estimates for the pressure and the Darcy velocity from the previous time step. After convergence, the pressure equation is solved only once. New values for the Darcy velocities are calculated from the pressure distribution. The salt mass fraction equations have to be solved again if a converged solution has not been obtained.

The matrix associated with the linearized pressure equations is symmetric and is solved by a conjugate gradient method using diagonal scaling as preconditioning (Pini and Gambolati, 1990). The matrix associated with the linearized salt mass fraction equation is non-symmetric and is solved by the Bi-CGSTAB method (Van der Vorst, 1990).

The flow domains used in the simulations are all 2 m long and 1 m high. The width values used in the 3-D simulations were 0.1, 0.5 and 1.0 m. The contaminant solutions were introduced from a source on top of the saturated porous media with a constant leachate velocity. A horizontal pressure gradient was imposed on the domain, forcing the ambient groundwater to move from the left to the right. Each simulation consisted of two parts. In the first part, a tracer solution with an initial concentration of 10^{-2} g/l was introduced in the flow domain. This concentration doesn't significantly affect the density of contaminant plumes. After a steady-state neutral tracer plume has developed, the leachate concentration was increased to the desired value while everything else was kept constant. Throughout the simulations, the grid Peclet numbers in the near source area were always smaller than 2. The maximum time step was chosen a priori and was based on the expected maximum velocity for each simulation and the grid size. The Courant numbers during the simulations were always smaller than 1.

RESULTS AND DISCUSSION

2-D plumes

The simulations show that when the density difference between the contaminant solution and the ambient groundwater is increased, the liquid density gradients in the near source area increase and the plumes sink deeper into the flow domains, and are more likely to become unstable. The nearly neutral plume is transported in the upper part of the flow domain while dense unstable plumes may eventually reach the bottom of the aquifer. Examples of this behavior are shown in Fig. 1. In Fig. 1a., a nearly neutral plume (c_0=1 g/l) is shown, while in Fig. 1b. a dense plume is shown with initial concentration, c_0=50 g/l, corresponding to a relative density difference of 3.5%.

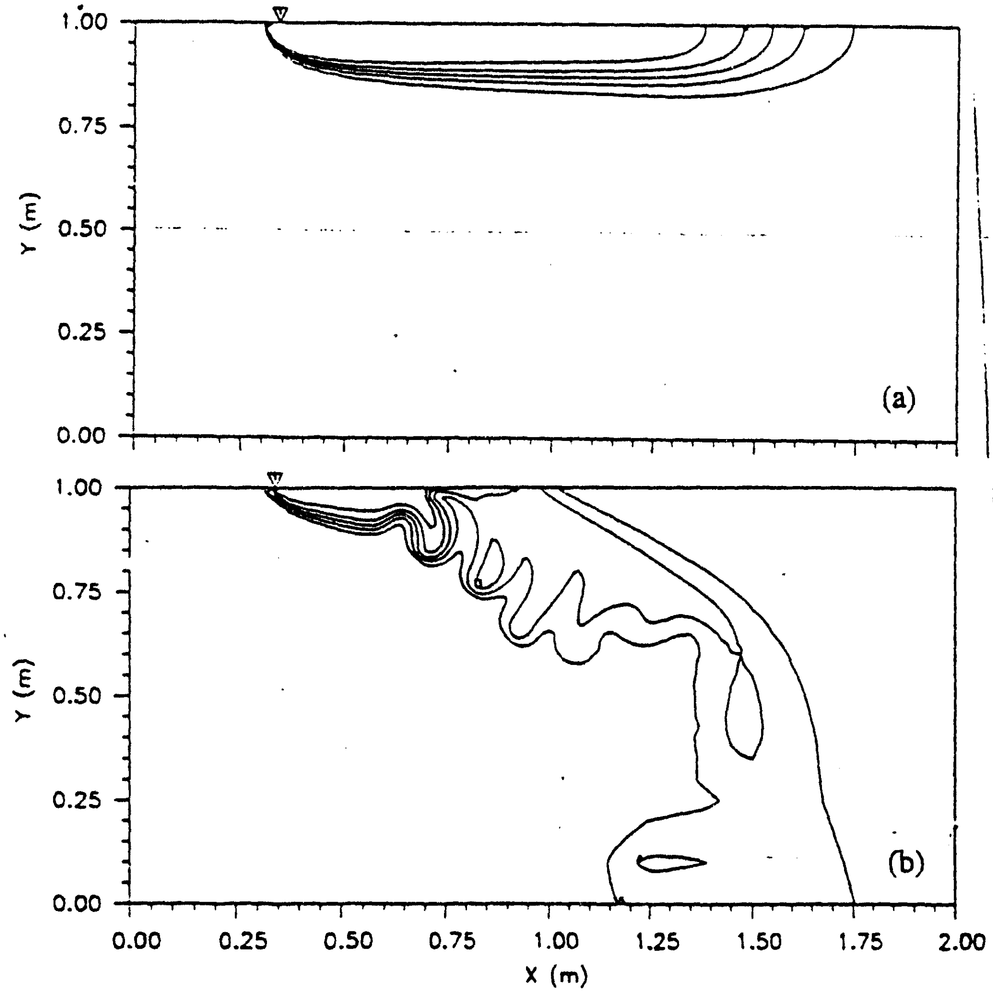


Fig. 1. Concentration contours of a) a neutral plume (c_0=1g/l), and b) a dense plume (c_0=50 g/l) after 12 hours with a horizontal Darcy velocity q_x=0.78 m/day. Shown are the 10, 30, 50, 70, and 90% contours of the c_0.

Other simulations indicated that larger Darcy velocities, as a result of higher horizontal pressure gradients, tend to stabilize dense plumes. A twofold increase in the flow rate almost completely stabilized the 50-g/l dense plume depicted in Fig. 1b, except for a small dip of the front edge of the plume (Fig. 2).

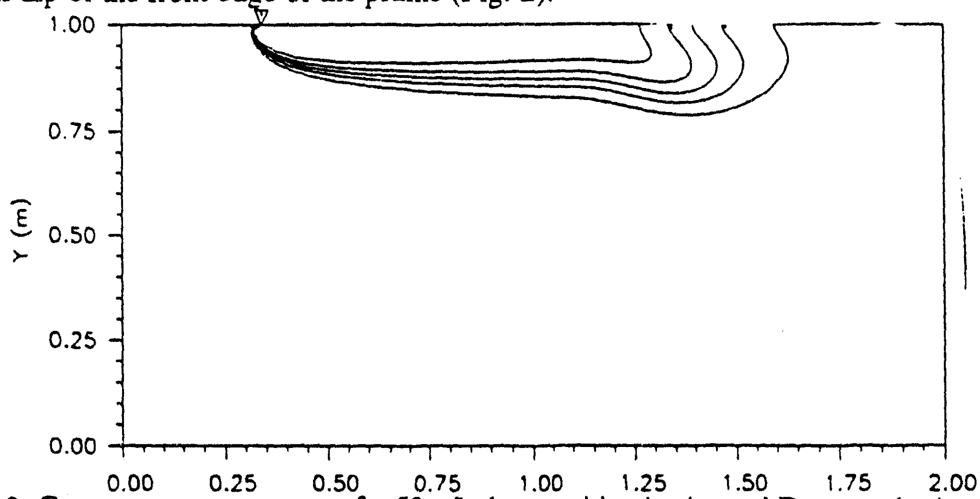


Fig. 2. Concentration contours of a 50 g/l plume with a horizontal Darcy velocity q_x=1.56 m/day. Shown are the 10, 30, 50, 70, and 90% contour of c_o.

Increases in the saturated hydraulic conductivity, while keeping the Darcy velocity constant, resulted in deeper-penetrating and generally more unstable plumes. These effects are related to near source behavior of the leaking contaminant solution. Since the leakage rates are the same in these simulations, dense plumes in media with larger conductivity values initially move faster in the vertical direction.

More mixing, realized in the simulations by using larger longitudinal or transverse dispersivity values, decreases the density gradients. Plumes with comparable density differences showed decreasing signs of unstable behavior with increasing dispersivity values.

Deeper-sinking plumes and an increased likelihood of unstable behavior when the density difference between the plume and the ambient groundwater increases or when the flow velocity in the flow domain decreases, have also been observed in the flow experiments described by Oostrom et al. (1992a,b) and Hayworth (1993).

3-D plumes

The dense plumes in the simulations emanated from either a centered point source or from line sources with various lengths. Plumes that developed from the point source did not show instabilities under conditions similar to the simulations in the 2-D flow domains. Contaminant concentrations exceeding 200 g/l were necessary to induce mild unstable patterns. These dense plumes did show, however, that plume penetration depth increases with increasing leaching rate and density difference. Relative-concentration contour lines for a plume resulting from a 100-g/l contaminant solution emanating from a point source into a 50-cm-wide flow domain are shown in Fig. 3a. This plume sinks rather deeply into the aquifer but remained stable at all times. A log-velocity plot of a y-z cross section (Fig. 3b) just downstream of the source shows water currents flowing downward below the plume and subsequently sideways and up. This circulatory flow pattern keeps the plume stable.

In contrast, a 100-g/l plume emanating from a 25-cm-wide line source showed instabilities in the longitudinal direction and also a totally different velocity profile downstream (Fig. 4a and b.) In this case, the ambient groundwater is unable to wrap around the plume to keep it from developing unstable patterns. These simulations clearly show the impact the source configuration has on dense plume behavior.

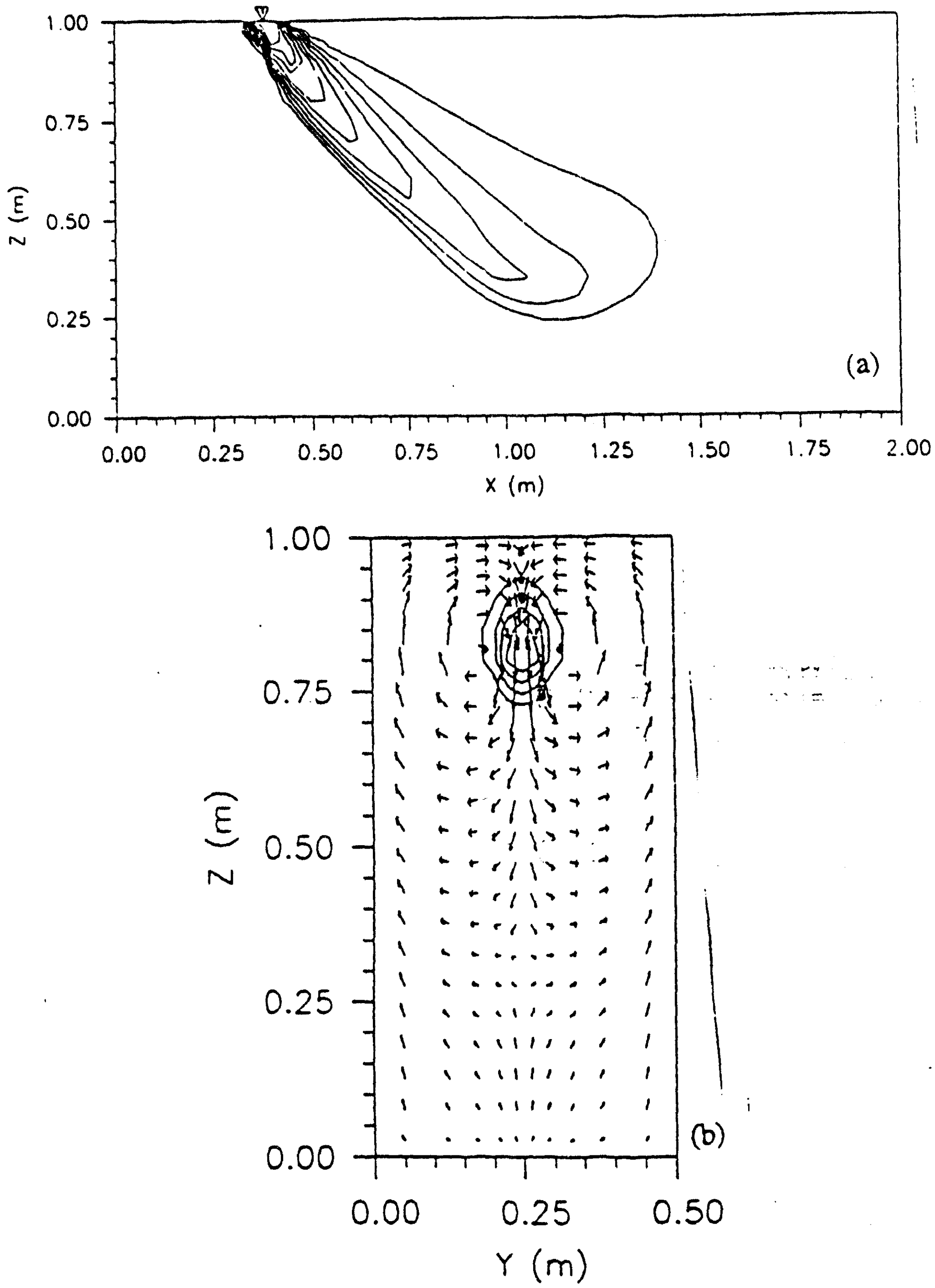
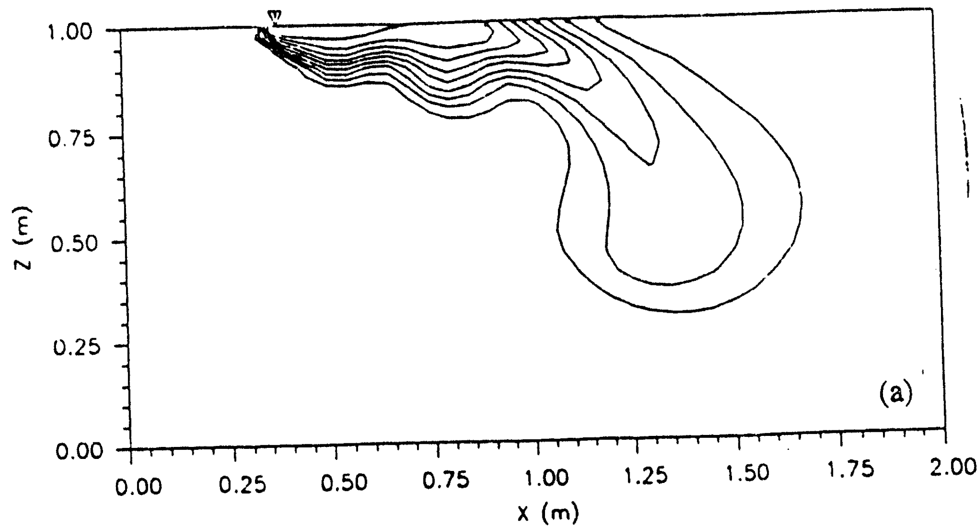


Fig. 3. a) Concentration contours, and b) log-velocity profiles at x=0.5 m of a 100-g/l plume emanating from a point source. The contours shown are the 10, 20, 30, 40, 50, 60, 70, 80, and 90% contours of c_0.



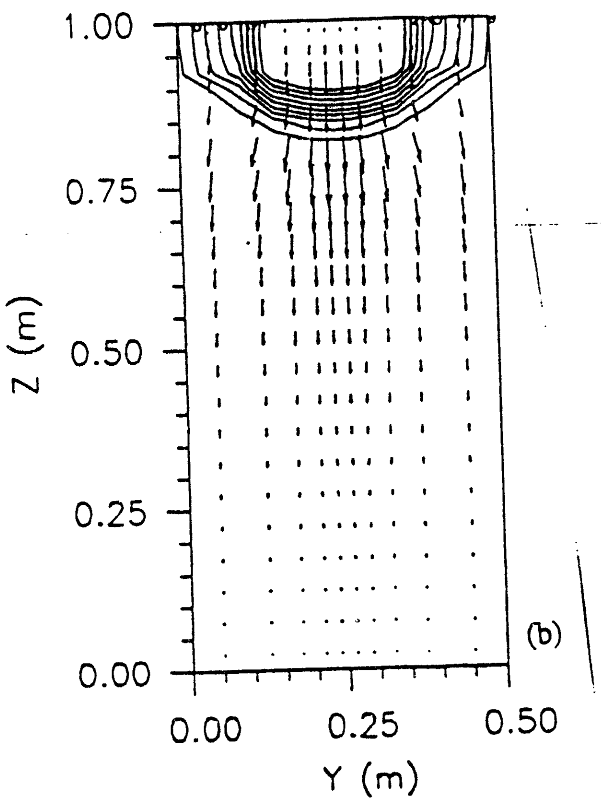


Fig. 4. a) Concentration contours, and b) velocity profiles at x=0.5 m of a 100-g/l plume emanating from a 25-cm-wide line source. The contours shown are the 10, 20, 30, 40, 50, 60, 70, 80, and 90% contours of c_o.

CONCLUSIONS

The simulations in the 2-D and 3-D flow domains support in a qualitative sense the experimental results reported by Oostrom et al. (1992a,b) and Hayworth (1993). The simulations show that dense plumes are more likely to penetrate deeper into homogeneous aquifers and eventually become unstable with increasing density difference, saturated hydraulic conductivity, leakage rate of the contaminant solution, and source width. The significance of density effects decreases with increasing longitudinal and vertical dispersivity values. Large differences are observed between plumes in 2-D and 3-D flow domains under similar conditions. In general, 3-D groundwater flow patterns have a stabilizing effect on dense contaminant plume behavior.

Dense plume experiments in fully saturated homogeneous and heterogeneous porous media are currently being conducted at Auburn University, Alabama. The results will be used to further test the METROPOL -3 code. Additional numerical simulations are planned to investigate the phenomena that initiate and develop instabilities.

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