Lawrence Berkeley National Laboratory

Recent Work

Title

Modeling the Density-Driven Movement of Liquid Wastes in Deep Sloping Aquifers

Permalink

<https://escholarship.org/uc/item/5cf476w4>

Journal

Ground Water, 29(5)

Authors

Dorgarten, H.-W.
Tsang, Chin-Fu

Publication Date

1990-08-01

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

Submitted to Ground Water

Modeling the Density-Driven Movement of Liquid Wastes in Deep Sloping Aquifers

H.-W. Dorgarten and C.-F. Tsang

August 1990

1 LOAN COPY
1 Circulates
1 for 2 weeks

Bldg. 50 Library.
Copy 2

LBL-30209

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Modeling the Density-Driven Movement of Liquid Wastes in Deep Sloping Aquifers

Hans-Wilhelm Dorgarten and Chin-Fu Tsang†*

*Hochtief AG, Technische Abteilung Tiefbau
Rellinghauser Str. 53-57, D-4300 Essen 1
Federal Republic of Germany
(Formerly with Aachen University of Technology)

†Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

August 1990

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Engineering and Geosciences Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the Office of Drinking Water, U.S. Environmental Protection Agency under EPA Interagency Agreement No. DW89931336-01. The first author was supported in part by a post-doctoral scholarship awarded by the NATO Scientific Committee through the German Academic Exchange Service, Bonn, Federal Republic of Germany.

Abstract

One method for the disposal of hazardous liquid wastes is by injection into deep aquifers. Although these aquifers may be separated from underground sources of drinking water by thick formations of low permeability, their mobility due to different migration mechanisms has to be studied carefully, since the injected wastes remain toxic over periods of thousands of years. One possible mechanism for waste movement is density-driven flow and transport, due to density differences between the waste and the surrounding water in the injection zone. In the present paper the importance of this phenomenon is studied mathematically by means of analytical and numerical calculations for typical deep injection conditions. The analytical estimates reveal that density-driven movement of liquid wastes in sloping aquifers can be much stronger than plume migration due to natural hydraulic gradients. This finding is emphasized by the results of a two-dimensional vertical finite element model, which is applied for detailed numerical simulations. Results show that during the initial stage, waste can be expected to spread into all directions due to density-induced stratification effects. Later on, it mainly moves laterally along the slope of either aquifer top or aquifer bottom, depending on the waste density. If regional ground-water flow is directed the same way, transport is accelerated. If regional ground-water flow is in the opposite direction, on the other hand, transport to both sides must be expected to occur. Thus, the aquifer slope and regional hydraulic gradient may be equally significant factors in estimating potential migration of disposed liquid wastes.

1. Introduction

Disposal of industrial wastes into deep aquifers started in the 1950s in the U.S., and has continuously increased since then (Donaldson et al., 1974; Moffett et al., 1986). It is considered as an appropriate method for isolating highly toxic material from underground sources of drinking water. Typically, injection zones are at depths of 1,000 to 2,000 m below the ground surface. Sufficient permeabilities and porosities are required to allow high injection rates under reasonable pressures. Injection zones predominantly consist of sand or sandstone formations, which are confined by layers of low permeabilities above and below. Most of the injected hazardous wastes are either acids or organics dissolved in water at average concentrations of 3 to 4 % (EPA, 1985). However, concentrations as high as 10 % or more are possible, as reported by Donaldson et al. (1974) from several case histories.

In order to protect underground sources of drinking water, especially over periods of thousands of years, the injection wells must be properly located, in addition to adhering to a proper program of construction, operation, and monitoring. The selection of suitable locations for injection wells requires the full understanding of all possible migration mechanisms. Questions have been raised about the possibility of hazardous waste migration due to their different densities in comparison to water. Such migration might derive from two effects: density stratification and subsequent horizontal spreading within an aquifer, and lateral displacement if the aquifer is sloping. Both phenomena might lead to a significant lateral movement of waste, which must be considered when selecting the injection sites. Otherwise, the waste might be transported into regions far away from the injection zone that have not been investigated for possible vertical pathways, such as abandoned wells, fracture zones, or faults.

Density-driven flow and transport phenomena have been studied and modeled intensively in the field of contaminant hydrogeology. There are many situations, where concentrations are sufficiently high to influence fluid densities, and subsequently fluid flow. Originally, numerical modeling of such phenomena mainly dealt with the problem of salt-water intrusion into coastal aquifers (e.g., Segol et al., 1975; Frind, 1982). Only recently, the importance of density-driven movement of organic

vapors in the unsaturated zone has become evident, and has been studied by many authors (Sleep and Sykes, 1989; Falta et al., 1989; Mendoza and Frind, 1990; Dorgarten and Tsang, 1990).

A general overview of modeling of deep injection systems was given by Prickett et al. (1986), who had to conclude that, up to then, very little work had been done in that field, except on a relatively simple basis. The problem of density-driven movement of injected wastes was addressed by Miller et al. (1986). Their calculations, however, were limited to the behavior during the injection phase and to horizontal formations, i.e. they did not include the influence of the aquifer slope. The objective of the present paper is to study the various phenomena related to density-driven movement of injected wastes, especially in sloping aquifers.

2. Formulation of Density-Driven Flow and Transport

Ground-water flow is described by combining the fluid continuity equation with a generalized form of Darcy's law. In the case of variable densities, the continuity equation can be formulated as (Bear, 1972)

$$\frac{\partial}{\partial t}(\rho\phi) + \frac{\partial}{\partial x_i}(\rho q_i) + \bar{\rho}Q = 0 \quad (1)$$

Here, ρ is the fluid density (kg/m^3), ϕ is the porosity of the porous medium (-), q_i is the Darcy velocity (m/s), and Q represents external sinks and sources ($\text{m}^3/\text{s}/\text{m}^3$). $\bar{\rho}$ denotes the density of the sink/source fluid, which may differ from the fluid density in the porous medium. Formulating a generalized Darcy's law in terms of fluid pressures yields

$$q_i = -\frac{k_{ij}}{\mu} \left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j} \right) \quad (2)$$

where k_{ij} is the intrinsic permeability tensor of the porous medium (m^2), μ is the dynamic viscosity ($\text{Pa}\cdot\text{s}$), p is the fluid pressure (Pa), g is the gravitational constant (m/s^2), and z is the vertical spatial coordinate (m). Inserting eq. (2) into eq. (1) results in the density-dependent ground-water flow equation

$$\frac{\partial}{\partial t}(\rho\phi) - \frac{\partial}{\partial x_i} \left[\frac{\rho k_{ij}}{\mu} \left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j} \right) \right] + \bar{\rho}Q = 0 \quad (3)$$

In this formulation, the fluid density can be a general function of pressure, temperature, solute concentrations, or any other parameter. In many ground-water problems, however, density changes over space and time are small, and only pressure dependence is taken into account by means of the fluid compressibility, if at all. In the present problem, in contrast, the density may vary significantly with the concentration, both in space and time, and this dependence cannot be neglected.

Transport of contaminants in ground water is generally described as a convective-dispersive process. The continuity formulation for the contaminant leads to the transport equation (Bear, 1972)

$$\frac{\partial}{\partial t}(R\phi C) + \frac{\partial}{\partial x_i}(q_i C) - \frac{\partial}{\partial x_i}\left(\phi D_{ij} \frac{\partial C}{\partial x_j}\right) + Q\tilde{C} = 0 \quad (4)$$

where C is the contaminant concentration (kg/m^3), D_{ij} is the tensor of hydrodynamic dispersion (m^2/s), and R is the retardation factor ($-$) that accounts for adsorption of contaminants to the soil surface. D_{ij} covers both mechanical dispersion and molecular diffusion. Mechanical dispersion is represented by the conventional approach as defined by Scheidegger (1961), depending on the ground-water flow velocity $v_i = q_i/\phi$ (m/s), and molecular diffusion is represented by the tortuosity concept as defined by Millington (1959). The tensor of hydrodynamic dispersion is then given by

$$D_{ij} = \delta_{ij}\alpha_t|v| + (\alpha_l - \alpha_t)\frac{v_i v_j}{|v|} + \delta_{ij}\phi^{1/3}D_0 \quad (5)$$

where α_l and α_t are longitudinal and transversal dispersivities (m), D_0 is the molecular diffusivity in water (m^2/s), and δ_{ij} is the Kronecker delta symbol ($\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$).

The ground-water flow equation (3) and the contaminant transport equation (4) are coupled by a constitutive relationship that defines the fluid density as a function of the contaminant concentration. If other dependences are small in comparison to the influence of the concentration, the fluid density can be formulated as

$$\rho(C) = \rho_o + \gamma C \quad (6)$$

where ρ_o is the ambient density at zero concentration, and the dimensionless factor γ is equal to the partial derivative $\partial\rho/\partial C$.

In deep formations, as they are studied here, the fluid density is influenced not only by the concentrations, but also by some other parameters. Increasing pressures and increasing salinities cause a density increase with depth, while increasing temperatures cause a density decrease with depth. The relative importance of these effects has been investigated by Oberlander (1989), who also discussed their impact on fluid potentials. Within the present problem, the influence of these parameters can be represented by the ambient density ρ_o , unless they change significantly within the injection zone.

3. Analytical Estimation of Density-Driven Movement in Sloping Aquifers

Density variations within fluids result in natural convection. If a fluid of density ρ can freely move in an ambient fluid of a different density ρ_o , it flows vertically unless the flow is prevented by a confining layer. If this confining layer is sloping, the fluid flows along this impervious boundary, and its Darcy velocity can be calculated as the component of eq. (2) along the slope

$$q_\ell = -\frac{k}{\mu} \left(\frac{\partial p}{\partial \ell} + \rho g \frac{\partial z}{\partial \ell} \right) \quad (7)$$

where ℓ is the spatial coordinate along the slope (m), and k is the component of the permeability tensor in ℓ direction. Eq. (7) can be modified by introducing the fluid head ψ (m) instead of the fluid pressure

$$\psi = \frac{p}{\rho_o g} + z \quad (8)$$

and the hydraulic conductivity K (m/s) instead of the permeability

$$K = \frac{\rho_o g k}{\mu} \quad (9)$$

In addition, the slope can be expressed in terms of the angle φ , with $\sin \varphi = \partial z / \partial \ell$. Then, one obtains the Darcy velocity along the slope as

$$q_\ell = -K \left[\frac{\partial \psi}{\partial \ell} + \left(\frac{\rho}{\rho_o} - 1 \right) \sin \varphi \right] \quad (10)$$

This formulation of Darcy's law allows the comparison of the convective transport due to regional ground-water flow and due to density-driven flow in a sloping aquifer, respectively. The relative importance of the sloping effect for lateral movement of liquid wastes in deep aquifers can be estimated by the ratio

$$\left(\frac{\rho}{\rho_o} - 1\right) \sin \varphi / \frac{\partial \psi}{\partial \ell} \quad (11)$$

Figure 1 gives this ratio as a function of the slope and the hydraulic gradient for density differences of 2 %, 5 %, and 10 %. Results indicate that even for a relatively high natural hydraulic gradient of 10^{-3} and for an aquifer slope of only one degree, density-driven flow can be stronger than regional ground-water flow. As hazardous wastes are mostly injected into aquifers with very slow regional ground-water flow, natural hydraulic gradients will generally be much smaller than 10^{-3} . Thus, lateral transport of liquid wastes due to density-driven flow can be expected to be much stronger than migration due to regional ground-water flow, even with small aquifer slopes.

Additionally, eq. (10) can be used to estimate the convective transport distance L (m) that results both from regional and from density-driven ground-water flow

$$L = \frac{q\ell T}{R\phi} = -\frac{KT}{R\phi} \left[\frac{\partial \psi}{\partial \ell} + \left(\frac{\rho}{\rho_o} - 1\right) \sin \varphi \right] \quad (12)$$

where T is the time interval (s). This equation has been applied to calculate the convective transport distance due to density-driven flow in a sloping aquifer over a period of 10,000 years. Figure 2 shows the results for a zero natural gradient as a function of aquifer slope and the ratio $K/R\phi$, again for density differences of 2 %, 5 %, and 10 %. For typical injection zone parameters, the convective transport distance can be as large as kilometers or even tens of kilometers. While restrictions on the injection pressures do not allow injection into aquifers with small permeabilities, these results indicate that very large permeabilities are also not acceptable for the injection of hazardous liquid wastes, unless density-driven migration is hindered by a favorable structure of the geological formation.

It should be noted that the previous analytical estimates are limited to the post-closure phase when regional ground-water flow depends on the natural hydraulic gradient, which generally is very

small. They do not cover waste movement during the injection phase when in the near-field flow is dominated by the injection itself and gradients may be higher than those used in Figure 1. In the numerical calculations, in contrast, waste movement in both periods will be taken into account and discussed.

4. Numerical Analysis

After the analytical estimates demonstrated that density-driven movement of liquid wastes in sloping aquifers can be important, more detailed numerical studies were performed. They account for several additional phenomena that were neglected in the analytical considerations, namely the effects of density stratification, multidimensionality, anisotropy, and dispersive and diffusive transport, on the plume behavior during and after waste injection. Additionally, the numerical calculations are capable of handling heterogeneities and irregular geometries.

A two-dimensional vertical finite element model was used for the simulations. It should be mentioned that two-dimensional models tend to overestimate density-induced movement slightly, since spreading of waste in the third dimension is neglected. As the scope of the present paper is to analyze and compare the significance of certain phenomena, this model effect is acceptable within this theoretical study. For the simulation of real injection sites, however, a fully three-dimensional model should be preferred. The present model is based on a recently developed multiphase flow and transport code (Dorgarten and Tsang, 1990), which was reduced for the single-phase problem formulated in Section 2. Since numerical simulation of single-phase, density-dependent flow and transport is considered to be standard, we omit the discussion of further details of the code.

A typical deep injection system was chosen for the numerical studies. The modeled aquifer lies in a medium depth of 1500 m and has a thickness of 100 m; its slope was chosen to be 5 %, i.e. the angle φ is about 2.86° . The geometry of the system is shown in Figure 3, together with the finite element mesh that was used for the simulations. The parameters that were selected to specify the problem are listed in Table 1. Most of them represent typical values according to the

case histories reported by Donaldson et al. (1974), especially the soil parameters. The regional hydraulic gradient and the waste density were varied during the simulations, in order to study their effect on the waste movement.

The injection well was assumed to penetrate the upper half of the aquifer, where the liquid waste was assumed to be disposed over a period of 20 years. Other boundary conditions of the flow field are hydrostatic pressures at the left and the right boundary, and zero flux along aquifer top and aquifer bottom. For the concentration field, zero dispersive flux is prescribed along all outer boundaries.

4.1 Base Case

The base case was designed to examine the different flow and transport phenomena that take place during and after waste injection. During the injection period flow and transport are predominantly controlled by the injection itself, while density effects are insignificant. The injected fluid is pushed nearly symmetrical to both sides, as indicated by the Darcy velocities in Figure 4a. Additional flow components are directed vertically downwards, because the injection well penetrates the aquifer only partially. According to these flow conditions, convective-dispersive transport of the waste results in the concentration distribution shown in Figure 4b at the end of the injection period. (It should be noted that all concentrations are plotted upon the horizontal mapping of the model area, due to the limited capabilities of the contouring program.)

As long as the regional hydraulic gradient is negligible, density-driven flow is the only mechanism that induces further ground-water motion after the injection has stopped. Therefore, the fluids tend to stratify according to their different densities. The heavier waste plume moves downwards in the injection zone, while the lighter surrounding water is pushed outwards and upwards, as shown by the Darcy velocities after 100 years (Figure 5a). This results in typical natural convection cells, which induce lateral spreading of the injected waste along the bottom of the aquifer (Figure 5b). The Darcy velocities as well as the concentration distribution clearly demonstrate

that the lateral spreading goes in both directions, i.e. not only downslope but also upslope. This symmetry indicates that the stratification effect dominates over the sloping effect in this early stage of density-driven flow.

With increasing time, the waste gets more and more stratified along the aquifer bottom. Therefore, the driving force for further density stratification decreases, and the relative importance of the sloping effect increases. This is demonstrated by the simulation results at 1000 years (Figure 6). Now the downslope natural convection cell is both larger and stronger than the upslope one (Figure 6a). According to this asymmetry of the velocity field, the plume has moved about 100 m farther downslope than upslope (Figure 6b). This asymmetry will further increase when the waste is further stratified along the aquifer bottom. Then the sloping effect remains as the only driving force that results in a continuous downslope movement of the plume.

4.2 Effect of Density Differences

The essential impact of the waste's density on its movement in sloping aquifers is shown by Figure 7, where Figure 7c represents the base case. If the density difference is negative, i.e. the injected fluid is lighter than the ambient ground water, the waste moves upslope along the aquifer top (Figure 7a). Since the waste is injected into the upper part of the aquifer, the fluids are already arranged according to their densities, and the stratification effect in this case is weaker than in the base case. Therefore, the lateral movement along the slope starts earlier, and the asymmetry after 1000 years is even stronger than in the base case. If the injected waste has the same density as the ambient ground water, there is neither convective nor dispersive transport after the injection has stopped. Molecular diffusion remains as the only transport mechanism, and the plume spreads only insignificantly (Figure 7b).

Apparently, the case with waste lighter than water is the most serious one in regard to the risk of an upward movement of liquid waste into underground sources of drinking water. The lower density of the waste relative to the surrounding water results in an upward buoyancy force with the

result that the waste plume is in contact with a significant area of the overlying formation. Now in addition, if the sloping effect results in a significant lateral movement of the waste plume, the region of potential vertical migration increases. Therefore, the potential vertical pathways in the overlying formation should be studied thoroughly especially if light liquid wastes are to be injected.

4.3 Effect of Regional Ground-Water Flow

The impact of regional ground-water flow on waste movement in sloping aquifers was determined with hydraulic gradients of $5 \cdot 10^{-4}$. In conjunction with the other parameters, this corresponds to a retarded, convective transport velocity of about 0.05 m per year. Flow was considered in the same and in the opposite direction of the slope, respectively, and compared to the base case without regional ground-water flow. Figure 8 shows the effect on the predicted waste concentrations after 1000 years, where Figure 8b represents the base case.

If the regional ground-water flow is directed downslope, this accelerates transport of the waste plume in that direction (Figure 8a). The difference with the base case in Figure 8b is mainly a horizontal shift of about 50 m, which corresponds to the retarded transport velocity mentioned above. The plume, however, spreads a little more because the higher velocities cause a stronger dispersion. Obviously, this case with the same transport direction from both effects is relevant when the largest transport distances are to be determined.

In the case of upslope ground-water flow, the results are more complicated. During the initial stage and even after 1000 years, transport upwards along the slope is stronger than downwards (Figure 8c), since the upslope migration derives both from regional ground-water flow and from density stratification. But when the stratification effect diminishes, the sloping effect proves to be stronger than transport by regional ground-water flow. Then migration downslope starts to dominate, as demonstrated by the results after a simulation period of 2000 years (Figure 9).

The plot of the Darcy velocities (Figure 9a) helps to explain the transport mechanisms at this later stage: a flat natural convection cell in the lower part of the aquifer causes transport downwards

along the slope, while the regional ground-water flow causes transport to the opposite side at the same time. Due to these mechanisms, the waste is continuously transported in both directions, which results in the concentrations shown in Figure 9b. This case with different transport directions from both effects must be considered as most uncertain, since waste migration to both sides must be expected to occur simultaneously. Apparently, the two effects do not neutralize each other, but work separately. In a natural, homogeneous aquifer with irregular slopes, this will lead to even more complicated and less predictable transport mechanisms than in the homogeneous aquifer simulated here.

4.4 Comparison of the Numerical Results with the Analytical Estimates

Since the final case with regional ground-water flow in the upslope direction combines all studied effects, it was selected for a comparison of the numerical calculations with the analytical estimates. Of course, only a limited comparison is possible, because the analytical estimates contain many simplifications, and do not account for a number of effects that are included in the numerical studies.

First, the flow field is compared by means of the Darcy velocities, where the analytical values can be estimated by applying eq. (10). With the regional hydraulic gradient of $5 \cdot 10^{-4}$, the aquifer slope of -2.86° , and the maximum density of 1050 kg/m^3 , it yields a Darcy velocity of $4.90 \cdot 10^{-9} \text{ m/s}$ for the migration downslope, while inserting the minimum (ambient) density of 1000 kg/m^3 yields $1.22 \cdot 10^{-9} \text{ m/s}$ for the migration upslope. In Table 2 these estimates are compared to the maximum Darcy velocities at the aquifer bottom from the numerical modeling. It is apparent that the numerical calculations yield much higher velocities during the initial stage, because the water is pushed both upslope and downslope along the aquifer bottom by the stratification effect, which is neglected in the analytical estimates. With increasing time, analytical and numerical results approach each other. At later times, the numerically calculated downslope migration becomes slower than the analytical value because the concentrations, and thus the density differences, slowly decrease due to the spreading of the plume.

A comparison of the numerically calculated transport distances with the analytical estimates is even more difficult than for the velocities. One problem is, for example, how to define the front of the waste plume from the calculated concentrations. Here, the front is (somewhat arbitrarily) defined as the place, where the concentration at the aquifer bottom is 1 % of the initial concentration, i.e. 1 kg/m^3 . In Table 2 these transport distances are compared to the estimates derived from eq. (12). It can be seen that the values determined numerically are much larger than the analytical estimates. This results from two phenomena that tend to accelerate waste migration during the early stage, but are neglected in the estimates: the forced convection during the injection phase, and the lateral spreading due to the stratification effect. Additionally, the plume spreads significantly due to dispersion, which also is not taken into account by the analytical estimates. At later times, in contrast, the downslope movement becomes slower than the estimates, since density-driven flow is reduced because of the smaller density differences.

Depending on the nature of the contaminant, much lower concentrations than 1 kg/m^3 may be of prime environmental concern. Such concentrations will occur much farther from the injection site than the distances given in Table 2. Hence, the analytical equations then will underestimate transport distances even more.

The comparisons show that analytical considerations are useful to give rough estimates of the importance of density-driven waste movement. But they should not be used for detailed calculations of flow velocities, transport distances, or waste concentrations. The complexity of the transport mechanisms requires the application of numerical models, such as finite difference and finite element models, which are becoming more and more widely used in contaminant hydrogeology.

5. Conclusions

The possibility of the migration of hazardous liquid wastes due to density-driven transport mechanisms in sloping aquifers has been studied mathematically by means of analytical and numerical calculations for the case of typical deep injection systems. Analytical estimates reveal that in

sloping aquifers, migration by density effects can be much stronger than transport by regional ground-water motion, and can result in significant transport distances. Due to the complexity of the transport mechanisms, the exact evaluation of flow velocities, transport distances, and waste concentrations requires detailed numerical analyses. Simulations with a finite element model were performed to identify the typical transport mechanisms, and to determine the sensitivity towards certain parameters. Their results show that in the case of density differences, waste initially spreads into all directions due to density-induced stratification effects. Later on, it mainly moves laterally along the slope of either aquifer top or aquifer bottom, depending on the waste density.

The risk of potential upward migration is highest, when the waste plume is lighter than the ambient ground water. Such conditions are very likely when fluid densities within the injection zone are large due to high salinities. Because of the resulting upward buoyancy force, the contact area between the waste plume and the overlying, confining formation will significantly increase. This fact should be considered when defining the "area of review", as required by the Underground Injection Control regulations.

Simulations with different natural hydraulic gradients demonstrated possible interactions between density-driven movement and regional ground-water flow in deep injection systems. If both effects are directed the same way, transport is accelerated. If they are directed to opposite sides, on the other hand, they do not neutralize each other, but work separately, and simultaneous transport into different directions must be expected to occur. Thus, the aquifer slope and regional hydraulic gradient may be equally significant factors in estimating potential migration of disposed liquid wastes.

The numerical analyses emphasize the need for field data to validate the model predictions. As waste movement is dominated by the injection itself as long as waste is injected, however, only data from post-closure conditions can be helpful to determine the effects of aquifer slope and natural hydraulic gradient in the field. Then, the extension of the numerical analyses to fully three-dimensional modeling is recommended to avoid the effect of model dimensionality.

Acknowledgements

This work was made possible by the support of a post-doctorate scholarship, awarded to the first author by the NATO Scientific Committee through the German Academic Exchange Service (DAAD), Bonn, Federal Republic of Germany. Part of the work was jointly supported by the Office of Drinking Water, U.S. Environmental Protection Agency and by the Director, Office of Energy Research, Office of Basic Energy Sciences, Engineering and Geosciences Division of the U.S. Department of Energy under contract No. DE-AC03-76SF00098. We would like to thank Helmut Daniels from Aachen for contributing many valuable comments, as well as Jahan Noorishad and Ronald Falta from Berkeley for reviewing this manuscript.

Notation

α_l	m	longitudinal dispersivity
α_t	m	transversal dispersivity
C	kg/m ³	concentration
D_{ij}	m ² /s	hydrodynamic dispersion tensor
D_0	m ² /s	molecular diffusivity
g	m/s ²	gravitational constant
k_{ij}	m ²	permeability tensor
K	m/s	hydraulic conductivity
ℓ	m	sloping coordinate
L	m	transport distance
p	Pa	pressure
q_i	m/s	Darcy velocity
Q	m ³ /s/m ³	sink/source flux
R	–	retardation factor
t	s	time
v_i	m/s	flow velocity
x_i	m	cartesian coordinates
z	m	vertical coordinate
δ_{ij}	–	Kronecker delta symbol
μ	Pa·s	dynamic viscosity
ρ	kg/m ³	density
ρ_o	kg/m ³	ambient (reference) density
φ	degree	sloping angle
ϕ	–	porosity
ψ	m	hydraulic head

References

- Bear, J. 1972. Dynamics of Fluids in Porous Media. American Elsevier, New York. 764 pp.
- Donaldson, E.C., R.D. Thomas, and K.H. Johnston. 1974. Subsurface waste injection in the United States: fifteen case histories. U.S. Bureau of Mines, Information Circular 8636, Washington, D.C., 72 pp.
- Dorgarten, H.-W. and C.-F. Tsang. 1990. Three-phase simulation of organic contaminations in aquifer systems. In K.U. Weyer (Editor): Proceedings, Conference on Subsurface Contamination by Immiscible Fluids, April 18-20, 1990, Calgary, Alberta, Canada, A.A. Balkema, Rotterdam (in press).
- EPA. 1985. Report to Congress on injection of hazardous wastes. Office of Drinking Water, U.S. Environmental Protection Agency, Report No. EPA 570/9-85-003, Washington, D.C., 265 pp.
- Falta, R.W., I. Javandel, K. Pruess, and P.A. Witherspoon. 1989. Density-driven flow of gas in the unsaturated zone due to the evaporation of volatile organic compounds. Water Resources Research, v. 25, no. 9, pp. 2159-2169.
- Frind, E.O. 1982. Simulation of long-term transient density-dependent transport in groundwater. Advances in Water Resources. v. 5, no. 2, pp. 73-88.
- Mendoza, C.A. and E.O. Frind. 1990. Advective-dispersive transport of dense organic vapors in the unsaturated zone, 1. model development. Water Resources Research, v. 26, no. 3, pp. 379-387.
- Miller, C., T.A. Fischer II, J.E. Clark, W.M. Porter, C.H. Hales, and J.R. Tilton. 1986. Flow and containment of injected wastes. Proceedings, International Symposium on Subsurface Injection of Liquid Wastes, March 3-5, 1986, New Orleans, LA, Water Well Journal Publ. Co., Dublin, OH, pp. 520-559.
- Millington, R.J. 1959. Gas diffusion in porous media. Science, v. 130, no. 3367, pp. 100-102.

- Moffett, T.B., P.E. LaMoreaux, J.Y. Smith, and M.B. Dismukes. 1986. Management of hazardous wastes by deep-well disposal. The University of Alabama Environmental Institute for Waste Management Studies, Open File Report No. 11, Tuscaloosa, AL, 272 pp.
- Oberlander, P.L. 1989. Fluid density and gravitational variations in deep boreholes and their effect on fluid potentials. *Ground Water*, v. 27, no. 3, pp. 341-350.
- Prickett, T.A., D.L. Warner, and D.D. Runnells. 1986. Application of flow, mass transport, and chemical reaction modeling to subsurface liquid injection. Proceedings, International Symposium on Subsurface Injection of Liquid Wastes, March 3-5, 1986, New Orleans, LA, Water Well Journal Publ. Co., Dublin, OH, pp. 447-463.
- Scheidegger, A.E. 1961. General theory of dispersion in porous media. *Journal of Geophysical Research*, v. 66, no. 10, pp. 3273-3278.
- Segol, G., G.F. Pinder, and W.G. Gray. 1975. A Galerkin finite element technique for calculating the transient position of the saltwater front. *Water Resources Research*, v. 11, no. 2, pp. 343-347.
- Sleep, B.E. and J.F. Sykes. 1989. Modeling the transport of volatile organics in variably saturated media. *Water Resources Research*, v. 25, no. 1, pp. 81-92.

Figure 1. Ratio between density-driven flow and regional ground-water flow as a function of aquifer slope, density difference, and regional hydraulic gradient.

Figure 2. Convective transport distance due to density-driven flow within 10,000 years as a function of aquifer slope, density difference, and the ratio $K/R\phi$.

Figure 3. Geometry of the studied system with finite element discretization.

Figure 4. Base case results after 20 years: (a) Darcy velocities; (b) waste concentrations.

Figure 5. Base case results after 100 years: (a) Darcy velocities; (b) waste concentrations.

Figure 6. Base case results after 1000 years: (a) Darcy velocities; (b) waste concentrations.

Figure 7. Effect of the waste density on transport in a sloping aquifer: waste concentrations after 1000 years for (a) $\bar{\rho}_{inj} = 950 \text{ kg/m}^3$; (b) $\bar{\rho}_{inj} = 1000 \text{ kg/m}^3$; (c) $\bar{\rho}_{inj} = 1050 \text{ kg/m}^3$ (base case).

Figure 8. Effect of the regional hydraulic gradient on transport in a sloping aquifer: waste concentrations after 1000 years for (a) $\partial\psi/\partial x = -5 \cdot 10^{-4}$; (b) $\partial\psi/\partial x = 0$ (base case); (c) $\partial\psi/\partial x = 5 \cdot 10^{-4}$.

Figure 9. Results with regional ground-water flow ($\partial\psi/\partial x = 5 \cdot 10^{-4}$) after 2000 years: (a) Darcy velocities; (b) waste concentrations.

Table 1. Data Specification for the Deep Injection Simulations

<i>Parameter</i>	<i>Specified value</i>
<i>Soil parameters</i>	
Horizontal permeability, k_{xx}	$2.5 \cdot 10^{-13} \text{ m}^2$
Vertical permeability, k_{zz}	$0.5 \cdot 10^{-13} \text{ m}^2$
Porosity, ϕ	0.25
<i>Fluid parameters</i>	
Ambient density, ρ_o	1000 kg/m ³
Viscosity, μ	$1.0 \cdot 10^{-3} \text{ Pa}\cdot\text{s}$
Injection rate, Q_{inj}	$2.5 \cdot 10^{-5} \text{ m}^3/\text{s}/\text{m}$
Injection period, T_{inj}	20 years
Injected waste concentration, $\tilde{C}_{inj}$	100 kg/m ³
<i>Transport parameters</i>	
Longitudinal dispersivity, α_l	20 m
Transversal dispersivity, α_t	1 m
Molecular diffusivity in water, D_0	$5.0 \cdot 10^{-10} \text{ m}^2/\text{s}$
Retardation factor, R	3.0
<i>Base values of varied parameters</i>	
Regional hydraulic gradient, $\partial\psi/\partial x$	0.0
Density factor, γ	0.5
i.e. density of injected fluid, $\tilde{\rho}_{inj}$	1050 kg/m ³
<i>Numerical model parameters</i>	
Number of nodes	2121 (21 by 101)
Number of elements	4000
Simulation period	1000 years
Time step	2 years

Table 2. Comparison between Numerical Results and Analytical Estimates

<i>Time</i>	<i>Downslope</i>		<i>Upslope</i>	
	<i>Num.</i>	<i>Anal.</i>	<i>Num.</i>	<i>Anal.</i>
<i>Darcy velocities (10^{-9} m/s)</i>				
1000 years	8.73	4.90	6.58	1.22
2000 years	6.06	4.90	4.14	1.22
3000 years	4.64	4.90	3.06	1.22
4000 years	3.88	4.90	2.45	1.22
5000 years	3.43	4.90	2.12	1.22
<i>Transport distances (m)</i>				
1000 years	542	206	560	52
2000 years	719	412	718	103
3000 years	840	619	829	155
4000 years	944	825	912	206
5000 years	>1000	1031	>1000	258

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
INFORMATION RESOURCES DEPARTMENT
BERKELEY, CALIFORNIA 94720