

Journal of Hydrology 258 (2002) 69-82



www.elsevier.com/locate/jhydrol

Dynamic stabilization of heat-generating liquid waste plume in a sloping aquifer

V.I. Malkovsky^a, A.A. Pek^a, C.-F. Tsang^{b,*}

^aInstitute of Geology of Ore Deposits, Petrography, Mineralogy, and Geochemistry, Staromonetny per., 35, Moscow 109017, Russian Federation

^bEarth Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

Received 29 February 2000; revised 24 August 2001; accepted 19 October 2001

Abstract

Contaminant transport by groundwater in a sloping aquifer is considered in the case when contaminant plume has a salinity (and density) different from that of the groundwater, and is heat generating. Forced convection is present due to regional groundwater flow and natural convection is also expected to develop due to concentration differences and thermal changes. Such a situation takes place in deep-well disposal of liquid radioactive waste, in which the heat generation is caused by the radioactive decay.

Flow and contaminant transport in the aquifer were calculated in 2D approximation in the plane of the aquifer, and the process of heat conduction in confining rocks was described by a 3D model. The set of equations governing flow, heat and mass transfer in the system was solved numerically with use of finite differences technique. Accuracy of numerical solution was checked by comparison with an original analytical solution of the flow problem for concentration-driven convection.

It was shown that the influence of the natural convection component could cause acceleration as well as slowing down of the contaminant plume movement depending on system parameters. Results of numerical solution were approximated by a dimensionless analytical expression, which can be used for estimation of the relative impact of different driving forces exerting influence on the contaminant plume movement. Published by Elsevier Science B.V.

1. Introduction

One method of isolating liquid hazardous waste from the biosphere is through injection of the waste into deep permeable layers confined at the top and bottom by low permeable rocks (Fried, 1975; Apps and Tsang, 1996). This technique is also used in Russia for the disposal of liquid

Generally, the liquid wastes injected into the disposal zone have density which differs noticeably from the density of formation ground water in that zone. Also, the disposal zone is not horizontal in the general case. That is why when the salinity of formation water is less than the solute mass concentration of injected waste, the contamination plume can sink down the dip of the aquifer (Dorgarten and Tsang, 1991). An additional factor exerting an influence on the flow of this

0022-1694/02/\$ - see front matter Published by Elsevier Science B.V. PII: S0022-1694(01)00556-X

radioactive waste (Spitsyn et al., 1978; Laverov et al., 1991; Foley et al., 1993; Rybalchenko et al., 1994; Rybalchenko, 1998; Rybalchenko et al., 1999).

^{*} Corresponding author. Tel.: +1-510-486-6726; fax: +1-510-486-5686

E-mail address: cftsang@lbl.gov (C.-F. Tsang).

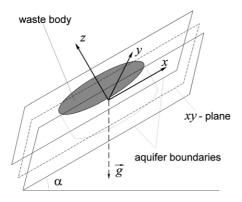


Fig. 1. Scheme of waste disposal.

contamination plume appears when the injected waste contains a radioactive component. Heat generation caused by radioactive decay leads to heating of the injected liquid and, hence, to a decrease in its density. As a result, components of buoyancy forces governing the movement of a contamination plume can vary in magnitude and can even reverse their direction, causing an up-dip movement of the injected liquid. One should take into account the fact that heat generation rate decreases with time and, therefore, the influence of this factor on plume movement decreases as well.

One of the main requirements imposed upon selection of waste disposal site is low velocity of a regional flow of ground water in the aquifer destined for waste disposal. Therefore, buoyancy forces can exert a significant influence on the groundwater flow. Thus, movement of the injected plume in the aquifer is governed by both of the following factors: buoyancy forces (caused by the difference between densities of injected liquid and native formation water) and regional flow of ground water in the aquifer. Joint action of these factors can lead to acceleration or, conversely, deceleration of contaminant migration. From the viewpoint of disposal safety, conditions should be chosen whereby these driving forces suppress each other, so that the displacement of the contamination plume from the injection location is minimal.

A mathematical model is considered which describes transport of an injected liquid waste plume in a sloping aquifer confined from top and bottom by low permeable rocks. This model is used for estimations of the influence exerted by different driving forces on the contaminant plume movement.

Results of these estimations can be used for a preliminary selection of an injection site where displacement of the contamination plume is minimal. One more application of these estimations should be mentioned. A sufficiently reliable safety assessment for a particular injection site calls for a more precise computer simulation of the contaminant transport process with account for site-specific features of a geological medium including a heterogeneity of medium properties (Malkovsky et al., 1999). Solution of such site-specific problems, which account for all driving forces exerting influence on the contaminant plume movement can represent a very complicated problem. The obtained approximate estimations permit the identification of components of driving forces that can be neglected, thus greatly simplifying the computer simulation problem (Malkovsky et al., 1999).

2. Problem formulation

Let us introduce some simplifying assumptions. The aquifer is considered to be flat and the movement of ground water parallel to the aquifer boundaries. As the duration of the injection period is much less than that for which prediction of contaminant migration should be obtained, we will consider only the time interval since the completion of waste injection. It is assumed that the contaminant migration process can be described satisfactorily by Boussinesq's approximation (Gebhart et al., 1988), i.e. the thermophysical properties of the medium are constant except for density in the gravity force term in the momentum equation.

Further, let us assume that the initial waste plume has the form of a cylinder with circular bases at the top and bottom aquifer boundaries (Fig. 1). It is assumed that the cylinder radius is much more than the aquifer thickness. The Cartesian coordinates system x, y, z can be introduced as shown in Fig. 1; here the plane xy is positioned equidistant from the upper and lower aquifer boundaries (with z as normal to the aquifer boundaries), and y axis is perpendicular to the vector of gravity force. A 2D model is considered with the distributions of temperature and concentration within the aquifer independent of z.

Then the ground water flow can be described by

Gebhart et al., 1988:

$$u_x = -\frac{k}{\mu} \left\{ \frac{\partial p}{\partial x} + \rho g \sin \alpha [1 - \beta_T (T - T_0) + \beta_C C] \right\},\tag{1}$$

$$u_{y} = -\frac{k}{\mu} \frac{\partial p}{\partial y},\tag{2}$$

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0. {3}$$

Here u_x , u_y are components of flow velocity field, p is pressure, T is temperature, C is solute mass concentration (i.e. fraction by weight), and ρ , μ are density and dynamic viscosity of water at the initial temperature T_0 . Further,

$$\beta_T = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_{p,C}; \qquad \beta_C = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial C} \right)_{p,T},$$
 (4)

k is permeability of the aquifer, g is acceleration due to gravity, and α is an angle of the aquifer plane with the horizon.

It is taken that the injected waste plume consists of two components. The first represents non-radioactive substances and the second component represents radionuclides which are responsible for heat generation. Mass concentration of the second component is referred to as K and thus the mass concentration of the non-radioactive component is equal to C - K. Let us assume that the velocity of convective transport of components is equal to the ground water flow velocity, and that the dispersion coefficients for both components are equal, and $K \ll C$. Then distributions of K and C satisfy equations of transient convective mass transfer

$$\frac{\partial C}{\partial t} + \frac{1}{\varphi} \left(u_x \frac{\partial C}{\partial x} + u_y \frac{\partial C}{\partial y} \right) = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right), (5)$$

$$\frac{\partial K}{\partial t} + \frac{1}{\varphi} \left(u_x \frac{\partial K}{\partial x} + u_y \frac{\partial K}{\partial y} \right)$$

$$= D\left(\frac{\partial^2 K}{\partial x^2} + \frac{\partial^2 K}{\partial y^2}\right) - \kappa K,\tag{6}$$

where φ is porosity, $\kappa = \ln 2/t_{\rm d}$ (when $t_{\rm d}$ is the effective half-life of the radioactive component), D is effective diffusivity of the solute.

Substitution of the Darcy's velocity components, Eqs. (1) and (2), into continuity Eq. (3) gives the Poisson equation for pressure

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = \rho g \sin \alpha \left(\beta_T \frac{\partial T}{\partial x} - \beta_C \frac{\partial C}{\partial x} \right). \tag{7}$$

Boundary conditions for pressure and concentrations can be presented in the form

$$p - p_0 + \frac{v_x \mu x}{k} + \frac{v_y \mu y}{k} + \rho gx \sin \alpha \to 0,$$

$$as|x|, |y| \to \infty \quad K \to 0, \quad C \to 0,$$
(8)

where v_x , v_y are the velocity components of regional flow, i.e. forced components of the flow velocity field, p_0 is the hydrostatic pressure at x = y = z = 0 in the absence of contamination.

Boundary condition (8) reflect a decrease of the waste plume influence on pressure and concentration distributions with increasing distance from the plume (Slattery, 1981).

Initial (at t = 0) conditions for concentrations can be written as

$$\sqrt{x^2 + y^2} \le r_{\text{in}}, \quad C = C_0, \quad K = \gamma C_0;$$

$$\sqrt{x^2 + y^2} > r_{in}, \quad C = K = 0,$$
(9)

where $r_{\rm in}$ is the initial radius of the plume.

It is assumed that heat transfer in the system caused by heat generation of the radioactive component in the waste plume is governed by conductive heat dissipation into the confining rock. Then, heat flux normal to the aquifer boundaries dominates. Further, if the temperatures within the aquifer are close to some z-average values (i.e. T = T(t, x, y) within the aquifer), then the temperature field in the surrounding rocks satisfies the equation

$$\frac{\partial T}{\partial t} = a_{\rm r} \frac{\partial^2 T}{\partial z^2},\tag{10}$$

with the following initial and boundary conditions

$$t = 0, T = T_0, (11)$$

$$z = \pm \frac{h}{2}, \qquad \lambda_{\rm r} \frac{\partial T}{\partial z} = \mp \varphi K \rho \frac{h}{2} \omega + \frac{h \lambda_{\rm r}}{2 a_{\rm r}} \frac{\partial T}{\partial t};$$

$$|z| \to \infty, \qquad \frac{\partial T}{\partial z} \to 0.$$
(12)

Here h is aquifer thickness, ω is heat generation rate per unit mass of the radioactive component, λ_r , a_r are respectively thermal conductivity and thermal diffusivity of the surrounding rocks.

Let us introduce the dimensionless variables:

$$X = \frac{x}{L}, \quad Y = \frac{y}{L}, \quad Z = \frac{z - h/2}{L}, \quad \tau = \frac{t}{t_{\rm m}},$$

$$\xi = \frac{C}{C_0}, \qquad \eta = \frac{K}{\gamma C_0},$$

$$P = \frac{k}{u_{\rm m}\mu L} \left(p - p_0 + \frac{v_x \mu x}{k} + \frac{v_y \mu y}{k} + \rho gx \sin \alpha \right),$$

$$\theta = \frac{T - T_0}{T_{\rm m}},$$

where

$$u_{\rm m} = \frac{k}{\mu} \rho g \beta_C C_0 \sin \alpha, \qquad L = \frac{D\varphi}{u_{\rm m}},$$

$$t_{\rm m} = D \left(\frac{\varphi}{u_{\rm m}}\right)^2, \quad l = \sqrt{a_{\rm r}t_{\rm m}}, \quad T_{\rm m} = \frac{\varphi l \gamma C_0 \rho h \omega}{2\lambda_{\rm r}}.$$

Then equations of fluid flow (7), heat (10) and mass transfer (5) and (6), can be rewritten in dimensionless variables as

$$\frac{\partial^2 P}{\partial X^2} + \frac{\partial^2 P}{\partial Y^2} = F \frac{\partial \theta}{\partial X} - \frac{\partial \xi}{\partial X},\tag{13}$$

$$\frac{\partial \xi}{\partial \tau} + U_X \frac{\partial \xi}{\partial X} + U_Y \frac{\partial \xi}{\partial Y} = \frac{\partial^2 \xi}{\partial X^2} + \frac{\partial^2 \xi}{\partial Y^2},\tag{14}$$

$$\frac{\partial \eta}{\partial \tau} + U_X \frac{\partial \eta}{\partial X} + U_Y \frac{\partial \eta}{\partial Y} = \frac{\partial^2 \eta}{\partial X^2} + \frac{\partial^2 \eta}{\partial Y^2} - D_c \eta, \quad (15)$$

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial Z^2},\tag{16}$$

where

$$F = rac{T_{
m m}eta_T}{C_0eta_C}, \qquad D_{
m c} = \kappa t_{
m m},$$
 $U_X = V_X - rac{\partial P}{\partial X} - \xi + F heta, \qquad U_Y = V_Y - rac{\partial P}{\partial Y},$ $V_X = rac{v_x}{u_x}, \qquad V_Y = rac{v_y}{u_x}.$

Initial conditions (9) and (11) in dimensionless form are written as

$$\tau = 0, \qquad \theta = 0,$$

$$\begin{cases} \sqrt{X^2 + Y^2} \le R_{\text{in}}, & \xi = \eta = 1; \\ \sqrt{X^2 + Y^2} > R_{\text{in}}, & \xi = \eta = 0. \end{cases}$$
(17)

Boundary conditions (8) and (12) take the form

$$|X|, |Y| \to \infty, \qquad P, \xi, \eta \to 0; \qquad Z = 0,$$

$$\frac{\partial \theta}{\partial Z} = -\eta + \frac{I}{2} \frac{\partial \theta}{\partial \tau}; \qquad Z \to \infty, \qquad \frac{\partial \theta}{\partial Z} \to 0.$$
(18)

Here

$$R_{\rm in} = \frac{r_{\rm in}}{L}, \qquad I = \frac{h}{l}.$$

It should be mentioned that the functions

$$\xi$$
 and $\eta e^{D_c \tau}$

satisfy Eq. (14) and the same initial and boundary conditions, i.e. it is not necessary to solve the problem for η because

$$\eta = \xi e^{-D_c \tau}$$
.

It can be seen that the governing equation set (13)–(16) and boundary and initial conditions (17) and (18) include 6 dimensionless parameters

$$F, D_c, V_V, V_V, R_{in}, I.$$

F determines a ratio between buoyancy force components caused by nonhomogeneous distributions of

temperature and those caused by concentration. D_c determines a ratio between time scales for convective mass transfer and for radioactive decay. Dimensionless variables V_X , V_Y characterize the ratio between regional flow velocity and velocity of density-driven flow. $R_{\rm in}$ is an analog of Peclet number and characterizes relative contributions of convection and dispersion to the mass transport. I characterizes the thermal capacity of the aquifer in the process of heat exchange with the confining rock beds.

3. Modeling results

The center of mass position of the plume can be calculated as

$$X^{\text{mass}}(\tau) = \frac{\int \int X\xi(X,Y,\tau) dX dY}{\int \int \xi(X,Y,\tau) dX dY},$$

$$Y^{\text{mass}}(\tau) = \frac{\int \int Y\xi(X, Y, \tau) dX dY}{\int \int \xi(X, Y, \tau) dX dY}$$

and the components of average plume velocity as

$$U_X^{\mathrm{mass}}(au) = rac{X^{\mathrm{mass}}(au)}{ au}, \qquad U_Y^{\mathrm{mass}}(au) = rac{Y^{\mathrm{mass}}(au)}{ au}.$$

These are important characteristics of contaminant migration in the aquifer.

First, let us consider the case when the waste does not contain a radioactive component. The flow problem at low τ can be solved analytically. This analytical solution is very important because it is exact at $\tau=0$, and its comparison with a numerical solution of the flow problem at $\tau=0$ permits to estimate accuracy of the numerical solution.

It is worthwhile to introduce dimensionless cylindrical coordinates R, ϑ such that $X = R \cos \vartheta$, $Y = R \sin \vartheta$.

Initial condition at $\tau = 0$ can be rewritten as,

$$\xi = \begin{cases} 1, & R \le R_{\text{in}}; \\ 0, & R > R_{\text{in}}, \end{cases}$$

when

$$\frac{\partial \xi}{\partial \vartheta} = 0, \qquad \frac{\partial \xi}{\partial R} = -\delta(R - R_{\rm in}),$$

where δ is Dirac's δ -function.

Then the momentum Eq. (13) can be rewritten at

low τ as

$$\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial P}{\partial R}\right) + \frac{1}{R^2}\frac{\partial^2 P}{\partial \vartheta^2} = \delta(R - R_{\rm in})\cos\vartheta.$$

If P is represented as $P = P_1 \cos \vartheta$ then

$$\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}R}\left(R\frac{\mathrm{d}P_1}{\mathrm{d}R}\right) - \frac{1}{R^2}P_1 = \delta(R - R_{\mathrm{in}}).$$

With the introduction of a new variable $\zeta = \ln(R/R_{\rm in})$, and taking into account

$$\delta(R - R_{\rm in}) = \delta(\zeta - \zeta(R_{\rm in})) \frac{\mathrm{d}\zeta}{\mathrm{d}R},$$

we obtain

$$\frac{\mathrm{d}^2 P_1}{\mathrm{d}\zeta^2} - P_1 = R_{\mathrm{in}} \delta(\zeta). \tag{19}$$

 P_1 should be finite at $\zeta \to \pm \infty$. Then

$$P_1 = \begin{cases} s_1 e^{\zeta}, & \zeta < 0; \\ s_2 e^{-\zeta}, & \zeta > 0. \end{cases}$$

Since Eq. (19) is satisfied (Vladimirov, 1971) at

$$P_1(-0) = P_1(+0), \qquad P'(+0) - P'(-0) = R_{in},$$

it follows that

$$s_1 = s_2 = -\frac{R_{\rm in}}{2},$$

and the net result is

$$P = \begin{cases} -\frac{1}{2}R\cos\vartheta = -\frac{X}{2}, & R \le R_{\text{in}}; \\ -\frac{1}{2}\frac{R_{\text{in}}^2}{R}\cos\vartheta, & R > R_{\text{in}}. \end{cases}$$

Therefore, we obtain for $R \leq R_{in}$

$$U_X = -\frac{\partial P}{\partial X} - \xi = -\frac{1}{2}.$$

and

$$U_X^{\text{mass}} = -\frac{1}{2}, \qquad U_Y^{\text{mass}} = 0 \tag{20}$$

at small τ

The solution obtained is precise only at the beginning of the process when the liquid waste plume is of a circular shape, and its concentration or density is constant (equal to initial concentration C_0). Later,

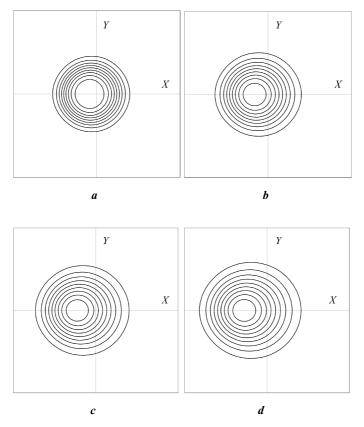


Fig. 2. Contamination plume movement at $R_{\rm in}=10$. Heat generation in the waste and regional flow in the aquifer are absent. $a-\tau=5, b-\tau=10, c-\tau=15, d-\tau=20$.

the dissolved component is transported not only by convection but also by diffusion (dispersion). The smaller the radius of the plume, the greater is the relative influence of diffusion on the overall mass transfer process. This is because the amount of dissolved component carried by convection per unit time is proportional to the plume volume (for 2D model— πR^2), and amount of the substance conveyed per unit time by diffusion is proportional to the area of the interface between formation water and the plume (for 2D model— $2\pi R$). That is why the greater the radius of the injected waste plume, the longer it retains a near-circular shape and the smaller is a relative width of dispersion halo of the dissolved component relative to the size of the central region where concentrations are close to the initial value C_0 .

Modeling of the process at arbitrary τ was carried out by computer simulation using the finite differences method. Successive overrelaxation method

(Roache, 1976) was used to solve the momentum Eq. (13) (with regard for boundary condition (18)). Alternating direction method with upwind differencing (Roache, 1976) was used with minor modifications for the integration of the equation of transient convective mass transfer (14). Eq. (16) (in the case of $F \neq 0$) was integrated with use of the Crank–Nicolson method.

Results of computer simulation at $V_X = V_Y = 0$, F = 0 are shown in Fig. 2 for $R_{\rm in} = 10$, and in Fig. 3 for $R_{\rm in} = 100$. Changes in the distribution of dimensionless concentration ξ are shown by isolines family ($\xi/\xi_{\rm max} = 0.1,...,0.9$) and support the inference about the impact of $R_{\rm in}$ on the contaminant transport process.

A plot of U_X^{mass} obtained numerically as a function of τ is given in Fig. 4 (points). One can see from Figs. 2–4 that the smaller the R_{in} value, the larger is the diffuseness of the plume boundary and the faster is

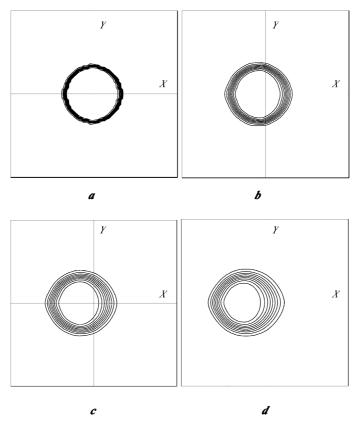


Fig. 3. Contamination plume movement at $R_{\rm in}=100$. Heat generation in the waste and regional flow in the aquifer are absent. $a-\tau=10$, $b-\tau=50$, $c-\tau=100$, $d-\tau=150$.

the decrease in the average center-of-mass velocity of the plume $U_X^{\rm mass}$. Rather simple explanation for this effect can be offered. The larger the diffuseness of the plume, the less is its average density, and therefore, the less is the magnitude of the density-induced force, which causes the movement of the plume down the dip of the aquifer. This leads to a decrease in the velocity of this movement.

Let us introduce a variable

$$R_{\rm mass}(\tau) =$$

$$\frac{3}{2} \frac{\int \int \sqrt{[X - X^{\text{mass}}(\tau)]^2 + [Y - Y^{\text{mass}}(\tau)]^2} \xi(X, Y, \tau) dX dY}{\int \int \xi(X, Y, \tau) dX dY}$$

as a characteristic of the effective size of the plume. It follows from initial condition (9) that

$$R_{\text{mass}}(0) = R_{\text{in}}.\tag{21}$$

Analysis of computer simulation results shows that

$$U_X^{\text{mass}}(\tau)R_{\text{mass}}(\tau) \approx \text{const}$$
 (22)

at each value of $R_{\rm in}$. Taking into account initial conditions (20) and (21), it follows from Eq. (22) that

$$U_X^{\text{mass}} = -0.5 \frac{R_{\text{in}}}{R_{\text{mass}}(\tau)}.$$
 (23)

It is seen from Fig. 4 that the values of $U_X^{\rm mass}$ obtained numerically and the values of $U_X^{\rm mass}$ determined by Eq. (23) are in satisfactory agreement. The function $R_{\rm mass}(\tau)$ (different at different $R_{\rm in}$) which enters into Eq. (23) was determined numerically. To make it possible to use Eq. (23) immediately (i.e. without numerical calculations) for the evaluation of $U_X^{\rm mass}(\tau)$, it is necessary to find an approximating analytical expression for $R_{\rm mass}(\tau)$ at different $R_{\rm in}$. From a fit of the computer simulation results in

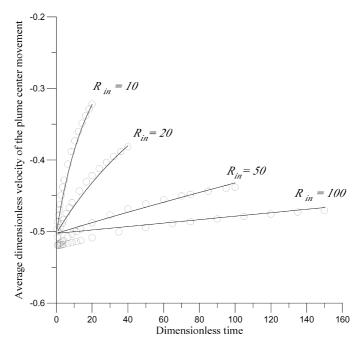


Fig. 4. Time dependence of average dimensionless velocity of the plume center movement. Heat generation in the waste and regional flow in the aquifer are absent, but there is an initial density difference between the injected liquid and the formation water. Values of U_X^{mass} obtained numerically are shown by circles. Solid lines correspond to U_X^{mass} values calculated from Eq. (23).

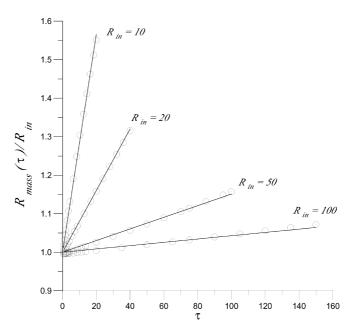


Fig. 5. Comparison between $R_{\text{mass}}(\tau)$ obtained numerically (circles) and calculated from the approximating expression (24) (solid line) at F = 0.

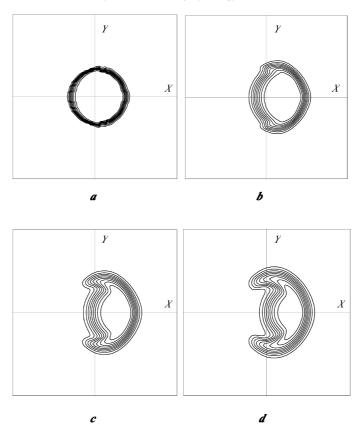


Fig. 6. Contamination plume movement at heat generation in the waste volume. F = 2, $D_c = 0.1$, $V_X = V_Y = 0$, I = 1, $R_{in} = 100$.

Fig. 5, the following expression was obtained

$$\frac{R_{\text{mass}}(\tau)}{R_{\text{in}}} = 1 + \frac{1.87}{R_{\text{in}}^{1.82}} \tau. \tag{24}$$

It can be seen from Fig. 5 that approximating expression (24) and computer simulation results are in satisfactory agreement.

In the case of nonzero V_X , the problem is reduced to the considered one through the substitution of X by the new variable $X_1 = X - V_X \tau$. Therefore, it can be written in general case for F = 0,

$$U_X^{\text{mass}}(\tau) = V_X - 0.5 \frac{R_{\text{in}}}{R_{\text{mass}}(\tau)},$$
 (25)

where $R_{\text{mass}}(\tau)$ is determined by approximating expression (24).

This type of contamination plume movement will be modified in the case when the waste contains a radioactive component, which causes heat generation

 $(F \neq 0)$. As one can see from the computer simulation results presented in Figs. 6 and 7, the following situation can take place. The plume moves first down the dip of the aquifer $(U_X^{\text{mass}} < 0$, see Fig. 7), driven by the initial excess in waste density over the formation water density. Later on, the heat generation caused by radioactive component in the waste leads to temperature increase (see Fig. 8), with a resulting decrease in solution density. When the density of the injected liquid becomes less than the density of formation water, the plume starts to move in the opposite direction, that is, up the dip of the aquifer and rises in the up-dip direction above the initial position ($U_X^{\text{mass}} > 0$, see Fig. 7). However because of the inhomogeneity in temperature and solute concentration distributions, the resulting effect of concentration and thermal convection is different in central part of the plume and at its periphery, which leads to a deformation of initial circular shape (see Fig. 6). Whereas the central

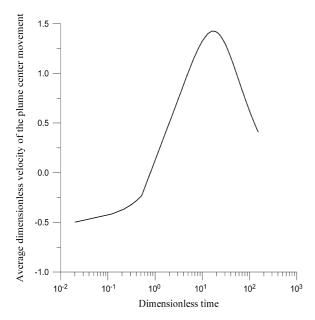


Fig. 7. Time dependence of U_X^{mass} at heat generation in the waste volume. F = 2, $D_c = 0.1$, $V_X = V_Y = 0$, I = 1, $R_{\text{in}} = 100$.

part of the plume continues to move up the dip of the aquifer (being driven by thermal convection currents which are sustained by the heat accumulated in the rock matrix at the location of the initial position of the plume), 'tongs' appear at the two sides of the plume, which move down the dip of the aquifer. At a later time, when the temperature in the aquifer declines to a level such that thermal convection is not able to oppose concentration induced convection, the up-dip movement of the plume in the central part is also overcome and it gives way to the down-dip movement.

To gain insight into how the average velocity of the contaminant plume movement depends on dimensionless governing parameters F, $R_{\rm in}$, V_X , V_Y , $D_{\rm c}$, and I, computer simulation of contaminant transport is carried out for several parameter sets. These sets are given in Table 1 and combine parameter values which correspond to conditions of high-level liquid radio-active waste injection in Russia (Rybalchenko et al., 1994). Time dependencies of $U_X^{\rm mass}$ for the different parameter sets from Table 1 are shown in Fig. 9.

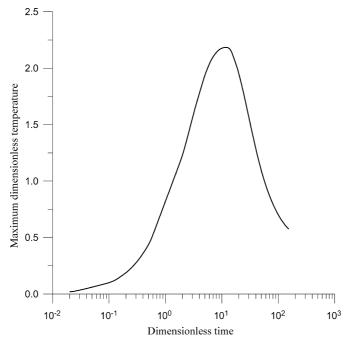


Fig. 8. Time dependence of maximum θ in the aquifer. F = 2, $D_c = 0.1$, $V_X = V_Y = 0$, I = 1, $R_{in} = 100$.

Table 1 Values of governing parameters for curves in Fig. 9

Curve number in Fig. 9	F	$R_{ m in}$	V_X	V_Y	D_{c}	I
1	1	10 ³	0	0	10^{-3}	10 ²
2	0	10^{3}	0	0	10^{-3}	10^{2}
3	0.5	10^{3}	0	0	10^{-3}	10^{2}
4	2	10^{3}	0	0	10^{-3}	10^{2}
5	1	10^{3}	0	0	10^{-4}	10^{2}
6	1	10^{3}	0	0	10^{-3}	2×10^{2}
7	1	10^{3}	0	0	10^{-3}	5×10^{2}
8	1	2×10^{3}	0	0	10^{-3}	10^{2}
9	1	10^{3}	- 0.5	0	10^{-3}	10^{2}

From a fit of the computer simulation results in Fig. 9 the following approximate analytical expression was obtained

$$\delta U_X^{\text{mass}} = U_X^{\text{mass}} - U_X^{\text{mass}}|_{F=0} = 0.5545 \frac{F}{I} \frac{\Phi_1^{0.867}}{1 + \Phi_2 \Phi_3},$$
(26)

$$\Phi_1 = \frac{1 - \exp(-0.35D_{\rm c}\tau)}{0.35D_{\rm c}},$$

$$\Phi_2 = \frac{(F/I)^{1.726}}{1.520 \times 10^{-3} + (F/I)^{1.726}},$$

$$\Phi_3 = 4.838 \times 10^{-4} \frac{\tau^2}{R_{\rm in}^{0.8}}.$$

 $U_X^{\text{mass}}|_{F=0}$ is the value of the average dimensionless velocity at F=0 calculated from Eqs. (24) and (25). Auxilliary functions Φ_1 , Φ_2 , and Φ_3 describe a change of a thermoconvective component of the

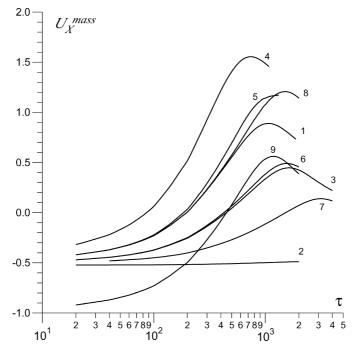


Fig. 9. Influence of the governing parameters on a character of the time dependence of U_X^{mass} at heat generation in the waste volume. Values of the governing parameters corresponding to a certain curve are given in Table 1.

flow at different stages of the simulated process. Φ_1 characterizes the initial stage when the temperature increases due to the heat generation. Φ_2 is a function of F/I and, hence, reflects the influence of thermal capacity of the aquifer on the thermoconvective flow. Φ_3 decreases with a decrease of $R_{\rm in}$ and an increase of τ and, therefore, can be considered as a function which describes the influence of a heat carried away from the aquifer at the initial stage of the process due to thermoconductive heat transfer and accumulated in the enclosing rocks on the thermoconvective flow at later stages when the heat generation exhausts.

Discrepancy between the numerical calculation results and the approximate analytical expression (26) does not exceed 25%.

Naturally, Eq. (26) is not universal and can be used for an approximate evaluation of the average velocity of the waste plume movement only in the case when the governing parameters have the same orders of magnitude as corresponding values in Table 1. However this limitation on applicability of expression (26) is not excessively strict for two following reasons. First, the ranges of the dimensionless parameters in Table 1 are determined in accordance with actual conditions characteristic to radioactive waste injection sites, in particular, the range of heat generation rate embraces possible values for liquid radioactive waste (Spitsyn et al., 1978; Rybalchenko et al., 1994). Second, the expression (26) can be used for a rough estimation of the influence exerted by the heat generation on the contaminant plume movement. This estimation can show in a particular case whether this influence can be neglected what is very important for simplification of rather complicated site-specific models.

4. Discussion

The main mechanisms governing convective transport of an injected waste plume are: (1) forced convection caused by the regional ground water flow, (2) concentration induced convection caused by the difference in salinity and hence in density between the formation water and the injected liquid, and (3) thermal convection caused by heat generation when the injected waste contains a radioactive component. The joint action of these processes can lead to an acceleration or, conversely, to deceleration

of contaminant migration along the injection zone of the aquifer. Therefore, in the design of a liquid waste injection disposal system, it is advisable from safety considerations to realize conditions such that the joint action of these processes brings about maximum spatial stability of the contamination plume in the aquifer, i.e. its minimum spatial displacement relative to the injection well.

For a rough estimation of the rate of injected waste migration, the above introduced parameter for the average mass velocity $U_X^{\rm mass}$ of the contamination plume can be utilized. With its use, an injection site selection criterion can be defined as $U_X^{\rm mass}(\tau_{\rm lim})\approx 0$ where $\tau_{\rm lim}$ is the specified time of safe isolation of the waste from the biosphere. This condition can be used as one of the criteria for the selection of disposal sites.

When the waste does not contain a radioactive component and heat generation is absent (F=0), the plume shape remains convex, and the function $R_{\rm mass}(\tau)$ (Eq. (24)) can be used for an estimation of the change in plume size. Then, the condition $U_X^{\rm mass}(\tau_{\rm lim}) \cong 0$ is a criterion of disposal site selection, and $R_{\rm mass}(\tau)$ characterizes the degree of disposal safety. The values of $U_X^{\rm mass}(\tau)$ and $R_{\rm mass}(\tau)$ can be calculated with use of expressions (24) and (25).

When heat generation exists $(F \neq 0)$, the problem of disposal safety assessment is more complicated. The values of $U_X^{\text{mass}}(\tau)$ can be calculated from Eq. (26) (if the governing parameters belong to the region represented in Table 1). But it is important to bear in mind that $U_X^{\rm mass}(\tau)$ characterizes only a preferential direction of convective transport of the waste but does not describe the oppositely directed flows at local parts of the plume which can occur for $F \neq 0$ (as can be seen from a comparison of Fig. 6c and d. In this case, the central part of the plume moves up the dip of the aguifer under the action of thermal convection, but the colder liquid at the two sides of the plume moves down under the action of concentrationinduced convection. These local flows can cause a significant deformation of the initial plume shape such that $R_{\text{mass}}(\tau)$ cannot adequately characterize the changes in the plume shape.

In conclusion, it is noted that the considered model describes the process of contaminant migration only when the aquifer is thin, i.e. at $h \ll r_{\rm in}$. Otherwise it is necessary to take into account plume movement normal

to the aquifer boundaries (Charny, 1963; Dorgarten and Tsang, 1991) and consider a general 3D model.

5. Conclusion

Underground disposal of liquid wastes is sometimes carried out through their injection into deep aquifers confined from top and bottom by low permeable rocks.

One of the possible options for the enhancement of the long-term safety of such waste disposal system lies in the selection of disposal sites where geochemical conditions provide sequestration of the injected waste. The process of sequestration develops through precipitation, co-precipitation and sorption of contaminant in the rock formation resulting in geochemical sequestration of the disposed wastes.

Another possible option for the enhancement of long-term safety of the liquid waste disposal lies in minimizing plume movement caused by an interaction among the different convective transport processes. For an examination of this approach, the 2D model of mixed (forced, concentration, and thermal) convection in the aquifer was considered. The preliminary investigation of the model presented in this paper shows that a contributory factor for enhancing long-term safety of the liquid waste disposal is a preliminary selection of the injection formation where the interaction between the processes of forced, concentration, and thermal convection can be designed to minimize the waste migration, thus resulting in spatial stabilization of the contamination plume in the aquifer. This can be accomplished by an adjustment of the injected waste density and the portion of its radioactive component (e.g. through addition of nontoxic components to the waste).

From a generalization of the computer simulation results, approximate analytical expressions are obtained which can be used for this purpose. This expression can be used to reveal cases where the influence of heat generation on the contaminant plume movement can be neglected. Such estimations permit to simplify significantly site-specific problems and substantiate applicability of available simulators for solving them. Because chemical retardation due to reactions between waste components, rocks, and formation water are not taken into account in the model, disposal safety assess-

ments obtained are conservative, i.e. corresponding to the worst variant of the process.

Results of computer simulations show that in the case when the injected liquid waste contains an amount of radioactive component causing heat generation in the waste volume, the mechanism of contaminant transport process changes that can lead to an essential deformation of the initial plume shape, with changes in velocity (and even direction) of the plume movement.

References

Apps, J.A., Tsang, C.-F. (Eds.), 1996. Deep Injection Disposal of Hazardous and Industrial Waste Academic Press, San Diego.

Charny, I.A., 1963. Underground Fluid Dynamics. Gostoptechizdat, Moscow (in Russian).

Dorgarten, H.-W., Tsang, C.-F., 1991. Modeling the density-driven movement of liquid wastes in deep sloping aquifers. Ground Water 29 (5), 655–662.

Foley, M.G., Hoover, K.A., Bradley, D.J., Devary, J.L., Wurstner, S.K., Williams, M.D., Vorvick, C.A., 1993. West Siberian Basin regional hydrogeology—toward a continent-scale model. In: Eckstein, Y., Zaporozec, A. (Eds.), Proceedings of the American Institute of Hydrology. Second USA-CIS Joint Conference on Environmental Hydrology and Hydrogeology. Water Environment Federation, Alexandria, Virginia, pp. 145–167.

Fried, J.J., 1975. Groundwater Pollution. Elsevier, Amsterdam. Gebhart, B., Jaluria, Y., Mahajan, R.L., Sammakia, B., 1988. Buoyancy Induced Flows and Transport. Hemisphere, Washington.

Laverov, N.P., Kantsel, A.V., Lisitsyn, A.K., Omelianenko, B.I., Pek, A.A., Seltsov, B.M., Filonenko, Yu.D., 1991. Main problems of radiogeology concerning disposal of radioactive waste. Atomnaya Energiya 71 (6), 523–534 (in Russian).

Malkovsky, V., Pek, A., Velichkin, V., Parker, F., 1999. Prediction of contaminant plume movement from the deep-well injection of liquid radioactive waste (LRW) at the Krasnoyarsk disposal site. Hydrological Science and Technology Journal 15 (1-4), 145-171.

Roache, P.J., 1976. Computational Fluid Dynamics. Hermosa Publ, Albuquerque.

Rybalchenko, A.I., Pimenov, M.K., Kostin, P.P., Balukova, V.D., Nosukhin, A.V., Mikerin, E.I., Egorov, N.N., Kaimin, E.P., Kosareva, I.M., 1998. Deep Disposal of Liquid Radioactive Wastes. IzdAT, Moscow in Russian, English translation published by Battelle Press, Columbus, Ohio.

Rybalchenko, A.I., 1998. Experience in site selection and characterization for the deep well injection of liquid radioactive waste in Dimitrovgrad. In: Proceedings of the International Conference on Radioactive Waste Disposal, DisTec'98 (September 9–11, 1998), Hamburg.-Congress Centrum Hamburg. pp. 162.

Rybalchenko, A.I., Pimenov, M.K., Kurochkin, V.M., Zubkov, A.A., Sigayev, B.P., Ladzin, A.S., 1999. Disposal of liquid radioactive waste—practical results and consequences for the environment. Geoecologiya 2, 128–132 (in Russian).

Slattery, J.C., 1981. Momentum, Energy, and Mass Transfer in Continua. R.E. Krieger, Huntington, New York.

Spitsyn, V.I., Pimenov, M.K., Balukova, V.D., Leontichuk, A.S.,

Kokorin, I.N., Yudin, F.P., Rakov, N.A., 1978. Main prerequisites and practice of use of deep aquifers for disposal of liquid radioactive waste. Atomnaya Energiya 44 (2), 161–168. Vladimirov, V.S., 1971. Equations of Mathematical Physics. Nauka, Moscow (in Russian).