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Computer Simulation of Radionuclide Transport through Thermal Convection of Groundwater from Borehole Repositories

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Abstract

Results are presented of numerical modeling of radionuclide transport by thermal convection of groundwater from a single well repository of high level waste. Because the problem possesses cylindrical symmetry, the process is described by a system of 2-D transient equations for momentum, convective heat transfer and convective mass transfer (taking into account hydrodynamic dispersion and radionuclide decay). Results of computer simulations for a selected range of system parameters were generalized by approximating analytical relationship, which can be used for safety assessment of a radioactive waste repository.

The problem of the reciprocal relationship between thermoconvective transport processes and well spacing in an underground repository with a regularly spaced set of the waste-loaded wells is examined using a two-well model as an example. In this case, the transport problem becomes three-dimensional. A solution to this problem was obtained using a special system of orthogonal coordinates, which simplifies the computational algorithm and enhances accuracy. It is shown that thermoconvective transport of radionuclides in the vicinity of each well can be considered to be independent at well separations of the order of 100 m when reasonable values of other repository parameters are assumed.

1. Introduction

High level radioactive wastes (HLW) should be disposed of in deep geological formations. Such a strategy is now accepted in all countries with a mature nuclear power industry [1-3]. The goal of disposing of HLW underground is to isolate radioactive wastes until their radioactivity decreases to an ecologically safe level. But isolation of HLW from the biosphere would not be absolute even in the case of the deep geological disposal.

The principal process, which can bring about HLW leakage from the underground repository, is radionuclide transport by groundwater. Geological conditions are, therefore, of paramount importance in the selection of a repository site. The general requirement, placed upon the geological conditions, is the minimization of the risk of HLW leakage from the repository to the biosphere by groundwater regional

flow. Well developed methods of computer simulation of hydrogeological systems with forced convection of groundwater can be used for assessments of such risk [4].

Besides forced convection, processes involving free convection are also of importance in HLW geological disposal. HLW as opposed to other types of waste generates substantial amounts of heat. Consequently, a HLW repository triggers thermal convection of the groundwater. This spontaneous process is one of the primary potential hazards for the long-term safety of the repository site [5]. Therefore, a reasonably achievable decrease of the risk caused by thermoconvective transport of radionuclides is one of the repository design requirements [2,6].

Mined and well repositories are the principal types of repository considered for geologic HLW disposal [2,3,6]. In mined repositories, canisters containing HLW are emplaced in the short boreholes drilled in the floor or walls of the underground drifts. In well repositories, canisters containing HLW are stacked along the axis in the lower part of each well. The mined repository option is of primary interest in the USA because retrievability is required by law. From the technical point of view, the retrievability requirement is easily satisfied in the case of a mined repository. But well repositories have particular advantages. They are much simpler in design and construction, and are less expensive.

In this paper the authors present the results of computer simulations of HLW leakage from a well repository by thermal convection of groundwater. The maximum concentration of radionuclides at the Earth's surface was accepted as a criterion for the safety evaluation. The problem is to obtain numerically the value of this maximum concentration and to find an approximating expression for the dependence between the maximum concentration and system parameters for a preliminary safety analysis of various well repository configurations.

2. Formulation of the Problem

Two conceptual models were considered (Fig. 1). The first one represents the case of a single well repository (Fig. 1a). The second model with two wells (Fig. 1b) was examined for assessment of reciprocal influence between thermoconvective transport processes and the distance between the wells.

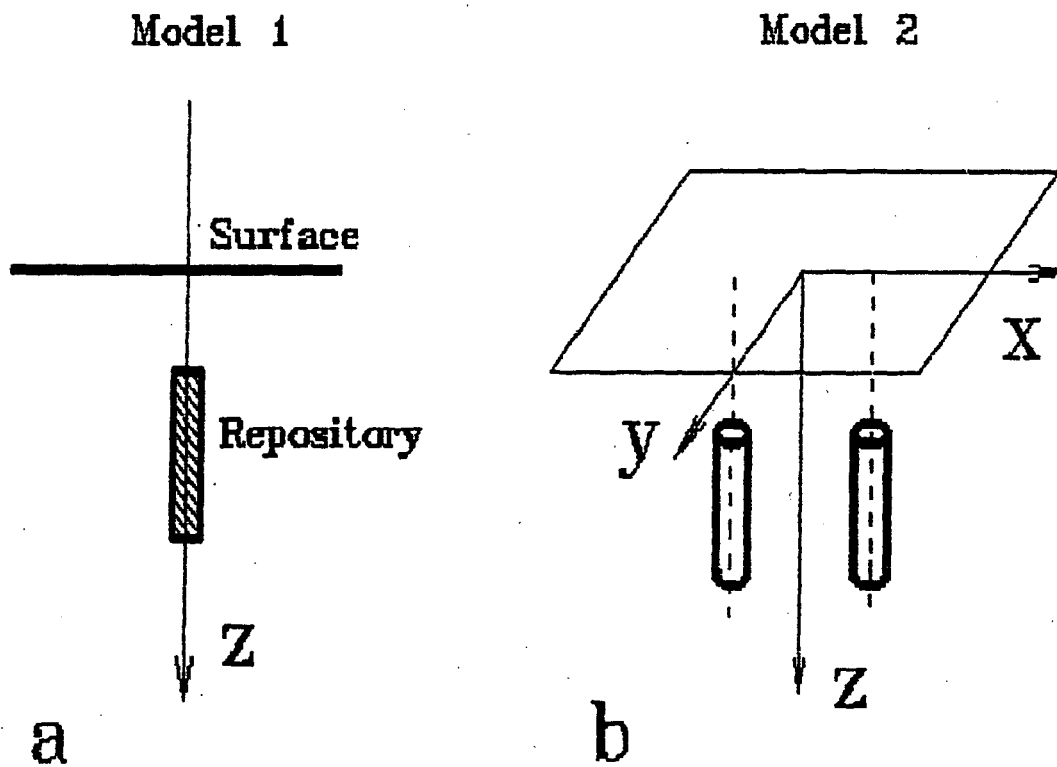


Fig.1 Conceptual models.
 a - single well model;
 b - two wells model.

In both models, wells of depth z_2 and of radius r_d are assumed to be vertical. Waste loaded canisters are emplaced in the lower parts of the wells over the interval $l = z_2 - z_1$. At the initial time $t = 0$, the waste specific heat generation is ω_0 , which decreases exponentially with time. Heat generated in the waste loaded canisters warms the enclosing rocks. As a result, free thermal convection of groundwater develops, and transports radionuclides leached from the waste towards the Earth's surface.

In order to taking a conservative approach regarding safety, the extreme case is considered where all the canisters are damaged initially. The radionuclide concentration at the surface of the waste is assumed to be limited by the solubility of the waste form. Radionuclides leached from the waste form are transported away by convective flow. Radionuclide transported in the groundwater will be retarded by sorption and by chemical reactions. These processes are not taken into account here, i.e., it is assumed that dissolved components move with the same velocity as the groundwater. Diffusion and hydrodynamic dispersion are taken into account, however, as well as the gradual decrease of radionuclide concentration in the groundwater due to radioactive decay. As noted above, the maximum acceptable concentration of radionuclides at the Earth's surface is taken as the safety criterion.

3. Mathematical Formulation of the Problem

It is assumed that the thermophysical properties of the pore fluid (except density in the expression for gravitational force) and of the enclosing rocks are constant. The fluid phase is assumed to be a single phase liquid in thermal and chemical equilibrium with the enclosing rocks.

Let us initially consider the model with a single well. In assuming cylindrical symmetry for the problem, the system of equations for convective heat and mass transfer can be written in cylindrical coordinates as follows [7,8]:

The continuity equation

$$\frac{\partial u}{\partial z} + \frac{1}{r} \cdot \frac{\partial}{\partial r} (rv) = 0$$

Darcy's equations in Boussinesq's approximation

$$u = -\frac{k}{\mu} \left\{ \frac{\partial p'}{\partial z} - \rho g [1 - \beta(T - T_0)] \right\}, \quad v = -\frac{k}{\mu} \frac{\partial p'}{\partial r}$$

The heat transfer equation

$$\frac{\rho_r c_r}{\rho c} \frac{\partial T}{\partial z} + u \frac{\partial T}{\partial z} + v \frac{\partial T}{\partial r} = \frac{\lambda_r}{\rho c} \left[\frac{\partial^2 T}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) \right]$$

The mass transfer equation

$$\frac{\partial C}{\partial t} + \frac{1}{\phi} \left(u \frac{\partial C}{\partial z} + v \frac{\partial C}{\partial r} \right) = \frac{\partial}{\partial z} \left(d_{zz} \frac{\partial C}{\partial z} + d_{zr} \frac{\partial C}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \left(d_{rr} \frac{\partial C}{\partial r} + d_{rz} \frac{\partial C}{\partial z} \right) \right) - \kappa C$$

where z, r are cylindrical coordinates (z axis runs along the well axis with $z = 0$ at the Earth's surface). u, v are vertical and horizontal components of the fluid flow velocity field respectively; k — permeability of enclosing rocks; μ, ρ, β, c — viscosity, density, coefficient of thermal expansion and specific heat of fluid, ρ_r, λ_r, c_r — density, thermal conductivity and specific heat of enclosing rocks, p' — pressure, g — acceleration due to gravity, T — temperature, T_0 — initial temperature, C — concentration, t — time, $d_{zz}, d_{zr}, d_{rr}, d_{rz}$ — dispersion coefficients, $\kappa = \ln 2 / \Delta t_d$, where Δt_d is the average value of the half-life for the waste isotopes, ϕ — porosity.

Values of hydrodynamic dispersion coefficients were defined according to [7]

$$d_{zz} = D + \alpha_L \frac{u^2}{\phi w} + \alpha_T \frac{v^2}{\phi w} ; \quad d_{rr} = D + \alpha_L \frac{v^2}{\phi w} + \alpha_T \frac{u^2}{\phi w} ; \quad d_{zr} = d_{rz} = (\alpha_L - \alpha_T) \frac{u}{\phi}$$

where D is the molecular diffusivity, α_L, α_T — linear parameters of dispersion.

$$w = \sqrt{u^2 + v^2}$$

In order to exclude the pressure from the momentum equation it is worthwhile introducing the stream function, ψ , such that

$$u = -\frac{1}{r} \frac{\partial}{\partial r} (r\psi) , \quad v = \frac{\partial \psi}{\partial z}$$

The continuity equation therewith is satisfied automatically. After substitution of u and v we obtain the momentum equation in the following form

$$\frac{\partial^2 \psi}{\partial z^2} + \frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial}{\partial r} (r\psi) \right] = \frac{kg\beta\rho}{\mu} \frac{\partial T}{\partial r}$$

For the well repository $r_d/l \ll 1$. This permits us to neglect the well diameter in the calculation of the fluid velocity field. Assuming that the radioactive element release is governed by dissolution of the waste matrix, the initial and boundary conditions for ψ and C can be written as

$$r=0, \frac{\partial \psi}{\partial z} = 0 ; z \notin [z_1, z_2] , \frac{\partial C}{\partial r} = 0 , z \notin [z_1, z_2] , C = \gamma C_{sat}(T) ;$$

$$z=0 , \frac{\partial \psi}{\partial z} = 0 ; \frac{\partial C}{\partial z} = 0 ;$$

$$r \rightarrow \infty, \frac{\partial \psi}{\partial z} , \frac{\partial \psi}{\partial r} , \frac{\partial C}{\partial r} \rightarrow 0 ;$$

$$z \rightarrow \infty, \frac{\partial \psi}{\partial z} , \frac{\partial \psi}{\partial r} , \frac{\partial C}{\partial z} \rightarrow 0 .$$

where γ is the concentration of radionuclides in the waste matrix, $C_{sat}(T)$ — temperature dependent saturation concentration of matrix components in the aqueous solution at a specified temperature, z_2 and z_1 — are depths of the top and bottom of the waste loaded interval within the well, respectively.

The situation with the heat transfer equation is more complicated, because the one-dimensional stationary solution of the thermal conductivity problem for an infinite region tends to infinity at $r_d \rightarrow 0$ for the case of cylindrical symmetry. This obstacle is especially important, because boundary conditions for concentration depend on the temperature in the loaded part of the well. In this connection we have to take into account a value of r_d that is different from zero for the problem of heat transfer, and the initial and boundary conditions for T should be written as

$$r=0 , z \notin [z_1, z_2] , \frac{\partial T}{\partial r} = 0 ;$$

$$r=r_d , z \in [z_1, z_2] , \frac{\partial T}{\partial r} = -\frac{M\omega}{2\pi\lambda_r} ;$$

$$r \rightarrow \infty , \frac{\partial T}{\partial r} \rightarrow 0 ;$$

$$z=0, T=T_0; z \rightarrow \infty, T \rightarrow T_0;$$

$$t=0, T=T_0,$$

M — waste mass per unit length of the loaded part of the well, ω — heat generation rate per unit of waste mass.

We introduce the dimensionless variables

$$R = \frac{r}{l}, z = \frac{z}{l}, \tau = \frac{t\Psi_M}{l^2}, U = \frac{ul}{\Psi_M}, V = \frac{vl}{\Psi_M}, \Psi = \frac{\psi}{\Psi_M}, \theta = \lambda_r \frac{T - T_0}{M\omega_0}, K = \frac{C}{\gamma C_{sat}(T_0)}$$

where

$$\Psi_M = \frac{kg\beta\rho l M \omega_0}{\mu \lambda_r}, \quad \omega_0 = \omega(0).$$

The system of momentum, heat and mass transfer equations can now be written as

$$\frac{\partial^2 \Psi}{\partial Z^2} + \frac{\partial}{\partial R} \left[\frac{1}{R} \frac{\partial}{\partial R} (R\Psi) \right] = \frac{\partial \theta}{\partial R},$$

$$\frac{\rho_r c_r}{\rho c} \frac{\partial \theta}{\partial \tau} + U \frac{\partial \theta}{\partial Z} + V \frac{\partial \theta}{\partial R} = \frac{1}{Pe} \left[\frac{\partial^2 \theta}{\partial Z^2} + \frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial \theta}{\partial R} \right) \right],$$

$$\frac{\partial K}{\partial \tau} + U \frac{\partial K}{\partial Z} + V \frac{\partial K}{\partial R} = \frac{1}{Pe_d} \left[\frac{\partial}{\partial Z} \left(D_{ZZ} \frac{\partial K}{\partial Z} + D_{ZR} \frac{\partial K}{\partial R} \right) + \frac{1}{R} \frac{\partial}{\partial R} R \left(D_{ZR} \frac{\partial K}{\partial Z} + D_{RR} \frac{\partial K}{\partial R} \right) \right] - \nu K.$$

$$Pe = \frac{\rho c \Psi_M}{\lambda_r}, Pe_d = \frac{Pe C_\lambda}{Le}, \nu = \frac{\ln 2 \cdot l^2}{\Delta t_d \Psi_M}, C_\lambda = \frac{\lambda_r}{\lambda}, Le = \frac{D \rho c}{\lambda}, D_{ij} = \frac{d_{ij}}{D}.$$

The dependence $C_{sat}(T)$, according to [9], may be given as

$$\ln C_{sat}(T) = 2.303 \frac{T - T_0}{\Delta T} + B$$

where ΔT is the temperature range within which C_{sat} changes by an order of magnitude. The transformation to dimensionless variables for the set of initial and boundary conditions is evident.

Let us now consider the model with two wells (Fig. 1b). This problem has two planes of symmetry. The first plane (Π_1) passes through axes of both wells, the second one (Π_2) runs between them so that points on this plane are equidistant from both axes. Let us introduce a Cartesian coordinate system, xyz ,

with the vertical z axis being the line of intersection of Π_1 and Π_2 planes and horizontal x and y axes lying in the Π_1 and Π_2 planes, respectively, so that x, y, z axes form the right angles.

The momentum equations in this system are written in the form

$$v_x = -\frac{k}{\mu} \frac{\partial p}{\partial x}, \quad v_y = -\frac{k}{\mu} \frac{\partial p}{\partial y}, \quad v_z = -\frac{k}{\mu} \left(\frac{\partial p}{\partial z} + \rho g \beta T \right).$$

v_x, v_y, v_z are components of velocity field, $p = p' - \rho g$, $T = T' - T_0$.

Taking into account the continuity equation

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0$$

we obtain the momentum equation in the form

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} = -\rho g \beta \frac{\partial T}{\partial z}.$$

The temperature distribution satisfies the equation of transient convective heat transfer

$$\frac{\rho_r c_r}{\rho c} \frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} = \frac{\lambda_r}{\rho c} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right).$$

For the sake of simplicity, it is assumed that $\alpha_L = \alpha_T = \alpha$. Then the distribution of concentration

satisfies the equation

$$\frac{\partial C}{\partial t} + \frac{1}{\varphi} \left(v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \right) = \frac{\partial}{\partial x} \left(d \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(d \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(d \frac{\partial C}{\partial z} \right) - \kappa \cdot C.$$

$$d = D + \frac{\alpha \cdot w}{\varphi}.$$

The boundary conditions in this system can be written as

$$x=0, \quad \frac{\partial p}{\partial x}; \quad z=0, \quad p=0;$$

$$x \rightarrow \infty, \quad \frac{\partial p}{\partial x} \rightarrow 0; \quad z \rightarrow \infty, \quad \frac{\partial p}{\partial z} \rightarrow 0;$$

$$y \rightarrow \infty, \quad \frac{\partial p}{\partial y} \rightarrow 0; \quad y=0, \quad \frac{\partial p}{\partial y} = 0;$$

$$z \leq z_2, \quad (x-h)^2 + y^2 = r_d^2, \quad \frac{\partial p}{\partial n} = 0;$$

where h is the half distance between the two wells, and n is the external normal to the boundary surface.

The boundary conditions for temperature and concentration take the form

$$\begin{aligned} x=0 \quad , \quad \frac{\partial T}{\partial x} = \frac{\partial C}{\partial x} = 0 \quad ; \quad z=0 \quad , \quad T=0 \quad , \quad \frac{\partial C}{\partial z} = 0 \quad ; \\ x \rightarrow \infty \quad , \quad \frac{\partial T}{\partial x} \rightarrow 0 \quad , \quad \frac{\partial C}{\partial x} \rightarrow 0 \quad ; \quad z \rightarrow \infty \quad , \quad \frac{\partial T}{\partial z} \rightarrow 0 \quad , \quad \frac{\partial C}{\partial z} \rightarrow 0 \quad . \\ y \rightarrow \infty \quad , \quad \frac{\partial T}{\partial y} \rightarrow 0 \quad , \quad \frac{\partial C}{\partial y} \rightarrow 0 \quad ; \quad y=0 \quad , \quad \frac{\partial T}{\partial y} = 0 \quad , \quad \frac{\partial C}{\partial y} = 0 \quad . \\ z \in [z_1, z_2] \quad , \quad (x-h)^2 + y^2 = r_d^2 \quad , \quad -\frac{\partial T}{\partial n} = \frac{M\omega}{2\pi r_d \lambda_r} \quad , \quad C = \gamma C_{sat}(T_0) e^{AT} \quad . \end{aligned}$$

It is evident that the problem is essentially three-dimensional. The form of the regional boundary is rather complicated. Taking into account the fact that the well radius is much less than the characteristic dimension of the region, it is clear that an exact description of the regional boundary presents a problem for any net partition of the region. To solve this problem, it is worthwhile adopting a special coordinate system that permits us to transform the regional boundary to a surface of simpler form. For example, the horizontal cross section of the region considered can be transformed to rectangle (as is shown in Fig. 2a).

This transformation is achieved by coordinate conversion from $\{x,y\}$ to $\{\xi,\eta\}$.

$$\begin{aligned} \xi = \ln R_1 + \frac{1}{2} \ln \left[\frac{(x^2 + y^2 - r_1^2)^2 + 4 \cdot r_1^2 y^2}{(x+r_1)^2 + y^2} \right] \quad , \quad \eta = \arctan \left(\frac{2 \cdot r_1 y}{x^2 + y^2 - r_1^2} \right) \quad . \\ r_1 = \sqrt{h^2 - r_d^2} \quad , \quad R_1 = \frac{h+r_d+r_1}{h+r_d-r_1} \quad . \end{aligned}$$

ξ,η coordinate lines in Cartesian coordinates (x,y) are shown in Fig. 2b.

The metric tensor of $\{\xi,\eta\}$ -system

$$\begin{aligned} \begin{bmatrix} G_{\xi\xi} & G_{\xi\eta} \\ G_{\eta\xi} & G_{\eta\eta} \end{bmatrix} \quad , \\ G_{\xi\xi} = \left(\frac{\partial x}{\partial \xi} \right)^2 + \left(\frac{\partial y}{\partial \xi} \right)^2 \quad , \quad G_{\xi\eta} = G_{\eta\xi} = \frac{\partial x}{\partial \xi} \frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi} \frac{\partial y}{\partial \eta} \quad , \quad G_{\eta\eta} = \left(\frac{\partial x}{\partial \eta} \right)^2 + \left(\frac{\partial y}{\partial \eta} \right)^2 \end{aligned}$$

is of spherical type, because of mapping analyticity,* that is

* This means that the derivative of the complex function $\xi + i\eta = f(x + iy)$ is direction-invariant (the definition of analytical function: complex function is analytical if its derivative exists and is direction-invariant).

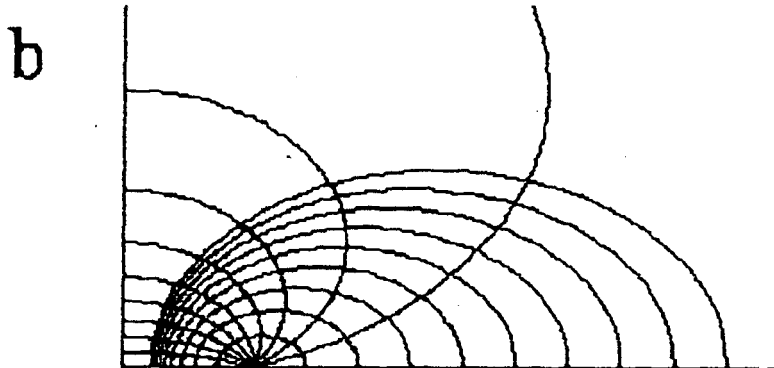
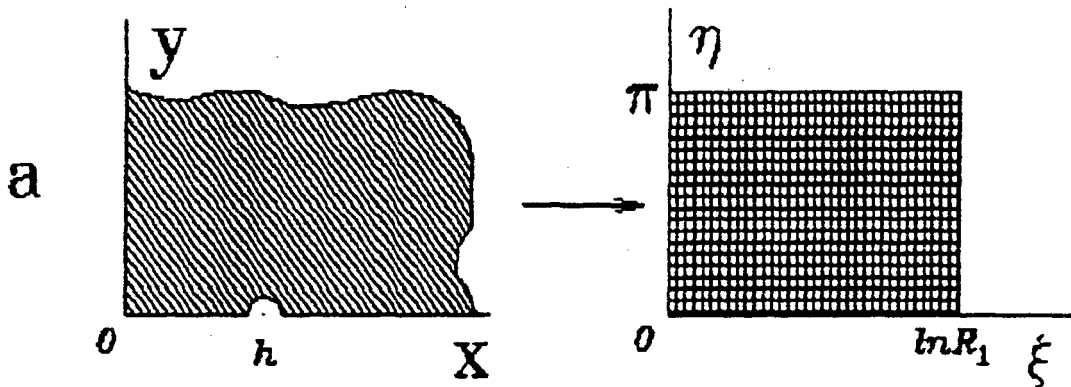


Fig.2. Transition to the new coordinate system.
 a - conformal mapping of horizontal cross section
 of the considered region,
 b - new coordinate lines in Cartesian coordinates.

$$G_{\xi\xi} = G_{\eta\eta} \quad , \quad G_{\xi\eta} = 0 \quad .$$

The momentum equation is, therefore, rewritten for $\{\xi, \eta, z\}$ coordinates in the form

$$\frac{\partial^2 p}{\partial z^2} + \frac{1}{\sqrt{G}} \left[\frac{\partial^2 p}{\partial \xi^2} + \frac{\partial^2 p}{\partial \eta^2} \right] = -\rho g \beta \frac{\partial T}{\partial z}$$

where $G = G_{\xi\xi} G_{\eta\eta}$.

Likewise, heat and mass transfer equations are rewritten in the form

$$\begin{aligned} \frac{\partial T}{\partial t} - \frac{\rho c k}{\rho_r c_r \mu} \left[\left(\frac{\partial p}{\partial z} + \rho g \beta T \right) \frac{\partial T}{\partial z} + \left(\frac{\partial p}{\partial \xi} \frac{\partial T}{\partial \xi} + \frac{\partial p}{\partial \eta} \frac{\partial T}{\partial \eta} \right) \frac{1}{\sqrt{G}} \right] \\ = \frac{\lambda_r}{\rho_r c_r} \left[\frac{\partial^2 T}{\partial z^2} + \frac{1}{\sqrt{G}} \left(\frac{\partial^2 T}{\partial \xi^2} + \frac{\partial^2 T}{\partial \eta^2} \right) \right] \quad , \end{aligned}$$

$$\begin{aligned} \frac{\partial C}{\partial t} - \frac{k}{\mu} \left[\left(\frac{\partial p}{\partial z} + \rho g \beta T \right) \frac{\partial C}{\partial z} + \left(\frac{\partial p}{\partial \xi} \frac{\partial C}{\partial \xi} + \frac{\partial p}{\partial \eta} \frac{\partial C}{\partial \eta} \right) \frac{1}{\sqrt{G}} \right] = \\ \frac{\partial}{\partial z} d \frac{\partial C}{\partial z} + \frac{1}{\sqrt{G}} \left(\frac{\partial}{\partial \xi} d \frac{\partial C}{\partial \xi} + \frac{\partial}{\partial \eta} d \frac{\partial C}{\partial \eta} \right) - \kappa C \quad . \end{aligned}$$

The boundary conditions take the form

$$\xi = 0 \quad , \quad \frac{\partial p}{\partial \xi} = 0 \quad , \quad \frac{\partial T}{\partial \xi} = - \left[\frac{x-h}{r_d} \frac{\partial x}{\partial \xi} + \frac{y}{r_d} \frac{\partial y}{\partial \xi} \right] \frac{M\omega}{2\pi r_d \lambda_r} \quad , \quad C = \gamma C_{sat}(T_0) e^{AT} \quad ;$$

$$\xi = \ln R_1 \quad , \quad \frac{\partial p}{\partial \xi} = 0 \quad , \quad \frac{\partial T}{\partial \xi} = 0 \quad , \quad \frac{\partial C}{\partial \xi} = 0 \quad ;$$

$$\eta = 0, \pi \quad , \quad \frac{\partial p}{\partial \eta} = 0 \quad , \quad \frac{\partial T}{\partial \eta} = 0 \quad , \quad \frac{\partial C}{\partial \eta} = 0 \quad .$$

4. Results of Calculations

Both problems were solved numerically by finite difference methods.

A. The Single Well Model

The momentum equation was solved by the successive over relaxation method [10], the equation of heat transfer was solved by the alternate directions method [10], and the equation of mass transfer was

integrated by a modified method of alternate directions with explicit determination of the second mixed spatial derivatives. The Courant condition was obtained from the Neumann's analysis of the last method for Cartesian coordinates in the absence of convection as

$$\Delta\tau \leq \left| \frac{\Delta_z \Delta_R}{D_{ZR}} \right|$$

where Δ_z, Δ_R are internodes R and Z distances, respectively, $\Delta\tau$ is a step of integration with respect to τ .

The boundary conditions for K depend on the value of θ at $R = R_d = r_d/1$. The r_d value is several orders of magnitude less than the radial dimension of the region under consideration. But use of a nonuniform net, as a rule, complicates the finite differences relationships or brings about a decrease of the accuracy with respect to Δ_R . For this reason, an approach similar to the one implemented in [11] was used. The equation of heat transfer was solved in two stages for each step of integration. Initially the solution was obtained for a rough net (with internode distance Δ_R), then for a finer net in the region $R \leq \Delta_R$. Examples of the flow lines and isoconcentration lines are given in Figs. 3 and 4.

An analysis of the system parameters shows that Pe , C_λ , and δ_z vary the most. These three dimensionless parameters include rock properties (permeability, thermal conductivity), heat generation rate per unit well length and geometrical parameters (the distance from the Earth's surface and the length of waste loaded part of the well).

Calculations were carried out for the following ranges for the dimensionless parameters

$$1 \leq Pe \leq 4 \quad , \quad 1.5 \leq C_\lambda \leq 6 \quad , \quad 0.5 \leq \delta_z = z_1 / 1 \leq 1.5$$

at

$$Le = 0.038 \quad , \quad \frac{\alpha_L}{1} = \frac{\alpha_L}{1} = 0.005 \quad , \quad \frac{\Delta T \lambda_r}{M \omega_0} = 0.45 \quad , \quad \frac{\Delta \tau_d}{Pe} = 0.0325 \quad .$$

The dependence of $\ln(K_{\max})$ (where K_{\max} is maximum dimensionless concentration of radionuclides in the groundwater at the Earth's surface) on Pe , C_λ , and δ_z was approximated numerically by the least squares method as

$$\ln(K_{\max}) = A_1 C_\lambda^{A_2} \delta_z^{A_3} \left(1 + A_4 \frac{\delta_z^{1.5}}{C_\lambda^{0.2}} + A_5 \frac{\delta_z^3}{C_\lambda^{0.3}} \right)$$

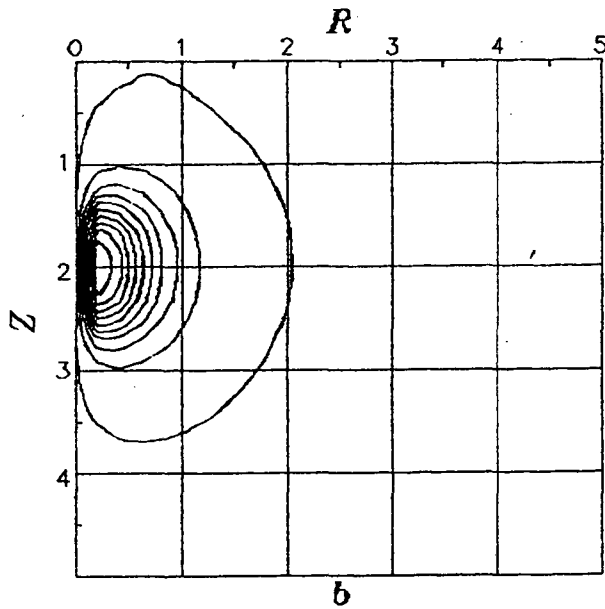
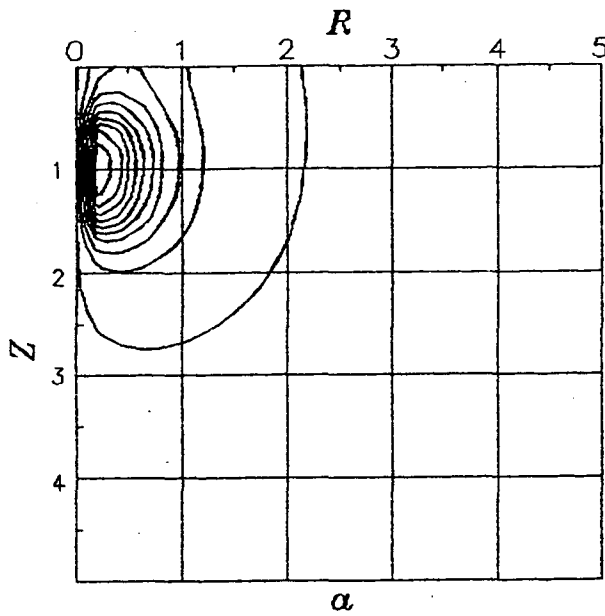


Fig.3. Stream lines. Flow function levels are taken from $0.01 \cdot \Psi_{\max}$ to Ψ_{\max} with a step $0.1 \cdot \Psi_{\max}$

$$Pe=20, r_d/l=0.002, \varphi=0.03, \alpha_T=\alpha_L=0.005 \cdot l,$$

$$\Delta\tau_d/Pe=0.02, \Delta T \cdot \lambda_r / (M\omega_0) = 0.45, \tau=0.6$$

$$a) Z_1=0.5, Z_2=1.5. \quad b) Z_1=1.5, Z_2=2.5$$

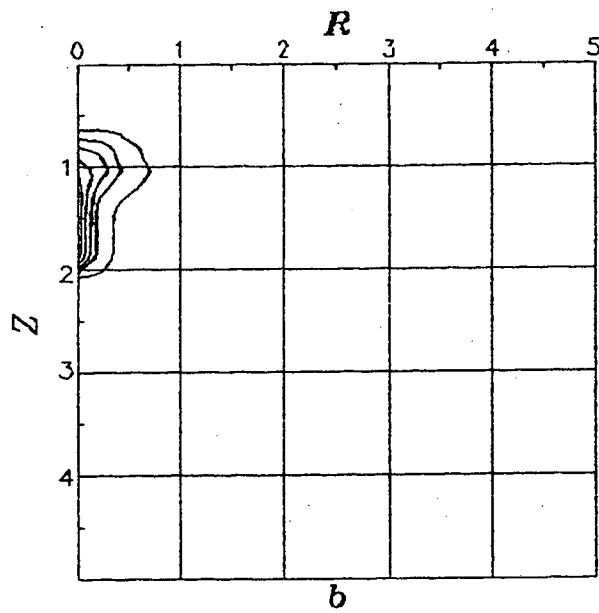
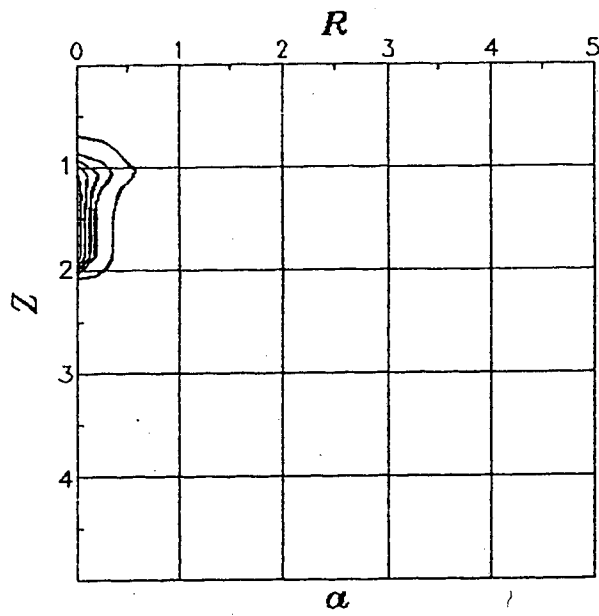


Fig.4. Equal concentration lines. Concentration levels are taken from $0.05 \cdot C_{\max}$ to C_{\max} with a step $0.2 \cdot C_{\max}$

$Pe=20$, $r_d/l=0.002$, $\varphi=0.03$, $\alpha_T=\alpha_L=0.005 \cdot l$,
 $\Delta\tau_d/Pe=0.02$, $\Delta T \cdot \lambda_T / (M\omega_0) = 0.45$, $Z_1=1$, $Z_2=2$;

a) $\tau=0.2$, b) $\tau=0.4$.

$$A_1 = 25.318 - 1.9137Pe - 0.07033Pe^2 + 0.01301Pe^3 ,$$

$$A_2 = 0.30793 - 0.08736Pe + 0.00911Pe^2 ,$$

$$A_3 = 1.2295 + 0.28938Pe - 0.01575Pe^2 ,$$

$$A_4 = 0.05194 - 0.01874Pe + 0.00540Pe^2^3 ,$$

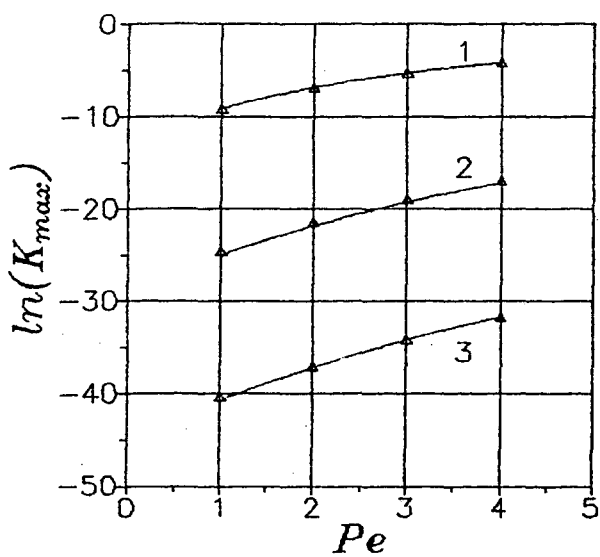
$$A_5 = -0.04893 - 0.01877Pe .$$

The results of the numerical calculations, when compared with the approximate analytical relationship are presented in Fig. 5. The approximation errors do not exceed 2.5%.

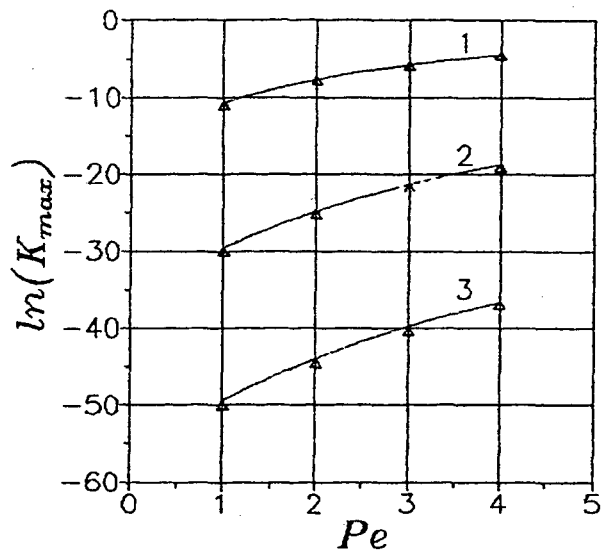
B. The Two Wells Model

Thermo convective transport processes occur when the wells are close to each other. An example of this effect is shown in Fig. 6. Isotherms are slightly extended in the direction of the second well (in the single well model isotherms are concentric with the well axis). But it is so only in that part of the region under consideration, which is affected by thermal perturbations from the second well. Thus, for the same parameter set, the temperature field in the vicinity of the first well (at a greater distance from the second well) is almost the same as for the single well. In particular, the maximum temperatures in the loaded part of the well (Fig. 7) are almost equal for the case of $h = 50$ m and $h = 1000$ m.

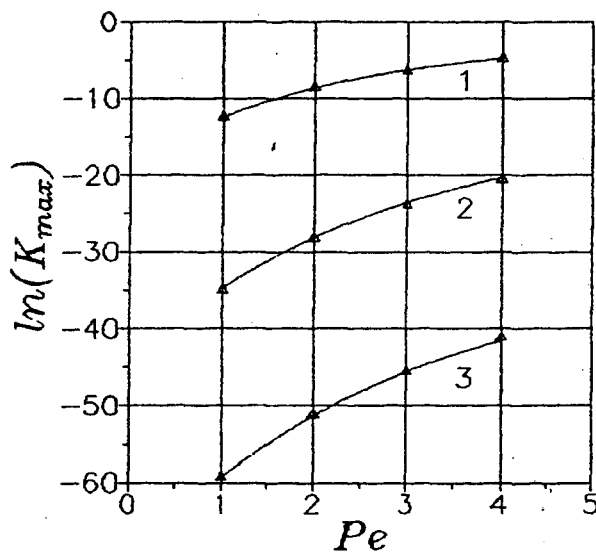
As is mentioned above, the maximum concentration of radionuclides at the Earth's surface, C_{max} , was accepted as a safety criterion. The plot given in Fig. 8 shows the relation of C_{max} for the two well model to C_{max} for single well ($h \rightarrow \infty$) model. It can be seen that processes of thermoconvective transport of radionuclides in the near field of the wells can be considered as practically independent for well separations of more than 100 m. In such a situation, an approximating expression obtained for the single well model can be used also for safety assessments for a repository represented by a regular set of the wells loaded with waste.



a



b



c

Fig.5. Comparison of approximating expression with the results of numerical modeling

1 - $\delta_2=0.5$, 2 - 1.0, 3 - 1.5;

a) $C_\lambda=1.5$, b) 3, c) 6

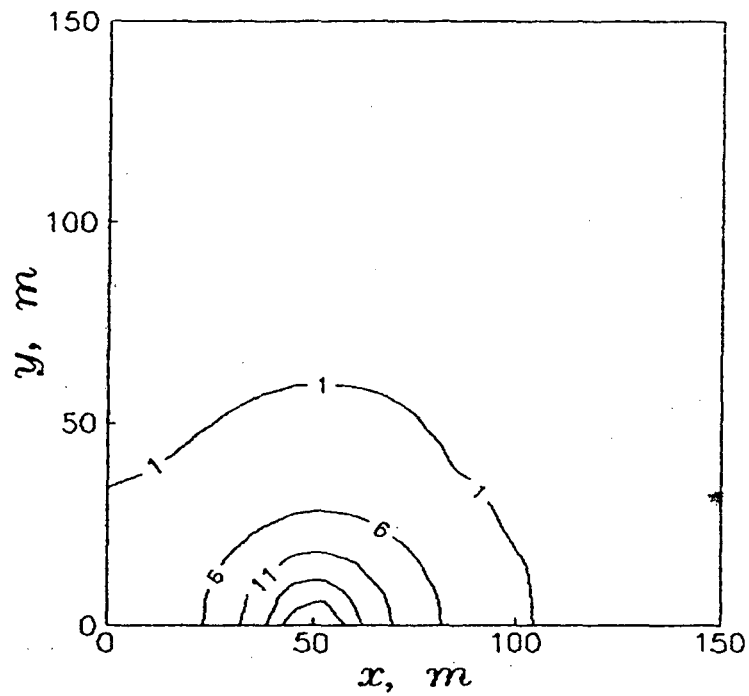


Fig.6. Isotherms in the plane $z=(z_1 + z_2)/2$ (horizontal section passing through the middle of the loaded part).

$$h=50\text{ m}, M\omega_0=250\text{ W/m}, z_1=l=500\text{ m},$$

$$k=10^{-16}\text{ m}^2, t=44.4\text{ years}$$

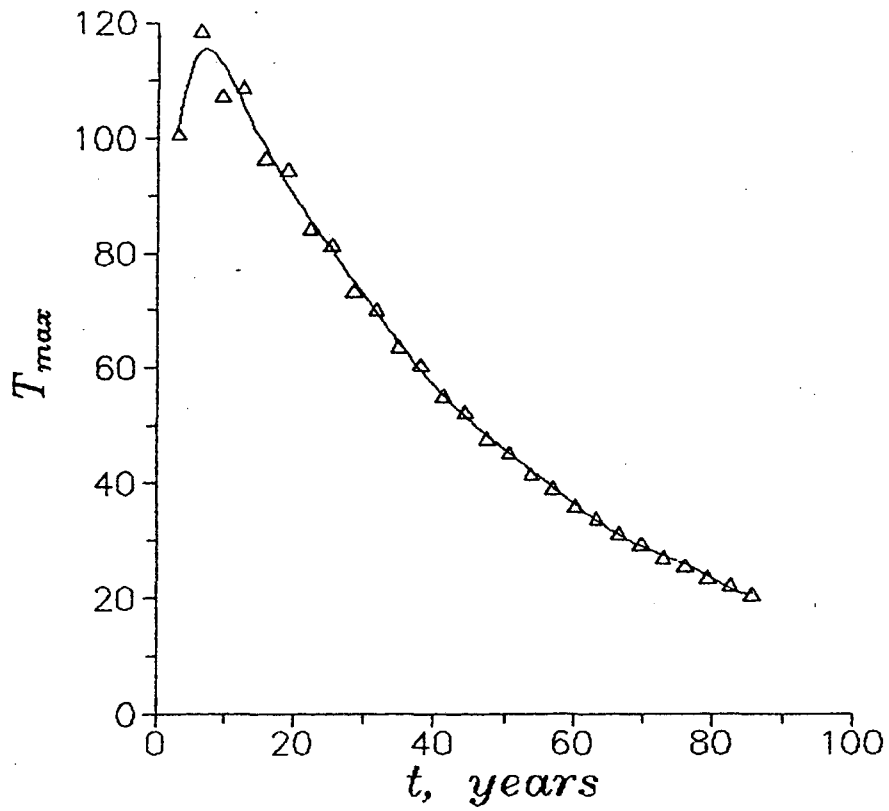


Fig.7. Time dependence of the maximum temperature in the loaded part of the well

$$M\omega_0 = 250 \text{ W/m}, k = 10^{-16} \text{ m}^2, z_1 = l = 500 \text{ m}, h = 50 \text{ m}.$$

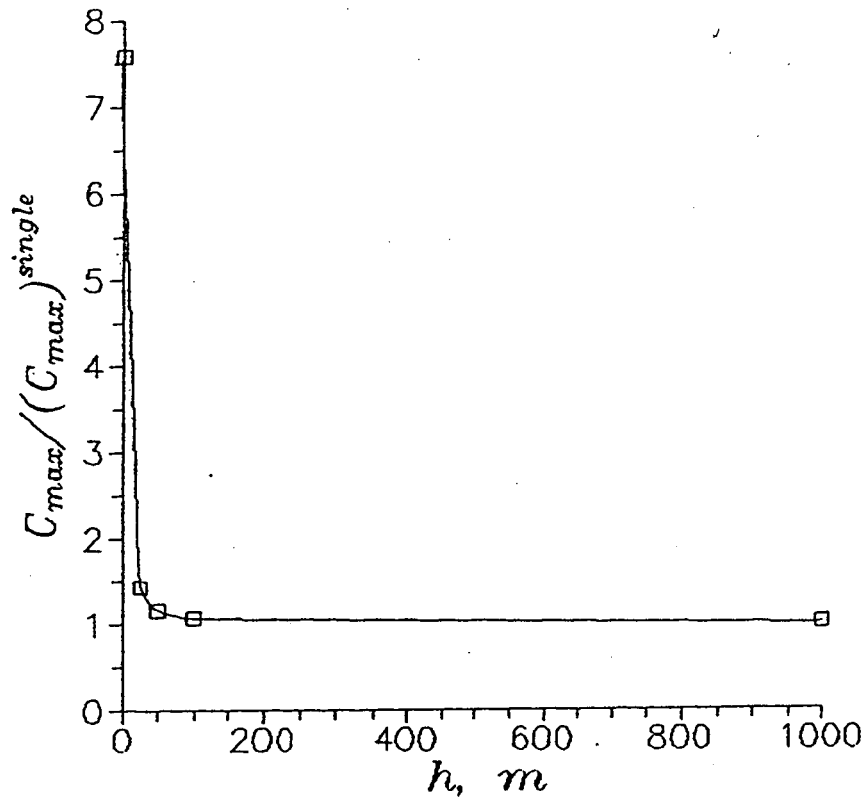


Fig.8. Inverse relationship of well spacing on radionuclide release

$$M\omega_o = 250 \text{ W/m}, z_1 = l = 500 \text{ m}.$$

5. Calculated Examples

It is worthwhile giving an example to show how the approximating expression could be applied for repository safety assessment. Let us consider the following case. Assume that the region of a repository site is given and, thus, the properties of the enclosing rocks are known. Let us assume that the waste loading per canister, the number of canisters emplaced in the well and the well depth are also known. Then the approximating expression permits calculation of the distance z_1 from the top level of waste disposal to the Earth's surface for the given set of safety criterion.

We assume that tuff is the enclosing rock. According to [5], the permeability, k , of tuffs is usually within the range 10^{16} – 10^{17} m^2 . Let us assume that $k = 10^{-16}$ m^2 . The thermophysical properties of water are taken from [5,15]

$$\rho = 10^3 \text{ kg / m}^3, c = 4200 \text{ J / kg} \cdot \text{K}, \beta = 15 \cdot 10^{-4} \text{ 1 / K}, \mu = 5 \cdot 10^{-4} \text{ Pa} \cdot \text{s},$$

$$\lambda_r = 1.26 \text{ W / m} \cdot \text{K}, \lambda = 0.6 \text{ W / m} \cdot \text{K}$$

whence $C_\lambda = 2.1$.

The dispersion parameters α_L, α_T and porosity ϕ are the same as in previous calculations (see subscripts to Figs. 3 and 4).

Waste heat generation at $t = 0$ is assumed, as in [5], to be equal to 2.16 kW/canister. Then if the repository is loaded in such a way that each canister occupies 2 m of well length, we obtain $M\omega_0 = 1080$ W/m. Suppose, also, that the number of canisters in the well is 250. Then $l = 500$ m and $Pe = 1.4$.

The dependence of K_{\max} on δ_z may be determined by using the approximating formula. A plot of this last dependence is presented in Fig. 9 (curve 1).

Let us assume further that the maximum concentration of radionuclides in the groundwater at the Earth's surface must not exceed the limiting concentration C_{lim} . Let us define K_{lim} as the quotient of C_{lim} divided by the scaling factor $\gamma C_{\text{sat}}(T_0)$.

$$K_{\text{lim}} = \frac{C_{\text{lim}}}{\gamma C_{\text{sat}}(T_0)}$$

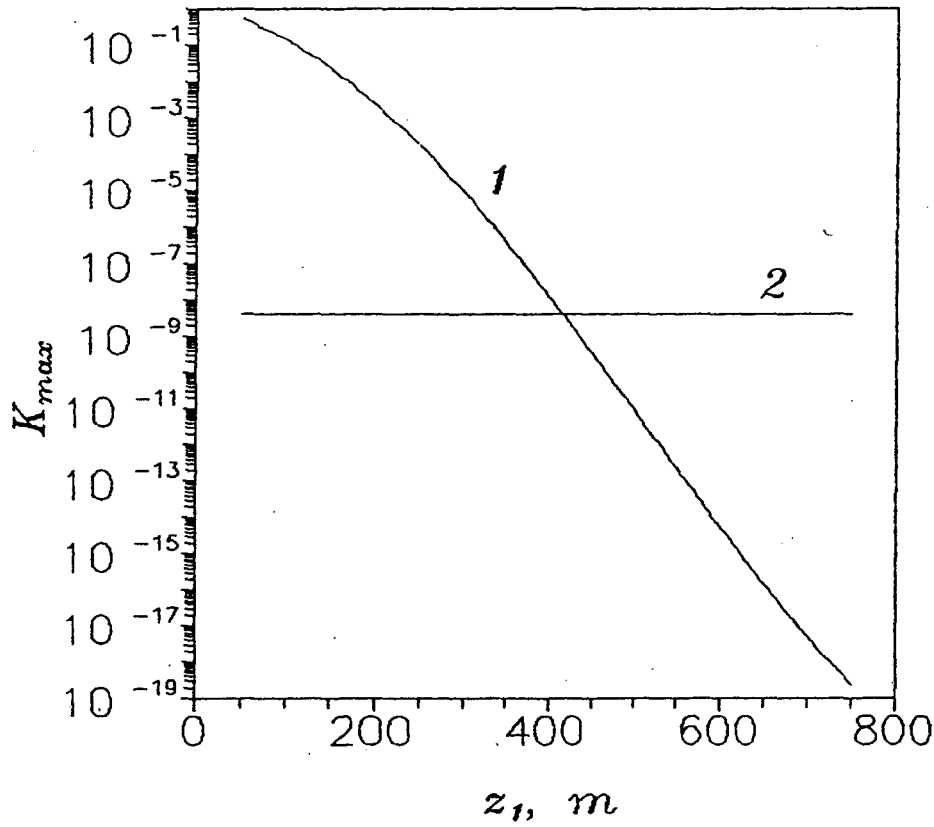


Fig.9. Calculation example.

1 - approximating expression,

2 - $K_{max} = K_{lim}$.

Let us select the isotope ^{90}Sr as an example. According to [14], the HLW weight fraction in the waste form is usually 10–35% and, according to [15], the weight fraction of ^{90}Sr in the HLW is about 5%. Then for ^{90}Sr we have $\gamma = 0.005 - 0.0165$. Assume that $\gamma = 0.01$ in our case.

From [9], $C_{\text{sat}}(T_0) = 5 \cdot 10^{-5} \text{ g/cm}^3$ at $T_0 = 20^\circ\text{C}$. For ^{90}Sr , $C_{\text{lim}} = 2 \cdot 10^{-15} \text{ gm/cm}^3$. Then $K_{\text{lim}} = 4 \cdot 10^{-9}$. Horizontal line 2 in Fig. 9 corresponds to this value. According to accepted safety criteria, the inequality

$$K_{\text{max}}(Pt, C_\lambda, \delta_z) \leq K_{\text{lim}}$$

should be satisfied.

It can be seen from the Fig. 9 that lines 1 and 2 cross each other at $z_1 \cong 430 \text{ m}$. This implies that the safety criterion is fulfilled when the top level of the waste loaded interval of the well lies at a depth greater than 430 m. Therefore, the depth of the well when $l = 500 \text{ m}$ must be more than 930 m.

6. Discussion

The example given above shows how the approximating expression obtained in this paper can be used for preliminary calculations in the design of an underground well repository for HLW. It is worthwhile mentioning that the model considered in this paper is “conservative” in that there is an added measure of “safety assurance” because the computer simulation was carried out for the most unfavorable case. All the canisters were assumed to be damaged, radionuclide retardation by an engineered barrier between the canisters and the wall of the well (e.g., bentonite, vermiculite, etc.), and sorption by the enclosing host rocks was not taken into account. Incorporation of these factors in a computer simulation could be readily achieved, but would make it impractical to generalize the results.

The models are an initial step in computer simulations of thermoconvective transport of radionuclides from a well type repository. The specific feature of the process as revealed by the above results is that the radionuclides concentration difference between the boundary of the well and the Earth’s surface differs by about ten orders of magnitude. This places rigorous requirements on the precision of calculations. For future developments of the model, therefore, it is reasonable to use the variable $\ln C$ instead of C (taking into account a nonzero background value of C) for calculation of radionuclide concentrations. The precision of the calculations will be much higher in such a case, because the range of $\ln C$ variation is much

less than that of C . But with such a substitution the equation of mass transfer becomes nonlinear with respect to $\ln C$ and the computational time increases, because an iterative procedure would be needed. Refinements should also be introduced in the formulation of the boundary conditions of the model. The rate of waste form leaching depends on the fluid flow velocity in the near-field of the repository. Therefore, the concentration of radionuclides in the fluid at the well boundary can differ from the concentration determined from the equilibrium condition of the waste matrix component.

Acknowledgments

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Figure Captions

- Fig. 1. Conceptual models. (a) Single well model. (b) Two well model.
- Fig. 2. Transformation to the new coordinate system. (a) Conformal mapping of the horizontal cross section of the considered region. (b) New coordinate lines in Cartesian coordinates.
- Fig. 3. Stream lines. Flow function levels are taken from $0.01 \psi_{\max}$ to ψ_{\max} with a step $0.1 \cdot \psi_{\max}$.
 $Pe = 20$, $r_d/l = 0.002$, $\varphi = 0.03$, $\alpha_T = \alpha_L = 0.005 \cdot l$, $\Delta\tau_d/Pe = 0.02$, $\Delta T \cdot \lambda_r / (M\omega_0) = 0.45$, $\tau = 0.6$.
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- Fig. 4. Equal concentration lines. Concentration levels are taken from $0.05 \cdot C_{\max}$ to C_{\max} with a step $0.2 \cdot C_{\max}$. $Pe = 20$, $r_d/l = 0.002$, $\varphi = 0.03$, $\alpha_T = \alpha_L = 0.005 \cdot l$, $\Delta\tau_d/Pe = 0.02$, $\Delta T \cdot \lambda_r / (M\omega_0) = 0.45$, $Z_1 = 1$, $Z_2 = 2$. (a) $\tau = 0.2$. (b) $\tau = 0.4$.
- Fig. 5. Comparison of the approximating expression with the results of numerical modeling. $1 - \delta_2 = 0.5$, $2 - 1.0$, $3 - 1.5$. (a) $C_\lambda = 1.5$. (b) 3. (c) 6.
- Fig. 6. Isotherms in the plane $z = (z_1 + z_2)/2$ (horizontal section passing through the middle of the loaded region). $h = 50$ m, $M\omega_0 = 250$ W/m, $z_1 = l = 500$ m, $k = 10^{-16}$ m², $t = 44.4$ years.
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- Fig. 8. Inverse relationships between well spacing on radionuclide release. $M\omega_0 = 250$ W/m, $z_1 = l = 500$ m.
- Fig. 9. An example of a calculation. 1 – Approximating expression, 2 – $K_{\max} = K_{\lim}$.

Nomenclature

C	concentration
C_λ	relative thermal conductivity of rock
c	specific heat
D	molecular diffusivity of nuclides in underground water
D_{ij}	dimensionless components of dispersion tensor
d_{ij}	components of dispersion tensor
g	free fall acceleration
K	relative concentration
k	permeability
l	length of loaded part
Le	Lewis number
M	waste mass per well length unit (for loaded part)
p	pressure
Pe, Pe_d	respective Peclet number for heat and mass transfer
r, z	cylindrical coordinates
t	time
Δt_d	half decay time
T	temperature
u, v	velocity coordinates

Greek Letters

α_L, α_T	longitudinal and transverse dispersion coefficients
B	coefficient of expansion
γ	mass part of nuclide in the matrix
δ_z	dimensionless distance between repository and Earth's surface
ϑ	$\ln 2 / \Delta t_d$ —decay intensity
α	dimensionless decay intensity
λ	thermal conductivity
μ	viscosity
ω	heat production of wastes per mass unit
ψ	flow function
θ	dimensionless temperature
ρ	density
τ	dimensionless time
φ	porosity

Subscripts

M	scaling factor, r - rock, O - initial, sat - saturated
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