

Conceptual and numerical modelling of density induced migration of radioactive contaminants at the Lake Karachai waste disposal site

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Abstract A modelling analysis of the major hydrodynamic mechanisms governing subsurface transport of brine containing radionuclides is performed for the Lake Karachai Waste Disposal site (Russia). Some results regarding the induced-density wave, and some indications regarding the media heterogeneity and relief of the base of the aquifer obtained by comparing simulation results and field measurements of the radioactive plume concentration, are presented.

PROBLEM DESCRIPTION

A radioactive waste disposal pond known as Lake Karachai serves as a major source of groundwater contamination in one of the South Ural provinces in Russia (Drozhko *et al.*, 1997a; Petrov *et al.*, 1994). The site under study is characterized by an unconfined volcanic-rock reservoir. The aquifer is recharged primarily by precipitation. The groundwater discharge area is associated with the river plains and lakes.

The water bearing rocks must be considered as a highly heterogeneous media. The transmissivity varies from 1 to 800 m² day⁻¹. Fractured porosity values at depths 0–100 m vary from 0.017 to 0.002 (0.005 on the average) (Belkin & Petrov, 1993; Drozhko *et al.*, 1997a,b). The porosity of the rock matrix ranges 0.2–0.7 % (Rumynin *et al.*, 1998).

The rate of leakage from the lake over the period of waste management has varied from tens to hundreds of cubic metres per day. The total volume of leakage is about 3.6 × 10⁶ m³. The wastes are radioactive and of high density. The latter is due to their salt content (mainly sodium nitrates) causing density variations from 1.01 to 1.09 g cm⁻³. The more dangerous radionuclides are: Sr-90, Cs-137, Co-60, and Ru-106.

The high-density of the waste, aquifer heterogeneity, and double porosity with no well-developed aquitard, have resulted in a complex three-dimensional (3-D) spreading of the plume. The plume moves towards the zones of groundwater discharge threatening surface water and groundwater well fields.

A GENERAL CONCEPT FOR MODELLING ANALYSIS

A comprehensive field study of the above-mentioned characteristics is difficult, time consuming, and very expensive. The use of mathematical models is probably one of

the very few viable options for bridging the gap between our incomplete knowledge of the site, and our capability for making predictions of future scenarios. Some strong *a priori* assumptions were introduced, based on indirect geological and structural information, such as the form of the base of the aquifer, as well as construction of a hydraulic conductivity profile with the help of pumping tests and borehole logging.

A set of alternative models incorporating different ideas on flow-parameters and geological and structural features of the strata seem to be a viable option for studying the contamination in the Mayak site. In our evaluation, both sharp interface DENSFLOW (Rumynin & Konosavsky, 1999) and complete mixing models, such as CODESA-3D (Gambolati *et al.*, 1999; Lecca, 1999), TOUGH2 (Pruess, 1991), and HST3D (Kipp, 1987) were used. The last three models were evaluated and furnished consistent results on benchmark problems (Gallo & Leonardi, 1999).

As previously mentioned, many processes are concurrent in determining the transport of the salty brine and radionuclides. The mass-transport potential is determined mostly by the bulk salt flux, which characterizes the content of the total dissolved solids and bulk density. Among the various dissolved salts, nitrate concentration is the dominant species, which affects brine density and serves as a major non-reactive marking component.

The calibration/validation procedures are aimed at identifying the parameters governing the bulk flow and brine transport, and those controlling radionuclide transport/retardation. This paper deals mainly with the first issue. This creates a basis for the further radionuclide transport analysis and forecasting.

For studying the brine migration a 3-D subarea ("window" model) was selected within the frame of a regional modelling domain (Fig. 1, Rumynin *et al.*, 1998). The domain is 10 250 m long, 9250 m wide, and 100 m high on average. In constructing the 3-D window model we assumed that eight zones of transmissivity (established on the basis of a geostatistical analysis of 200 pumping test data), were present. At this stage,

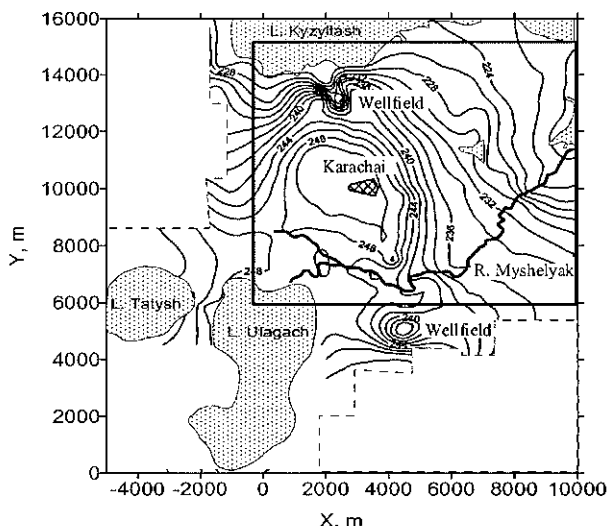


Fig. 1 The frame of the regional model and the area selected for the local ("window") model (elevations are metres above sea level).

the domain was assumed to be vertically homogeneous, leaving vertical heterogeneity for future work. The bottom of the domain was assumed not to be flat, given the depth of weathering variation over the area, i.e. the subsurface interface between the domain considered and the semi-permeable underlying aquitard undulates according to the surface elevation. Finally, we assumed that storage capacity is determined by both fractured and matrix porosity.

ANALYSIS OF THE DENSITY-FACILITATED TRANSPORT USING A SHARP-INTERFACE MODEL

The initial stage of modelling was based on an original computer code DENSFLOW (Rumynin & Konosavsky, 1999), which is a sharp-interface numerical simulator. This simulator is based on the solution of a coupled system of two PDE equations, one describing freshwater flow over the brine body, and the other modelling brine flow. The two equations are coupled together through the Ghyben-Herzberg relationship (Bear, 1972). The calibration of the flow/transport model was based on hydrodynamic and geochemical data of the regime of groundwater within the contaminated site.

Results indicated (Fig. 2) that the calculated freshwater potentiometric surface was in good agreement with experimental measurements, thus confirming that the transmissivity field and recharge rate distribution over the area are close to the actual hydrogeological characteristics of the site. The relief of the aquifer base and the structure of soil heterogeneity are the major factors controlling preferential flow paths of the brine movement. The combination of these factors forces the brine to move southwards, in the direction of the river valley (Fig. 2). The velocity of the advancing front of the plume for the transmissivity field given, is controlled by the effective porosity which was found to equal 1.5%, in close agreement with the sum of the fractured and matrix

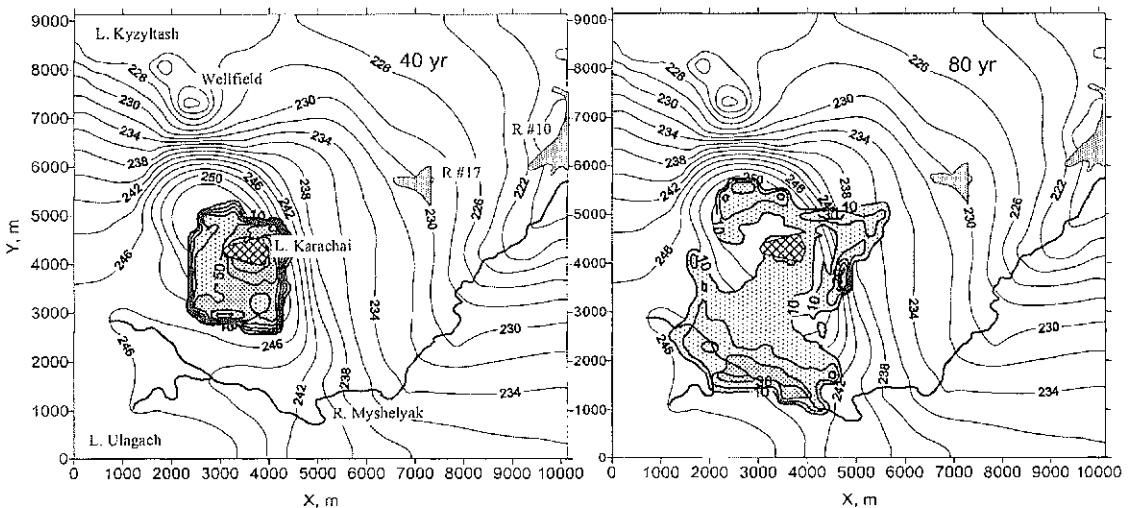


Fig. 2 The plume spreading as a result of DENSFLOW simulation for $t = 40$ and 80 (40 years after interruption of the brine leakage) years. The plume contours are thickness (m) of the brine body; the potentiometric surface of groundwater is represented in elevation (m) above sea level.

porosity of the domain. It should be noted, however, that limitations of the sharp-interface approach could lead to an excessively optimistic prediction of salt spreading. For example, vertical movement of the interface near the river valley cannot be simulated properly and this may lead to some errors in evaluation of the discharge of brine into the river. This motivated the use of a mixing model, as discussed below.

ANALYSIS OF THE BRINE TRANSPORT USING MIXING MODELS

Preliminary two-dimensional simulations of the plume spreading (homogeneous stratum test case) were performed using the CODESA-3D simulator (Gambolati *et al.*, 1999; Lecca, 1999). The CODESA-3D calculations were validated against those produced by TOUGH-2 (Pruess, 1991) and HST3D (Kipp, 1987) in a set of simulations under different conditions and using different grid resolutions. Results produced by the three codes were mutually consistent and the main concentration patterns were reproduced correctly. A few differences were found in terms of artificial dispersion introduced in the concentration isolines.

The Lake Karachai zone was schematized as in Fig. 1 (a detailed description of the test case can be found in Gallo & Leonardi, 1999). At this stage, a simplified contamination history has been considered: a contamination phase, during the first 40 years, a constant inflow of contaminant was considered to correspond to Lake Karachai. Then, for the following years, no inflow of contaminant is accounted for. Boundary conditions for the flow are partially described in Fig. 1; the bottom aquifer is assumed to be impermeable (its hydraulic conductivity is several order of magnitude less than that of the overlying layers). On the boundary of the domain a prescribed head is imposed. These values were obtained from previous regional modelling results in which parameter calibration was performed. At the top of the domain under study, a distributed natural recharge is considered.

The objectives of the numerical simulation are: mathematical 3-D description of a hydrogeological situation at the Lake Karachai site with respect to the nitrate groundwater contamination; and simulation of the spreading of the dense brine plume using a window model.

Initially the TOUGH2/EOS7 simulator was applied. The numerical scheme (EOS7 modular) is based on higher-order differencing methods, which minimize grid effects and smearing of concentration fronts from artificial (numerical) dispersion. Such methods can provide much better accuracy for modelling solute transport. However, the modular ignores the physical dispersion. The window model domain was discretized in 41 blocks along the x direction, 37 blocks in the y direction and 16 blocks in the z direction. Only horizontal heterogeneity was accounted for and only a single homogeneous physical layer was considered.

Figure 3 shows the evolution of the brine spreading at time $t = 40$ years, respectively, for the top and bottom layers. As expected, the plume reaches the bottom of the aquifer and begins to spread horizontally. The influence of the basal relief is quite evident (as also found using the sharp-interface model) and the plume tends to spread southward during the contamination period.

After interrupting the contaminant "injection", the brine continues to migrate preferentially in a southerly direction discharging into the river, although there is a weakly

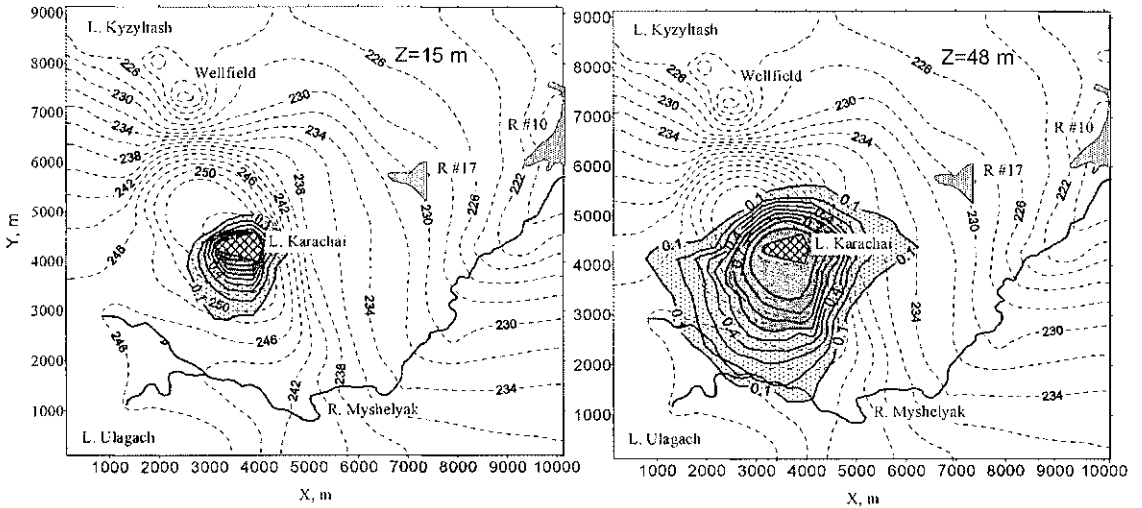


Fig. 3 The plume spreading as a result of TOUGH2 simulation for $t = 40$ years: left frame, $z = 15$ m below the surface; right frame, $z = 48$ m below the surface. The plume contours (solid lines) are dimensionless concentration of the brine; dashed lines are the potentiometric surface of groundwater in elevation (m) above sea level.

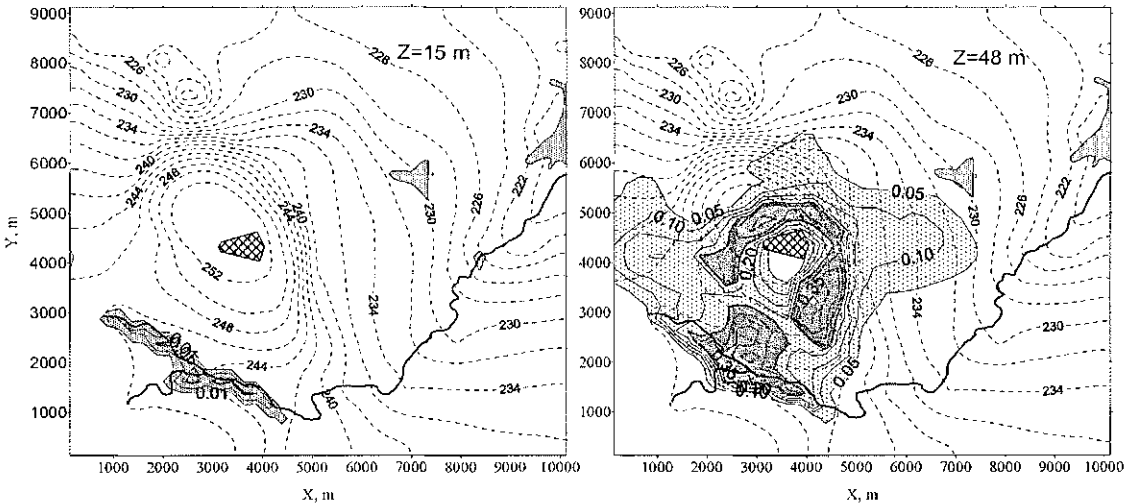


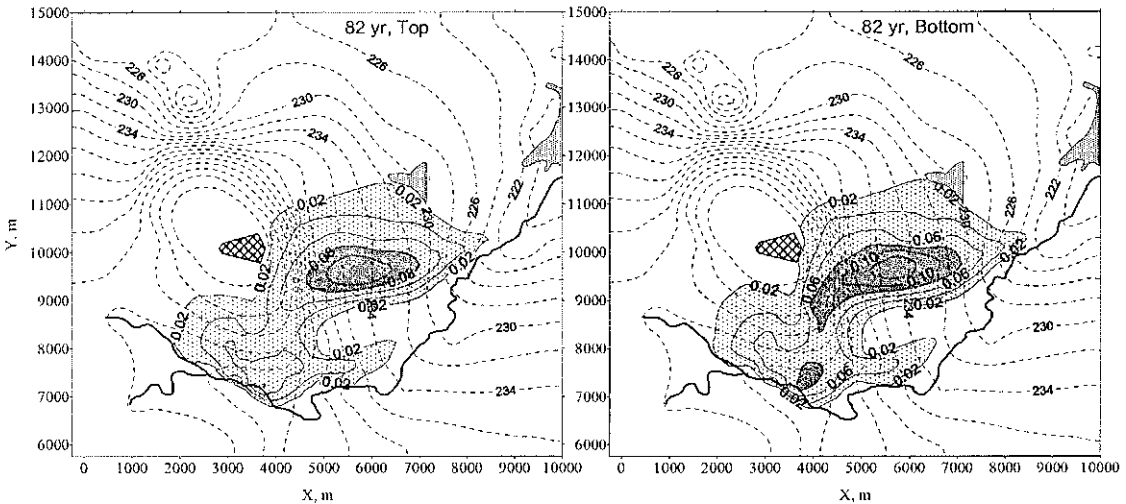
Fig. 4 The plume spreading as a result of TOUGH2 simulation for $t = 70$ years: left frame, $z = 15$ m below the surface; right frame, $z = 48$ m below the surface. The plume contours (solid lines) are dimensionless concentration of the brine; dashed lines are the potentiometric surface of groundwater in elevation (m) above sea level.

contaminated area (with low brine concentrations) which spreads eastwards (Fig. 4). There is a strong cross-sectional differentiation of the brine concentration due to the gravitation factor.

Then CODESA-3D code was used to show how large-scale dispersion phenomenon (values of the longitudinal and transverse dispersivity constants were assumed to be 100 and 20 m) could affect the transport process. The domain has been discretized

using a regular mesh with 82 subdivisions in the x direction, 74 subdivisions in the y directions, and 10 layers in the vertical direction, by means of a structured triangular mesh; 68 475 nodes and 364 080 tetrahedral elements composed the complete 3-D domain. So, a relatively high resolution of the model domain discretization was applied.

As Fig. 5 shows, the plume tends to dilute due to hydrodynamic dispersion and the brine concentration decreases. As long as the time advances, the salt concentration decreases and thus density effects caused by density differences between the brine and freshwater tend to fade and the plume spreads eastwards (Fig. 5). The dispersion effects noticeably smooth the brine concentration differences in the cross-section as well, and suppress the gravitation factor.



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