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DEVELOPMENT OF A MATHEMATICAL MODEL FOR CONTAMINATION MIGRATION IN THE AREA OF THE SULPHUR-TAR SLUDGE WASTE POOLS IN INCUKALNS, LATVIA

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Abstract: Mathematical modelling is a part of the remediation program approved by the Ministry of Environmental Protection and Regional Development of Latvia for two hazardous waste pools located in the vicinity of Incukalns, Latvia. The spatial model of contamination migration in groundwater from the pools has been developed by the team of the Environment Modelling Centre (EMC) of the Riga Technical University. Software tools used and results obtained are discussed.

Introduction

The hazardous acid sulphur-tar sludge was a refining process waste created from 1956 until 1981 by the Oil Processing Factory of Riga. Annually, about 16,000 tonnes of this liquid were transported 35 km out of Riga, and discarded into two abandoned sand pits situated between the Gauja River and its tributary Straume in the vicinity of the Incukalns village (Fig.1). As a result, these pits became open waste pools, each covering 1 - 1,5 ha. The two waste pools are informally referred to the Incukalns area Northern and Southern pools. In the centre of the plumes of the pools, pH is between 3 and 4, chemical oxygen demand reaches 1,800 mg/L, biological oxygen demand exceeds 100 mg/L, surface active compounds, which are the contaminant of concern, exceed 100 mg/L and SO_4 reaches 4,500 mg/L.

Both waste pools are situated in the important dune area characterized by high infiltration capacity from which considerable amount of groundwater originates. The dissolved waste species leak downward into the upper Devonian *D3gj2* and *D3gj1* sandstone aquifers used for drinking water supply (see Fig.2). Furthermore, dissolved pollutants in these aquifers migrate downgradient towards the Gauja River. The damage already done to the hydrogeological environment is enormous. The waste pools are located in the centre of the area where the best possible prospective well fields for supplying Riga with drinking water, should have been constructed (Spalvins et al. editors, 1996).

During the period following cessation of the liquid waste discharging, some investigations of the contaminant migration in groundwater were done and attempts made to lessen the environmental impact of Northern and Southern waste pools (Semjonovs, 1995; VIOGEM, 1991). For example, the Northern pool was covered by sand and during 1989-1991, about 90,000 m^3 of waterdiluted waste mixture from the Southern pool was injected into the lowest geological structures. Results of previous investigations, regarding both pools, were summarised and some new findings discovered, within the Latvian - Danish project (Aleksans et al., 1992; Aleksans et al., 1994; Levins et al., 1994).

To investigate the contaminant migration in groundwater in the Incukalns area, some hydrogeological models (HM) have been constructed (VIOGEM, 1991; Aleksans, 1995). The dissolved contaminant transport models (TM) and HM reported in this paper have been developed by the EMC team. They must serve as tools for planning and optimising remediation measures taken to clean-up the contaminated areas at Incukalns (RTU, 1998). These models are mainly based on materials provided by the above mentioned Latvian - Danish project, the report (Aleksans, 1995), and (Prols, 1998). As drivers for TM, three HM have been created: regional HM for the Incukalns area, and local HM for each pool.

The REMO system (Spalvins et al., 1996; Janbickis and Lace, 1997) developed by the EMC team was used for creating all three HM reported. The MT3D'96 code (Papadopulos, 1996) was applied for running TM, within the environment of the Groundwater Vistas (GV) program (ES, 1997). Advantages and limitations of the three above mentioned software tools are explained and obtained simulation results discussed.

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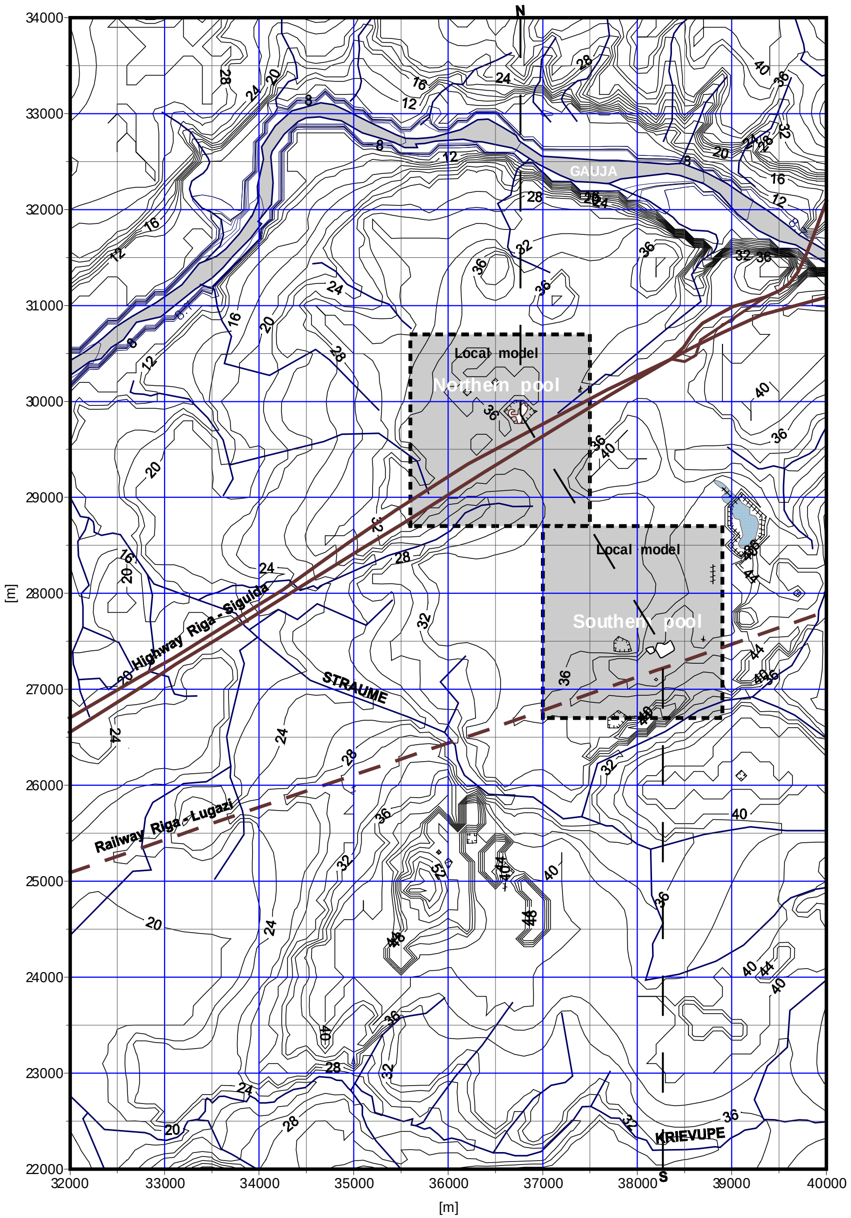

Fig.1. The area of the Incukalns regional hydrogeological model. Relief isolines and hydrographical network are shown.

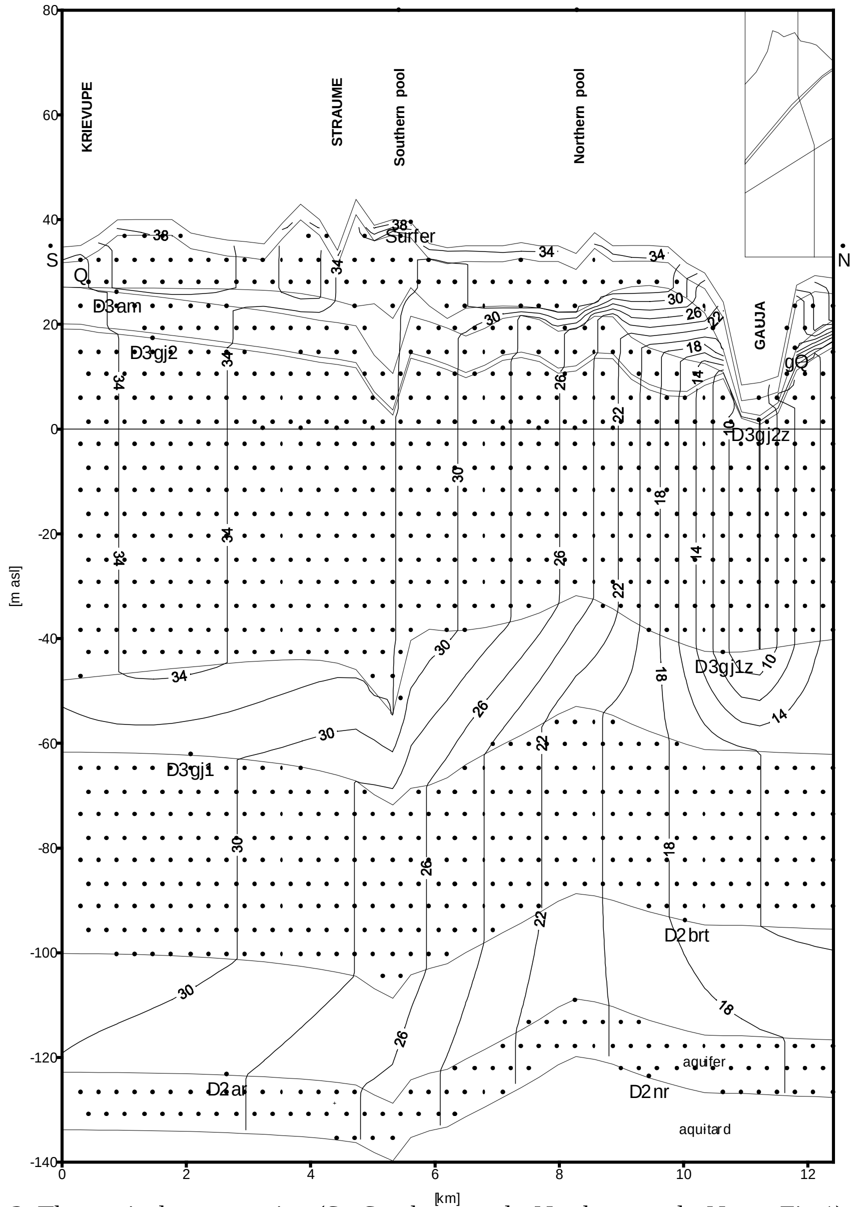

Fig.2. The vertical cross section (S - Southern pool - Northern pool - N, see Fig.1) of the Incukalns hydrogeological model. Isolines of hydraulic heads are shown.

Hydrogeological models

Regional HM covers an 8 km × 12 km area shown in Fig.1. In the vertical direction (see Fig.2), the quasi-three dimensional (3D) approximation scheme is used (Papadopulos, 1996): regional HM contains six joined rectangular planes accounting for four aquifers (*Q*, *D2am*, *D3gj2*, *D3gj1*) and two boundary condition surfaces (maps of the landscape relief *relh* elevations ψ_{rel} and the head distribution ψ_{D2ar} of the *D2ar* aquifer) on the HM top and bottom, respectively. Each of the planes is approximated by the uniform 81 × 121 grid of 100 m × 100 m blocks. Therefore, the 3D grid of HM contains 81 × 121 × 6 = 58806 nodes. On the four vertical sides of HM - the shell shaped by edges of the HM planes, the corresponding heads, as boundary conditions, are specified.

The REgional MOdel (REMO) "Large Riga" of the central part of Latvia (Spalvins et al., 1996) provided basic data regarding the conditions: ψ_{shell}, ψ_{D2ar} and properties of the Devonian sandstone aquifers *D3am* , *D3gj2* , *D3gj1* . HM of the Incukalns area includes exactly 24 blocks of 2 km × 2 km from the "Large Riga". Now, the abbreviation REMO is conditionally applied to the modelling system which has been developed by the EMC team during the "Large Riga" project (Janbickis and Lace, 1996; Janbickis and Lace, 1997), and applied within the reported project.

On the regional HM base, more detailed local HM for each of the pools have been created (see Fig.1). Both of them cover 1.9 km × 2.0 km areas approximated by 20 m × 20 m grid blocks. Each local HM contains 96 × 101 × 6 = 58176 nodes.

In REMO, the steady state mean annual head distribution φ in nodes of the HM grid is found as the solution of the following algebraic equation system:

$$A\,\varphi = b\ , \qquad A = A_{xy} + A_z - G\ , \qquad b = -\,G\,\psi + \beta \tag{1}$$

where the matrices A_{xy} , A_z and G represent transmissivities of aquifers, vertical grid links accounting for influence of aquitards and elements connected with piezometric boundary conditions ψ , respectively; β is the vector of water withdrawal in wells. In REMO, this vector does not include the infiltration flow through the unsaturated aeration zone *aer* which is represented by a formal aquitard (Fig.2). The infiltration flow there is driven by the difference between the ground surface *relh* elevations ψ_{relh} and heads φ_Q of the unconfined quaternary sand aquifer Q.

Elements a_{xy} , a_z of the matrices A_{xy} , A_z of (1) are computed by using digital maps of thickness (m , m_0) and permeability (k , k_0) of aquifers and aquitards, correspondingly:

$$a_{xy} = km\ , \qquad a_z = h^2\, l\ , \qquad l = m_0 / k_0 \tag{2}$$

where h is the uniform grid plane step; l is the leakance of an aquitard.

The thickness (m , m_0) - distributions should be obtained as the difference between the elevations of the neighbouring bottom surfaces of geological strata. The full set of these maps describes the geometry of HM.

The Geological Data Interpolation (GDI) program developed as a part of REMO (Spalvins and Slangens, 1994) was applied for creating digital maps of: permeability (k , k_0), the HM geometry and the boundary condition ψ distributions of (1). For example, the ψ_{relh} map (Fig.1) is created by GDI, using elevation isolines and the hydrographical network as information carriers.

When the system of (1) for any HM of Incukalns is prepared, its solution can be obtained in tens of seconds if a Pentium II type (166 MHz) personal computer is used.

Because all three HM for the Incukalns case were created by using the REMO system, the following problem arose: to run corresponding TM, it was necessary to insert these HM into the environment of the GV code which joins MODFLOW (represents HM) and MT3D'96 (serves as TM) programs. The export of REMO data to the GV system does not go smoothly, because the leakance l - distribution of (2) may get seriously damaged during this process. This fault of GV is due to the outdated zone principle used there for saving a computer memory. In GV, roughly 10,000 zones are available for storing maps of the HM geometry, permeability k and leakance l distributions. In all HM of Incukalns, the leakance of aquitards varies nearly 10^6 - fold, throughout HM. Therefore, no guaranty exists that such l - distributions will be properly repeated in GV by MODFLOW.

There is no principal need to use the REMO code, as a pre-processor for the GV program, because MODFLOW may be applied to the creation of all HM involved. However, REMO was applied because of the following advantages provided by this system:

- all maps of HM can be obtained from initial data by the GDI program which is in perfect synchronism with REMO; consequently, the impact of human caused errors is greatly reduced;
- all initial data (points, lines, areas) are presented in a most general grid independent vectored form;
- irregularly located data can be interpolated from/to nodes of an HM grid (Lace et al., 1995);
- boundary conditions, on the HM shell surface, are mostly generated and concorded by the system itself;
- vertical cross sections can be built, along a line of any form chosen (see Fig 2).

We are going to comment, in more details, the above mentioned problems of creating boundary conditions on the shell of HM, and of the vertical cross sections.

When one deals with a complex hydrogeological situation, then piezometric boundary conditions ψ_{shell} , on the shell of HM, cannot be specified directly on the whole surface, because of the following reasons:

- the values of ψ_{shell} , along the edge of an aquifer, are not always known for the full length of the edge;
- an uncertain situation arises when, within some fragments of the edge, an aquifer or aquitard cease to exist ($m = 0$ or $m_0 = 0$).

In REMO, the above problem is solved by converting the shell of HM into a universal interpolation device which computes the unknown distribution ψ_{shell} , in all nodes of the shell, by applying the known values ψ_{shell} , as initial data. The matrix G of (1) is also accounted for during this process.

One can notice that, in Fig.2, all isolines of the head are vertical within an aquifer, as it should be, if the vertical head gradient there is assumed to be nil. The isolines have their breaking points, on interfaces of aquifers and aquitards, as it should be, in accordance with the groundwater flow hydraulics. None of this two proper features of this REMO product are present in the vertical cross sections created by the GV code. This fault may have some influence on simulation processes of the mass transportation in groundwater.

Transport models

The MT3D'96 code, driven by various HM of Incukalns, was used for simulating TM (Papadopulos, 1996). By computing concentration c - distribution versus time t , this code accounts for the following elements of the dissolved mass transport in groundwater: advection, sorption, destruction and diffusion. The method of characteristics (MOC) was chosen, as the optimal one, for all TM of Incukalns. No diffusion was accounted for, because the MOC method itself possesses a considerable numerical dispersion. The following TM regimes were tested for both waste pools in regional and local HM: advection only, as the worst possible case; sorption with the retardation coefficient $R = 8.2$; sorption ($R = 8.2$) and the first order destruction (half life time $t_{0.5} = 6000$ days). Both values ($R = 8.2$ and $t_{0.5} = 6000$) were taken from (Semjonovs, 1995), as the characteristics of rather conservative surface active constituents (detergents) of the acid waste.

During the last five years, the concentration of dissolved waste products in the close vicinity of both pools, has decreased about ten times. This fact may be explained by a possible natural encapsulation of the pools due to the reduction of the permeability of *Q* and *D3am* aquifers there. This phenomenon was accounted for, in the MT3D'96 code, by a gradual lowering of the relative concentration values of both pools from $c = 100$ % to 10 %. Regional TM was applied for making long term contamination migration prognoses for both waste pools. Modelling confirmed the rough estimate (Aleksans, 1995; Aleksans, 1996) that at the area of the Northern pool, directions of the contaminant migration in *Q* and *D3gj2* aquifers are almost apposite (see Fig.3). At the area of the Southern pool, directions of the contaminant movement in *Q* and *D3gj2* aquifers almost coincide (see Fig.3). In the vicinity of this pool, heads φ_Q and φ_{D3gj2} are practically equal due to the influence of hydrogeological windows, in the aquitards *gQ* and *D3gj2z* there. Modelling shows that the contamination risk of the *D3gj1* aquifer, due to the downward recharge, is higher in the case of the Southern pool. Moreover, it is shown in Fig.2 that the aquitard *D3gj1z* there has a rather deep local lowering. It has been observed (Aleksans et al., 1994) that, within this underground pit, a pool of dense sulphates has formed, due to the gravitational sedimentation of waste species. This process in no way is accounted for by the MT3D'96 code, because it ignores the influence of the dissolved waste density.

The principal danger caused by both waste pools, is the downgradient migration of pollutants towards the Gauja River, in the *D3gj2* aquifer. In the most pessimistic case (only advection accounted for), dissolved waste species may reach Gauja, in about 50 and 150 years for the Northern and Southern pools, respectively. In Fig.3, the computed relative concentration distributions formed within 10,000 days in the *D3gj2* aquifer, are shown. Results of (RTU, 1998) confirm that, practically, no dissolved waste species can reach the Gauja River, if sorption and destruction processes are accounted for.

Local TM of waste pools may be used for investigating processes in smaller areas which are connected with simulation of various clean-up processes and protective barriers. However, no attempt was made, within the reported project, to simulate various remediation schemes proposed (Aleksans, 1996).

The following limitations of the MT3D'96 code were observed when the MOC method of the mass transport simulation was applied:

- the contaminant mass balance is unsatisfactory;
- no prognoses longer than for 15,000 days may be obtained, because then computations are stopped automatically, when some of stability criteria (usually, unknown to modeller) are not met;
- even before the computations are cut, obvious indications of the solution instability can be observed: irregular oscillations of computed concentrations at observation wells, appearance of isolated non-zero concentration spots, abrupt jumps of mass balance parameters.

However, in spite of difficulties mentioned above, the results provided by the MT3D'96 code were quite reasonable. They may be used, as a guide, for planning remediation measures for the contaminated Incukalns area.

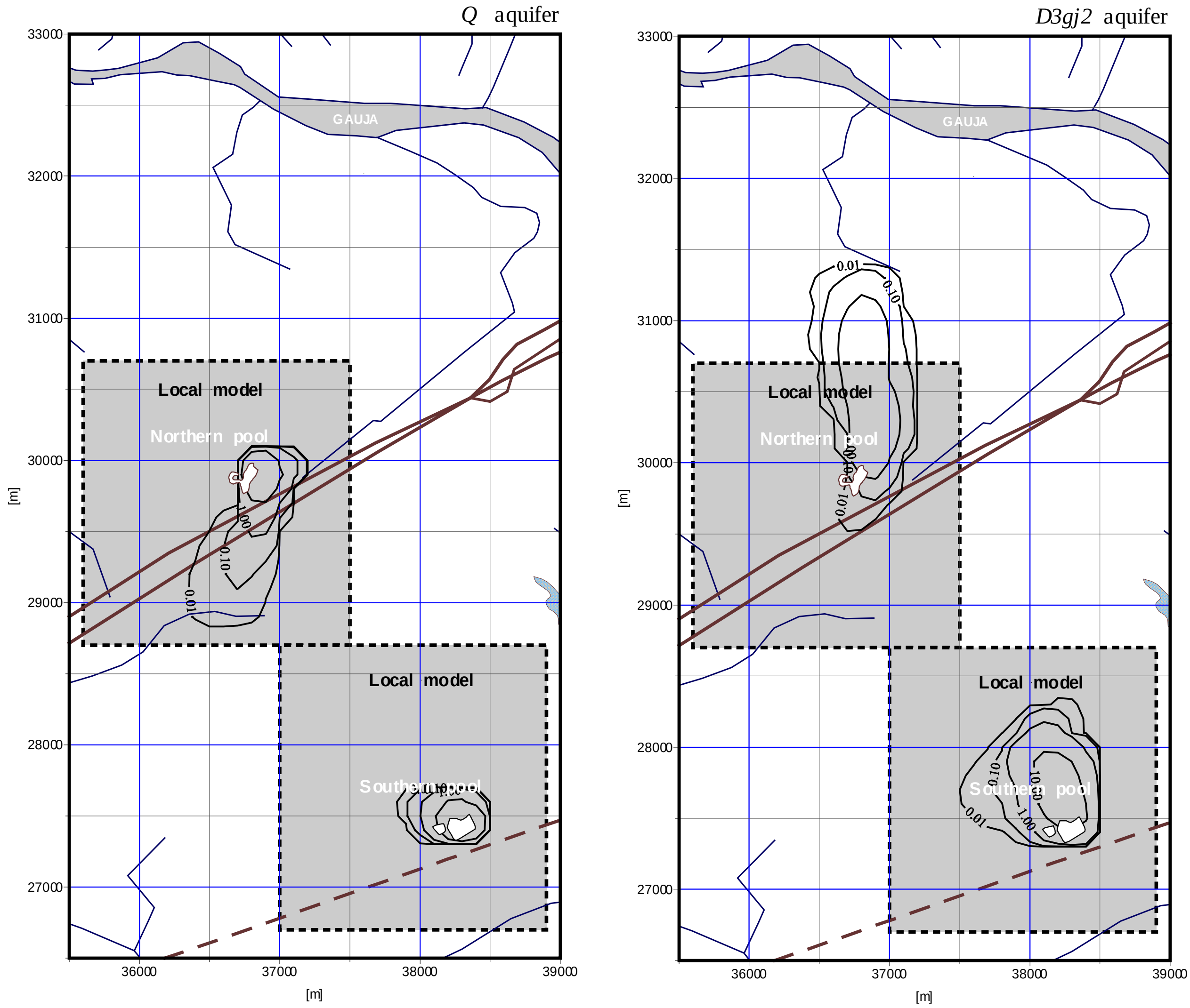

Fig.3. Relative concentration distributions in *Q* and *D3gj2* aquifers after 10,000 days, if only advection is accounted for. The logarithmic scale for contouring isolines c = 10, 1, 0.1 and 0.01 is used.

Conclusions

Regional and local hydrogeological and transport models have been developed for investigating contamination of groundwater by various dissolved acid sulphur-tar components in the area of Incukalns, Latvia.

These models considerably improve understanding of hydrogeological processes in this area, and will serve as tools for planning and optimising remediation measures.

Hydrogeological and transport models are open for possible corrections and improvements. For example, within the regional hydrogeological model, the local models of constructed waste storage places can be created. Their degree of risk may be evaluated on regional and local scales.

The REMO system developed by the Environment Modelling Centre of the Riga Technical University has proved to be an excellent software tool for creating hydrogeological model of complex objects.

The Groundwater Vistas and MT3D'96 codes were used to run simulation processes of the contaminant migration in groundwater. However, it was necessary to check-up these simulation results regularly, in order to sort out the uncertain ones caused by some limitations and faults of both codes.

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