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Numerical Modelling of the Contaminated Former Black Fuel Storage Area Effect in Latvia: a Case Study

A. Spalvins, I. Lace, K. Krauklis, D. Pipira, S. Karusa, I. Retike, M. Mame, L. Fibiga

Abstract – *In the town Valmiera of Latvia, the abandoned former black fuel storage area was not inspected before on the area contamination and its effect on the quality of groundwater at the storage environs. In 2016-2017, the storage area was investigated. In 2017, the quality of groundwater in the area environs was estimated and the oil contamination migration was explored by means of numerical modelling. The local hydrogeological model was developed jointly by specialists of the Latvian Environment, Geology and Meteorology Centre and Riga Technical University. The model was created by extracting information from the HM of Latvia LAMO4 and by supplying and reshaping its regional data by detailed information on the model area. The results of modelling ensure that in the closest storage area environs the groundwater quality has been only slightly worsened and no pollution of the nearby river should happen. Methods of developing and using the local hydrogeological and contaminant migration models may be useful for specialists dealing with groundwater contamination problems.* ***Copyright © 2020 Praise Worthy Prize S.r.l. - All rights reserved.***

Keywords*:* *Contaminated Groundwater, Dissolved Oil Products, Hydrogeological Model, Modelling Of Contaminant Migration*

Nomenclature

HM	Hydrogeological Model
LAMO4	HM of Latvia
GV	Groundwater Vistas - 6
x, y, z	Coordinates for 3-dimensional space [m] for x, y; [m asl] for z
h	Plane step of HM grid [m]
u	Number of layers in HM grid
i	Number in turn of i-th layer
δ, δ_i	Thickness of geological layer, of i-th layer [m]
k, k_i	Permeability of geological layer, of i-th layer [m/day]
K_i, j=1,2,3,4	Factors of k-map [m/day]
z_0, z_i	Elevation of HM top surface, of i-th layer bottom [m asl]
φ, φ_i	Vector of piezometric head which components are found in nodes of HM grid, in i-th layer of HM [m asl]
ψ, ψ_{rel}, ψ_{river}	Vector of boundary conditions for piezometric head, for relief, for long profile of river [m asl]
β	Vector of boundary conditions for flows [m^3/day]
A, A_{xy}, A_z	Matrix of hydraulic conductivities for links of HM grid, for horizontal and vertical links [m^2/day]
a_{xy}, a_z	Elements of A_{xy} and A_z [m^2/day]
G, G_{river}, G_{Aer}	Matrix (part of A) that assembles links connecting nodes of HM grid with boundary conditions ψ, with ψ_{river} , with ψ_{rel} [m^2/day]
V	Volume [m^3]
C	Contaminant concentration [mg/m^3]
C_r	Relative contaminant concentration [%]
$BTEX$	(Benzene, Toluene, Ethylbenzene, Xylenes) oil contamination marker [mg/m^3]
M	Mass of contaminant [g]
MCL	Maximal concentration level above which a contaminant poses a health concern [mg/m^3]
$MCLG$	Maximal concentration level goal at which adverse health effects would not occur [mg/m^3]
q_x, q_y, q_z, q_{river}, q_{Aer}	Flows of a grid block, base flow of river, flow in aeration zone Aer [m^3/day]
γ_x, γ_y, γ_z	Flow velocities on surfaces of a grid block [m/day]
v_z	Infiltration [mm/year]
p	Porosity
t	Time [day]
$t_{0.5}$	Half-life time of contaminant [day]

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I. Introduction

Computer modelling is applied for predicting effects of groundwater contamination [1]. The abandoned former black fuel storage area in the town Valmiera of Latvia (Fig. 1) was chosen as the pilot site for groundwater contamination modelling. The research was carried out jointly by the Latvian Environment, Geology and Meteorology Centre (LEGMC) and Riga Technical University (RTU) as the part of the Central Baltic project INSURE (Innovative Sustainable Remediation) [2]. The storage area is situated in the town southern part named Kaugurmuiza (Fig. 2). The river Gauja which may be polluted is located ~1800 m far from the storage. In 2016-2017, the company "Vides konsultaciju birojs" (VKB) investigated the area and provided data on the area contamination by oil products and on the site hydrogeological features [3]. To carry out the research, the local HM was developed by specialists of LEGMC and RTU. The HM size was 2500 m×2800 m (Fig. 2).

The information obtained by VKB, the borehole data provided by LEGMC and the regional data extracted from LAMO4 [4], [5] were used. The local HM, like LAMO4, was run in the modelling system GV [6] environment where its parts MODFLOW [7], MODPATH [8] and MT3D [9], accordingly, supported HM, simulated the contamination movement and transportation in the groundwater flow. For visualization of simulation results and the initial data processing, the program SURFER12 [10] was applied.

In Fig. 3, the VKB investigated area of the trapezium form is shown. It covers ~15000 m^2. The area was divided in four polygons A_1-A_4 where two kinds of wells U and DZ were established. In the Quaternary aquifer Q, the wells (U_1, U_2,…, U_{11}) were used for monitoring the groundwater contamination and head. The deeper wells DZ_1, DZ_2, DZ_3 were used for monitoring groundwater head in the primary sandstone aquifer D2brt. By using the local HM and by applying MODPATH and MT3D programs, it was found out that the groundwater from the contaminated area fled towards the river Gauja and the oil products could reach it in ~60 years. Then the BTEX concentration due to the dilution in groundwater, may decrease ~2000 times. The river Gauja will not be endangered even if the initial storage area contamination has been much larger then presently.

Fig. 1. The area of HM LAMO4 and location of the town Valmiera

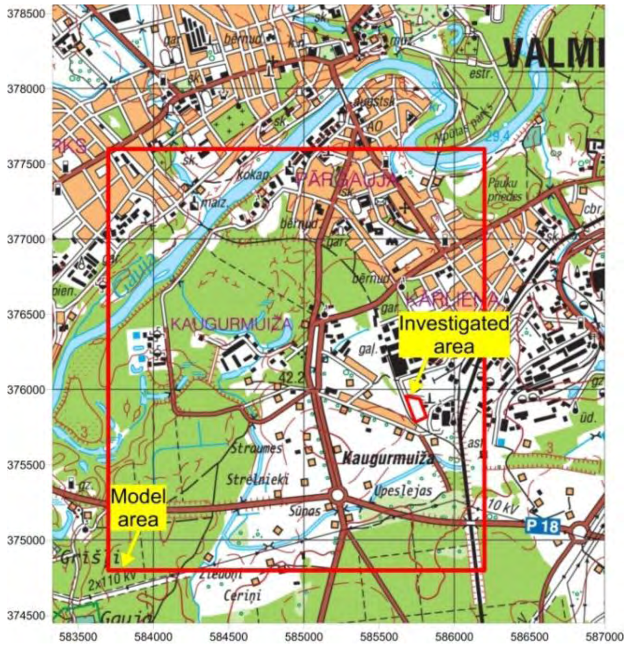


Fig. 2. The HM location in the town Valmiera

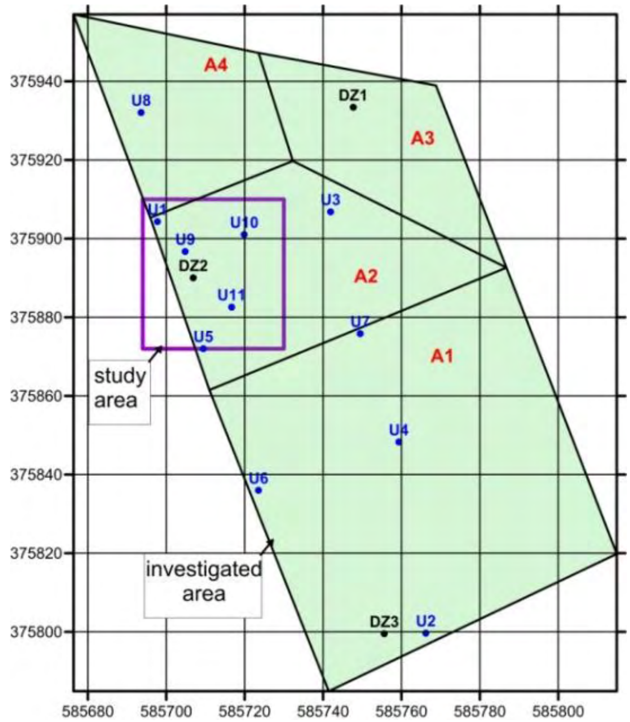


Fig. 3. Locations of the investigated and study areas. The arrangement of wells U, DZ and of the polygons A1, A2, A3. A4 are shown

For the groundwater samples, complex analyses including BTEX were done.

The permeability k_Q of the aquifer Q was estimated [3]. The BTEX data within the study area were used as the initial ones for modelling.

In Sections II and III of the paper, accordingly, the HM construction and calibration are described. The results provided by HM by using the MODPATH and MT3D programs are reported in Sections IV and V, correspondingly.

Section VI presents the discussion on the research results.

The paper ends with the Conclusion (Section VII), Acknowledgements, Authors biographies, References and the Appendix. In the Appendix, complex figures are presented.

They are related to the Section II (groundwater head and infiltration distributions, flow balance of HM) and to Section V (concentration distributions after 25 and 60 years, concentration hydrographs in monitoring posts).

II. The Hydrogeological Model Construction

By applying the 3D finite-difference approximation of the geological environment, the xyz-grid of HM was built.

It contained the ($h\times h\times\delta$) sized blocks (h=10 metres was the constant plane approximation step, δ was the variable thickness of a geological layer).

The grid nodes were located in the block centres. In Table I, the HM vertical schematization is shown. The model included 11 grid planes.

To ensure credible results of the contaminant transport modelling, the aquifers Q and D2brt were divided in three subaquifers.

In the primary Devonian layers D2brt and D2ar, HM simulated the average hydrogeological situation. For the Quaternary aquifer Q, the summertime conditions in 2017 were used.

The MODFLOW program provided the 3D distribution of groundwater head for the boundary field problem that was approximated in nodes of the xyz-grid of HM as the solution φ of the algebraic equation system [4], [11]:

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

where φ is the groundwater head vector; β and ψ are the boundary flow and head vectors; A is the symmetric sparse hydraulic conductivity matrix for geological layers; it contained horizontal and vertical conductivities A_{xy} and A_z of layers, accordingly.

The values of their elements a_{xy}, and a_z for the i-th plane of the HM grid were obtained by using the formulas [4]:

$$\begin{aligned} &a_{xyi} = k_i\delta_i,\ a_{zi} = h^2 k_i / \left(\delta_i + k_i\delta_{i+1} / k_{i+1}\right), \\ &\delta_i = z_{i-1} - z_i \geq 0,\ i = 1, 2, ..., u,\ u = 11 \end{aligned} \tag{2}$$

where u is the number of the HM grid planes; z_{i-1} and z_i are the digital elevation maps of the top and bottom surfaces, accordingly; z_0 represents the digital relief map which is also applied as the boundary condition of the head ψ_{rel} on the top surface of HM; the full set of the u+1=12 z-maps describes the geometry (stratigraphy) of the local HM; δ_i, k_i are the digital δ and k-maps of thickness and permeability, accordingly; δ_{i+1}, k_{i+1} are these maps for the next underlying (i+1)-th plane of the HM grid.

The digital relief map ψ_{rel} was obtained from of the Latvian Geospatial Information Agency (LGIA) [12] and the ψ_{D2ar} map was taken from LAMO4 [4], [5]. The diagonal matrix G (part of A) assembles the elements linking the grid nodes where φ must be found with the locations where ψ is given.

Appliance of the head maps as boundary conditions is reported also in [13], [14]. The top and bottom planes of HM were used for fixing the boundary conditions ψ_{rel} and ψ_{D2ar}, accordingly.

The thickness of the both aquifers was 0.02 m. These boundary condition ψ-maps were connected with the subaquifers Q3 and D2brt1 by the sets of vertical elements a_{z2} and a_{z10} of the aquitards Aer and D2arz, accordingly.

The flows q_{river} for the river Gauja and the Kaugurmuizas brook are simulated, as follows [4]:

$$q_{river} = G_{river}\left(\phi - \psi_{river}\right) \tag{3}$$

where G_{river} is the diagonal matrix (part of G) that assembles the elements linking the boundary conditions ψ_{river} (long profile of a river) with the nodes of the HM grid.

These links control the interaction of the HM body with rivers [15].

The flow q_{river} represents the groundwater inflow in a river as its base flow. The boundary condition for flows β was not applied to simulate the infiltration flow q_{Aer} on the HM top.

Due to appliance of the ψ_{rel} –map as the boundary condition the flow q_{Aer} is computed automatically by HM, as follows [4], [5], [13], [14]:

$$q_{Aer} = G_{Aer}\left(\psi_{rel} - \phi_{Q3}\right) \tag{4}$$

where G_{Aer} is the set of vertical elements a_{z2}; φ_{Q3} is the head distribution for the subaquifer Q3.

Initially, the right values of the G_{Aer} elements are unknown.

They must be found in the course of the HM calibration.

Then for the aeration zone which is used in HM as a formal aquitard, the fitting distributions of δ_{Aer} and k_{Aer} were obtained (Section III). The q_{Aer} map is the most complex one.

It includes areas of various ascendant and descendant flows.

Perhaps, no modeller is able to guess – work such a map, especially, if the β –flow boundary condition is used.

The appliance of the ψ_{rel} –map is allowable when the climate is humid.

Then mainly the earth surface controls the groundwater recharge and discharge.

TABLE I
VERTICAL SCHEMATIZATION OF THE HYDROGEOLOGICAL MODEL

HM plane No.	HM plane name	HM plane code	Permeability [m/day]	Thickness [m]	Notes
1	Relief	Rel	10.0	0.02	ψ_{rel} – map is boundary conditions
2	Aeration zone	Aer	7×10^{-3}–2×10^{-6}	0.5-14.0	Aquitard
3	Quaternary	Q3	0.3 and 3.0	0.1-5.8	Bed of Kaugurmuizas brook; For Gauja alluvium k=3.0 m/day
4	Quaternary	Q2	0.3 and 3.0	0.1-7.2	For Gauja alluvium k=3.0 m/day
5	Quaternary	Q1	0.3 and 3.0	0.1-7.2	Bed of Gauja river; For Gauja alluvium k=3.0 m/day
6	Quaternary	gQ	1.5×10^{-4}	0.02-4.8	Aquitard
7	Burtnieks	D2brt3	1.2-3.0	15.5-17.8	Bed of Gauja river; For Gauja alluvium k=3.0 m/day
8	Burtnieks	D2brt2	1.2-1.6	15.5-17.8	
9	Burtnieks	D2brt1	1.2-1.6	31.0-35.6	
10	Arukila	D2arz	2×10^{-3}	25.2-27.0	Aquitard
11	Arukila	D2ar	10.0	0.02	ψ_{D2ar} – map is boundary condition

For arid or permafrost conditions, the relationship (4) cannot be applied [14]. The MODFLOW program provides the set of velocities γ_x, γ_y, γ_z on the HM grid block surfaces. The velocities are used by the MODPATH and MT3D programs. The *q*-flows q_x, q_y, q_z are related to the corresponding velocities, as follows [7]:

$$q_x = h\delta y_x,\ \ q_y = h\delta y_y,\ \ q_z = h^2 y_z \tag{5}$$

The *q* –flows are ingredients in the solution process of (1). They are used for the mass balance calculations where the groundwater inflows in rivers and lakes are also included. The velocity γ_z –map presents the infiltration on the top surface of an HM plane. For the sake of perceptibility, the infiltration, like a precipitation, has the dimension mm/year. The dimension conversion from m/day into mm/year is defined by the formula:

$$v_z = 3.65\times10^5\gamma_z \tag{6}$$

where v_z is the notation for an infiltration given in mm/year. In HM, the k and δ-maps extracted from LAMO4 were used (Table I). By accounting for the borehole data provided by LEGMC, the top surface of the Devonian aquifer D2brt3 was adjusted. For the aquifers Q and D2brt3, the alluvium deposit (*k*=3.0 m/day) for the river Gauja was accounted for. For the sandy loam aquifer Q, *k*=0.3 m/day was used [3]. In the area where the aquitard gQ did not exist, the thickness δ_{gQ}=0.02 m was used. When for the GV system, the *k* and *z*-maps and the ψ–conditions were prepared, the MODFLOW program created HM which provided the necessary results. The most important of them are the φ and v_z – maps and the *q*–balances which, accordingly, as Fig. 1A, Fig. 2A and Fig. 3A are included in the Appendix. In Fig. 1A, the digital relief ψ_{rel} –map as the boundary condition is shown. The area in colour represents the river Gauja alluvium location. The φ_Q – map is presented for the aquifer Q. Within the area in colour, the aquitard gQ does not exist. The φ_{D2brt} –map for the aquifer D2brt is exposed. The ψ_{D2ar} –map, as the boundary condition for the HM bottom, is shown.

By comparing the φ_Q and φ_{D2brt} distributions, one can notice that within the area where the aquitard gQ does not exist, the above distributions practically coincide. In the part where the aquitard gQ exists, they differ considerably, because the Kaugurmuiza brook notably affects the φ_Q distribution there.

In Fig. 1A, the borehole U11 location is shown. There the maximal BTEX concentrations in groundwater were found.

In Fig. 2A, the infiltration v_z –maps for the HM planes Q3, D2brt3, D2brt2, D2arz are shown. For the planes Q3 and D2ar, due to constancy of q_z within aquitards, the infiltration maps coincide with the ones of the overlaying aquitards Aer and D2arz, respectively. By comparing the above v_z –maps, one can notice that downwards the positive and negative infiltrations, accordingly, decrease and increase.

This feature can be displayed numerically if the GV option "Mass balance" is used. The complete, abridged and local groundwater flow balances for HM and its planes are shown in Fig. 3A. The HM balance includes the elements: q_z–flow, q_{river}-flow and the q_{xy}-flow which represent the lateral groundwater flux through the HM area border.

The flow balance may also include q_{lake} for lakes and q_{wells} for groundwater extraction wells. These flows are not presented in HM. For the complete balance case (Fig. 3A), all elements for the plane top and bottom q_z –flows are exposed.

One can to find out that the downward (positive) flow gradually decreases from 2118.7 m^3/day on the top of Q3 to 11.6 m^3/day on the bottom of D2brt1. The upward (negative) flow increases from 4184.0 m^3/day to 170,1 m^3/day, accordingly, on the bottom of D2brt1 and on the top of Q3. For the abridged balance, the sums of flows on the plane top and bottom surfaces of subaquifers are found. They certify the resulting q_z–flows on these surfaces. For the local balance, the sum of top and bottom flows is found for each layer. The balance characterizes its groundwater transfer and consumption. By considering the abridged HM balance, one can conclude that the flows q_{river}=5514.1 m^3/day and q_{border}=609.9 m^3/day are supported by the infiltration flow q_{inf}=1948.6 m^3/day (~100 m^3/year) and the flow q_{D2ar}=4172.4 m^3/day from the aquifer D2ar. The flow q_{river} has three parts: 217.9 m^3/day of the Kaugurmuiza brook, 608.8m^3/day and 4687.4 m^3/day of the river Gauja from the subaquifers Q1 and D2brt3, correspondingly.

III. Calibration of the Hydrogeological Model

To create the local HM where h=10 m, the regional data provided by LAMO4 (h=250 m) were supplemented and reshaped by accounting for the detailed local information. It included the refined digital relief map ψ_{rel} that contained the Kaugurmuizas brook, the revised surface z_6 of the plane gQ was used, the river Gauja alluvial deposit (k=3.0 m/day) was implemented, the permeability k_Q=0.3 m/day for the aquifer Q was applied.

In the storage area, as the calibration targets, the groundwater heads φ_Q=46.0 m asl and φ_{D2brt}=43.5 m asl were used, accordingly, for the aquifers Q and D2brt.

The observed thicknesses δ_{Aer}=2.0 m and δ_Q=14.0 m were applied for the aeration zone Aer and for the saturated part of the aquifer Q, correspondingly. Due to this requirement, finding the z-maps for the HM Quaternary planes u=2, 3, 4 turned into the calibration task. By considering Table I, it can be found that the z-maps for the planes u=1, 2, …, 5 can be obtained, as follows:

$$\begin{aligned}&\delta_{Aer}=0.5,\quad \text{if } \Delta\phi<0 \quad K_3=\delta_{Aer}/0.5\\&z_1=\psi_{rel}-0.02,\;\; z_2=z_1-\delta_{Aer},\; z_3=z_2-4\delta_Q/14,\\&z_4=z_3-5\delta_Q/14,\;\; z_5=z_4-5\delta_Q/14,\;\; \delta_Q=z_2-z_5\end{aligned} \quad (7)$$

where the z_2 –map must be found by calibrating the variable thickness δ_{Aer} –map. The plane Q1, Q2, Q3 thicknesses share in 4/14, 5/14, 5/14, accordingly, was determined by their thicknesses δ_{Q3}=4 m, δ_{Q2}=5 m, δ_{Q1}=5 m, in the storage area. The calibration was carried out by finding the variable k-maps that matched the calibrations targets. The k-map was presented by the product of the factors K_j (j=1, 2, 3, 4) [16]:

$$K=K_1K_2K_3K_4 \quad (8)$$

where K_j were diagonal matrices. They controlled the permeability in the nodes of the HM grid planes. Values of their elements were 1 or any other ones if the node permeability remained invariable or it got changed, accordingly.

The unity matrix elements are 1. The factor K_1 is a variable scalar. Its value characterizes the primary quality of the plane permeability. The matrix K_2 accounts for specific local changes in k. The factor K_3 is used in the case when the m-maps must be altered.

The factor K_4 accounts for changes in k, which are caused by the calibration of infiltration flows. For the calibrated HM, the values of K_j elements are shown in Table II where the four variable factors are applied only for the aeration zone Aer. For the other HM planes, two or three factors are the unity matrices. The factor of K_1 has the dimension m/day but the factors K_2, K_3, K_4 are dimensionless The calibration was performed in three steps. For the first step, δ_{Aer} =0.5 m and δ_{Q2} = δ_{Q1} = 0.02 m. For the plane Aer, K_2 = 1.0 and 0.001, K_3 = K_4 =1.

The value 0.001 is used for the locations where the river Gauja and the Kaugurmuizas brook are attached to the plane Q1, in order to decrease there the influence of the relief ψ_{rel}. By using k_{Aer}=2×10^{-3} m/day, k_{gQ}=1.5×10^{-4} m/day and k_{D2brtz}=2×10^{-3} m/day, the targets for the groundwater heads were matched.

During the second step, the true thickness δ_{Aer} and the factor K_3 were found by using the procedure:

$$\delta_{Aer}=\Delta\phi,\quad \text{if } \Delta\phi>0 \quad \Delta\phi=\psi_{rel}-\phi_{Q3} \quad (9)$$

By using the formula (7), the true surfaces z_3, z_4, z_5 were found. To suppress in HM some unnaturally large flows q_{Aer}, the third calibration step is performed by finding the factor K_4:

$$\begin{aligned}&K_4=\left(2.5/\delta_{Aer}\right)^{0.9},\;\; if\ \delta_{Aer}>2.5;\\&K_4=1,\;\; if\ \delta_{Aer}<2.5\end{aligned} \quad (10)$$

In the hilly areas, before using the factor K_4, the infiltration v_{Aer} was above 700 mm/year.

IV. Results Provided by the MODPATH Program

The contaminant travel time depends both from the hydraulic conductivity matrix A of HM and from the porosity p [17]. For all layers of HM, the assumed porosity p=0.12 was used. The MODPATH program was applied to investigate the contaminant movement in groundwater from the well U11 in the plane Q3 towards the river Gauja. The program computed the pathline locations in time and space of the water particle that moved within the groundwater system simulated by the calibrated HM. The MODPATH program controls the particle movement by using the velocities γ_x, γ_y, γ_z of (5).

The results are shown in Fig. 4. During the first 15 years, the particle reaches the D2brt3 plane and makes only 40 metres. The velocity γ_{xy}=(γ_x^2+γ_y^2)$^{0.5}$~0.007 m/day is small, due to low k=0.3 m/day of the aquifer Q. For the next 45 years, the particle attains the river Gauja. Its track length is ~1800 m. In the D2brt3 plane, during the 35 years, the particle goes down due to the descending q_z (Fig. 2A, Fig. 4). There γ_{xy}~0.07 m/day. In the alluvium part of the D2brt3 plane, the particle climb is caused by the ascending q_z. During the last ten years, γ_{xy} ~0.22 m/day. The MODPATH program does not provide information on the contaminant concentration and the mass change in time and space. These data were obtained by the MT3D (Mass Transport 3D) program (Section V).

It evidently follows from considering the results shown in Fig. 4 that the MODPATH program provides the most important predicative information for a case to be investigated.

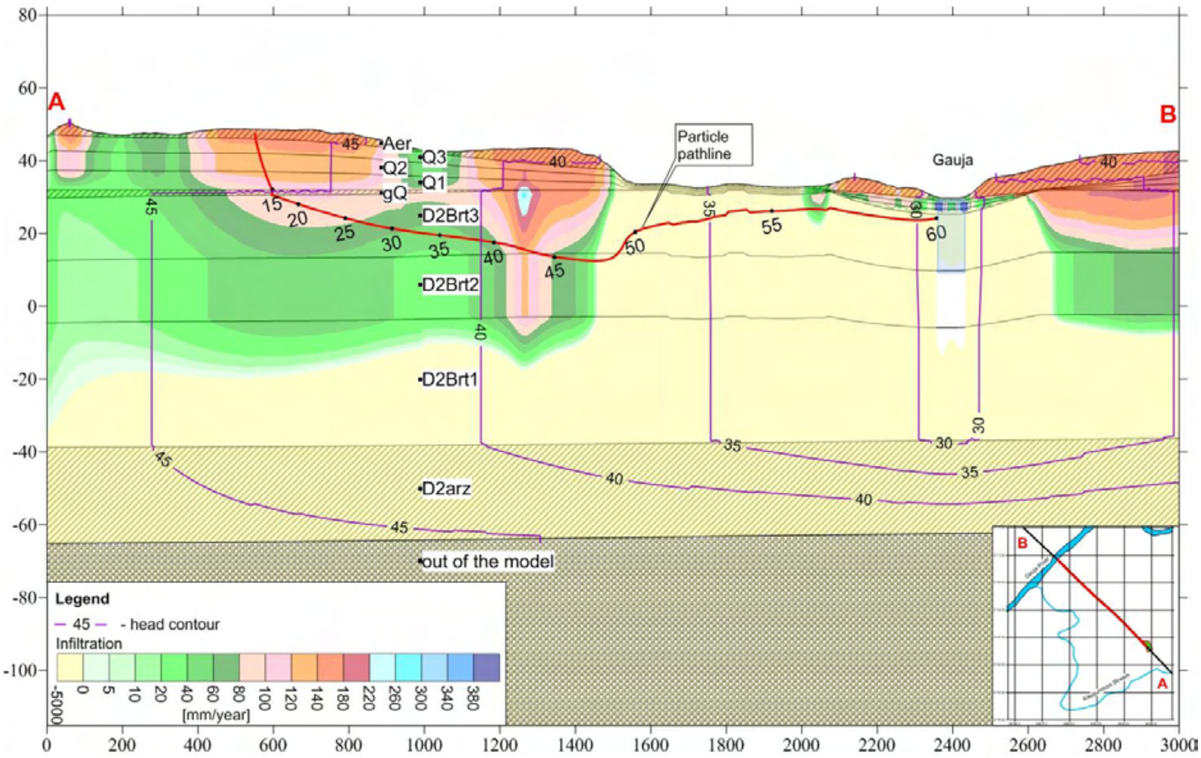


Fig. 4. The section A-B along the MODPATH pathline. The groundwater head isolines [m asl], the infiltration [mm/year] and the particle travel time [years] are shown

It was reported in [18] that appliance of the MODPATH program with the HM for the south-eastern part of Lithuania provided very impressive results on its geochemistry. In [19], the case of the Iecava river was investigated by using the MODPATH program with the HM of Latvia LAMO4 for searching sources of the river base flow. In [20] the MODPATH system was applied for investigation of pumping/injection wells.

Before any appliance of the most complex MT3D program, in order to organize properly its various control parameters, the MODPATH program must be used, because it roughly predicts the contaminant plume movement in time and space.

V. Results Provided by the MT3D Program

No information on contamination and spill accidents in the storage during its action (~30 years) and in its environs after the storage closure (~30 years) was available. For this reason, only computer modelling of the case by using the MT3D program, allowed to estimate the storage area effect on its environment [21].

TABLE II
VALUES OF ELEMENTS FOR THE FACTORS K_1, K_2, K_3, K_4

Factor code	No of HM planes 1	2	3, 4, 5	6	7	8,9	10	11
K_1	10.0	2×10^{-3}	0.3	1.5×10^{-4}	1.0	1.0	2×10^{-3}	10.0
K_2	1.0	1.0 and 0.001	1.0 and 10.0	1.0	1.2-3.0	1.2-1.5	1.0	1.0
K_3	1.0	1.0-27.8	1.0	1.0	1.0	1.0	1.0	1.0
K_4	1.0	0.2-1.0	1.0	1.0	1.0	1.0	1.0	1.0

For modelling, the BTEX concentration was used. Its component concentrations were found [3]. In [22]-[24], the appliance of BTEX as the important oil contamination marker for evaluation of the contamination effect, age and depletion rate is considered. To use the MT3D program, the actual data on the contaminant location and distribution must be applied. It was found out that only in the wells U_1, U_{10}, and U_{11} the concentration of the BTEX elements were above MCLG established by the regulations [25]. For this reason, within the study area of the size 36 m×38 m=1368 m^2 (Fig. 3), the concentrations in these wells were processed by the Kriging interpolation method [10].

The results are presented in Table III. $C_{\max}$ is the concentration [mg/m^3] in the well U_{11}; C_{mean} is the mean concentration [mg/m^3] in the study area; C_s is the concentration [mg/m^3] in the three contaminant source blocks located in the well U_{11} vicinity; M is the contaminant mass [g].

The study volume V in the plane Q3 has the size: V=1368 m^2 ×4 m×0.12=656.69 m^3 where 4 m –the plane Q3 thickness, 0.12 –porosity.

TABLE III
SUMMARY ON THE GROUNDWATER CONTAMINATION

Features	Benzene	Toluene	Ethylbenzene	Xylenes	BTEX
1	2	3	4	5	2+3+4+5
$C_{\max}$	5.30	1.60	1.80	12.80	21.50
C_{mean}	1.33	0.74	0.84	6.81	9.72
C_s	6.07	3.37	3.83	31.05	44.32
MCL	5.00	50.0	60.0	60.0	175.0
MCLG	0.20	0.50	0.50	0.50	1.70
M	0.87	0.49	0.55	4.47	6.38

The mass M of contaminants within V is obtained, as follows:

$$M = VC_{mean}10^{-3} \quad (11)$$

It is obvious from the data of Table III that the actual mean BTEX concentration 9.72 mg/m^3 is considerably smaller than the MCL=175.0 mg/m^3 defined by [25]. The BTEX mass is only M=6.38 grams. To simplify the contamination source which should be presented by the various interpolated BTEX concentrations in the 16 grid nodes within the study area, it contained only three nodes where the concentration $C_s = C_{mean} \times 1368/300=44.32$ mg/m^3. The source was located in the Q3 plane. In order to obtain general results, it was assumed that the relative source concentration C_{rs}=100%. Then the MT3D program computes the relative concentrations C_{rt} that can be used for obtaining the real C_t:

$$C_t = C_s C_{rt} 10^{-2} \quad (12)$$

If C_{rs} = 100% then for the MT3D program, M_{rs}=100 kg=10^5 g. The computed M_{rt} and the real M_t are related, as follows:

$$M_t = MM_{rt}10^{-5} = MR, \; R = M_{rt}10^{-5} \quad (13)$$

where R is the dimensionless parameter which graphs are shown in Fig. 5 for three numerical experiments. The summary on the numerical experiment features is presented in Table IV. It was assumed that if the contamination source was active, its concentration was kept constant. For the third experiment, the source was removed after the first 25 years. For the second experiment, the contaminant decay in groundwater was accounted for by using $t_{0.5}$=10 years. The dispersion option was not applied, because the method "finite difference" that was used to carry out the experiments, itself possessed the considerable numerical dispersion [9]. The "finite difference" method correctly simulated the contaminant mass changes in space and time. The time step 73 days (0.2 years) was used for all three experiments. It follows from considering the R–graphs of Fig. 5 that for the first and the second experiment, the source graph is the linear function which shows the increase of contamination amount injected in groundwater. The contaminant mass in groundwater is smaller than the injected one. For the first experiment, the R–graph becomes almost flat (R ~4.8) when the contamination plume enters the river Gauja after 60 years (as predicted by MODPATH). Some amount of contamination discharges in the alluvium area and reaches the ground surface after ~25 years (Fig. 4A). If the contaminant decay is accounted for (the second experiment) then the R–graph reaches R ~ 1.1 and does not change after the first 25 years. When the contaminant source is removed after the first 25 years (the third experiment) then the R–graph goes down due to the discharges in the alluvium area and in the river Gauja.

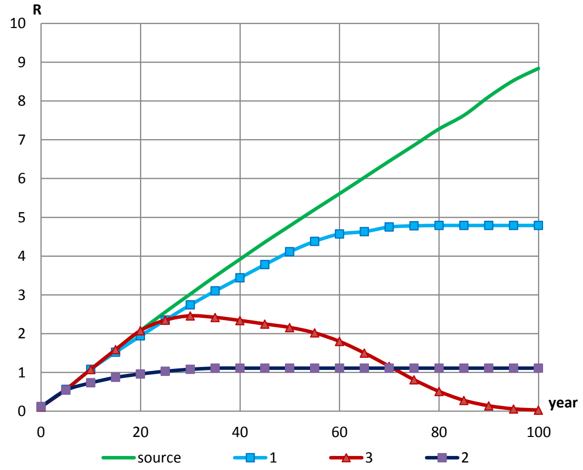


Fig. 5. Graphs of R versus time for three experiments on the contaminant motion

TABLE IV
FEATURES OF NUMERICAL EXPERIMENTS

Experiment No.	Source present for years	Advection used	Decay used	Dispersion used
1	100	yes	no	indirectly
2	100	yes	yes	indirectly
3	25	yes	no	indirectly

The results of the experiment acknowledge that the self-cleaning of the site environs may take at least 75 years after the storage area was remediated. For the first experiment, in Fig. 4A, the relative concentration distributions in the planes Q3 and D2brt3 after 25 and 60 years are shown.

After 25 years, in the plane Q3, the contaminant plume has appeared. It is located in the area, where the vertical flow q_z<0 (Fig. 2A shows the infiltration distributions in the plane Q3). On the plume back line, q_z=0. The plume occurrence in the plane Q3 was caused by the ascending flow q_z which discharges on the ground surface (Fig. 4).

After 60 years, the plumes in the planes Q3 and D2brt have reached the river Gauja. Because there the aquitard gQ is not present, the concentration distributions of the plumes are almost identical.

The R-graph of Fig. 5 predicts that during the next 10 years, the plumes should reach their stationary condition. To obtain data on the concentration changes along the plume centre line, the virtual monitoring posts were inserted in the HM planes 3(Q3), 4(Q2), 5(Q1) and 7(D2brt3).

Their locations 1, 2, 3 are shown in Fig. 4A. The posts 3.1, 4.1, 5.1, 7.1 were placed in the vicinity of the concentration source. The posts 5.2, 7.2 and 7.3 were situated, accordingly, in the alluvium deposit frontage and at the river Gauja left bank. In Fig. 5a, the relative concentration hydrographs in the monitoring posts are shown.

Because the hydrographs of the posts 5.2 and 7.2 are identical, the one for the post 5.2 is not exposed. The summary on the relative concentration hydrographs is presented in Table V.

It follows from considering of Table V and Fig. 5A that during the first 25 years, the hydrographs in the posts 3.1, 4.1, 5.1, 7.1 are similar for the three experiments.

After 25 years, the hydrographs for the first and the third experiment are different, because the contaminant source has been removed. However, the maximal values of the hydrographs for both experiments are almost identical.

For the first experiment, after 100 years, the relative concentration in the post 7.3 will be 0.05%. The concentration decrease in 2000=100/0.05 times is due to the contaminant dilution in groundwater. When the plume enters the river Gauja, its flow ~3.6×10^6 m^3/day [5] will also dilute the contaminant. The groundwater inflow in the Gauja river is 5514 m^3/day (Fig. 3A) from its bank of the length ~750 m (Fig. 4A).

The width of the contamination plume is ~250 m. The inflow of the contaminated groundwater is ~1840 m^3/day = 5514×250/750.

Due to the contaminant dilution in the river, its concentration will decrease ~$3.6\times10^6/1840=1.95\times10^3$ times. The resulting dilution will be ~$2.0\times10^3\times1.95\times10^3$ $=3.9\times10^6$ times.

Due to such enormous concentration decrease, the oil contaminated storage area cannot endanger the river Gauja.

For the first experiment, after 100 years, the BTEX mass that enters the river M_t equals: M_t=30.6=6.8×4.8 where M =6.8 grams (Table III), R=4.8 (Fig. 5). The intensity in mg/day of the contaminant source for all three experiments, was invariable: (6.38×9.0)/(100×365) ~1.6 mg/day where R=9.0 after 100 years (Fig. 5).

It is obvious that due to such a low intensity of the contaminant source, the quality of groundwater in the storage area close environs may be only slightly worsened.

TABLE V
THE RELATIVE CONCENTRATION SUMMARY IN MONITORING POSTS AFTER 25, 65 AND 100 YEARS

Monitoring post No.	Experiment No. 1	2	3
After 25 years			
3.1	55.00	52.40	55.00
4.1	24.10	21.80	24.10
5.1	9.00	7.00	9.00
7.1	1.60	0.74	1.60
7.2	0.00	0.00	0.00
7.3	0.00	0.00	0.00
After 65 years			
3.1	55.00	52.40	0.00
4.1	24.10	21.80	0.00
5.1	9.00	7.00	0.00
7.1	1.65	0.76	0.00
7.2	0.11	0.0044	0.12
7.3	0.04	0.0009	0.04
After 100 years			
3.1	55.0	52.40	0.00
4.1	24.10	21.80	0.00
5.1	9.00	7.00	0.00
7.1	1.65	0.76	0.00
7.2	0.13	0.0045	0.001
7.3	0.05	0.0010	0.004

VI. Discussion

Only recent results on the investigation of the contaminated abandoned black fuel storage area were available. The investigation was carried out only within the small area where the storage was located. No data were available about contamination of the environs of the storage and on the oil spill accidents during exploitation of the storage. However, due to appliance of the reported numerical modelling experiments, the necessary information on effects caused by the contaminated place has been obtained:

- Due to the low contamination concentration, the quality of groundwater in the close storage environs may be only slightly worsened;
- The contamination can reach the Gauja river in ~60 years; then due to dilution, its concentration may decrease at least ~2000 times. Therefore the river cannot be polluted even if the past contamination concentration was much larger then presently.

The experiments represented the adverse case when the source intensity did not change. In reality, due to the natural oil contaminant depletion, its mass decreases [23], [24]. The second experiment proved the notable effect of this phenomenon. No experiment directly accounted for the contaminant presence in groundwater.

It certainly existed in nature, because the storage area presented the contamination source during at least 60 years. Indirectly, this fact was simulated by the third experiment when the contaminant source was removed.

VII. Conclusion

The effect on environment of the former black fuel storage area in the town Valmiera was estimated by using the local HM.

It was established jointly by specialists of LEGMC and RTU. To create HM, the regional information extracted from LAMO4 was supplied and reshaped by detailed local data.

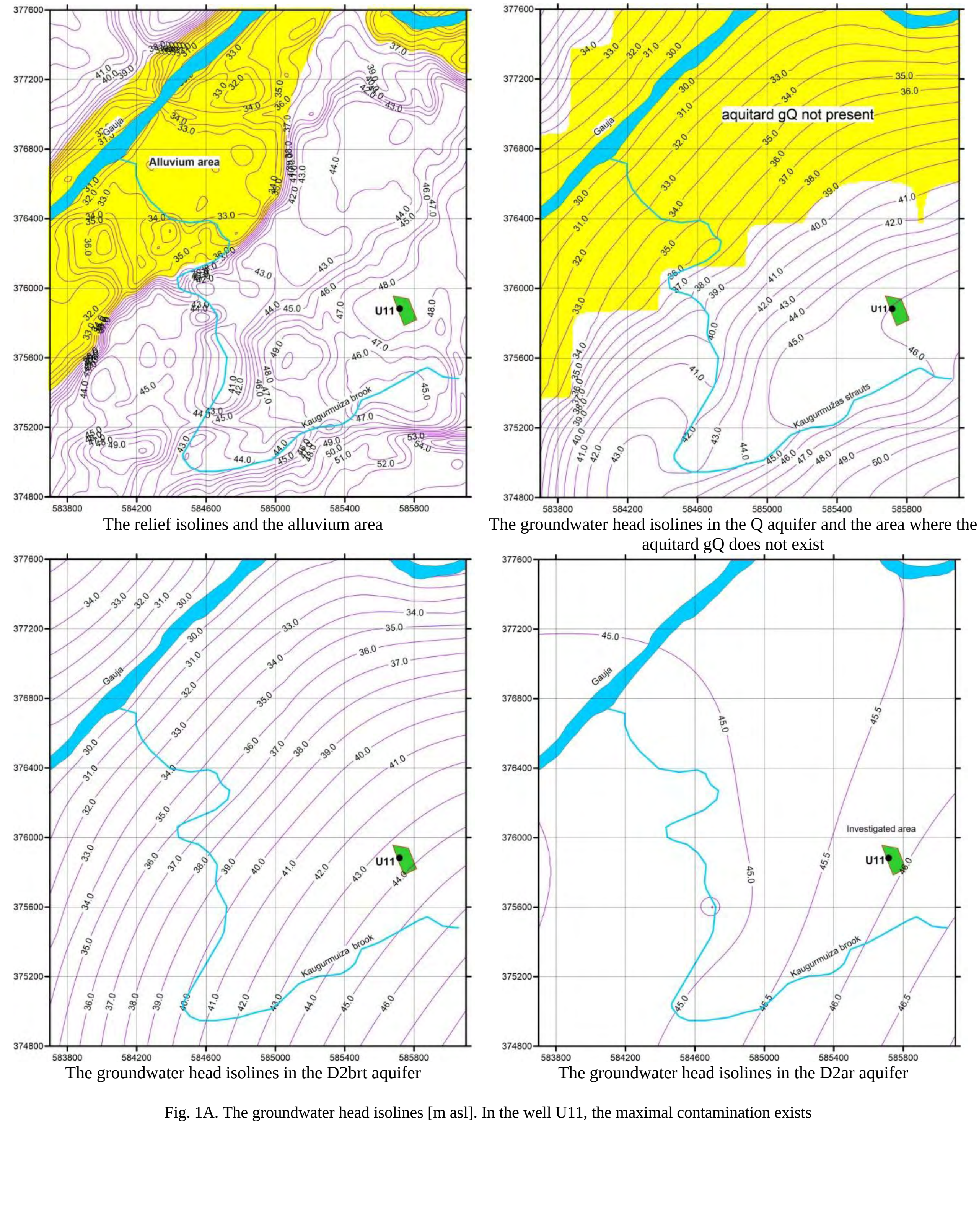
They were provided by LGIA (digital relief), LEGMC (borehole data on the place stratigraphy) and VKB (groundwater contamination, hydrogeological data on the storage area).

The contaminant movement and transport in groundwater were explored by using the MODPATH and MT3D programs.

It was found out that the contaminant plume may reach the river Gauja in about 60 years. The contaminant concentration in groundwater may decrease at least 2000 times.

The simulation results ensure that presently the storage area may only slightly worsen the groundwater quality in its close environs. Methods of developing and using the local HM and the contaminant migration models may be useful for specialists dealing with groundwater contamination problems.

Appendix



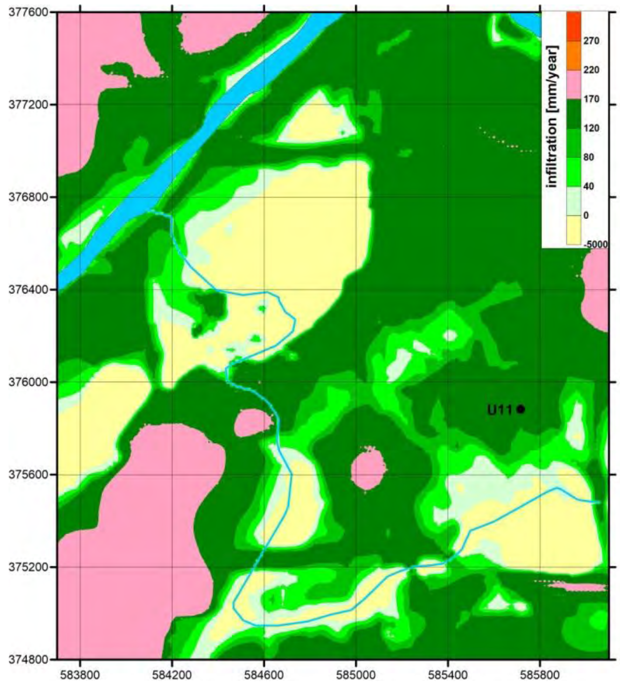
The relief isolines and the alluvium area

The groundwater head isolines in the Q aquifer and the area where the aquitard gQ does not exist

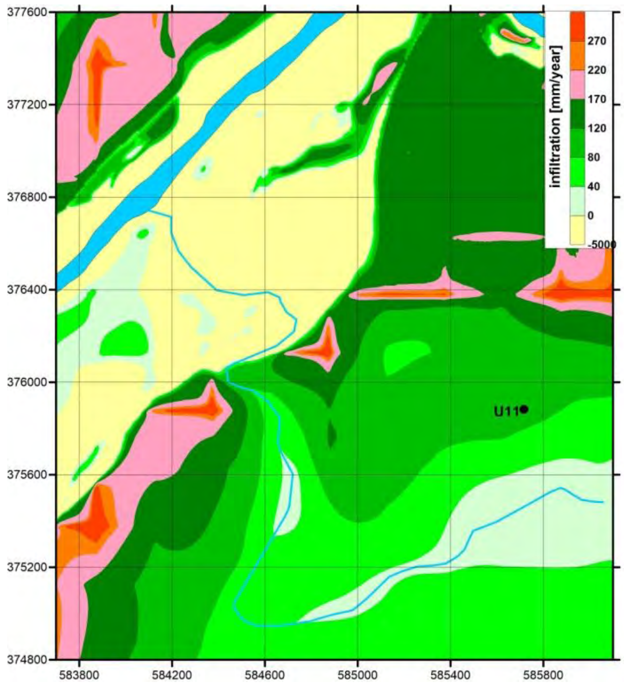
The groundwater head isolines in the D2brt aquifer

The groundwater head isolines in the D2ar aquifer

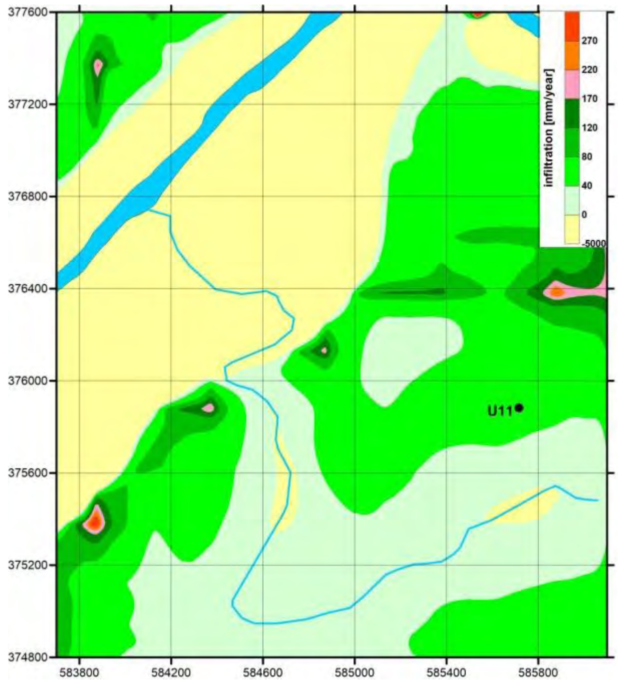
Fig. 1A. The groundwater head isolines [m asl]. In the well U11, the maximal contamination exists



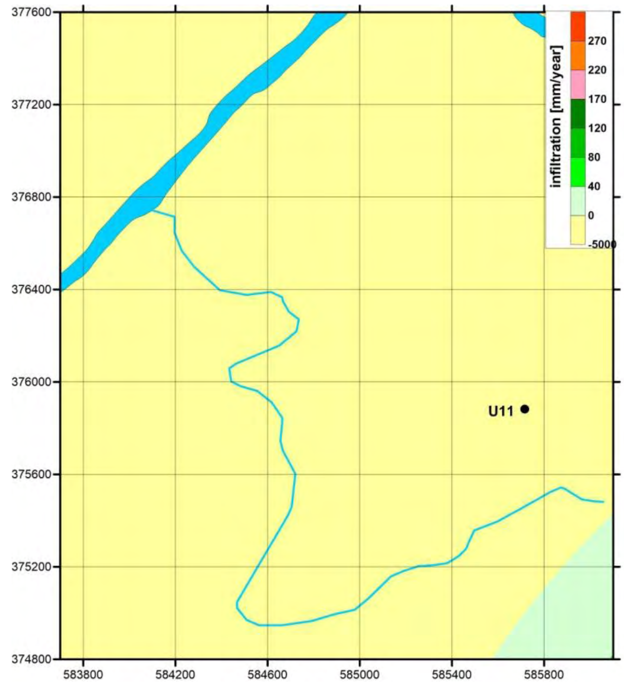
In the Q3 plane



In the D2brt3 plane



In the D2brt2 plane



In the D2arz plane

Fig. 2A. The infiltration [mm/year] distributions

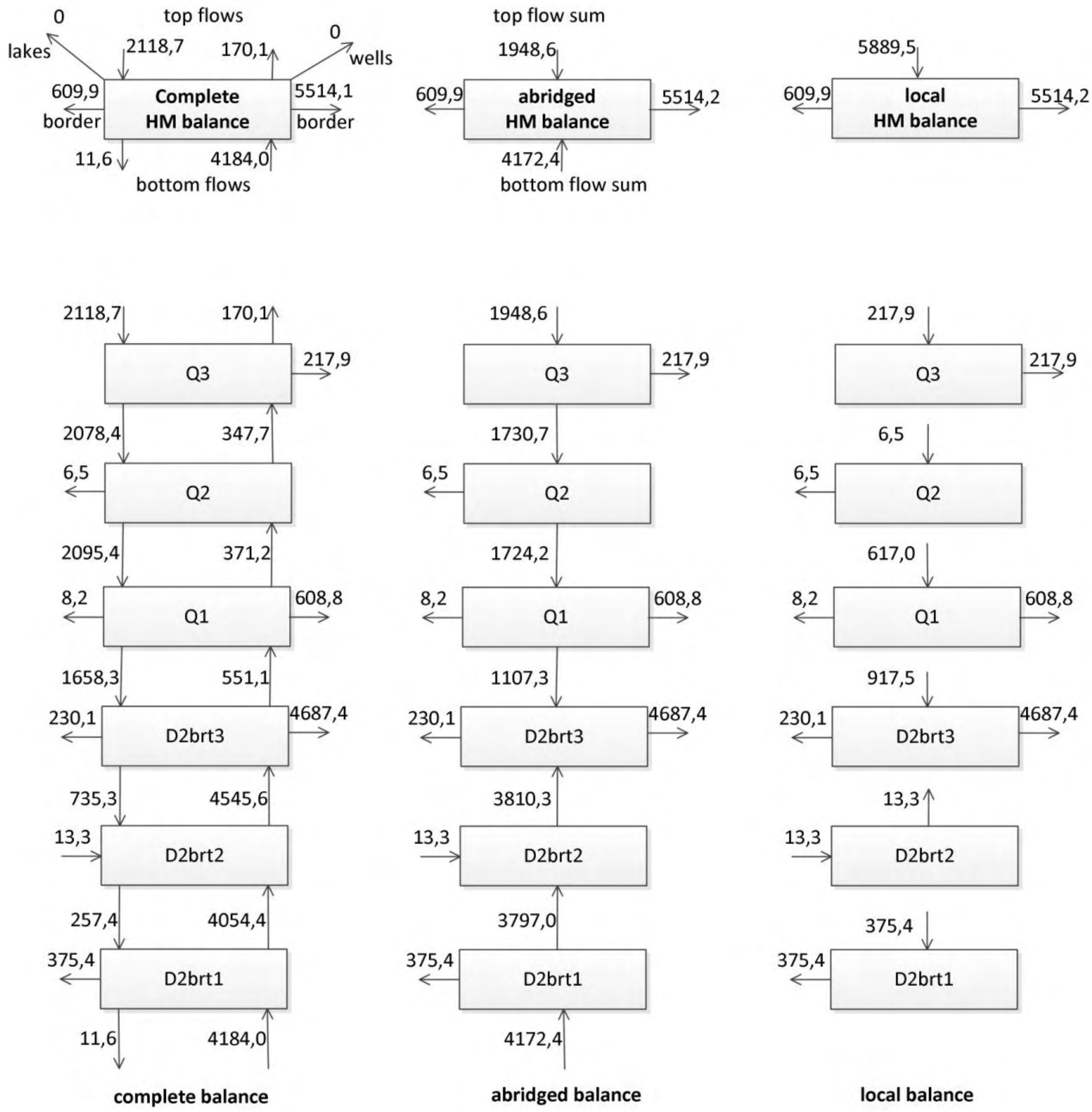
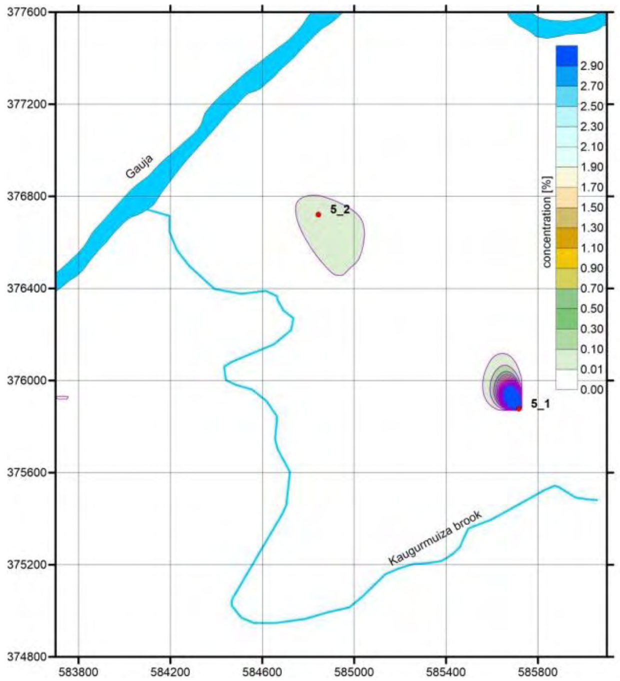
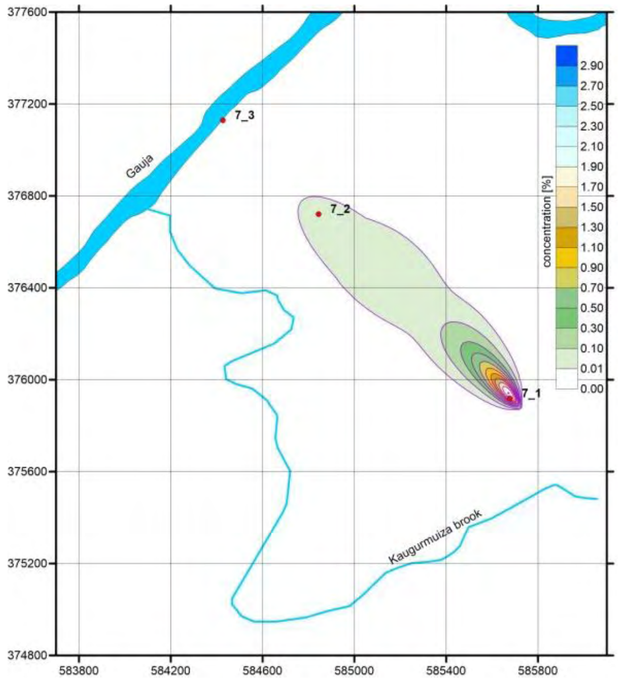


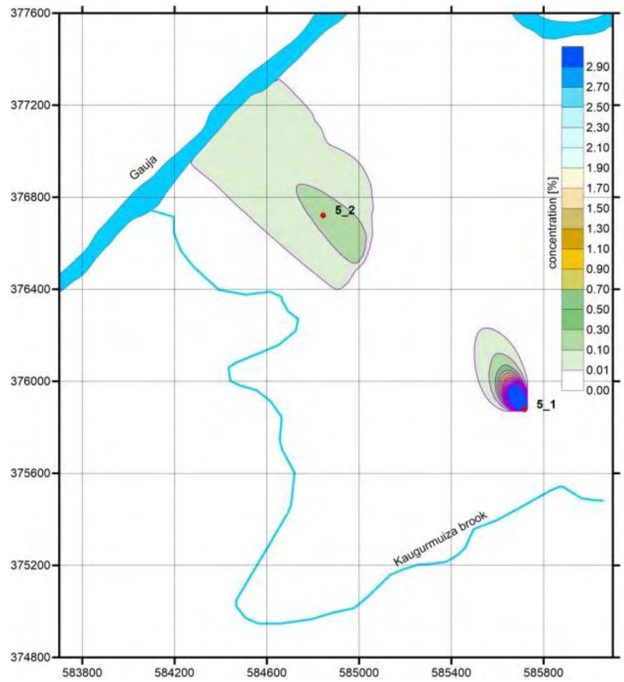
Fig. 3A. The graphical representation of complete, abridged and local groundwater flow balances [m^3/day] for HM and its planes



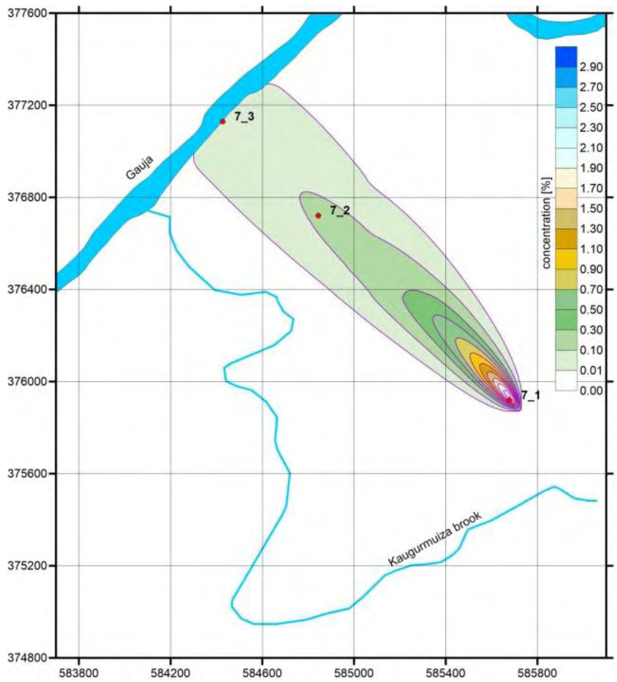
In the Q1 plane after 25 years



In the D2brt3 plane after 25 years

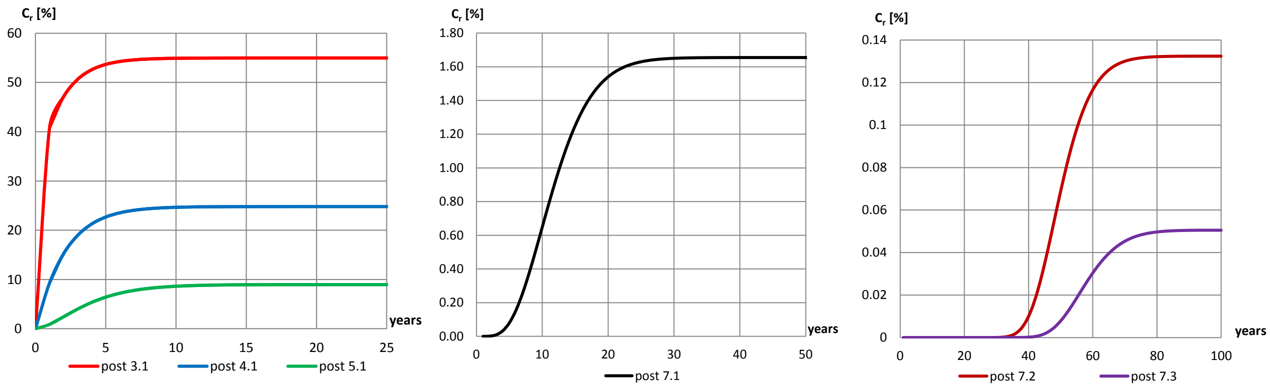


In the Q1 plane after 60 years

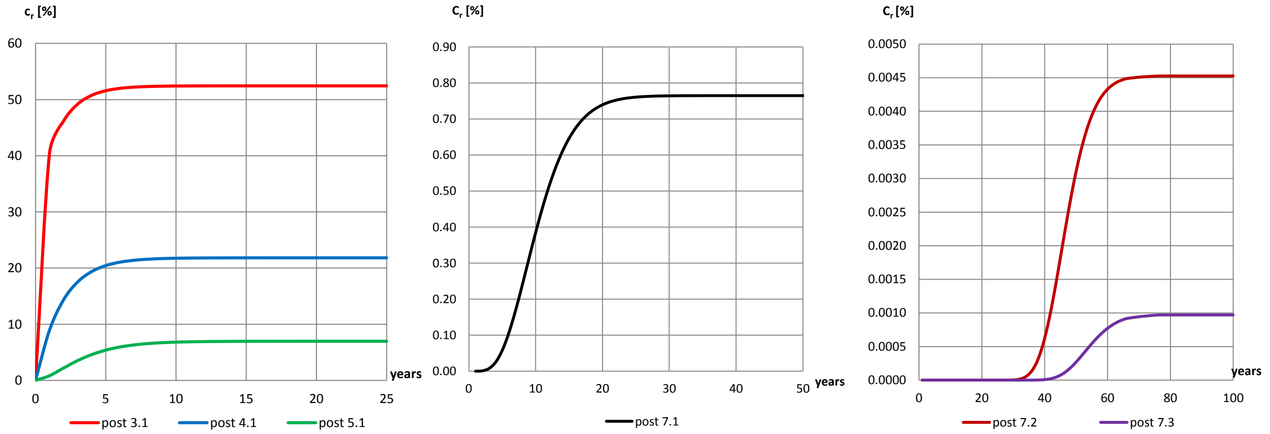


In the D2brt3 plane after 60 years

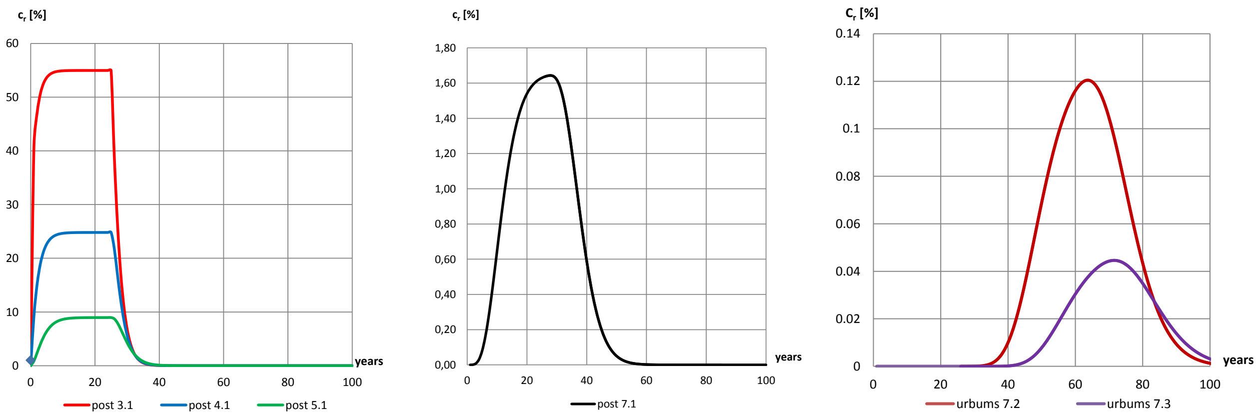
Fig. 4A. The first experiment. The relative concentration [%] distributions after 25 and 60 years



The first experiment



The second experiment



The third experiment

Fig. 5A. The relative concentration Cr [%] hydrographs in monitoring posts

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Authors' information

Aivars Spalvins, graduated in 1963 from the Riga Polytechnical Institute (since 1990 – Riga Technical University) as a Computer Engineer. A. Spalvins is the Head of the Environment Modelling Centre of RTU. His research interests include computer modelling of groundwater flows and migration of contaminants.
E-mail: aivars.spalvins@rtu.lv

Inta Lace graduated in 1971 from the Riga Technical University as a Computer Engineer. In 1995, I. Lace received the Master's degree in Applied Computer Science. Since 1991, she is a researcher at the Environment Modelling Centre of the Faculty of Computer Science and Information Technology, RTU.
E-mail: intalace@yahoo.com

Kaspars Krauklis received the Master's degree in Computer Systems from the Riga Technical University in 2007 and the Certificate in Teaching of Engineering Sciences from the Institute of Humanities of RTU in 2005. He is the researcher at the Environment Modelling Centre of RTU.
E-mail: kaspars.krauklis@rtu.lv

Daiga Pipira graduated from the University of Latvia as a Geologist in 2015, she received the PhD in field of Bedrock Geology. D.Pipira is the Head of the Subsoil Department at the State Ltd. "Latvian Environment, Geology and Meteorology Centre".
E-mail: daiga.pipira@lvgmc.lv

Sandra Karusa received the Master`s degree in Geology from University of Latvia in year 2016 and currently is a PhD student. S.Karusa is a hydrogeologist in Latvian Environment, Geology and Meteorology Centre (LEGMC) and deals with groundwater modelling, groundwater management issues and subsoil microbiology biodiversity and ecological services.
E-mail: sandra.karusa@lvgmc.lv

Inga Retike received the Master's degree in Environmental Science from University of Latvia (UL), Faculty of Geography and Earth Sciences in year 2012. Currently is a PhD student at UL and working as hydrogeology expert in Latvian Environment, Geology and Meteorology Centre. Main research topics are: groundwater status assessment in Latvia according to European legislation; groundwater hydrochemistry with respect to multivariate statistics and chemistry forecasting tools.
E-mail: inga.retike@lvgmc.lv

Madara Mame received the Master's degree in Geography from the University of Latvia in 2013. Works as a hydrogeologist in Latvian Environment, Geology and Meteorology Center from year 2016.
E-mail: madara.mame@lvgmc.lv

Linda Fibiga received the Master's degree in Heat, gas and water technology from the Riga Technical University in 2008. Currently she is working in Latvian Environment, Geology and Meteorology Centre (LEGMC) with river basin management issues.
E-mail: linda.fibiga@lvgmc.lv

