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MATHEMATICAL MODELLING OF THE INTER-COLLECTOR TRANSFER OF WATER CONTAMINANTS*

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Abstract. The contribution is devoted to the description and the application of the mathematical model of groundwater flow and transport based on the mixed-hybrid formulation of the finite element method. The model was applied on a problem of identification and evaluation of the transfer of contaminants between two aquifers divided by an aquitard in the area of Stráž pod Ralskem, Czech Republic, where the ISL mining of uranium was run. Originally impermeable low-turonian aquitard placed between cenomanian (the uranium deposit) and upper-turonian (the source of drinking water) aquifers was partially destroyed by the technological wells. First, it was necessary to define the vertical filtration coefficients of low-turonian semi-aquitard in the area of the interest. The measured values of the piezometric head were used to calibrate the model. An interval of the most probable values of the vertical filtration coefficient of low-turonian semi-aquitard was found. Then three model scenarios based on different level of cleaning up of cenomanian aquifer were calculated using calibrated model.

Key words. porous media, underground flow, transport of contaminants, finite element method

AMS subject classifications. 76S05, 76M10

1. Introduction. The uranium deposit Stráž was exploited by underground acidic leaching between 1968 and 1996. More than 14 000 tons of uranium were produced during this period. More than 4 million tons of H_2SO_4, 300 thousand tons of HNO_3, 120 thousand tons of NH_3 and other chemicals were injected in cenomanian sandstones. The chemical mining of uranium on the deposit Stráž has resulted in large contamination of groundwater of cretaceous collectors in Stráž block of North-bohemian cretaceous table and causes serious ecological problems.

The low cenomanian aquifer, where the uranium deposit was placed, is mainly afflicted. The total salinity of the cenomanian solutions reaches up to 80 g/l.

The upper laying turonian aquifer is a drinking water reservoir for larger region. Its contamination is weaker than in cenomanian aquifer and it is possible to remove it using conventional tools.

The contamination of cenomanian aquifer represents the potential risk for turonian drinking water sources. After finishing the remediation of Stráž deposit the cenomanian piezometric surface will arise on the original level before starting the mining activities. Such level will be higher than turonian water level in the area of Stráž deposit. Then the inter-collector transfer of the contaminated waters from cenomanian aquifer to turonian through low-turonian semi-aquitard which is weaken by large amount of wells and probably by natural non-homogenities can also happen.

2. Used models. The models are more precisely described in contributions "Mathematical Modelling of the Underground Transport of Contaminants" and "Solution of augmented systems from a mixed-hybrid finite element discretization of the potential fluid flow problem: asymptotic rates of convergence" in these Proceedings.

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The inter-collector transfer problem is a compilation of more problems – unsteady flow in saturated cenomanian aquifer and unsteady flow in partially unsaturated turonian aquifer. The communication between them is a separete problem. Besides these problems, the chemical transport and reactions have to be solved.

2.1. Unsteady unsaturated flow model. Unsteady flow problem is solved on fixed domain Ω, which includes both saturated and unsaturated zones. Let us call phreatic surface the area where both zones meet. The phreatic surface separates saturated zone $p \geq 0$ from unsaturated zone $p < 0$, where p is a pressure head. At the beginning the contact area is not a priori known. Unsteady unsaturated porous media flow is governed by the continuity equation and the Darcy law with mixed boundary conditions allowing to model the impermeable part of the boundary, the free water surface, and the part of boundary, where a defined inflow is set. The mixed-hybrid finite element method is applied to the system.

MH-model gives results on the faces of the elements and keeps mass balance on these faces. Such model is suitable for following using of the transport-reactive model.

Mixed-hybrid formulation leads to a solution of symmetrical but indefinite systems of large sparse linear equations with zero diagonal block. This structure allows use of different algorithms with variable effectiveness. Common is use of conjugate gradient method to solve system of Schur complement with symmetric positive definite (SPD) matrix. This was the method used to simulate substance migration in the neighbourhood of tailings pond. Another option is to consider the linear system to be complex and use the MINRES method. Symmetrization of indefinite system into SPD is just another method (see [3]).

2.2. Chemical substance transport model. The operator of the governing balance equation of each substance of the solution is decomposed to two parts – the convective and the reactive one. At first, the convective part is solved and the inter-element fluxes of particular species are computed. Then, the solution is 'virtually mixed' in each finite element and the reactive part of balance equation is solved in several steps (oxidation-reduction reactions, interaction between solution and the rock and actually sorption and desorption of the chemicals).

The chemical transport and reactions are much more fast than the development of flow. That is why the time step of solution of the flow problem is set much longer than the time step of the transport model computations.

3. Calculations.

3.1. Model mesh. The area of the interest is about 38 km^2. The southern boundary is created by Ploužnický stream, the western boundary is given by river Ploučnice and Panenský stream.

The northern boundary leads partially along the river Ploučnice and Stráž fault zone. The eastern part of the boundary is given by tectonic line of Jelení hills that has non-negligible influence on the hydrogeological situation of the modelled area.

The finite element mesh covering the area of the interest created by 1619 plain nodes and 3119 plain elements is shown on the figure 1. The mesh is vertically divided into 15 layers. The whole mesh consists of about 47000 spatial elements. The elements in the area of leaching fields are triangles with the edge of about 100 metres. In the western part the elements are twice larger and the largest elements are in the southern part. The edges of the elements here are not longer than 400 metres.

The vertical decomposition of the model mesh respects the main stratigraphical interfaces. The base of the model copies the impermeable crystalline rock. The top

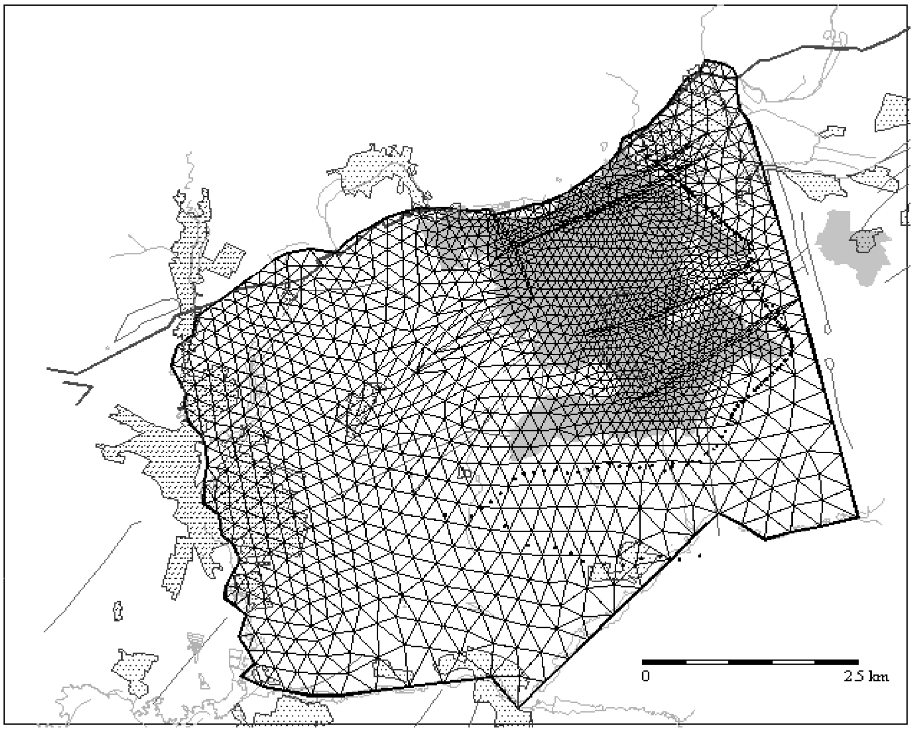

Fig. 1. *The finite element mesh*

of the model is given by the phreatic surface of turonian aquifer.

3.2. Calibration. The regional hygrogeological model was used for calibration calculations. The values of the vertical hydraulic conductivity of the low-turonian semi-aquitard obtained by solving of the iterative procedure of calibration were transformed into the contaminant transfer model mesh. The variant calculations of contaminant transfer from cenomanian aquifer to turonian aquifer were performed using this model.

For calibration the current measured piezometric heads in both cenomanian and turonian aquifers were used. The characteristics of low-turonian semi-aquitard obtained by small difference between water levels in aquifers are not unique. There exists an interval of possible values of vertical filtration coefficients. The certain decreasing of permeability due to remediation of the all wells has to be also considered. The water level in cenomanian aquifer after finishing all remediation activities cannot be predicted with sufficient reliability.

Combining possible values of filtration coefficients and water level it is possible to obtain large amount of variants. After initial benchmark calculations the two main scenarios - optimistic and pessimistic were formulated. The first one (I) combines the least auspicious parameters when the transfer of the contaminants is maximal. The second one (II) combines the most auspicious parameters. The coefficients of these scenarios are shown in the table 1 (the area was divided into four parts by expert suppositions made before the calibration and the conductivity coefficients of these parts were searched).

Scenarios	vertical hydraulic conductivity of low-turonian semi-aquitard [m/day]				cenomanian piezometric level
	LF with simple well casing	LF with wells with lift-pumps	LF with wells with pumps	main transfer area	
I	0.0006	0.0004	0.0002	0.08	+ 3 m
II	0.0004	0.00027	0.00013	0.04	before mining

LF = Leaching fields

TABLE 1
Definition of simulated scenarios.

3.3. Simulation. The three base model scenarios were created. Zero variant (considering current state of groundwater pollution), remediation variant - 10 g/l TDS (considering cleaning of cenomanian aquifer up to the level of average remaining concentration 10 g/l of the total dissolved solids) and remediation variant - 3 g/l TDS (considering cleaning of cenomanian aquifer up to the level of average remaining concentration 3 g/l of the total dissolved solids).

The inter-collector transfer of the contaminants was simulated in the time interval 1000 years. Such interval is suitable especially for predicting of the evolution of pollution of drinking water source in the Mimoň area and pollution of river Ploučnice by contaminants transferred from cenomanian aquifer to turonian. The results obtained by simulation were treated and stored with time step 50 years. The choice of a shorter sample period would not afford better set of data for following treatment (it is not too dynamical evolution) but the whole process of data treatment would be more complicated due to extremely large resulting data file.

For the simulation of transport the 15-day time step was chosen. Such value is optimal due to precision of computation (it is given by Courant number - relation between time step, flow velocity and spatial discretizing parameter) and also it is acceptable for performing of the complicated numerical operations with large data files.

4. Conclusions. The convective transport of the contaminants is given by character of groundwater flow in the area of Stráž block. The character of flow in both cenomanian and turonian aquifers was determined by solving the groundwater flow problem under conditions considered. The main flow heads in south-east direction in the both aquifers. In the turonian aquifer there are two main paths of the contaminants migration. The southern path, leading from the central part of the leaching fields, passes the southern hillside of volcanic massive Ralsko towards Mimoň, where the flow is influenced by abstraction from drinking water well MI-6. The northern path passes the northern hillside of Ralsko and leads along the Stráž fault zone, continues along the river Ploučnice towards Mimoň, where the well MI-6 influences the flow. The flow velocity in turonian aquifer is more than twice higher comparing the situation in cenomanian aquifer.

It follows from the modelling of the pessimistic scenario that 980 000 tons of TDS (20% of solids currently dissolved in the cenomanian solutions) will migrate from cenomanian aquifer to turonian. In the optimistic case it will be less than 6%. These numbers are significantly higher than it was assumed before the simulation.

The evaluation of the effect of the target parameters of remediation was performed under condition of the limit of NH_4^+ concentration - 3 mg/l (given by the standard

ČSN 757214) in the drinking water well MI-6.

For the extreme combinations of the both auspicious and inauspicious conditions the target parameters of remediation are 2 and 9 g/l TDS. It means that it is necessary to clean cenomanian aquifer up to average remaining concentration 2 or 9 g/l TDS. Because such extreme conditions are not too probable we can recommend the target parameters on the level of 3 - 5 g/l TDS.

The water quality in the river Ploučnice will not be seriously affected by transferred secondary contamination even in the case of current level of cenomanian contamination. It is also not probable that the contaminants migrating under Ploučnice riverbed in the area of Mimoň would later seriously affect water quality in Ploučnice in the area south-east from Mimoň.

The figures 2–6 show the time propagation of concentration of NH_4^+ computed with the more optimistic transfer scenario (II) with initial conditions set such a way that no remediation is made (the "zero" variant).

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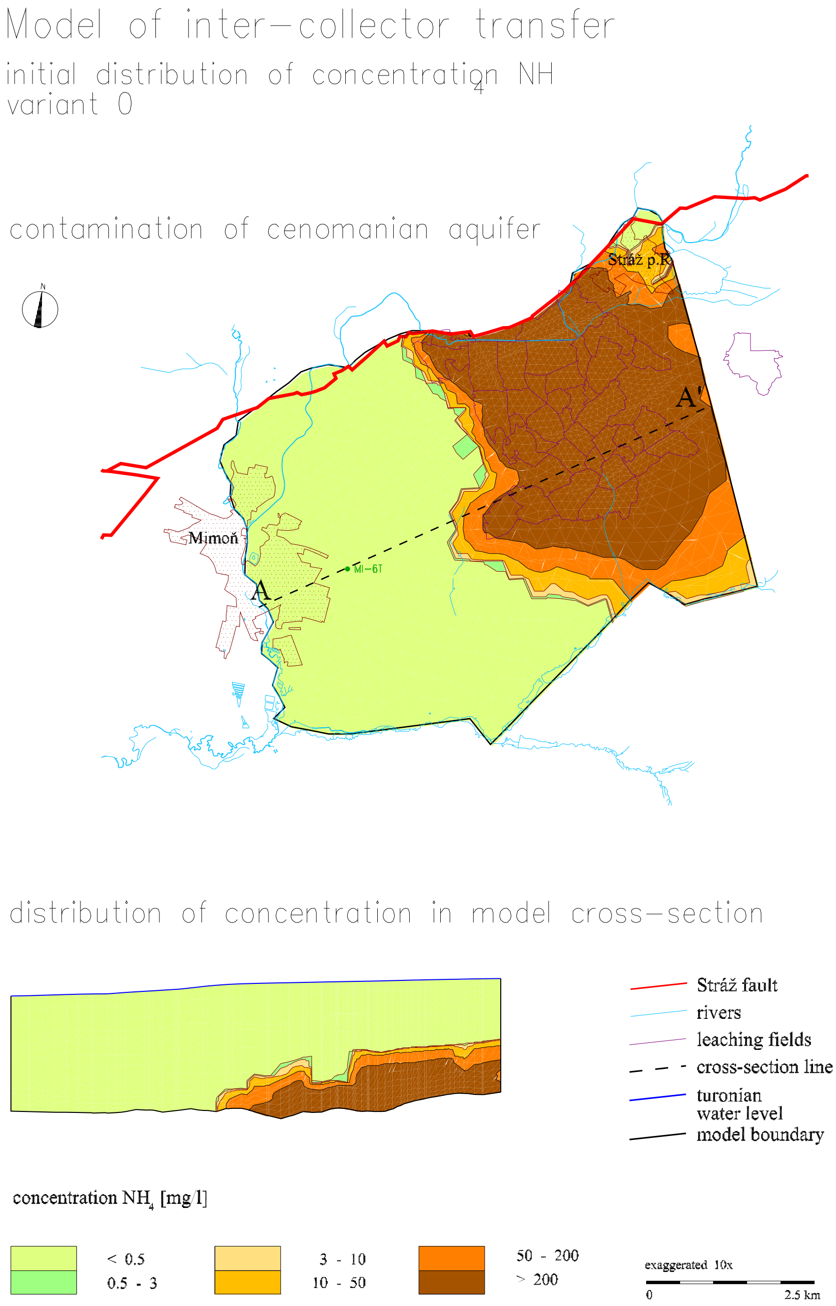

FIG. 2. *Initial distribution of concentration of NH_4. The "zero" variant (no remediation).* The cenomanian aquifer contamination above and the cross-section A–A' below. The z-axis scale is 10 times exagerrated.

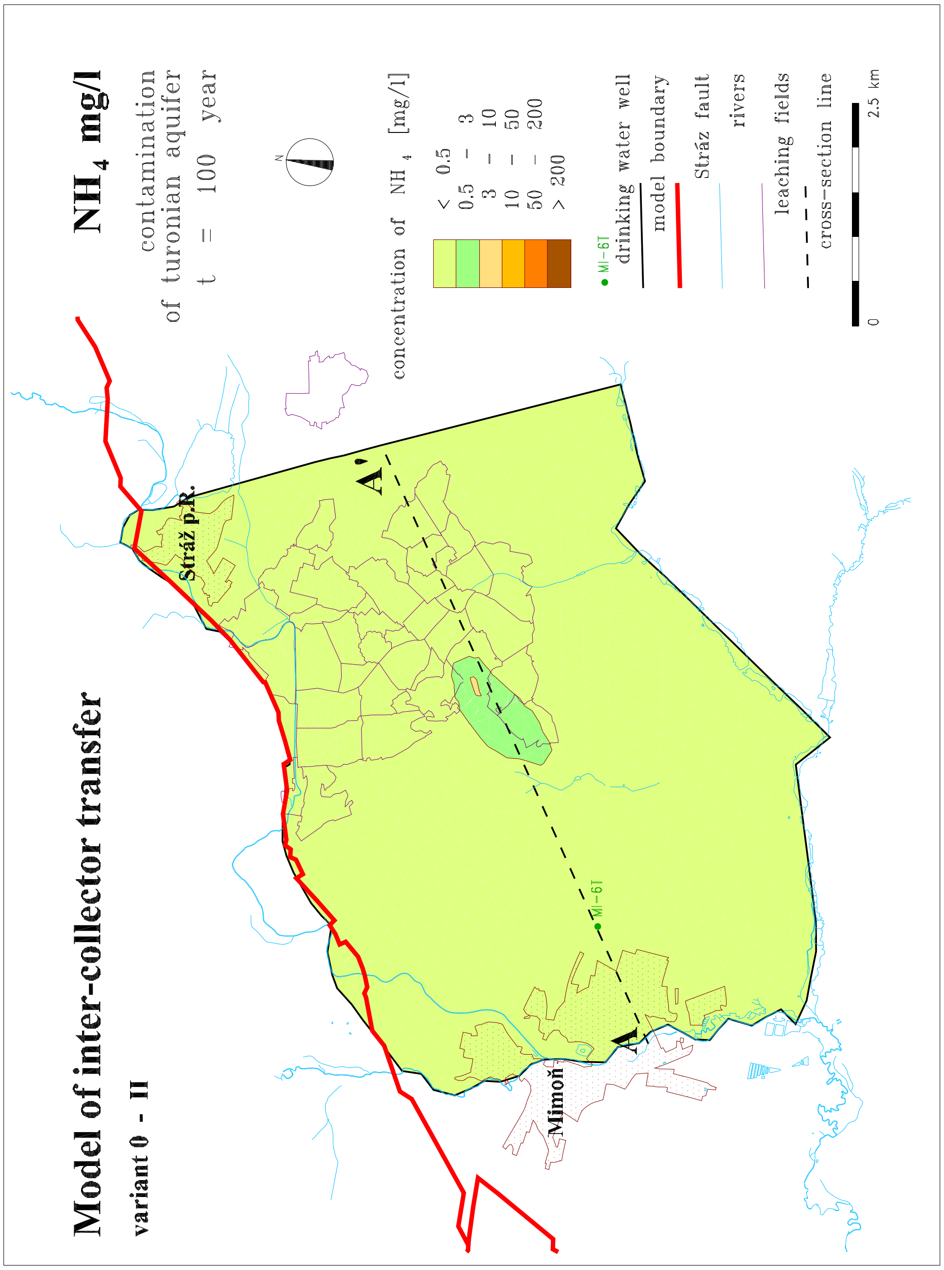

FIG. 3. *The distribution of concentration of NH_4 in turonian aquifer after 100 years.* The "zero" variant (no remediation), the "optimistic" scenario II of inter-collector conductivity coefficients.

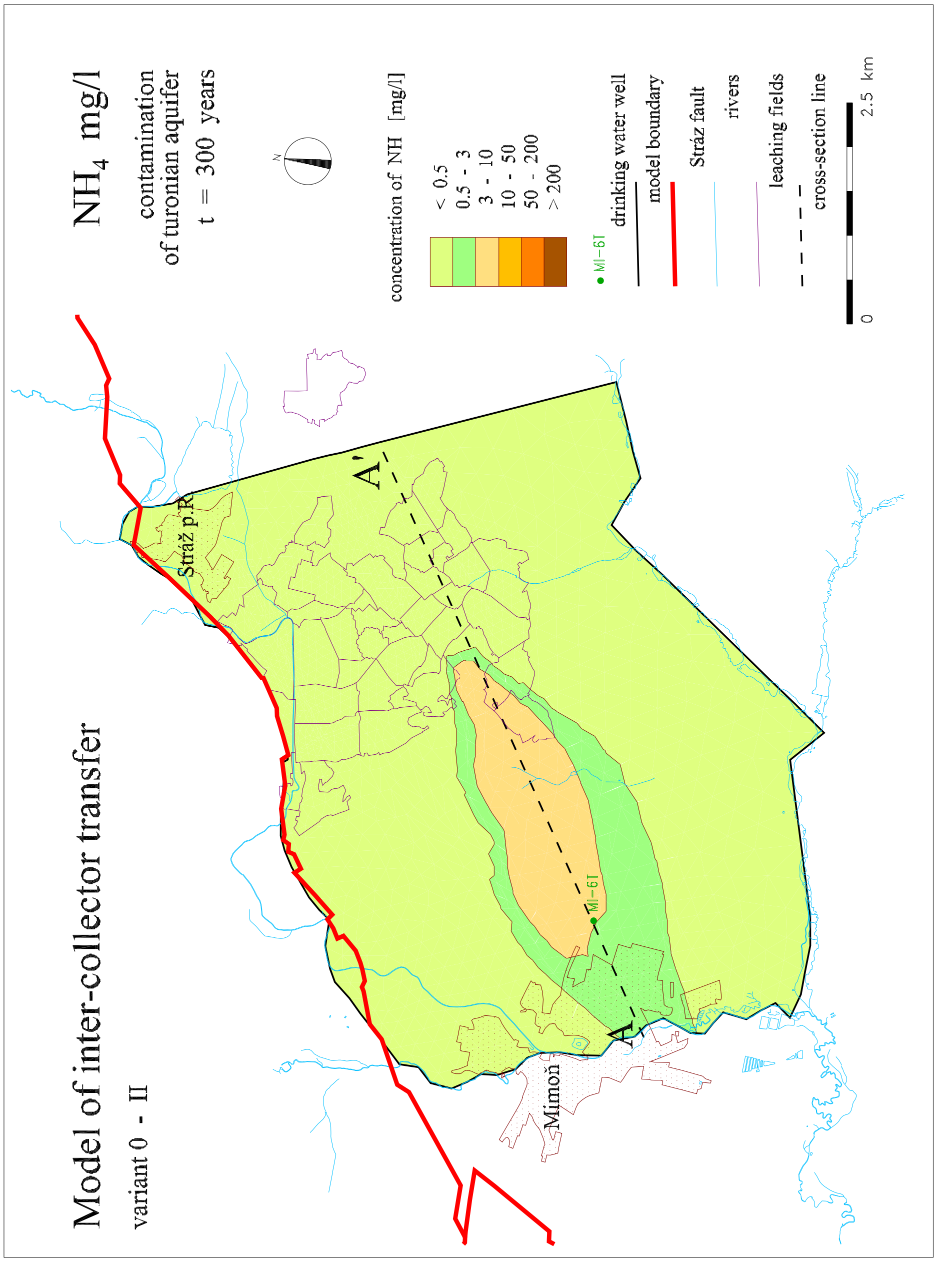

FIG. 4. *The distribution of concentration of NH_4 in turonian aquifer after 300 years.* The "zero" variant (no remediation), the "optimistic" scenario II of inter-collector conductivity coefficients.

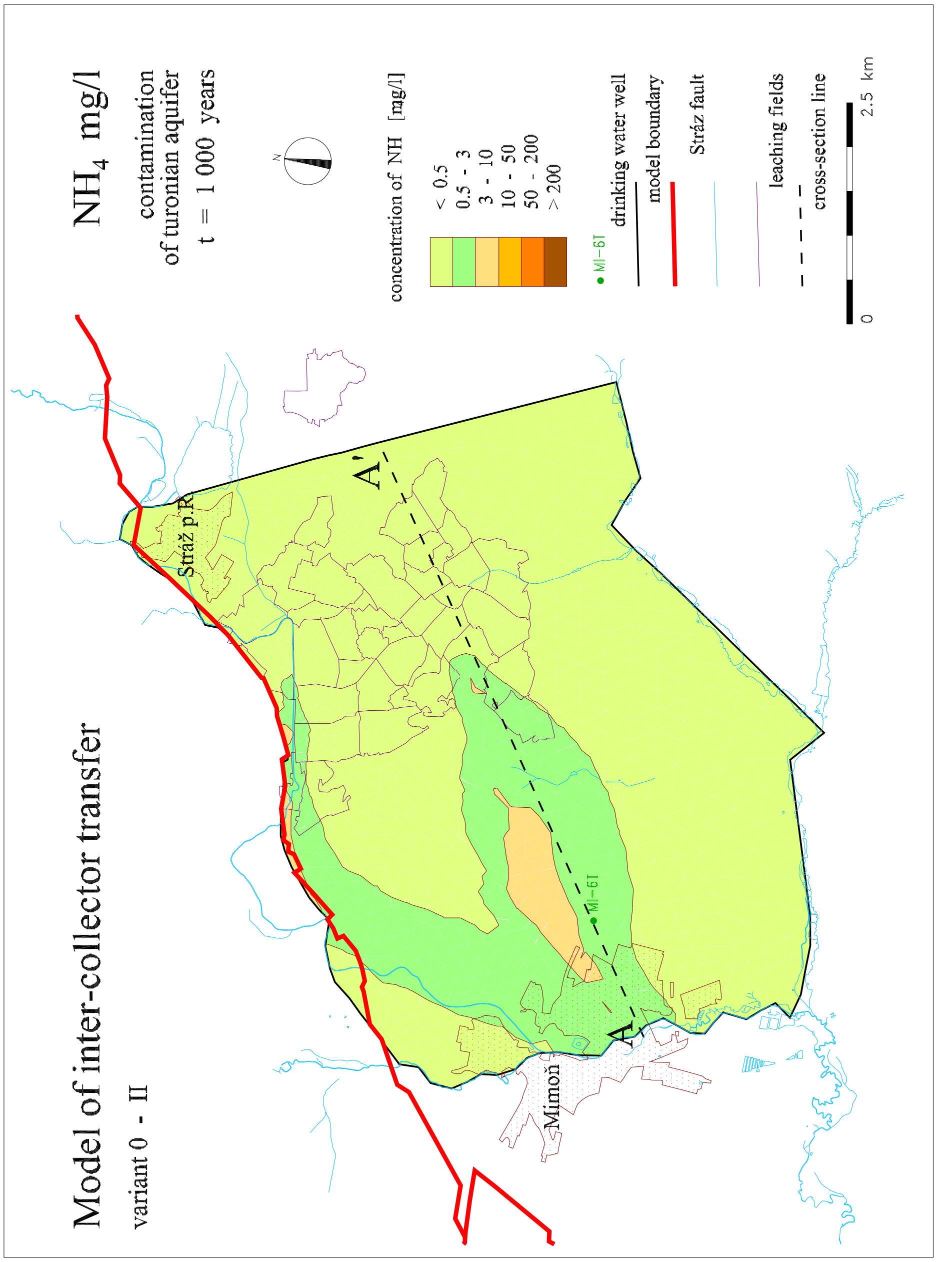

FIG. 5. *The distribution of concentration of NH_4 in turonian aquifer after 1000 years.* The "zero" variant (no remediation), the "optimistic" scenario II of inter-collector conductivity coefficients.

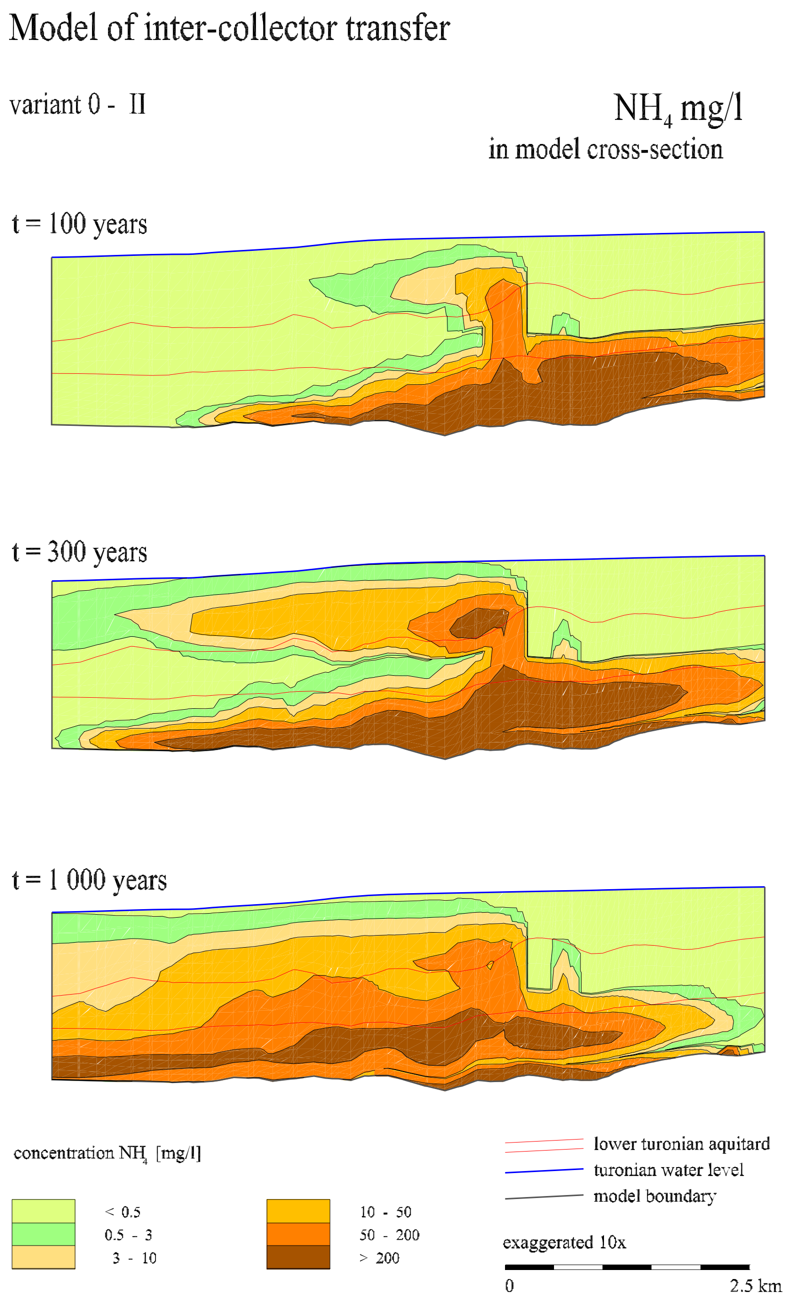

FIG. 6. *Time development of distribution of concentration of NH_4 in model cross-section A–A'.* The "zero" variant (no remediation), the "optimistic" scenario II of inter-collector conductivity coefficients. The z-axis scale is 10 times exagerrated.