Modelling of the Contaminants Transfer Between two Aquifers

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Abstract: The contribution is devoted to the description and the application of the mathematical model of groundwater flow and transport. 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 Straz pod Ralskem, Czech Republic, where the ISL mining of uranium was run. Originally impermeable Lower-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 Lower-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 Lower-Turonian semi-aquitard was found. Then three model scenarios based on different level of cleaning up of Cenomanian aquifer were calculated using calibrated model. The results of simulations show, that in the case of so-called "zero variant", i.e. scenario, where no remediation will be realized, the drinking water well MI-6 will be contamined by amonia ions in the time horizon of 500 years. In other scenarios the polution of this well has not been observed.

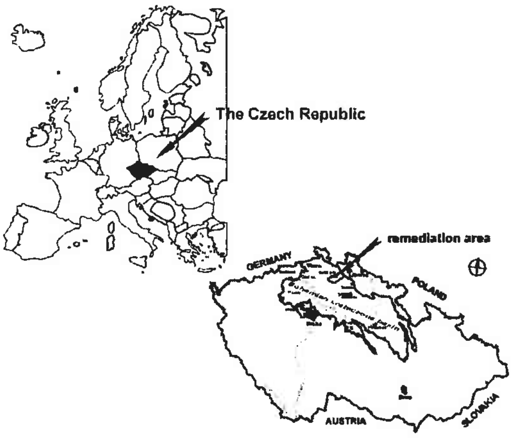
Keywords: Porous media; Transport of contaminants; Groundwater flow; Finite element method; Finite volume method

1. INTRODUCTION

The uranium deposit Straz 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 Straz has resulted in large contamination of groundwater of Cretaceous collectors in Straz block of Northbohemian Cretaceous table and causes serious ecological problems.

The Lower Cenomanian aquifer where the uranium deposit was placed is mainly affected. The total salinity of the cenomanian solutions reaches up to 80 g.L^{-1}.

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 Straz 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 Straz deposit. Then the transfer of the contaminated waters from Cenomanian aquifer to Turonian through the Lower-Turonian semi-aquitard which is weaken by large amount of wells and probably by natural non-homogenities can also happen.

2. BRIEF DESCRIPTION OF THE USED MODELS

The groundwater flow models [Bear] are based on primal (P-model) and mix-hybrid (MH-model) formulations of the finite element method. The areas of the interest are spatially discretized using the trilateral prismatic elements with vertical faces and generally non-horizontal bases.

P-model gives results (values of the piezometric head and filtration velocities) in the nodes of finite element mesh. This model is suitable for using in more extensive regional model. Input data is piezometric head in wells. Output are coefficients of permeability in elements. These are input to MH-model.

MH-model gives results on the faces of the elements and keeps mass balance on these faces.

Such model is more suitable for following using of transport model [Frydrych,2001], coupled with chemical reactive model, based on a finite volume method.

All used models are fully 3D.

The calculation of chemical changes represents the sequence of partial steps. There are two types of chemical reactions, immediate reactions calculated by the thermo-dynamic equilibrium rules and kinetic reactions. The immediate reactions are reactions between the components of solutions and the sorption of the substances on the surface of solid phase. It is supposed that the reactions run in the element in the time interval corresponding to the selected time step. Kinetic reactions are the reactions in solution and interaction between the components of solution and the minerals of hosting rock. Their slow process is longer then the time step.

2.1 Used mathematical theory

Steady flow problem is solved separately on two fixed domains Ω_1 (Cenomanian aquifer) and Ω_2 (Turonian aquifer). Both of them include 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.

Steady unsaturated porous media flow is governed by the following continuity equation:

$$\nabla \cdot \mathbf{u} = q \quad \text{in } \Omega_i \qquad (1)$$

where $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$, $\mathbf{u}$ denotes filtration velocity and function q describes solution source density.

The Darcy's law will be considered in the following form

$$\mathbf{u} = -k_r(\theta)\mathbf{K}\left(\nabla p + \nabla z\right) \quad \text{in } \Omega_i \qquad (2)$$

where $k_r(\theta) \approx \theta_e^3$ is a relative hydraulic conductivity (θ_e is effective water content) and tensor $\mathbf{K}$ represents environment hydraulic conductivity. The piezometric head equals to sum of $p+z$.

The mixed boundary conditions will be prescribed on the boundary of the domain Ω_i. An aquifer base is considered impermeable. Permeability of the domain cover depends on pressure head gradient and transfer coefficient σ. Thus following general Newton boundary condition is prescribed on this part of the boundary

$$\mathbf{u} \cdot \mathbf{n} - \sigma\left(p - p_D\right) = q_N \qquad (3a)$$

This condition allows even modelling of the impermeable part of the boundary letting $\sigma = q_N = 0$ respectively setting defined inflow $\sigma = 0$. On the free water surface Γ_D the non-homogenous Dirichlet boundary condition is prescribed:

$$p = p_D. \qquad (3b)$$

On the interface between domains Ω_1 and Ω_2 (Cenomanian and Turonian aquifer), the interface Newton boundary condition is prescribed:

$$\mathbf{u} \cdot \mathbf{n} - \sigma\left(p_1 - p_2\right) = q_N \qquad (3c)$$

where p_1 and p_2 are pressures of contaminated water in Cenomanian and Turonian aquifer respectively, and $\mathbf{u}$ is water flux between two aquifers.

2.2 The mixed-hybrid flow model

Let us consider the decomposition of the domain Ω into the system of subdomains E_h. The mixed-hybrid model (MH-model) [Maryska] we derive as a dis-cretized problem. The Darcy's law (2) we trans-form

$$R_r(p)\mathbf{A}\ \mathbf{u} = -(\nabla p + \nabla z) \qquad (4)$$

Where $R_r(p) = k_r^{-1}(p)$ is a relative resistance and $\mathbf{A} = \mathbf{K}^{-1}$ is a hydraulic resistance [Frydrych,1997]. The weak fulfilment of the transformed Darcy's law in the space $\mathbf{H}(div; E_h)$ leads to the following integral equation using Green's formula

$$\sum_{e \in E_h} \left\{ \left(R(p_{n-\varepsilon}^e)\mathbf{A}\ \mathbf{u}_n^e; \mathbf{v}^e \right)_e - \left(p_n^e; \nabla \cdot \mathbf{v}^e \right)_e + \left\langle \lambda_n^e; \mathbf{v}^e \cdot \mathbf{n}^e \right\rangle_{\partial e \cap \Gamma_F} \right\} =$$

$$= \sum_{e \in E_h} \left\{ -\left\langle p_D^e; \mathbf{v}^e \cdot \mathbf{n}^e \right\rangle_{\partial e \cap \Gamma_P} + \left(z_e; \nabla \cdot \mathbf{v}^e \right)_e - \left\langle z_{\partial e}; \mathbf{v}^e \cdot \mathbf{n}^e \right\rangle_{\partial e} \right\} \qquad (5)$$

We require the fulfilment of the equation (5) for all $\mathbf{v}^e$ from the space $\mathbf{H}(div; E_h)$. The weak fulfilment of the continuity equation of steady flow leads to the integral equation

$$\sum_{e \in E_h} \left\{ \left(\nabla \cdot \mathbf{u}_n^e; \phi^e \right)_e \right\} = \sum_{e \in E_h} \left\{ \left(q^e; \phi^e \right)_e \right\} \qquad (6)$$

its fulfilment we require for all ϕ^e from the space $L_2(\Omega)$. The final weak fulfilment of the balance equations on the structure Γ_h in the space $H^{1/2}(\Gamma_h)$ leads to the third integral equation

$$\sum_{e \in E_h} \left\{ \left\langle \mathbf{u}_n^e \cdot \mathbf{n}^e; \mu^e \right\rangle_{\partial e \cap \Gamma_h} - \left\langle \sigma^e \lambda_n^e; \mu^e \right\rangle_{\partial e \cap \Gamma_N} \right\} = \sum_{e \in E_h} \left\langle q_{N,n}^e - \sigma^e p_{D,n}^e; \mu^e \right\rangle_{\partial e \cap \Gamma_N} \qquad (7)$$

its fulfilment we require for all μ^e from the space $H^{1/2}(\Gamma_h)$.

The above-mentioned system of integral equations we call the weak solution of the MH-model (see [Kaasschieter]).

3. CALCULATION

3.1 Model Mesh

The area of the interest is about 50 km^2. The southern boundary is created by Plouznicky stream; the western boundary is given by river Ploucnice and Panensky stream.

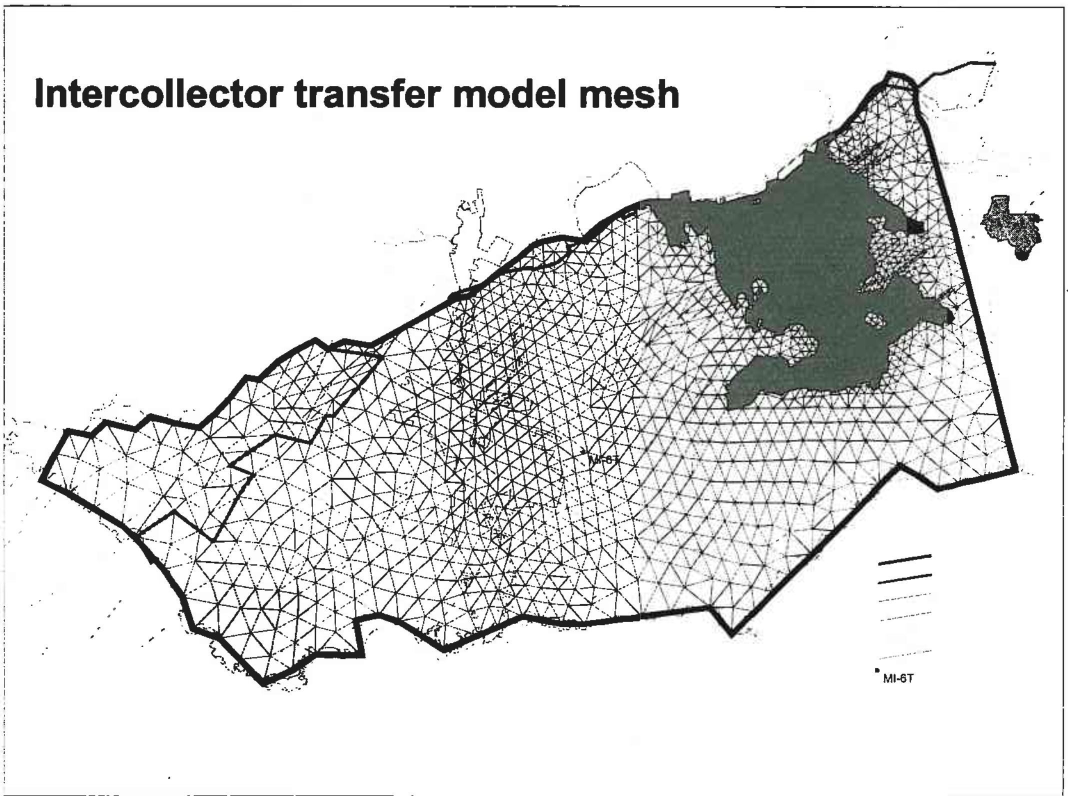


Figure 1. Plan view of the used FEM mesh.

The northern boundary leads partially along the river Ploucnice and Straz fault zone. The eastern part of the boundary is given by tectonic line of Jeleni 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 1 619 plain nodes and 3 119 plain elements was used for calculations. The mesh is vertically divided into 15 layers. The whole mesh consists of about 47 000 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 western 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 crystaline rock. The top of the model is given by the phreatic surface of the Turonian aquifer.

3.2 Simulation

The three base model scenarios were created [Muzak]. Zero variant (considering current state of groundwater pollution), remediation variant – 10 g.L^{-1} TDS (considering cleaning of Cenomanian aquifer up to the level of average remaining concentration 10 g.L^{-1} of the total dissolved solids) and remediation variant – 3 g.L^{-1} TDS (considering cleaning of cenomanian aquifer up to the level of average remaining concentration 3 g.L^{-1} of the total dissolved solids).

The transfer of the contaminants was simulated in the time interval of 1000 years. Such interval is suitable especially for predicting of the evolution of pollution of drinking water source in the Mimon area and pollution of river Ploucnice by contaminants transferred from Cenomanian aquifer to Turonian. The results obtained by simulation were treated and stored with time steps of 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.

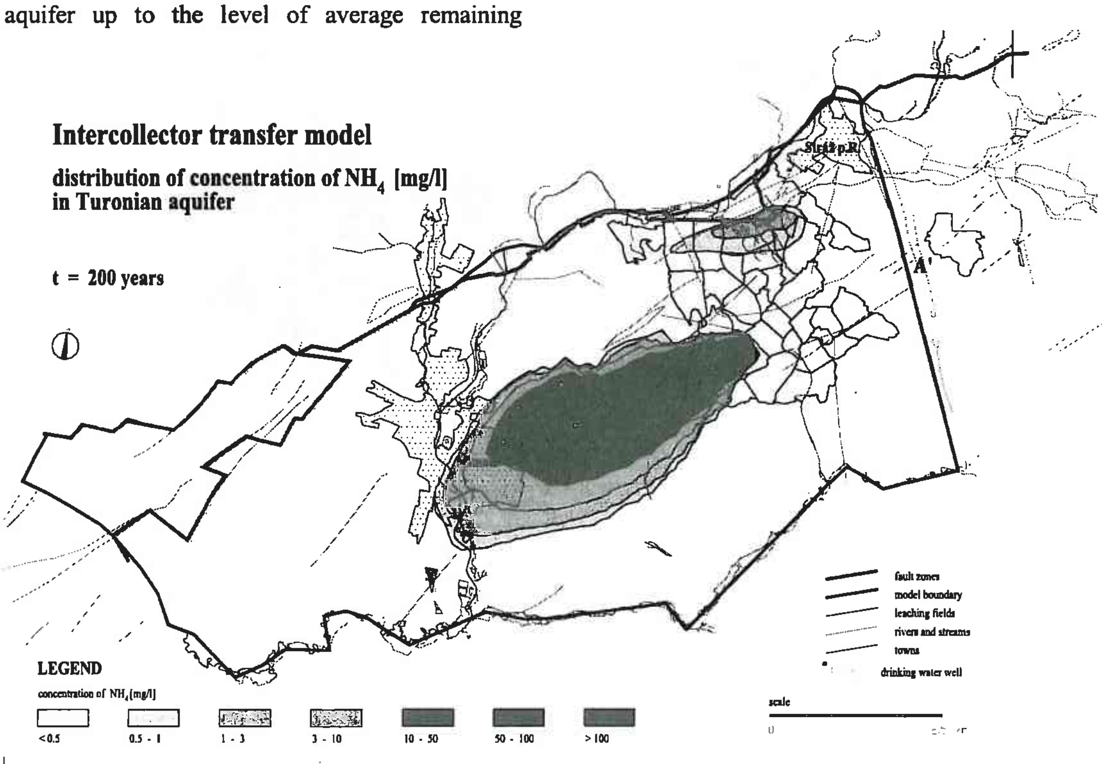


Figure 2. Distribution of NH_4 in Turonian aquifer, situation in 200 years.

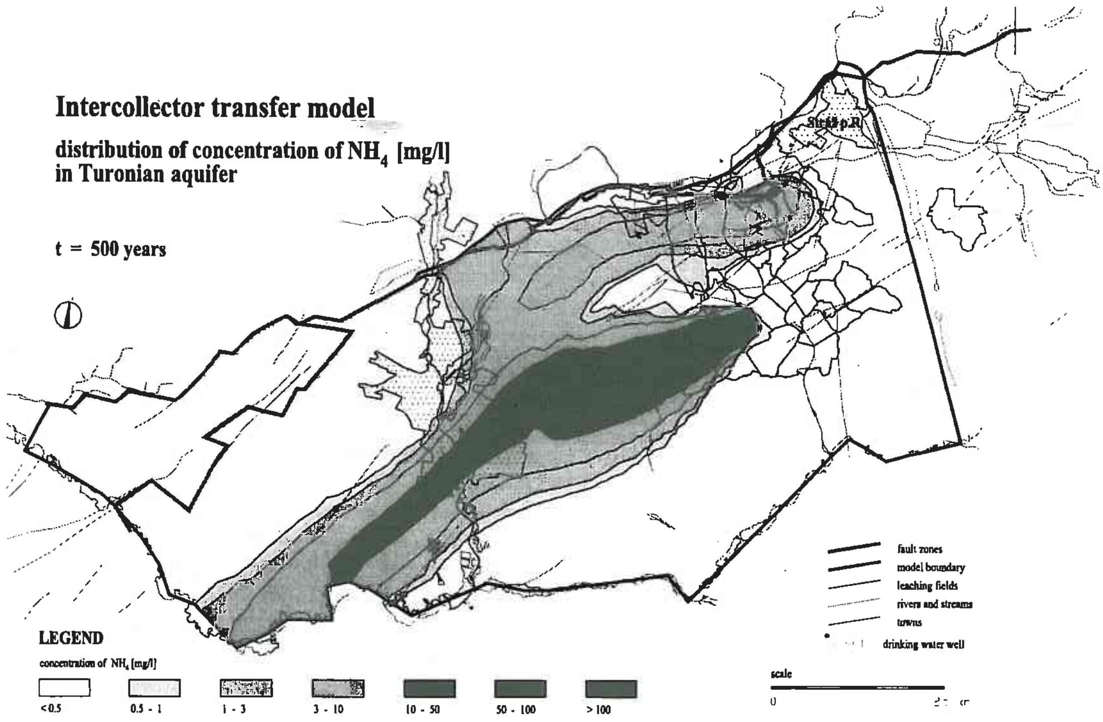


Figure 3. Distribution of NH_4 in Turonian aquifer, situation in 500 years.

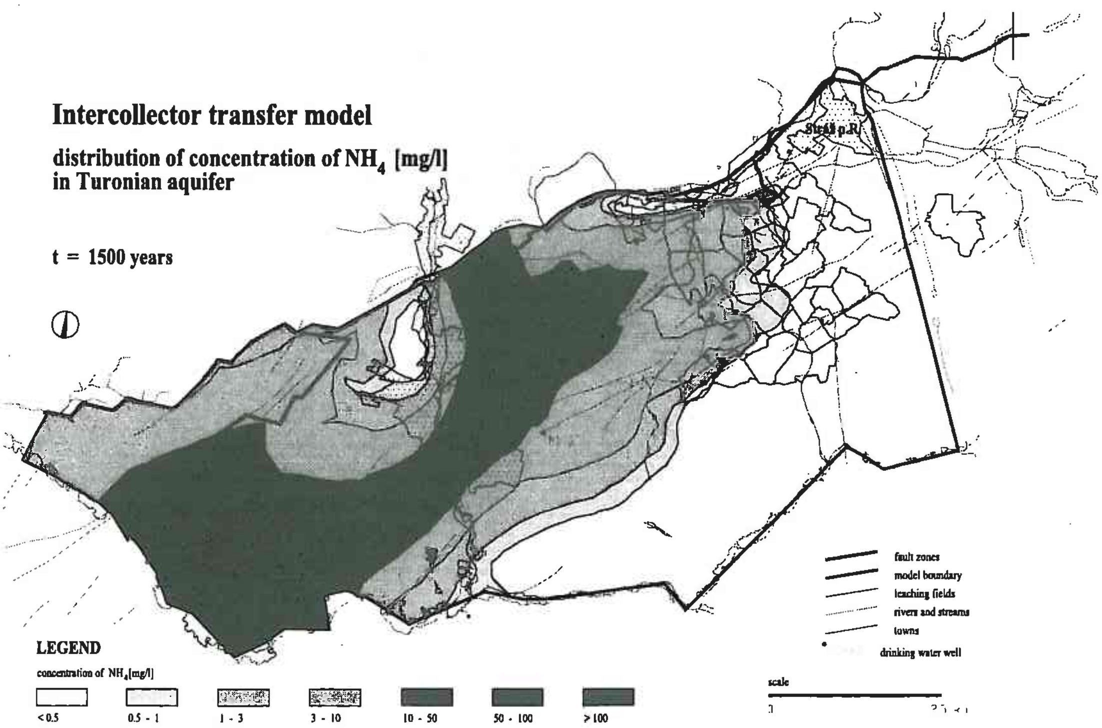


Figure 4. Distribution of NH_4 in Turonian aquifer, situation in 1500 years.

4. CONCLUSIONS

The convective transport of the contaminants is given by character of groundwater flow in the area of Straz 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-west direction in the both aquifers. In the Turonian aquifer there are two main paths of the contaminants migration. The south path leads from the central part of the leaching fields passes south hillside of volcanic massive Ralsko towards Mimon where the flow is influenced by abstraction from drinking water well MI-6. The north path passes the north hillside of Ralsko leads along the Straz fault zone continues along the river Ploucnice towards Mimon 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 then 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 $mg.L^{-1}$ (given by the standard CSN 757214) in the drinking water well MI-6.

For the extreme combinations of the both auspicious and inauspicious conditions target parameters of remediation are 2 and 9 $g.L^{-1}$ TDS. It means that it is necessary to clean cenomanian aquifer up to average remaining concentration 2 or 9 $g.L^{-1}$ TDS. Because such extreme conditions are not too probable we can recommend the target parameters on the level of 3 – 5 $g.L^{-1}$ TDS.

The water quality in the river Ploucnice 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 Ploucnice riverbed in the area of Mimon would later seriously affect water quality in Ploucnice in the area southeast from Mimon.

5. ACKNOWLEDGEMENTS

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