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MATHEMATICAL MODELLING OF A URANIUM MINE FLOODING.*

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Abstract. Mathematical model of unsteady unsaturated porous media flow is discussed. A compact expression of the governing equations is found. It is discretized by Rothe method in time and by mixed-hybrid finite element method in space. A sketch of an existence proof for the mixed-hybrid formulation is given. An iterative scheme for solution of the resulting nonlinear problem is proposed. An application to the model to modelling of flooding deep uranium mines after finishing the mining activities is considered.

Key words. porous media flow, mixed-hybrid finite elements, groundwater flow modelling

AMS subject classifications. 35J65, 65N30, 76S05

1. Introduction. The enormous contamination of the underground water in the Cenoman formation near Stráž pod Ralskem due to uranium exploitation is one of the most serious environmental problems in the Czech Republic. Since 1963 uranium ore was mined there and later, since 1969 uranium salts were leached. Both the methods strongly differ in their hydrogeological demands. Whereas for the classical mines the underground waters should be pumped out under the level of the mining tunnels, the leaching process needs as high level of the Cenoman underground waters as possible in order to simplify the procedure, but, at the same time, protecting the sources of potable water which are in the same region. The co-existence of both the mining techniques at the same place thus naturally induced a complicated hydrogeological situation in the region. The classical mining was stopped in 1993 and the mines are being filled with concrete. The leaching is beeing finished just now and this technique will be replaced by the remediation which will take approximately 30 years. Nowadays, the flooding of the mines will be started so that the escape of the pollutants from the leaching fields would be minimized. It will be controlled based on the results of the transport modelling. For the simulation purposes a model of the nonstationary flow based on the mixed and hybrid finite elements was developed which keeps the balances on the inner faces of the discretized region. Therefore, it is compatible with the transport model based on finite volume method.

Let us assume a porous-media flow in a neighbourhood of some resource of contaminated water and denote the domain of interest by Ω. A part of Ω is fully saturated and the rest is unsaturated.

Consider now the fixed domain Ω, where the unsaturated and saturated zones Ω_1, Ω_2 are separated by a contact surface Γ_α. This contact surface is defined by the distribution of saturation $S \in \langle S_{min}, 1\rangle$, $S_{min} > 0$. The unsteady filtration flow is

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governed by continuity equation

$$\frac{\partial \beta(S,\hat{p})}{\partial t} + \nabla \cdot \mathbf{u} \;=\; q \tag{1}$$

in both Ω_1 and Ω_2. Here $\mathbf{u}$ is filtration velocity and the accumulation term is assumed in the form:

$$\frac{\partial \beta(S,\hat{p})}{\partial t} = \delta\varepsilon(\hat{p})\,\frac{\partial \hat{p}}{\partial t} + \varepsilon(S)\,\frac{\partial S}{\partial t} \tag{2}$$

Its first part expresses the accumulation capacity of the porous medium dependency on pressure (it can be neglected for small water level variations) and the second term expresses the accumulation changes in the non-saturated zone. Here ε denotes the specific water capacity which is a soil water content differentiated by the pressure. The filtration velocity now depends also on capillarity effects and saturation gradient according to modified Darcy's law

$$\mathbf{u} \;=\; -\,k_r(S)\mathbf{k}\left(\frac{1}{\varrho g}\nabla\hat{p} + \lambda_c\frac{\nabla S}{S} + \nabla z\right), \tag{3}$$

where $\hat{p}$ is pressure, $\mathbf{k}$ is the permeability tensor and $k_r(S)$ is relative hydraulic conductivity expressing the influence of saturation on the permeability of porous media. The function k_r depending on the saturation S is increasing with values in $\langle k_{min}, 1\rangle$, $k_{min} > 0$. Usually, the functions of type S^κ are used in definition of k_r. The coefficient λ_c characterizes the capillarity forces.

On the boundary $\Gamma = \partial\Omega$ several types of conditions can be prescribed: the nonpermeable part of boundary Γ_N with $\mathbf{u}\cdot\mathbf{n} = 0$, the open water level (for example, the pond) is modelled by Dirichlet boundary condition $\hat{p} = 0$ on Γ_D, on the terrain level Γ_T on has rain dotation $\mathbf{u}\cdot\mathbf{n} = -u_R$ and on the vertical boundaries $\Gamma_{N'}$ the general Newton condition $\mathbf{u}\cdot\mathbf{n} = \sigma(\hat{p} - \hat{p}_D)$ is considered. The contact surface Γ_α beetwen saturation and unsaturation zones is characterized by condition $\hat{p} = 0$ and $S = 1$.

2. The governing equation. In the unsaturated zone Ω_1 one has $\hat{p} = 0$ and $S_{min} < S < 1$, therefore Darcy's law (3) reduces to

$$R_r(S)\,\mathbf{A}\,\mathbf{u} \;=\; -\left(\lambda_c\frac{\nabla S}{S} + \nabla z\right) \quad \text{in } \Omega_1\,, \tag{4}$$

where $R_r(S) = [k_r(S)]^{-1}$, $\mathbf{A} = \mathbf{k}^{-1}$. In the saturated zone Ω_2, $S = 1$ and Darcy's law simplifies to

$$\mathbf{A}\,\mathbf{u} \;=\; -\left(\frac{1}{\varrho g}\nabla\hat{p} + \nabla z\right) \quad \text{in } \Omega_2. \tag{5}$$

Introducing the function $p = \lambda_c \ln S + z$, equation (4) can be rewritten as

$$\mathcal{R}_r(p)\,\mathbf{A}\,\mathbf{u} \;=\; -\,\nabla p \quad \text{in } \Omega_1, \tag{6}$$

where

$$\mathcal{R}_r(p) = \frac{1}{k_r(e^{\lambda_c(p-z)})}.$$

Further, we introduce the substitution $p = \frac{\hat{p}}{\varrho g} + z$, equation (5) can be rewritten as

$$\mathbf{A}\,\mathbf{u} \;=\; -\nabla p \quad \text{in } \Omega_2, \tag{7}$$

If we define

$$\mathcal{R}_r(p) = \begin{cases} \frac{1}{k_r(e^{\lambda_c(p-z)})} & \text{for } p < 0 \\ 1 & \text{for } p \geq 0 \end{cases}, \tag{8}$$

then $\mathcal{R}_r(p)$ is a bounded function and it holds

$$1 \leq \mathcal{R}_r(p) \leq \frac{1}{k_{min}}. \tag{9}$$

Darcy's law can be now expressed in one formula for both saturated and unsaturated zones:

$$\mathcal{R}_r(p)\,\mathbf{A}\,\mathbf{u} \;=\; -\nabla p \quad \text{in } \Omega. \tag{10}$$

3. MH-model of the time disretized unsaturated porous media flow. The flooding problem will be solved in the time period $\langle 0, T\rangle$. This period will be equidistantly partitioned into N subintervals of the length $\Delta t = \frac{T}{N}$. Values of the state variables in the individual time moments will be denoted by subscripts. [1] We will consider the continuity equation (1) implicitly discretized as

$$\frac{\beta_n - \beta_{n-1}}{\Delta t} + \nabla\cdot\mathbf{u}_n \;=\; q_n \tag{11}$$

Consider the decomposition of the domain Ω into system of subdomains (elements) $\mathcal{E}_h$ such that

(i) $\overline{\Omega} \;=\; \cup_{e\in\mathcal{E}_h}\overline{e}$;
(ii) $e_i \cap e_j \;=\; \emptyset$, for $i \neq j$;
(iii) $e \in \mathcal{E}_h$ is open subset of Ω with a boundary ∂e smooth enough .

and denote $\Gamma_h \;=\; \cup_{e\in\mathcal{E}_h}\partial e\backslash\Gamma_D$ the system of interelement and Newton- or Neumann-type boundary faces of elements $\mathcal{E}_h$. We shall introduce the following functional spaces:

$$\mathbf{H}(div,\mathcal{E}_h) \;=\; \{\,\mathbf{v}\in\mathbf{L}^2(\Omega)\,;\ \nabla\cdot\mathbf{v}^e \in L^2(e)\,,\ \forall e\in\mathcal{E}_h\}\,, \tag{12}$$

$$H^{\frac{1}{2}}(\Gamma_h) \;=\; \{\mu : \Gamma_h \to R;\ \exists\varphi\in H^1_D(\Omega),\ \mu = \gamma_h\varphi\}\ , \tag{13}$$

$$\mathbf{W}(\mathcal{E}_h) = \mathbf{H}(div,\mathcal{E}_h)\times L^2(\Omega)\times H^{\frac{1}{2}}(\Gamma_h)\ , \tag{14}$$

where γ_h is the trace operator on Γ_h and the superscript e denotes the restriction on element e. Further we define the form

$$\begin{aligned}\mathcal{B}_n(\mathcal{E}_h,\mathcal{R}_r(p_n);\widetilde{\mathbf{w}}_n,\mathbf{w}) = \sum_{e\in\mathcal{E}_h}\{&(\mathcal{R}_r(p_n)\mathbf{A}\mathbf{u}^e_n,\mathbf{v}^e)_{0,e} - (p^e_n,\nabla\cdot\mathbf{v}^e)_{0,e} - \\ &-(\nabla\cdot\mathbf{u}^e_n,\phi^e)_{0,e} + \langle\lambda^e_n,\mathbf{v}^e\cdot\mathbf{n}^e\rangle_{\partial e\cap\Gamma_h} + \langle\mathbf{u}^e_n\cdot\mathbf{n}^e,\mu^e\rangle_{\partial e\cap\Gamma_h} - \\ &-\sigma^e\langle\lambda^e_n,\mu^e\rangle_{\partial e\cap\Gamma_{N'}} - \frac{\theta_n}{\Delta t}(p^e_n,\phi^e)_{0,e}\}\ ,\end{aligned} \tag{15}$$

[1] In some cases we will remove the subscripts for simplicity

and the functional

$$\mathcal{Q}_n(\mathcal{E}_h;\mathbf{w}) = \sum_{e\in\mathcal{E}_{h,\alpha_n}} \{-\langle\sigma^e p^e_{D,n},\mu^e\rangle_{\partial e\cap\Gamma_{N'}} - \langle p_{D,n},\mathbf{v}^e\cdot\mathbf{n}^e\rangle_{\partial e\cap\Gamma_D} -$$

$$-\langle u^e_{R,n},\mu^e\rangle_{\partial e\cap\Gamma_T} - (q^e,\phi^e)_{0,e} - \frac{\theta_n}{\Delta t}(p^e_{n-1},\phi^e)_{0,e}\} \tag{16}$$

where $(.,.)_{0,e}$ denotes scalar product in L_2 space, α_n is shape of free boundary in n-th time step, $\widetilde{\mathbf{w}}_n = (\mathbf{u}_n, p_n, \lambda_n) \in \mathbf{W}(\mathcal{E}_h)$, $\mathbf{w} = (\mathbf{v},\phi,\mu) \in \mathbf{W}(\mathcal{E}_h)$ $\theta_n = \delta\varepsilon(p_n)$ for $p_n \geq 0$ and $\theta_n = \varepsilon\lambda_c e^{\lambda_c(p_n-z)}$.

Definition 3.1. *The weak solution of time discretized of mixed-hybrid formulation of unsteady unsaturated flow problem given by (11) and (10), by the boundary conditions mentioned above and by the decomposition $\mathcal{E}_h$ of Ω is a Rothe's function*

$$\widetilde{\mathbf{w}}(t) = \widetilde{\mathbf{w}}_{n-1}\frac{t_n - t}{\Delta t} + \widetilde{\mathbf{w}}_n\frac{t-t_{n-1}}{\Delta t} \ , \quad t \in < t_{n-1}, t_n), \tag{17}$$

where a triplet $\widetilde{\mathbf{w}}_n = (\mathbf{u}_n, p_n, \lambda_n) \in \mathbf{W}(\mathcal{E}_h)$ satisfying

$$\mathcal{B}_n(\mathcal{E}_h, \mathcal{R}_r(p_n); \widetilde{\mathbf{w}}_n, \mathbf{w}) = \mathcal{Q}_n(\mathcal{E}_h;\mathbf{w}) \tag{18}$$

for all $\mathbf{w} = (\mathbf{v},\phi,\mu) \in \mathbf{W}(\mathcal{E}_h)$.

Remark 3.1. Let $\mathcal{R}_r(p)$ be an increasing bounded function satisfying (9), $p_D \in H^{\frac{1}{2}}(\Gamma_D \cup \Gamma_{N'}$, $u_R \in H^{-\frac{1}{2}}(\Gamma_T)$, $\sigma \in L_\infty(\Gamma_{N'})$ and $q \in L_2(\Omega)$. Then there exists solution of problem (3.1). The bilinear form

$$\mathcal{C}(\mathcal{E}_h;[p,\lambda],\mathbf{v}) = \sum_{e\in\mathcal{E}_h}\{\langle\lambda^e,\mathbf{v}^e\cdot\mathbf{n}^e\rangle_{\partial e\cap\Gamma_h} - (p^e,\nabla\cdot\mathbf{v}^e)_{0,e}\}$$

satisfies on $\mathbf{W}(\mathcal{E}_h)$ BB-condition and is bounded. The form

$$\mathcal{A}(\mathcal{E}_h,\mathcal{R}_r(p);\mathbf{u},\mathbf{v}) = \sum_{e\in\mathcal{E}_h}(\mathcal{R}_r(p)\mathbf{A}\mathbf{u}^e,\mathbf{v}^e)_{0,e}$$

is strictly monotone and bounded on $\mathbf{W}(\mathcal{E}_h)$, as the spectrum of bilinear form

$$\mathcal{A}_\ell(\mathcal{E}_h;\mathbf{u},\mathbf{v}) = \sum_{e\in\mathcal{E}_h}(\mathbf{A}\mathbf{u}^e,\mathbf{v}^e)_{0,e}$$

is contained within $(\frac{a_{min}}{h},\frac{a_{max}}{h})$ and function $\mathcal{R}_r(p)$ satisfies (9). Further, the bilinear form

$$\mathcal{S}(\mathcal{E}_h;p,\lambda,\mu) = -\sum_{e\in\mathcal{E}_h}\sigma^e\langle\lambda^e,\mu^e\rangle_{\partial e\cap\Gamma_{N'}} - \sum_{e\in\mathcal{E}_h}\theta^e\langle p^e,\phi^e\rangle_{0,e}$$

is bounded negative definite. It follows from these properties, that the form

$$\mathcal{B}(\mathcal{E}_h,\mathcal{R}_r(p);\widetilde{\mathbf{w}},\mathbf{w})$$

satisfies on $\mathbf{W}(\mathcal{E}_h)$ BB-condition uniformly and is bounded. Similarly, the functional $\mathcal{Q}(\mathcal{E}_h;\mathbf{w})$ is on $\mathbf{W}(\mathcal{E}_h)$ bounded.

4. Approximation by mixed-hybrid FEM. The solution of underground water flow problem in the real conditions must reflect complex geological structure of sedimented minerals. Layers of the stratified rocks with substantially different physical properties must be modelled using the appropriate discretization of the geological region. These geological characteristics can be correspondingly described by the mixed finite element method using trilateral prismatic elements with vertical faces and generally nonparallel bases.

Let index h be a discrete parameter of horizontal plane. Due to the characteristics of the problem, the vertical discretization parameter h' satisfies $h' \ll h$ since the flow domain is usually fairly large (several squared kilometers) in comparison to the vertical thickness of sedimented layers (several meters).

We assume that the chosen discretization $\mathcal{E}_h$ is compatible with boundary conditions, i.e. Γ_N, $\Gamma_{N'}$ and Γ_D is an unification of some faces of elements from $\mathcal{E}_h$.

Further, let

$$\mathbf{W}_h(\mathcal{E}_h) \;=\; \mathbf{RT}(\mathcal{E}_h) \times M^0_{-1}(\mathcal{E}_h) \times M^0_{-1}(\Gamma_h) \tag{19}$$

be the approximate finite dimensional function space defined in [3].

Definition 4.1. *A function $\widetilde{\mathbf{w}}_{n,h,k} \in \mathbf{W}_h(\mathcal{E}_h)$ is said to be an approximation of the weak solution of time discretized mixed-hybrid formulation of the* **linearized** *porous media flow problem if the following identity holds*

$$\mathcal{B}_{n,h}(\mathcal{E}_h, \mathcal{R}_r(p_{n,h,k-1}); \widetilde{\mathbf{w}}_{n,h,k}, \mathbf{w}_h) \;=\; \mathcal{Q}_{n,h}(\mathcal{E}_h; \mathbf{w}_h)\ , \quad \forall \mathbf{w}_h \in \mathbf{W}_h(\mathcal{E}_h)\ , \tag{20}$$

and

$$\|p_{n,h,k} - p_{n,h,k-1}\|_{0,\Omega} < \zeta\,, \tag{21}$$

where $\mathcal{B}_{n,h}$ and $\mathcal{Q}_{n,h}$ are the approximation of the the bilinear form $\mathcal{B}_n$ and functional $\mathcal{Q}_n$ in the space $\mathbf{W}_h(\mathcal{E}_h)$. and ζ is given accuracy limit. For detailed description of MH-approximation see [1].

5. The numerical scheme. Inserting the basis functions

$$(\mathbf{v}_i, \phi_j, \mu_\ell) \in \mathbf{RT}^0_{-1}(\mathcal{E}_h) \;\times\; M^0_{-1}(\mathcal{E}_h) \;\times\; M^0_{-1}(\Gamma_h)$$

into the identity (20) one can obtain the following system of equations:

$$\begin{array}{rcccl} \mathbf{R}_{n,k}\mathbb{A}\;\mathbf{u}_{n,k} & + \;\mathbb{B}\mathbf{p}_{n,k} & + \;\mathbb{C}\boldsymbol{\lambda}_{n,k} & = & \mathbf{q}_{1,n,k}\ , \\ \mathbb{B}^T\mathbf{u}_{n,k} & + \;\mathbb{H}_{n,k}\,\mathbf{p}_{n,k} & & = & \mathbf{q}_{2,n,k}\ , \\ \mathbb{C}^T\mathbf{u}_{n,k} & & + \;\mathbb{S}\,\boldsymbol{\lambda}_{n,k} & = & \mathbf{q}_{3,n}\ , \end{array} \tag{22}$$

Methods used for solving this system of equations are described in [4].

We propose the following iterative procedure:

1. Set $n = 1$, $k = 0$;
2. $p_{n,h,k}$ is given
3. Fill the system (22) for $\mathbf{R}_{n,k}$ and $\mathbf{q}_{1,n,k}$ computed from $\mathcal{R}_r(p_{n,h,k})$ and $\theta(p_{n,h,k})$;
4. Find $\mathbf{U}_{n,k+1}$, $\mathbf{P}_{n,k+1}$, $\boldsymbol{\Lambda}_{n,k+1}$ as values of the flows for faces, piezometric heads in the barycentra of the elements or faces of the decomposition;

5.
   - If $|P^i_{k+1} - P^i_k| < \zeta\frac{|e_i|}{|\Omega|}$, where $|e_i|$ is the volume of element e_i and $|\Omega|$ is the volume of domain Ω, then set $\tilde{\mathbf{W}}_n = (\mathbf{U}_{n,k+1},\ \mathbf{P}_{n,k+1},\ \mathbf{\Lambda}_{n,k+1})$ and if $n < N$ then n=n+1, k=0 and continue by step 2; if not computation is finished.
   - If exist such i that $|P^i_{k+1} - P^i_k| \geq \zeta\frac{|e_i|}{|\Omega|}$, then set

$$\hat{P}^i_{k+1} = \omega^i P^i_k + (1-\omega^i)P^i_{k+1}\ ;$$

6. Set $k = k+1$; $p_{h,k} = \sum_i \hat{P}^i_k \phi_i$ and continue by step 3.

The weights $\omega^i(P^i_k, P^i_{k-1}, \ldots)$ are adjusted with some hysteresis to prevent the oscillations of the iterative process.

REMARK 5.1. For the computation we will use the mean values of $R_r(p_{n,h,k})$ for the faces of the decomposition and the mean values of the specific water depositness $\theta_{n,h,k}$ in the elements.

6. Application of model in real-world problem. This model was used in the real-world application for the simulation of the flooding of the deep mine as described in the introduction. Location of remediation area in the Czech republic is shown on figure 1

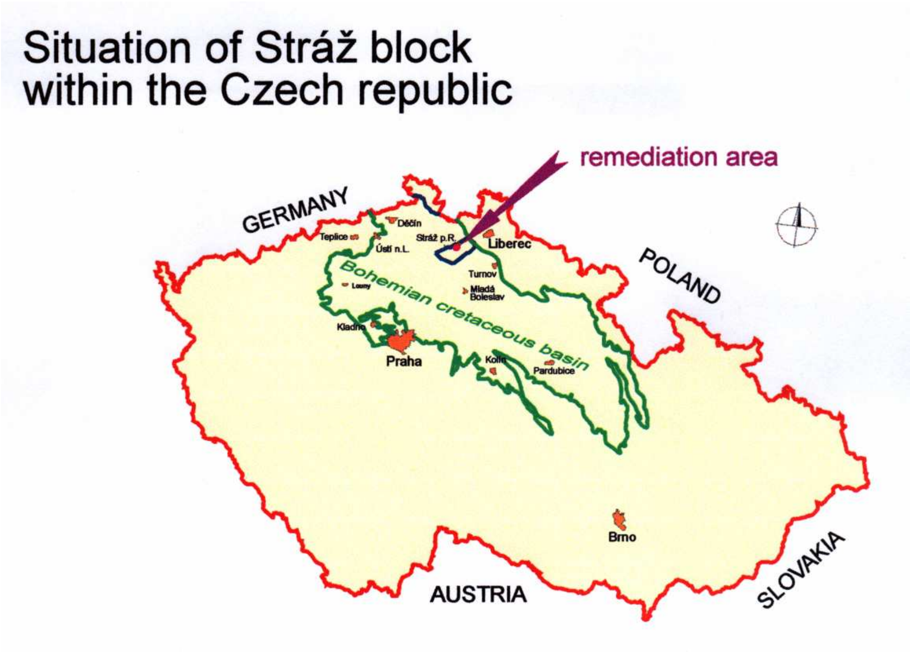

FIG. 1. *Localization of remediation area*

For numerical calculation of flow field and transport of chemical species FEM mesh was used. This mesh, shown on figure 2, contains more than 20000 trilateral prizmatic elements with nonparallel bases.

The flooding is beeing done by decreasing the activity of the water barrier situated between the two mines. For the flooding the used waters from the previous activities were used. It is well known for them that they do not react chemically with the

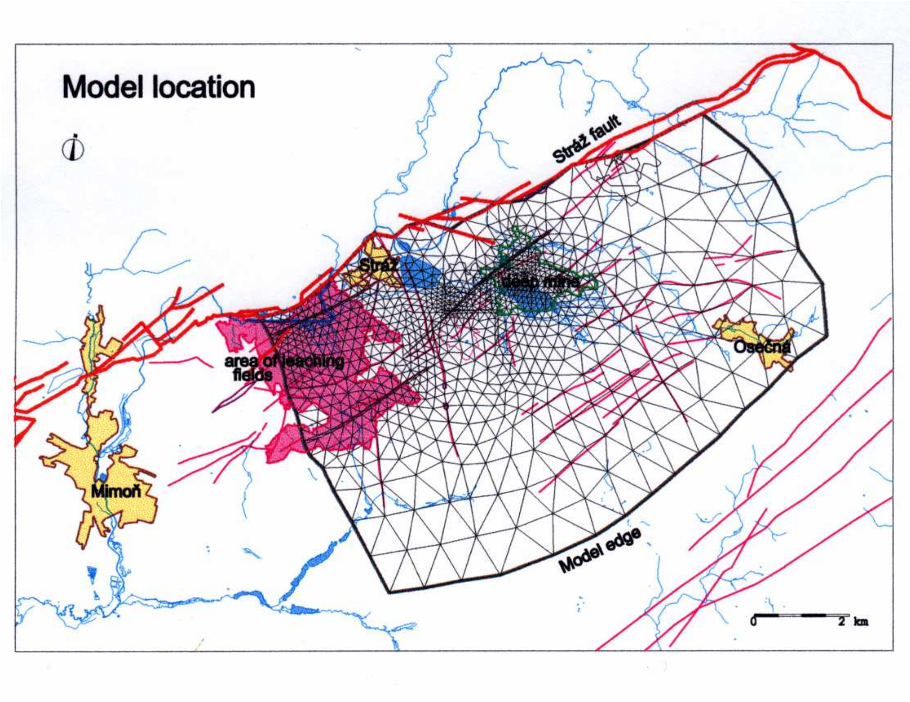

FIG. 2. *Model localization in Stráž area and FEM Mesh*

basic rock formation of the mines as well as with the other fresh water sources from the Lužice mountain area. The water level of the underground waters will rise by approximately 90 meters during the whole flooding.

Several different variants of flooding were calculated to find optimal mode of decreasing the activity of the barrier to minimalize the migration of acidic chemical species into the area of deep mine. The process of flooding was simulated for period of 2560 days (approx. 7 years) with timestep of 10 days. Figures 3 and 4 shows the state of flow field in time 0 and 500 days after begining of flooding.

Following two figures (5 and 6) shows results of transport model.

7. Conclusion. The main advantage of the approach taking into account the saturation is the use of a fixed grid. The computational cost of one iteration is relatively low in comparison with adaptive grid approach in phreatic-surface models. The mixed-hybrid formulation gives the flow field approximation suitable for finite-volume reaction-transport models.

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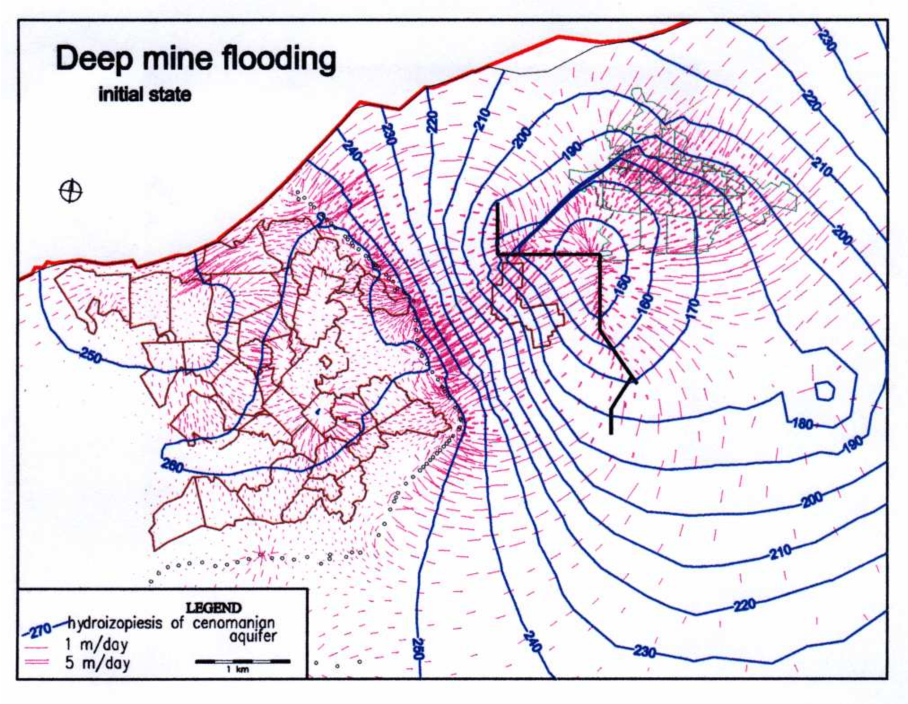

Fig. 3. *Deep mine flooding - initial state of flow field*

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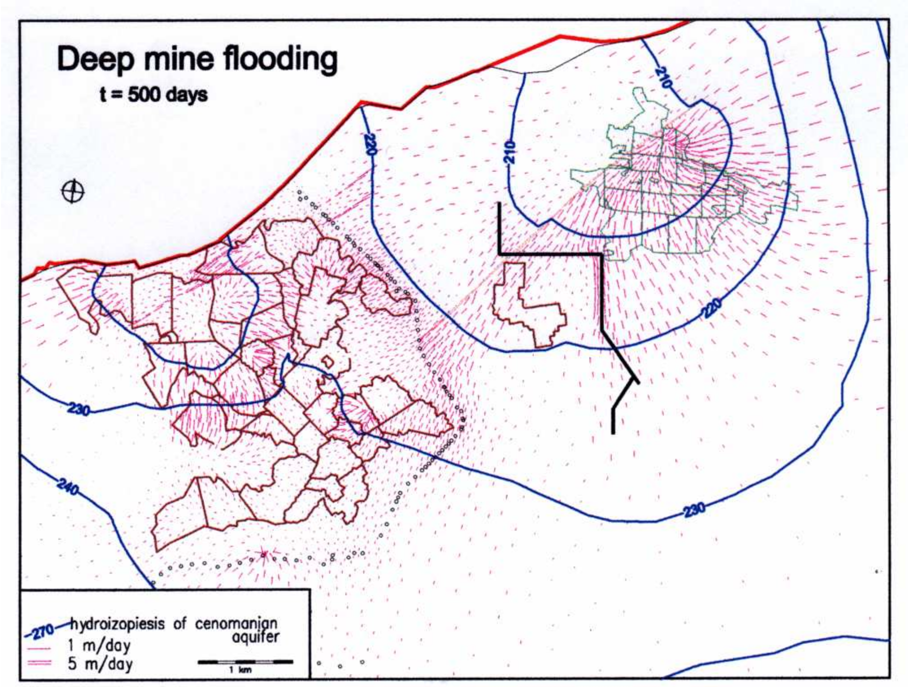

FIG. 4. *Deep mine flooding - state of flow field after 500 days*

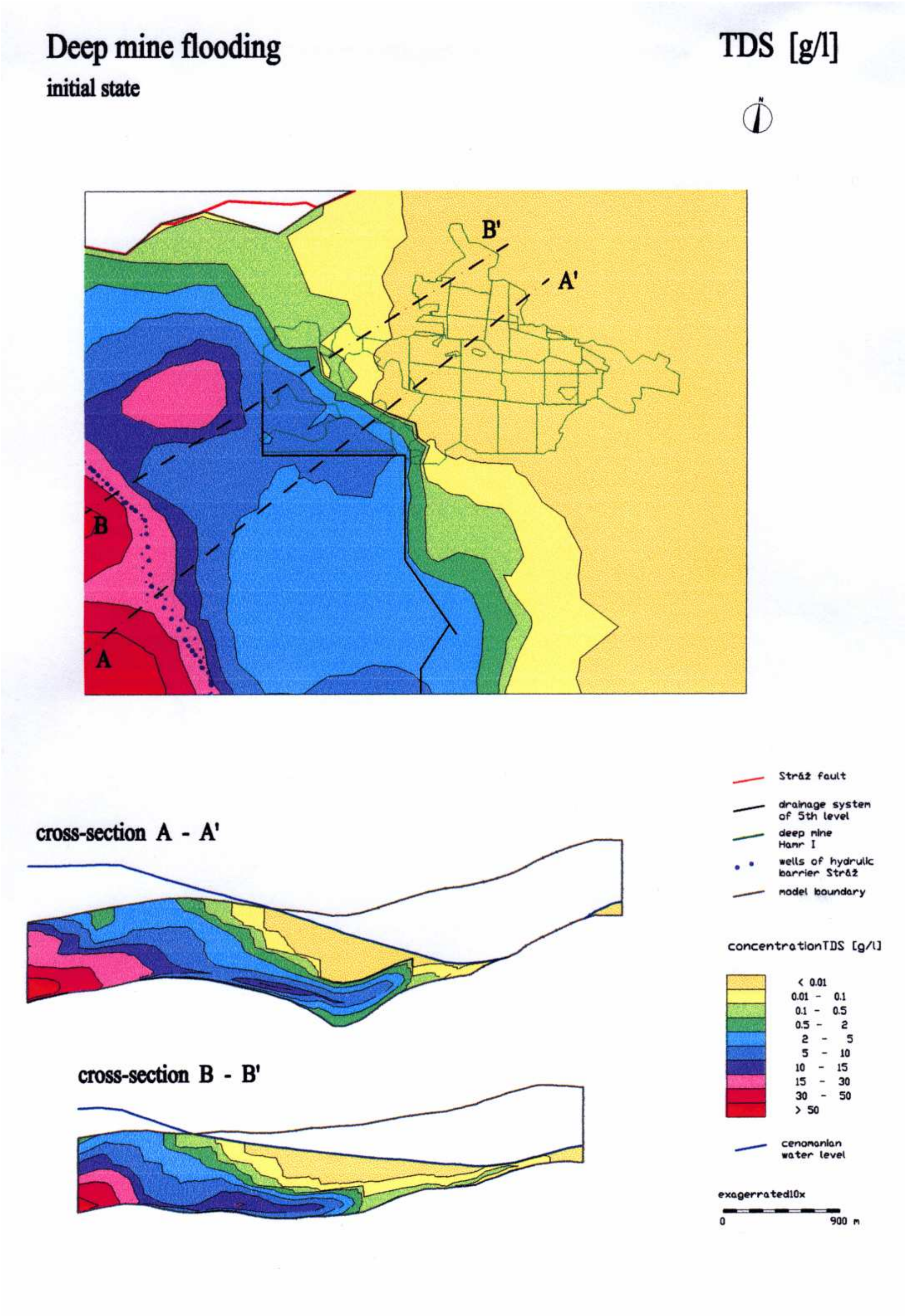

FIG. 5. *Deep mine flooding - initial state*

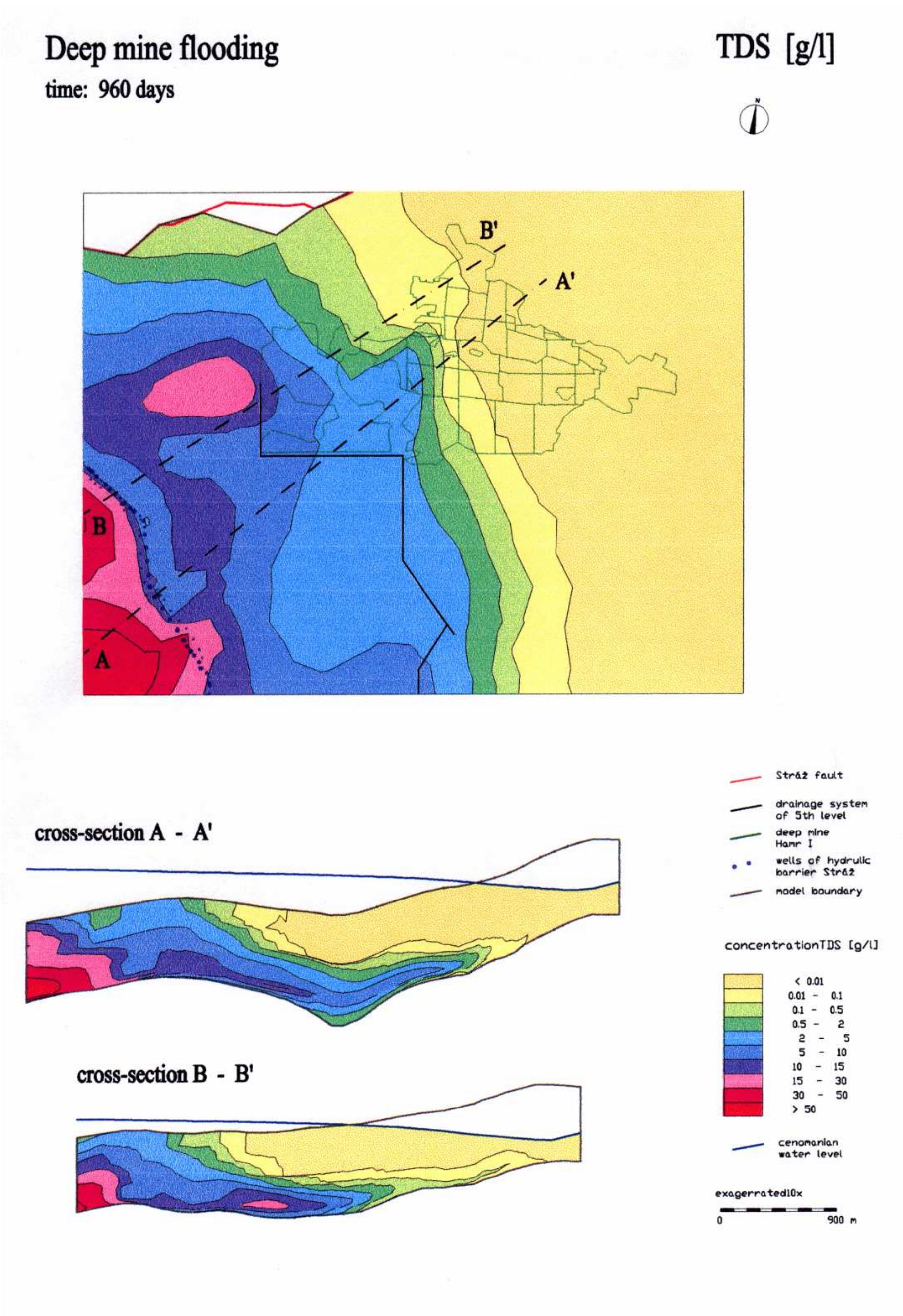

FIG. 6. *Deep mine flooding - after 960 days*