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MATHEMATICAL MODELLING OF THE UNDERGROUND WATER FLOW AND TRANSPORT OF CONTAMINANTS

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Abstract. Mathematical modelling of unsteady flow and transport in underground porous media is discussed. Governing equations in a compact form are introduced. They are discretized by Rothe method in time and by mixed-hybrid finite element method in space. We restrict our attention to methods which provide an easy and robust way to solve both the flow and transport problems with mixtures of reacting contaminants. In this paper, basic components of such approach are described. An iterative scheme for solution of the resulting nonlinear problem is proposed and the strategy of treating transport of contaminants is explained.

Key words. potential fluid flow problem, transport of chemical substances, governing equations, mixed-hybrid finite element approximation, symmetric indefinite linear systems

AMS subject classifications. 35J25, 65F10, 65F50

1. Introduction. The groundwater fluid flow problem in regions with a phreatic surface is sometimes tackled by dividing the domain into dry and saturated parts detached by a free boundary. We often need to treat both steady and unsteady filtration flow in different parts of the domain. In general, we may have four possible situations as follows. The saturated and steady flow is the simplest case and the nonsaturated unsteady flow is the most complicated one. In the following, we will treat mostly the latter case which includes the other situations as special cases. The unsteady flow plays an important role in processes with moving boundaries. Examples of such applications are published in this volume by other members of our research team.

A standard method of choice for solving the filtration flow in regions with both saturated and non-saturated part is an iterative procedure with a moving grid. The filtration flow is then defined only for a saturated part and the procedure with moving grid is often used to determine position of the free boundary. Nevertheless, there are good reasons for involving the unsaturated part into the model as well. It is desirable to include possible existence of two phreatic surfaces in a vertical cut in some cases. Another reason to avoid modelling only of the saturated part is faced in case of more general models of the regions where chemical changes of rain waters must be taken into account. These changes might be caused by slow water flow through a nonsaturated part of the domain. The same situation we face in cases of more explicit transport of chemicals through the domain.

In our case we discretize the whole domain using only one grid which covers both saturated and non-saturated parts. The finite element and finite volume techniques are then used for discretization in our generally unsteady saturated/non-saturated flow/transport code. It is only natural that from the numerical point of view, we meet troubles caused by grid deformations. One of the side effects of our method is a highly non-uniform grid close to the boundary. In particular, very thin elements should be used in these parts close to the free boundary. They increase conditioning

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of a system and oscillations in the iterative process are often observed. Therefore, the implementation should be coupled with a clever use of damping parameters against zigzagging effect similarly as it is done in the codes for solving constrained optimization rules based on active set strategies.

We will use the following notation. Denote by Ω_1 - saturated zone, by Ω_2 - unsaturated zone, by Ω_3 - vadose water (intermediate) zone and, finally, by Ω_4 - soil water zone. We will solve the filtration flow problem in $\Omega_1 \cup \Omega_2 = \Omega_\alpha$, where Ω_2 is detached from Ω_3 by the free boundary with the pressure level $p = p_{min}$; p_{min} is a negative function providing the capillar pressure which depends on the geometry of domain. The free boundary we will denote by $\Gamma_\alpha = \overline{\Omega_2} \cap \overline{\Omega_3}$.

2. Basic governing equations. The unsteady unsaturated porous media fluid flow problem is governed by a generalized continuity equation in the following form

$$\{C_\theta + c_{ls}(p)\} \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = q \quad \text{in} \;\; \Omega_\alpha,$$

where C_θ denotes the water content obtained by differentiating the retent curve of moisture by pressure, $c_{ls}(p)$ determines the coeficient of solid matrix compresibility, p is a pressure, $\mathbf{u}$ filtration velocity and q is a density of source or sink of water in domain (pumping and injection wells). Retent curve determines the dependence of moisture θ on negative capillar pressure. It is described by van Genuchten relation:

$$\theta = \theta_0 + \frac{\varepsilon - \theta_0}{(1 + \beta |p|^m)^{\frac{m-1}{m}}}.$$

Here β and m depend on a geometrical structure of the porous medium. Darcy's law expressing dependence of filtration velocity on the gradient of pressure is linear for saturated zone Ω_1 and it is given by

$$\mathbf{u} \; = \; -\mathbf{K} \; (\nabla p + \nabla z)\,;$$

where $\mathbf{K} = \varrho g \frac{\mathbf{k}}{\mu}$ denotes the tensor of hydraulical conductivity. For unsaturated zone Ω_2 is nonlinear and it is given by relation

$$\mathbf{u} \; = \; -k_r(\theta)\, \mathbf{K} \; (\nabla p + \nabla z),$$

where $k_r(\theta)$ is a coeficient of relative conductivity depending on moisture θ. Empirical relations were deduced for various rocks defining this dependence for which we have

$$k_r(\theta(p)) = \left[\frac{\theta - \theta_0}{\varepsilon - \theta_0}\right]^3 \qquad \text{for } p_{min} \le p < 0,$$

where p_{min} determines capillary pressure created by structure of rock as introduced above. Assume that

$$\mathcal{K}_r(p) = \begin{cases} k_r(\theta(p)) & \text{for } p_{min} \le p < 0 \\ 1 & \text{for } p \ge 0 \end{cases}$$

In general, we can use all the possible boundary conditions. We combine homogenous Dirichlet condition on the level of lakes, tailings ponds and in areas with wells $p = 0$ on Γ_D, we treat the rain dotation as a nonhomogenous Neumann boundary condition $\mathbf{n}.\mathbf{u} = -u_r$ on Γ_T on the terrain level. This condition is later transformed to an appropriate part of the phreatic surface Γ_α which divides unsaturated and intermediate zones. The nonhomogenous Dirichlet condition $p = p_{min}$ must be valid on the phreatic surface. The function p_{min} is obtained by monitoring the layers. Finally, on the rest part of boundary the general Newton condition is prescribed as $\mathbf{n}.\mathbf{u} - \sigma(p - p_D) = 0$ on Γ_N. If there is a part of the boundary impermeable we set there $\sigma = 0$.

3. Mixed-hybrid nonsaturated flow model. The mixed-hybrid model is based on the decomposition of domain Ω_α into collection of subdomains e_i. We denote this decomposition by $\mathcal{E}_\alpha$. Structure of interelement faces and faces with Neumann or Newton boundary conditions we denote by $\Gamma_{\mathcal{E}_\alpha}$.

$$\mathcal{E}_\alpha = \mathcal{E}(\Omega_\alpha) \quad ; \quad \Gamma_{\mathcal{E}_\alpha} = \bigcup_{e \in \mathcal{E}_\alpha} \partial e - \Gamma_D .$$

Darcy's law in the domain Ω_α is expressed in the form

$$\mathcal{R}_r(p)\,\mathbf{A}\,\mathbf{u} \;=\; -\,(\nabla p + \nabla z\,) \qquad \text{in } \Omega_\alpha ,$$

where $\mathbf{A} = \mathbf{K}^{-1}$, $\mathcal{R}_r(p) = \mathcal{K}_r(p)^{-1}$ for $p_{min} < p < 0$. $\mathbf{A}$ is a tensor of hydraulic resistance of porous media and $\mathcal{R}_r(p)$ is a relative hydraulic resistance in unsaturated zone.

We express the continuity equation discretized in time in an n-th time step as follows. Overlined symbols denote average values of the state variables in the n-th step. These values are set during iterative process.

$$\{C_\varepsilon(\overline{\theta_n}) + c_{ls}(\overline{p_n})\}\frac{p_n - p_{n-1}}{\Delta t} + \nabla \cdot \mathbf{u_n} = q_n\,, \quad \text{in} \;\; \Omega_\alpha$$

Let us introduce the function space $\mathbf{W}(\mathcal{E}_\alpha)$:

$$\mathbf{W}(\mathcal{E}_\alpha) = \mathbf{H}(div, \mathcal{E}_\alpha) \times L^2(\Omega_\alpha) \times H^{\frac{1}{2}}(\Gamma_{\mathcal{E}_\alpha})\ .$$

This function space is a Cartesian product of three spaces: the space $\mathbf{H}(div, \mathcal{E}_\alpha)$ of vector valued function whose divergence belongs to Lebesgue space $L^2(\Omega_\alpha)$, Lebesgue space $L^2(\Omega_\alpha)$ and $H^{\frac{1}{2}}(\Gamma_{\mathcal{E}_\alpha})$ of the trace of the function from Sobolev space $H^1(\Omega_\alpha)$ of functions defined on the structure of faces $\Gamma_{\mathcal{E}_\alpha}$. Denote $\widetilde{\mathbf{w}}_n$ a triple of functions $(\mathbf{u}_n, p_n, \lambda_n)$ from the space $\mathbf{W}(\mathcal{E}_\alpha)$ and similarly denote $\mathbf{w}$ a triple of test functions $(\mathbf{v}, \phi, \mu)$. We then get $\mathcal{B}_{\mathcal{E}_\alpha}(p_n; \widetilde{\mathbf{w}}_n, \mathbf{w})$ and nonlinear functional $\mathcal{Q}_{\mathcal{E}_\alpha}(p_n; \mathbf{w})$ as follows:

$$\mathcal{B}_{\mathcal{E}_\alpha}(p_n; \widetilde{\mathbf{w}}_n, \mathbf{w}) = \sum_{e \in \mathcal{E}_\alpha} \{(\mathcal{R}_r(p_n)\mathbf{A}\mathbf{u}_n, \mathbf{v})_{0,e} - (p_n, \nabla \cdot \mathbf{v})_{0,e} - (\nabla \cdot \mathbf{u}_n, \phi)_{0,e}$$

$$+\langle \lambda_n, \mathbf{v} \cdot \mathbf{n}^e \rangle_{\partial e \cap \Gamma_{\mathcal{E}_\alpha}} + \langle \mathbf{u}_n \cdot \mathbf{n}^e, \mu \rangle_{\partial e \cap \Gamma_{\mathcal{E}_\alpha}} - \sigma^{\partial e} \langle \lambda_n, \mu \rangle_{\partial e \cap \Gamma_N} -$$

$$- \;\frac{C_\varepsilon[\overline{\theta}(p_n)] + c_{ls}(p_n)}{\Delta t}\;(p_n, \phi)_{0,e}\,\}\ ,$$

$$\mathcal{Q}_{\mathcal{E}_\alpha}(p_n; \mathbf{w}) = \sum_{e \in \mathcal{E}_\alpha} \{-\,(q_n, \phi)_{0,e} - \langle u_{n,R}, \mu \rangle_{\partial e \cap \Gamma_T} + (z\ , \nabla \cdot \mathbf{v})_{0,e} - \langle z\ , \mathbf{v} \cdot \mathbf{n}^e \rangle_{\partial e}$$

$$-\sigma^{\partial e}\langle p_{D,n},\mu\rangle_{\partial e\cap\Gamma_N} - \frac{C_\varepsilon[\overline{\theta}(p_n)] + c_{ls}(p_n)}{\Delta t}\,(p_{n-1},\phi)_{0,e}\,\}.$$

Since for the function p_n the condition $p \geq p_{min}$ must hold in each time step we introduce also the convex set of functions $\mathbf{W}_*(\mathcal{E}_\alpha)$, where we seek for a solution:

$$\mathbf{W}_*(\mathcal{E}_\alpha) = \mathbf{H}(div,\mathcal{E}_\alpha) \times L^2_*(\Omega_\alpha) \times H^{\frac{1}{2}}(\Gamma_{\mathcal{E}_\alpha})\ ,$$

$$L^2_*(\Omega_\alpha) = \{\phi \in L^2(\Omega_\alpha)\ ;\quad \phi \geq p_{min}\}.$$

The weak solution of mixed-hybrid formulation of the n-th step of time discretized unsteady unsaturated flow problem given by continuity equation and Darcy's law, boundary conditions and by the decomposition $\mathcal{E}_\alpha$ of Ω introduced above is a triplet of functions $\widetilde{\mathbf{w}}_n = (\mathbf{u}_n, p_n, \lambda_n) \in \mathbf{W}_*(\mathcal{E}_\alpha)$ satisfying

$$\mathcal{B}_{\mathcal{E}_\alpha}(p_n;\widetilde{\mathbf{w}}_n,\mathbf{w}) = \mathcal{Q}_{\mathcal{E}_\alpha}(p_n;\mathbf{w}) \tag{1}$$

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

4. Mixed-hybrid finite elements for the flow problem. The flooding problem will be solved in the time period $\langle 0,T\rangle$. This period will be partitioned into N subperiods of the length $\Delta t = \frac{T}{N}$. Values of the state variables in the individual time steps will be denoted by subscripts. The Rothe method is used for time discretization and MH FEM for the space discretization.

The solution of ground 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 described by the mixed finite element method using trilateral prismatic elements with vertical faces and generally nonparallel bases. Let index h is 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 the sedimented layers (several meters).

On these prismatic elements we define the Raviart-Thomas space of vector valued functions. Parameters of these functions are determined so that each function defines unit flow through one face and zero flow through the remaining faces. For a prismatic element with nonparallel bases these functions have the following form:

$$\mathbf{v}_i^e = k_i^e\begin{bmatrix} 0 \\ 0 \\ x_3 - \alpha_{i3}^e \end{bmatrix}\quad,\quad \mathbf{v}_i^e = k_i^e\begin{bmatrix} x_1 - \alpha_{i1}^e \\ x_2 - \alpha_{i2}^e \\ \beta_i^e x_3 - \alpha_{i3}^e \end{bmatrix},$$

$$i\ =\ 1,2, \qquad\qquad i\ =\ 3,4,5.$$

The parameters of these functions are determined from equations

$$\int_{f_j^e} \mathbf{n}_j^e \cdot \mathbf{v}_i^e\, dS\ =\ \delta_{ij}\ ,\ i,j = 1,...,5.$$

Now we introduce the space $\mathbf{RT}^0(e)$ as a linear cover of the set of the introduced functions:

$$\mathbf{RT}^0(e) \ = \ \{\mathbf{v}^e \, ; \, \mathbf{v}^e(\mathbf{x}) = \sum_{i=1}^{5} V^j \mathbf{v}_j(\mathbf{x}) \ , \ \mathbf{x} \in e\, \}.$$

And finally we define also the Raviart-Thomas space of functions defined on whole decomposition $\mathcal{E}_\alpha$

$$\mathbf{RT}^0_{-1}(\mathcal{E}_h) \ = \ \{\mathbf{v} \in \mathbf{L}^2(\Omega)\, ; \ \mathbf{v}|_e \in \mathbf{RT}^0(e)\, , \forall e \in \mathcal{E}_h\}.$$

We introduce also spaces $M^0_{-1}(\mathcal{E}_h)$ and $M^0_{-1}(\Gamma_h)$ of piecewise constant trace function on each element or face, respectively, from Γ_h to aproximate pressure in the elements and on the faces.

If we introduce the base functions

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

to the formulation of the problem (1) introducing above we get the following system of nonlinear equations

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

This system is then solved iteratively by linearization. Then, e.g., a Schur complement transformation or a dual variable method coupled with conjugate residual solvers might be applied. Nevertheless, first we need to show, how to treat the nonlinearity which is inherently embedded into the system. The iterative procedure for a $n-$th time step we will show below. The initial conditions are given for real-world problems by a steady-state pressure field determined by a premature hydrogeological treatment.

In each iteration step, the computed and set variables are compared. Further, capillar pressure bounds are checked. In case that the current linear model do not provide acceptable results, new step of the nonlinear loop is started. Pressure values are combined with those from previous steps. The solvers are coupled with damping parameters to prevent oscillations.

5. General iterative procedure for unsteady non-saturated flow. In this section we will briefly summarize the iterative procedure to solve the nonlinear system (2) which we used in our implementations and which corresponds to the previous description.

1. Set $n = n+1$, $k = 0$ and $p_{h,n-1}$;
2. Assemble the system (2) for $\mathbf{R}_{n,k}$ computed from $\mathcal{R}_r(\lambda_{n,k})$ and $C_{n,k}$ computed from $C_\varepsilon(p_{n,k}) + c_{ls}(p_{n,k})$;
3. Find $\mathbf{U}_{n,k+1}, \ \mathbf{P}_{n,k+1}, \ \boldsymbol{\Lambda}_{n,k+1}$;
4. • If $|P^i_{n,k+1} - P^i_{n,k}| < \zeta \frac{|e_i|}{|\Omega|}$ & $P^i_{n,k+1} \geq P_{min}$, where $|e_i|$ is the volume of element e_i and $|\Omega|$ is the volume of domain Ω. If $|\Lambda^i_{n,k+1} - \Lambda^i_{n,k}| < \zeta \frac{|\partial e_j|}{|\Gamma_h|}$, where $|\partial e_j|$ is the area of face ∂e_j and $|\Gamma_h|$ is the area of the all faces from decomposition Γ_h, stop the computation;

- If there exists such i that $P^i_{n,k+1} < P_{min}$ then the i-th element leaves
- If exists i such that $|P^i_{n,k+1} - P^i_{n,k}| \geq \zeta \frac{|e_i|}{|\Omega|}$
  or if there exists j such that $|\Lambda^i_{n,k+1} - \Lambda^i_{n,k}| \geq \zeta \frac{|\partial e_j|}{|\Gamma_h|}$
  then set

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

$$\widetilde{\Lambda}^j_{n,k+1} = \omega^j \Lambda^j_{n,k} + (1-\omega^j)\Lambda^j_{n,k+1} \ ;$$

5. Set $k = k+1$; $p_{n,k} = \sum_i \widetilde{P}^i_{n,k}\phi_i, \quad \lambda_{n,k} = \sum_j \widetilde{\Lambda}^j_{n,k}\mu_j$ and continue by step 2.

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

6. Transport of chemical substances. Complex task of transport of chemical substances is defined by balance equations for each substance in the mixture and its general form for a l-th substance is:

$$(3) \ \frac{\partial c^l}{\partial t} + \nabla \cdot (\mathbf{u}c^l) - \nabla \cdot (\mathbf{D}\nabla c^l) + c^l q^- + r^{l,-}(c^l, c^i, \ldots) = c^{l*} q^+ + r^{l,+}(c^k, c^i, \ldots),$$

where D is tensor of diffusivity and dispersivity, which depends on molecular diffusivity of the l-th substance, longitudal and transversal dispersivity and filtration velocity according to following formula:

$$\mathbf{D} = D_m \delta_{ij} + \alpha_T |\mathbf{u}| \delta_{ij} + (\alpha_L - \alpha_T)\frac{u_i u_j}{|\mathbf{u}|}, \tag{4}$$

D_m is molecular diffusion coefficient, $\mathbf{u}$ is filtration velocity, α_L and α_T transversal dispersivity coefficients (see [4]). Homogenous boundary conditions are typically prescribed. Let us denote by $\partial\Omega^+$ the sum of inflow border faces. We will describe explicitly typical boundary conditions. If we assume uncontaminated water flows into the model area through inflow border faces, then a homogenous Dirichlet boundary condition $c^l = 0$ is prescribed. If the chemical composition is known, then a non-homogenous condition is given. Let us denote by $\partial\Omega^-$ the sum of outflow border faces. Homogenous Neumann condition

$$\mathbf{D}\nabla c^l \cdot \mathbf{n} = 0 \tag{5}$$

characterizes the case in which chemical components are taken out of model area only by convection (impact of diffusion is then neglected due to low concentrations) and this is applied to outflow border faces.

7. Time decomposition of transport operator. In this section we express the fact that different processes given in the summary equation in the previous section and different outcomes should be compared on basis of different time steps. They are also different from time steps of the previously mentioned Rothe method. Let us mention more in detail individual parts of the transport operator.

Dominant influence on transport progress in substance migration in tailings pond surrounds problem is caused by convection expressed in the following equation:

$$\frac{\partial c^l}{\partial t} + \nabla \cdot (\mathbf{u}c^l) + c^l q^- = c^{l*} q^+, \tag{6}$$

In this equation q^- denotes the output and q^+ injection output of misture with concentration c^{l*} of the l-th substance. This equation is explicitly discretized in time and solved in each time step. Chemical changes provide another important influence on the transport. There are two basic types of chemical changes which we consider in our models: 1. Chemical changes caused by a new balance of substances in the chemical solution. The following system of non-linear equations for separate solution components mathematically describes these changes:

$$G^m(c^l, c^i, c^k, \ldots) = 0,$$

for $l, i, k \in L_s$, where L_s denotes aggregate index of solution components. If there are major chemical changes within the current time step, multiple recalculation of the system is necessary due to the non-linearity in chemical balance expressions within this time interval. 2. Chemical changes caused by dissolve and precipitation reactions. These changes are much slower compared to previous case of reactions in solution. They are calculated from a kinetic model and described by following differential equations:

$$\frac{\partial c^l}{\partial t} + r^{l,-}(c^l, c^i, \ldots) = r^{l,+}(c^k, c^i, \ldots), \tag{7}$$

Function $r^{l,-}$ defines changes in concentration of the l-th substance as a result of precipitation reactions. Function $r^{l,+}$ defines input of the l-th substance caused by dissolving of substances from solid rock. Both functions include velocity coefficients set according to current chemical situation. Influence of diffusion and dispersion can be also taken into account in the model. It is mathematically described by following parabolic partial differential equation:

$$\frac{\partial c^l}{\partial t} - \nabla \cdot (\mathbf{D} \nabla c^l) = 0, l \in L_s. \tag{8}$$

The influence of diffusion and dispersion is often typically equal to the numerical diffusion of model and thus we can sometimes omit its consequences.

8. Solution of transport problem based on computed flow. The transport is solved in time steps using an inter-element transfer of the solution with dissolved solids. After the transfer, the balance of solids as well as the calculation of concentrations of the solution components are performed (see [3], [7]). The three-dimensional element of the shape of pentahedron, which is used in the mixed-hybrid formulation of the FEM (finite element method), has the total volume V_0. Part V_r of the total volume is filled with rock and part V_f is filled with solution. If ϵ is porosity, then:

$$V_f = \epsilon V_0, V_r = (1 - \epsilon) \cdot V_0,$$

The result of the calculation of mixed-hybrid formulation is the flow through all faces of the mesh elements. Let U_j^e, j=1,2,3,4,5 be flows (transfers through the element faces) of selected element e. Positive value of U_j^e represents a flow into the element and negative value a flow out of the element. The dimension of quantity U_j^e is a volume transferred per time unit (e.g.m^3/day). Transferring volume of the solution meets the condition on elements

$$\sum_{j=1}^{5} U_j^e = Q^e,$$

where Q^e is an intensity of the source (sink) residing in the element. The transport of substances is implemented with selected time step δt. Quantity of fluid flowing in the time step through the specific face is $\delta t U_j$. For all elements it must comply with the condition

$$\delta t \left(\frac{1}{2} \sum_{j=1}^{5} |U_j^e| + |Q^e| \right) \leq V_f.$$

The mentioned condition guarantees that in one time step there is no transfer through the element of a bigger quantity of fluid then the one represented by a volume of the element. The condition is an analogy of the control using a permissible value of the Péclet number in other models. It expresses connection of the model mesh geometry (size of elements), velocity of flow and size of time step. It is necessary to keep this in mind when preparing the conceptual model for solving a specific problem. Dissolved substances are transferred through the element faces with the fluid. It is assumed in the model that the substances concentrations are constant in the whole volume of the element. The quantity of every substance transferring through the element face is a product of the transferring volume and the concentration of the l-th substance in the element where the solution is coming from:

$$M_i^{e,l} = U_i^e \cdot C^{e,l},$$

$M_i^{e,l}$ is a quantity of substance being transferred through a face, e is index of the input element (there are 2 possibilities for every internal face of a chosen element). The quantity of substance which inputs/outputs into/out of the element from the source or through the boundary face of the model is a product of the fluid volume and concentration of the substance.

$$M_Q^{e,l} = Q \cdot \delta t \cdot C^{e,l}.$$

For the inflow into element the concentration $C^{e,l}$ is defined in the form of boundary condition. For the outflow the concentration is variable in time and corresponds to the current concentration in the element. For every observed substance the balance calculation is carried out in the beginning of time step

$$M_t^{e,l} = M_{t-1}^{e,l} + \sum_{i=1}^{5} M_i^{e,l} + M_Q^{e,l}.$$

where e is index of element, t is index of time step. New concentrations of the substances are

$$C_t^{e,l} = \frac{M_t^{e,l}}{V^e}.$$

If only transport is modelled then the time step for the element is finished after this calculation. After processing of all the elements it is possible to continue with the next step. In the case of transport-reactive model the calculated concentrations represent input values for chemical reactions. The numerical model of the systems of chemical reactions which we use in this case is described in [9], [8] .

9. Numerical solution of linearized equations. Mixed-hybrid formulation leads, in its ultimate step, to a solution of symmetric but indefinite systems of large sparse linear equations with a lower right zero diagonal block. This structure allows flexible choice from more algorithmic options as mentioned above. A separate paper in this volume is devoted to different algoritms and their asymptotic complexity. Therefore, we will not treat this task in this overview.

10. Conclusion. In this paper we explained our scheme for generally non-saturated and generally unsteady flow and transport. 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. This model was used in the real-world application for the simulation of the mines' flooding as it is shown in subsequent contributions from Liberec flow and transport modelling group from their Laboratory devoted to modelling of ecological processes.

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