APPLICATION OF NUMERICAL MODEL ON EXTRACTION OF UNDERGROUND CONTAMINATION: IDENTIFICATION OF DUAL-POROSITY PROPERTIES

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Abstract
We present a model of contaminant transport in a dual-porosity environment and solution of several problems of groundwater remediation and protection. The numerical methods for flow and transport are derived to fit the needs of solved problems. We determined the parameters of dual-porosity medium in the area by means of calibration. Then several scenarios of remediation for the next years are calculated, together with analysis of influence to the drinking water sources.

Additional Keywords: two-region model, non-equilibrium transport, parameter identification

Introduction
Computer modelling is standard tool for analyses of groundwater processes and the research in numerical methods for various physical problems is wide. Because of varying geological conditions and complexity of physical processes, a practical application of models is not just a routine: for larger problems it is always a question of approximation – choice of the most important processes and possibly a tailored numerical algorithm.

The presented problems and models are part of wider research connected with uranium leaching and groundwater remediation in the Stráž pod Ralskem area in the north of the Czech Republic, which is now important ecological problem in the local context (Novák, 2001). There were some non-standard technologies used (parallel operation of leaching and deep mine, vicinity of water sources, complicated geological structures) and thus the numerical methods were developed to fit the needs of technology. We deal with the following situation: There are two important aquifers, lower is the Cenomanian where the leaching was performed and contains the major contamination, the upper is the Turonian with isolated smaller “clouds” of contamination caused mostly by technical defects of well casings. In the paper we deal with planning the efficient remediation of the Turonian aquifer by extraction wells and protection of drinking water sources in the neighbourhood.

Concerning the model itself, we especially study the effect of dual porosity on the solute transport and globally on the process of decontamination. The influence of blind pores with immobile water was introduced in (Coats and Smiths 1964): the medium is represented by two zones (two values of porosity n_m, n_i and two unknown functions of concentration – mobile and immobile) and non-equilibrium linear mass transfer between them (“dual-continuum” or “two-region” model). To solve the governing system of equations, we use the operator splitting method as a straightforward generalisation of splitting in advection-dispersion equation (see below).

Model Description
The model is based on finite element and finite volume methods, on 3D mesh derived from unstructured horizontal triangulation (i.e. trilateral prisms ordered in columns and layers). We solve two physical problems: the fluid flow problem and solute transport problem including the mobile-immobile exchange.

In the solved problems, the fluid flow can be approximated by a sequence of steady states (the flow is either natural or determined by the pumping rates, which are constant during certain periods). The Darcy's Law and the mass balance equation (Bear and Verruijt, 1990) have the form

$$\nabla \cdot v = q_s^+ + q_s^- \ , \ \ v = -\frac{1}{n_m} K \nabla \phi,$$

where K is the tensor of permeability, ϕ is the piezometric head, v is the seepage velocity, $q^{+;s}>0$ is the fluid source intensity, and $q^{-;s}<0$ is the fluid sink intensity (volume per unit volume of mobile fluid and unit time). The system is numerically solved by the mixed-hybrid finite element method (Maryška *et al.,* 1995) on trilateral prismatic elements. The piezometric head is approximated by piecewise constant function (both in element volumes and on element sides) and the velocity by piecewise linear function. The improvement with respect to standard hydrogeological models (MODFLOW etc.) is in unstructured mesh topology and more accurate approximation of flow velocity, which is important for subsequent calculation of mass transport.

The advection-diffusion transport with non-equilibrium exchange between mobile and immobile zone is governed by the system of equations

$$\frac{\partial c_m}{\partial t} + \nabla \cdot (c_m v) - \nabla \cdot (D \nabla c_m) = \frac{1}{n_m} \alpha (c_i - c_m) + c^* q_s^+ + c_m q_s^- ,$$

$$\frac{\partial c_i}{\partial t} = -\frac{1}{n_i} \alpha (c_i - c_m) \ ,$$

where c_m, c_i are the unknown concentrations in the mobile and immobile zone, D is the matrix of hydrodynamical dispersion coefficients (functions of velocity, see e.g. (Bear and Verruijt, 1990), c^* is the injected solute concentration given and v is the seepage velocity, solution of the fluid flow problem. Below, we use an alternative coefficient for the mobile-immobile exchange $T_{1/2} = \ln 2/\alpha$ (characteristic time).

The mass transport is solved by the finite volume method (Eymard *et al*., 2000) with cell-centred representation, ie. two values (mobile and immobile concentration) in each cell. This is compatible with the discretisation for fluid flow, as the advection fluxes through volume/element sides can directly use the water fluxes resulting from the flow model. While standard numerical solution methods use the directly the coupled form or various techniques of decoupling the equations (Gallo *et al*., 1996), we applied the operator splitting method, known as an efficient tool for the advection-dispersion equation (Crandall and Majda, 1980) as well as for incorporation other interaction processes (Kačur and Frolkovič, 2002). The operator-splitting method lead to sequential solution of the processes (Figure 1) and the mobile-immobile interaction can be expressed in analytical form. The detailed description of the numerical procedure and results of test problems are given in (Hokr *et al*., 2003).

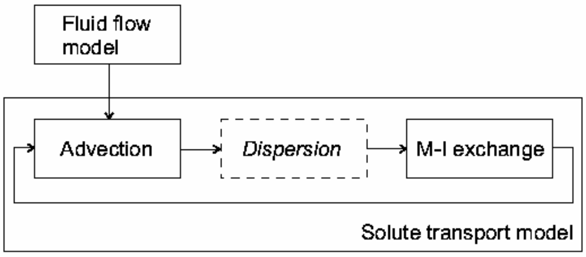

Figure 1. Block scheme of the operator-splitting approach for solution of the non-equilibrium dual-porosity transport.

Identification of Dual Porosity

Since the parameters in the dual-porosity model cannot be directly measured and the field methods are quite complicated (Casey *et al.,* 1999), we estimated the values by calibration in the sample area for the first two years of remediation, applying the measured values of concentrations in the extraction wells. We solved a problem of extraction from a single contamination cloud; the model domain has the horizontal dimensions about 1200 x 500 m and 60-90 m thickness (Figure 3). The time interval concerned is 18 months and it begins at the beginning of remediation drawing. There are 20 drawing wells in the area. The calculation is done with the mesh of about 12000 cells, ordered in 12 layers. The time step used was 3 days.

As the initial distribution of concentration could not be determined in sufficiently dense points, the significant variations are in the single wells, especially in the beginning of pumping. Therefore we used a global measure of fit: the sum of mass extracted from all wells in the month. Then the fit is expressed by sum of quadratic deviations in single months over the time interval. Minimizing the total deviation we obtained the approximate intervals for total porosity, mobile porosity and mass transfer coefficient (characteristic time of exchange), which were not unique (Table 1).

Solution of remediation and water protection problems

The model covers both the contaminated zone above the leaching domain and the clean zone with a drinking water well. The natural piezometric gradient is aimed from the contaminated area to the well, which means potential risk in the horizon of next tens or few hundreds years. The model domain and mesh is in Figure 3. The model with mobiles–immobile exchange showed expected behaviour: the concentration in the drawn solution decreases slower, mainly in the later period, when the model without the immobile pores forecasts almost zero concentration. In

Figure 2, we see a comparison of drawn concentrations in a chosen well. There is important good agreement in the later part of the period.

Table 1. Values of porosities and mass transfer coefficient – two possible combinations found by calibration

Mobile porosity n_m	Immobile porosity n_i	Mass transfer coefficent (characteristic time $T_{1/2}$)
< 0.2	0.07	>150
< 0.13	0.07	>100

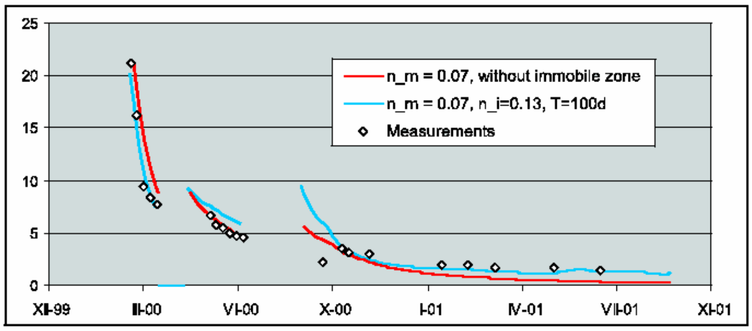

Figure 2. Extracted concentration vs. time (date) – comparison of model with measurement.

There are two phases modelled: the first is short-period decontamination and the second is long-period process of natural transport of the residual contamination. There are several scenarios for various amounts of extracted contaminants and we have to decide, how much percentage of total contamination must be extracted to keep the water source clean for next hundred years. There is a comparison for two scenarios in Figure 4. In this process, the dual porosity plays important role. For the initial analysis, the values from the smaller area are used (the reason is economical: the test pumping was performed only in a part of contaminated area) and we expect to perform running corrections during the next years.

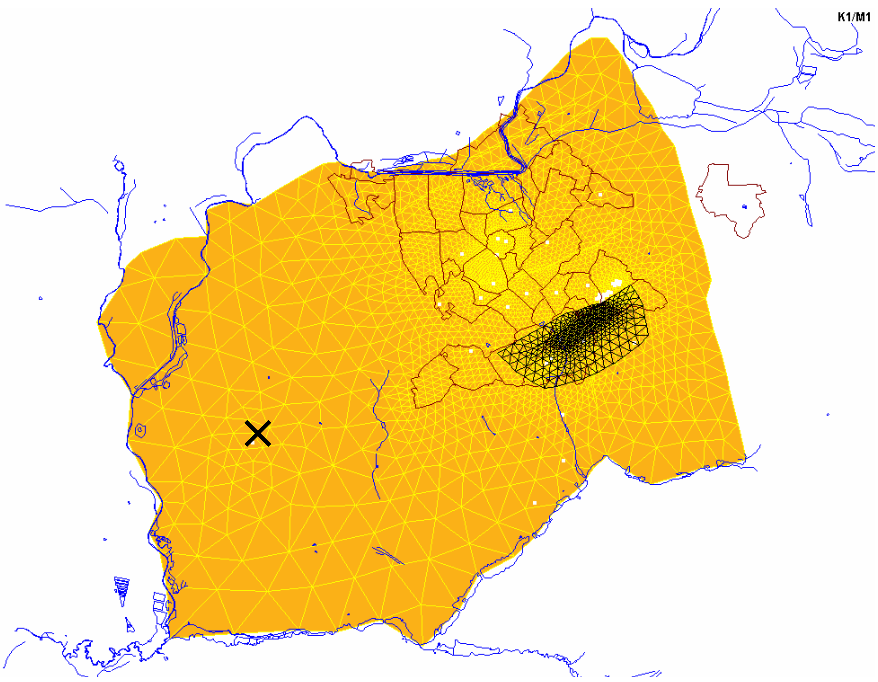

Figure 3. Model mesh, placement in the river network, and sub-model used for calibration of dual-porosity properties [black]. Position of the leaching fields (contamination) [brown] and position of the well [cross].

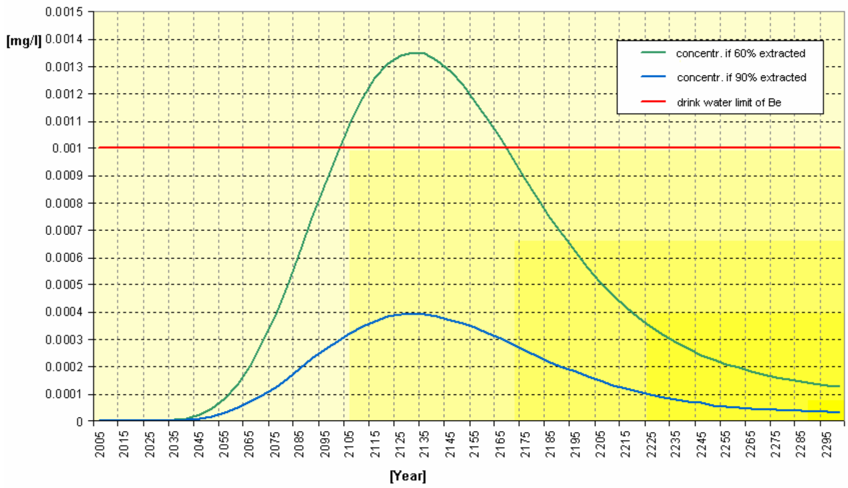

Figure 4. Run of the concentration of contaminant (beryllium) in the drink water well for two scenarios with different ratio of decontamination (percent of total initial mass).

Conclusions

The presented solute transport model, with incorporated kinetic exchange between mobile and immobile pores, appears to well represent the processes in studied area. The measurement do not allow to analyse spatial variability of the coefficients, but for global it is sufficient. The studies of the residual contamination spreading show the necessary amount of contamination to extract, to keep the observed water source within the limits.

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