Numerical Techniques for Radioactive Waste Repository Safety Assessment Based on Transport in Geological Media Models – 12083

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ABSTRACT

Radionuclide migration in geological media is considered within the framework of safety assessment of radioactive waste disposal facility. In this context groundwater flow and transport models are necessary. Computational technologies allowing for semiautomatic generation of unstructured meshes with different cell types, i.e. tetrahedra, hexahedra and pyramids and the subsequent solution of groundwater flow problems on these meshes are introduced. The application of methods is demonstrated in the groundwater flow model for a decommissioned subsurface reactor vessel, buried on its current location.

INTRODUCTION

After the adoption of the law regulating the radwaste management in the Russian Federation a number of new safety problems for RW repositories become a challenge. In most cases geological media will act as the principal safety barrier for the prospective repositories and existing legacy contaminated sites. Safety cases and safety assessments of these sites require appropriate numerical models allowing to predict the migration of isotopes in complicated geological conditions for a long time period (hundreds of thousands of years).

The present-day technological level and availability of parallel computers make it possible to create 3D numerical models with tens of millions of cells or vertices in the computational grid. Cutting edge computational schemes are required to solve problems featuring domain geometrical complexity, necessity of precise boundary representation and layer pinch-outs. To satisfy these requirements of precision and computational efficiency in our works we focus on the use of unstructured hybrid meshes with different types of cells as well as arbitrary polyhedral meshes. For example, we make use of grids containing hexahedra, tetrahedra and pyramids. An adaptive tetrahedral grid with prescribed cell size can be generated automatically in subdomains with complex boundaries while hexahedral mesh is the most appropriate for layered subdomains with simple boundaries. Transition from tetrahedra to hexahedra is performed by pyramidal cells.

The prediction of radionuclides migration comprises two joint tasks: groundwater flow and transport problems. The main tasks along their solution are the discretizations of the diffusion and advection operators in space. As long as arbitrary polyhedral grids are concerned we use finite volume methods [1] for the diffusion operator discretization. Herein linear multipoint flux approximation methods may be applied as well as the novel nonlinear methods [2], which guarantee solution non-negativity. For the advection operator discretization we consider using a finite volume scheme with piecewise-linear solution reconstruction providing second order accuracy and low numerical diffusion [3].

The application of the aforementioned computational technologies is demonstrated in the creation of a 3D groundwater flow model for a nuclear legacy site – decommissioned reactor vessel disposed of at its current location.

NUMERICAL TECHNOLOGY AND ITS APPLICATION

In case when the contaminant concentration doesn't significantly alter the groundwater density, density-driven convection may be neglected and groundwater flow and transport problems may be solved separately. In order to create a radionuclide migration model one shall generate the computational grid and numerically solve the groundwater flow and then the transport problem. The algorithm of a model groundwater flow problem solution with parameters close to reality is considered further.

The computational domain is quadrilateral in the horizontal XY-plane (see Fig. **3**), 100m high along the Z axis, with horizontal lower and upper boundaries, and vertical side boundaries. The reactor vessel building subsurface part, the shaft, is cut out of this domain, the computations are conducted only in the external media with respect to the shaft.

Stationary groundwater flow problem is to be solved. Fluxes are governed by the Darcy law. The mass conservation law is written in the following form:

$$-\nabla K(H,x,y,z)\nabla H = 0 \qquad \text{(Eq. 1)}$$

Here H is the hydraulic head (measured in meters of water column) to be computed. $K(H,x,y,z)$- is the symmetric positive definite hydraulic conductivity tensor assumed diagonal in this work:

$$K(H,x,y,z) = \begin{pmatrix} K_{xy}\left(H,x,y,z\right) & 0 & 0 \\ 0 & K_{xy}\left(H,x,y,z\right) & 0 \\ 0 & 0 & K_{z}\left(H,x,y,z\right) \end{pmatrix}. \qquad \text{(Eq. 2)}$$

As the groundwater flow occurs in the near-surface area, partially in the vadoze zone, the hydraulic conductivity tensor $K(H,x,y,z)$ is assumed to depend on the hydraulic head. The hydraulic conductivity coefficients decrease in the unsaturated zone with respect to saturated conditions. Here is a description of the computation of $K(H,x,y,z)$.

First the tensor is defined for saturated conditions. In this case it is assumed isotropic, say $K(H,x,y,z) = K(x,y,z) = k(x,y,z)I$, where I is 3x3 identity matrix. The hydraulic conductivity coefficient $k(x,y,z)$ is determined from the hydraulic transmissivity map [4] dividing it by the layer thickness and taking into account the location of the mesh cell, for which the coefficient is computed. It is assumed that the computational domain consists of two horizontal layers with different parameters, the upper layer (with higher permeability), and the lower layer (with lower permeability). This structure is stipulated by the dependence of rock fracturing on depth. The hydraulic transmissivity of these two layers is connected with the hydraulic conductivity coefficients by the following relation

$$T(x,y) = k_1(x,y)m_1 + k_2(x,y)m_2 , \qquad \text{(Eq. 3)}$$

where $T(x,y)$ is the hydraulic transmissivity, $m_1 = 60$ - upper layer thickness (m), $m_2 = 40$ - lower layer thickness (m), $k_1(x,y) = 10k_2(x,y)$ - the upper layer hydraulic conductivity coefficient is ten times higher that the lower. The index i denotes the upper ($i = 1$) or the lower ($i = 2$) layer, the coefficients $k_1(x,y), k_2(x,y)$ do not depend on z any longer. The hydraulic conductivity coefficients obtained from **Error! Reference source not found.** exhibit high spatial heterogeneity (approximately 5 orders, from $3.1 \cdot 10^{-5}$ to $1.6 \cdot 10^{1}$).

A simplified pseudo-unsaturated approach [5] is used to simulate groundwater flow in the vadoze zone. Its idea is to significantly decrease the hydraulic conductivity tensor components in unsaturated conditions. In order to let the precipitation seep till the saturated zone, the coefficient k_z is assumed constant, independent of H, say $k_{i,z}(x,y) = k_i(x,y)$. For the horizontal hydraulic conductivity coefficient $k_{i,xy}(H,x,y)$ the following approximation is used:

$$k_{i,xy}(H,x,y) = \begin{cases} k_i(x,y)/5 \ \text{ if } H \le H_{bot}, \\ \dfrac{k_i(x,y)}{5}\left(1 + \dfrac{4\left(H - H_{empty}\right)}{H_{full} - H_{empty}}\right) \ \text{ if } H_{bot} \le H \le H_{top}, \\ k_i(x,y) \ \text{ if } H \ge H_{top}. \end{cases} \qquad \text{(Eq. 4)}$$

In **Error! Reference source not found.** H_{bot} , H_{top} are the heights of the cell bottom and top points respectively. As a result the hydraulic conductivity coefficients $k_{i,xy}$ in every mesh cell depend on the saturation, defined by the hydraulic head and its Z-coordinates. If the cell saturation becomes sufficiently low, tensor horizontal component is substantially reduced thus limiting the flow associated with the given cell in horizontal directions.

The boundary conditions are based on the following considerations:

- the lower boundary - no flux boundary conditions. An impermeable clay layer is deposited 100 m deep.
- side surfaces – Dirichlet-type boundary conditions, based on the annual average water table map [4];
- top surface – Neumann-type boundary conditions, prescribed precipitation seepage defined by the annual average rainfall for the area with the assumption that 1/10 of the rainfall reaches the groundwater table;
- reactor shaft surface – the drainage system keeps the water level inside the shaft on a fixed point H_{sl} , the space of the shaft lower H_{sl} is filled by water. We set $H_{sl} = -21$ m.

In more detail the boundary conditions on the faces belonging to surface of the reactor shaft are defined by the following assumptions:

- if the mass center of the face is lower than the drainage level H_{sl} the flux through the face is proportional to the difference between the hydraulic heads inside the shaft and on the face itself. The factor of proportionality is defined as the hydraulic resistance of the concrete wall.
- if the mass center of the face is higher than the drainage level H_{sl} and higher than the computed hydraulic head on this face, the impermeability condition (zero flux) is imposed because the media is unsaturated;
- if the mass center of the face is higher than the drainage level H_{sl} but lower than the computed hydraulic head on this face, seepage face boundary condition is imposed (the flux is proportional to hydraulic head).

Formally the boundary conditions of the reactor shaft surface are written as follows:

$$\sigma_f = \begin{cases} \alpha\left(H_f - Z_f\right) \text{ if } Z_f \geq H_{sl} \text{ and } Z_f < H_f; \\ 0 \text{ if } Z_f \geq H_{sl} \text{ and } Z_f \geq H_f; \\ \alpha\left(H_f - H_{sl}\right) \text{ if } Z_f < H_{sl}; \end{cases} \qquad \text{(Eq. 5)}$$

Here $\sigma_f = -K\left(H, x, y, z\right)\nabla H \cdot \vec{n}_f$ - flux through the face f, n_f - external with respect to the computational domain unit normal vector to the face; Z_f-height of the face f mass center; H_f - computed hydraulic head on f; $\alpha = 2 \cdot 10^{-3}$ day^{-1} – the hydraulic resistance of a concrete wall 0.5m thick.

The Picard method is applied to solve the nonlinear problem **Error! Reference source not found.**:

$$\nabla K\left(H^i, x, y, z\right)\nabla H^{i+1} = 0 \qquad \text{(Eq. 6)}$$

The boundary conditions on the side, top and bottom surfaces of the computational domain do not change along the iterative process **Error! Reference source not found.**. The boundary conditions on the shaft surface must be defined on each iteration. On the first iteration the flux through a face f on the reactor shaft surface is defined as follows

$$\sigma_f = \begin{cases} \alpha\left(H_f^1 - Z_f\right) \text{ if } Z_f \geq H_{sl}; \\ \alpha\left(H_f^1 - H_{sl}\right) \text{ if } Z_f < H_{sl}, \end{cases} \qquad \text{(Eq. 7)}$$

where H_f^1- is the value of the initial guess H^1 on the face f. On all the subsequent iterations the following expressions are used to determine the fluxes through faces of the shaft surface:

$$\begin{cases} \sigma_f = \alpha\left(H_f^i - Z_f\right) \text{ if } Z_f \geq H_{sl} \text{ and } Z_f < H_f^{i-1}; \\ -K\left(H^{i-1}\right)\nabla H^i \cdot \vec{n}_f = 0 \text{ if } Z_f \geq H_{sl} \text{ and } Z_f \geq H_f; \\ \sigma_f = \alpha\left(H_f^i - H_{sl}\right) \text{ if } Z_f < H_{sl}, \end{cases} \qquad \text{(Eq. 8)}$$

The hydraulic conductivity tensor on the first iteration is the same value as if it were under fully saturated conditions. On each subsequent iteration it is recalculated using the values $H^i,\ i = 2,3,\ldots$ according to formula **Error! Reference source not found.**.

A mixed grid containing hexahedral, pyramidal and tetrahedral cells is generated for the discretization of the problem in the given domain.Here is the mesh generation algorithm step-by-step:

1) The user creates the initial coarse conformal grid, containing quadrilaterals, in the footprint of the computational domain in the XY plane.

2) The quadrilateral grid is automatically uniformly refined and converted into a 3D conformal hexahedral mesh by addition of a sufficient number of identical horizontal layers. The user sets the necessary parameters of refinement in the horizontal plane and along the vertical axis.

3) A parallelepiped containing the reactor vessel shaft with a margin of several tens of meters on every side is cut out of the hexahedral grid.

4) The tetrahedral grid and the intermediate layer are constructed. This procedure comprises the following substeps:

- Sorting of the nodes lying on the planes in the cut-out area. Node coordinates serve as sorting parameters.
- Addition of new nodes to the mesh. These nodes will be the vertices of the pyramids built on the faces belonging to the planes in the cut-out area.
- Addition of pyramidal cells to the mesh.
- Addition of tetrahedral cells filling the space between the pyramids. Thus, the intermediate layer is formed, containing pyramids and tetrahedra.
- Generation of surface triangular grid on the reactor vessel shaft basing on its CAD (computer-aided design) model. The *surface_CGM_model* function from *Ani3D* package is used (see Fig. **1**).
- Generation of a surface triangular grid on the top plane of the computational domain between the nodes of the intermediate layer and the nodes in the surface grid of the reactor shaft. *mesh_2d_aft_cf* function from the *Ani2D* package is used [6].
- Generation of a tetrahedral grid in the subdomain enclosed by the reactor shaft, the top boundary of the computational domain and the intermediate layer taking

as input the existing surface grid. Function *mesh_3d_aft_cf* [6] from *Ani3D* package is used.

5) Merging the grids (hexahedral, intermediate layer and tetrahedral) in one – mixed grid (Fig. **2**).

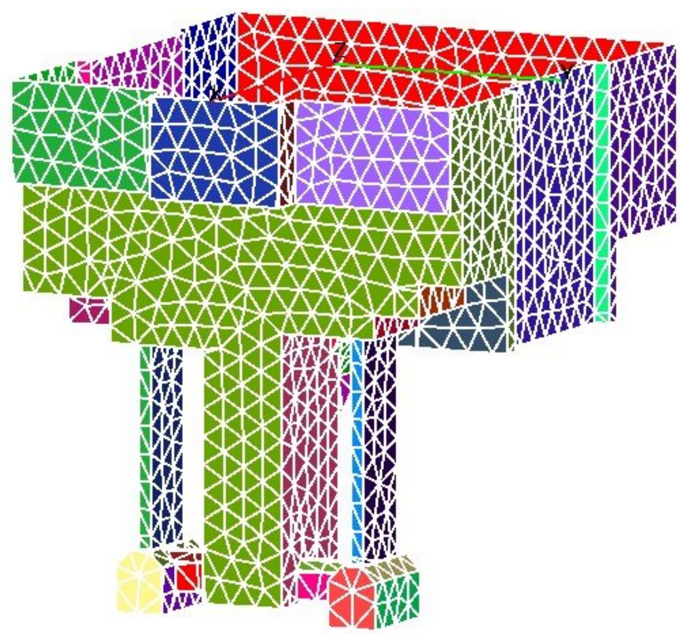

Fig. 1. Surface grid of the reactor vessel shaft.

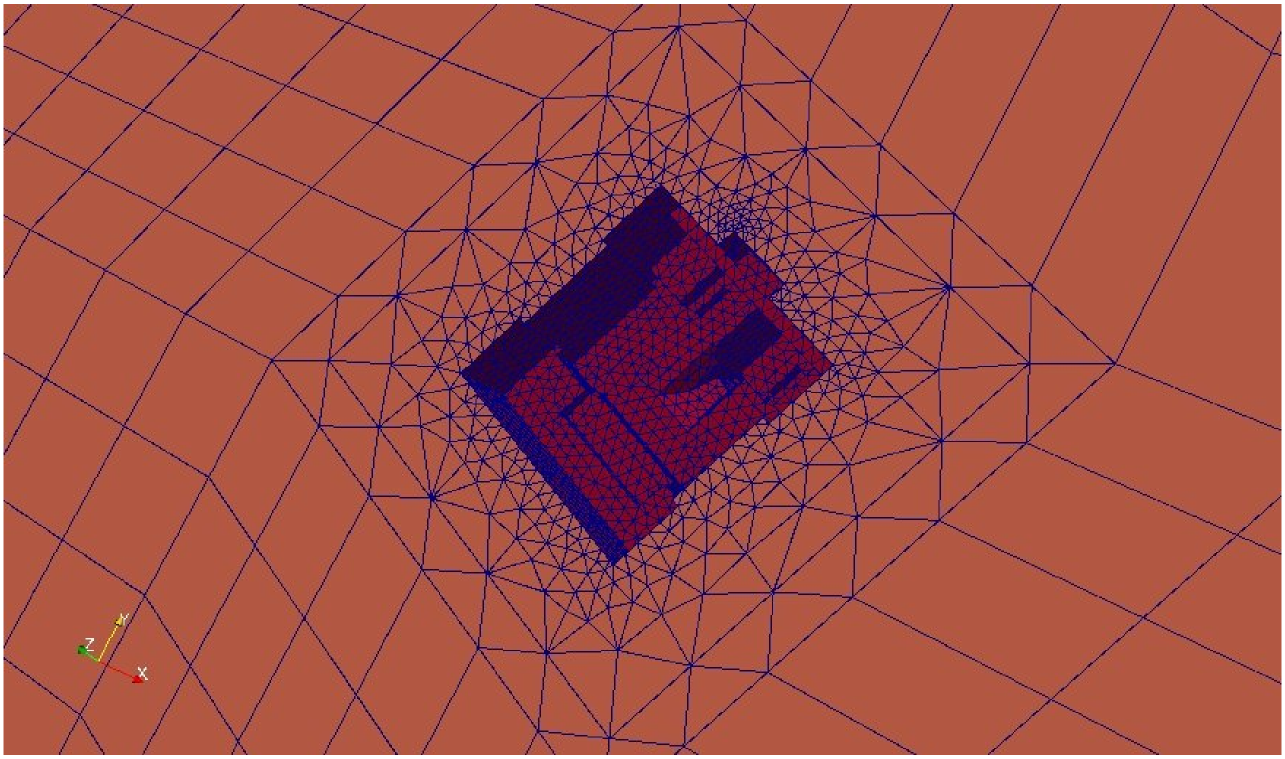

Fig. 2. Final mixed grid.

The diffusion equation discretization is provided by the finite volume method (FV). FV allows to obtain the expression for the left-hand-side of **Error! Reference source not found.** in terms of hydraulic head in the cell mass centers and mass centers of the boundary faces with non-Dirichlet-type boundary conditions. The O-scheme with multipoint flux approximation [7,8] was chosen from the variety of linear FV methods. Convergence of the O-scheme was proved on triangular and tetrahedral grids [9]. In the tests the scheme exhibits second order convergence for the hydraulic head and first order for the fluxes.

The stabilized bi-conjugate gradient (BiCGSTAB) method along with the nonsymmetric version of ILU2 [10] preconditioner is used for the solution of arising linear systems

RESULTS AND DISCUSSION

The stopping criterion for the external (Picard) iteration loop was chosen as the maximum norm of the difference in two solutions, obtained on subsequent iterations:

$$\left\| H^{i} - H^{i-1} \right\|_{\infty} < \varepsilon \quad \text{(Eq. 9)}$$

with parameter $\varepsilon = 10^{-5}$. The experiment was conducted on a grid with 32617 cells. Fig. **3** shows the hydraulic head distribution in the computational domain (in meters of the water column) on the plane $Z = 0$. One can see that the reactor vessel shaft does not influence the groundwater fluxes structure in the computational domain. The hydraulic head has two-dimensional structure in most of the domain, except for the close vicinity of the shaft, where it depends on Z coordinate. Fluxes in the vicinity of the shaft and on its surface are depicted by arrows on Fig. **4**. It can be seen that the shaft acts as a local drainage in the area, and the fluxes are directed into the shaft.

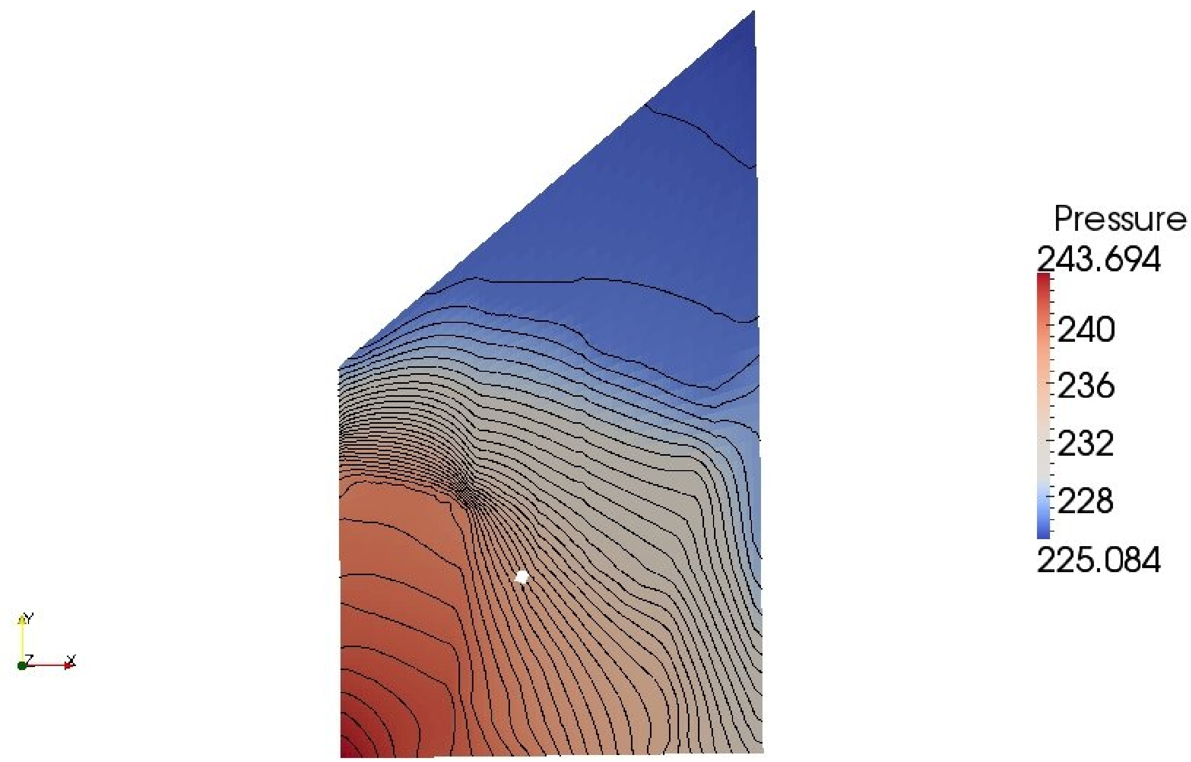

Fig. 3. Hydraulic head distribution in the domain.

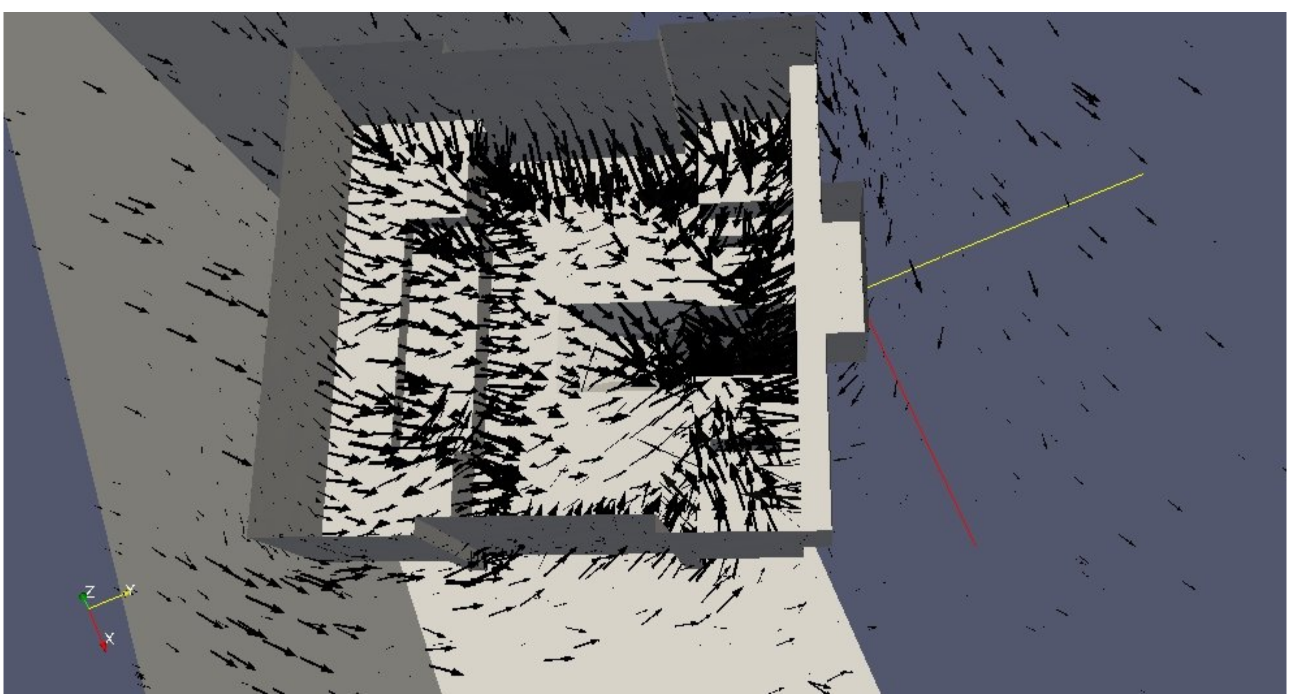

Fig. 4. Fluxes in the vicinity of the reactor shaft.

It must be noted, that there exists a problem of convergence of the internal iteration loop (linear systems solution), namely it takes more than 300 internal loop iterations to reduce the residual down to $res = 10^{-9}$ on each step of the Picard method. Note, that if the stopping criterion res is to be increased, the external Picard iterative process fails to converge because of the low precision of the linear system solution. The primary root of the problem is the mesh. The irregularities in the reactor shaft CAD model lead to strongly elongated cells in the surface grid and subsequently in the spatial grid as well. Hydraulic conductivity tensor heterogeneity (almost 5 orders) and its anisotropy also deteriorate convergence. The most simple and evident way to ensure the convergence of the internal and external loops is the proper modification of the reactor shaft CAD model. Also the application of another discretization method and another preconditioner is worth consideration in the future.

REFERENCES

1. Eymard R., Gallouet T., Herbin R. Finite volume methods (2000). // Handbook of numerical analysis / Ed. by P. Ciarlet, J. Lions - Amsterdam, North Holland - Vol. 7. - Pp. 713–1020.

2. Danilov A.A.,.Vassilevski Yu.V. A monotone nonlinear finite volume method for diffusion equations on conformal polyhedral meshes. (2009). // Russ. J. Numer. Anal. Math. Modelling - Vol. 24, № 3 - Pp. 207-227.

3. Nikitin K., Vassilevski Yu. A monotone finite folume method for advection-diffusion equations on unstructured polyhedral meshes in 3D. (2010). // Russ. J. Numer. Anal. Math. Modelling. Vol. 25, no. 4. Pp. 335–358.

4. Reservoir-9 – liquid radwaste storage and its impact on the geological media // Drojko E.G., Samsonova B.G. eds. – Moscow-Ozersk - 2007, 250 p, in Russian.

5. Diersch H.-J.G. FEFLOW finite element subsurface flow and transport simulation system - User's Manual/ White Paper. Release 5.0. (2004). WASY Ltd, Berlin.

6. Ani3D software home page http://ani3d.sourceforge.net/ .

7. Aavatsmark I., Barkve T., Boe O., Mannseth T. Discretization on unstructered grids for inhomogeneous, anisotropic media. Part I: Derivation of the methods. (September 1998). SIAM J. SCI. COMPUT. Vol. 19, No. 5, pp. 1700–1716.

8. Aavatsmark I. An introduction to multipoint flux approximations for quadrilateral grids. (2002). Computational Geosciences 6: 405–432.

9. Agelas L., Masson R. Convergence of the finite volume MPFA O scheme for heterogeneous anisotropic diffusion problems on general meshes. (2008). Comptes Rendus Mathematique. Vol.346. Iss.17-18. Pp.1007-1012.

10. Kaporin I. High quality preconditioning of a general symmetric positive definite matrix based on its $U^TU + U^TR + R^TU$ -decomposition. (1998). // Numer.Linear Algebra Appl. Vol. 5. Pp.483–509.

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