Development of Models to Forecast Radionuclide Migration in the Geological Environment for Safety Cases of Radioactive Waste Repositories in the Russian Federation - 11269

L.A. Bolshov[*,**], I.I. Linge[*], I.V. Kapyrin[*], Yu.V. Vassilevski[*], A.V. Rastorguev[*], **S.S. Utkin**[*]

*Nuclear Safety Institute of Russian Academy of Sciences (NSI RAS), 52 Bolshaya Tul'skaya St., 115191 Moscow, Russia

**Moscow Institute of Physics and Technology (State University), 9 Institutskii per., Dolgoprudniy, 141700 Moscow Region, Russia

ABSTRACT

This paper provides a brief review of the existing models in the Russian Federation to forecast radionuclide migration in the geological environment, as well as experience of the Nuclear Safety Institute in this field. The prospective codes are considered, which are aimed at describing three-dimensional groundwater flow and advective-diffusive transport of radioactive substances taking into account for sorption and decay. The discretizations to deal with unstructured mixed cell type meshes. The main prospective numerical techniques are novel finite volume methods, transport schemes with low numerical diffusion and operator-splitting schemes.

INTRODUCTION

Until recently the radwaste (RW) management in the Russian Federation was based mainly on the deferred decisions applied to the most problematic waste. In the next 5-10 years the situation will essentially change. According to the draft of the federal law «On the Radioactive Waste Management» the special RW management system will be created and aimed at timely RW disposal. Now it is planned that at least one repository for high-level RW and five to seven repositories for intermediate- and low-level RW will be needed for disposal. For some RW repositories, in-situ disposal can be implemented (for example, conservation of open liquid RW storage reservoirs and storage facilities for solid RW, generated from defense activities). Existing foreign experience shows that the

[*] The presenter, e-mail: uss@ibrae.ac.ru

lack of reliable safety estimations and/or lack of public acceptance led to the freezing of building of the disposal facilities at stages close to completion.

Until recently the development of geologic environment radionuclide migration models in the Russian Federation was focused on such unique objects as surface RW repositories in the form of reservoirs (first of all – lake Karachay) and places of liquid RW deep ground discharge. The principal feature of these models is the possibility to use monitoring data (100 to 200 or more boreholes). Some models were developed for other conditions, but these were the individual research activities. Numerical hydrogeological modeling work performed by Russian scientific institutions can be summarised as follows:

- GEON-3D regional model [1], which is specifically developed for the calculation of groundwater flow and radionuclide transport at PA "Mayak" site and its surroundings. This two-dimensional model with local three-dimensional zooms uses a porous conducting medium approach.
- Calculations for groundwater flow and radionuclide migration for Karachay lake [2].
- Survey at Leningrad Radon Special Combine site (Lenspetskombinat) in Sosnovy Bor [3].
- Modeling radionuclide propagation in deep aquifers (injection of liquid radioactive waste into the aquifer at Mining and Chemical Combine) [4]. Two-dimensional models for the porous medium have been developed.
- Studies on the description of heterogeneous porous and fractured media by effective parameters [5].
- Studies on the development of migration models for fractured carbonate media and geochemical models [6].
- Modeling radionuclide migration with assessment of sensitivity to input parameters using MODFLOW (U.S. Geological Survey) and MT3DMS (The University of Alabama). The example of such modeling for the radioactive waste storage facilities located at the territory of RSC "Kurchatov Institute" is given in [7].

Due to the appearance of many new practical problems that require a robust calculation for the safety case, the requirements to models increase significantly. It is necessary to use software that allows calculating of radionuclide migration for a long time period, taking into account, among other things, the presence of highly heterogeneous spatial and temporal characteristics of the geological environment, the complex geometry of the computational domains, geochemical and biochemical aspects of radionuclide transport.

EXPERIENCE AND THE PROSPECTIVE DIRECTIONS OF MODEL DEVELOPMENT

With regard to modeling radionuclide migration in groundwater NSI RAS focuses on two main areas: numerical and mathematical models. Analysis of a large volume of accumulated field data shows, that in some cases it is impossible to describe transport of radionuclides in the geological environment using classical models - the difference can reach several orders of magnitude. In this regard non-classical radionuclide transport models are developed [8].

Numerical models are the main tool to make sound long-term (up to million years) forecasts of contaminant propagation in groundwater. Numerical models differ in dimension (1D, 2D, 3D), type of conducting medium representation (porous or fractured) and extent to which physical effects are taken into account. The main physical processes reflected in the models are one- or two-phase (water-air) groundwater flow based on Darcy's law, advection and dispersion. The effects of molecular diffusion, sorption, radioactive decay, heat transfer, chemical and biological transformations are taken into account optionally.

Porous media models are suitable to describe the processes occurring in plastic and loose/granular media for which fracturing is not typical. For example, their use is appropriate for waste disposal in clay layers or transport in sand layers. On the contrary fractured medium models are suitable for modeling processes in rock massifs, which have very low intrinsic rock permeability and the transport is carried out through the fractures. Models of the second type either use direct simulation of individual fractures or are reduced to the first type model through upscaling and use of dual porosity and dual permeability concepts.

Up to now we've gained certain experience in creation of two- and three-dimensional groundwater flow and radionuclide transport models. The process of model building is based on the following key technologies:

1. Computational grid generation methods;
2. Temporal and spatial discretization methods;
3. Solvers for linear and nonlinear systems.

Automatic and semiautomatic methods are used for computational grid generation. For automatic generation of tetrahedral (in 3D) or triangular (in 2D) grids the **aniAFT** library from **ani3d** software package [9] is used. This makes it possible to build a grid, which approximates two- and three-dimensional boundaries of the computational domain with a specified accuracy, to refine it in subdomains, where high accuracy of calculations is needed, and to coarsen it outside of such subdomains. Specification of the computational domain boundaries and the desired resolution parameters is required to build the grid. The boundary of the computational domain can be defined in a CAD system, thus the use of a CAD model for nuclear and radiation hazardous facilities makes the grid generation process almost completely automated.

The use of mixed grids, based on hexahedra and tetrahedra with the use of prisms and pyramids as intermediates in the transition from hexahedra to tetrahedra, seems to be the most promising trend in grid generation for groundwater flow and radionuclide migration problems. Hexahedra shall be built in subdomains, where the boundaries don't have singularities, and tetrahedra - in subdomains, where it is important to approximate the boundary with high accuracy. For example, in the calculations for some localized nuclear and radiation hazardous facility with a complex geometry the grid is tetrahedral in the vicinity of the facility (with a scale of tens or hundreds of meters) and hexahedral outside this vicinity (usually the radius of the computational domain in the horizontal plane is tens of kilometers).

Solving the problem of radionuclide transport in the geological environment is usually divided into two subproblems: groundwater flow and transport, based on the advection-diffusion equation. For spatial discretization an approximation of two operators is required: diffusion (also suitable for groundwater flow) and advection. It is necessary to take into account that permeability and diffusion tensors can be heterogeneous, anisotropic, the flow field can strongly vary in space, and grids can be unstructured, anisotropic, lacking the properties of K-orthogonality and Delaunay. Models developed at NSI RAS can be used for the diffusion operator mixed finite elements method, multipoint finite volume methods as well as the new nonlinear finite volume method [10, 11]. The advantages of the new method are the following:

- scheme monotonicity in terms of non-negativity of the obtained solutions;
- possibility to be used on grids with mixed cells;
- efficient solution of arising linear systems by conventional methods;
- high order of convergence (not less than second).

Monotonicity of the method becomes especially important when calculating chemical reactions and radioactive decay, it provides conservation of mass and correct calculation of chemical transformations.

For the temporal discretization of the transport equation the operator-splitting over physical components scheme is used [12, 13]. This allows, in contrast to the explicit or implicit schemes, choosing the most appropriate approximation for each of the spatial operators as well as using different time steps for the calculation of advection and diffusion terms. The diffusion operator is approximated implicitly, the advection is approximated by the explicit predictor-corrector scheme. The diffusion step, which requires significant computational efforts, can be performed much less frequently than the fast advective step. Overall scheme stability depends on the Courant number, that is feasible in terms of front tracking. In future a fully implicit scheme can be used for cases, when precise front tracking is not required.

Spatial discretization of the advection operator is based on the discontinuous finite elements method with slope limiters [13]. It has low numerical diffusion and exhibits high-order accuracy (second-order accuracy for smooth solutions).
Linear systems formed in the process of task solving can have a large condition number. They are solved by iterative methods in Krylov subspaces (conjugate gradients, biconjugate gradient, generalized minimum residual) using modern incomplete factorization preconditioners [14]. As an alternative to incomplete factorization multi-level preconditioners are considered, implementation of which will be especially important for code parallelization. Nonlinear systems generated by new finite volume method are solved by the Picard method.
Along with the saturated porous media models the research is conducted in the area of saturated-unsaturated groundwater flow. For safety assessments of near-surface RW repositories a one-dimensional unsaturated groundwater flow model has been developed and used. It allows assessing the groundwater flow in unsaturated zone. Prospects for the development of this research are associated with three-dimensional saturated-unsaturated groundwater flow models based on Richards' equation and models of two-phase flow of air and water.
Two-dimensional models, developed in NSI RAS, were used to estimate the groundwater flow component of water balance of Techa cascade at PA "Mayak", to forecast radionuclide migration from old RW repositories of Kirovo-Chepetsk Chemical Combine, for scoping calculations of the planned RW storage facility in the North-West region of Russia. A three-dimensional model was used for calculations of groundwater flow and radionuclide migration of the prospective HLW deep repository in France. Models were verified against ModFlow and other codes on a number of test problems.

SUMMARY

Concerning the current level of modeling of radionuclide migration in geological media, we can conclude that Russian scientists have gained significant experience in creating models that can handle saturated flow and transport in porous media. However to the best of our knowledge fractured media models and unsaturated (and multiphase) flow models have not been applied in Russian safety cases and need to be developed. Prospects for the development of groundwater flow and radionuclide migration models in the Russian Federation are associated with the following developments:

1. Improvement of numerical methods and grid generators;
2. A wider range of used models (saturated-unsaturated groundwater flow, anomalous non-classical transport, chemical and biological transformations etc);
3. Models verification and cross-verification;
4. Interrelations of problems arising in radwaste repositories building: the development of mathematical models for safety cases, practical design, long-term monitoring etc.

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