COMPUTATIONAL CODES FOR THE HYDROGEOLOGICAL MODELING IN THE SAFETY ASSESSMENT OF NUCLEAR FACILITIES

Kapyrin I. V.[1, 2]

[1]**Nuclear Safety Institute of the Russian Academy of Sciences, Moscow, Russia**
[2]**Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences, Moscow, Russia**

Article received on May 16, 2022

The paper analyzes modern trends in the development and use of software for three-dimensional hydrogeological modeling. It provides an analytical overview of most recent and widely used software products, their development process, the implemented models and the numerical methods applied. The study specifies a range of typical tasks addressed by Russian nuclear industry requiring the development of numerical groundwater flow and transport models. To demonstrate the use of modern computational technologies, calculations in the GeRa software package performed for LRW DDF are considered. The paper identifies the trends for further software evolution taking into account the Russian needs in the development of near-surface and deep RW disposal facilities, decommissioning, as well as the accumulated experience in the operation of RW storage facilities and global trends in the code development.

Keywords: *hydrogeological modeling, radionuclides transport, software packages, groundwater flow, multiphysics models, radioactive waste.*

Introduction

Hydrogeological modeling is currently viewed as a key element in the safety assessment of radioactive waste disposal facilities (RWDF) and nuclear legacy facilities (NLF), since potential radionuclide transport with groundwater flows is considered as the main way of radionuclide release into the environment. Today, the standard approach provides for the development of hydrogeological models using specific software fitted with relevant model preparation tools and enabling numerical calculations of the corresponding groundwater flow, mass and heat transfer equations and the analysis of the results obtained. These models evaluate the structure of groundwater flow and the rate of contaminant transport with groundwater, thus, the transport of substances and the effects from the implementation of relevant engineering solutions (waterproofing and attenuating barriers, caps, drainage systems, etc.) can be predicted.

This article overviews current trends in the development of hydrogeological modeling software based on global cutting-edge developments and urgent tasks for the safety assessment of nuclear facilities facing nuclear industry in Russia.

It should be noted that in addition to 3D modeling software, the so-called chamber models implemented in such codes as ECOLEGO (certified software), AMBER and GoldSim are often used in the safety assessment of nuclear facilities. They are very easy to master, which makes it simple to build complex chains of contaminant transport from its source up to the biosphere and population considering the time-varying parameters of the environments and facilities considered, as well as to assess the uncertainties in a rapid manner. However, their limitations should be clearly understood: the flows carrying the contaminants should be calculated using external software tools; contaminant concentrations are averaged within each chamber, which may result in a calculated concentration at the end point underestimated by orders of magnitude.

This paper focuses on the software designed for three-dimensional hydrogeological modeling. The article is structured as follows: the first section provides an overview of modern software tools for hydrogeological modeling used in the safety assessment of nuclear facilities (NF); the second section considers the urgent tasks faced by the Russian nuclear industry requiring hydrogeological modeling; based on the first two sections, the third section states the main areas of focus for further software development and provides some common examples of their application; to summarize, conclusions are drawn about the prospects of their development.

3D hydrogeological modeling software tools

3D hydrogeological modeling software tools have been first developed at least five decades ago. Thus, the development of the most commonly used software tools in the world was started in the 1970s (FEFLOW[1]) and 1980s (MODFLOW[2], TOUGH[3] family).

The MODFLOW software was developed by the United States Geological Survey (USGS). This work was started in 1981 with the first version released in 1984. Today, this software is most commonly used to evaluate groundwater reserves, to support the decision-making on the establishment of sanitary protection zones for water intakes and to address other problems related to water use. Such widespread use can be explained by a number of factors. First, the software is built on a modular basis. Early in its development, it involved two types of modules: "problem statements", in which mathematical models were discretized, and "solvers" providing solution to linear and nonlinear problems stated in the modules of the first type. Later, when it became necessary to integrate transport and calibration calculations, models of individual processes became the software modules. Such an approach with uniform rules for module programming and clear interfaces for their interaction made it easy to add new features to it using separate modules. Secondly, the source code of the software has always been open, therefore, different specialists were able to develop their own specialized modules, graphical user interfaces and software tools that involved MODFLOW as a computational core. Most famous among them are: MT3D used to solve mass transfer problems, MODPATH used to build particle pathlines, SEAWAT used to solve variable density flow problems, graphical interfaces Visual MODFLOW, Processing MODFLOW, Groundwater modeling system (GMS). It should be emphasized that unlike the MODFLOW computational core itself, modern graphical interfaces are commercial software tools.

Currently, USGS supports two core MODFLOW versions: MODFLOW-2005 and MODFLOW 6. The first is considered the main operating software which is a classic version based on the discretization of groundwater flow and transport problems using the control volume finite differences method with rectangular hexahedral meshes. The second is under active development: it provides opportunities for flow and transport calculations based on unstructured meshes, parallel calculations using MPI and integrates a module designed to calculate variable density flows. MODFLOW 6 was developed from scratch based on object-oriented approach and allows the user to combine different processes both via successive solution of individual subtasks and by combining them into a common system of equations. In addition to the two core versions, USGS supports several advanced specialized packages: MODFLOW-USG — for calculations on unstructured meshes; MOFLOW-NWT — for calculations providing solution to groundwater flow problems in unconfined conditions using the Newton method and by smoothing non-linear dependencies; GSFLOW — for joint modeling of groundwater and surface water flows; MT3D-USGS — to calculate the contaminant transport; SEAWAT — to calculate flows of solutions with variable densities, etc. Upon finetuning the computational technologies within such software, they eventually become part of the core version.

Also widely used among hydrogeologists is the FEFLOW software [1] considered a most successful commercial hydrogeological code. Its development was started in the late 1970s. Discretization in FEFLOW is based on the finite element method with either layered prismatic or fully unstructured tetrahedral meshes. The software is fitted with a convenient graphical user interface, a large amount of educational literature and scientific publications, as well as high-quality demonstration and training videos available in the public domain, which, along with the wide modeling capabilities, paved the way to its success. FEFLOW is geared to the use of personal computers (systems with shared memory) allowing the application of a multi-core processor architecture. It implements groundwater flow calculations under variable saturation, heat and mass transfer conditions, also taking into account chemical interactions based on coupling with PHREEQC [4]. It provides opportunities for joint calculation of groundwater and surface water dynamics when paired with MIKE software. Cracks and faults are accounted for using a conduit tool (fast channels).

Within the topic of safety assessment of nuclear facilities, a wide-range simulation software COMSOL Multiphysics [5] has gained ground. Among its advantages is its ability to build a wide range of multiphysics models (mechanics, hydrodynamics, heat transfer, etc.) and a highly developed graphical interface. COMSOL implements the finite element method, including the Discontinuous Galerkin method and unstructured meshes with a mixed cell type (tetrahedra, hexahedra, prisms, pyramids). It provides some interfaces enabling its coupling with the PHREEQC geochemical module [6], [7].

In terms of numerical modelling, TOUGH is believed to be a most advanced software [8], which has been developed since the early 1980s by the Berkeley Laboratory, USA, and was designed to simulate multiphase multicomponent flows. The Newton method with an approximate numerical calculation of the Jacobian applied to solve nonlinear problems allowed to introduce a large number of complex models into TOUGH. Basic features of TOUGH provide the use of either Cartesian (rectangular) meshes or radially symmetrical ones. Moreover, some external mash generators are available in it allowing the user to build unstructured meshes for calculations. Discretization is based on the integral finite difference method. The use of the implicit Euler method and the simplest upwind approximation of the convective terms, while providing unconditional stability, results in high numerical dispersion of computational models. The latest version of the software, TOUGH3 [9], focuses on the computational efficiency: massively parallel calculations and efficient linear solvers. Basically, this software is very difficult to master, input-output is implemented using files. The graphical interface is not included into the basically delivered TOUGH package. However, there are some commercial versions of the graphical interface offered by third parties.

To model groundwater flow and transport processes under saturated-unsaturated conditions, the HYDRUS software [10] can be used. Basically, it is designed to simulate the flow, mass and heat transfer in the vadose zone (mainly to address agricultural problems). It is primarily focused on hydrological and physical properties of rocks, the features of root water uptake from the soil by plants. HYDRUS software was mainly designed for personal computers, is based on the finite element method involving meshes with a mixed cell type. HYDRUS has necessary capacities to consider fracturing of the medium based on the dual porosity and dual permeability models. Since this software is mainly designed to solve flow and transport problems in the soil layer, it is difficult to build three-dimensional geological models of complex layered structures in it.

Along with the above developments dating back to over three decades ago, some newer software tools that have not yet gained such popularity, but nevertheless based on most advanced programming and computational approaches should be noted as well.

For example, the Amanzi software package (https://amanzi.github.io) has been developed in the USA since 2010 as part of the US Department of Energy (US DOE) ASCEM project aimed at addressing the problems associated with radioactive waste disposal and cleanup of sites run by DOE. A number of US national laboratories (LANL, LBNL, ORNL, PNNL) have been engaged in its development. Nuclear Safety Institute (IBRAE RAS) has also taken part early in the ASCEM project. Amanzi is designed to simulate non-isothermal groundwater flow and transport processes under variable saturation conditions using personal and massively parallel computers [11]. The software package provides flexible tools for multiphysics modeling, for example, it is possible to connect external modules PFLOTRAN and CrunchFlow for geochemical calculations. Discretization is performed on meshes with polyhedral cells in various ways: linear and nonlinear finite volume methods, the mimetic finite difference method. Its development mainly seeks to apply most advanced packages aimed at massively parallel problem solving: MSTK framework for meshes and data on them; packages of efficient linear solvers Trilinos, PETSc (https://petsc.org) and HYPRE. Amanzi's code is open source. Subsequently, it was interfaced with the ATS software, which enabled joint modeling of groundwater and surface water flow dynamics [12], including the freezing and thawing processes [13]. Most recently Amanzi capabilities were extended: now it’s possible to calculate flow and transport in a fractured-porous medium based on the DFM approach (Discrete Fracture and Matrix) [14]. Amanzi was used to perform calculations for a number of nuclear and radiation hazardous facilities (NRHF) in the US (Nevada, Savannah River).

PFLOTRAN [15] is another leading open-source software tool supported by a group of US national laboratories (Los Alamos, Oak Ridge, Pacific Northwest, Sandia) and several other organizations. It is primarily geared to massively parallel computers. To date, it has been tested in calculations involving hundreds of thousands (2^{18}) nodes performed to solve problems on meshes containing up to 2 billion cells. PFLOTRAN is designed to simulate multi-phase multi-component flows with chemical interactions in porous media and discrete fracture network (DFN). To calculate the transport assuming relevant chemical interactions, both a fully-implicit scheme with the Newton method and a splitting scheme can be used. Currently, capabilities providing the coupling of underground and surface water flows, geomechanics and multicontinuum models are being developed. As far as the author knows, PFLOTRAN does not have its own graphical interface. Discretization is done based on the finite volume method using a two-point flux approximation scheme on structured and unstructured mashes.

The OpenGeoSys software is being developed by an international community with most of its developers working in Germany. The latest version of this software has been developed since 2011, when certain difficulties associated with further development of the previous OpenGeoSys version were faced, namely, those faced when attempting to modify the software for users by repeated code duplication [16]. OpenGeoSys is designed to simulate thermal-hydro-mechanical-chemical processes (THMC) in porous and fractured media. It has been repeatedly used to address the tasks related to the safety of RW disposal facilities (for example, in the MoMaS, DECOVALEX, SEALEX, Mont Terri projects, see [17] and other books in this series). For discretization purposes, the finite element method and unstructured meshes are used [18]. OpenGeoSys is a computational kernel launched from the command line. Separate preprocessors were proposed to be used to make it easier to address practical tasks at hand: third-party packages designed to build computational meshes GMSH (www.gmsh.info) and TetGen (www.berlios.de/software/tetgen), PETSc providing effective solution for systems of linear algebraic equations (SLAE), the ParaView postprocessor (www.paraview.org) used to visualize the results. OpenGeoSys is distributed under a BSD license, therefore, its source code can be freely used to develop commercial applications.

Scientific publications (for example, [19, 20]) often mention the ParFlow software (https://parflow.org). It was mainly designed to simulate the water balance of large areas, including groundwater and surface water flows, precipitation, and evapotranspiration. To date, ParFlow calculations are performed on orthogonal structured meshes and it is basically geared to massively parallel calculations. Parallel efficiency has been demonstrated when running on more than 100,000 computing cores. ParFlow was used to build continental hydrological models for the US and the Western Europe, models of large watersheds. It couples groundwater flow with variable saturation based on the Richards equation and surface runoff based on the shallow water equations. The software has been developed for over two decades under large international cooperation engaging 10 scientific and educational organizations from Europe and the US. Its source code is open. Text script files are used for problem setting at hand for ParFlow, whereas the results obtained are visualized in an external software, which is VisIt (https://visit-dav.github.io). Currently, ParFlow is being further developed to introduce adaptive meshing technologies, particle pathlines calculations by the Lagrangian method and a transport model with chemical interactions based on high-resolution schemes for advection and the CRUNCH geochemical module.

The latter three software tools mentioned (PFLOTRAN, OpenGeoSys and ParFlow) despite their very powerful computational capacities, currently appear to be more of research application and are mainly used by scientists either to develop computational technologies or solve rather unique and specific problems, rather than working tools for hydrogeologists.

Among the Russian software used in hydrogeological modeling, two can be noted in particular: these are currently being actively developed and used in practice: GeRa (http://gera.ibrae.ac.ru, developed by IBRAE RAS and INM RAS since 2012) and NIMFA (http:// nimfa.vniief.ru, developed by FSUE RFNC-VNIIEF and FSBI Hydrospetsgeologiya since 1998). Several versions of these software products have been certified by Rostekhnadzor (the Russian regulator) authorizing their use for the safety assessment of nuclear facilities. They are geared to the application of unstructured computational meshes, finite volume methods for spatial discretization purposes and can be used to perform calculations both on personal and parallel computers. At present time, these software products have necessary capabilities to simulate groundwater flow, mass and heat transfer processes in porous media. Spatial discretization of problems in NIMFA is implemented based on three-dimensional unstructured meshes and the finite volume method [21]. Its certified capabilities include groundwater flow models both under confined-unconfined and unsaturated conditions, convective-diffusive-dispersive transfer models taking into account equilibrium sorption governed by isotherms and radioactive decay. NIMFA also involves a hydrological module providing surface runoff and flow calculations in open channels of a rectangular shape, but nevertheless not accounting for their interaction with groundwater.

The GeRa code, the author of this article being its development leader, is mainly distinguished by its certified capabilities of reactive transport model (for this purpose, modern geochemical module PHREEQCRM [4] was used), the coupled model of groundwater flow and surface runoff [22] and the model of two-phase water–gas flow. The GeRa code also provides relevant opportunities for accounting rather specific effects: the dependence between the contaminant distribution factor and the concentration of a major component (for example, nitrate ion), radioactive decay chains, radiogenic heat release, time-varying parameters of the media (the latter is important when the near field of a nuclear facility is simulated). GeRa has a user-friendly graphical interface providing complete solution of safety assessment problems for nuclear facilities when it comes to potential groundwater contamination: from building a geological model to calculating the radioactive exposure of the population. Hydrogeological conditions are set on the model in a mesh-independent way, which makes it easy to change them if necessary. Parallelization is implemented using the MPI library [23]. Freely distributed software framework INMOST (www.inmost.org, [24], [25]) developed by INM RAS is used to provide effective simultaneous operations with meshes and data on them, as well as to build and solve SLAE. The first version of GeRa was certified by Rostekhnadzor, the Russian nuclear regulator, in 2018 and included basic capabilities designed to model groundwater flow and transport processes in porous media with variable saturation. It also allowed to consider density-driven convection and chemical interactions in the water–rock system (both based on isotherm and by calculating relevant chemical reactions). The second version, certified in 2021, was complemented with the ability of simulating dual porosity media, thermal processes, two-phase flow and surface runoff processes. These software tools provided successful implementation of models simulating various facilities at the sites of FSUE PA Mayak, FSUE MCC, JSC SCC and many others (examples of their application were discussed in [26], [27]). GeRa/V3, which is currently under development, can be used to model groundwater flow and transport in fractured media [28]. It is also geared to the safety assessment tasks at hand for the DGR planned to be constructed at the Yeniseiskiy site, as well as more advanced chemical and hydrological models, convenient user tools that can be used to handle the applied problems.

If one endeavors to compare the codes developed in Russia and abroad, a general conclusion can be made: Russian software is being developed in accordance with the global trends. However, in Russian practice, the development of open-source programs has not become widespread at all, although its important advantages are already recognized in the US and Europe. These are multiple comprehensive verification of codes and documentation, which increases the confidence in the results obtained; third-party specialists may be involved in the development, testing of these software products and handling of complex problems based on them, as well as relevant research resulting in scientific publications; use of advanced ready-made open source packages distributed under copyleft licenses.

Current tasks currently of the nuclear industry

Hydrogeological modeling software is mainly used in the nuclear industry to assess the safety of RW disposal and storage facilities, as well as decommissioned nuclear facilities and cleanup efforts performed at contaminated sites [29]. In terms of modeling needs, four categories of facilities can be distinguished.

The first category includes storage facilities and near-surface RW disposal facilities. They are usually characterized by a relatively short (hundreds of years) timeframe considered in the safety assessment which is associated either with a short period of potential hazard or the lifetime of the considered facility. These facilities commonly involve an engineered barriers system (EBS) driving the need for the development of a separate model representing the near field of the facility, which, in turn, usually requires the consideration of processes taking place in the unsaturated zone.

The second category refers to facilities being decommissioned based on the in-situ isolation or disposal option: production uranium-graphite reactors (PUGR) [30, 31]; industrial storage liquid radioactive waste (LRW) reservoirs [32], [33]; buildings contaminated due to past operations. Since all these facilities are located at the near-surface level, geological environment usually cannot be considered as a reliable safety barrier. At the same time, these facilities can be characterized by long periods of time while they may remain hazardous due the long-lived radionuclides contained therein. Their immobilization can be achieved through the installation of EBS limiting radionuclide release and transport [34]. In this case, modeling should consider much longer periods compared to the first category, while EBS evolution and chemical processes occurring over a long time period should be taken into account as well.

The third category includes LRW deep disposal facilities (LRW DDF): Zheleznogorskiy, Severskiy, Dimitrovgradskiy [35], [36]. They are characterized by a large volume of waste injected over the years of operation (millions, tens of millions of cubic meters), complex chemical and biological processes occurring in the reservoirs, density-driven and thermal convection, which should be evaluated and considered in relevant models. Despite being developed for many decades, models describing these unique facilities require further elaboration, since, to date, full-fledged demonstration of their long-term safety has been provided only considering relatively short-lived radionuclides [35].

The fourth category involves the DGR to be sited at the Yeniseiskiy site (Krasnoyarsk Territory), the designs of which are currently under development [37]. In this case the key challenges involve the fractured structure of the gneiss rock mass, available faults and the paucity of available initial data on both the boundary conditions and the properties of the host rocks. The flow in the rock mass is confined to fractures and faults, which requires the development of appropriate numerical models based on the DFN, DFM, EPM and SCM approaches.

Trends in the development of hydrogeological modeling software

Summing up the above analysis focused on available software and tasks facing the hydrogeological modeling, one can single out some focus areas being considered crucial for further software development. These are discussed below. Almost all software products are geared to unstructured computational meshes (Figure 1) providing certain flexibility in adjusting their spatial discretization by refining the mesh in those subdomains where high accuracy solutions are required (for example, in the areas where a contaminant plume is expected to be present) or accounting for geometrically complex objects. At the same time, in other areas, the mesh remains coarse enough so that the calculations do not take too much time.

Another focus area requiring further development are the capacities providing the calculations on massively parallel computers suggesting that the problems are solved on finer meshes (both in space and time), calculations are speeded up by orders of magnitude, inverse problems can be solved and the model uncertainties can be estimated, which requires them to be run repeatedly. Parallelization provides certain advantages: capabilities of modern multi-core PC processors can be used effectively and calculations aimed at solving some large-scale problems can be run on remote clusters.

Actively developed are multiphysics models accounting for the processes that were not previously taken into consideration. In particular, THMC models are required to model the near field of a RW disposal facility [38]. In certain cases, traditional models for contaminant sorption represented by isotherms appear to be inadequate due to the chemical conditions that can change significantly with time and the mutual influence of individual substances. Models representing transport by means of chemical and biological interactions are being developed: their development and application is possible only in case of interdisciplinary experts engagement, namely, specialists in hydrogeology, numerical methods and geochemistry [39]. Such models are especially relevant for DGR and LRW DGR. The latter, for example, are characterized by high salt content in the injected solutions decreasing the sorption capacity of the rock. At the same time, in the long term, biological processes, such as nitrate

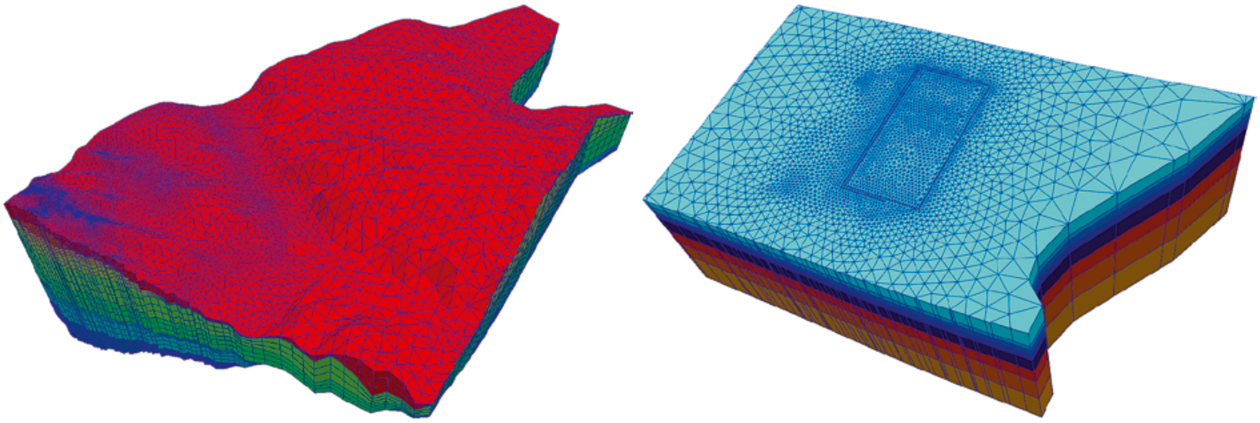

Figure 1. Adaptive unstructured meshes: on the left – mesh cross-section of a LRW DGR model providing certain thickening towards injection wells; on the right – fragment of a mesh representing a regional model taking into account a double wall in the subsoil surrounding the industrial reservoirs

reduction, provide groundwater treatment from the nitrate ion. In the future, these processes should be taken into account in models applied in the course of LRW DGR safety assessment. If freezing and thawing processes are considered, hydrogeological problems in the Arctic zone can be therefore solved.

The problem of high-density LRW transport at the Zheleznogorskiy site calculated using the GeRa code and discussed in [40] is presented below as a case study of parallel computations on adaptive meshes implemented for a complex model covering multiple coupled processes. The model takes into account density-driven convection, double porosity of the medium, flow in unconfined conditions. The computational grid contains about 2.2 million cells. To increase the accuracy in accounting the density-driven convection, the mesh was refined vertically in the 9th model layer (first operating aquifer) and horizontally in the vicinity of the injection wells. The task at hand appeared to be quite complex: simulation of a 44-year time period took a day assuming parallel calculation run on 80 cores. For this purpose, an INM RAS cluster with Arbyte Alkazar R2Q50 G5 computing nodes was used: each node involved two 20-core Intel Xeon Gold 6230@2.10GHz processors. The high complexity of the problem was associated with high inhomogeneity of the parameters (the hydraulic conductivity varied by 6 orders of magnitude) and the iterative nature of the approach implemented to solve nested nonlinear problems (density convection and flow in a unconfined conditions) using the Picard's method. The main calculation time was spent on solving the SLAE required at each iteration of the nonlinear solver of the groundwater flow problem. This was, firstly, due to a very complex preconditioner used to provide the convergence of the process and, secondly, to its slow convergence (this required from tens to several hundred iterations of the linear solver). To solve the SLAE, the restarted iterative method GMRES (30) was used involving a parallelization according to the additive Schwarz method ASM (3) with three layers of overlapping subdomains. Within each of them, an incomplete triangular decomposition ILU (8) was applied. To evaluate the parallelization effectiveness, calculations were performed for a time period of 5 years on 10, 20, 40 and 80 computing nodes.

Figure 2 shows the acceleration gained due to an increased number of applied computing nodes; a linear relationship is given for comparison purposes as an ideal option. This task was quite effectively parallelized: 8-fold increase in the core number has provided a 5.76-time acceleration. It should be emphasized that the calculation involving 160 nodes with the chosen parameters of the linear solver could not be carried out, since the preconditioning quality turned out to be insufficient to provide the convergence. Figure 3 presents the calculation.

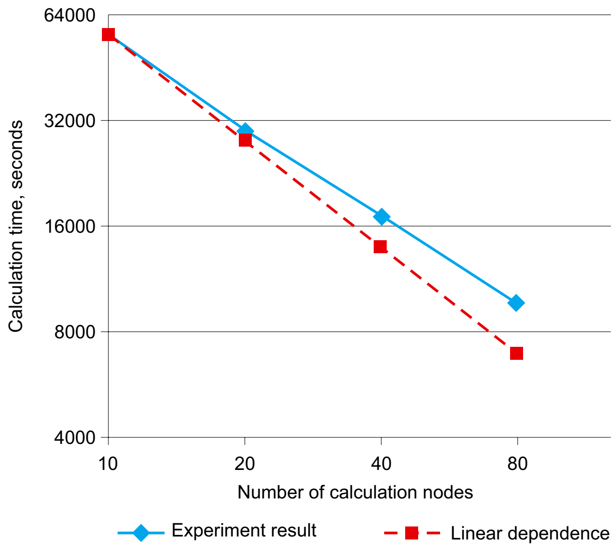

Figure 2. Accelerated calculations for a density-driven convection model in the Zheleznogorskiy LRW DGR performed on a multiprocessor computer

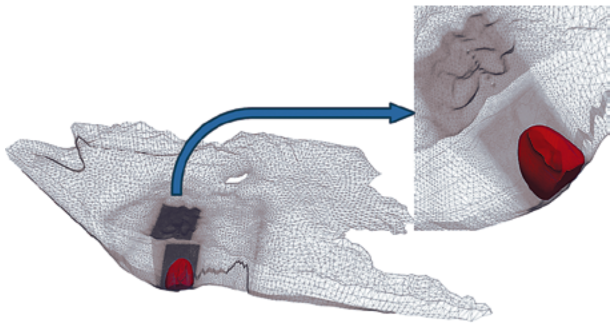

Figure 3. Calculated plume showing the spread of a high-density nitrate ion solution in the operating aquifer (scaled 10 times vertically)

The above case study clearly demonstrates another important trend: the search for efficient robust solvers of linear and nonlinear problems. The use of unstructured meshes, anisotropy and heterogeneity of filtration parameters, vertical-horizontal anisotropy of mesh cells and changing relative permeability of the medium due to variable saturation results in extremely ill-conditioned SLAE matrices. To solve them, high-quality parallelizable preconditioners are required. Non-linear problems emerging when groundwater flow in variable saturation modes is simulated (Richards equation or two-phase flow equations) and their solution appears to be quite challenging. Thus, a review article [41] states that today no common method is available that could provide robust solution and sufficient accuracy for the entire spectrum of media parameters, initial and boundary conditions encountered in practice. Due to the inhomogeneity in the parameters of the media and derivative discontinuities in the constitutive relations one should choose unacceptably small-time steps, while in some cases it appears even impossible to solve nonlinear problems using Newton's or Picard's methods. Therefore, to improve the convergence of nonlinear solvers MODFLOW-NWT offers the smoothing of piecewise linear functional dependencies [42], whereas, FEFLOW developers have proposed a method involving primary variable switching technique [1]. Several operations have been performed in GeRa to solve such problems using the continuation method [43]. However, the search of robust and efficient nonlinear solvers remains an urgent task to be addressed.

The crystalline host rock proposed for DGR siting requires the development of specifically-tailored models that would adequately describe the flow and transport processes occurring in the fractured-porous media. Since it is not always possible to represent such a medium as an equivalent porous one (this depends on whether a representative elementary volume of a required size is available), the DFN (Discrete Fracture Network) and DFM (Discrete Fracture and Matrix) models are being developed. Using these models, fractures can be explicitly taken into account. Based on the fractured medium modeled on a small scale, its characteristics in an elementary volume can be calculated. DFN models assume fluid flow and transport only along a system of fractures (faults), while DFM also considers the flow and transport in the rock matrix, moisture and mass transfer between fractures and the matrix. In these models, cracks are represented by two-dimensional surfaces.

Particular attention should be paid to the development of models, which are essentially required to simulate radionuclide transport processes in the EBS, including colloidal transfer models [44] accounting for possible radionuclide transport on suspended particles constituting to clay EBS, irreversible sorption models and models with time-varying parameters of the media. Although it was identified that colloidal transport plays an important role at certain sites (for example, the Severskiy LRW DGR, see [44]), the use of such numerical models is currently limited to one-dimensional models and theoretical studies. Therefore, these are not applied during actual nuclear safety assessments. Models with variable media parameters are already used to describe the near field in GeRa; in particular, it is possible to take into account time-varying hydraulic conductivity and distribution coefficient due, for example, to the chemical degradation of concrete EBS. Models allowing to account for the changes in the porosity properties of rocks over time are viewed as a much more complex challenge. It should be noted that when chamber models are applied, the ease of taking into account the variation in the material porosity over time is fraught with the danger of either violating the mass conservation law or non-physical concentration jumps in the chambers and requires an in-depth analysis.

Usually, the safety assessment of nuclear facilities ultimately results in a peak level of radionuclide specific activity calculated for the intended water use location. Numerical diffusion effect, which is usual for the transport operator discretization schemes, causes an underestimation of the calculated peak value relative to the actual one. For example, IBRAE RAS, jointly with the St. Petersburg Branch of the Geoecology Institute of RAS (IGE RAS), compared the solutions provided by the GeRa code for the problem of convective radionuclide transport with the analytical solution obtained by the IGE RAS experts [45]. The calculations covered a time period of 2.7 million years considering a profile with a fine mesh (cell size 5×5 m) involving an implicit scheme with a step of 27 years (100,000 steps in total). It was shown that even given the chosen detailed problem discretization (and a very long time required for its solution), the calculated peak specific activity levels of radionuclides in water at the exit from the computational domain turned out to be approximately two times lower than the analytical ones.

To abate the effect of numerical diffusion, the mesh may be refined in space, the time step may be reduced and high-resolution numerical schemes can be applied. The latter, however, are usually explicit and require the use of sufficiently small time steps determined based on the grid Courant number to provide stability. Since very long timeframes should be accounted for in the calculations, the use of explicit schemes becomes prohibitively time-consuming. Therefore, the task of developing computationally efficient discretization methods with low numerical diffusion still remains to be addressed.

Conclusion

Hydrogeological modeling software products developed both in Russia and abroad (both legacy and the most recent developments) have been analyzed to identify the key trends for further development in this area. In terms of numerical methods, these trends provide for an increased efficiency and accuracy of calculations that can be attained through the use of unstructured meshes, massively parallel calculations, new solvers of nonlinear and linear systems of algebraic equations and the development of low-dissipation stable computational models. As regards the studied processes, further development is thought to be associated with multiphysics modeling combining many coupled processes: hydrogeological, hydrological, thermal, mechanical, chemical and biological (coupled models of underground and surface runoff, THMC models, etc.). Another key focus area in the evolution of the software stands for the development and verification of groundwater flow and transport models in fractured media, which is especially important for the DGR to be sited in crystalline host rocks.

The Russian-designed GeRa software development is guided precisely by the above-mentioned global trends. Perhaps the only exception is that the developers have refused to open the source code, which, according to the experience of foreign colleagues, provides tangible advantages in the quality and speed of development. At the same time, developers of Russian software products have greatly benefited from the massive experience gained by the nuclear industry in the development, operation and monitoring of RW repositories, LRW DGR and safety barriers.

References

1. Diersch H. J. G. FEFLOW: finite element modeling of flow, mass and heat transport in porous and fractured media. — Springer Science & Business Media, 2013.

2. McDonald M. G., Harbaugh A. W. The history of MODFLOW. Groundwater, 2003, vol. 41, no. 2, pp. 280—283.

3. Pruess K., Oldenburg C. M., Moridis G. J. TOUGH2 user's guide version 2. — Lawrence Berkeley National Lab. (LBNL), Berkeley, CA (United States), 1999. — No. LBNL—43134.

4. Parkhurst D. L., Wissmeier L. PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC. *Advances in Water Resources,* 2015, vol. 83, pp. 176—189. DOI: 10.1016/j.advwatres.2015.06.001.

5. Li Q. et al. COMSOL Multiphysics: A novel approach to ground water modeling. *Groundwater,* 2009, vol. 47, no. 4, pp. 480—487.

6. Nardi A. et al. Interface COMSOL-PHREEQC (iCP), an efficient numerical framework for the solution of coupled multiphysics and geochemistry. *Computers & Geosciences,* 2014, vol. 69, pp. 10—21.

7. Wissmeier L., Barry D. A. Simulation tool for variably saturated flow with comprehensive geochemical reactions in two-and three-dimensional domains. *Environmental Modelling & Software,* 2011, vol. 26, no. 2, pp. 210—218.

8. Pruess K. TOUGH2-A general-purpose numerical simulator for multiphase fluid and heat flow. 1991. 102 p.

9. Jung Y. et al. TOUGH3: A new efficient version of the TOUGH suite of multiphase flow and transport simulators. *Computers & Geosciences,* 2017, vol. 108, pp. 2—7.

10. Šimůnek J., Van Genuchten M. T., Šejna M. Recent developments and applications of the HYDRUS computer software packages. *Vadose Zone Journal,* 2016, vol. 15, no. 7, p. vzj2016. 04.0033.

11. Freedman V. L. et al. A high-performance workflow system for subsurface simulation. *Environmental Modelling & Software,* 2014, vol. 55, pp. 176—189.

12. Coon E. T. et al. Coupling surface flow and subsurface flow in complex soil structures using mimetic finite differences. *Advances in Water Resources,* 2020, vol. 144, p. 103701.

13. Jan A. et al. An intermediate-scale model for thermal hydrology in low-relief permafrost-affected landscapes. *Computational Geosciences,* 2018, vol. 22, no. 1, pp. 163—177.

14. Hyman J. D. et al. Flow and Transport in Three-Dimensional Discrete Fracture Matrix Models using Mimetic Finite Difference on a Conforming Multi-Dimensional Mesh / arXiv preprint arXiv:2112.12592. 2021.

15. Hammond G. E., Lichtner P. C., Mills R. T. Evaluating the performance of parallel subsurface simulators: An illustrative example with PFLOTRAN. *Water resources research,* 2014, vol. 50, no. 1, pp. 208—228.

16. Bilke L. et al. Development of open-source porous media simulators: principles and experiences. *Transport in porous media,* 2019, vol. 130, no. 1, pp. 337—361.

17. Kolditz O. et al. Thermo-Hydro-Mechanical Chemical Processes in Fractured Porous Media: Modelling and Benchmarking. Vol. 25. — Berlin : Springer, 2016.

18. Wang W. et al. A parallel finite element method for two-phase flow processes in porous media: OpenGeoSys with PETSc. *Environmental Earth Sciences,* 2015, vol. 73, no. 5, pp. 2269—2285.

19. Jones J. E., Woodward C. S. Newton–Krylov-multigrid solvers for large-scale, highly heterogeneous, variably saturated flow problems. *Advances in Water Resources,* 2001, vol. 24, no. 7, pp. 763—774.

20. Maxwell R. M. A terrain-following grid transform and preconditioner for parallel, large-scale, integrated hydrologic modeling. *Advances in Water Resources,* 2013, vol. 53, pp. 109—117.

21. Butnev O. I. et al. "NIMFA" software complex for solving problems of nonlinear single-phase fluid flows and heat-and-mass transport in porous media.

Voprosy Atomnoi Nauki i Tekhniki. Ser.: Math. Model. Phys. Process, 2018, no. 2, pp. 3—13.
22. Novikov K., Kapyrin I. Coupled Surface–Subsurface Flow Modelling Using the GeRa Software. Lobachevskii Journal of Mathematics, 2020, vol. 41, no. 4, pp. 538—551.
23. Bagaev D. et al. Improving parallel efficiency of a complex hydrogeological problem simulation in GeRa. *Russian Supercomputing Days.* Springer, Cham, 2019. Pp. 265—277.
24. Terekhov K., Vassilevski Y. INMOST parallel platform for mathematical modeling and applications. *Russian Supercomputing Days.* Springer, Cham, 2018. Pp. 230—241.
25. Konshin I., Kapyrin I. Scalable computations of GeRa code on the base of software platform INMOST. *International Conference on Parallel Computing Technologies.* Springer, Cham, 2017. Pp. 433—445.
26. Suskin V. V., Kapyrin I. V., Rastorguyev A. V. Programmnoye sredstvo «GEOPOLIS»: geofil'tratsionnoye modelirovaniye punkta glubinnogo zakhoroneniya zhidkikh radioaktivnykh otkhodov poligona "Severnyy" [GEOPOLIS software tool: geofiltration modeling of a deep disposal facility for liquid radioactive waste at the Severniy site]. *Gornyy zhurnal — Mining Journal,* 2021, no. 5, pp. 91—97. DOI: 10.17580/gzh.2021.05.12.
27. Suskin V. V., Kapyrin I. V., Grigorev F. V. Otsenka effektivnosti bar'yera «stena v grunte» pri sozdanii pripoverkhnostnykh punktov konservatsii i zakhoroneniya RAO [Assessing the efficiency of a "buried wall" barrier in the establishment of near-surface long-term storage and disposal facilities for RW]. *Radioaktivnyye otkhody — Radioactive Waste,* 2021, no. 1 (14), pp. 96—105. DOI: 10.25283/2587-9707-2021-1-96-105.
28. Grigorev F. V., Kapyrin I. V., Plenkin A. V. Discrete Fracture Matrix Model Applied to the Computation of Water Flow Through the Underground Facility. *Lobachevskii Journal of Mathematics,* 2020, vol. 41, no. 4, pp. 526—532.
29. *Problemy yadernogo naslediya i puti ikh resheniya* [Nuclear Legacy Challenges and Ways to Address Them]. / Under general edt. of A. M. Agapov, L. A. Bolshov, E. V. Evstratov, N. P. Laverov, I. I. Linge. Vol. 1. — Moscow, Energopromanalitika Publ., 2012. 356 p.
30. Belkin D. Yu., Ivanov I. A., Tananayev I. G. Kontseptsiya po vyvodu iz ekspluatatsii promyshlennykh uran-grafitovykh reaktorov (PO "Mayak", Chelyabinskaya oblast') [Decommissioning Concept for Production Uranium-graphite Reactors (PA Mayak, Chelyabinsk region)]. *Vestnik Dal'nevostochnogo otdeleniya Rossiyskoy akademii nauk — Bulletin of the Far Eastern Branch of the Russian Academy of Sciences,* 2016, no. 3 (187), pp. 58—65.
31. Talitskaya A. V., Zakharova Ye. V., Andryushchenko N. D., Bochkarev V. V. Otsenka dolgovremennoy bezopasnosti ob"yekta okonchatel'noy izolyatsii radioaktivnykh otkhodov, sozdavayemogo pri vyvode iz ekspluatatsii promyshlennogo uran-grafitovogo reaktora [Long-term safety assessment of the final radioactive waste disposal facility established during the decommissioning of a production uranium-graphite reactor]. *Yadernaya i radiatsionnaya bezopasnost' — Nuclear and Radiation Safety,* 2017, no. 2, pp. 54—60.
32. *Vodoyom-9 — khranilishche zhidkikh radioaktivnykh otkhodov i vozdeystviye yego na geologicheskuyu sredu* [Reservoir-9 - storage facility for liquid radioactive waste and its impact on the geological environment]. Edited by Drozhko E. G., Samsonov B. G. — Moscow, 2007. 250 p.
33. Zakharova Ye. V., Andryushchenko N. D. et al. Inzhenernyye bar'yery bezopasnosti pri vyvode iz ekspluatatsii ob"yektov yadernogo toplivnogo tsikla [Engineered safety barriers for the decommissioning of nuclear fuel cycle facilities]. *ARGILLASTUDIUM-2017. Materialy Pyatoy Rossiyskoy Shkoly po glinistym mineralam* [Proceedings of the Fifth Russian School on Clay Minerals], 2017, Pp. 50—54.
34. Linge I. I., Ivanov A. Yu., Kazakov K. S. O sistemnykh merakh po rasshireniyu primeneniya glinyanykh materialov na ob"yektakh atomnoy otrasli [On comprehensive approach to use clay materials as nuclear facilities safety barriers]. *Radioaktivnyye otkhody — Radioactive Waste,* 2018, no. 4 (5), pp. 33—41.
35. Laverov N. P., Velichkin V. I. et al. *Izmeneniye okruzhayushchey sredy i klimata: prirodnyye i svyazannyye s nimi tekhnogennyye katastrofy. T. 5: Izolyatsiya otrabotavshikh yadernykh materialov: geologo-geokhimicheskiye osnovy* [Environmental and Climatic Changes: natural and man-induced disasters. Vol. 5: Final disposal of spent nuclear materials: geological and geochemical fundamentals]. — Moscow, IGEM RAN, IPE RAS Publ., 2008. 280 p.
36. Rybal'chenko A. I., Pimenov M. K., Kostin P. P. et al. *Glubinnoye zakhoroneniye zhidkikh radioaktivnykh otkhodov* [Deep Disposal of Liquid Radioactive Waste]. — Moscow, IzdAT Publ., 1994. Vol. 256.
37. Dorofeev A. N., Bolshov L. A., Linge I. I., Utkin S. S., Saveleva E. A. Strategicheskiy master-plan issledovaniy v obosnovaniye bezopasnosti sooruzheniya, ekspluatatsii i zakrytiya punkta glubinnogo zakhoroneniya radioaktivnykh otkhodov [Strategic Master Plan for R&D Demonstrating the Safety of Construction, Operation and Closure of a Deep Geological Disposal Facility for Radioactive Waste]. Radioaktivnyye otkhody — Radioactive Waste, 2017, no. 1, pp. 32—41.
38. Birkholzer J. T., Bond A. E., Hudson J. A. et al. DECOVALEX-2015: an international collaboration

for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. *Environ Earth Sci,* 2018, vol. 77, p. 539.
39. Carrera J., Saaltink M. W., Soler-Sagarra J., Wang J., Valhondo C. Reactive transport: a review of basic concepts with emphasis on biochemical processes. *Energies,* 2022, vol. 15, no. 3, p. 925.
40. Kapyrin I. V. Assessment of density driven convection effect on the dynamics of contaminant propagation on a deep well radioactive waste injection disposal site. *Journal of Computational and Applied Mathematics,* 2021, vol. 392, p. 113425.
41. Farthing M. W., Ogden F. L. Numerical solution of Richards' equation: A review of advances and challenges. *Soil Science Society of America Journal,* 2017, vol. 81, no. 6, pp. 1257—1269.
42. Niswonger R. G., Panday S., Ibaraki M. MODFLOW-NWT, a Newton formulation for MODFLOW-2005. *US Geological Survey Techniques and Methods,* 2011, vol. 6, no. A37, p. 44.
43. Anuprienko D. Comparison of nonlinear solvers within continuation method for steady-state variably saturated groundwater flow modelling. *Russian Journal of Numerical Analysis and Mathematical Modelling,* 2021, vol. 36, no. 4, pp. 183—195.
44. Rumynin V. G. *Geomigratsionnyye modeli v gidrogeologii* [Geomigration models in hydrogeology]. Saint-Petersburg, Nauka Publ., 2011. 1158 p.
45. Rumynin V. G., Sindalovskiy L. N., Nikulenkov A. M., Leskova P. G. Effect of anisotropy and depth-dependent hydraulic conductivity on concentration curve response to nonpoint-source pollution. *Journal of Hydrology,* 2020, vol. 591, p. 125319.

Information about the author

Kapyrin Ivan Viktorovich, Ph.D., Head of Laboratory, Nuclear Safety Institute of the Russian Academy of Sciences (52, Bolshaya Tulskaya st., Moscow, 115191, Russia), Senior Researcher, Marchuk Institute of Numerical Mathematics of the Russian Academy of Sciences (8, Gubkina st., Moscow, 119333, Russia), e-mail: kapyrin@ibrae.ac.ru.

Bibiliographic description

Kapyrin I. V. Computational Codes for the Hydrogeological Modeling in the Safety Assessment of Nuclear Facilities. *Radioactive Waste,* 2022, no. 2 (19), pp. 105—118. DOI: 10 25283/2587-9707-2022-2-105-118. (In Russian).