Finite element code FENIA verification and application for 3D modelling of thermal state of radioactive waste deep geological repository

R A Butov¹, N I Drobyshevsky¹, E V Moiseenko¹, U N Tokarev¹
¹Nuclear Safety Institute of Russian Academy of Sciences (IBRAE RAN), 52, B. Tulskaya str., Moscow, 115191, Russia

E-mail: bra@ibrae.ac.ru, dni@ibrae.ac.ru, moi@ibrae.ac.ru, tyn@ibrae.ac.ru

Abstract. The verification of the FENIA finite element code on some problems and an example of its application are presented in the paper. The code is being developing for 3D modelling of thermal, mechanical and hydrodynamical (THM) problems related to the functioning of deep geological repositories. Verification of the code for two analytical problems has been performed. The first one is point heat source with exponential heat decrease, the second one - linear heat source with similar behavior. Analytical solutions have been obtained by the authors. The problems have been chosen because they reflect the processes influencing the thermal state of deep geological repository of radioactive waste. Verification was performed for several meshes with different resolution. Good convergence between analytical and numerical solutions was achieved. The application of the FENIA code is illustrated by 3D modelling of thermal state of a prototypic deep geological repository of radioactive waste. The repository is designed for disposal of radioactive waste in a rock at depth of several hundred meters with no intention of later retrieval. Vitrified radioactive waste is placed in the containers, which are placed in vertical boreholes. The residual decay heat of radioactive waste leads to containers, engineered safety barriers and host rock heating. Maximum temperatures and corresponding times of their establishment have been determined.

1. Introduction
To date, a large amount of radioactive waste has been accumulated in the world. The concept of radioactive waste management assumes its burial in deep geological repositories [1].

Deep geological repository of radioactive waste is intended for final disposal of radioactive waste without the intention of extracting them in the future. The repositories are designed to be located in the host rock at a depth of several hundred meters. Rock type may be different, but usually it is selected from one of three types: crystalline, salt or clay [2].

Radioactive wastes that are intended for disposal are divided into several classes, according to their activity level [3]. The thermal state is primarily influenced by high-level waste (HLW) and intermediate-level waste (ILW, later in the article ILW and HLW are considered to be HLW), which is a source of heat for hundreds of years. Specific heat of HLW can exceed several kW/m³.

Isolation of the HLW from the environment is provided by so-called engineered barriers (EBS), which consist of vitrified HLW, insulating containers, low-permeability material (e.g. bentonite) and void filling materials [2]. HLW in combination with engineered barriers are arranged in vertical or horizontal boreholes in the host rock.
Determination of the thermal state is an important task, due to the influence of temperature on many physical and chemical processes in the repository. The code FENIA (Finite Element Nonlinear Incremental Analysis) is being developed to determine the state of the repository itself and host rock [4]. Its current version is capable of thermal state modeling, while further models for other processes will be included, primarily – for thermal state mechanics and groundwater flows. Thus full THM coupling will be attained.

2. FENIA code
The FENIA code is a finite element solution for thermal problems. Isoparametric finite elements of various configurations with first- and second-order shape functions can be used. The PETSc library is used to solve systems of algebraic equations [5, 6, 7].

Presently, the code solves the 3D nonhomogeneous time-dependent equation of energy conservation:

$$\rho(t, X)c(t, T, X)\frac{\partial T}{\partial t} - \frac{\partial}{\partial x_i} \left( \lambda_{ij}(t, T, X) \frac{\partial T}{\partial x_j} \right) = q(t, X), i, j = 1..3, X = (x_1, x_2, x_3),$$

(1)

where $\rho$ – density, $t$ – time, $X$ – spatial coordinates, $c$ – specific heat, $T$ – temperature, $\lambda$ – thermal conductivity tensor, $q$ – heat source. The dependencies of the coefficients in the equation can have discontinuities, e.g. at the material boundaries.

The code is being developed as a part of the simulation complex for modelling of various chemical and physical processes in the repository, which will be used for the substantiation of long-term safety of radioactive waste disposal. The results of the thermal state calculations will be used by other modules of the complex in modelling of corrosion, radionuclide propagation, etc. Also, the FENIA code will receive data from other modules, for example, heat generation of HLW, depending on its composition or heat resulting from chemical processes.

3. Verification
The dependence of the heat from the HLW on time is well described by an exponential law. To verify the solution of the heat equation, the problem with an exponentially decreasing heat source was selected:

$$q(t) = q_0 e^{-t/t_0},$$

(2)

where $q$ - current heat generation, $W$; $t$ - time, $s$; $q_0$ - initial heat generation, $W$; $t_0$- time during which the heat generation decreases by $e$ times, $t_0/s$.

Two problems were chosen for verification: with point and linear heat sources. A point heat source can be treated as an approximation for a single container with HLW, while a linear source – for a filled borehole. Analytical solutions for these problems have been obtained by the authors from the common solution for the time-dependent heat transfer equation for homogeneous isotropic medium [8].

3.1. Analytical solution
The analytical solution for the temperature field from the point source in spherical symmetry is expressed by the formula:

$$T(r, t) = T_0 + \frac{q_0}{4 \pi \alpha r} \sum_{n=0}^{\infty} \frac{I_n}{n!} \left( \frac{r^2}{4 \alpha^2 t} \right)^n,$$

(3)

where $T$ - temperature, $K$; $T_0$ - initial temperature; $K$; $r$ – distance from the center of the sphere, $m$; $q_0$ - initial heat generation; $W$; $\alpha$ - thermal diffusivity, $m^2/s$; $I_n$ - coefficients calculated from the recurrence relation:

$$I_{n+1} = \frac{1}{2n+1} \left[ 2 \sqrt{\pi} \left( \frac{r^2}{4 \alpha^2 t} \right)^{-n-1/2} \exp \left( - \frac{r^2}{4 \alpha^2 t} \right) - 2I_n \right], n = 0, 1, 2, \ldots,$$

(4)

where
\[
I_o = \text{erfc}\left(\frac{r}{2a\sqrt{t}}\right).
\]  
(5)

The analytical solution for the temperature field from the infinitely long straight-line source in axial symmetry is expressed by the formula:

\[
T(r,t) = T_0 + \frac{q_0 \exp(-t/t_0)}{4\pi a^2} \sum_{n=0}^{\infty} \frac{(t/t_0)^n}{n!} E_{n+1} \left(\frac{r^2}{4a^2 t}\right),
\]  
(6)

where \(T\) - temperature, K; \(T_0\) - initial temperature; K; \(r\) - distance from the axis, m; \(q_0\) - initial heat generation; W; \(a\) - thermal diffusivity, m\(^2\)/s; \(E_{n+1}\) - exponential integral:

\[
E_n(x) = \int_1^{\infty} \frac{\exp(-xs)}{s^n} ds.
\]  
(7)

The values of thermal diffusivity and other parameters are given below.

3.2. Numerical solution

The simulation domain for the case of spherical symmetry was taken as a ball with a radius of 10 m. The domain for the axial one is a cylinder with a radius of 150 m. The size of the domain was chosen so that the conditions on the external boundary did not influence the solution. For each geometry, several computational meshes with different number of cells along the radius have been constructed to test the convergence. Examples of the meshes for each problem are shown in Figure 1. The construction of the meshes was performed with gmsh program [9].

![Figure 1. Computational mesh examples: a - ⅛ ball with 30 cells along the radius, b - cylinder with 40 cells along the radius.](image)

Thermal properties of the material were chosen to be close to those of crystalline rock [10] and are indicated in the Table 1.

| Density \(\rho\), kg/m\(^3\) | Specific heat \(c\), W/(m\(^3\)·K) | Thermal conductivity \(\lambda\), W/(m·K) | Thermal diffusivity \(a = \lambda/\rho c\), m\(^2\)/s |
|-----------------|----------------------------------|----------------|----------------------------------|
| 840             | 2700                             | 2.91           | 1.28 · 10\(^{-6}\)              |
The heat release is specified in the cells immediately adjacent to the center of the sphere and the cylinder. For the spherical case ¼ of the whole domain was used. On the symmetry planes of the sphere, as well as on the top and bottom surfaces for the cylinder, the conditions of the 2nd kind (Neumann) with zero flux are given. On the external boundaries others - of 1st kind (Dirichlet). The parameters used in the calculations are given in Table 2.

| Table 2. Parameters for the calculation. |
|------------------------------------------|
| Spherical initial heat \( q_0 \), W      | Cylindrical initial heat \( q_0 \), W/m | Time \( t_0 \), years | Initial temperature, °C | Temperature on the outer surface, °C |
|------------------------------------------|
| 591.3                                    | 303.57                                   | 40                      | 9                        | 9                                       |

3.3. Comparison

Figures 2-3 show comparisons of the analytical and numerical solutions for various meshes. Solid lines denote an analytical solution, dashed - numerical. One should note that the analytical solutions for both problems have discontinuity at the heat source, where it grows infinitely. On the meshes with small amount of cells the numerical solution differed considerably from the analytical one near the heat source. However, with mesh refinement the solutions tend to converge, and as it can be seen from the graphs, on finer meshes the numerical solution is close to the analytical one, even near the singular point.

The presented results were obtained with the first-order shape functions. The same simulations were performed with the shape functions of the second order, but no significant increase in accuracy was observed. The tests with meshes made of hexahedral elements were done as well and showed the same accuracy. Thus, the solution quality does not depend on the mesh type.

![Figure 2. Point heat source, mesh with 30 cells, a - temperature field after 250 days, b - time dependence of the temperature in 4 points](image)

![Figure 3. Straight-line source, mesh with 40 cells, a - temperature field after 5000 days, b - time dependence of the temperature in 4 points](image)
4. Thermal state of deep geological repository of radioactive waste

Prototypic repository is supposed to be located in the rock at the depth of several hundred meters. Type of rock is crystalline [10]. Repository has two horizontal levels connected with boreholes. The boreholes are filled with HLW containers. Boreholes are divided into two groups according to the density of their location as shown in Figure 4. Engineered barriers consist of metal containers, bentonite, and thixotropic slurry.

![Repository horizontal level layout.](image)

The first (dense) group of boreholes will be filled with HLW with an initial heat generation of 1.0 kW/m³. In the second group - 1.5 kW/m³. Heat generation decreases exponentially. The decrease rate was supposed to be the same as in the verification problems ($t_0 = 40$ years).

Repository is filled at a rate of 1 row/year starting from the second group of boreholes. Thus, repository will be filled in about 30 years. The calculation was performed for the period from the start of filling up to 10000 years. After 3500 years, the temperature inside the repository was almost equal to the initial temperature of the host rock.

The computational domain volume includes repository itself and the host rock at a distance of 400 meters in all directions. Due to the double symmetry of the problem, the calculation was performed on $\frac{1}{4}$ of total volume. The mesh was created in gmsh program [9]. The number of cells is about 15 million.

Initial repository and host rock temperature was taken equal to $9 \, ^\circ C$. Boundary condition of the first kind (Dirichlet) was applied on the external computational domain boundaries with $9 \, ^\circ C$ temperature as well. Neumann conditions with zero heat flux were set at the symmetry planes.

Some simplifications have been made:

- HLW heat production was considered to be uniformly distributed over the entire length of the boreholes;
- engineered barriers (except for the HLW glass matrix) were simulated as one material with the averaged thermal properties;
- the tunnels were considered to be filled from the beginning of calculation and their thermal properties were taken to be the properties of the host rock.

Temperature field after 55 years is shown in Figure 5. The lower cross-section - the middle of boreholes, the middle - their tops, the upper one - the middle of boreholes + 100 m.
5. Conclusions
The performed verification calculations for the heat transfer equation with a heat source with an exponential decrease confirm that the FENIA code can be used for modelling thermal state of prototypic radioactive waste repository. Good agreement between numerical and analytical solution was obtained. According to the calculation of the thermal state of a prototypic repository and host rock for a period of 10,000 years, the maximum temperature within the repository reached 110 °C after 55 years. After 3500 years, the temperature returns to its original value. The temperature change at the surface of the area is insignificant and practically equal to 0. At the same time, several assumptions were made in the calculation, and the simulations for the actual repository project will require further analysis.

References
[1] IAEA 2011 Disposal of radioactive waste. Specific Safety Requirements SSR-5 (Vienna: International Atomic Energy Agency)
[2] Pusch R 2009 Geological storage of highly radioactive waste: current concepts and plans for radioactive waste disposal (Berlin: Springer Science & Business Media)
[3] IAEA 1994 Classification of radioactive waste: a safety guide (Vienna: International Atomic Energy Agency)
[4] FENIA 2017 project web pages https://sites.google.com/view/fenia/home
[5] Balay S et al 2001 {PETSc} {W} eb page
[6] Balay S et al 2014 Petsc users manual revision 3.5 (Argonne, IL: Argonne National Laboratory)
[7] Balay S et al 1997 Efficient management of parallelism in object-oriented numerical software libraries Modern software tools for scientific computing (Boston: Birkhäuser) 163-202
[8] Vladimirov V S 1976 Equations of mathematical physics (Moscow: Izdatel Nauka)
[9] Geuzaine C Remacle J F 2009 Gmsh: A 3-D finite element mesh generator with built-in pre- and post-processing facilities International Journal for Numerical Methods in Engineering 79 1309-1331
[10] Anderson E B, Belov S V, Kamnev E N, et al 2011 Underground Disposal of Radioactive Wastes (Moscow: Gornaya Kniga)