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THREE-DIMENSIONAL NUMERICAL MODELING OF THE THERMAL STATE OF THE DEEP RADIOACTIVE WASTE DISPOSAL FACILITY IN THE NIZHNEKANSK GRANITOID MASSIF

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A problem of calculation of the thermal state of the deep radioactive waste disposal facility in the Nizhnekansk granitoid massif (DRWDF) is considered. A 3D-finite-element code FENIA (Finite Element Nonlinear Incremental Analysis) has been developed to model the thermal processes in DRWDF. The obtained results describe the spatial and time evolution of temperature within DRWDF and surrounding rock for the period of up to 10,000 years. The results show that nearly entire heat will be absorbed by surrounding rocks without substantial increase of temperature. Nevertheless, during short periods of time, the temperature inside DRWDF will exceed 100°C.

Keywords: *radioactive waste, deep disposal, mathematical modeling, temperature mode.*

Introduction

Isolation in deep geological formations is currently considered to be the most reliable method of high-level waste disposal, capable of minimizing the effect on human and environment for the period of potential hazard of the waste. Projects of disposal facilities exist in a number of countries: Finland, Sweden, USA, Belgium, France, etc. [1]. The current stage of these projects varies: from research stage in Belgium to the facility being already under construction in Finland. The project of a deep radioactive waste disposal facility (DRWDF) for RW of 1 and 2 classes is being developed in Russia [2]. DRWDF is planned to be constructed at the depth of approximately 500 m in the Nizhnekansk rock massif (NKM).

For RW placed in deep geological disposal facilities, the containment function is implemented by engineered safety barriers, which minimize the release of radionuclides out of the facility, while confinement function is ensured by natural barriers limiting the impact of waste on human and biosphere. The natural barriers are represented by rocks, mainly of the following three types: crystalline, salt or clay-sediment. The Russian project deals with the crystalline rocks composed of granites, gneiss and diorites. Engineered barriers include the conservation matrix, steel claddings, layers of concrete, bentonite and other materials. In accordance with the regulatory documents, the engineered barriers should maintain their integrity for at least 1000 years.

The range of studies required for the long-term safety case of DRWDF is unprecedentedly broad and is connected with processes having the highest effect on the condition of the facility at various stages of its lifecycle, which may be as long as million years (Fig. 1). This also defines the priorities of the required studies.

During the first several hundred years of operation, the key issues are connected with heat impact. These issues also affect the selection of a disposal concept (facility geometry) and safety concept (system of safety barriers).

The highest temperatures will be observed in the first decades after the closure; however there is the highest probability of the integrity of protective barriers for this period. For the range of intermediate temperatures and time periods above 300 years, there will be inevitable water ingress to safety barriers and increase of the intensity of corrosion, gas

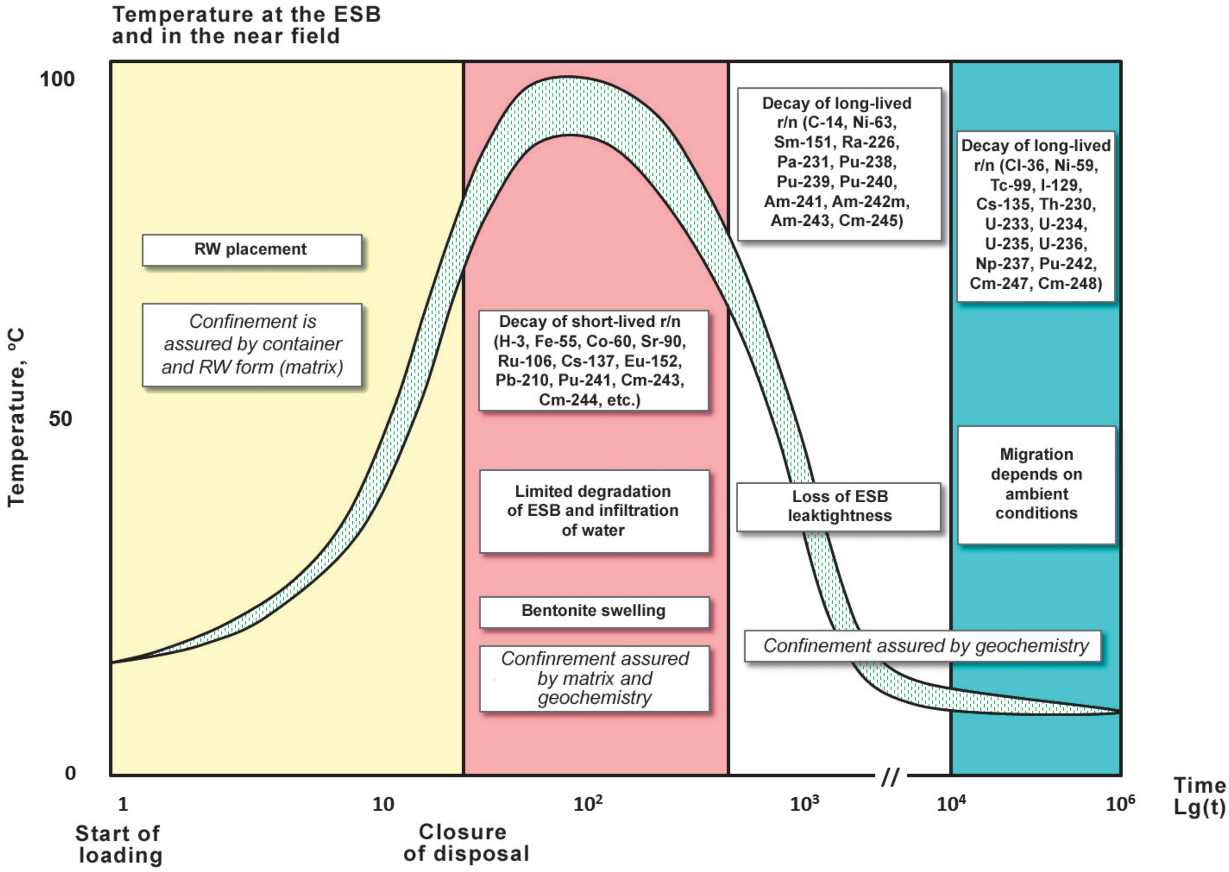


Fig. 1. Dynamics of major processes and temperature mode

generation and other processes. However, the significance of these processes is considerable for longer-lived radionuclides. For most of the time periods, the DRWDF system, including the near field, will experience relatively low ambient temperatures close to natural ones.

This example already shows the importance of the safety concept formulation as it will, in fact, serve as terms of reference for the future research.

In our case, HLW is characterized by a high heat generation — up to 2 kW/m^3. The thermal conditions of DRWDF depend on a number of factors, including configuration of the disposal facility, schedule of its filling, RW heat generation, and thermal physical properties of materials.

Time-dependent thermal fields will have significant effect on the rate and intensity of various chemical and physical processes in DRWDF, many of them being interconnected. The temperature gradients at the walls will change the stress state (SS) and affect the flows of fluids and gases in engineered barriers and host rock.

SS will affect the permeability of the medium for water and gases. Water flow will serve as an additional heat transport mechanism and will lead to bentonite swelling. Adequate assessment of such phenomena requires coupled solution of the heat transport, stress-strain and porous medium hydraulic equations (the so-called "THM Coupling" [3]). FENIA (Finite Element Nonlinear Incremental Analysis) program was developed as a tool for simultaneous solution of these equations. Discretization of equations is done using the finite elements method and the specially developed library of finite elements of the first and second order. Implicit difference schemes are used for temporal integration. Solution of linear and non-linear algebraic equation systems is performed using PETSc libraries [4].

The heat calculations are required because of the considerable effect of temperature on the mechanical strength, corrosion strength and other physical and chemical properties of barriers. At the same time, the currently available assessments of the DRWDF thermal conditions have been carried out either for a single borehole with symmetrical conditions for the side boundaries, i. e. without taking into account the schedule of facility filling, or by superposition of analytical solutions obtained for a borehole as a linear heat source located in uniform homogeneous medium [5].

FENIA program is used in the present work for numerical simulation of the thermal conditions of the DRWDF in the Nizhnekansk rock massif. The developed meshing takes into account all boreholes filled with RW and prolonged schedule of their filling. The calculations provided the estimates for change of temperature field inside DRWDF and in the surrounding rock massif for the period of up to 10,000 years. Such assessments of the thermal conditions will contribute to optimization of the

DRWDF project by their application to specification of boreholes configuration, schedule of filling, selection of engineering materials.

Method of heat condition calculation

Finite element code FENIA is used to simulate the DRWDF thermal conditions. The code calculates the 3D heat conductivity equation:

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

where ρ — density, t — time coordinate, **X** — vector of spatial coordinates, c — heat capacity, T — temperature, λ— heat conductivity tensor, q — heat source. The calculation meshes include, as a rule, tetrahedral or hexahedral elements, but, in general, any shape of convex finite elements may be used.
Form functions of the first or second order can be used for the problem solution.
The dependence of coefficients in (1) on spatial and temporal coordinates and on temperature is taken into account. Dependence of heat capacity and temperature conductivity of materials on temperature can be given as a database of materials or as user input.
Since equation (1) is solved for the entire area including the DRWDF and the surrounding rock, the functions $\rho(\mathbf{X})$, $c(\mathbf{X})$, $\lambda(\mathbf{X})$, $q(\mathbf{X})$ have discontinuities at the boundaries of the materials. Another source of the spatial dependence of the thermal properties of host rock is the process of excavation works, since the material properties in the excavation disturbed zone (EDZ) can differ from the properties of the overall rock massif.

The main source of heat is its generation due to RW decay and chemical reactions in engineered barriers caused by, e.g., solidification of concrete. Some of the time dependences of parameters will be exported from external calculations, e.g. heat flows due to heat and mass transport with ground waters or chemical reactions in engineered barriers.

It is also planned to add solution of the equilibrium equation for simulation of the stress states and the liquid motion equation for simulation of ground water flows in the future. Upon implementation of these models, simulation of processes at DRWDF within a joint THM (thermal-hydraulic-mechanical) model will be possible. The need for such coupling arises from the close relation of these processes, which was demonstrated, in particular, in the series of DECOVALEX projects [3].

The FENIA code is planned to be used for simulation of objects of various sizes. The smallest of them will be small experimental installations or single RW packages, while the largest one is to be the whole DRWDF and the adjoining rock massif. Thus, the characteristic dimensions of the considered model area range from tens of centimeters to hundreds of meters. At the boundary of the calculation area, the conditions of the first, second or third kind can be set. Also, the boundary conditions may describe re-radiation in the cavity or radiation to the ambient environment. A combination of various boundary conditions can also be used.

Verification of the code was performed for two non-stationary analytical problems: with point and distributed heat sources, where the authors had obtained analytical solutions [6]. It was assumed that the heat generation decreases exponentially:

$$q(t)=q_0\,\mathrm{e}^{-t/t_0}, \tag{2}$$

where q —current heat generation, W; t —time, s; q_0 — initial heat generation, W; t_0 — time period, for which the initial heat generation decreases by a factor of *e, s*.

The problem with a point heat source was solved in a spherical calculation area, and with a distributed source — a cylindrical one. The calculation area for the point source was 1/8 of a sphere with a radius of 10 m, and for distributed source — a cylinder with a radius of 150 m. The dimensions of the area were selected in such a way that the conditions at the external boundaries do not affect the solution. The thermal properties of the material were selected close to those characteristic for the host rock (gneiss for NKM) [7] and are given in Table 1. The calculation areas for the problem are shown in Fig. 2.

The conditions of the second kind with a zero heat flow are set for the planes of symmetry of the sphere and for the upper and lower surfaces of the cylinder. The conditions of the first kind are set for other planes. Parameters used for calculations are given in Table 2.

Verification is described in more detail in [6]; here we will demonstrate only the curves showing the comparison of the results obtained by numerical calculations using the FENIA code with analytical solution. Time dependence of temperatures for several points located at different distances from the point heat source is shown in Fig. 3a, from the distributed source — in Fig. 3b.

A fairly good agreement of the results for all considered points for both problems is observed.

Geometrical model of DRWDF

According to the DRWDF design documents, the vitrified HLW will be located in vertical 75 m deep boreholes between the horizontal drifts (+5 m and -70 m).

Table 1. Thermal physical properties of the material

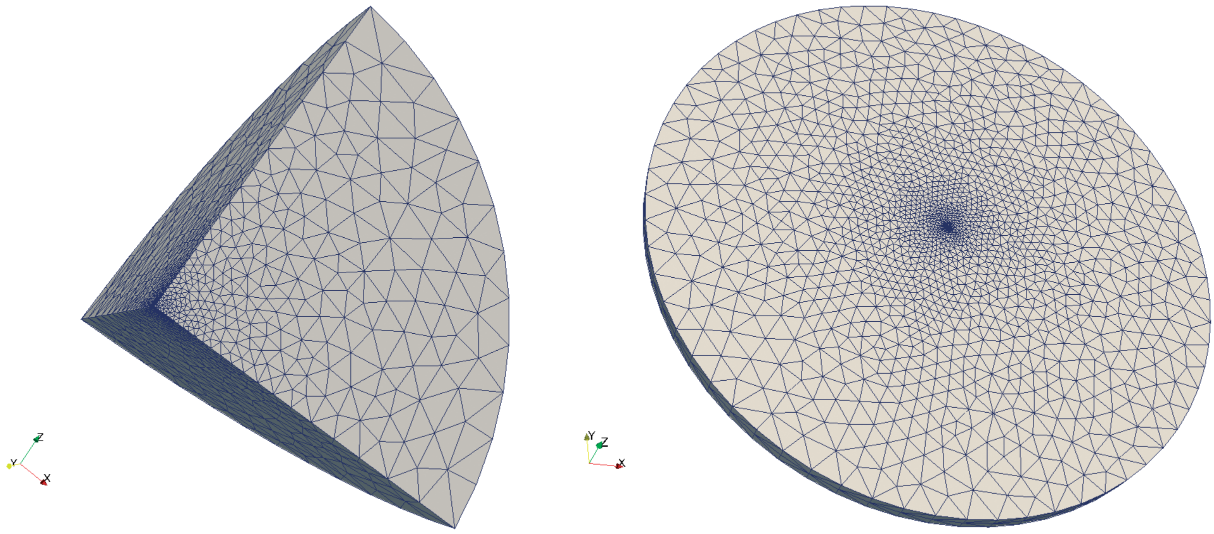
Density ρ, kg/m^3	Heat capacity c, W/(kg·K)	Heat conductivity λ, W/(m·K)	Temperature conductivity a = λ/(ρc), m^2/c
2700	840	2.91	$1.28\cdot10^{-6}$

The boreholes are located in 28 disposal chambers, each 360 m long, with ends of the chambers connected by transport and technological shafts. The disposal facility will be divided into two sections. The first one will be used for storing the waste accumulated before 2010 and having initial heat generation of approximately 1 kW/m^3; and the second one will store waste accumulated after 2010 with initial heat generation of approximately 1.5 kW/m^3. Therefore, the disposal of waste will be more sparse in the second section: while the first 14 disposal chambers (section 1) would have 20 boreholes located at 15 m from each other, the remaining ones (section 2) will have 13 boreholes at the distance of 23 m. The distance between disposal chambers in the first section will be 23 m, and 26 m — in the second section, thus the overall dimensions of the disposal facility will be approximately 360x700 m. It is presumed that one borehole will host 27 tons of HLW. The overall number of boreholes is 462. The plan of the simulated part of the +5 m level is given in Fig. 4

Once the boreholes will be filled with 1 class RW, the disposal chambers will be used for disposal of

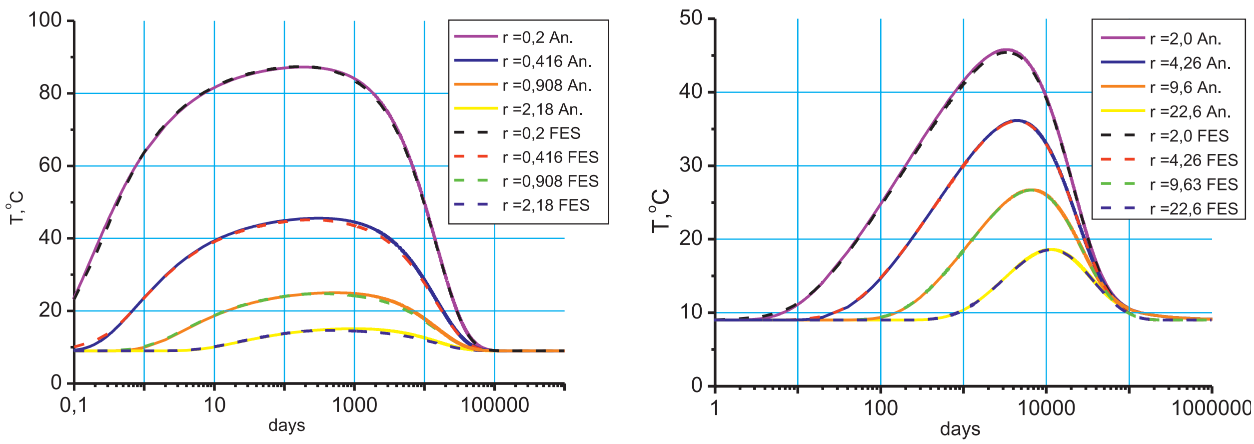
Table 2. Calculation parameter

Initial heat generation for sphere q_0, W	Initial linear heat generation density for cylinder q_0, W/m	Time t_0, years	Initial temperature, °C	Temperature at surfaces with boundary conditions of the 1st type, °C
591.3	303.57	40	9	9



a) **b)**

Fig. 2. Calculation meshes: a — 1/8 of a sphere with 30 cells along the radius; b — cylinder with 40 cells along the radius



a) **b)**

Fig. 3. Comparison of FENIA code numerical calculations with analytical solution, distance r is given in meters: a — for a point source; b — for a distributed source

2 class RW. Their heat generation is not taken into account in the current calculation, along with other relatively weak heat sources: concrete in process of solidification, other chemical reactions in safety barriers, etc.

Engineered barriers (packages and containers) are constructed of several layers of steel, separated by concrete or bentonite. The space between the container and the borehole wall is filled with thixotropic slurry.

The host rock is represented by granitoids: granites, gneiss, diorites. The temperature of the host rock at the depth of 400—500 m is 5—10°C. Average annual temperature at the surface is 0°C.

DRWDF calculation model

A mesh model of the underground section of the disposal facility and the host rock was developed for calculation. The mesh includes approximately 17.5 million tetrahedral finite elements and covers the disposal facility and 400 m of host rock in each direction. As the disposal facility has two planes of symmetry, the mesh models one fourth of the DRWDF and has the dimensions of 1500×550×450 m. The mesh for the calculation area is shown in Fig. 5.

Several simplifications were applied in setting up the calculation area. For example, the heat generation was considered to be uniform along the well, the materials of engineered barriers (bentonite, concrete, container walls) were grouped in one element with averaged properties, the difference of thermal physical properties at EDZ was not taken into account. All corridors and galleries were considered to be filled with rock from the start of the calculation (in reality they will be filled with 2 class RW and excavated rock after the disposal facility is filled). The rock properties were assumed corresponding to gneiss for temperatures of 20—100°C [7]. The thermal physical properties of materials used in calculation are given in table 3. Gradual filling of DRWDF was simulated, with wells of one disposal chamber being filled over one year. Thus, the overall filling time is equal to 27 years. The initial temperature across the calculation area was taken equal to 9°C. Boundary conditions of the first type also with the temperature of 9°C were assigned for the boundaries of the area. It was assumed that the heat generation power of HLW reduces exponentially with time (2). The value of initial power was taken equal to 1 kW/m^3 for section 1, and 1.5 kW/m^3 for section 2; parameter t was taken equal to 40 years, i.e. it was considered that the heat generation power drops by e times over 40 years, or by approximately 2.5% per year that is similar to verification problems.

Results of the thermal state calculations

The values of temperature field inside the disposal facility and in the surrounding rock massif for the period of up to 10,000 years were obtained.

An example of calculation of 3D temperature field is given in Fig. 6 for the time moment t = 55 years from the start of disposal. One can see that, by this moment, the rock within section 1 (left side) has noticeably been heated, and the temperature exceeds 100 °C; within section 2, the similar temperatures correspond to the matrix with HLW and confining container, but only in those parts that are located closer to the middle of the disposal facility and were filled in earlier; the rock itself as well as the last of the disposed containers have not warmed up yet. The dependence of the temperature for the central part of internal boreholes of sections 1 and 2, shown in Fig. 7, demonstrates that the maximum temperatures are reached within 50—70 years from the start of DRWDF operation. It should be noted that

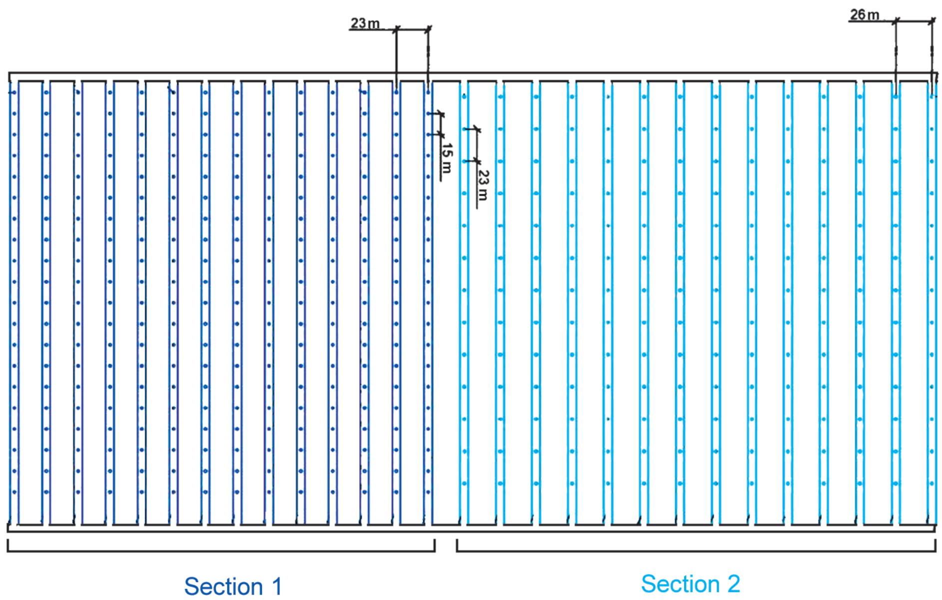


Fig. 4. Diagram of the modeled part of the +5 m-layer of DRWDF

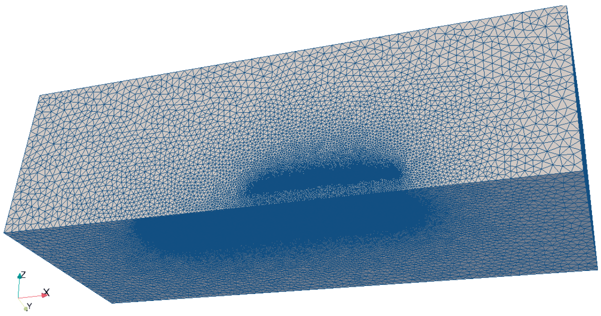


Fig. 5. Mesh spacing for DRWDF modeling

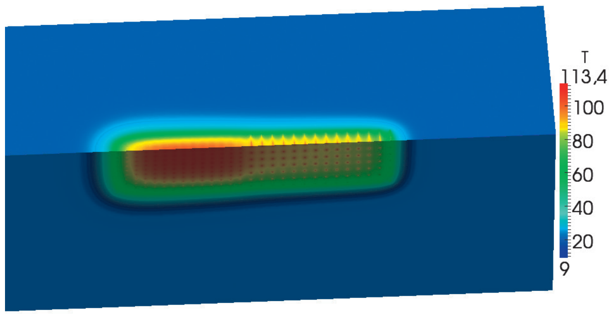


Fig. 6. Calculated temperature field for DRWDF in 55 years from the start of disposal

Table 3. Thermal physical properties of materials used in the calculation

Material	Heat conductivity, W/(m·K)	Heat capacity, W/(kg·K)	Density, kg/m^3
Vitrified HLW	2.4	800	2500
Host rock	2.91	840	2700
Engineered barriers	8.1	1500	2800

for section 2, which starts to be filled after 14 years, the maximum temperatures are reached within approximately the same time frame as for section 1 due to the higher heat generation. Afterwards, both the containers and host rock start to cool down, and within 7—10 thousand years, the temperature for the whole calculation area returns to initial values.

The change of spatial profiles of temperature with time at the stage of DRWDF heating is given in Fig. 8. The Fig. 8a shows the temperature profiles along the horizontal axis of symmetry at DRWDS. The curves corresponding to time moments t = 8 years and t = 14 years from the start of HLW placement show the extent of filling of DRWDF for these time moments — the temperature of the empty area has initial value, while the temperature in the filled area is the higher the earlier the waste was placed. Time moment t = 28 years corresponds to complete filling of DRWDF, temperatures close to the maximum are observed for the time moment t = 55 years.

The more abrupt peaks for section 2 are due to the fact that the axis of symmetry passes directly through the boreholes (there is an odd number of boreholes in section 2), while it passes between the boreholes in section 1. Naturally, the temperature inside the heat generating matrix is higher than in the surrounding rock. Fig. 8b shows the temperature profiles along the vertical line passing through the centre of section 1 — through the centre of the eighth disposal chamber. Within 55 years from the start of DRWDF filling, the rock layer of approximately 200 m from the horizontal symmetry plane is heated, corresponding to approximately 160 m from the top of the boreholes (+5 m level). Once the HLW boreholes will be plugged, it is planned to fill the disposal chambers with intermediate-level waste. Therefore, the thermal conditions at the respective levels are an important aspect of DRWDF operation. The temperature profiles along the horizontal line passing across the tops of the boreholes of the eighth chamber in the disposal section 1 (level + 5 m) show that in approximately a year after the filling of this chamber with HLW (t = 8 years), the temperature will rise to approximately 20°C. By the time of completion of the first section filling (t = 14 years), the temperature will reach 25—35°C, and for the moment of filling of entire DRWDF (t = 28 years), it will reach 60°C. At the same time, the calculated temperature inside the transport and technological tunnels ($y \approx 180$ m) will remain below 30°C up to the moment of t = 55 years.

Spatial profiles of temperature with time at the stage of DRWDF cooling are given in Fig. 9. Within 100 years from the start of filling, the temperature inside DRWDF stabilizes at 90—95°C, and within 3500 years, as mentioned above, returns to values that are close to the initial ones. Temperature inside the transport and technological tunnels (Fig. 9c, $y \approx 180$ m) will remain about 30°C up to the moment of t = 274 years, and then starts to decrease gradually. It should be noted that close to the outside boundaries of the calculation area there is no noticeable temperature rise, i.e. there are no heat flows through the boundaries of the area.

Conclusion

The knowledge about the thermal state is required for all stages of facility operation, starting from RW loading, and is one of important aspects of DRWDF safety case. Temperature has a strong impact on various properties of engineered safety barriers and host rock: strength, transport, chemical properties, etc. The developed 3D finite-element code FENIA provides calculation of temperature field evolution in DRWDF and host rock for any time

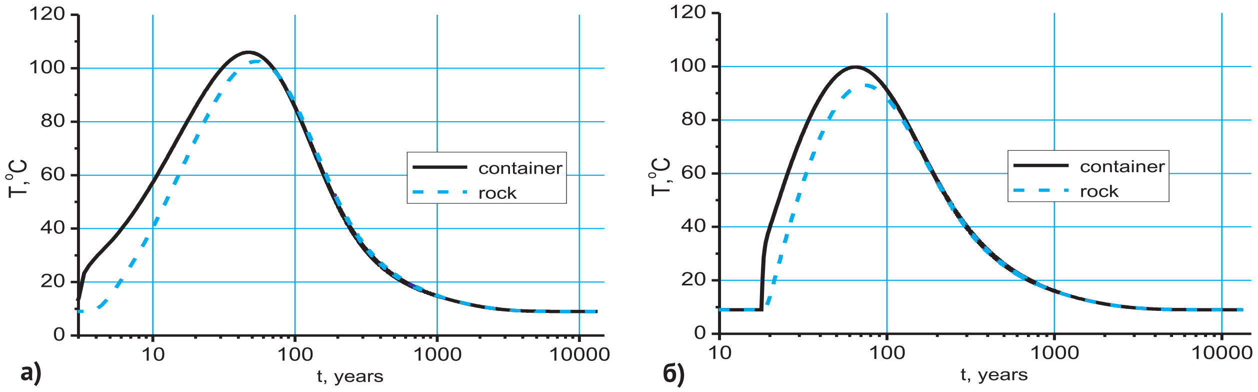
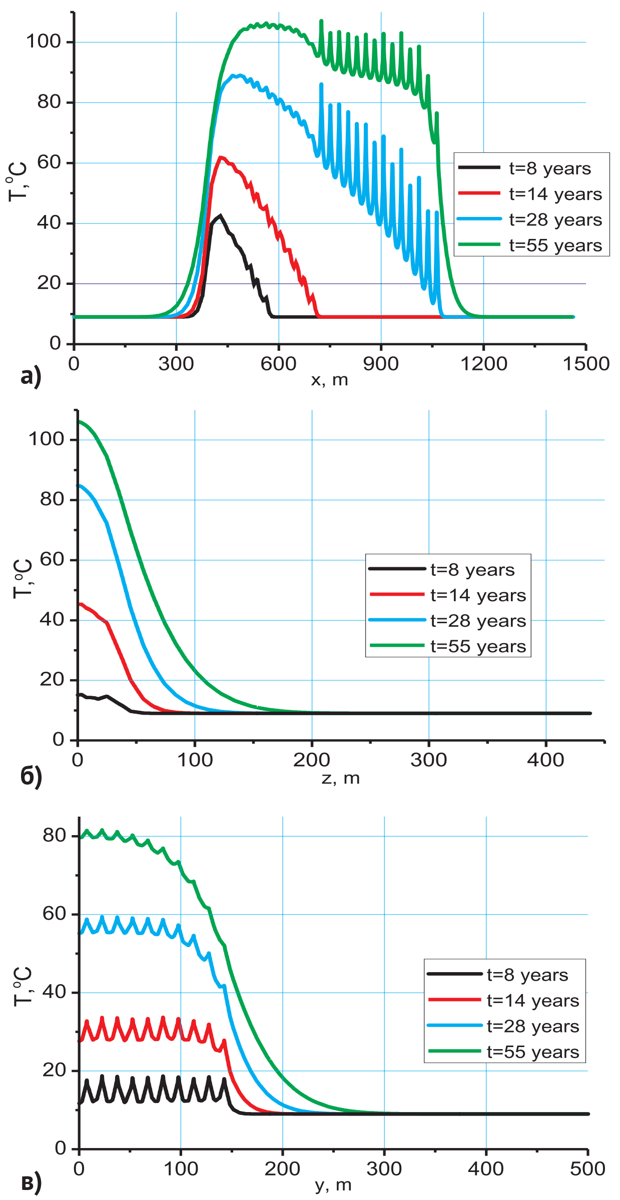


Fig. 7. Time dependences of temperatures for the centre of an internal well: a — section 1; b — section 2



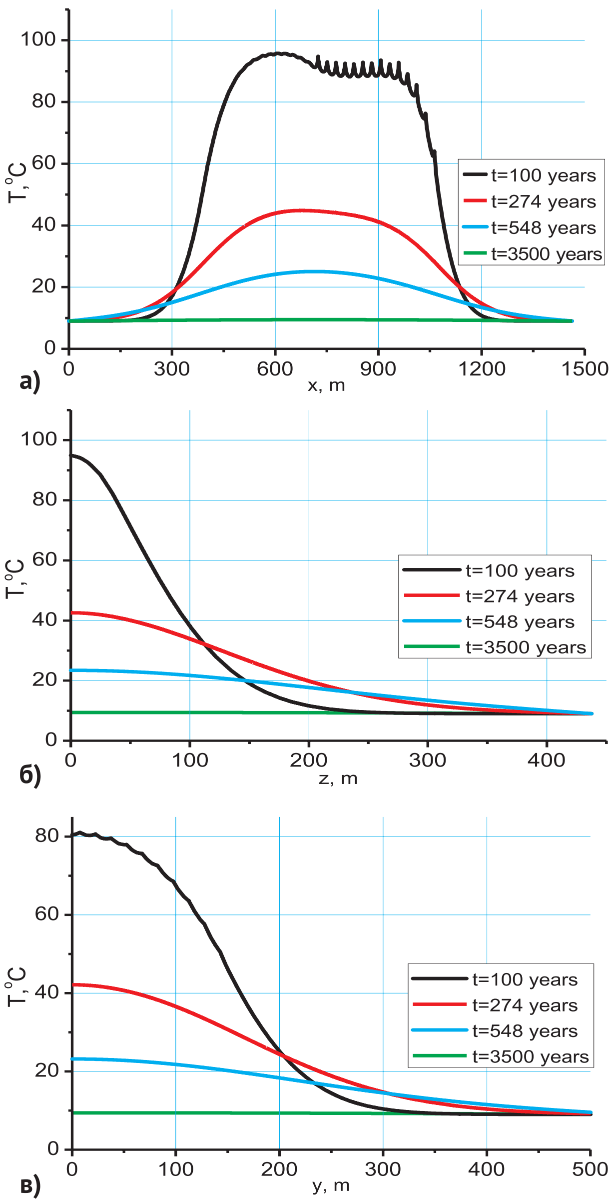


Fig. 8. Spatial profiles of temperatures at the stage of DRWDF heating: a — along horizontal axis of symmetry at DRWDS; b — along the vertical line crossing the centre of the eighth chamber of the disposal section 1; c — along the horizontal line crossing the tops of boreholes in the eighth chamber of disposal section 1

Fig. 9. Spatial profiles of temperatures at the stage of DRWDF cooling: a — along horizontal axis of symmetry at DRWDS; b — along the vertical line crossing the centre of the eighth chamber of the disposal section 1; c — along the horizontal line crossing the tops of boreholes in the eighth chamber of disposal section 1

interval. Verification of the code performed for the tasks relevant for the temperature field modeling at the deep RW disposal facility has demonstrated a good agreement of numerical calculations using FENIA code with reference ones.

The described calculations represent only one of research stages; they do not take into account all the mechanisms of heat transport. The more accurate assessment of the thermal conditions and upgrade of the FENIA code for simulation of these processes, as well as solution of the conjugate problem will be performed in the future. The presented assessment of the thermal conditions gives an understanding of the limits of temperature changes in the disposal facility, provides better justification for decisions to select protective barrier materials (bentonite, slurry, concrete), and to optimize the configuration of boreholes at DRWDF and the procedure of their filling.

At present, there is a considerable uncertainty of design solutions and selection of materials for DRWDF. There is no final decision on the materials of engineered barriers, first of all bentonite-containing filling and slurry, as well as concrete of the isolating containers. On the other hand, the uncertainties of input data are related to inhomogeneity of geological structures, since the thermal physical properties of granitoids of the Nizhnekansk massif differ substantially. For example, the specific heat conductivity of rock samples taken at distances of several hundreds of meters from each other may differ by more than three times [7]. Elaboration of input data for the calculations is required to obtain more accurate assessments of the DRWDF thermal state evolution. First of all, this concerns the properties of materials, which can be studied during geologic surveys, laboratory studies and, after construction of the underground research laboratory (URL) at NKM, — in experimental in-situ studies. It would certainly be impossible to completely eliminate the uncertainties; however, the reduction of uncertainty range and conduct of multivariate calculations will provide realistic assessments, while keeping the reasonable level of conservatism.

The performed assessment of the thermal conditions allows selection of conditions for model experiments, which will be performed at URL for containers with heat sources emulating the RW heat generation. The power of these sources and their configuration shall be defined prior to start of the experiments using pretest simulations, and FENIA code can be used for these purposes. The results of in-situ experiments at URL will enhance our knowledge regarding the conditions of safety barriers and the DRWDF host rock, will provide data for additional verification of the model, and specification of the used numerical and mesh models.

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