Eurasian Journal of Physics and Functional Materials

2022, 6(3), 198-212

Feasibility study mixed oxide fuel tests in the impulse graphite reactor

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DOI: **10.32523/ejpfm.2022060305**
Received: 01.09.2022 - after revision

The article presents the results of computational studies to substantiate the possibility of testing the fuel of the Multipurpose hYbrid Research Reactor for a High-tech Applications reactor (MYRRHA) in the Impulse Graphite research Reactor (IGR). A scheme for conducting experiments is proposed, which allows simulating the operating conditions of MYRRHA fuel elements in a wide range of changes in their thermohydraulic parameters, including the conditions of accidents with the destruction of fuel pellets, blocking the flow area and stopping the coolant flow. A method for thermohydraulic calculations has been developed, implemented in the software environment of the computational fluid dynamics (CFD) code. A computational model of the experimental device is developed, optimized according to the spatial partitioning grid. A turbulence model for determining the parameters of convective heat and mass transfer in a eutectic lead-bismuth alloy is selected and substantiated.

Keywords: MYRRHA reactor; mixed-oxide fuel; fuel pellet destruction; research Impulse Graphite Reactor; thermohydraulic parameters

Introduction

In the safety analysis of fast sodium reactors, local destruction of fuel elements are considered as possible initiating events for severe accidents [1]. The destruction (cracking) of the fuel at nominal operating conditions occurs due to thermal stresses and gas swelling as one of the significant burnout effects. Local destruction of fuel can cause destruction of neighboring fuel elements if conditions for their cooling are violated. One of the reasons for the deterioration of the cooling

conditions for fuel elements is a blockage of the flow area of the coolant caused by the release of fuel outside the fuel elements in case of overheating [1]. Such a situation may arise as a result of errors in loading fuel elements with fuel pellets with a higher than required content of fissile isotopes. As a result of blocking the flow area, sodium boiling and void formation are possible, which, in turn, will cause local power surges due to the manifestation of a positive effect of reactivity on the coolant density.

In reactors with a lead or lead-bismuth liquid metal coolant, local destruction is not accompanied by local power surges, since such reactors have, though not large, but a negative effect of reactivity in terms of the coolant density and a higher boiling point [2]. The worst hypothetical result of local damage is a subsequent increase in the number of destroyed fuel elements in fuel assemblies, which occurs due to blocking of the flow section of the coolant with fuel fragments extending beyond the fuel elements destroyed at the previous stage of the accident evolution.

In the safety assessment of the Multipurpose hYbrid Research Reactor for a High-tech Applications reactor (MYRRHA), described scenario of the fuel element destruction and leaching of fuel from them is simulated by calculation [3], while within the framework of the Seventh Framework Program (FP7) of the European Commission in a project entitled Methodology, Analysis and Experiments for the "Safety In MYRRHA Assessment" (MAXSIMA) considered the possibility of carrying out real experiments tests at the Impulse Graphite Reactor (IGR) to study severe accidents with damage to the MYRRHA reactor core.

The National Nuclear Center of the Republic of Kazakhstan (NNC RK), operating the IGR reactor, has significant experience in such studies [4]. The technical characteristics of the IGR make it possible to carry out in-reactor research aimed at obtaining information about the processes occurring in the elements of nuclear reactors in transient and emergency modes. An important task when testing model fuel elements and fuel assemblies in the IGR reactor is the implementation of a given power release. It, with high accuracy, is provided thanks to a number of developed methods which are aimed for the determining the tests energy parameters [5, 6], location and mass of fuel composition inside the test device [7, 8] and impurity gas releasing from the fuel during the irradiation [9]. IGR technical possibilities as well as the developed methodical base made it possible to launch the ambitious international experimental programs EAGLE (Experimental Acquisition of Generalized Logic to Eliminate re-criticalities) [10, 11] and SAIGA (Severe Accident In-pile experiments for Gen-IV reactors and the Astrid prototype) [12].

For computational and analytical substantiation of a possibility of conducting experiments at the IGR reactor to study the destruction (cracking) of fuel pellets of the MYRRHA research reactor, an experimental scheme was developed and justified by calculation. The computational model of the experimental device and calculation algorithms made it possible to simulate the behavior of fuel pellets in emergency modes. When describing heat transfer in the experimental device, there was no forced movement of the coolant, which corresponded to the conditions of the accident with termination of the coolant flow. In this case,

it was assumed that heat transfer at the boundaries of solids with a coolant is carried out due to the convective movement of the coolant.

As part of improving the computational approaches to thermohydraulic modeling, the relevance of which is long overdue [13], it was proposed to use the computational fluid dynamics (CFD) code to describe convective heat transfer in the numerical simulation of spatial hydrodynamic effects. Such codes allow one to describe both laminar and turbulent flows in order to obtain correct results, while the correct choice of the space-time parameters of the computational grids is important.

This article describes the results of thermohydraulic modeling using the ANSYS Fluent CFD code of the experimental device and the scheme of the experiment to study the cracking of fuel pellets of the MYRRHA research reactor at the IGR reactor.

Design of an in-pile experimental device

The scheme of the in-pile device with a MYRRHA fuel element was developed in accordance with the requirements [14] for the experimental device and was supposed to accommodate the model fuel element and coolant of the considered reactor.

For this purpose, a capsule is provided, which is a sealed structure and placed inside a protective casing (Figure 1).

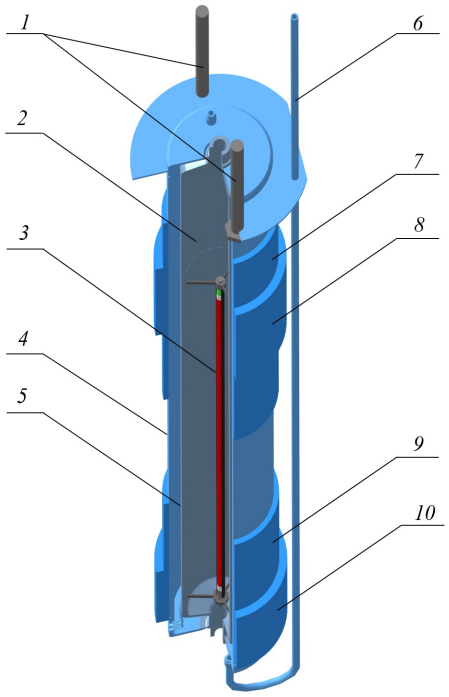

Figure 1. Experimental device sketch: 1 – bar, 2 – cavity for filling with eutectic, 3 – model fuel element, 4 – protective cover, 5 – capsule, 6 – cooling system pipeline, 7, 8, 9, 10 - additional absorbers of neutron flux.

On surface of the capsule, in the upper and lower parts, there are steel thickening (7, 8, 9, 10), which act as additional absorbers and are designed to provide the required height profile of energy release in the fuel element.

A cable heater is installed on the outer surface of the capsule to preheat the elements to a temperature of 400 K during the experiment. The model fuel element (3) consists of cylindrical fuel pellets with a diameter of 5.42 mm and a height of 6.5 mm, installed in a stainless-steel cladding. The gap between the column of fuel pellets and the cladding is filled with helium. Mixed-oxide (MOX) fuel (uranium oxide and plutonium oxide) is used as a material for fuel pellets.

The fuel element is immersed in the coolant volume (44.5% Pb, 55.5% Bi) without ensuring its forced movement. The coolant level in the capsule must be at least 50 mm above the upper end of the fuel element.

Experiment conditions

In the experiment it was supposed to investigate the early cracking of fresh fuel pellets caused by thermal loads with a sharp increase in power to the rated value and further operation of the reactor at rated power with a blocked coolant flow. Thermal cracking factor determines the upper limit of the sizes of fuel fragments, which are most likely to lead to blocking of the coolant section in the fuel assembly. Thus, the conservative case of the initiating event was considered, which could lead to the development of an accident situation caused by violation of the fuel assembly cooling conditions.

When experiment preparations, the capsule must be heated up to 400 K by electric heaters in order to transfer the eutectic into a liquid state, then the IGR reactor is started up with the implementation of the specified power change diagram. During the experiment, stationary power of the IGR is maintained until the start of fuel cracking.

The specified energy release in the fuel element is provided by the experimental device design, its position in the central experimental channel and implementation of the required IGR power diagram [15].

Analysis of the thermohydraulic parameters of the experiment

Computational model

The calculation of the thermohydraulic characteristics of the experimental device during the experiment in the IGR reactor was carried out using the ANSYS Fluent software package [14]. Based on the conditions of the axial symmetry of the device, for the computational modeling, a segment 1/12 of the device part was chosen, which includes a model fuel element located in the volume of the eutectic alloy, the capsule casing, cooling path and the cooling jacket. The fuel in the fuel element was divided into 143 equal volumes (13 elements in height and 11 elements radially) (Figure 2). On the upper and lower surfaces of the model, adiabatic conditions of heat transfer with the external environment were established.

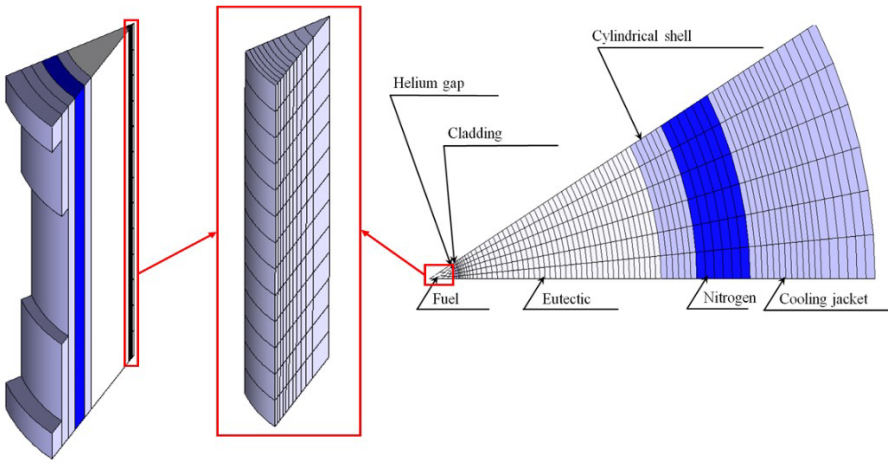

Figure 2. Computational model.

The main requirement for grid methods is, first of all, to ensure a small numerical error of the results obtained with the minimum required computational resource. Therefore, it is very important to correctly choose the parameters for solving the problem, which affect the accuracy and duration of the numerical model calculation. The main parameter is the grid step.

Based on preliminary calculations, the total number of quadrangular prismatic elements contained in the spatial grid was selected, which was 285150. This number of elements is the optimal choice for calculating the device, has sufficient accuracy and adequate consumption of computing resources. Splitting into more elements was not advisable, since the relative deviation from data with a denser grid is less than 2%.

Constitutive equation

The main dependences underlying the calculations:

Continuity (flow) equation:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho_i u_i) = 0 \tag{1}$$

where ρ – is the density of the medium; x_i – coordinates x, y, z; u_i – components of the average velocity of the medium u, v, w, corresponding to the x, y, z axes.

Equation for momentum transfer:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_i}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right)\right] - \frac{\partial(\rho\overline{u_i u_j})}{\partial x_j} \tag{2}$$

where μ – coefficient of dynamic viscosity of the medium; δ_{ij} – Kronecker symbol.

Energy conservation equation in a medium:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}[u_i(\rho E + p)] = \frac{\partial}{\partial x_i}\left(k_{eff}\frac{\partial T}{\partial x_i} - \sum_j h_j J_j + (\overline{\overline{\tau_{eff}}} u_i)\right) \tag{3}$$

where E – total energy; k_{eff} – effective thermal conductivity coefficient ($k + k_t$, where k_t is turbulent thermal conductivity); T – medium temperature; $\sum_j h_j J_j$ – diffusion of components; $\tau_{eff} u_i$ – dissipation of energy due to viscous forces; p – medium pressure.

Energy conservation equation in a solid region:

$$\frac{\partial(\rho h)}{\partial t} = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + S_h \tag{4}$$

where S_h – enthalpy source, and enthalpy h is the dependent variable:

$$h = \int_T^0 C_p \, dT \tag{5}$$

where C_p – specific heat.

The calculations took into account the natural convective motion of the eutectic alloy, which arises as a result of the occurring of a temperature gradient in the volume of the eutectic during its heating and affects the heat removal from the fuel element.

In issues with natural convection, the Reynolds number is not a characteristic of the flow. The dimensionless parameter characterizing the flow regime and determining the behavior of the fluid under the influence of the temperature gradient is the Rayleigh number:

$$Ra = \frac{g\beta\Delta T L^3}{\nu\chi} \tag{6}$$

where g – acceleration of gravity; L – characteristic size of the fluid region; ΔT – temperature difference between walls and liquid; ν – kinematic fluid viscosity; χ – thermal diffusivity of liquid; β – thermal expansion coefficient of liquid

Rayleigh-Benard convection in a closed cavity is a classical solution in numerical methods used in various computational fluid dynamics codes. At high Rayleigh numbers, the flow pattern becomes turbulent, and depending on the constriction of the cavity, it can have a complex unsteady circulation structure. The Navier-Stokes equations used in modern CFD codes describe well both laminar and turbulent flows [16], but depending on the complexity of the issue, it is implied the need for accurate resolution of all space-time scales of turbulence, which means the use of very small grids and time steps in combination with high-precision flux approximation schemes [17].

During the preliminary calculation, the value of the Rayleigh number was $Ra \sim 10^{11}$. Consequently, in the numerical simulation of the heat transfer in this model under conditions of natural convection, it is necessary to take into account the turbulent flow regime of the medium [18–20].

The (κ-ε)-model was used as a turbulence model. In addition to the equations of continuity and momentum transfer, this model includes two additional equations: for turbulent kinetic energy κ and turbulence dissipation rate ε.

The equation for the κ transfer (turbulent kinetic energy):

$$\frac{\partial(\rho\kappa)}{\partial t}+\frac{\partial(\rho u_i\kappa)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_T}{\sigma_\kappa}\right)\frac{\partial\kappa}{\partial x_j}\right]+2\mu_T E_{ij}E_{ij}+G_b-\rho\varepsilon \tag{7}$$

where μ_T - turbulent viscosity coefficient.

The generation of turbulence due to temperature (density) stratification is determined from the formula:

$$G_b=\beta g_i\frac{\mu_i}{Pr_i}\frac{\partial T}{\partial x_i} \tag{8}$$

where g_i – component of the gravity vector in the i-th direction; β – thermal expansion coefficient.

The equation for the transfer ε (the rate of dissipation of turbulent kinetic energy):

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho u_i\varepsilon)}{\partial x_i}=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{\kappa}(2\mu_T E_{ij}E_{ij}+C_{3\varepsilon}G_b)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{\kappa} \tag{9}$$

where μ_T – turbulent viscosity coefficient.

In equation (9) there is a $C_{3\varepsilon}$ coefficient associated with the buoyancy forces, calculated from the following relation:

$$C_{3\varepsilon}=tanh\left|\frac{\nu}{u}\right| \tag{10}$$

where ν – component of the current velocity that is parallel to the gravity vector; u – component of the current velocity that is perpendicular to the gravity vector.

To take into account the radiant heat transfer between the fuel core and the cladding of the fuel element, the method of effective thermal conductivity [21] was applied, the essence of which is to introduce a correction that takes into account the contribution of radiant heat transfer to the total heat transfer to the thermal conductivity coefficient of helium filling the gap:

$$\lambda_{eff}=\lambda+\lambda_{rad}=\lambda+C_{red}\frac{\left[(\frac{T_1}{100})^4-(\frac{T_2}{100})^4\right]}{(T_1-T_2)}\sigma \tag{11}$$

where λ – thermal conductivity of helium; λ_{rad} – radiation coefficient of thermal conductivity; C_{red} – reduced emissivity; T_1 – temperature on the fuel surface; T_2 – temperature on the inner cladding of a fuel element; σ – helium gap thickness.

This approach made it possible to significantly optimize the calculation, and its correctness was confirmed by preliminary studies, during which the deviation of the calculation results using the proposed method from the results of detailed modeling of radiant heat transfer in the calculation program was no more than 2%.

Boundary conditions

During the calculations, the following boundary conditions were set:

- on the outer surface of the capsule, conditions of convective heat exchange with the environment with a temperature of 300 K at a heat transfer coefficient of 5 $W/(m^2 * K)$ are determined;

- the initial temperature of all structural elements was taken equal to 400 K;

- implementation time of the reactor power diagram – 100 s;

- the thermophysical characteristics of MOX-fuel in the $(U, Pu)O_2$ composition were determined using the dependences given in [22], the properties of the remaining materials were taken from the literature [23];

- the energy release in the fuel pellets of the fuel element was set in accordance with the results of calculating the neutronic parameters of the device.

The calculation of the neutron-physical characteristics [24] of the "IGR reactor - experimental device" system was carried out using the combined computational model [25], which fully corresponds to the real design and takes into account the true distribution of the uranium concentration in the graphite blocks of the core. The calculation results showed that in experiments with a given configuration of the experimental device, the required height profile of the power in the fuel element [26] can be provided (Figure 3). In a fuel element with MOX fuel, a significant irregularity of radial energy release will be observed. This is due to the fact that the neutron spectrum in IGR, in contrast to fast reactors, is predominantly thermal.

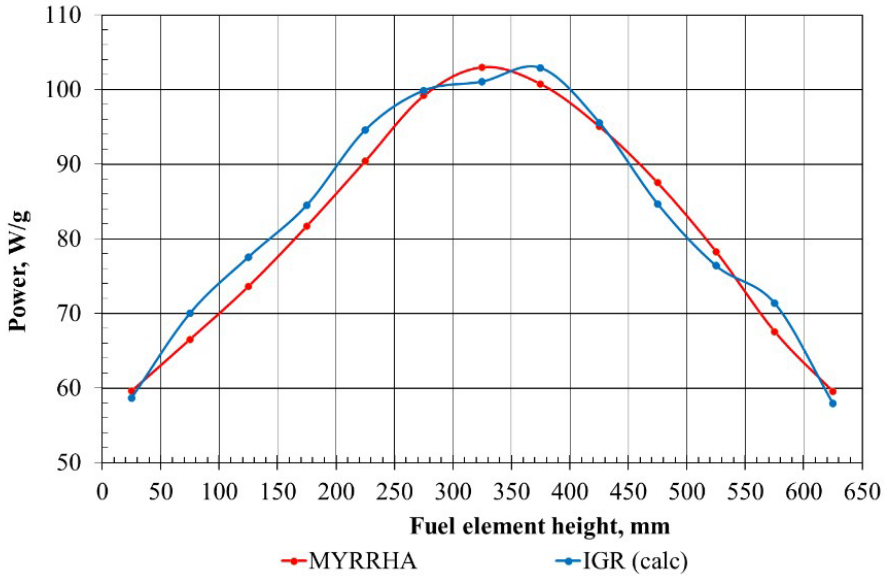

Figure 3. Height distribution of the power in a fuel element.

Calculation results

There is not much information in open publications about experimental studies of convective heat transfer in a liquid metal located in a closed region with a local source of energy release. Therefore, there are difficulties in choosing the correct approach to solving problems of the spatial hydrodynamic effects of convective heat and mass transfer in closed regions, which depend on many factors, such as

the volume of the coolant, shape of the reservoir with the coolant, location of the local source of energy release, etc.

It is known that with a small temperature difference between the coolant and the local source of energy release, the problem of convective heat transfer will be solved in the laminar approximation, and an increase in the temperature difference leads to the formation of turbulent flow regimes. In this regard, based on the analysis of similar studies in [27, 28], a number of thermohydraulic calculations were carried out using ANSYS Fluent with turbulence models of the $\kappa-\varepsilon$ family. The models differ in the method for calculating the turbulent viscosity, in the method for setting the turbulent Prandtl numbers in the diffusion fluxes $\kappa-\varepsilon$, in terms of generation and dissipation. Based on the results of the calculations and the analysis of similar studies, the Realizable $\kappa-\varepsilon$ turbulence model was used for further calculations.

Calculations to determine the thermophysical parameters of a device with a MOX fuel element were carried out for two cases of energy release distribution in a fuel element. In the first case, the radial energy release was assumed to be uniform and only the height distribution of the energy release was taken into account. This situation is closest to the operating conditions of a fuel element in the MYRRHA reactor. In the second case, actual distribution of power release was considered under test conditions in the IGR (Figure 3), taking into account both altitudinal and radial irregularities. The rise in the power of a fuel element upon reaching the stationary mode is modeled by a jump from zero to the nominal value. When simulating the experiment, there was no forced cooling in order to conservatively estimate the maximum heating of the outer walls of the experimental device. In fact, during the experiment at the IGR reactor, the forced cooling system will be activated.

Figure 4 shows the graph of the temperature change of the fuel pellet in the section with the highest fuel temperature, located at a height of 390 mm from the lower end of the fuel column, within 100 s from the moment of power increase.

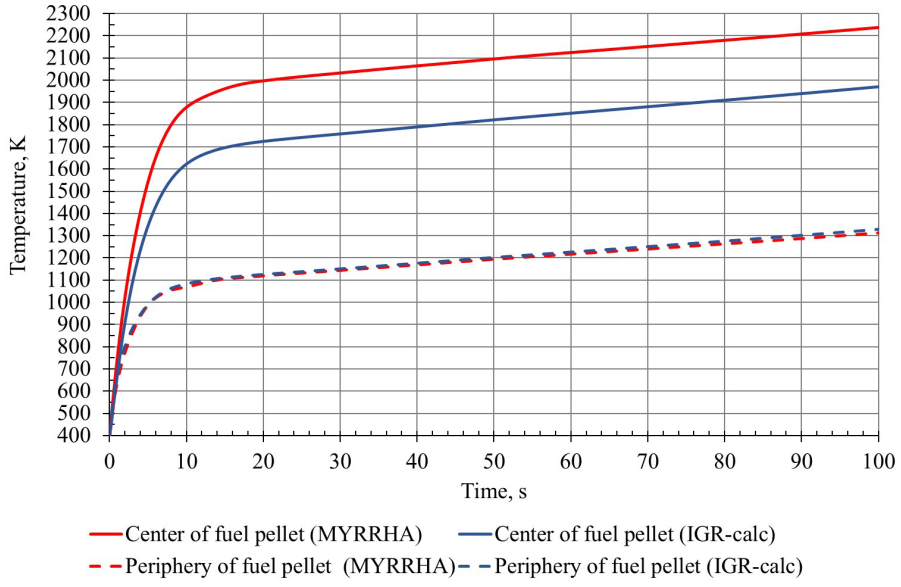

Figure 4. Change in fuel temperature during experiment.

During operation of the MYRRHA reactor at rated power, the maximum fuel temperature is $\sim$ 2073 K.

This is due to the fact that the melting point of MOX-fuel decreases with an increase in the proportion of plutonium oxide and with an increase in burnup. When fresh MOX-fuel $(U_{0.7}Pu_{0.3})O_2$ is used, the melting point is 3000 K. With a calculated burnup of 100 MW day/kg of heavy metal, the melting point will decrease to 2680 K. The design maximum temperature must be below these limits. In order to keep the fuel far enough from the plastic state, maximum operating temperature is usually chosen below $0.9 * T_m$ [29].

In calculations with a uniform radial distribution of the energy release at 35 s from the beginning of the experiment, i.e. time of intensive heating completion, the temperature in the center of the fuel is $\sim$ 2051 K, which corresponds to the maximum operating temperature of the MYRRHA reactor during normal operation. With an uneven radial distribution of energy release for 35 s from the beginning of the experiment, the temperature in the center of the pellet will be $\sim$ 1780 K (Figure 4). The steady-state mode of fuel heating in the experiment for both cases of radial energy release distribution is achieved by about 15 seconds of the experiment, after which heating continues at a rate of about 2.5 K/s. Figure 5 shows the temperature distribution in the fuel at 100 seconds of the experiment.

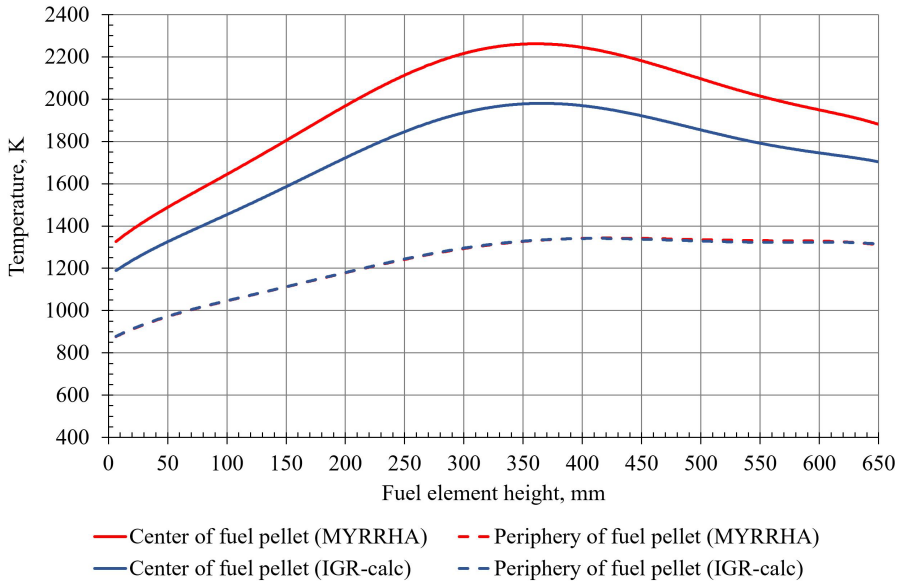

Figure 5. Temperature distribution in the fuel at 100 seconds of the experiment.

The temperature gradient in the fuel pellet $(U_{0.7}Pu_{0.3})O_2$ will be $\sim$ 600–650 K for the case of a real radial profile of the energy release. In this case, the maximum pellet temperature by the end of the experiment will not exceed 1995 K.

The temperature field of the eutectic at different times is shown in Figure 6.

The maximum temperature in the eutectic alloy for 100 s of the experiment reaches a value equal to 957 K, which does not exceed its boiling point. Boiling point is about 1000 K (T_{boil} = 1911 K) [23].

The velocity field due to the convective motion of the eutectic alloy during its heating is shown in Figure 7.

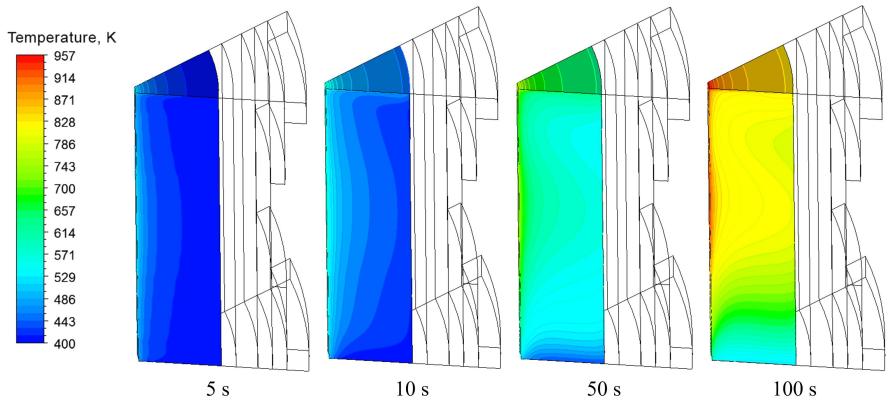

Figure 6. Temperature distribution in the device eutectic.

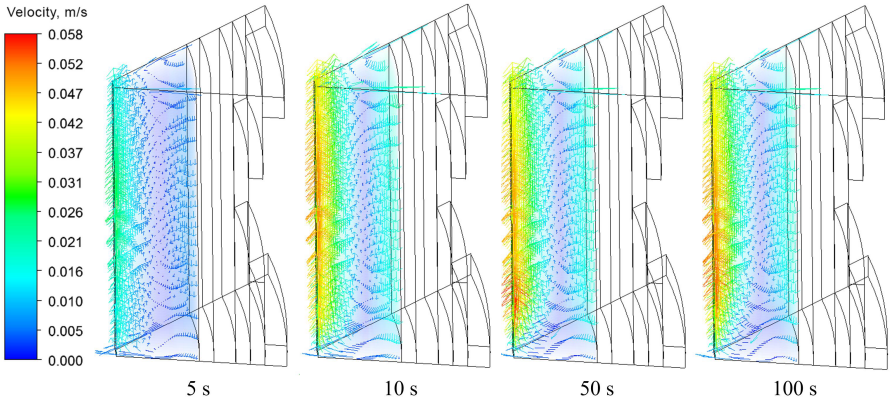

Figure 7. Velocity vector in the eutectic alloy of the device at different times.

The maximum temperature of steel structures reaches 833 K, i.e. the necessary margin is provided up to the melting temperature (T_m = 1700 K) [22], which guarantees the preservation of the integrity of the experimental device even in the absence of forced cooling (Figure 8).

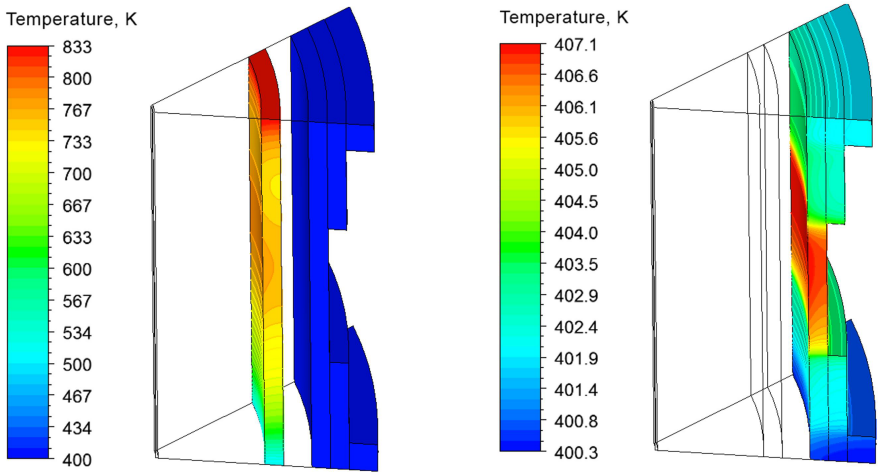

Figure 8. Temperature distribution in the steel structures of the device for 100 s of the experiment.

The main calculated parameters of the experiment are presented in Table 1.

Table 1.
Main calculated parameters of the experiment.

Parameter	**Value**
Coolant material	44.5 % Pb, 55.5 % Bi
Fuel rod material	$(U_{0.7}Pu_{0.3})O_2$
Experiment time, s	100
Initial temperature of the fuel rod and coolant, K	400
Average energy release in the fuel element, W/g	77.27
Maximum temperature in the fuel element, K	1995
Temperature gradient in the fuel pellets, K	600–650
Maximum temperature in the coolant, K	957
Maximum temperature of steel structures of the device, K	833
Average velocity in coolant layers, m/s	0.02
Energy target value, kJ	172 [30]

Estimation of a time for starting of MOX-fuel pellets cracking

The estimation of the time required for destruction (cracking) of MOX-fuel pellets for cases of uniform and non-uniform distribution of radial energy release was made on the basis of the assumption that thermal destruction of fresh fuel after intensive reaching the nominal operating mode depends on the amount of energy absorbed by the fuel as a result of its irradiation in the IGR and does not depend on the input mode of this energy.

The results of previous experiments on research reactors aimed at establishing threshold loads in fresh fuel under conditions of an RIA accident [30-32], enables estimating the amount of energy that must be invested in the fuel to achieve pellet cracking.

In the case of a uniform radial distribution of the energy release, cracking of fuel pellets in the energy-stressed fuel-element pellet itself begins at $\sim$ 40 s of the experiment, in the case of an actual distribution – at $\sim$ 45 s. By about 65 seconds from the start of the experiment, almost all the fuel pellets in the fuel element will be cracked, after which it will be possible to shutdown the IGR reactor.

Conclusion

A set of calculations was carried out, the thermal hydraulic parameters of the experimental device with a MYRRHA fuel element were determined during the planned tests.

As a result of the research, the most suitable method for obtaining the calculated data necessary for the qualitative preparation of the experiment and ensuring its safety has been determined. The optimal number of computational grid elements has been selected for the implementation of sufficient accuracy of calculations and adequate consumption of computing resources. To simulate

thermal convective heat and mass transfer in a eutectic alloy, various turbulence models of the $(\kappa-\varepsilon)$ family were tested in the developed device model.

Calculations have shown that the temperature gradient in the fuel pellet $(U_{0.7}Pu_{0.3})O_2$ will be $\sim$ 600-650 K for the case of a real radial profile of energy release and the maximum pellet temperature by the end of the experiment will not exceed 1995 K.

The eutectic alloy surrounding the fuel element, due to convective heat exchange with the surface of the fuel element, heats up to 957 K by 100 s from the experiment.

The outer walls of the experimental device heat up insignificantly even without activating the forced cooling system of the device, therefore, their integrity will be ensured, and the thermal effect on the IGR reactor is negligible.

In the case of a uniform radial distribution of the energy release, cracking of fuel pellets in the energy-stressed fuel-element pellet itself begins at $\sim$ 40 s of the experiment, in the case of an actual distribution – at $\sim$ 45 s. By about 65 seconds from the start of the experiment, almost all the fuel pellets in the fuel element will be cracked, after which it will be possible to shutdown the IGR reactor.

Thus, the results of the computational and analytical substantiation demonstrated the applicability of the adopted approach for predicting thermohydraulic parameters and confirmed the possibility of safely conducting reactor tests with MYRRHA fuel elements to study the destruction (cracking) of fuel pellets and simulate an emergency situation with the cessation of coolant flow.

Acknowledgments

This study was financially supported by the Ministry of Energy of the Republic of Kazakhstan on the topic "Development of nuclear energy in the Republic of Kazakhstan" (BR09158470), and main initial data for the study was obtained within the framework international MAXSIMA program (Methodology, Analysis and Experiments for the "Safety In MYRRHA Assessment, the fifth section of the work on the project (WP5)" Fuel safety for MYRRHA "Task 5.3" Development of the concept of an experiment in the IGR reactor".

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