Conference Paper

Modeling of Analytical-Experimental Benchmark on Irradiation of Nitride Fuel in BN-600 Reactor in the SCALE6 code

V. Y. Shorov, S. N. Ryzhov, M. Y. Ternovykh, and G. V. Tikhomirov

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, Moscow, 115409, Russia

Abstract

In this work was carried out the simulation in the SCALE6 code of an experiment on the BN-600 reactor on irradiating of fuel assemblies, containing samples of mixed nitride uranium-plutonium fuel. A comparison of the results for SCALE6 on the results of other codes is presented. The results of an estimation of uncertainties in the calculated data connected with uncertainties of an irradiation of an experimental sample and used neutron cross-sections library. Discussion of possible differences between analytical and experimental results is given.

Keywords: fast reactor, mixed nitride uranium-plutonium fuel, spent fuel, analytical-experimental benchmark.

1. Introduction

Currently, some researches are underway to form the next-generation technologies to be used in the transition of nuclear power to a closed nuclear fuel cycle and creation of safer conditions for the operation of reactors through the introduction of natural safety systems. Within the framework of these directions, research is being carried out on a new type of fuel, which is planned to be used in the new generation reactors: mixed nitride uranium-plutonium (MNUP) fuel. The first experiments with samples of MNUP fuel at the BN-600 reactor were completed.

The purpose of this work is to conduct a detailed calculation analysis in the SCALE6 code \[1\] of the experiment with irradiated nitride fuel for verification of codes and libraries of constants used in the substantiation of projects of reactors with liquid-metal coolant with MNUP fuel. The possibility of using the SCALE6 code for the calculation of fast neutron reactors was analyzed in [2, 3].

At the present time, the first stage of radiochemical researches of MNUP fuel sample irradiated in the BN-600 reactor and calculations of the experiment for various Russian
codes has been completed. It is planned to create an international benchmark on the basis of an analysis of the calculated and experimental results.

Scope of the benchmark is MNUP fuel with burnup up to 5.5%, to substantiate the projects of nuclear facilities in the physics of reactors in the burnup process and from the point of view of the accumulation of radiation-hazardous nuclides. To correctly model the results of radiochemical researches of spent fuel assemblies with MNUP fuel, three tasks are distinguished in the benchmark:

- Three-dimensional neutron-physical calculation of the BN-600 reactor.
- Neutron-physical calculation of fuel assemblies with MNUP fuel.
- Calculation of the nuclide kinetics of fuel assemblies with MNUP fuel.

In calculations of neutron-physical characteristics, the characteristics of neutron irradiation of fuel elements with MNUP fuel are determined by the developed benchmark model, with reception of spectra and density of a stream of neutrons in investigated zones, the average blocked sections of neutron reactions according to a mode of an irradiation.

In calculations of nuclide kinetics based on neutron-physical calculations, calculations of the composition of the irradiated sample with MNUP fuel are performed in accordance with the irradiation regime and the history of post-reactor studies.

2. Materials and Methods

The reactor core of the BN-600 reactor consists of 136 small enrichment fuel assemblies, 94 medium enrichment fuel assemblies and 139 large enrichment fuel assemblies. Fuel assemblies have a hexagonal cover made of steel, 127 fuel rods are located in the fuel assemblies in 8 mm increments. The fuel rod is a thin-walled steel tube with a diameter of 6.9 mm with a wall thickness of 0.4 mm. The fuel rod is filled with pellets that form a fuel core. The design of the fuel element provides for the combination of both the lower and the upper end reflectors in one shell.

The experimental assembly consists of 123 fuel rods with the standard uranium oxide fuel for the BN-600 reactor and four fuel rods with MNUP fuel, one of which is the central. Experimental fuel assembly with MNUP fuel was irradiated in the reactor core of the BN-600 reactor during three micro-campaigns (time intervals between reactor overloads), then it was transferred to the in-reactor storage. After exposure for one micro-campaign, it was unloaded into the drum of the spent assemblies and after a while entered the experiment.
By the time the experiment began, the history of the BN-600 reactor had more than 60 micro-campaigns. Benchmark models were developed on the basis of complete models for all microcampaigns within the ModEx calculation complex [4] from the BN-600 reactor fuel archive. This complex describes in detail each assembly of the active zone and the side screen: 11 compositions for the height of the core and 3 compositions in the upper and lower end screens, in which burnout is calculated. In addition, the composition and movement of the regulatory and protective organs are described in detail - for each rod there are more than 40 physical zones. Thus, the complete reactor model counts from 15 to 20 thousand zones of different compositions. The calculation tool is TRIGEX [5] with the constants ABBN-93 [6].

For the computational benchmarks, simpler models were compiled, the number of compositions in which varies from 36 to 52 with the condition that the model is informative in relation to the calculation of the fuel rods characteristics with MNUP fuel.

Reactor control and safety system rods are exposed in an intermediate position from the real displacement in such a way as to reproduce the average level of the total flow in the volume of interest for the micro-campaign. This option is standard for cross-verification of codes. For a correct comparison with experiment in the benchmark, the positions of the reactor control and safety system rods are set, which allow us to estimate the effect of the motion of the reactor control and safety system rods on the results of calculations and comparison with experiment in the calculation.

The developers of the benchmark have identified differences related to simplifications and approximations, which can be used as corrections. In particular, the correction for a detailed model in the spectra and the magnitude of the total flux was obtained as the ratio of the results of calculations of these characteristics by the full model to similar calculations for the benchmark model. It was found from the calculations that the correction for the neutron flux density is no more than 2% in the main energy groups of the neutron spectrum upon irradiation in the core in each of the three micro-campaigns under consideration. In the store, the correction is 3-4%, which does not play a significant role due to the smallness of the neutron flux in this area.

With the TRIUM [7] complex, the simplified model for the TRIGEX code was uniquely translated into the MMKK/MMKC code [8], which calculates using the Monte Carlo method. Thus, the “kinetic” correction was defined as the ratio of transport calculation to diffusion.

The next simplification of the benchmark model is the homogeneous representation of a real heterogeneous experimental fuel assembly. To account for this factor, all the
fuel rods of the fuel assemblies (separately central with the experimental section) were identified in the MMKK/MMKC code, the remaining fuel elements with MNUP fuel and uranium fuel rods. The neutron flux in the central fuel rod (the selected section) and the average flux over the specified fuel assembly were compared in two calculations, the ratio of which is interpreted as a “heterogeneous correction”. Note that in the development of three-dimensional and two-dimensional models for the SCALE6 code, the experimental fuel assembly was described without geometric simplifications and, when obtaining the results, the “heterogeneous correction” was not used.

When constructing a fuel assembly model with MNUP fuel for solving the problem of nuclide kinetics a heterogeneous model was used by the recommendation of the benchmark developers, in which only the central rod with MNUP fuel is left, the remaining 126 - with oxide uranium fuel. Thus, the model represents an infinite grid of fuel elements in the “environment” of heat-transfer materials. When compiling the model, it is proposed to limit the composition of the core only. Boundary conditions - reflection in all directions. When carrying out calculations using the SCALE6 code, both the proposed model and the model heterogeneously describing the fuel rod cover and shells were considered.

3. Results

The three-dimensional neutron-physical calculation of the BN-600 reactor by the SCALE6 code for the three microcompanies in question was conducted in a homogeneous layer-by-layer description of all fuel assemblies except for the experimental one. In the benchmark of the model, the experimental fuel assembly is described by a beam of fuel cores set at a given step. The diameter of the cores is equal to the inner diameter of the shell. The remaining volume is filled with a mixture of sodium and steel. Concentrations of nuclides for homogeneously described regions are specified for each micro-campaign. Heterogeneous concentrations of fuel assemblies with MNUP fuel are set at the beginning of the first micro-campaign. Further, the nuclide concentrations for all micro-campaigns should be obtained as a result of calculating the nuclide kinetics of the experimental fuel assembly.

To solve the first problem, a three-dimensional model of the BN-600 reactor was created to perform calculations using the Monte Carlo method in the SCALE6 code. The special opportunity was used in SCALE6 to define a hexagonal cartogram that allowed describing the active zone, the fuel assembly of the reflector and the area of exposure.
of irradiated fuel assemblies in the model. The main parameters of the model for each microcampaign are: 14 different types of fuel assemblies, up to 10 different layers in the description of the structure of each fuel assembly for the height of the core, 35 different material compositions. Figure 1 shows a 3-D section of the model constructed by the visualizer SCALE6.
Based on the results of the calculations of each micro-campaign, the calculated parameters of irradiation of fuel rods with MNUP and fuel rods with oxide fuel were obtained: 28 group neutron spectra, the density of the total neutron flux, and single-group cross sections for calculating nuclide kinetics. For the purposes of cross-verification and analysis of results using the SCALE6 code, a number of additional parameters were obtained at the beginning of the micro-campaign:

- effective multiplication factor;
- axial distributions of energy release in the form of a linear load;
- radial distributions at the center of the test sample in the form of a linear load.

The main interesting volume is the experimental fuel assembly. The neutron flux density is determined by normalizing to the nominal thermal power of the reactor. For calculating the burn-up, the average thermal capacity for the fuel assembly with the MNUP fuel is used for the microcampaign. In accordance with the recommendations of the benchmark developer, the calculations took into account the heat release in all neutron reactions without considering the transfer of gamma quanta.

The control over the model created in the SCALE6 code is based on the number of fuel assemblies of various types given in the benchmark, the calculated values of the effective multiplication factor, and the isotope loading in the entire calculation model for micro-campaigns.

The results of the SCALE6 code comparison with the results of other codes obtained at the current stage of the design analysis of the experiment were compared. The difference in the effective multiplication factor does not exceed 0.5%. This result can be considered good given the special simulation in the SCALE6 code of data on effective fission fragments 235U and 239Pu. Data on effective fission fragments are available in the ABBN-93 library, are used in calculations of fast reactors for various codes, the concentration of effective fission fragments are the initial data of the benchmark.

When analyzing the calculation of the energy release in fuel assemblies at the level of the center of the test sample with MNUP fuel, three microcircuits differ from the results for the other codes. The maximum difference does not exceed 3%. The characteristics of micro-campaigns and the differences obtained are presented in Tab. 1.

The characteristics of micro-campaigns and the obtained differences obtained are presented in Tab. 1.

To solve problem of the nuclide kinetic of the MNUP fuel in the SCALE6 code, a 2-D fuel assembly model was developed for calculations by the $S_N$-method using neutron
TABLE 1: The characteristics of micro-campaigns.

<table>
<thead>
<tr>
<th>micro-campaigns</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Irradiation, days.</td>
<td>139</td>
<td>165</td>
<td>141</td>
<td>163</td>
</tr>
<tr>
<td>Uncertainty in average power,% fuel cooling, days.</td>
<td>3</td>
<td>1,6</td>
<td>2,2</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>41</td>
<td>10</td>
<td>541</td>
</tr>
</tbody>
</table>

TABLE 2: The difference in the masses of the elements in the irradiated sample with MNUP fuel.

<table>
<thead>
<tr>
<th>Element</th>
<th>Difference from the results other codes,%</th>
<th>Uncertainty associated with nuclear data,%</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>0,3</td>
<td>0,2</td>
</tr>
<tr>
<td>Np</td>
<td>1,4</td>
<td>1,9</td>
</tr>
<tr>
<td>Pu</td>
<td>0,6</td>
<td>0,9</td>
</tr>
<tr>
<td>Am</td>
<td>1,9</td>
<td>2,2</td>
</tr>
<tr>
<td>Cm</td>
<td>4,7</td>
<td>5,6</td>
</tr>
</tbody>
</table>

TABLE 3: Uncertainty in the masses of the elements in the irradiated sample with MNUP fuel.

<table>
<thead>
<tr>
<th>Element</th>
<th>Uncertainty associated with the uncertainty of energy release in the sample,%</th>
<th>Uncertainty associated with the uncertainty of the irradiation regime of the sample,%</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>0,3</td>
<td>0,1</td>
</tr>
<tr>
<td>Np</td>
<td>1,7</td>
<td>0,3</td>
</tr>
<tr>
<td>Pu</td>
<td>1,1</td>
<td>0,2</td>
</tr>
<tr>
<td>Am</td>
<td>2,8</td>
<td>0,6</td>
</tr>
<tr>
<td>Cm</td>
<td>5,4</td>
<td>1,2</td>
</tr>
</tbody>
</table>

constants in the 238-group approximation. In Fig. 2 shows a two-dimensional model of a fuel assembly zone with samples of MNUP fuel constructed by the visualizer SCALE6. To ensure the reliable construction of the spatial computational grid, the possibility of repeating the spatial hexagonal elements realized in SCALE6 was used.

A comparison was made of the nuclide compositions of the irradiated sample with SNPP fuel by SCALE6 code with the results for the other codes. An estimate of the possible error associated with various libraries of neutron cross sections is made. The data from the ENDF / B-V, VI and VII libraries were used for evaluation. The results of a comparison of the elemental composition of the irradiated sample are presented in Tab. 2.
In the framework of this paper, estimates are made of the uncertainties in the calculated data related to the uncertainties of the burnup depth and the irradiation regime of the experimental sample. The uncertainty associated with the magnitude of fuel burnup in the sample was estimated for an uncertainty of 3%. The uncertainty associated with the sample irradiation regime was estimated for an uncertainty of power by micro-campaigns of no more than 3% with a constant value of the fuel burn-up depth. The uncertainty values calculated for the SCALE6 code in the elemental composition of the irradiated sample are presented in Tab. 3.

4. Discussion

Based on the analysis of the experimental and calculated results of the benchmark at the present stage of its conduct, the following conclusions can be drawn. Good agreement was obtained for the calculation of various codes (including code SCALE6) for the key isotopes of uranium, plutonium and fission fragments. A significant difference in the experimental and calculated results is shown (up to 20% in some key isotopes). To explain these differences, it is planned to conduct additional experimental work with the irradiated sample and additional estimated estimates of the uncertainties in the results.

Based on the results of the calculations in the future, it is planned to prepare recommendations for adjusting and supplementing the programs of experimental and calculated studies on nitride fuel. In addition to the direct goal, it is also planned to use a benchmark for cross-verification of codes. To this end, a number of additional design characteristics have been introduced into the benchmark.

5. Conclusion

Based on the work done and analysis of the results obtained, the following conclusions can be drawn:

Effective three-dimensional and two-dimensional models of the BN-600 reactor have been developed for solving complex stationary problems and problems of nuclide kinetics.

It is shown that the SCALE6 code gives a good agreement with the benchmark calculations for Russian codes and can be used as an independent tool for their verification.
The estimated uncertainties of the results obtained may exceed the difference between the results of different codes and in some cases require clarification of the formulation of the calculated benchmark.

Acknowledgments

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References