

# **INVESTIGATION OF SOME MODELS AND APPROXIMATIONS APPLIED AT CALCULATION OF GT-MHR FUEL ASSEMBLIES**

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## **ABSTRACT**

Main neutron-physical models applied in RRC Kurchatov Institute as design models on the stage of fuel assembly calculations of GT-MHR are described, namely, model for calculation of fuel burnup, model for calculation of depletion of burnable poison isotopes, model for calculation of fuel assemblies for fixed values of burnup. All models were realized by using WIMS-D code modernized slightly in OKFTI RRC KI. Model task for study of some calculational approximations is proposed. The following problems were studied: selection of 51-group neutron spectrum used for preparing few-group fuel assembly cross sections; influence of the graphite of the reflector, the number of energy groups and spatial discretization on the calculation of some neutron-physical characteristics; fuel burnup. Result of this study is step-by-step model for preparing the group homogeneous cross sections of fuel assembly.

*Key Words:* GT-MHR, fuel assembly, neutron-physical models, WIMS-D

## **1. INTRODUCTION**

For several years, neutron-physical calculations of different variants of Gas Turbine Modular Helium Reactor (GT-MHR) have been carried out in OKFTI RRC KI. WIMS-D [1] and JAR [2] codes are used as design codes. The first code is used for preparing the group homogeneous cross sections of the Fuel Assemblies (FA-s) and their parts. The second code is used for solving the 3-dimension group diffusion equation. This report is devoted to the models applied for the first part of the calculation. Step-by-step method for preparing the group homogeneous cross sections of the FA-s with using WIMS-D code was elaborated. This method is described in detail in this report. Model task for study of the calculational approximations is proposed. Some calculational approximations is studied and described in this report.

Topic: Physics and Methods of Gas-Cooled Reactor.

## **2. STEP BY STEP METHOD FOR PREPARING THE GROUP HOMOGENEOUS CROSS SECTIONS OF THE FA**

Code WIMS-D is a design code applied in OKFTI RRC KI for preparing the group homogeneous cross sections of the FA-s. The following two restrictions do not allow using the WIMS-D for calculation FA-s directly. First, geometry of FA-s is very complex and second, there are essential limitations connected with simultaneous taking into account resonance shielding of

fuel and burnable poison isotopes when they are placed in different zones. Therefore, the step-by-step method for preparing the group homogeneous cross sections of the FA was elaborated.

### 2.1. Model for Calculation of the Fuel Burnup

On this calculational stage, three-dimensional, hexagonal in the plane the cell of the fuel compact with pitch equaled 1.9 cm is separated in a FA. Infinite on height, cluster cell of the fuel compact with equivalent on square cylindrical external boundary and with  $N$  cylindrical fuel rods covered by four layers of coat is chosen as a model for previous cell. Diameter of the fuel rods is chosen from the condition of the conservation of the average chord in fuel. Then, this diameter of the fuel rods is increased a little to get the nearest entire number of fuel rods under the condition of the conservation of the fuel volume. Many-layer clad is ‘smeared’ layer by layer on the fuel rods under the condition of the conservation their volumes in fuel compact. Obtained cluster cell has one central rod and three rows of rods. External radius of fuel compact is  $R_1$  (0.625 cm). External zone of the cluster cell of fuel compact consists of the graphite of block ( $\gamma=1.73\text{g/cm}^3$ ) and its external radius is  $R_2$  (0.997571 cm). Extended cluster cell of the fuel compact has two additional zones (see Figure 1). The first additional zone ( $R_3$ ) consists of the helium, burnable poison, and additional graphite of the FA pertaining to one fuel compact. The second additional zone ( $R_4$ ) consists of the graphite of the external and internal reflector pertaining to one fuel compact.

Transport calculation of such a cluster cell is carried out by WIMS-D code in 43 energy groups with maximum division of the energy scale in vicinity of resonance of  $^{240}\text{Pu}$  ( $\sim 1\text{eV}$ ). This constructed cell is used for the calculation of the fuel burnup but not the depletion of the burnable poison isotopes, though the isotopes of the burnable poison are burning up too.

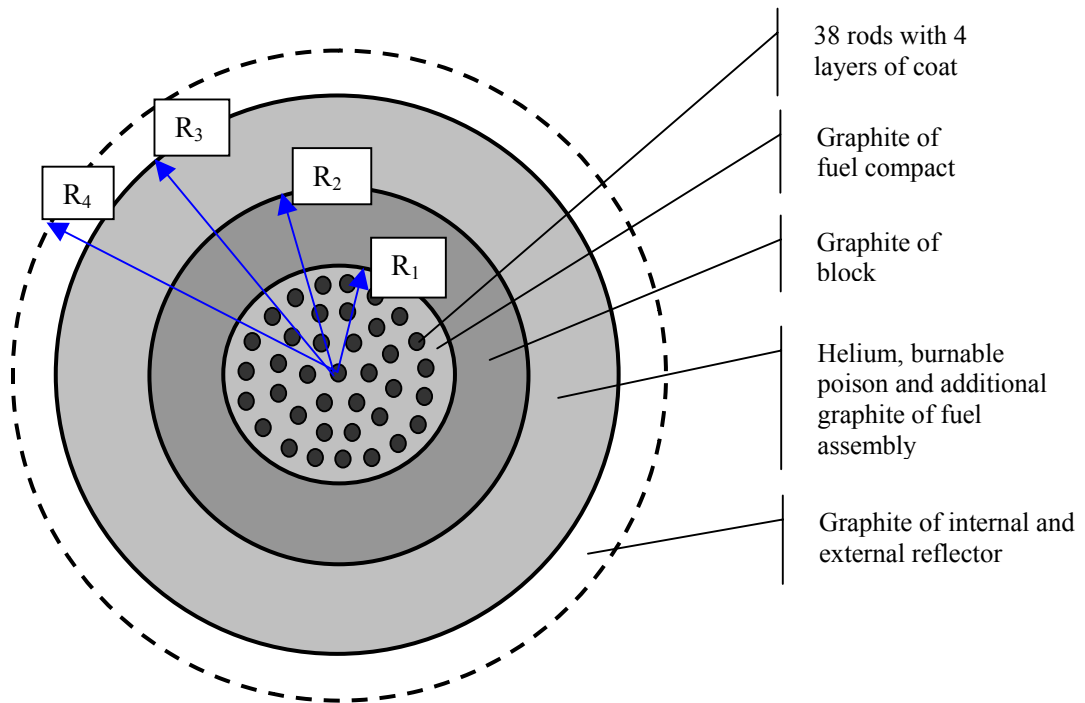
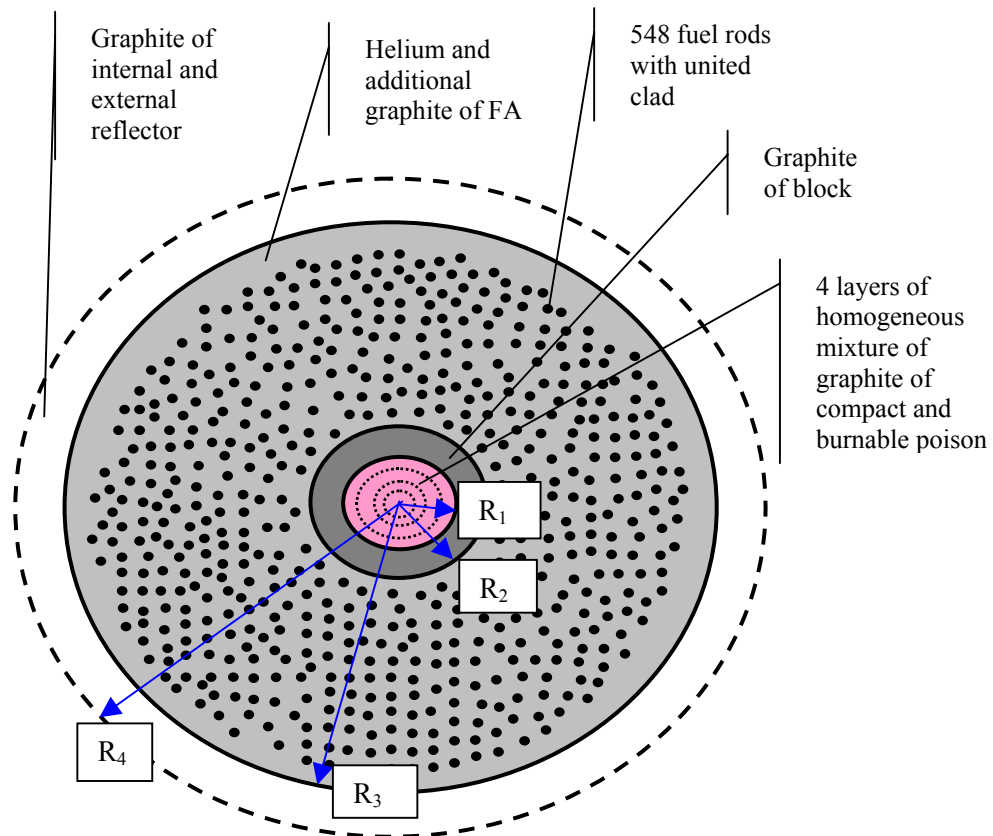


Figure 1. Extended cluster cell of fuel compact

## 2.2. Model for Calculation of the Depletion of the Burnable Poison Isotopes.

On this calculational stage, the model of the supercell (Figure 2) for the calculation of the depletion of the burnable poison isotopes is constructed. The cell of the compact with burnable poison is placed in the center of the supercell. Compact with the burnable poison ( $R_1=0.625$  cm) is placed in the center of the last cell.



**Figure 2. Supercell for calculation of the depletion of the burnable poison isotopes**

The burnable poison and the graphite of the compact matrix ( $\gamma=1,7$  g/cm<sup>3</sup>) are homogeneously mixed in this compact. Under calculations, this zone is divided in a few sub-zones (ordinary 4 sub-zones). External zone ( $R_2$ ) of the cell of the compact with burnable poison consists of the graphite of block ( $\gamma=1.73$ g/cm<sup>3</sup>).

Then the numbers of the cells of fuel compact, the cells with helium channel and the quantity of the additional graphite of the FA pertaining to one cell of the compact with burnable poison are calculated. All these materials are located in the next zone of the supercell with external radius  $R_3$ . All the fuel rods with the united clad placed in the cells of fuel compacts are located in the background material of this zone consisting of the homogeneous mixture of helium and graphite.

The last zone of the supercell with external radius  $R_4$  consists of the graphite of the external and internal reflector pertaining to one compact with burnable poison.

Transport calculation of such a supercell is carried out by WIMS-D code in 51 energy groups with maximum division of the energy scale in vicinity of the resonance of  $^{167}\text{Er}$  ( $\sim 0.5$  eV).

This constructed supercell is used for calculation of the depletion of the burnable poison isotopes but not fuel burnup, though the isotopes of the fuel are burning up too.

### **2.3. Model for Calculation of the Group Homogeneous Cross Sections of the FA for Fixed Values of Burnup.**

On this calculational stage, model of the FA for calculation of it for fixed values of burnup is constructed. Firstly, the cluster cell of fuel compact is replaced by the cylindrical cell of fuel compact with central fuel rod with united clad and with one fuel ring with united clad in internal and external rings joined to fuel ring. Place and thickness of the fuel ring are chosen separately for each value of burnup from the condition of equality of  $k_\infty$  in these two cells. Isotope composition of the fuel in the cylindrical cell is taken identical in central fuel rod and in fuel ring and equaled to isotope composition averaged on all the fuel rods in the cluster cell of fuel compact.

Then, in calculational model of FA, chosen cylindrical fuel compacts replace cluster fuel compacts. FA is taken with cylindrical external boundary. For each value of burnup, resonance cross sections of all resonance isotopes are taken from outside. Resonance cross sections of the isotopes placed in fuel are taken from the calculation of the extended cluster cell of fuel compact averaged on all the fuel rods. Isotope composition of the burnable poison and resonance cross sections of the burnable poison isotopes are taken from the calculation of the supercell averaged on all zones with burnable poison.

Transport calculation of such a model of FA is carried out by WIMS-D code (option PIJ-PERSEUS) in 51 energy groups and used for preparing the few-group homogeneous cross sections of the FA. It should be noted that for correct forming the neutron spectrum in FA the graphite placed in reflector should be taking into account.

## **3. CALCULATIONAL INVESTIGATION OF 2D MODEL TASK**

### **3.1. 2D Model Task**

2D section of GT-MHR (Figure 3), consisting of two types of assemblies, was chosen as an object for research. The first type of FA is standard FA without the hole for control rod (Figure 4) and with burnable poison compacts. The second type of FA is the graphite assembly without the hole for control rod. Clearance between FA-s is 0.25 cm, and the temperature of all materials is 1200°K. All investigations were carried out with weapon grade plutonium fuel.

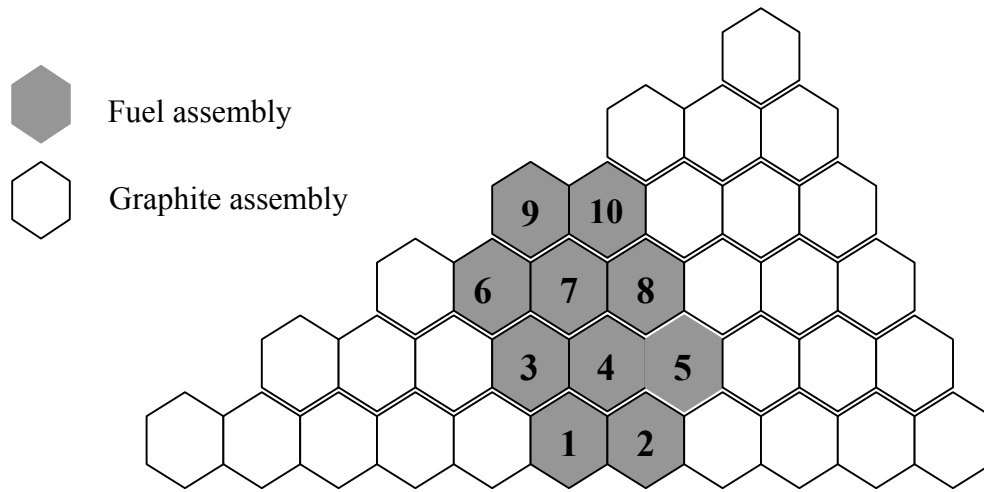


Figure 3. 2D section of GT-MHR (30°)

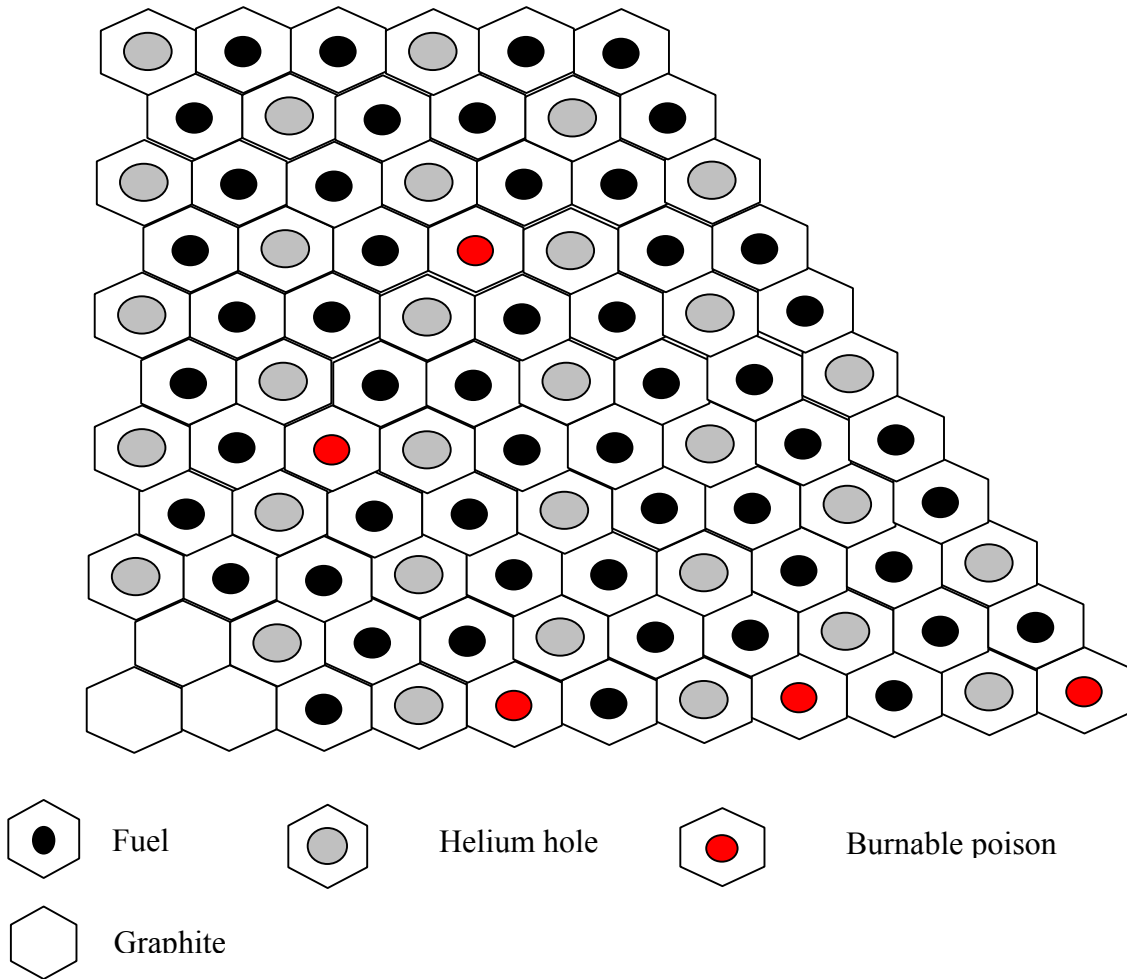


Figure 4. Fuel assembly of GT-MHR (90°)

### 3.2. 51-Group Neutron Spectra for Calculation of the Homogeneous FA Cross Sections

Spectra, by which 51-group cross sections are condensed to group ones with lower number of groups, have to take into account both the influence of the graphite located outside the core and the value of  $k_{ef}$  of calculated object. When operating reactor is such an object it is supposed that  $k_{ef}=1$ . In our case, it is not truth.

Denote  $R_c$  as an external radius of additional graphite layer round the fuel assembly. For given value  $R_c$  after 'Pin-cell' option of WIMS code we have 51-group cross sections for all materials of considered FA. The following three tasks are solved by WIMS code with these cross sections.

Task 1. 51-group calculation of heterogeneous FA with additional layer round the fuel assembly. 51-group spectrum (spectrum 1) in homogenized FA is obtained from this calculation.

Task 2. 51-group calculation of homogeneous infinite medium with 51-group homogeneous cross sections obtained in task 1 (task searching  $k_{\infty}$ , spectrum 2).

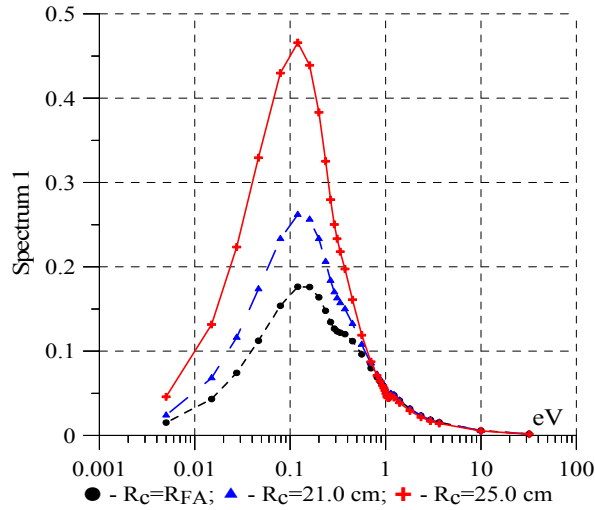
Task 3. 51-group calculation of homogeneous medium with 51-group homogeneous cross sections obtained in task 1 and with critical 'buckling' ( $k_{ef}=1$ , spectrum 3).

All three tasks give the different 51-group neutron spectra in homogenized FA. Figures 5-7 show these spectra normalized on unity (integral of neutron spectrum on all energies equals 1) with different thickness value of additional graphite layer. The following conclusions can be obtained from the analysis of these figures.

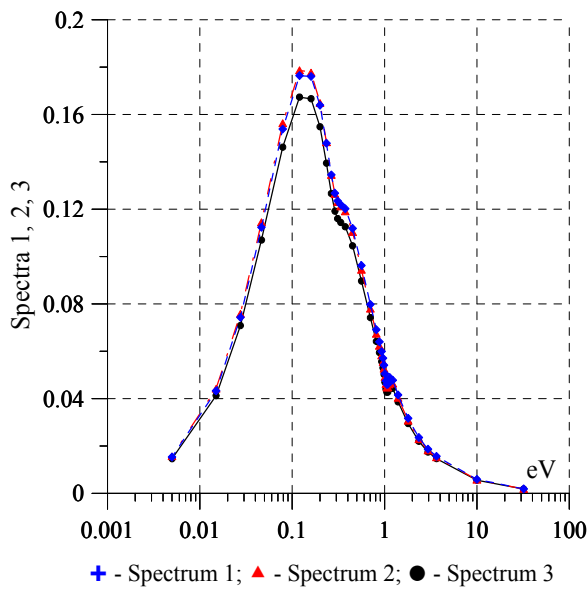
- Neutron spectra in task 3 do not practically depend on availability of additional graphite layer round the fuel assembly.
- Neutron spectra in tasks 2 and 3 are very close.
- Spectrum 1 significantly differs from spectra 2 and 3 and this difference is more essential for more thickness value of additional graphite layer round the FA.

### 3.3. Taking into Account the Graphite of Reflector

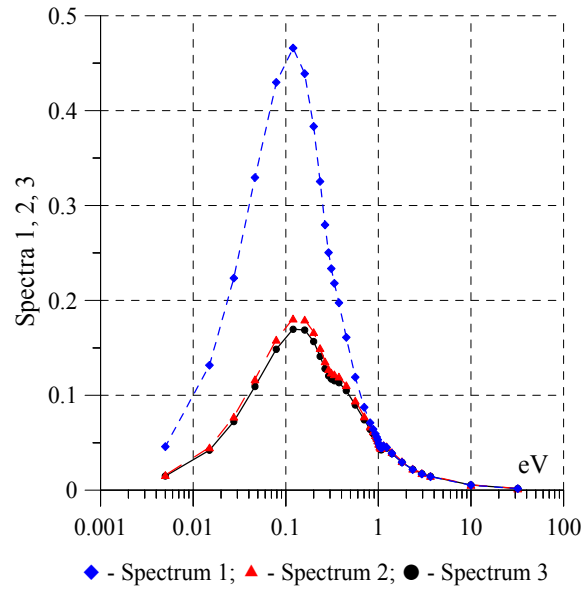
In general case, value of external radius  $R_c$  of the additional graphite layer round the fuel assembly will be different for each FA of a core. Choice of the different values of  $R_c$  for each FA is enough complex procedure and is not necessary because of presence of others not less serious calculational approximations. Therefore, we will try to choose one value of  $R_c$  for all the fuel assemblies of a core, which give us the average neutron spectrum in a core. The following criterion for choosing value of  $R_c$  is proposed. The most close two calculations are chosen. The first calculation is 51-group calculation of the heterogeneous FA with additional graphite layer searching its  $k_{\infty}$  (task 1 in subdivision 3.2). The second calculation is 51-group calculation of 2D section of GT-MHR, consisting of two types of homogenized assemblies, searching its  $k_{\infty}$ . 51-group cross sections of homogenized FA are taken from calculation 1. 51-group cross sections of



**Figure 5. Neutron spectrum 1 in homogenized FA**



**Figure 6. Neutron spectra in FA with  $R_c = R_{FA}$ .**



**Figure 7. Neutron spectra in FA with  $R_c = 25.0$  cm.**

the graphite are identical in both calculations. The second calculation is carried out by Surface Harmonics Method (SHM) [3] with three trial functions and with 331 spatial meshes per each FA. Denote  $k_0^{(i)}$  as a ratio of fission reaction to absorption reaction in FA in task 'i'. Choosing value of  $R_c$  is done from the condition of equaling values of  $k_0$  in calculations 1 and 2. Figure 8 shows that only  $k_0^{(1)}$  in task 1 can be equal  $k_0$  in 2D section of GT-MHR under definite value of  $R_c$ , and namely, under  $R_c=22.10$  cm. Taking into account that calculation 2 with six trial

functions for such an object can increase value of  $k_0$  up to 0.3% we obtain that chosen value of  $R_c$  equals 22.24 cm.

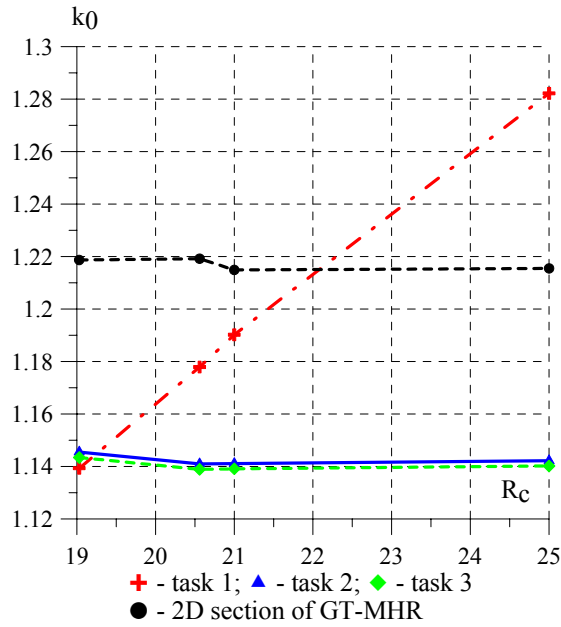


Figure 8.  $k_0$  in FA and in 2D section of GT-MHR

### 3.4. Spatial Discretization

For study of the spatial discretization the 51-group calculations of the 2D section of GT-MHR were used. Three types of calculations were carried out. The first type is calculation with one mesh per each FA. Both the second and third calculational types were carried out by SHM, in so doing, the SHM worked as a nodal method and the calculations were carried out by two stages. First, many-group trial matrices were calculated for all types of FA-s. Each FA was divided in 7 hexagons in the second calculation type and in 331 hexagons in the third one, in so doing the volumes of FA-s were conserved and the integration was carried out on real boundary of FA. All calculational types used 51-group spectrum from task 1. Table 1 presents the values of  $k_{ef}$  and Table II presents the values of energy release in FA-s for all calculated cases.

Table I. Values of  $k_{ef}$  in 51-group calculations of 2D section of GT-MHR.

| Number of meshes per FA | $R_c$          |                |
|-------------------------|----------------|----------------|
|                         | 21.0 cm        | 25.0 cm        |
| 1                       | 1.0976 (-2.5)* | 1.0984 (-2.5)* |
| 7                       | 1.1248 (-0.1)  | 1.1255 (-0.1)  |
| 331                     | 1.1260         | 1.1266         |

\* Percent deviation from corresponding value in calculation type 3 (331 meshes).



**Table II. Energy release in FA-s in 51-group calculations of 2D section of GT-MHR**

| Number of FA \ $R_c$ | 1 mesh per FA |       | 7 meshes per FA |       | 331 meshes per FA |        |
|----------------------|---------------|-------|-----------------|-------|-------------------|--------|
|                      | 21.00         | 25.00 | 21.00           | 25.00 | 21.00             | 25.00  |
| 1                    | 2.58*         | 2.57* | 0.12*           | 0.12* | 1.0436            | 1.0438 |
| 2                    | 4.10          | 4.08  | 0.32            | 0.32  | 0.8946            | 0.8949 |
| 3                    | -5.17         | -5.15 | -0.41           | -0.41 | 1.2307            | 1.2302 |
| 4                    | 11.80         | 11.70 | 0.75            | 0.75  | 0.8333            | 0.8340 |
| 5                    | -8.81         | -8.79 | -0.50           | -0.50 | 1.0097            | 1.0092 |
| 6                    | -6.17         | -6.15 | -0.47           | -0.46 | 1.2377            | 1.2372 |
| 7                    | 11.90         | 11.80 | 0.74            | 0.74  | 0.8550            | 0.8556 |
| 8                    | -2.94         | -2.93 | -0.11           | -0.11 | 0.9543            | 0.9541 |
| 9                    | 11.80         | 11.80 | 0.74            | 0.74  | 0.8610            | 0.8616 |
| 10                   | -2.60         | -2.60 | -0.10           | -0.10 | 0.9797            | 0.9796 |
| Max. dev.            | 11.90         | 11.80 | 0.75            | 0.75  | ---               | ---    |

\* Percent deviation from corresponding values in calculation with 331 meshes per FA.

One can see that the calculation by SHM with seven meshes per FA has enough accuracy: deviation in  $k_{ef}$  does not exceed 0.1% and deviation in energy release in FA-s does not exceed 0.8%.

### 3.5. Number of Energy Groups

Calculations of the 2D section of GT-MHR with maximum spatial discretization (331 meshes per FA) were carried out in 2, 13, and 51 groups. Table III presents percent deviation of  $k_{ef}$  and Table IV presents percent deviation of energy release in FA-s in 2- and 13-groups calculations from corresponding values calculated in 51 groups.

One can see that the calculation in 2 groups has not enough accuracy: deviation in  $k_{ef}$  reaches up to 7.0% and deviation in energy release in FA-s reaches up to 17.5%. Whereas, calculation in 13 groups has enough accuracy for design calculations: deviation in  $k_{ef}$  reaches up to 0.4% and deviation in energy release in FA-s reaches up to 0.7%.

**Table III. Percent deviation of  $k_{ef}$  in 2- and 13-group calculations from corresponding values calculated in 51 groups**

| Number of groups | $R_c$   |         |
|------------------|---------|---------|
|                  | 21.0 cm | 25.0 cm |
| 2                | 0.07    | 7.09    |
| 13               | -0.12   | 0.39    |

**Table IV. Percent deviation of the energy release in FA-s in 2- and 13-group calculations from corresponding values calculated in 51 groups**

| Number of FA | 2 groups    |        | 13 groups |       |
|--------------|-------------|--------|-----------|-------|
|              | $R_c$ 21.00 | 25.00  | 21.00     | 25.00 |
| 1            | 3.02        | 2.80   | 0.03      | -0.03 |
| 2            | 4.29        | 4.08   | -0.01     | -0.06 |
| 3            | -6.91       | -6.66  | -0.22     | -0.18 |
| 4            | 16.50       | 15.70  | 0.62      | 0.44  |
| 5            | -13.60      | -13.00 | -0.61     | -0.44 |
| 6            | -6.62       | -6.28  | -0.01     | 0.02  |
| 7            | 17.30       | 16.50  | 0.67      | 0.49  |
| 8            | -4.99       | -4.73  | -0.27     | -0.18 |
| 9            | 17.50       | 16.70  | 0.70      | 0.51  |
| 10           | -4.42       | -4.21  | -0.25     | -0.15 |
| Max. dev.    | 17.50       | 16.70  | 0.70      | 0.49  |

### 3.6. 13-group Calculation with 7 Meshes per FA

Up to these investigations, we used the 13-group calculations with six triangular meshes per FA executed by JAR code as design calculations. 13-group calculations with seven meshes per FA executed by SHM (WIMS and SUHAM-2D [4] codes) and described in former section is very close to design calculations. Table V presents percent deviation of  $k_{ef}$  and energy release ( $\delta E$ ) in FA-s in 13-group calculation with 7 meshes per FA from corresponding values calculated in 51 groups with 331 meshes per FA.

One can see that accuracy of the 13-group calculations with seven meshes per FA of such an object is quite enough: up to 0.3% in  $k_{ef}$  and up to 1.5% in energy release in FA

## 4. CALCULATION OF FUEL BURNUP

Model for calculation of fuel burnup was described in section 2.1. In this section, influence of the graphite of reflector and burnable poison on depletion of fuel isotopes is studied. Three types of calculational models were used. Configuration presented in Figure 1 was used as the basis for these models. In the first model the cell was limited by external boundary  $R_3$ , in so doing, burnable poison was not taking into account in the third zone. The second model differs from the first model by adding the fourth zone (external radius  $R_4$ ) taking into account the graphite of reflector. The third model differs from the second model by taking into account burnable poison in the third zone.

As a demonstration, Figures 9, 10 present curves of changing the nuclear densities of  $^{240}\text{Pu}$  and  $^{241}\text{Pu}$  in these three model calculations. One can see that both the graphite of reflector and the

burnable poison essentially influence on the depletion of the fuel isotopes. This statement is the real one for another fuel isotopes and actinides appearing in fuel up to  $^{245}\text{Cm}$ , too.

**Table V. Percent deviation of  $k_{\text{ef}}$  and energy release in FA-s in 13-group calculation with 7 meshes per FA from corresponding values calculated in 51 groups with 331 meshes per FA**

|                            | $R_c$ | 21.00          | 25.00 |
|----------------------------|-------|----------------|-------|
| $\delta k_{\text{ef}}, \%$ |       | 0.03           | -0.03 |
| <b>Number of FA</b>        |       | $\delta E, \%$ |       |
| 1                          |       | 0.18           | 0.11  |
| 2                          |       | 0.34           | 0.28  |
| 3                          |       | -0.67          | -0.61 |
| 4                          |       | 1.47           | 1.26  |
| 5                          |       | -1.19          | -1.01 |
| 6                          |       | -0.53          | -0.47 |
| 7                          |       | 1.51           | 1.30  |
| 8                          |       | -0.40          | -0.31 |
| 9                          |       | 1.54           | 1.32  |
| 10                         |       | -0.37          | -0.27 |
| Max. dev.                  |       | 1.54           | 1.32  |

## 5. CONCLUSIONS

Main neutron-physical models applied in RRC Kurchatov Institute on the stage of FA calculations of GT-MHR as design models were described, namely, model for calculation of fuel burnup, model for calculation of depletion of burnable poison isotopes, model for calculation of fuel assemblies for fixed values of burnup. All models were realized by using WIMS-D code modernized slightly in OKFTI RRC KI. Model task for study of some calculational approximations was proposed. The following problems were studied: selection of 51-group neutron spectrum used for preparing the few-group fuel assembly cross sections; influence of the graphite of the reflector, the number of the energy groups and the spatial discretization on the calculation of the different neutron-physical characteristics; fuel burnup. Result of this study is step-by-step model for preparing the group homogeneous cross sections of FA.

The main conclusions of the carried out studies are the following.

- When choosing the many-group (51) spectrum in FA used for preparing few-group FA cross sections it is necessary to take into account graphite of the internal and external reflector.
- For calculations of the object as in considered test task (lack of the absorber rods, initial isotope composition for all fuel compacts) 13-group calculations with six meshes per FA used as design calculations have quite enough accuracy: up to 0.3% in  $k_{\text{ef}}$  and up to 1.5% in energy release in FA-s. Cases with the more strong heterogeneity need in additional studies.

- Two-group calculations used as design calculations in the earliest time of study are not admissible: errors in energy release reach 20%. In cases with the more strong heterogeneity these errors can be much more.
- Both the graphite of reflector and the burnable poison essentially influence on the depletion of the fuel isotopes.

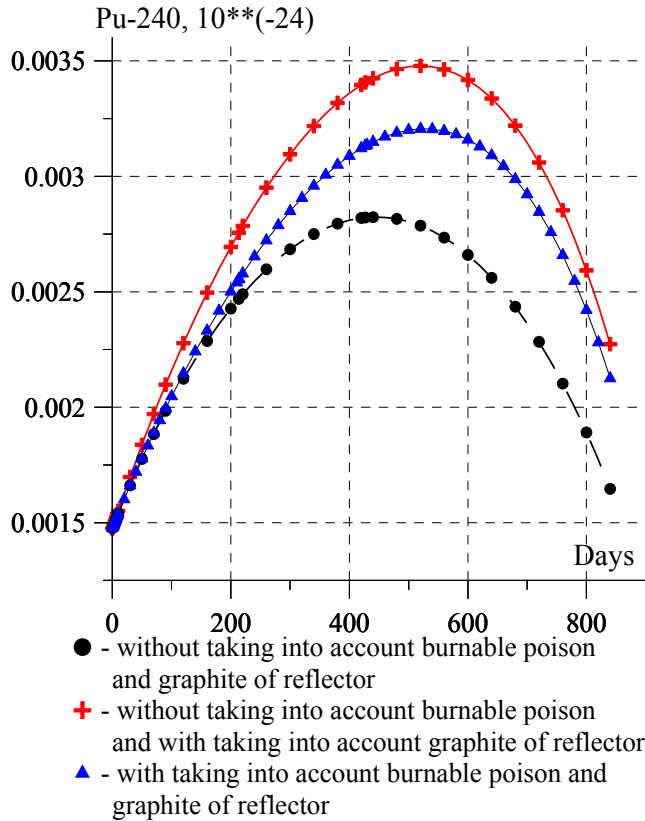


Figure 9. Nuclear densities of <sup>240</sup>Pu

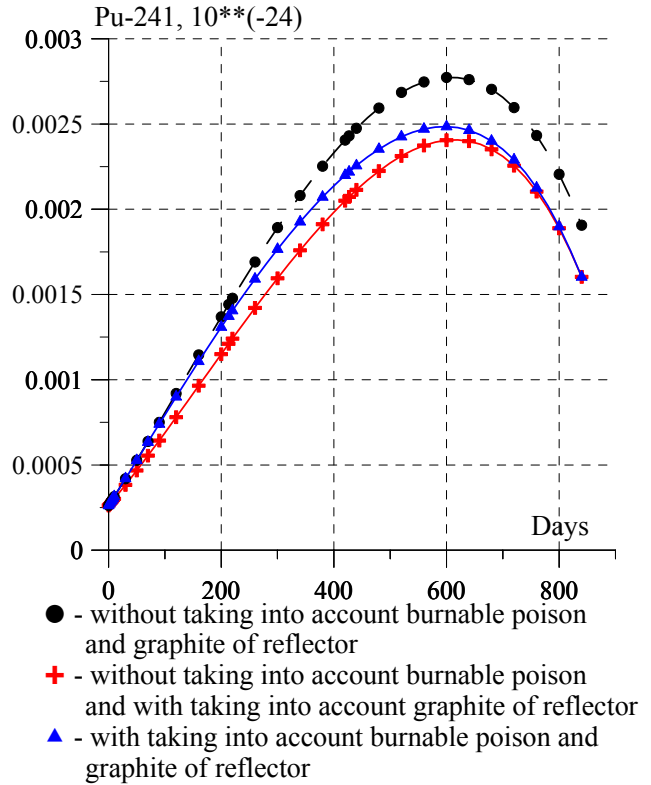


Figure 10. Nuclear densities of <sup>241</sup>Pu

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