Influence of accounting the distribution parameters of the fuel assembly (FA) and dynamic operating characteristics on the fuel nuclide composition of a VVER-1000 spent fuel assembly (SFA)

M M Albrek, M Y Ternovykh and V Y Shorov
National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe shosse, 115409 Moscow, Russia
E-mail: mustafaalbreak@yahoo.com, vlad_shorov@mail.ru, MYTernovykh@mephi.ru

Abstract. On the basis of the obtained results, the uncertainty of the isotopic composition was studied, which is associated with the uncertainty of operational characteristics and dynamic changes in the average burnup depth in the core of the WWER-1000 reactor.

1. Introduction
The isotopic composition knowledge of nuclear fuel in spent fuel assemblies (SFA) is necessary for accurate assessment of its neutron-physical properties. On the basis of this knowledge, the multiplication factor of the SFA is calculated and the radiation and nuclear safety procedures for handling them are justified.

At present, there is no global precise way for characteristics determination of the SFA. Such characteristics as the energy release and the isotopic composition are determined by using tables of approximated values that are obtained with precision programs. At the moment there are a huge number of programs for neutron-physical calculation, which are actively used to simulate the nuclide composition of SF [1].

Thus, in the modeling process of a particular nuclear installation, arises a question about the choosing and the correct consideration of the optimal parameters of the used calculation code and of the accounting need for these parameters when irradiating fuel assemblies so that the nuclide composition uncertainties in the SFA do not exceed the technological ones that cannot be completely excluded [2].

In order to obtain more accurate results in modeling the irradiation process of FA, the consideration of physical parameters is of importance and an uncertainty component will appear. Another component of uncertainty is associated with the irradiation of a specific fuel assembly in a specific reactor. The rearrangement of fuel assemblies in the reactor core during fuel shuffling causes different situations in which the assembly data operates in different modes. The change in the power and ambient parameters affects the neutron spectrum in the fuel assembly. The main sources of this type of uncertainty are:

1) Fuel mass
2) Average burnup depth
3) Density and temperature of the moderator
2. Calculation results

Let us consider each source of uncertainty and its contribution to the total one separately based on the results of modeling the VVER-1000 irradiated (burnup depth of 70 MWd/kg) fuel assembly using the SCALE software package [3, 4, 5, and 6].

Tables 1 and 2 show the uncertainty results of the nuclide composition calculations of the irradiated FA (TBCA-12) to, where the uncertainty in fuel density is from 10.4 to 10.7 (g/cm³). (Δm/m =% is the deviation of the fuel mass to fuel density).

Table 1. Masses (g/t) and uncertainty in the nuclide composition (NCU) of the SF due to the uncertainty in the fuel mass

| Nuclide | Mass at NCU in the fuel mass | Mass at NCU in the fuel mass | Mass at NCU in the fuel mass | NCU % nuclide composition due to NCU in the fuel mass |
|---------|----------------------------|----------------------------|----------------------------|-----------------------------------------------------|
|         | Δm = 0                     | Δm = 1.4                   | Δm = -1.4                  |                                                     |
| U       | 9.0849E+05                 | 9.0871E+05                 | 9.0836E+05                 | 0                                                   |
| Pu      | 1.7333E+04                 | 1.7160E+04                 | 1.7507E+04                 | 1.0                                                 |
| Np      | 1.0570E+03                 | 1.0530E+03                 | 1.0610E+03                 | 0.4                                                 |
| Am      | 5.7479E+02                 | 5.7420E+02                 | 5.7533E+02                 | 0.1                                                 |
| Cm      | 3.6025E+02                 | 3.5914E+02                 | 3.6135E+02                 | 0.3                                                 |
| Nd      | 7.8278E+03                 | 7.8299E+03                 | 7.8258E+03                 | 0.0                                                 |
| Eu      | 3.2975E+02                 | 3.2944E+02                 | 3.3005E+02                 | 0.1                                                 |
| Cs      | 5.8884E+03                 | 5.8827E+03                 | 5.8951E+03                 | 0.1                                                 |
| Ce      | 5.4351E+03                 | 5.4372E+03                 | 5.4350E+03                 | 0                                                   |
| Sm      | 1.4364E+03                 | 1.4359E+03                 | 1.4368E+03                 | 0                                                   |
| Gd      | 4.0069E+02                 | 4.0066E+02                 | 4.0084E+02                 | 0                                                   |
**Table 2.** Plutonium vectors (w %) and isotopic composition uncertainty (ICU) of the SF due to the uncertainty in the fuel mass

| Isotope | Isotope w% at ICU in the fuel mass | Isotope w% at ICU in the fuel mass | Isotope w% at ICU in the fuel mass | ICU (Pu w%) due to ICU % in the fuel mass |
|---------|-----------------------------------|-----------------------------------|-----------------------------------|------------------------------------------|
|         | $\Delta m/m = 0$                  | $\Delta m/m = 1.4$                | $\Delta m/m = -1.4$               |                                           |
| Pu-236  | 0.0                               | 0.0                               | 0.0                               | 0.3                                      | -0.2                                    |
| Pu-238  | 4.0                               | 4.0                               | 4.0                               | -0.1                                     | 1.0                                     |
| Pu-239  | 50.1                              | 49.9                              | 50.3                              | 0.4                                      | -0.4                                    |
| Pu-240  | 22.8                              | 22.9                              | 22.7                              | -0.4                                     | 0.4                                     |
| Pu-241  | 15.5                              | 15.5                              | 15.5                              | 0.0                                      | 0.0                                     |
| Pu-242  | 7.7                               | 7.8                               | 7.5                               | -1.6                                     | 1.6                                     |

**Table 3.** Masses (g / t) and the nuclide composition uncertainty of spent fuel due to the burnup depth $\Delta B$

| $\Delta B\%$ | -3 | -1 | +1 | +3 |
|--------------|----|----|----|----|
| Mass Nuclide | Mass g/t | NCU % | Mass g/t | NCU % | Mass g/t | NCU % | Mass g/t | NCU % |
| U           | 9.1090E+05 | -0.3 | 9.0932E+05 | -0.1 | 9.0766E+05 | 0.1 | 9.0610E+05 | 0.3 |
| Pu         | 1.7093E+04 | 1.4 | 1.7256E+04 | 0.4 | 1.7411E+04 | -0.4 | 1.7564E+04 | -1.3 |
| Np         | 1.0330E+03 | 2.3 | 1.0490E+03 | 0.8 | 1.0650E+03 | -0.8 | 1.0800E+03 | -2.2 |
| Am         | 5.4550E+02 | 5.1 | 5.6498E+02 | 1.7 | 5.8459E+02 | -1.7 | 6.0425E+02 | -5.1 |
| Cm         | 3.2837E+02 | 8.8 | 3.4944E+02 | 3.0 | 3.7126E+02 | -3.1 | 3.9386E+02 | -9.3 |
| Nd         | 7.6087E+03 | 2.8 | 7.7565E+03 | 0.9 | 7.9023E+03 | -1.0 | 8.0471E+03 | -2.8 |
| Eu         | 3.2119E+02 | 2.6 | 3.2694E+02 | 0.9 | 3.3254E+02 | -0.8 | 3.3803E+02 | -2.5 |
| Cs         | 5.7415E+03 | 2.5 | 5.8398E+03 | 0.8 | 5.9370E+03 | -0.8 | 6.0355E+03 | -2.5 |
| Ce         | 5.2831E+03 | 2.8 | 5.3847E+03 | 0.9 | 5.4874E+03 | -1.0 | 5.5881E+03 | -2.8 |
| Sm         | 1.3943E+03 | 2.9 | 1.4224E+03 | 1.0 | 1.4504E+03 | -1.0 | 1.4784E+03 | -2.9 |
| Gd         | 3.7382E+02 | 6.7 | 3.9161E+02 | 2.3 | 4.0991E+02 | -2.3 | 4.2855E+02 | -7.0 |
From the obtained results, it can be concluded that the deviation of the fuel mass from the nominal value makes a small contribution to the isotopic composition uncertainty calculation. It is also erroneous to assume that each fuel rod has a maximum mass deviation, since their production is controlled by a special quality system of product manufacturing. Therefore, we can assume that the contribution of this source of uncertainty to the overall calculation error is minimal.

Particular interest in modeling is accounting the average burnup depth. It is determined, as a rule, by tracking the reactor operation history, which depends on the power load of a particular electrical grid. During a long period of operation, the electricity generation is affected by many factors: fuel shuffling, maintenance problems, etc. Thus, the determination of the burnup depth is a noticeable error source, which can be seen from the data shown in tables 3 and 4, as well as in figure 1 (these results were obtained for uncertainty in the burnup depth of ± 1% and ± 3% of the average burnup depth (70 MWd/kg).

Table 4. Plutonium vectors (w %) and isotopic composition uncertainty of the SF due to the burnup depth

| Isotope | ∆B% | ICU % | w% | ICU % | w% | ICU % | w% | ICU % |
|---------|-----|-------|----|-------|----|-------|----|-------|
| Pu-236  | 0   | 4.3   | 0  | 1.5   | 0  | -1.4  | 0  | -4.3  |
| Pu-238  | 3.8 | 3.6   | 3.9| 1.2   | 4.0| -1.2  | 4.1| -3.6  |
| Pu-239  | 50.7| -1.1  | 50.3| -0.4 | 49.9| 0.4   | 49.6| 1.1   |
| Pu-240  | 22.7| 0.4   | 22.8| 0.1  | 22.8| -0.1  | 22.9| -0.3  |
| Pu-241  | 15.4| 0.3   | 15.5| 0.1  | 15.5| -0.1  | 15.5| -0.3  |
| Pu-242  | 7.4 | 3.5   | 7.6| 1.1   | 7.7| -1.1  | 7.9| -3.4  |

Figure 1. Uncertainties % of U, Pu, Pu-239, and Pu-241 due to various parameters uncertainties of: Burnup depth ∆B, Fuel mass uncertainty, Absence of gap (He), and Selected irradiation mode of fuel assembly during the simulation.
Of no less serious interest is the source of uncertainty that arises when considering the moderator density and temperature during the simulation (in this reactor it is presented in the form of water with boric acid). As an example, consider various 2D and 3D models with an average enrichment of 4.6% UO2 fuel and burnup depth of 70 MWd/kg (assuming a linear moderator temperature and density distributions) [7,8,9].

In the first 2D model, a simple unit cell was chosen that contains fuel, a clad, and a moderator. In the second and third 3D models the fuel rod was selected with the same dimensions of the unit cell used in the first model but with a height of 3.54 m. The difference between the second and the third models is the partitioning of the third model into 10 layers with different mean moderator’s density each. The main characteristics of the models are shown in figure 2.

The results of calculating the uncertainties in the isotopic composition of all three models are presented in tables 5 and 6.

While working with a nuclear reactor, in order to increase the burnup efficiency, the fuel is rearranged (shuffled) in the core each cycle. The different arrangement of fuel in the core as it burns up has its own power values and ambient parameters that differ from the mean values. Accordingly, the question arises for the need to take into account the irradiation regimes (modes) of FA, which affects the overall uncertainty of the isotope composition of SF.

Using the SCALE program code, two cases of fuel shuffling schemes were simulated to a burnup depth of 70 MWd/kg:

The first scheme moves FA from the center of the core (1.13 times the mean specific power) to the periphery of the core passing through intermediate position (0.87 times the mean specific power). The second shuffling scheme performs the process of reversing the previous scheme. In both schemes, the shuffling time (30 days) after each cycle is considered.

![Figure 2. Models in the problem of studying the water density along the height of the fuel rod.](image)

(A): 2-D model of a unit cell with a constant average density of water.
(B): 3-D model of a fuel rod with a constant average density.
(C): 3-D model with distributed water density over the height of a fuel rod.
Table 5. Masses (g/t) and nuclide composition uncertainty of the SF for the unit cell model and the 3D models

| Nuclide | Mass (g/t) 3D fuel rod with 10 layers | Mass (g/t) 3D fuel rod of one layer | Mass (g/t) of a unit cell | NCU % of 3D fuel rod | NCU % of a unit cell |
|---------|-------------------------------------|-------------------------------------|--------------------------|----------------------|----------------------|
| U       | 9.0793E+05                          | 9.0753E+05                          | 9.0849E+05               | 0.0                  | -0.1                 |
| Pu      | 1.8093E+04                          | 1.8271E+04                          | 1.7333E+04               | -1.0                 | 4.2                  |
| Np      | 1.0780E+03                          | 1.0910E+03                          | 1.0570E+03               | -1.2                 | 1.9                  |
| Am      | 5.9649E+02                          | 5.9923E+02                          | 5.7479E+02               | -0.5                 | 3.6                  |
| Cm      | 3.8032E+02                          | 3.7586E+02                          | 3.6025E+02               | 1.2                  | 5.3                  |
| Nd      | 7.7801E+03                          | 7.8023E+03                          | 7.8278E+03               | -0.3                 | -0.6                 |
| Eu      | 3.2919E+02                          | 3.3440E+02                          | 3.2975E+02               | -1.6                 | -0.2                 |
| Cs      | 5.8825E+03                          | 5.9130E+03                          | 5.8884E+03               | -0.5                 | -0.1                 |
| Ce      | 5.2902E+03                          | 5.4245E+03                          | 5.4351E+03               | -2.5                 | -2.7                 |
| Sm      | 1.4184E+03                          | 1.4380E+03                          | 1.4364E+03               | -1.4                 | -1.3                 |
| Gd      | 3.9846E+02                          | 3.9869E+02                          | 4.0069E+02               | -0.1                 | -0.6                 |

Table 6. Plutonium vectors (w %) and the isotopic composition uncertainty of spent fuel of the unit cell model and the 3D models.

| Nuclide | w% 3-D 3D fuel rod with 10 layers | w% 3-D fuel rod of one layer | w% of a unit cell | ICU (Pu w%) 3D fuel rod of one layer | ICU (Pu w%) of a unit cell |
|---------|----------------------------------|------------------------------|-------------------|-------------------------------------|---------------------------|
| Pu-236  | 0                                | 0                            | 0                 | 0.6                                 | -5.9                      |
| Pu-238  | 3.9                              | 3.9                          | 4.0               | -0.3                                | -0.8                      |
| Pu-239  | 51.3                             | 51.3                         | 50.1              | 0                                   | 2.3                       |
| Pu-240  | 21.6                             | 21.6                         | 22.8              | 0.3                                 | -5.4                      |
| Pu-241  | 15.8                             | 15.8                         | 15.5              | -0.6                                | 1.8                       |
| Pu-242  | 7.4                              | 7.4                          | 7.7               | 0.5                                 | -3.3                      |
| U-235   | 0.7                              | 0.6                          | 0.6               | 2.4                                 | 8.4                       |
| U-233   | 0.0                              | 0.0                          | 0.0               | -0.5                                | 2.1                       |
On the basis of the obtained results, it can be concluded that, in 2D modeling, the isotopic composition uncertainty has a higher value, in contrast to the other two models, where the Monte Carlo method was used [10]. It should also be noted that the behavior of the mean relative power ($W/W_{av}$, where $W_{av}$ is the average power) and burnup ($B_z$) with fuel rod height differs somewhat from the theoretical cosine dependence; it is shown in figure 3.

![Graph](image)

**Figure 3.** Mean relative power (dimensionless) and burnup of 70 MWd/Kg with fuel rod height.

The results of calculating the nuclide composition uncertainty depending on the irradiation regime for the two described schemes were compared to a model that does not take into account this source of uncertainty. The results of the calculation are presented in tables 7 and 8.

It should be noted that considering the irradiation regime leads to more realistic modeling of the FA and obtains more accurate data for the nuclide composition of SF.

Moreover, it is worth mentioning that another uncertainty source of such importance related to the nuclide composition of SF is the concentration of the absorber (boron) in the moderator. Since the absorption of neutrons in boron occurs mainly in the thermal energy range, this leads to an increase in the fast spectrum. As a result, the transmutation of U-238 and the accumulation of plutonium are enhanced by the use of thermal neutron absorbers, and therefore the fission of U-235 decreases. Both of these factors can significantly increase the reactivity of SF and have a serious impact on the isotopic composition of SF.
Table 7. Masses (g / t) and Nuclide composition uncertainty of spent fuel for the selected irradiation regime of fuel assemblies (one month of reactor shutdown per each shuffle)

| Nuclide | Mass considering the first scheme | Mass considering the second scheme | Mass Without considering shuffle | NCU % compared to the first scheme | NCU % compared to the second scheme |
|---------|----------------------------------|----------------------------------|-------------------------------|--------------------------------|----------------------------------|
| U       | 9.0850E+05                       | 9.0849E+05                       | 9.0849E+05                    | 0.0                             | 0.0                              |
| Pu      | 1.7455E+04                       | 1.7468E+04                       | 1.7333E+04                    | 0.7                             | 0.8                              |
| Np      | 1.0730E+03                       | 1.0720E+03                       | 1.0570E+03                    | 1.5                             | 1.4                              |
| Am      | 5.9016E+02                       | 5.7696E+02                       | 5.7479E+02                    | 2.6                             | 0.4                              |
| Cm      | 3.5398E+02                       | 3.5569E+02                       | 3.6025E+02                    | -1.8                            | -1.3                             |
| Nd      | 7.8922E+03                       | 7.8443E+03                       | 7.8278E+03                    | 0.8                             | 0.2                              |
| Eu      | 3.2951E+02                       | 3.2942E+02                       | 3.2975E+02                    | -0.1                            | -0.1                             |
| Cs      | 5.8479E+03                       | 5.8740E+03                       | 5.8884E+03                    | -0.7                            | -0.2                             |
| Ce      | 5.3844E+03                       | 5.4366E+03                       | 5.4351E+03                    | -0.9                            | 0.0                              |
| Sm      | 1.4329E+03                       | 1.4259E+03                       | 1.4364E+03                    | -0.2                            | -0.7                             |
| Gd      | 4.0900E+02                       | 4.0787E+02                       | 4.0069E+02                    | 2.0                             | 1.8                              |

Table 8. Plutonium vectors (w %) and isotopic composition uncertainty of the SF for the selected irradiation regime of fuel assemblies (one month of reactor shutdown per each shuffle)

| Isotope | w% considering the first scheme | w% considering the second scheme | w% Without considering shuffle | ICU (Pu w%) compared to the first scheme | ICU (Pu w%) compared to the second scheme |
|---------|--------------------------------|--------------------------------|-------------------------------|--------------------------------|--------------------------------|
| Pu-236  | 0                              | 0                              | 0                             | -4.1                           | 0.2                           |
| Pu-238  | 4                              | 4                              | 4.0                           | 1.1                            | -0.8                          |
| Pu-239  | 50                             | 51                             | 50.1                          | 0.6                            | 0.9                           |
| Pu-240  | 23                             | 23                             | 22.8                          | -0.5                           | -0.8                          |
| Pu-241  | 15                             | 15                             | 15.5                          | -1.4                           | -0.6                          |
| Pu-242  | 8                              | 8                              | 7.7                           | -0.7                           | -0.7                          |
Let's consider two models of different behaviors in boron concentration change (figure 4) and compare them with the model where this uncertainty source (presence of boron in the water) is not taken into account (tables 9 and 10).

**Figure 4.** Concentration of boron in two different variants (constant and variable boron concentration during irradiation) operating modes in the modeling process

It should be noted from the obtained results that in modeling the dynamic change in boron concentration, more accurate results will be obtained for the nuclide composition of SF since, it approaches to more realistic situation when working with the reactor.

Consider the modelling of a full-scale fuel assembly using the VVER-1000 fuel assembly: U46G2 (TBCA-12).

The fuel in this fuel assembly is held in a hexagonal grid. Light water, used as a moderator and coolant, is passed under very high pressure through the active zone, in a high-pressure housing of about 14 m in height and 4 m in diameter. The reactor's core includes, in common with 211 assemblies: 163 fuel assemblies identical by design, but differing in fuel enrichment and 48 reflector assemblies. In the axial direction, the core is divided into 10 layers 35.5 cm high each, which sums up to a total active height of 355 cm. Both upper and lower axial reflectors have a thickness of 23.6 cm. The active zone (core) is divided radially into hexagonal cells in increments of 23.6 cm, each of which corresponds to a single fuel assembly, plus a radial reflector of the same size. Fuel assembly VVER-1000 is a hexagon contains 312 fuel cells. It contains 18 guide tubes and 1 central tube, carries the fuel load. Tubes are also useful for supporting the assembly that guarantees the right space between fuel cells. The head of the fuel assembly and the lower mesh hold the guide tubes. In the central tubes there are control rods and sensors for monitoring neutrons and temperature. To improve physical characteristics and safety, some fuel nuclides are filled with pellets containing gadolinium oxide (Gd2O3) content of 5.0 w%. The fuel assembly characteristics are shown in table 11.
## Table 9. Masses (g / t) and nuclide composition uncertainty of the SF due to the change in boric acid concentration \( \rho_B \)

| Nuclide | Mass (g/t) With varying boric acid concentration | Mass (g/t) With constant boric acid concentration | Mass (g/t) without considering boric acid concentration | NCU % of constant boric acid concentration | NCU % without considering boric acid concentration |
|---------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| U       | 9.0848E+05                                    | 9.0876E+05                                    | 9.0917E+05                                    | 0.0                                          | -0.1                                          |
| Pu      | 1.7378E+04                                    | 1.7078E+04                                    | 1.6689E+04                                    | 1.7                                          | 4.0                                           |
| Np      | 1.0600E+03                                    | 1.0480E+03                                    | 1.0340E+03                                    | 1.1                                          | 2.5                                           |
| Am      | 5.7529E+02                                    | 5.7177E+02                                    | 5.6716E+02                                    | 0.6                                          | 1.4                                           |
| Cm      | 3.6021E+02                                    | 3.5816E+02                                    | 3.5462E+02                                    | 0.6                                          | 1.6                                           |
| Nd      | 7.8257E+03                                    | 7.8331E+03                                    | 7.8406E+03                                    | -0.1                                         | -0.2                                          |
| Eu      | 3.2924E+02                                    | 3.2879E+02                                    | 3.2738E+02                                    | 0.1                                          | 0.6                                           |
| Cs      | 5.8958E+03                                    | 5.8786E+03                                    | 5.8619E+03                                    | 0.3                                          | 0.6                                           |
| Ce      | 5.4342E+03                                    | 5.4393E+03                                    | 5.4425E+03                                    | -0.1                                         | -0.2                                          |
| Sm      | 1.4372E+03                                    | 1.4353E+03                                    | 1.4336E+03                                    | 0.1                                          | 0.2                                           |
| Gd      | 4.0031E+02                                    | 4.0144E+02                                    | 4.0250E+02                                    | -0.3                                         | -0.5                                          |

The first model is a full-scale fuel assembly model with three enrichments (4.7%, 4.4% and 3.6% + Gd). The second model is a full-scale model with averaged enrichment (4.6%) without taking into account the presence of Gd. The third model is a unit cell with enrichment (4.6%) without taking into account the presence of Gd. The fourth model is a unit cell with enrichment (4.6%) with a homogeneous distribution of Gd in fuel rods within assemblies. The fifth model is a unit cell with enrichment (4.6%) and longer pitch (pitch = 1.336 cm) instead of (pitch = 1.275 cm) in the previous unit cell models, taking into account the presence of a larger amount of moderator in FA.

In order to show how the value of uncertainty behaves in one or other models of a single fuel assembly, five different variants were created.

The results of calculation of the nuclide composition of SFA and the quantity of plutonium isotopes are shown in tables 12 and 13.
Table 10. Plutonium vectors (w %) and isotopic composition uncertainty of spent fuel due to the change in boric acid concentration $\rho_B$

| Nuclide | w% With varying boric acid concentration | w% With constant boric acid concentration | w% without considering boric acid | ICU (Pu w%) of constant boric acid concentration | ICU (Pu w%) without considering boric acid |
|---------|------------------------------------------|------------------------------------------|----------------------------------|-----------------------------------------------|------------------------------------------|
| Pu-236  | 0                                        | 0                                        | 0                               | -1.4                                          | 1.7                                      |
| Pu-238  | 4.0                                      | 4.0                                      | 4.0                             | -1.3                                          | 0.2                                      |
| Pu-239  | 50.0                                     | 50.9                                     | 49.2                            | -1.7                                          | 1.7                                      |
| Pu-240  | 22.9                                     | 23.1                                     | 23.4                            | -1.0                                          | -2.3                                     |
| Pu-241  | 15.5                                     | 15.7                                     | 15.3                            | -1.6                                          | 0.7                                      |
| Pu-242  | 7.7                                      | 7.8                                      | 8.1                             | -1.5                                          | -5.3                                     |
| U-235   | 0.6                                      | 0.6                                      | 0.6                             | 1.5                                           | 7.2                                      |
| U-233   | 0                                        | 0                                        | 0                               | 1.2                                           | 7.0                                      |

Figure 5. 2D fuel assembly model created with the SCALE code for further calculation.
Table 11. Characteristics of the fuel assembly TVCA-12 (U46G2) [33]

| Characteristics                                      | Value                        |
|------------------------------------------------------|------------------------------|
| Average enrichment of FA fuel,%                      | 4.6                          |
| Description of fuel Nuclides (UO2 weight,%, pcs)     | U46G2                        |
| Fuel 1 (UO2)                                         | 4.7%. 240 pcs                |
| Fuel 2 (UO2)                                         | 4.4%. 60 pcs                 |
| Fuel 3 (95% UO2 + 5% Gd2O3)                          | 3.6%. 12 pcs                 |
| TVEL / TVEG (fuel+Gd)                                | 1.275                        |
| Pitch between fuel rods, cm                          | 0.91/0.793                   |
| Outer diameter / inner diameter of the fuel cladding, cm | 0.91/0.773                   |
| Cladding material                                    | Zirconium                    |
| Fuel pellets Fuel1,2/Fuel+Gd                         |                              |
| Mass of fuel (UO2) in fuel, g                        | 1750±25                      |
| Mass of fuel (UO2 + Gd2O3), g                        | 1620                         |
|Density of fuel in fuel/Fuel+Gd, g/cm³               | 10.55/10.5                   |
| Fuel 3 (95% UO2 + 5% Gd2O3), g                       | 1.1252/0.96                  |
| Central tube                                         |                              |
| Outer diameter / inner diameter, cm                  | 1.1252/0.96                  |
| Guide tube                                           |                              |
| Outer diameter / inner diameter, cm                  | 1.26/1.09                    |
| Moderator                                            | Borated Water (H2O+H3BO3)   |
Table 12. Masses (g / t) and nuclide composition uncertainty of the SF when using models compared to the full-scale fuel assembly model

| Nuclide | Mass of the model FA 4.7%, 4.4% & 3.6%+Gd | Mass of the model FA 4.6% UO2 | Mass of the unit cell model With 4.6% UO2 | Mass of the unit cell model +Gd UO2 | Mass of the new unit cell model h pitch = 1.336 cm | NCU % of using FA with 4.6% UO2 | NCU % of using a unit cell with 4.6% UO2 | NCU % of using a new unit cell model |
|---------|------------------------------------------|-------------------------------|------------------------------------------|---------------------------------|-------------------------------------------------|-------------------------|-----------------------------------|----------------------------------|
| U       | 9.1034E+05                              | 9.1035E+05                   | 9.0849E+05                               | 9.0846E+05                     | 9.0959E+05                                      | 0                      | 0.2                               | 0.2                              | 0.08                             |
| Pu      | 1.5699E+04                              | 1.5680E+04                   | 1.7333E+04                               | 1.7379E+04                     | 1.6192E+04                                      | 0.1                    | -10.4                             | -10.7                           | -3.14                            |
| Np      | 1.0160E+03                              | 1.0150E+03                   | 1.0570E+03                               | 1.0590E+03                     | 1.0260E+03                                      | 0.1                    | -4.0                              | -4.2                             | -0.98                            |
| Am      | 5.7872E+02                              | 5.7804E+02                   | 5.7479E+02                               | 5.7561E+02                     | 5.6644E+02                                      | 0.1                    | 0.7                               | 0.5                              | 2.12                             |
| Cm      | 3.5811E+02                              | 3.5807E+02                   | 3.6025E+02                               | 3.6070E+02                     | 3.5274E+02                                      | 0                      | -0.6                              | -0.7                             | 1.50                             |
| Nd      | 7.8223E+03                              | 7.8258E+03                   | 7.8278E+03                               | 7.8233E+03                     | 7.8470E+03                                      | 0                      | -0.1                              | 0.0                              | -0.32                            |
| Eu      | 3.2591E+02                              | 3.2548E+02                   | 3.2975E+02                               | 3.3021E+02                     | 3.2650E+02                                      | 0.1                    | -1.2                              | -1.3                             | -0.18                            |
| Cs      | 5.8123E+03                              | 5.8084E+03                   | 5.8884E+03                               | 5.8918E+03                     | 5.8478E+03                                      | 0.1                    | -1.3                              | -1.4                             | -0.61                            |
| Ce      | 5.4352E+03                              | 5.4370E+03                   | 5.4351E+03                               | 5.4332E+03                     | 5.8478E+03                                      | 0                      | 0                                 | 0.0                              | -7.59                            |
| Sm      | 1.4273E+03                              | 1.4274E+03                   | 1.4364E+03                               | 1.4362E+03                     | 1.4335E+03                                      | 0                      | -0.6                              | -0.6                             | -0.44                            |

Based on the obtained data, it can be concluded that ignoring the influence of high-absorbing materials like Gd in the modeling process does not impose high uncertainty results if the same geometric model is used. A more complex model used in the analysis of isotopic composition requires more geometry and composition details in the modeling process and an increase in time costs. Also, the best choice of the geometric model during the modeling process has a significant effect on the obtained isotopic composition results.
Table 13. Plutonium vectors (w %) and isotopic composition uncertainty of spent fuel using the unit cell model and the model of the average fuel enrichment

| Isotope | w% of the model FA 4.7% | w% of the model FA 4.6% & 3.6%+Gd | w% of the new unit cell model With pitch = 1.336 cm | w% of the unit cell model With pitch = 4.6% UO2 | ICU of (Pu w%) FA 4.6% UO2 | ICU of (Pu w%) of using a unit cell with 4.6% UO2 | ICU of (Pu w%) of using a new unit cell model+Gd | ICU of (Pu w%) of using a new unit cell model |
|---------|-----------------|-------------------------------|---------------------------------|---------------------------------|-----------------|---------------------------------|---------------------------------|---------------------------------|
| Pu-236  | 0               | 0                             | 0.0                            | 0.0                             | -8.7            | -8.7                            | -8.6                            |
| Pu-238  | 4.0             | 4.0                           | 4.0                            | 4.0                             | -0.1            | 1.4                             | 1.4                             | 0.4                             |
| Pu-239  | 47.9            | 50.1                          | 50.2                           | 48.5                            | -4.5            | -4.6                            | -1.3                            |
| Pu-240  | 23.3            | 22.8                          | 22.8                           | 23.6                            | -0.1            | 2.2                             | 2.4                             | -1.3                            |
| Pu-241  | 15.7            | 15.5                          | 15.5                           | 15.4                            | 0.1             | 1.1                             | 1.1                             | 1.6                             |
| Pu-242  | 9.1             | 7.7                           | 7.6                            | 8.4                             | -0.1            | 15.7                            | 15.9                            | 7.1                             |

3. Conclusion

Based on all the results above as well as the choice of methodological parameters (the first point), we can formulate a number of important conclusions:

- During the burnup calculations in the fuel assembly model, it is recommended to use these parameters (NxNy = 16x16, SN = 4, V7-238, N = 2, ΔB = 18). In this case, the errors in the masses of Pu-239 < 0.2%, in Cm < 0.7%, in Pu < 0.9% and in U < 0.1% (based on the modelling experience).
- Not considering the boron in the moderator during the simulation leads to an error in the masses of Pu-239 = 1.7%, in Cm = 1.6%, and in Pu < 4%. Not taking into account the dynamic changes in boron concentration during the irradiation time, leads to an error in the masses of Pu-239 = 1.7% and in Pu < 1.7%.
- Not taking into account the axial dependence of the density and temperature of the moderator during the simulation leads to errors in the masses of Pu = 1% and 4.2% of the 3D fuel rod and the unit cell, respectively.
- Ignoring the energy release distribution with the shuffling process and reloads of fuel assemblies during burnup modelling leads to errors in the masses of Pu = 0.7% and in Pu-239 = 0.6%.
- The use of the geometric unit cell model to model a full-scale fuel assembly leads to errors in the masses of Pu = 10.4% and in Pu-239 = 4.5%. Taking into account the excess concentration of the moderator in the unit cell model, minimize the error in the masses of Pu = 3.14% and in Pu-239 = 1.3%.
Ignoring the gap and centered-holes of the fuel rod in the unit cell model leads to an error in the masses of Pu-239 = 0.3%

References

[1] Baranov V G, Ternovyk M Y, Tikhomirov G V and Khlunov A V 2008 Simulation of nuclear-physical processes in the surface layer of a fuel kernel with a consumable absorber. Atomic Energy 105(6) 391-396

[2] Deev V I, Kutsenko K V and Lavrukhin A A et al. 2014 Heat-transfer modeling in supercritical pressure water using other media. Atomic Energy 115(4) 260-266

[3] SCALE: A modular code system for performing standardized computer analyses for licensing evaluation. 1993 NUGER/CR-0200 CCC-545

[4] Ternovykh M, Tikhomirov G, Khomyakov Y and Suslov I 2017 Determination of equilibrium fuel composition for fast reactor in closed fuel cycle. EPJ Web of Conferences 153

[5] Shorov V Y, Ryzhov S N, Ternovykh M Y and Tikhomirov G V 2017 Modeling of Analytical-Experimental Benchmark on Irradiation of Nitride Fuel in BN-600 Reactor in the SCALE6 code. KnE Engineering 490–499

[6] Dehart M D and Bowman S M 2011 Reactor physics methods and analysis capabilities in scale. Nuclear Technology 174 196–213

[7] Ternovykh M, Saldikov I, Tikhomirov G and Gerasimov A 2017 Prediction of the Material Composition of the VVER-type Reactor Burned Pellet with Use of Neutron-Physical Codes. 15th Int. School-Conference “New materials – Materials of innovative energy: development, characterization methods and application” KnE Materials Science 32–43

[8] ELLIS R J 2000 Analyses of weapons-grade MOX WER-1000 neutronics benchmarks: pin-cell calculations with SCALE/SAS2H. ORNL/TM-2000/4 april 2000

[9] Neutronics benchmarks for the utilization of mixed-oxide fuel: joint U.S./Russian progress report for fiscal year. ORNL 1997

[10] Saldikov I, Tikhomirov G, Ternovyk M and Gerasimov A 2017 Computation methods and techniques for solution of coupled multiphysics problems in precision calculations of VVER type reactors. Proceedings of the 7th International Conference on Coupled Problems in Science and Engineering. “Coupled Problems 2017” 1031-1041