Investigation of the effect of spatial discretization and burnup steps on the neutron characteristics of VVER-1000 fuel assembly using MCU code

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Abstract. A fundamental knowledge of the fuel assembly behaviour in different situations of burning is required for safe and economic nuclear power generation. Due to the importance of a fuel rod behaviour modelling in high burnup, in this paper, the spatial discretization used for the fuel assembly and burnup calculations influences significantly the results. The effective multiplication factor, total radial atomic distribution during the burnup of uranium dioxide (UO₂) fuel, fission products and actinides total atomic density and their variations besides the speed of calculations by increasing burnup and the burnup steps were studied for different spatially discretized models of fuel assemblies for VVER-1000 reactor in an operational cycle using the MCU Monte Carlo code. The effects of spatial discretization and the number of burnup steps appear slightly with the increasing of the discretization layers and the steps numbers.

1. Introduction
A successive change in the power density, fission products and distribution of fissile material within the UO₂ fuel pellets when it is subjected to irradiation and taken into operation. In fresh fuel, U-235 isotope is uniformly distributed in the fuel pellets as a fissile material, with a relatively small variation of both power and fission products generated along the fuel pellet radius. However, with increasing burnup through resonance capture by U-238 and subsequent of decays, there is a non-uniform buildup of fissile plutonium isotopes [1]. The fission products, fission rate and distributions of fissile material will develop marked peaks at the pellet surface as fuel burnup increases, because the neutron capture takes place mainly at the pellet surface. Different models of equivalent cell and fuel assembly in the beginning of fuel cycle were calculated. Besides the pellet radius, the neutron energy spectrum of the reactor fuel initial content of U-235 and the shapes of these distributions are dependent on irradiation time.

An interest in performing burnup dependent core analysis has increased in recent [2]. Because highly dependency of the mechanical and thermal analyses on the configuration of fuel pellet that varies with burnup, the prediction of fuel rod behavior in a LWR at high burnup is difficult [3]. In other hand, material concentrations in fuel pellet vary with burnup especially in the rim region by the generation of Pu-239, which must be taken into account in fuel rod thermal analyses when the burnup increasing.

Some potentials have been conducted to achieve an accurate understanding of radial burnup and isotopic distribution in fuel pellets during the burnup. A 3D burnup calculations of the Uranium Oxide (UOX) LWR spatially discretized cell using HELIOS 1.9 code showed a significant effect of the
different spatial discretization cases on the flux distribution, which leads to different isotopic densities, $K_{eff}$ value, and different calculating time for each case [4]. Using MCNPX code in order to investigate the influence of the number of burnup steps and radial burnup calculations in a geometrical radial nodes fuel pellets of a VVER-1000 reactor show that as the number of nodes increase the accuracy of the calculation approaches the benchmarks, besides the increasing of the calculation time [5].

Due to precisely accurate calculations of MCU code, this work performed and the cases (input files) designed to fit with the requirements of this code. In this study, a forward step to investigate the influence of the discretization and the number of burnup steps on the radial burnup calculations, the change in the isotopic composition and the calculation time of a different spatially discretized fuel assembly in the base of the design of LEU fuel type in the process of operation in the VVER-1000 reactor was calculated. The fuel burnup was calculated for an infinite fuel assembly grid using precision Monte Carlo code MCU with five year reactor operating cycle.

2. Models description

The VVER-1000 reactor produces 3000 MW at full power core operation and consists of 163 LEU hexagonal shaped fuel assemblies, each one contains 331 rods of four different types. Besides the main characteristics LUE fuel assembly of VVER-1000, the reactor core shown in the tables 1–3 [6]. Figure 1 shows the configuration of the study’s fuel assembly model. Fuel rods supposed at 1200 K and other elements of fuel assemblies at 578 K. In this model, the moderator includes light water with density of 0.7153 g/cm$^3$ at 578 K. In order to show the effect of spatial discretization clearly, we removed the soluble boron from the moderator while the number of poison fuel rods have been increased to 30 instead of 18 in the 35ZSH fuel assembly design, which is the original design we referred to. Parallel computing used for speeding up Monte Carlo neutron transport and nuclide transmutation calculations. The MCU package allows running multiple processes for the same task [7].

In this work, to estimate the effect of spatial discretization on the neutron characteristics, and the isotopes radial atomic density distributions, the whole fuel assembly (includes fuel rods and the rods contain the burnable absorber) discretized into 5, 10, 15, 20 and 25 identical layers, besides the original case with no discretization.

The irradiation time of the fuel assembly was 1650 effective days includes 5 reloading periods with 30 days for each. Indeed, what is important in this study is the value of burnup and its radial distribution within the fuel pellet.

A model of the TVS-2M finite fuel assembly with black and mirror boundary conditions used for the calculations, which executed by means of supercomputers in National Research Nuclear University MEPHi (Moscow Engineering Physics Institute), which have a distributed memory system with 128 cores and 120 GB hard drive.

The description of the fuel rod, poison rod, the guide channel, the used fuel assembly model and the study models shown in figures 1-5, and tables 1-3. Figure 1 and figure 2 obtained using the office tool included in the MCU code.
Figure 1. VVER-1000 LEU fuel assembly model (35ZSUH) used in the study.

Figure 2. Study models based on different discretization layers number, where:
1- Fuel rod (3.6% 235 U),
2- Fuel rod with gadolinium (2.4% 235 U, 8% Gd),
3- Central tube,
4- Guide channel.
Table 1. Characteristics of burnable absorber rod.

| Characteristics             | Details                     |
|-----------------------------|-----------------------------|
| Burnable absorber material  | Gadolinium oxide            |
| Appearance                  | White odourless powder      |
| Number of rods              | 30                          |
Absorbing material stack height, cm 353  
Molecular weight (g/mol.) 362.50  
Apparent density (g/cm3) 7.407  
Solubility in water Insoluble  
Melting point (C) ~2350  
Solubility Soluble in acid  
Specific gravity (g/cc at 15 C) 7.407  
Crystal structure Monoclinic, cubic  
Cladding material Alloy Zr + 1% Nb

Table 2. Characteristics of VVER-1000 fuel assembly used in the study.

| Characteristics                        | Details                  |
|----------------------------------------|--------------------------|
| FA form in a plan                      | Hexagonal                |
| Arrangement of fuel rods               | Triangle                 |
| Fuel                                   | Dioxide (UO₂)            |
| Fuel enrichment                        | 3.3%; 3.6%               |
| Burnable absorber                      | Gadolinium               |
| Burnable absorber enrichment           | 8%                       |
| Number of guide channels               | 18                       |
| Number of central channel              | 1                        |
| Number of U-235 3.3% fuel channel      | 66                       |
| Number of U-235 3.6% fuel channel      | 216                      |
| Number of U-Gd channel                 | 30                       |
| Moderato density, g/m³                 | 0.7153                   |

Table 3. Description of study Models.

| Case Name | Number of Burnup steps | Number of discretized layer |
|-----------|------------------------|-----------------------------|
|           |                        | 3.3% | 3.6% | U-Gd |
| 0105      | 5                      | 1    | 1    | 1    |
| 0505      | 5                      | 5    | 5    | 5    |
| 1005      | 5                      | 10   | 10   | 10   |
| 1505      | 5                      | 15   | 15   | 15   |
| 2005      | 5                      | 20   | 20   | 20   |
| 2501      | 1                      | 25   | 25   | 25   |
| 2505      | 5                      | 25   | 25   | 25   |
The numeration of the study cases follows a strategy that identifies the number discretized layers by the first two digits, and the number of burnup steps by the second two digits. For example, the case “1505” corresponds to the case where all rods within the mentioned fuel assembly were discretized into fifteen symmetrical layers in thickness with five burnup steps according to the terms “15” and the term “05”.

3. MCU Code
MCU is the universal computer code for simulation of three-dimensional systems transport particle (positrons, photons, neutrons, electrons) and projected on practical use, with an accuracy that is practically limited only by the accuracy of the neutron data used, by means of the Monte Carlo method. The MCU includes models for depletion and thermal analysis beside other different versions of the codes of the MCU5 family [8].

The codes of the MCU family allowed continuous, pointwise and stepwise description of the nuclear reaction cross sections. The data banks were developed using evaluated Russian libraries (RUSFOND, BNAB-78, 90, and 93, LIPAR and etc.), and different international files of evaluated neutron data and nuclear data libraries (ENDF/B, JENDL, JEF and etc.).

The executable codes of the MCU family have their own specific features and application fields specially for simulating three-dimensional system of almost any complexity. The code has the ability to use of a multiprocessor computer cluster.

4. Results
The results of Monte Carlo calculations using MCU code for each case of study are compared to each other in order to estimate the effect we tested for a whole fuel assembly described previously. Figure 6 presents the change of $K_{\text{eff}}$ values of the fuel assembly during the burnup for different cases in the base of the number of spatial discretized layers. As shown, the burnup starts with dramatically decrement due to a resulted high absorbing fission products. Then, it followed by a significant increment of the reactivity until the burnable absorber (Gd) consumed totally and then a slight gradual decrease over the full burnup. On the other hand, the effect of the number of spatial discretized layers appears significantly as shown in the figure 6 especially at the burnup 10 – 20 MWd/kgHM (the largest difference between the minimal and maximal $K_{\text{eff}}$ values was about 5.38E-2 at 15.7 MWd/kgHM). The $K_{\text{eff}}$ values approach to each in the rest of the burnup cycle. The effect of the burnup steps is illustrated in figure 7 which shows the change of $K_{\text{eff}}$ values of the fuel assembly during the burnup for different cases in the base of the number of burnup steps. The effect of burnup steps number appears significantly during burnup up to 20MWd/kgHM as shown in the figure 7. The $K_{\text{eff}}$ values approach to each in the rest of the burnup cycle with fluctuations about the reloading periods for both effects.
Figure 6. Calculated $K_{\text{eff}}$ values versus burnup for different study cases using MCU code for different spatial discretized layers

Figure 7. Calculated $K_{\text{eff}}$ values versus burnup for different study cases using MCU code for different burnup steps

In the operated reactors with the Uranium dioxide fuel, U-238 and U-235 precisely the significant fission isotopes in the fresh fuel. During the operation, the atomic density of U-235 decreases as the burnup increases. The plutonium isotopes appear as a result of the consumption of the U-238 isotope by absorption and decay. Figure 8 – 11 present the total atomic distribution of the U-235 and U-238 isotopes for different study cases based on the number of burnup steps (figures 8 and 10) and the number of spatial discretized layers (figures 9 and 11).
Figure 8. Variation of radial U-238 total atomic density distribution for different number of burnup steps

Figure 9. Variation of radial U-238 total atomic density distribution for number of spatial discretized layers
Figure 10. Variation of radial U-235 total atomic density distribution for different number of burnup steps

![Graph showing variation of radial U-235 total atomic density distribution for different number of burnup steps]

Figure 11. Variation of radial U-235 total atomic density distribution for number of spatial discretized layers

![Graph showing variation of radial U-235 total atomic density distribution for number of spatial discretized layers]

After the reactor operation, the plutonium isotopes have an important influence on the consumed fuel in the intermediate and final storage. The total amount of plutonium built during the operating time. In order to reprocess and produce the MOX fuel, the possibility of using the plutonium isotopes for the design of fuel cycle strategies [9; 10].
The radial distribution of the total atomic density of Pu-239 in the fuel assembly calculated using MCU code during the burnup for study cases as shown in figures 12 and 13. As presented in the figure 12, the number of burnup steps effects the MCU code results. And, increasing the number of discretized layers effects the total atomic density of the Pu-239 accumulated at the rim region (figure 13).

**Figure 12.** Variation of radial Pu239 total atomic density distribution for different number of burnup steps

**Figure 13.** Variation of radial Pu239 total atomic density distribution for number of spatial discretized layers
Using the gadolinium isotopes as a burnable absorber due to their high neutron capture helps the reactivity control aims. Increasing the U-Gd rods instead of using the boron in the moderator leads to increasing the amount of atomic density of the gadolinium isotopes at the begging of the cycle.

Figures 14 – 17 present the change of the total atomic distribution of the Gd-155 and Gd-157 isotopes during the burnup for different study cases based on the number of burnup steps (figure 14 and 16) and the number of spatial discretized layers (figure 15 and 17). Figures 14 and 16 show that the increasing the number of burnup steps leads to rapid depletion of the gadolinium isotopes within the burnup cycle. As shown, the depletion of the gadolinium isotopes about 20 MWd/KgHM for the case of 5 burnup steps and less than that for the case of 15 burnup steps. Figures 15 and 17 show that, increasing the number of discretized spatial layers increases the total atomic density at the beginning of the burnup cycle. With the conserving of the depletion point for the all cases, increasing the number of discretized spatial layers lead to a rapid depletion of gadolinium isotopes.

![Figure 14](image1.png)
**Figure 14.** Atomic density values for Gd155 versus burnup for different number of burnup steps

![Figure 15](image2.png)
**Figure 15.** Atomic density values for Gd155 versus burnup for different spatial discretized layers
In addition to the evaluated accumulation of the plutonium isotopes, and due to their strong influence on the safety of the reactor core, two other minor actinides are important to be investigated for the reactor calculations.

Figures 18 – 21 show the total atomic density radial distribution based on different numbers of burnup steps and discretized spatial layers. Figures 18 and 20 show that increasing the burnup steps affected significantly the calculations by increasing the total radial isotopic density for both Xe-135 and Sm-149. In the other side, as the number of discretized spatial layers, the isotopic densities in the rim region increase as shown in the figures 19 and 21.
Figure 18. Variation of radial Xe135 total atomic density distribution for different number of burnup steps

Figure 19. Variation of radial Xe135 total atomic density distribution for number of spatial discretized layers
Figure 20. Variation of radial Sm149 total atomic density distribution for different number of burnup steps

Figure 21. Variation of radial Sm149 total atomic density distribution for number of spatial discretized layers

Other comparison has been performed to investigate the effect of increasing the discretized layers and the burnup steps on the calculating time. Figures 21 and 22 illustrate the effects of the spatial discretized layers and the burnup steps on the calculations time. As shown, increasing the number of discretized layers and the burnup steps leads to a slightly increment of the calculation time on the MCU code, which means that the calculation speed depends clearly on both, the number of the spatial discretized layers and the burnup steps number.
5. Conclusion
In this study the model of fuel assembly of VVER-1000 reactor was developed to investigate the effect of discretization and the burnup steps on the effective multiplication factor, total fission products and actinides atomic distribution besides the speed of calculations using the MCU Monte Carlo code. The study has been performed on the nine different cases. Obtained results showed a significant effect of the increasing of discretized layers number and the burnup steps number on the effective multiplication factor (especially within 10 – 20 MWd/KgHM), total radial atomic distribution during the burnup of Uranium dioxide (UO$_2$) fuel, fission products and actinides total atomic density and their variations besides the speed of calculations of the fuel assembly of VVER-1000 reactor using MCU Monte Carlo code.

References
[1] Duderstadt J J and Hamilton L J 1976 Nuclear Reactor Analysis Wiley New York.
[2] Hadad K, Ayoobian N and Piroozmand A 2009 Quantitative accuracy analysis of burnup calculations for BNPP fuel assemblies using FFTBM method Prog. Nucl. Energy 51 170-76.
[3] Lassmann K, O’Carroll C, van de Laar J and Walker C T 1994 The radial distribution of plutonium in high burnup UO$_2$ fuels J. Nucl. Mater 252 71-78.

[4] Merk B 2009 On the influence of spatial discretization in LWR-burnup calculations with HELIOS 1.9 – Part I: Uranium oxide (UOX) fuel Annals of nuclear energy 36 151-67.

[5] Gurevich M I and et al. 2009 Adaptation of MCU-PD code to parallel computing on multiprocessor computer Questions of atomic science and technology Ser. Phys. Nucl. React. 4 66–77.

[6] Pirouzmand A and Roosta F 2016 Calculation of radial burnup and nuclides atom density distributions in a VVER-1000 fuel rod using Monte Carlo method Progress in Nuclear Energy 88 321–31.

[7] U. S. Nuclear Regulatory Commission 2003 Final Safety Analysis Report of BNPP-1 Chapter 4 Reactor 49.BU.10.0.OO. FSAR. RDR001.

[8] Kalugin M A, Oleynik D S and Shkarovsky D A 2015 Overview of the MCU Monte Carlo software package Annual of Nuclear Energy 82 54-62.

[9] Merk B and Broeders C H M 2008 Auswirkungen von politischen Optionen auf die anfallenden Aktinidenmengen im deutschen Reaktorpark Atomwirtschaft 6.

[10] Kessler G and et al.1999 Wohin mit dem deutschen Plutonium Atomwirtschaft 3.