Neutronic calculations for the VVER-1000 LEU and MOX assembly computational benchmark using the GETERA code

T M Abuqudaira and Y V Stogov
Department of Theoretical and Experimental Physics of Nuclear Reactors, National Research Nuclear University MEPhI, Kashirskoe highway, 31, Moscow 115409, Russia

E-mail: thabitne@gmail.com

Abstract. Disassembling nuclear warheads require the deployment of mixed oxide fuel \((UO_2+PuO_2)\) for the utilization of Plutonium from warheads. For this purpose, the Nuclear Energy Agency has proposed a computational benchmark consisting of two VVER-1000 assemblies: LEU and MOX; to study their physics and the main differences between them. GETERA code which is based on the collision probability method was used to study the neutronic characteristics of these assemblies at different reactor states. The aim of this work is to test the accuracy of the GETERA code and its nuclear data library BNAB-93 against previously obtained solutions. Burnup calculations were conducted up to 40 MWd/kgHM. Calculations of the infinite multiplication factor, average isotopic composition, several reactivity effects and the radial variation of isotopic composition in Uranium–Gadolinium (UGD) pins were performed. Comparison of our results with the benchmark mean results was performed and was shown to give a very good agreement.

1. Introduction
Benchmarks are used to validate computer codes and test nuclear data libraries [1]. Also, they play as an educational tool for engineers to be capable of performing neutronic calculations for nuclear reactors. The Russian Federation and the United States have studied the modifications that may be required to use MOX fuel in nuclear reactors [2]. An international experts group at the OCED/NEA has proposed a VVER-1000 LEU and MOX computational benchmark to facilitate the sharing of existing information and experience about the future designs of VVER-1000 fuel assemblies [3].

The Benchmark was studied using six codes received from five institutions. Two of the solutions are based on continuous energy Monte Carlo methods: MCU and MCNP-4B codes. The remaining four solutions are based on collision probability (or similar) methods: TVS-M, WIMS8A, HELIOS, and MULTICELL codes. The average value from the results obtained using these codes is described as “Benchmark mean” throughout this paper. Furthermore, the benchmark was studied using different codes and different data libraries. These studies were performed using: EXCELL [4], APOLLO2 and TRIPOLI4 [5], SCALE and SERPENT [6], MCNPX [7], and VISWAM [8].

The GETERA code is intended for calculation of neutron space-energy distribution in nuclear reactor cells and polycells by the collision probability method in multigroup approximation[9]. It uses the nuclear
The benchmark model consists of two typical assemblies of the advanced designs for the VVER-1000 reactor: LEU Assembly and a profiled MOX Assembly. Each assembly consists of 331 cell locations in a hexagonal array. 12 pins with 4 wt% burnable absorber in the form of Gd₂O₃ are located in each assembly. The UGD pins in both assemblies are in the same location and have the same content. The LEU assembly is shown in figure 1. The average $^{235}$U enrichment in the assembly is $\approx 3.7\%$. The MOX assembly is shown in figure 2. The average fissile Pu content in the assembly is $\approx 3.3\%$.

The assembly lattice pitch is 23.6 cm and the hexagonal cell pitch is 1.275 cm. Unit cell dimensions are shown in figure 3. The clad and structural materials are composed of a Zr-Nb alloy. The number densities of nuclides in the assemblies are reported in the benchmark report [3].
The benchmark has been studied with five different reactor states. Reactor states are listed in table 1. For the operating poisoned state S1, the fuel has been depleted at a constant power density of 108 MW/m³ up to a burnup of 40 MWD/kgHM. 80 depletion steps were used; 50 steps of 0.2 MWd/kgHM followed by 30 steps of 1.0 MWd/kgHM. Calculations for other reactor states have been performed at zero burnup.

4. Results and discussion

4.1. Infinite multiplication factor

The infinite multiplication factor versus burnup for both assemblies at the operating poisoned state S1 is shown in figures 4 and 5. GETERA results are compared with the benchmark mean value. For the LEU assembly, the burnup increases reactivity at the beginning of cycle because of the buildup of ²³⁹Pu and the rapid burn out of gadolinium isotopes. For the MOX assembly, this is not seen due to the harder neutron spectrum. Hardness of neutron spectrum [14], defined as the ratio of the flux of neutrons with (E_n>1 eV) to the flux of neutrons with (E_n<1 eV) is determined at specific burnup steps and is shown in table 2.

| Table 1. Reactor states. |
|--------------------------|
| State | Description | Fuel Temp. (K) | Non-fuel Temp. (K) | ¹³⁵Xe and ¹⁴⁹Sm Conc. | Boron Concentration (ppm) |
| S1 | Operating poisoned state | 1027 | 575 | Equilibrium conc. | 600 |
| S2 | Operating non-poisoned state | 1027 | 575 | 0 | 600 |
| S3 | Hot state | 575 | 575 | 0 | 600 |
| S4 | Hot state without Boron acid | 575 | 575 | 0 | 0 |
| S5 | Cold state | 300 | 300 | 0 | 0 |

| Table 2. Hardness of neutron spectrum. |
|--------------------------|
| Burnup (MWd/kgHM) | LEU Hardness | MOX Hardness |
|------------------|-------------|--------------|
| 0 | 5.96 | 10.85 |
| 10 | 6.45 | 10.27 |
| 20 | 6.79 | 9.62 |
| 30 | 6.94 | 9.12 |
| 40 | 7.00 | 8.69 |
The deviation of the GETERA results from the mean values for specific burnup points and comparison of results with WIMS8A code (which is also based on collision probability method) is listed in table 3. Results show good agreement with the benchmark mean value. However, at high burnup GETERA showed deviations, this may be due to the absence of some gadolinium isotopes in the used data library (\(^{152}\)Gd, \(^{158}\)Gd, and \(^{160}\)Gd).

**Table 3.** \(K_{inf}\) with burnup for the operating poisoned state.

| Burnup (MWd/kgHM) | GETERA   | Benchmark Mean (BM) | WIMS8A[3] | \(\Delta k\) (GETERA-BM).10\(^5\) |
|-------------------|----------|---------------------|-----------|---------------------------------|
| LEU               |          |                     |           |                                 |
| 0                 | 1.13559  | 1.1350              | 1.1328    | 59                              |
| 20                | 1.04384  | 1.0411              | 1.0383    | 274                             |
| 40                | 0.91807  | 0.9065              | 0.9088    | 1157                            |
| MOX               |          |                     |           |                                 |
| 0                 | 1.15792  | 1.1566              | 1.1494    | 132                             |
| 20                | 1.01804  | 1.0160              | 1.0127    | 204                             |
| 40                | 0.91295  | 0.9015              | 0.9048    | 1145                            |

For S2-S5 reactor states, \(K_{inf}\) has been determined at zero burnup. Results show a very good agreement and it is listed in table 4. Comparison of our results with the results obtained by MCNPX [7] that uses ENDF-VII nuclear data library confirms the validity of the model used in GETERA and its nuclear data library BNAB-93.
Table 4. $K_{inf}$ at zero burnup for S2-S5 states.

| State | GETERA | Benchmark mean (BM) | MCNPX[7] | $\Delta K$ (BM-GETERA).10^5 |
|-------|--------|---------------------|----------|-----------------------------|
| LEU   |        |                     |          |                             |
| S2    | 1.17568| 1.1754              | 1.171    | -28                         |
| S3    | 1.18947| 1.1891              | 1.183    | -37                         |
| S4    | 1.24901| 1.2489              | 1.252    | -11                         |
| S5    | 1.3177 | 1.3175              | 1.322    | -20                         |
| MOX   |        |                     |          |                             |
| S2    | 1.18641| 1.1899              | 1.194    | 349                         |
| S3    | 1.19986| 1.2073              | 1.213    | 744                         |
| S4    | 1.23383| 1.2422              | 1.254    | 837                         |
| S5    | 1.31213| 1.3209              | 1.331    | 877                         |

4.2. Reactivity effects
Reactivity effects have been determined based on the $K_{inf}$ results for different reactor states and it is listed in table 5. Results show a very good agreement for all effects for LEU assembly. However, for MOX assembly, relative deviation of 14.4% was observed for the poisoning effect and 22.9% for the Doppler effect. It is shown that the reactivity effect of $^{135}$Xe and $^{149}$Sm poisoning and soluble boron is less negative in the MOX assembly, this can be explained by its harder neutron spectrum.

Table 5. Reactivity effects at zero burnup.

| Initial state | Final state | Effect                             | LEU | MOX |
|---------------|-------------|------------------------------------|-----|-----|
|               |             |                                    | GETERA | Benchmark mean | GETERA | Benchmark mean |
| S1            | S2          | $^{135}$Xe and $^{149}$Sm poisoning| -4.01| -4.04| -2.85| -3.33 |
| S2            | S3          | Fuel temperature (Doppler)        | -1.38| -1.37| -1.35| -1.75 |
| S3            | S4          | Soluble boron                     | -5.95| -5.98| -3.39| -3.48 |
| S4            | S5          | Moderator temperature             | -6.87| -6.86| -7.83| -7.87 |

4.3. Isotopic composition change with burnup
The average concentrations of 11 nuclides in the assemblies have been determined with burnup. On overall, a very good agreement was observed for nuclides concentration in both assemblies at low burnup. Assemblies average nuclides concentration with burnup is shown in figures 6-14. At high burnup, deviations were increased but for most nuclides good agreement was observed. At burnup of 40 MWd/kgHM, $^{155}$Gd concentration was under-predicted with a relative deviation from the benchmark mean value by 46% in the MOX assembly. For the LEU assembly, Deviations were observed and reached the maximum at a burnup of 40 MWd/kgHM for $^{238}$U, $^{240}$Pu and $^{155}$Gd with relative deviations of: 70%, 69%, and 49% respectively. However, for main fuel isotopes $^{235}$U, $^{238}$U and $^{239}$Pu results show very good...
agreement in both assemblies, relative deviations for the LEU assembly do not exceed 7%, 0.09% and 3.5% respectively. For MOX assembly, relative deviations are 4%, 0.04% and 4.8% respectively.

Figure 6. $^{235}$U assembly average concentration versus burnup.

Figure 7. $^{236}$U assembly average concentration versus burnup.

Figure 8. $^{238}$U assembly average concentration versus burnup.

Figure 9. $^{239}$Pu assembly average concentration versus burnup.
4.4. Radial variation of isotopic composition

For the UGD pins, the variation of the isotopic composition averaged over all UGD pins with radius has been determined at specific burnup step, 2 MWd/kgHM for $^{155}$Gd and $^{157}$Gd and 40 MWd/kgHM for $^{235}$U, $^{239}$Pu. Concentration of nuclides averaged over each sub-region of the five annular sub-regions of the pin is plotted versus radius in Figures 17-20.
Figure 14. $^{149}$Sm assembly average concentration versus burnup.

Figure 15. $^{155}$Gd assembly average concentration versus burnup.

Figure 16. $^{157}$Gd assembly average concentration versus burnup.

$^{155}$Gd and $^{157}$Gd showed a decreasing of concentration with the radius of the pin; this can be explained by the self-shielding of the gadolinium isotopes. For $^{157}$Gd shows higher variation with radius than $^{155}$Gd, this is because of the higher absorption cross section of $^{157}$Gd. As shown, $^{239}$Pu concentration increased with radius, mainly due to the self-shielding of the $^{238}$U [15]. For $^{235}$U, the concentration is lower in the outer regions from the inner ones, this is due to the higher fission rate at the outer regions [16].
Although the Benchmark results for the isotopic composition with radius have calculated for a specific UGD pin, our results agree in principle (showed the same behavior) with the benchmark results.

**Figure 17.** $^{155}$Gd concentration versus radius of UGD pins.

**Figure 18.** $^{157}$Gd concentration versus radius of UGD pins.

**Figure 19.** $^{235}$U concentration versus radius of UGD pins.

**Figure 20.** $^{239}$Pu concentration versus radius of UGD pins.

5. Conclusion

Neutronic calculations have been carried out for the VVER-1000 LEU and MOX assembly benchmark using the GETERA code with nuclear data library BNAB-93. It was shown that the main difference between assemblies is the harder neutron spectrum in the MOX assembly that leads to less negative reactivity effects of $^{135}$Xe and $^{149}$Sm poisoning and soluble boron addition. The calculated results were compared with the benchmark mean value and with different results obtained by different codes. The
comparison shows good agreement and confirms the ability of GETERA to obtain good solutions not only for one cell geometries but also for geometries containing multi-cells. An improvement for the code will be made if isotopes of gadolinium: $^{152}$Gd, $^{158}$Gd, and $^{160}$Gd will be added.

References
[1] Alhassan E, Sjostrand H, Duan J, Helgesson P, Pomp S and El. S et al. 2014 Selecting benchmarks for reactor calculations PHYSOR 2014, Role React. Phys. Towar. a Sustain. Futur.
[2] Ghein J, Carbajo J and Ellis R 2004 Issues in the Use of Weapons-Grade MOX Fuel in VVER-1000 Nuclear Reactors: Comparison of UO2 and MOX Fuels Oak Ridge Natl. Lab. 223
[3] OECD NEA 2002 A VVER-1000 LEU and MOX Assembly Computational Benchmark
[4] Thiagam L, Sunil Sunny C, Jagannathan V and Subbaiah K V. 2009 A VVER-1000 LEU and MOX assembly computational benchmark analysis using the lattice burnup code EXCEL Ann. Nucl. Energy 36 505–19
[5] Petrov N, Todorova G and Kolev N P 2013 APOLLO2 and TRIPOLI4 solutions of the OECD VVER-1000 LEU and MOX assembly benchmark Ann. Nucl. Energy 55 93–107
[6] Mercatali L, Venturini A, Daebel M and Sanchez V H 2015 SCALE and SERPENT solutions of the OECD VVER-1000 LEU and MOX burnup computational benchmark Ann. Nucl. Energy 83 328–41
[7] Louis H K and Amin E 2016 The Effect of Burnup on Reactivity for VVER-1000 with MOXGD and UGD Fuel Assemblies Using MCNPX Code J. Nucl. Part. Phys. 6 61–71
[8] Khan S A, Jagannathan V, Kannan U and Mathur A 2016 Study of VVER-1000 OECD LEU and MOX Computational Benchmark with VISWAM Code System Nucl. Energy Technol. 2 312–34
[9] Belousov N, Bichkov S, Marchuk Y, Prianichnikov A, Savander V and Fyodorov I 1992 The Code GETERA for Cell and Polycell Calculations. Models and Capabilities Proc. of the 1992 Topical Meeting on Advances in Reactor Physics (Charleston Sheraton, Charleston, SC, USA) pp 2-516-2–523
[10] Pryanichnikov A 2009 (In Russian) Description of the GETERA code Probl. At. Sci. Technol. Ser. Nucl. React. Phys. 3 63–77
[11] Dawahra S, Khattab K and Saba G 2015 Calculation of fuel burnup and radionuclide inventory in the 10 MW MTR type research reactor using the GETERA code Ann. Nucl. Energy 78 89–92
[12] Khattab K and Dawahra S 2011 Calculation of fuel burnup and radionuclide inventory in the 10 MW MTR type research reactor using the GETERA code Ann. Nucl. Energy 38 1442–6
[13] Prabha H, Karthikeyan R, Lajoie M A, Marleau G and Hébert A 2017 Multiplication factors of single pin hexagonal cells and VVER-1000 reactor assembly Ann. Nucl. Energy 109 720–5
[14] Badalov A F and Kononov S L 1988 (In Russian) The results of Monte-Carlo calculations of light water lattices characteristics for different water ratio Probl. At. Sci. Technol. Ser. Phys. 3 24–9
[15] Mura L F L, dos Santos A, Domingos D B, Rossi P C R and Jerez R 2017 The experimental determination of the238U(n,γ) and total fission reaction rates along the pellet radius of the IPEN/MB-01 reactor Ann. Nucl. Energy 99 399–409
[16] 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 Prog. Nucl. Energy 88 321–31