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Inter-Code Comparison of Computational VERA Depletion Benchmark Using OpenMC, OpenMC-ONIX and DRAGON

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ABSTRACT

This research focuses on the comparative analysis of the PWR fuel assembly based on VERA depletion benchmark problems using community-developed open source Monte Carlo code OpenMC, python based burnup code system ONIX (a coupling interface for Monte Carlo code OpenMC), and deterministic DRAGON code. The depletion analysis was performed using OpenMC and ONIX with ENDF/B-VII.1 nuclear data library, and DRAGON with SHEM-361 based DRAGLIB format library (ENDF/B-VII.1). The code-to-code analysis on the evolution of k_{eff}, atom number density, and power distribution as a function of burnup has been performed and the result shows a good agreement with the maximum difference within 200 pcm at EOC. However small discrepancy around 90 pcm has been observed in k_{eff} calculated by DRAGON compared to OpenMC in the presence of integral fuel burnable absorbers (IFBA). The above-mentioned codes have been validated successfully for the first time against PWR fuel assembly based on VERA depletion benchmark problems. It can be concluded that initial implementation of these codes at the Department of Nuclear Science and Engineering under Military Institute of Science and Technology, Dhaka, was successful and that further research works are to be performed to utilize these codes for depletion/neutronics calculation of existing 3MW TRIGA Mark-II research reactor and VVER-type power reactor that is to be commissioned in Bangladesh

INTRODUCTION

To predict and assess the safety and operational parameters of research and power nuclear reactors, it has become more important to accurately calculate the isotopic depletion/burnup of nuclear fuel in reactors in order to assess reactor behavior in both normal and abnormal conditions [1,2]. Computational code that is capable to accurately determine neutronics and fuel burnup-related parameters required to analyze reactor safety is essential. Hence, computational code for nuclear reactor must be verified and validated on a variety of cases to demonstrate its reliability and accuracy [2]. Many research performed code verification with different benchmark problems to ensure that their results are accurate with the benchmark data. Different types of computer codes such as MCNP [3], ORIGEN [3], SCALE [4], OpenMC [5-6], WIMS-CITATION [7], and DRAGON5 [8] are being widely used for neutronics analysis as well depletion calculation for different research and power nuclear reactors. Fuel burnup or depletion analysis plays a vital role on both research and power nuclear reactor since reactor safety, cost-effective utilization and core lifetime are depending on fuel burnup/depletion process during operation. The objective of this study is to validate the open source codes OpenMC, ONIX-OpenMC [9] and DRAGON against the PWR fuel assembly based on VERA depletion/burnup benchmark problems for the first time. The purpose of burnup calculation is to determine the characteristics of the core that vary with time and improve the safety and performance of the core. The calculation of time-dependent material compositions in fuel requires the solution to the decay and transmutation equations. Burnup equations that describe the time rate of change of isotopic

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composition form a system of first-order linear differential equations. Chebyshev Rational Approximation Method (CRAM) is the currently most widely used method due to its stability for solving the equations with many isotopes and large time steps [9].

The VERA depletion benchmark problems [10-11] were proposed by the Consortium for Advanced Simulation of Light Water Reactor (CASL) from Oak Ridge National Laboratory (ORNL), with detailed guidelines including the burnup chain, fission Q-value for a depletion analysis. The depletion calculations of the VERA depletion benchmark suite were performed using Monte Carlo codes OpenMC, ONIX [9] and deterministic code DRAGON. OpenMC calculation result is considered as a standard solution due to explicit geometry modeling capability in 2D and 3D, usage of continuous energy cross-sections and with only a limited number of approximations for physics interaction and six dimension phase of a neutron such as the location, energy, and direction. To perform this study with OpenMC code, ENDF/B VII.1 data library was utilized to generate data set in HDF5 format for OpenMC at 565 K, 600 K, 900 K, and 1200 K temperatures utilizing NJOY2016, while DRAGLIB [9] format for DRAGON was processed using PyNJOY 2016 to obtain the cross section at specific temperatures. In this paper, 2D results of VERA depletion problems are reported. For fair comparison the same recoverable energies of fissionable isotopes were used in all three codes.

METHODOLOGY

Computational benchmark description

Code-to-code comparative analysis of the VERA depletion benchmark problem was performed using open source Monte Carlo and deterministic codes. It includes 10 fuel pins and 16 fuel assembly problems with four different fuel temperatures (565 K, 600 K, 900 K, and 1200 K). Each assembly consists of a 17×17 rectangular lattice array of fuel pins with different types of burnable absorber (IFBA, Pyrex) which are widely used in LWRs during the initial part of the cycle with the assembly pitch of 21.5 cm. There are four ^{235}U enrichments in the model: 2.1, 3.1, 3.6, and 4.6 wt%. The isotopic composition of the fuel, burnable absorber, and structural material can be found in the benchmark specifications [10-11]. For the depletion intra-zone sensitivity test, problem 1C was selected as a representative case problem. Depletion calculations were carried out using a power density of 40 W/gU and 40 burnup steps from 0 to 60 MWd/kgU as per suggestions in the benchmark report [10]. The detailed specifications of each problem are given in Table 1.

Table 1. Fuel pin and assembly depletion benchmark problems.

Problem	Description	Temperature (K)			Moderator density (g/cm^3)	U^{235} wt.%	Power density (w/gU)
		Moderator	Clad	Fuel			
1A	Pin (3.1 w/o)	565	565	565	0.743	3.1	40.0
1B	Pin (3.1 w/o)	600	600	600	0.700	3.1	40.0
1C	Pin (3.1 w/o)	600	600	900	0.700	3.1	40.0
1D	Pin (3.1 w/o)	600	600	1200	0.700	3.1	40.0
1E	Pin (IFBA)	600	600	900	0.700	3.1	40.0
1F	Pin (2.1 w/o)	600	600	900	0.700	2.1	40.0
1G	Pin (3.6 w/o)	600	600	900	0.700	3.6	40.0
1H	Pin (4.6 w/o)	600	600	900	0.700	4.6	40.0
1I	Pin (Gadolinia)	600	600	900	0.700	1.8	40.0
1J	Pin (3.1 w/o)	600	600	600/900/1200	0.700	3.1	40.0
2A	FA (No poison)	565	565	565	0.743	3.1	40.0
2B	FA (No poison)	600	600	600	0.700	3.1	40.0
2C	FA (No poison)	600	600	900	0.700	3.1	40.0
2D	FA (No poison)	600	600	1200	0.700	3.1	40.0
2E	FA (12 Pyrex)	600	600	900	0.700	3.1	40.0
2F	FA (24 Pyrex)	600	600	900	0.700	3.1	40.0
2G	FA (24 AIC*)	600	600	900	0.700	3.1	40.0
2H	FA (24 B_4C)	600	600	900	0.700	3.1	40.0
2I	FA (Instrumentation Tube)	600	600	900	0.700	3.1	40.0
2J	FA (24 Pyrex)	600	600	900	0.700	3.1	40.0
2K	FA(Zoned, 24 Pyrex)	600	600	900	0.700	3.1/3.6	40.0
2L	FA (80 IFBA)	600	600	900	0.700	3.1	40.0
2M	FA (128 IFBA)	600	600	900	0.700	3.1	40.0
2N	FA (104 IFBA,20 WABA*)	600	600	900	0.700	3.1	40.0
2O	FA (12 Gadolinia)	600	600	900	0.700	3.1/1.8	40.0
2P	FA (24 Gadolinia)	600	600	900	0.700	3.1/1.8	40.0

*WABA: Wet Annular Burnable Absorber,
*AIC: Ag-In-Cd rod

Algorithm for solving depletion equation

The rate of change of number density or concentration with respect to time in each isotope of interest is equal to its net production rate per unit volume subtracted with its removal rate per unit volume. Productions are available through: direct fission, neutron nuclear reactions of target isotope, decay of parent isotope. Removal can happen through: fission if the interested isotope is

fissionable isotope, neutron reactions and self-decay to a daughter isotope. A system linear first-order differential equations can be developed for all isotopes that be considered in the burnup problem. The general form of depletion equation [2] of each specific isotope in the burnup problem is given in Eq. (1):

$$\frac{dN_i}{dt} = \sum_j \gamma_{ji}\,\sigma_{f,j} N_j \phi + \sum_k \sigma_{x,k\to i}\, N_k \phi + \sum_l \lambda_{l\to i}\, N_l - \left(\sigma_{f,i} N_i \phi + \sigma_{x,i} N \phi + \lambda_i N_i\right) \quad (1)$$

where,

$\frac{dN_i}{dt}$ is the time rate of change in number density of isotope i

$\sum_j \gamma_{ji}\,\sigma_{f,j} N_j \phi$ is the production rate of isotope i from fission of all fissionable nuclides,

$\sum_k \sigma_{x,k\to i}\, N_k \phi$ is the production rate of isotope i from neutron transmutation of all isotopes including (n, 2n), (n, γ), (n, p),

$\sum_l \lambda_{l\to i}\, N_l$ is the production rate of isotope i from decay of all isotopes including α, β+, β-

$\sigma_{f,i} N_i \phi$ is the removal rate of isotope i by fission,

$\sigma_{x,i} N \phi$ is the removal rate of isotope i by all reaction except fission,

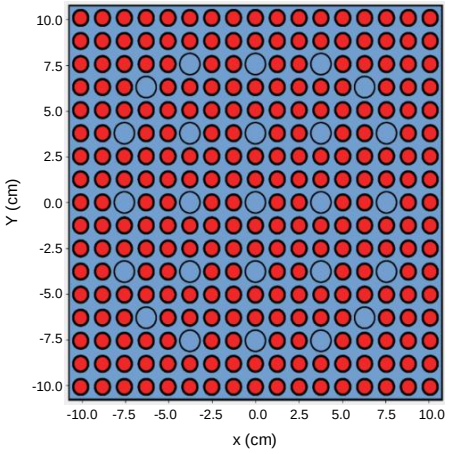
$\lambda_i N_i$ is the removal rate of isotope i by decay

In the equation, N_i is number density of isotope i in atoms/cm^3, t is time in seconds, γ_{ji} is the fission yield fraction for the production of isotope i from fission of isotope j, $\sigma_{f,i}$ is the microscopic fission cross section for isotope i in cm^2, $\sigma_{x,i}$ is the microscopic capture cross section (all reactions minus fission) for isotope i in cm^2, ϕ is the neutron flux in n/cm^2.s, and λ_i is the decay constant for isotope i in 1/s. Reaction rates of these reactions multiplication factor are calculated by using these codes.

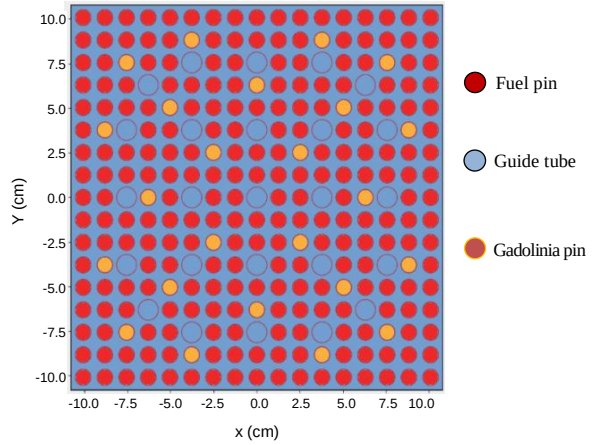
CODE DESCRIPTIONS

OpenMC

OpenMC is an open source continuous energy Monte Carlo neutron transport code. The code was used as a State-of-the-Art Monte Carlo tool for the VERA depletion benchmark problem with fuel burnup capability using CRAM [3] method to solve depletion equations. OpenMC uses a native HDF5 format to store nuclear data. Rich Python API and modern portable input/output file format enable programmatic pre and post-processing in the more efficient way. The source code of OpenMC is written in C++ for high performance computing. OpenMC is capable of simulating neutrons, photons, electrons and positrons either in fixed source or k-eigenvalue problems. OpenMC uses legacy Constructive Solid Geometry (CSG) capability to build arbitrarily complex three-dimensional models. In all cases, the reflective boundary conditions are used. Configurations of fuel and Gd pins in the FA are shown in Fig. 1.



(a) Case: 2C



(b) Case: 2P

Fig. 1. Configuration of FA problem.

ONIX

ONIX (OpeNIsotopiX) is a Python language-based open-source depletion code that uses CRAM method to solve the decay and transmutation equation of nuclides. In this study, to carry out burnup calculation, ONIX was coupled with OpenMC because of its distribution as an open-source code. During depletion run, problem-dependent cross-section data are needed e.g. one

group absorption cross-section, and it can be obtained from OpenMC. Salamèche used a 16th order CRAM method to solve the depletion equations over each of the time intervals. **Passport** object was used to store problem-specific data e.g isotopic density, decay, and fission yield (FPY) of each individual isotope of depleted material. All Passport objects were handled by **Passlist** class. To store the volume of each depleted material cell, **BUCell** object was used. Finally, for each BUCell, individual nuclides data was processed by the System object and stores parameters such as k_{eff}, atom density, and reaction rate at each burnup step in a text file.

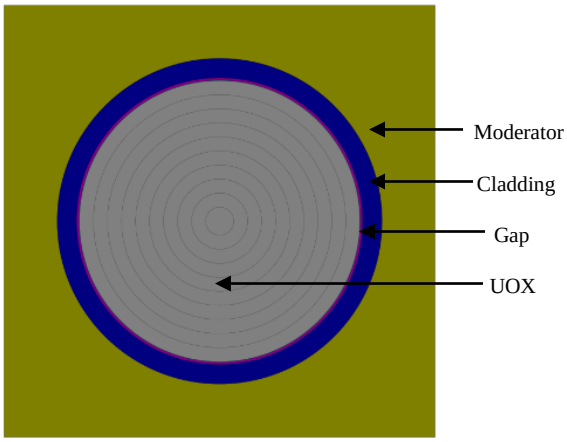


Fig. 2. Configuration of Pin Cell.

DRAGON

DRAGON is a lattice cell code which is developed by École Polytechnique de Montréal. The calculations were performed with the latest release version DRAGON -V 5.0.7 using the ENDF-B VII.1 nuclear data library. SHEM 361 energy groups ENDF/B-VII-based libraries were chosen for all calculations. DRAGON is a linked list of modular code and modules are linked together by the GAN generalized driver. The self-shielding calculations were performed using the **SHI** module based on the generalized Stammler method with Livolant and Jeanpierre (LJ) option [13] and WIMS-style transport correction was applied to the cross-sections. Depletion calculations were performed using the **EVO** module and for the time integration, fifth-order Cash-Karp algorithm was used. The DRAGON5 depletion calculations were conducted on a much finer time discretization and employed a fifth-order Cash-Karp algorithm for the time integration. **PSP** module was used to generate a PostScript image for 2D geometry. In all cases, the reflective boundary conditions were used. Figure 2 shows the configuration of fuel pin (1C) of a VERA depletion benchmark problem using the **PSP** module.

RESULTS AND DISCUSSION

This section presents the results which were obtained from running the OpenMC, ONIX, and DRAGON codes. In the burnup calculation, the accuracy of the solution greatly depends on the number of zones in fuel pins. The fuel rod inside the pin and assembly cells were split into several rings for accurate estimation of absorption of major isotopes. To get consistent depletion results, intra-zone sensitivity tests were performed for both normal UOX and Gd pins. A normal UOX pin was divided into several rings e.g. 3, 5, and 10 volumetric zones.

Figure 3 shows the relative deviation of k_{eff} with three and five depletion intra-volumetric zone compared to ten zones. It is clear that for the UOX fuel pin, three depletion intra-zones are quite enough to produce a converged solution for both OpenMC and ONIX but in the case of DRAGON at least five depletion intra-zones are required. To achieve the best comparison, the Gd pin was divided into ten rings as shown in Fig. 4. It should be noted that, there is still a significant difference from 0 to 20 MWd/kg and this can be reduced by applying a refined number of burnup steps.

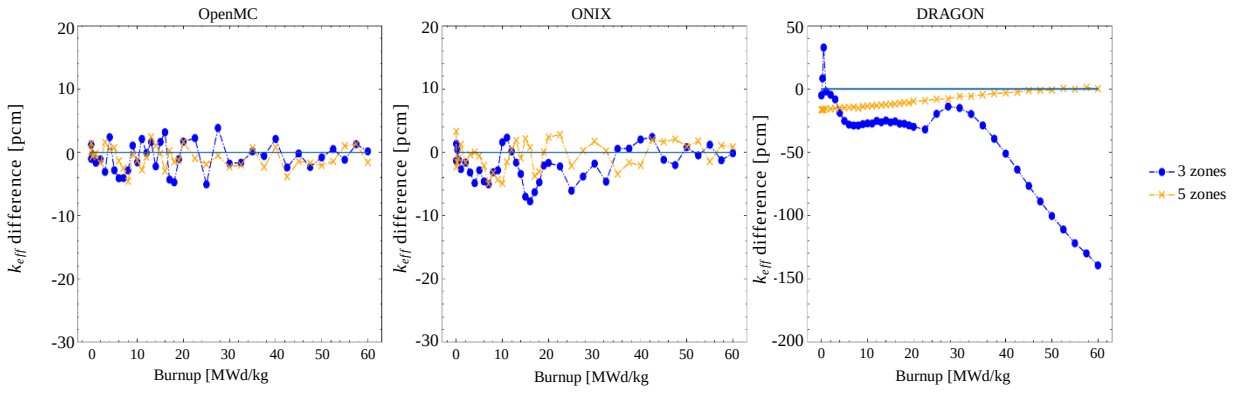


Fig. 3. Depletion intra-zone sensitivity test for UOX fuel (1C).

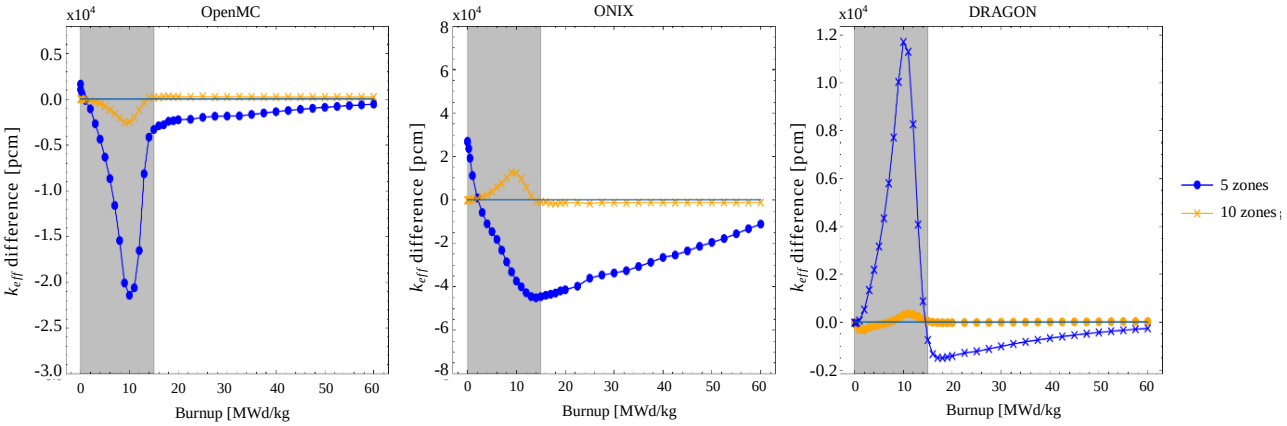


Fig. 4. Depletion intra-zone sensitivity test for problem 1I.

Table 2. k_{eff} values at BOC.

ID	Description	KENO-CE (k_{eff})	OpenMC (k_{eff})	Error (pcm)	DRAGON (k_{eff})	Error pcm
1A	Pin 3.1w/o TF=565K	1.18704±0.00005	1.18699±0.00019	4.21215797	1.18793	-74.976411
1B	Pin 3.1w/o TF=600K	1.18428±0.00017	1.18419±0.00021	7.59955416	1.18479	-43.064140
1C	Pin 3.1w/o TF=900K	1.17393±0.00016	1.17399±0.00018	-5.1110372	1.17365	23.8515073
1D	Pin 3.1w/o TF=1200K	1.16516±0.00013	1.16501±0.00024	12.8737684	1.16579	-54.0698273
1E	Pin IFBA 3.1w/o TF=600K	0.76521±0.00022	0.76529±0.00020	-10.454646	0.76321	261.366160
1F	Pin 2.1w/o TF=900K	1.05835±0.00017	1.05829±0.00018	5.66920206	1.05801	32.1254783
1G	Pin 3.6w/o TF=900K	1.21335±0.00018	1.21346±0.00022	-9.0658095	1.21363	23.076606
1H	Pin4.6w/o TF=900K	1.27094±0.00018	1.27089±0.00025	3.93409602	1.27119	-19.670480
1I	Pin Gadolinia rod (5 %Gd_2O_3)	0.21820±0.00010	0.21817±0.00023	13.7488542	0.21801	-87.076077
1J	Pin 3.1w/o TF=600/900/1200K	1.17451±0.00014	1.17444±0.00022	5.95993223	1.17469	-15.32554001
2A	FA No Poisons TF=565K	1.18218±0.00002	1.18208±0.00021	8.45894872	1.18259	-34.68168976
2B	FA No Poisons TF=600K	1.18240±0.00012	1.18231±0.00024	7.61163735	1.18207	27.90933694
2C	FA No Poisons TF=900K	1.17354±0.00014	1.17359±0.00027	-4.2606131	1.17303	43.45825451
2D	FA No Poisons TF=1200K	1.16543±0.00015	1.16530±0.00019	11.1546811	1.16517	22.30936221
2E	FA 12 Pyrex	1.06072±0.00016	1.06079±0.00016	-6.5992910	1.06021	48.08054906
2F	FA 24 Pyrex	0.96541±0.00017	0.96529±0.00022	12.4299520	0.96476	67.32890689
2G	FA 24 AIC	0.83443±0.00017	0.83448±0.00019	-5.9921143	0.83489	-55.12745227
2H	FA 24 B_4C	0.77337±0.00021	0.77345±0.00025	-10.344337	0.77376	-50.42864347
2I	FA Instrument Thimble	1.17256±0.00012	1.17246±0.00026	8.52834823	1.17209	40.08323668
2J	FA Instrument+24 Pyrex	0.96476±0.00017	0.96487±0.00023	-11.401799	0.96503	-27.98623492
2K	FA Zoned+24 Pyrex	1.00886±0.00019	1.00879±0.00025	6.93852467	1.00811	74.34133577
2L	FA 80 IFBA	1.01133±0.00018	1.01125±0.00019	7.91037545	1.01107	25.7087202
2M	FA 128 IFBA	0.93205±0.00017	0.93215±0.00024	-10.729038	0.93169	38.62453731
2N	FA 104 IFBA+20 WABA	0.86123±0.00020	0.86118±0.00017	5.8056500	0.86066	66.18441067
2O	FA 12 Gadolinia	1.04004±0.00017	1.04009±0.00026	-4.8075074	1.03960	42.30606515
2P	FA 24 Gadolinia	0.91993±0.00016	0.91977±0.00019	17.3926277	0.91910	90.22425619

Table 2 shows the k_{eff} value at BOC calculated using OpenMC and DRAGON for all the cases. For pin cell problems (1A-1J), OpenMC calculations were performed using 10,000 source neutrons per cycle, 200 active cycles, and 25 inactive cycles. For the assembly case (2A-2P), it was 50,000 neutrons per cycle and the number of active and inactive cycle was 250 and 25 respectively. Inactive cycles were applied for fission source convergence in each case problem. OpenMC and Dragon calculated results with the ENDF/B-VII.1 library are in a very good agreement with the reference continuous energy (CE) Monte Carlo code KENO-CE [14].

DRAGON depletion calculations were conducted using a multi-group cross section library based on SHEM-361 multi-group structure [15]. Case problem 1C is selected as a representative case problem for comparative analyses because of available data [15] from the literature and McCARD [16] Monte Carlo code calculated value is used as a reference solution. To achieve the best comparison, the same recoverable energies of fissionable isotopes were used in burnup calculation. Figure 5 shows the evolution of the effective multiplication factor calculated by OpenMC, ONIX and DRAGON codes. The result is consistent at all burnup points. The relative difference in the calculated ^{235}U number density compared to McCARD value is provided in Fig. 6. In both OpenMC and ONIX calculated values, the relative difference is less than 100 pcm, while the highest discrepancy is seen at EOC with a 150 pcm error in DRAGON code. Figure 7 shows the change in one-group fission reaction rate of ^{235}U at each burnup step. Figure 8 depicts the relative difference in number density of major actinide isotopes at 60 MWd/kg compared to the McCARD code. It is clear that the computed number density in OpenMC and ONIX is quite similar to the McCARD value, with a relative difference of less than 0.5 % in both codes. From the DRAGON calculated value, ^{239}Pu and ^{241}Am are the worst performing isotopes and reach a relative error of approximately 0.93 %.

To complete the code-to-code comparison, multigroup scalar flux, pin power distribution, particle number density (PND) , one group fission, and absorption reaction rates are calculated using ONIX and DRAGON codes.

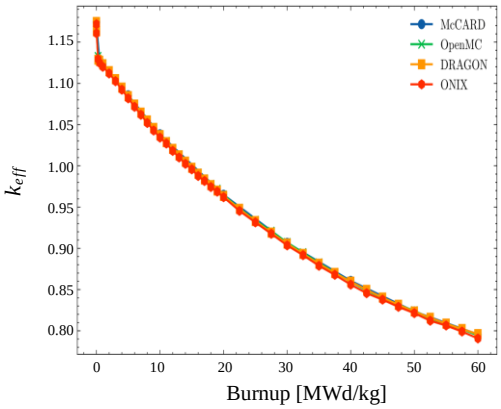


Fig. 5. Comparison of k_{eff} for VERA pin 1C.

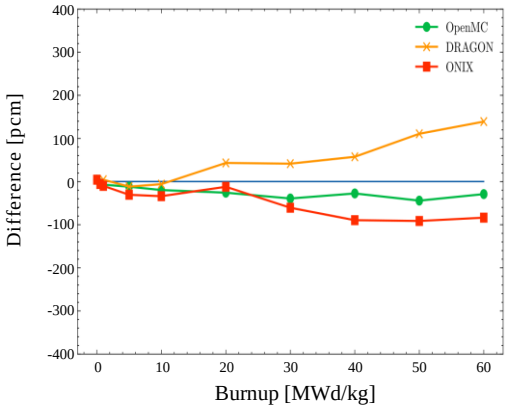


Fig. 6. Comparison of ^{235}U number density for VERA pin 1C.

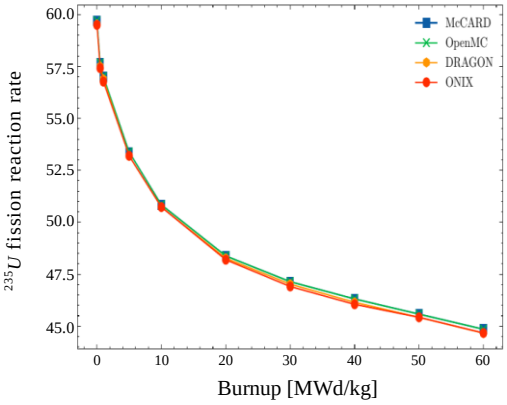


Fig. 7. Comparison of fission reaction rate of ^{235}U for problem 1C

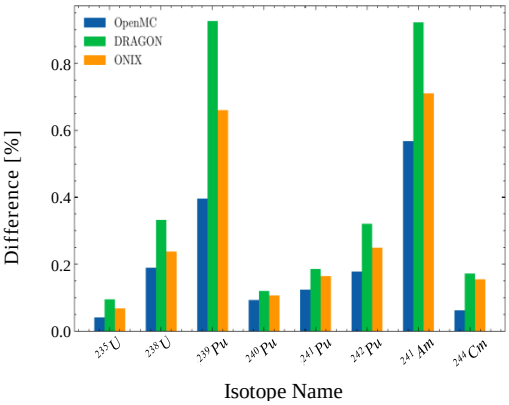


Fig. 8. Relative error of isotopic densities at 60 MWd/kg for problem 1C.

Multi-group scalar flux

Multi-group neutron fluxes per unit lethargy at 1 MWd/kg for pin cell problems 1C and 1H have been studied. Figures 9-10 show a comparison of multi-group scalar neutron flux among OpenMC, ONIX, and DRAGON with the two different energy structures. OpenMC and ONIX calculated neutron flux is obtained with pre-defined multi-group (47-groups) energy structure as stated in the benchmark problem [9] whereas DRAGON computed neutron flux obtained using SHEM-361 energy group structure. The results reveal that neutron flux in the thermal energy region is well agreed upon in both models obtained using OpenMC, ONIX, and DRAGON codes. However, the neutron flux is slightly depressed in the epithermal and fast energy regions due to absorption resonances, which are much more visible in the DRAGON calculated value due to the higher number of energy groups and different energy bin structure in these areas. The results of OpenMC, DRAGON, and ONIX are consistent with a relative difference of around 0.3 %.

Particle number density (PND)

The evolution of the number density of ^{239}Pu, ^{240}Pu and ^{241}Pu during burnup for case problem PIN-1C is reported in Figs. 11-13 respectively. As it can be seen, the results are consistent between OpenMC, ONIX and DRAGON calculated values. In the case of ^{239}Pu buildup, it can be concluded that the ^{239}Pu content with a burnup exceeding 40 MWd/kg falls within a flat range with nearly a factor of 1.5 between the minimum and maximum concentration. In addition, the radial density distribution of ^{235}U at 60 MWd/kg has been calculated for each radial zone. The results are shown in Fig. 14. It is obvious that ONIX and DRAGON computed values are nearly equal to OpenMC values after splitting the UOX fuel pellet into several rings as previously discussed in the intra zone depletion sensitivity analysis.

Xenon-135 is the most important saturating fission product because of its high neutron absorption cross section on the order of millions of barns, but has a half life of ~9 hours. On the other hand, another important fission product Samarium-149, has a half life ~320 days, reaches an equilibrium steady value which depends on the flux level in the core. Figures 15-16 display the buildup of ^{135}Xe and ^{149}Sm in the UOX fuel pin. ONIX calculated number density of ^{135}Xe and ^{149}Sm is quite low at high burnup compared to OpenMC and DRAGON calculated value and the maximum relative error peaks at around 9 %.

The evolution of the atomic density of ^{155}Gd and ^{157}Gd isotopes during burnup for case PIN-1I is presented in Figs. 17-18. Because of the high neutron capture cross section (n, γ) of around 7000 barn compared to ^{155}Gd capture cross section (5000 barn) as computed by OpenMC, ^{157}Gd depletes more rapidly than ^{155}Gd. After 20 MWd/kg, both isotopes reach an equilibrium level of very low density. However, ONIX computed results show that both gadolinium isotopes burn more rapidly compared to the OpenMC and DRAGON code values, which will be examined later in the pin power distribution section.

To demonstrate code reliability in nuclear data processing capability, assembly case 2A has been selected for isotopic number density comparison with OpenMC, ONIX and DRAGON code. NJOY data processing code was used to process ACE data into HDF5 format for OpenMC and DRAGLIB format for DRAGON code. Average number density plots of high actinide isotopes (^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu) for assembly case 2A are reported in Fig 19 and Fig 20. For the y-axis, a twin axis has been employed to depict the side-by-side buildup and decay of high actinides in the assembly. A consistent result is obtained at all burnup points.

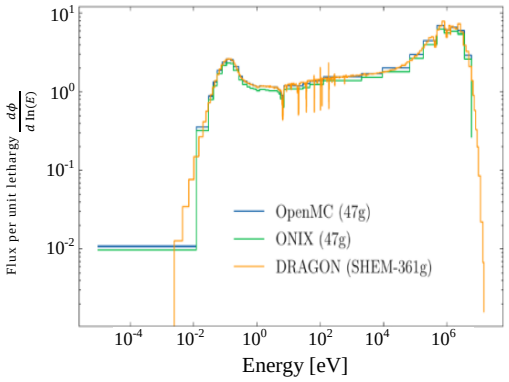


Fig. 9. Comparison of normalized neutron flux per lethargy at 1 MWd/kg for pin 1C.

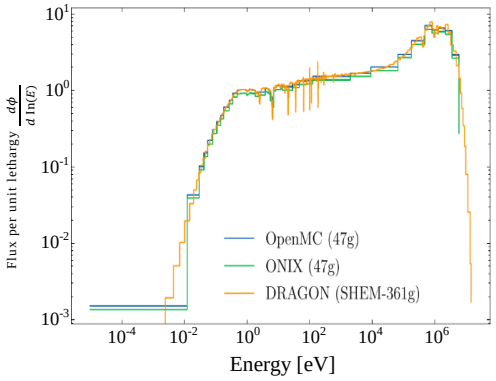


Fig. 10. Comparison of normalized neutron flux per lethargy at 1 MWd/kg for pin 1H.

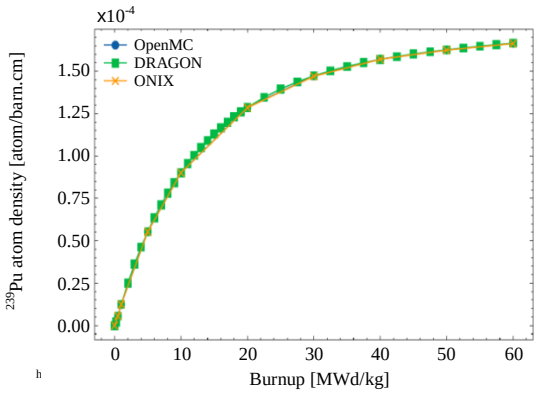


Fig 11. Atomic density of ^{239}Pu (PIN 1C).

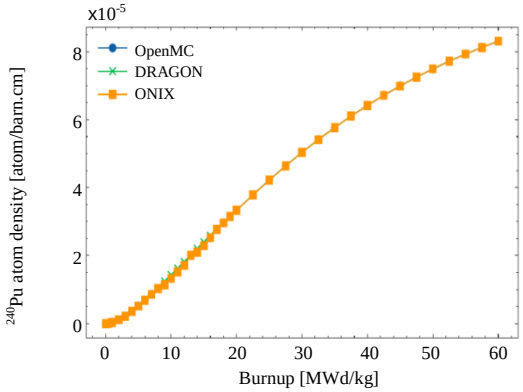


Fig. 12. Atomic density of ^{240}Pu (PIN 1C).

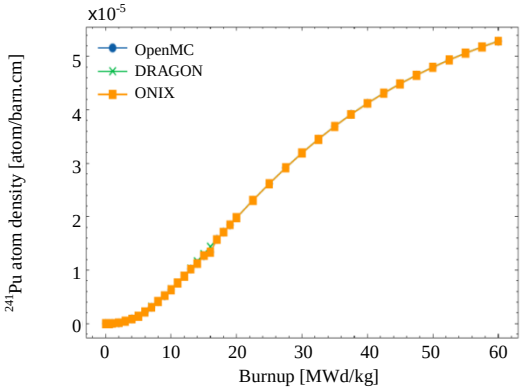


Fig. 13. Atomic density of ^{241}Pu (PIN 1C).

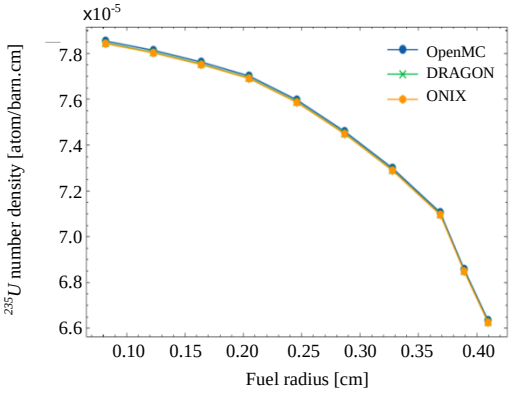


Fig. 14. Atomic density of ^{235}U along the radial direction at 1 MWd/kg (PIN 1C).

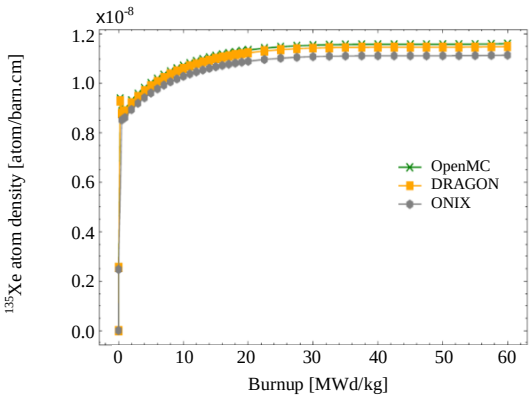


Fig. 15. Number density of ^{135}Xe (1C).

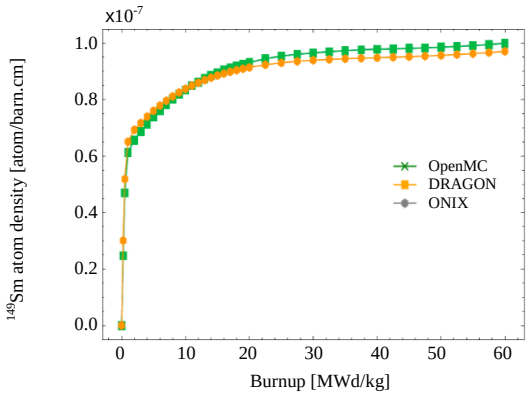


Fig. 16. Number density of ^{149}Sm (1C).

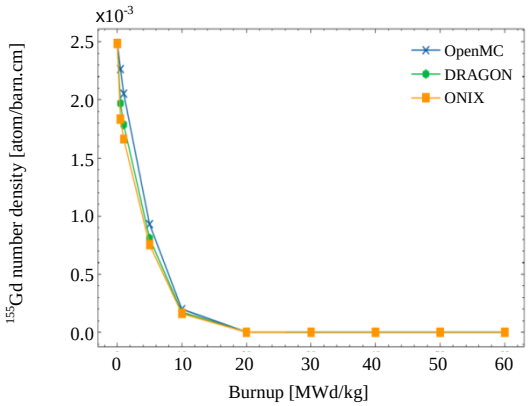


Fig. 17. Number density of ^{155}Gd (1I).

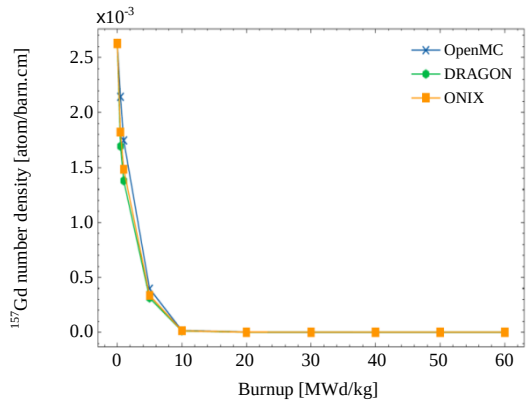


Fig. 18. Number density of Gd isotopes.

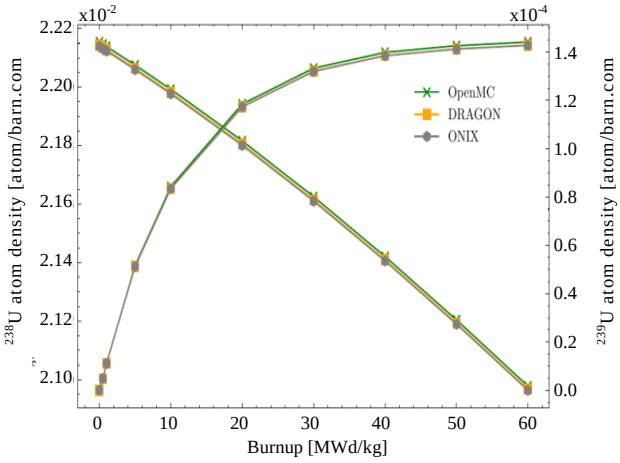


Fig. 19. Assembly average number density of ^{238}U and ^{239}Pu.

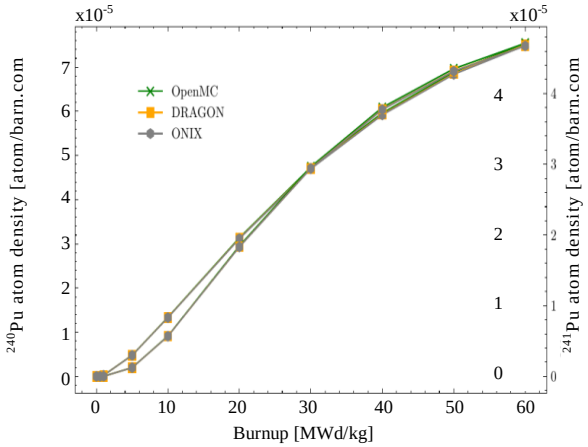


Fig. 20. Assembly average number density of Pu isotopes.

Reaction rate

The one group fission (n,f) and capture reaction (n, γ) rates of some major actinides and fission products are calculated at burnup point 1 MWd/kg for case 1C as stated in benchmark specification with a list of nuclide IDs. DRAGON calculated reaction rates are condensed into one group for a fair comparison with OpenMC and ONIX calculated values. Figure 21 presents the relative difference of fission reaction rate value between ONIX and DRAGON compared to OpenMC calculated value. Overall, plutonium isotopes are the worst-performing isotopes that show an error of around 0.4 % during burnup calculation. Figure 22 shows the relative error of the one group absorption reaction rate for major actinides and fission product isotopes and all errors are below 0.7 %.

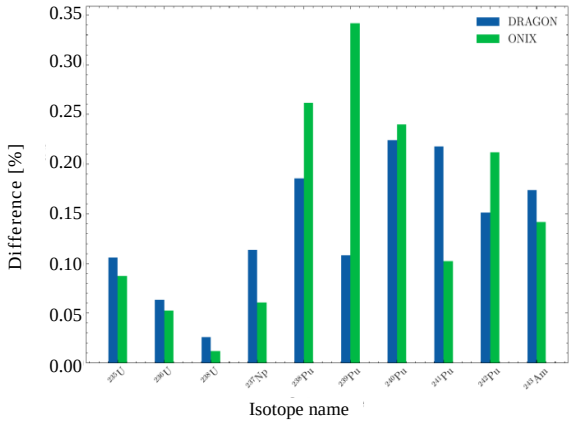


Fig. 21. Relative discrepancies in the fission reaction at 1 MWd/kg for problem 1C.

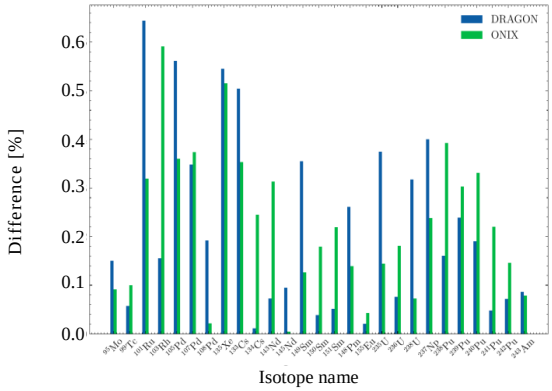


Fig. 22. Relative discrepancies in the capture reaction at 1 MWd/kg for problem 1C.

Pin power distribution

To compare pin power distributions in ONIX and DRAGON codes, case problems 2C and 2P were selected as specified in the benchmark specification. A 3D contour map with a 17x17 grid in the XY plane was utilized to represent typical PWR assembly, where Z represents the relative statistical difference in pin-wise power distribution compared to the OpenMC calculated value. Figs. 23-24 present the comparison of the radial power distribution at burnup point 1 MWd/kg. For case 2C, all power profiles are loaded with a relative statistical error lower than 2.9 %. However, in the presence of gadolinia pins, the differences are relatively significant. The maximum relative error peaks at ~8.9 % in the gadolinia pin. When comparing isotopic number density in the presence of burnable absorber with fuel matrix, this explains why both gadolinium isotopes burn rapidly in ONIX compared to OpenMC and DRAGON code. Nonetheless, excellent agreement is observed for the central part of the assembly (~1 %).

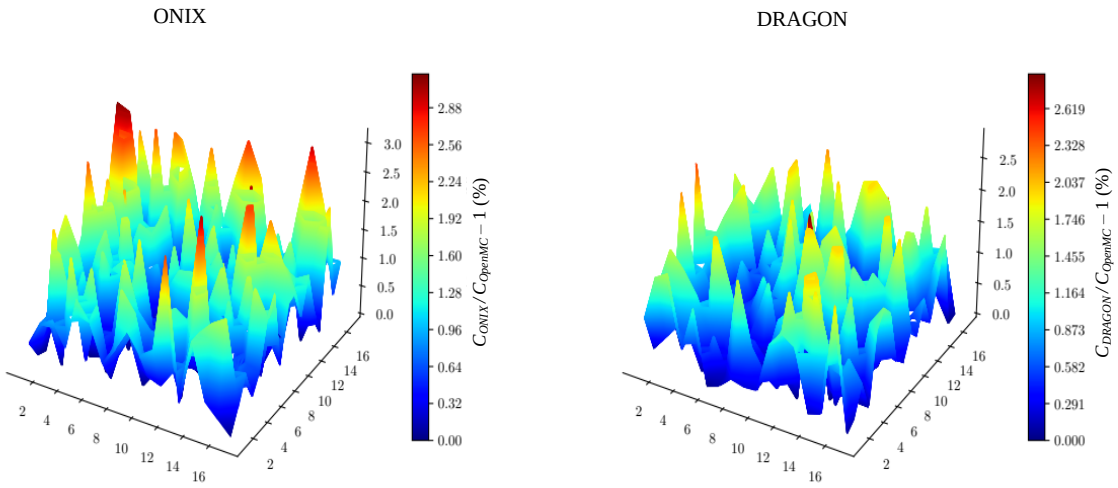


Fig. 23. Comparison of power distribution at 1 MWd/kg for VERA problem 2C.

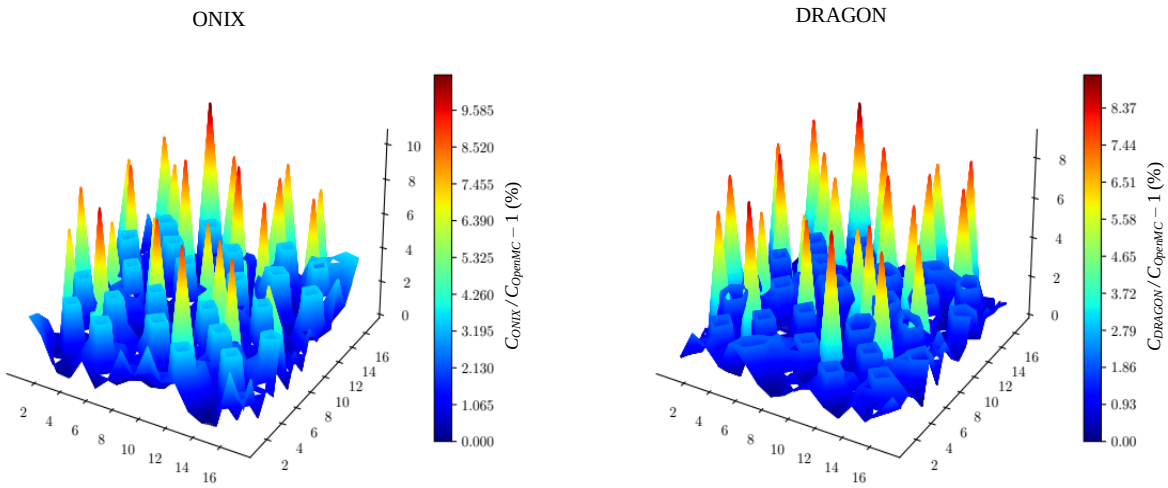


Fig. 24. Comparison of power distribution at 1 MWd/kg for problem 2P.

CONCLUSION

In the present study, the VERA depletion benchmark problem suite has been studied for validating the depletion capability of open source nuclear reactor computational codes. Monte Carlo code OpenMC, an open-source depletion code ONIX (coupled with neutron transport code OpenMC), and deterministic code DRAGON have been used in this work for a detailed analysis of neutronic and depletion parameters. The validation results are presented by comparing effective multiplication factor, atomic densities, multi-group normalized scalar neutron flux, one group fission/capture reaction rates, and pin by pin power distribution at different burnup steps. It is evident that the CRAM method is capable of providing a robust and accurate solution even with smaller time steps. By comparing the calculated results with McCARD, it was found that the results show excellent agreement for pin-cell problems. The k_{eff} deviations from the McCARD values are observed to be less than 250 pcm. The atomic densities inside fuel rings of some transuranic isotopes show relative errors of around 0.8 %. Fission and capture rates show less than 1 % of maximum relative error for both ONIX and DRAGON codes. The comparisons of k_{eff} at BOC and pin power distribution at 1 MWd/kg show that the results are in satisfactory agreement in assembly calculation with UOX fuel pins. This study shows that the presence of Gd isotopes causes overall assembly-wise degradation for both ONIX and DRAGON codes. The maximum relative error in normalized power distribution peaks at 8.9 % compared to OpenMC value. From this study, the obtained results show the capability of neutronic and depletion analysis of open source OpenMC, ONIX, and DRAGON.v5 codes. Each code has some limitations. In spite of such limitations, the OpenMC, OpenMC-ONIX, and DRAGON are

capable of performing neutronics and depletion calculations. In the future study, these open source codes will be used for the neutronic and depletion analysis of the existing 3 MW TRIGA MARK-II research reactor. Further, the full fuel cycle of LEU core of the forthcoming light water power reactor (VVER-type) to be commissioned in Bangladesh will be selected with detailed operating time and core configurations. Moreover, these codes are being used for practical demonstration of nuclear core management principles under the course title NSE475: In-core Fuel Management [17] for students of nuclear science and engineering at the Department of Nuclear Science and Engineering, Military Institute of Science and Technology, Dhaka, Bangladesh.

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AUTHOR CONTRIBUTION

A. Islam: study conception and modeling design, data analysis, draft manuscript preparation, T. A. Rahim: literature reviews, resources, writing manuscript, A. S. Mollah: Conceptual design idea, review and editing, interpretation of results, supervision. All authors reviewed the results and approved the final version of the manuscript.

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