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Development of an MCNP5-ORIGEN2 coupling scheme for burnup calculation of VVER-1000 fuel assemblies

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Abstract: The paper aims to develop an MCNP5-ORIGEN2 coupling scheme for burnup calculation. Specifically, the Monte Carlo neutron transport code (MCNP5) and the nuclides depletion and decay calculation code (ORIGEN2) are combined by data processing and linking files written in the PERL programming language. The validity and applicability of the developed coupling scheme are tested through predicting the neutronic and isotopic behavior of the "VVER-1000 LEU Assembly Computational Benchmark". The MCNP5-ORIGEN2 coupling results showed a good agreement with the k-inf benchmark values within 600 pcm during the entire burnup history. In addition, the differences of isotopes concentration at the end of the burnup (40 MWd/kgHM) when compared with benchmark values were reasonable and generally within 6.5%. The developed coupling scheme also considered the shielding effect due to gadolinium isotopes and simulated well the depletion of isotopes as a function of the radial position in gadolinium bearing fuel rods.

Keywords: *MCNP5, ORIGEN2, burnup, coupling, VVER-1000 LEU.*

I. INTRODUCTION

In the field of reactor core management, which consists of nuclear fuel burnup calculation, deterministic and Monte Carlo methods are widely used to solve the neutron transport equation. Each method has advantages and weaknesses. Deterministic method (e.g., collision probability method) has major advantage of the short computer time needed to find solutions while the disadvantages are related to the energy groups collapsing or the ability dealing with complicated reactor core geometries, which may lead to significant errors in the results. Whereas, the Monte Carlo based codes such as MCNP can model an arbitrary geometry and use continuous energy libraries. For that reason, they will provide high accurate solution to the neutron transport equation. However, the Monte Carlo method requests to use a large number of neutron histories and consequently this can be time consuming. For example, a simulation with multiple runs may be of little practical value if each run requires days or weeks. Such weakness is no longer a too difficult problem because nowadays, computers are able to perform simulations much more efficiently and quickly than before. For this reason, the Monte Carlo based codes are being widely used in nuclear reactors calculation.

In recent decades, a number of Monte Carlo burnup calculation code systems have been developed worldwide thanks to the advancement of computer science. Some Monte Carlo codes were added with an auxiliary module which has the function of depletion calculation such as MVP-BURN [1] and BURNCAL [2] while several ones were coupled with a special depletion and decay calculation code such as the MCNP-ORIGEN coupling strategy based codes, which are

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regularly used. In detail, MCNP [3] performance provides some parameters such as multiplication factor, neutron flux distribution, and neutron cross sections for a given compositional model while ORIGEN [4] calculates time-dependent fuel material compositions via irradiation, transmutation, activation, fission, and decay in the nuclear reactor environment. The first MCNP-ORIGEN coupling program was created in 1995 by the Idaho National Engineering and Environmental Laboratory (INEEL) with the name MOCUP (MCNP-ORIGEN Coupling Utility Program) [5]. MOCUP was written in ANSI C programming language and had a friendly interactive interface which was based on the portable X11 window environment and the Motif tool kit. MOCUP, however, only accounted for 17 actinides (ACT) and 41 fission products (FP). Four years later (1999), the Los Alamos National Laboratory (LANL) released their version of an MCNP-ORIGEN coupler, MONTEBURNS [6], written in FORTRAN and PERL. MONTEBURNS used a simple predictor-corrector method to improve the accuracy of the ORIGEN depletion calculation. In 2001, the Massachusetts Institute of Technology (MIT) distributed another MCNP-ORIGEN combined program, MCODE (MCNP-ORIGEN DEpletion program) [7], written in ANSI C. In MCODE, there are 39 actinides and 100 fission products considered in the burnup calculations, which account for more than 99% of neutron absorptions. In 2007, a burnup simulation system was developed at CIEMAT (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas), Spain with the name EVOLCODE (Burn-up EVOLution Simulation CODE) [8]. In EVOLCODE, MCNPX was coupled with two point-depletion codes, ORIGEN and ACAB [9], to enlarge the number of nuclear reactions taken into account by the irradiation calculations. In 2013, another MCNP-ORIGEN burnup calculation code system, named MCORE (MCNP and ORIGEN burn-up Evaluation code) [10], was developed at Xi'an Jiaotong University, China. In MCORE, besides the investigation of the reactivity effects and isotopic inventory as a function of burnup, it is also capable of simulating the fuel shuffling process after burnup calculation. In general, these MCNP-ORIGEN burnup calculation code systems, which are mentioned above, have a special attention in ORIGEN depletion calculation. The fact is that the cross sections and neutron flux values vary continuously throughout reactor operation time, thus beginning-of-time-step values are not fully representative of the entire time step, unless the time step is extremely small. For instance, in MOCUP, cross sections and flux values at beginning-of-time-step are assumed constant over the entire time step. With such simple method, the user needs small enough time steps to obtain high accurate results. After the development of MOCUP, other MCNP-ORIGEN coupling codes used a predictor-corrector algorithm for the depletion calculation in ORIGEN. This integrated algorithm allows the user to create larger time steps.

In Vietnam, combining a Monte Carlo based code with a depletion and decay code to realize burnup calculations, has received much attention in recent years. Typically, a REBUS-MCNP linkage system was used for core and fuel management of the Dalat Nuclear Research Reactor (DNRR) [11][12]. Moreover, a depletion calculation code using Radau IIA Implicit Runge Kutta method was developed in combination with MCNP5 and named MCDL (Monte Carlo Depletion for Light Water Reactor) to investigate burnup of DNRR [13]. However, the study on the combination of Monte Carlo code and depletion code for burnup calculation of commercial reactors such as VVER-1000 has not yet been done. For this reason, the aim of this study is to develop a coupling scheme between MCNP5 and ORIGEN2 codes to perform burnup calculation of VVER-1000 fuel assemblies, in which we used the simple approach adopted in MOCUP, for the sake of simplicity. To validate the MCNP5-ORIGEN2 coupling program, a VVER-1000 LEU benchmark assembly [14] was calculated and analyzed. The obtained calculation results showed a good agreement with the benchmark.

II. METHODOLOGY

A. Depletion and decay calculation

In a nuclear reactor environment, formation of new isotopes comes primarily from fission, neutron capture, and decay. Likewise, destruction of isotopes also comes from these processes. An equation for modeling isotopic depletion is expressed as follows:

$$\frac{dN_i}{dt} = \sum_j \gamma_{ji}\sigma_{f,j}N_j\Phi + \sum_k \sigma_{c,k\to i}N_k\Phi + \ldots + \sum_l \lambda_{l\to i}N_l - (\sigma_{f,i}N_i\Phi + \sigma_{a,i}N_i\Phi + \lambda_i N_i) \quad (1)$$

where $\frac{dN_i}{dt}$ is the rate of change in concentration of isotope i, $\sum_j \gamma_{ji}\sigma_{f,j}N_j\Phi$ the production rate per unit volume of isotope i from fission of all fissionable isotopes, $\sum_k \sigma_{c,k\to i}N_k\Phi$ the production rate per unit volume of isotope from neutron transmutation of all isotopes, $\sum_l \lambda_{l\to i}N_l$ the production rate per unit volume of isotope i from decay of all isotopes, $\sigma_{f,i}N_i\Phi$ the removal rate per unit volume of isotope i by fission, $\sigma_{a,i}N_i\Phi$ the removal rate per unit volume of isotope i by neutron absorption, and $\lambda_i N_i$ the removal rate per unit volume of isotope i by decay.

To solve the equation (1) one need to gather information of important parameters such as neutron fluxes and cross sections. Such parameters are in fact not constant over the entire cycle. That is why the cycle needs to be divided into a number of small time steps, during which the coefficients such as cross-sections and neutron fluxes are assumed to be constant. These constant coefficients can be calculated by the MCNP5 program for a specified geometry at a certain time step, and then used in ORIGEN2 calculations to provide the material compositions for the next time step. The calculations are repeated till the final time step. The coupling procedure between the MCNP5 and ORIGEN2 codes is presented in the next section.

B. Description of MCNP5-ORIGEN2 coupler

The developed MCNP5-ORIGEN2 coupler was written in the PERL programming language. The coupler consists of PERL files, which can generate the MCNP5 and ORIGEN2 input files, modify and update the cross-section library of ORIGEN2 during burnup, and process the data in the MCNP5 and ORIGEN2 output files automatically.

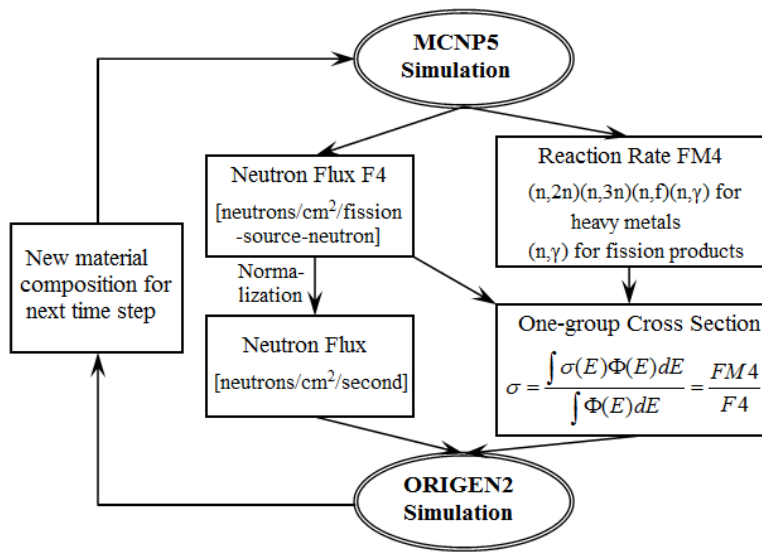

Fig. 1. MCNP5-ORIGEN coupling flow diagram

This coupler provides full capabilities of the Monte Carlo code MCNP5 and the versatile nuclides depletion and decay code ORIGEN2. It makes use of the tally information of MCNP5 to get neutron fluxes and nuclides cross-sections, which are processed to obtain input information of ORIGEN2 for every active cell. After running ORIGEN2, the coupler exploits the depletion and decay information from ORIGEN2 output files and provides the material compositions of all active cells for the next time step. The coupling procedure is illustrated in Fig. 1. The normalization of the neutron flux values obtained by MCNP5 and the generation of the one-group cross sections for performing ORIGEN2 calculations are presented in sections 2.3 and 2.4, respectively.

C. Neutron flux normalization

Since all tallies in MCNP5 are normalized as per fission source neutron, the flux values are in units of (number-of-neutrons)/(fission-source-neutron)/cm^2, which needs to be multiplied by a constant factor to convert into (number-of-neutrons)/(cm^2.second) for using in ORIGEN2. The constant factor can be calculated based on the power of the system. The system producing power P needs $\frac{P}{w_f}$ fissions per second, where w_f denotes effective energy released per fission event. Although the value of w_f will vary somewhat with the type of reactor and the detailed core composition, it is typically taken by 198 MeV for steady state condition. This fission rate produces $\frac{P\bar{\upsilon}}{w_f}$ neutrons per second, where $\bar{\upsilon}$ denotes the average number of neutrons released per fission. For subcritical and supercritical systems, one should multiply the above result by $\frac{1}{k_{eff}}$ to maintain the critical i.e. steady-state power level system (k = 1). Accordingly, the following equation (2) [15] should be used to normalize the F4 flux tally (Φ_{F4}):

$$\Phi\left[\frac{neutron}{cm^2 s}\right]=\frac{P[W]\bar{\upsilon}\left[\frac{neutron}{fission}\right]}{\left(1.6022\times10^{-13}\frac{J}{MeV}\right)w_f\left[\frac{MeV}{fission}\right]}\frac{1}{k_{eff}}\Phi_{F4}\left[\frac{1}{cm^2}\right] \quad (2)$$

where Φ denotes the actual total neutron flux in the system.

D. Cross-section calculation

ORIGEN2, unlike MCNP5, uses one-group cross sections which are averaged for all energies, whereas in MCNP5, cross sections are available for all energy points. Therefore one can use MCNP5 to generate a mean cross section for all energies, which can be used in the ORIGEN2 code to update the one-group cross-section library. Such MCNP5 calculation can be done by using the F4 and FM4 tallies. The F4 tally gives neutron flux in a cell while the FM4 tally can multiply flux by cross sections in all energy points for each isotope and each reaction. Finally, the dividing FM4 value by F4 value can give a one-group cross section for that isotope and for all important reactions. The Eq. (3) shows how the above approach will be done.

$$\sigma=\frac{\int_E \sigma(E)\Phi(E)dE}{\int_E \Phi(E)dE}=\frac{FM4}{F4} \quad (3)$$

For fission products, only neutron capture cross sections are calculated since their principal effect is due to neutron absorption. For actinides, four type of cross sections are considered including (n,γ), (n,f), (n,2n), and (n,3n) reactions because actinides are important in terms of generating fission source neutrons and transforming into higher-mass actinides (see Eq.(1)).

Because of the excessive computer time and the unavailability of many MCNP5 cross-sections, only a limited set of libraries of

important nuclides, 24 actinides and 61 fission products, were updated by using MCNP5 as shown in Table I. In ORIGEN2 depletion calculations, the cross sections, which are not provided by MCNP5, are taken from the ORIGEN2 one-group cross section library PWRU.LIB (PWR library, thermal spectrum) which includes 129 actinides and 879 fission products. The cross sections for most of the isotopes are obtained from ENDF/B-IV, ENDF/B-V, and ENDF/B-VI, while for the others, data from libraries evaluated at different laboratories are used. Because the MCNP5 cross section libraries are only available at certain temperatures (293, 600, 900, 1200K), libraries of U-235, U-238, Pu-239 were created from JEFF3.2 at 1027K (the required benchmark temperature) by the NJOY99 code [16] in order to consider the Doppler broadening of resonance cross sections of these three important isotopes.

Table I. List of nuclides were updated the one-group cross sections library using MCNP5

24 Actinides	U-234, U-235, U-236, U-237, U-238, U-239, Np-236, Np-237, Np-238, Np-239, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Pu-243, Am-241, Am-242, Am-243, Cm-242, Cm-243, Cm-244, Cm-245, Cm-246
61 Fission products*	Kr-83, Y-89, Zr-91, Zr-92, Zr-93, Zr-94, Zr-96, **Mo-95**, **Tc-99**, **Ru-101**, Ru-103, **Rh-103**, **Rh-105**, Pd-104, **Pd-105**, Pd-106, **Pd-108**, **Ag-109**, Cd-110, Cd-111, Cd-112, Cd-113, I-127, I-129, **I-135**, Xe-130, **Xe-131**, Xe-132, Xe-134, **Xe-135**, Xe-136, **Cs-133**, **Cs-134**, Cs-135, Cs-137, Ba-138, **Pr-141**, **Nd-143**, **Nd-145**, Nd-147, Nd-148, **Pm-147**, **Pm-148**, **Pm-149**, **Sm-147**, **Sm-149**, **Sm-150**, **Sm-151**, **Sm-152**, Eu-151, Eu-152, **Eu-153**, **Eu-154**, **Eu-155**, **Gd-152**, **Gd-154**, **Gd-155**, **Gd-156**, **Gd-157**, **Gd-158**, **Gd-160**
Library in MCNP5	JEFF3.2 (U-235, U238, Pu-239) (Created by NJOY99) ENDL92 (Np-236, Np-238) LANL (U-239) ENDF/B-IV, ENDF/B-V, ENDF/B-VI (other nuclides)
Library's temperature	1027K (U-235, U-238, Pu-239) (Created by NJOY99) 880.8K (Xe-135) 293.6K, 300K (other nuclides)

*34 FPs shown in bold characters are important in reactivity prediction [17]. These 34 FPs were used for criticality calculation in MCNP5.

III. BENCHMARK ANALYSIS

The MCNP5-ORIGEN2 coupling scheme was validated through predicting the neutronic and isotopic behavior of a VVER-1000 LEU benchmark assembly [14]. The results of coupling calculations were compared with those of several burnup codes including MCU, TVS-M, WIMS8A, HELIOS, Multicell and to the Benchmark Mean (BM) values. Each MCNP5 run was done with 50 millions neutron histories that lead to a statistical error of about ±10 pcm (±1σ) for *k-inf*. This section presents the specification of the VVER-1000 LEU assembly (section 3.1) and the analysis and discussion about the calculated results (sections 3.2-3.4).

A. VVER-1000 LEU assembly benchmark specification

The VVER-1000 LEU hexagonal assembly consists of one central tube, 18 guide tubes, and 312 fuel pin locations (12 of which are gadolinium rods - UGD). The hexagonal lattice pitch of the assembly is 23.6 cm. The fuel pins, which are cylindrical and cladded with Zirconium alloy have a pitch of 1.275 cm. The benchmark assembly is shown in Fig. 2 and consists of fuel rods with 3.7 wt.% enrichment. Cell numeration in the 1/6 of the fuel assembly for simulating different isotopic composition is as shown in Fig. 3.The 12 UGD pins have a ^{235}U enrichment of 3.6 wt.% and a Gd_2O_3 content of 4.0 wt.%. Descriptions of material composition of fuel pins, cladding and moderator are given in Table II.

The calculations are performed under hot operating poisoned condition, i.e. at T_{fuel} = 1027K, $T_{moderator}$ = 575K with equilibrium ^{135}Xe and ^{149}Sm concentrations, a power density of 108 MWt/m^3 up to a burnup of 40 MWd/kgHM. The burnup calculation is realized with 30 steps of 0.5 MWd/kgHM and 10 step of 2.5 MWd/kgHM. The Gd rods are divided into 10 annuli of equal area in order to account for the shielding effect due to gadolinium isotopes. This permits us to easily calculate the nuclides concentrations as a function of the radial position (5 regions required in benchmark document [14]).

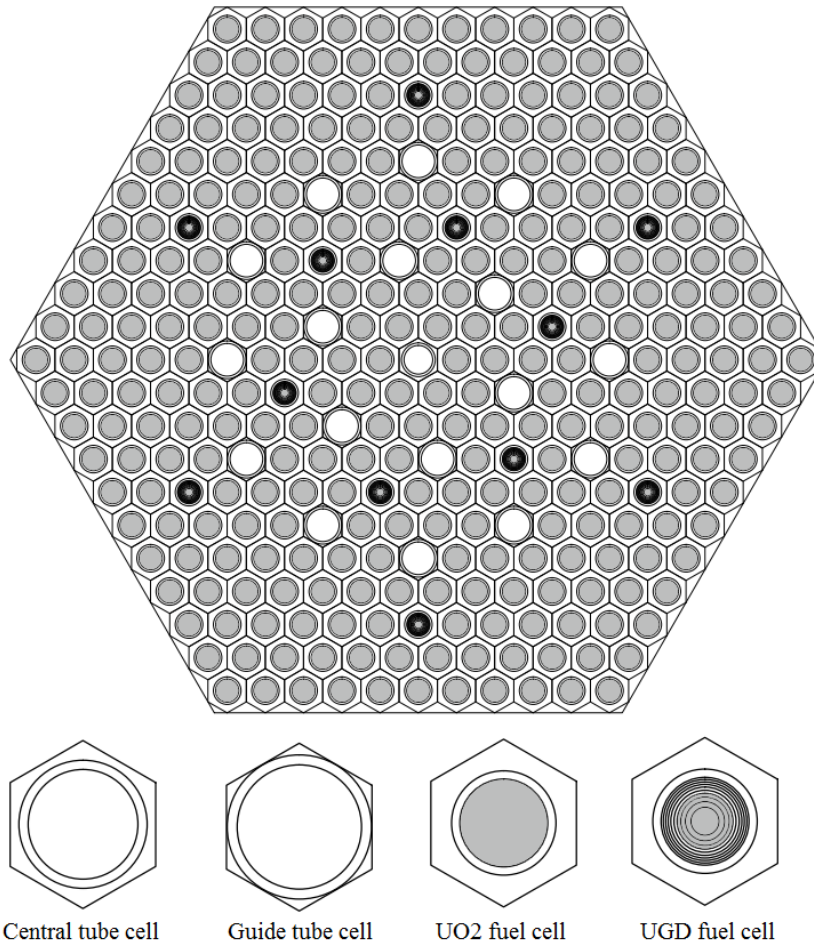

Fig. 2. MCNP5 model of the VVER-1000 LEU benchmark assembly

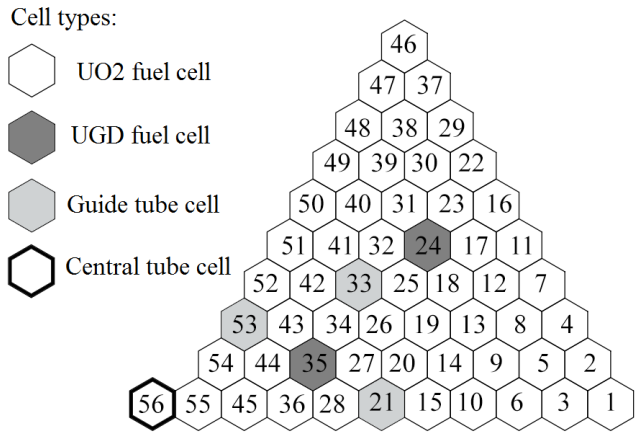

Fig. 3. Cell numeration in the 1/6 of the benchmark assembly

Table II. Material composition of the VVER-1000 LEU benchmark assembly

Material name	Comment	Isotopic content (atoms/barn-cm)			
UO2	LEU fuel 3.7 w/o enrichment	^{235}U	8.6264E-4	^{16}O	4.6063E-2
		^{238}U	2.2169E-2		
UGD	LEU fuel of 3.6 w/o of ^{235}U containing 4 w/o of Gd_2O_3	^{235}U	7.2875E-4	^{155}Gd	1.8541E-4
		^{238}U	1.9268E-2	^{156}Gd	2.5602E-4
		^{16}O	4.1854E-2	^{157}Gd	1.9480E-4
		^{152}Gd	2.5159E-6	^{158}Gd	3.0715E-4
		^{154}Gd	2.7303E-5	^{160}Gd	2.6706E-4
Cladding	Zirconium alloy	Zr	4.259E-2	Hf	6.597E-6
		Nb	4.225E-4		
Moderator	Light water with 0.6 g/kg of boron, Tm = 575K, d = 0.7235 g/cm^3	H	4.483E-2	^{10}B	4.794E-6
		^{16}O	2.422E-2	^{11}B	1.942E-5

B. K-inf versus burnup

The infinite multiplication factor (*k-inf*) of the VVER-1000 LEU Benchmark Assembly was calculated with respect to burnup using MCNP5-ORIGEN2 coupling scheme and compared with those obtained by the aforementioned burnup codes as shown in Fig.4 The differences in the *k-inf* values of these codes from benchmark mean values are also shown separately in Table III.

Table III shows that, the k-inf results obtained using MCNP5-ORIGEN2 are in satisfactory agreement with the results estimated by the rest of burnup codes. The k-inf values between MCNP5-ORIGEN2 coupling scheme and the BM values are slighly different in beginning burnup steps and then the difference increases in later ones. The maximum of the deviation with BM values are 440, 400, 460, 260, 360, 585 pcm for MCU, TVS-M, WIMS8A, HELIOS, MULTICELL, and MCNP5-ORIGEN2, respectively. As can be seen in Figure 4, at the beginning, the reactivity slightly increases with burnup due to the use of Gd_2O_3 in UO2 for core reactivity control. As the gadolinium isotopes burn out, the reactivity starts to decrease with burnup in a roughly linear manner due to the effect of fissile material depletion and neutron-absorber accumulation. It is obviously seen that the effect on reactivity of the gadolinium absorber is well simulated by the MCNP5-ORIGEN2 coupling scheme.

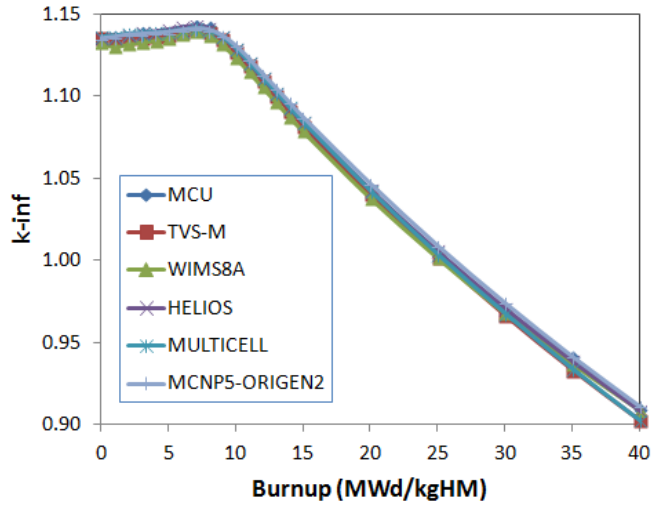

Fig. 4. Variation of k-inf with burnup for VVER-1000 LEU Benchmark Assembly

Table III. Deviation of k-inf values from benchmark mean values

Burnup (MWd/kgHM)	Deviation from BM Values, pcm					
	MCU	TVS-M	WIMS8A	HELIOS	MULTICELL	MCNP5-ORIGEN2
0	30	30	-220	50	130	14
1	150	-40	-460	120	210	117
2	-30	-20	-390	200	250	167
3	180	-110	-400	170	160	84
4	40	-80	-320	220	160	111
5	50	-100	-270	220	90	44
6	70	-110	-210	200	30	12
7	140	-100	-210	170	10	-24
8	210	-100	-290	140	40	51
9	-30	-10	-290	180	160	228
10	70	-40	-370	140	180	315
11	-70	0	-350	180	240	432
12	30	-40	-380	160	210	413
13	-60	-20	-360	180	230	485
14	80	-50	-380	160	200	471
15	20	-40	-350	180	210	489
20	-80	-60	-280	240	160	585
25	30	-140	-190	250	50	556
30	140	-240	-80	250	-80	546
35	440	-390	10	200	-280	466
40	260	-400	230	260	-360	493

C. Isotopic composition versus burnup

Figs. 5-15 display the MCNP5-ORIGEN2 calculations for the isotopic composition variation as a function of burnup of nuclides ^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{135}Xe, ^{149}Sm, ^{155}Gd and ^{157}Gd, respectively in cell-1 and cell-24 of the VVER-1000 LEU benchmark assembly in comparison with the benchmark mean values [14], where we can see a good agreement. It should be noted that the deviations obtained from the comparison mentioned above at the end of the burnup (40 MWd/kgHM) are generally within 6.5% as shown in Table IV.

As can be seen in Figs. 14-15, the depletion of the burnable absorbers ^{155}Gd and ^{157}Gd is well simulated in the MCNP5-ORIGEN2 coupling scheme. The figures show that ^{157}Gd depletes faster than ^{155}Gd due to its higher absorption cross section ($^{155}\sigma_a$ = 60,801 barns and $^{157}\sigma_a$ = 253,929 barns at thermal neutron 0.0253 eV). Despite the deviation from BM values of ^{157}Gd isotope in gadolinium bearing fuel rod exceeds 15%, this percentage of the small concentration of ^{157}Gd (1.469E-7 atoms/barn-cm at the end of cycle) is negligible in the burnup calculation. The results from MCORE, an MCNP4C-ORIGEN2.1 coupling code, developed by Meiyin Zheng et. al. in 2013 [10] showed a better agreement with the BM values. In MCORE's results, the deviation from BM value at 40 MWD/kgHM is only -2.0% for ^{157}Gd when compare with -15.07% in this research. One of the reason is MCORE considered 37 actinides and 101 fission products in burnup calculations when compare with 24 actinides and 61 fission products in this work. In MCORE, the NJOY system code was also used to process the source evaluated nuclear data files into libraries useable for MCNP code. Another reason for the more accurate results in MCORE is that the code considered (n,γ), (n,2n), (n,α) and (n,p) reactions for updating fission product's libraries while this study only considered (n,γ). Besides, MCORE obtained more reliable results due to the burnup calculation was realized with 60 steps of 0.25 MWD/kgHM and 50 steps of 0.5 MWD/kgHM when compare with only 30 steps of 0.5 MWD/kgHM and 10 steps of 2.5 MWD/kgHM in this work.

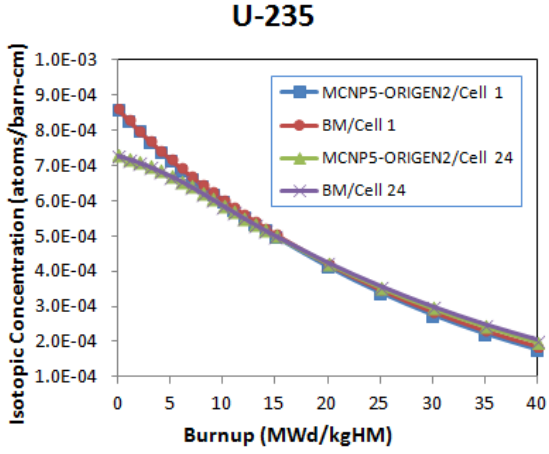

Fig. 5. ^{235}U isotopic composition as a function of burnup

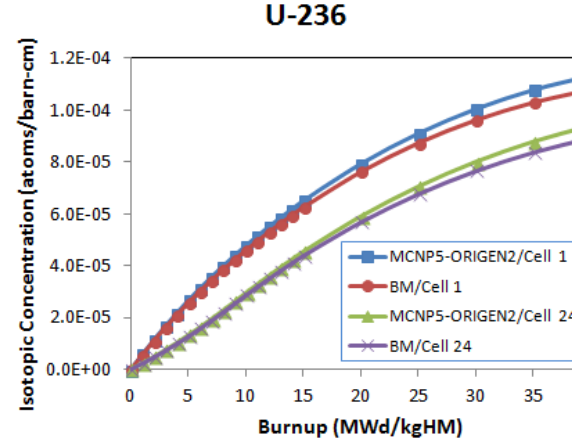

Fig. 6. ^{236}U isotopic composition as a function of burnup

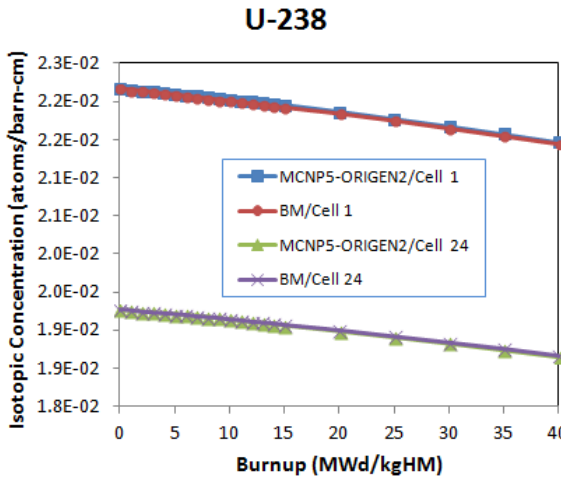

Fig. 7. ^{238}U isotopic composition as a function of burnup

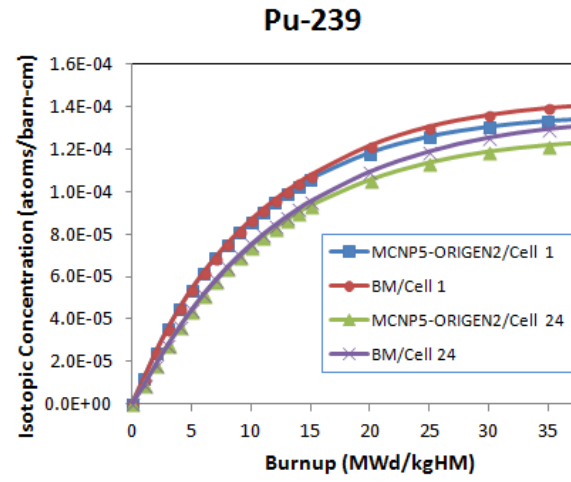

Fig. 8. ^{239}Pu isotopic composition as a function of burnup

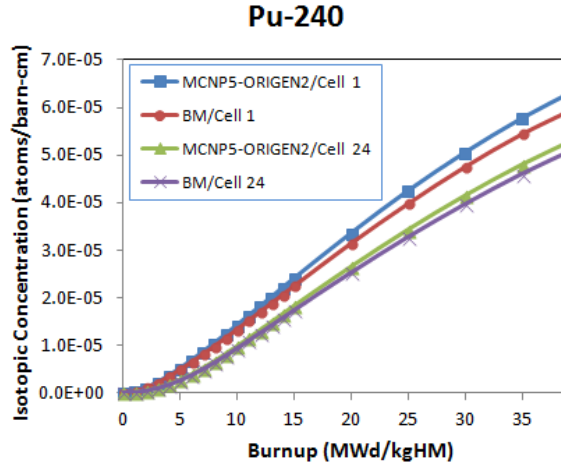

Fig. 9. ^{240}Pu isotopic composition as a function of burnup

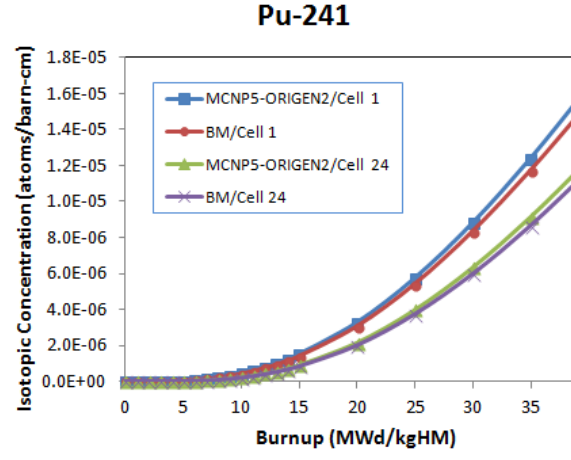

Fig. 10. ^{241}Pu isotopic composition as a function of burnup

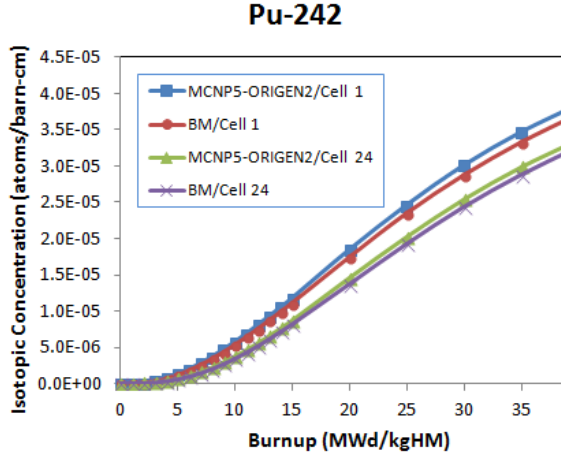

Fig. 11. ^{242}Pu isotopic composition as a function of burnup

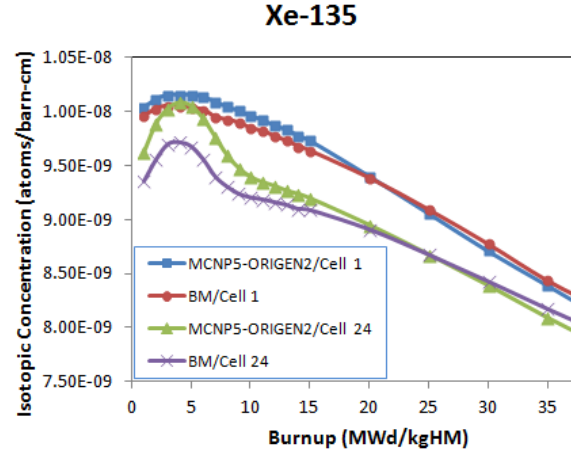

Fig. 12. ^{135}Xe isotopic composition as a function of burnup

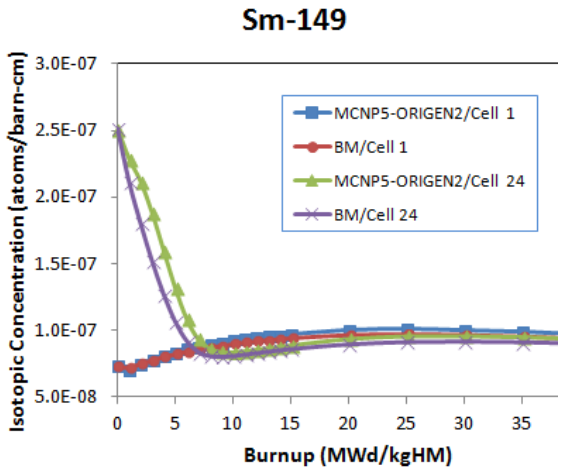

Fig. 13. ^{149}Sm isotopic composition as a function of burnup

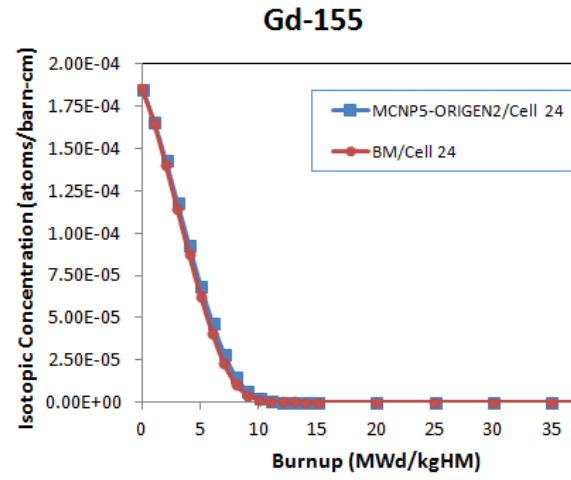

Fig. 14. ^{155}Gd isotopic composition as a function of burnup

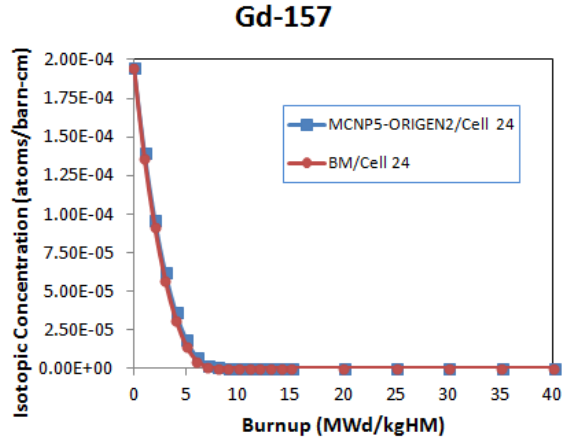

Fig. 15. ^{157}Gd isotopic composition as a function of burnup

Table IV. Isotopic composition error (%) compared to BM values at 40 MWd/kgHM

Isotope	^{235}U	^{236}U	^{238}U	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{135}Xe	^{149}Sm	^{155}Gd	^{157}Gd
Cell 1	-4.82	4.99	0.07	-4.69	6.29	3.78	6.20	-1.07	3.52		
Cell 24	-3.30	4.89	-0.09	-6.14	3.81	3.18	5.50	-1.45	4.16	-1.42	-15.07

D. Isotopic composition versus fuel volume radius

As mentioned in section 3.1, every UGD rod has radial sub-divisions (10 rings) in order to take into account the shielding effect due to gadolinium. In this section, the concentration of some isotopes in 5 zones (each zone consists of 2 rings) of cell 24 (see Fig. 3) were calculated and compared with benchmark mean values. The isotopic compositions in five fuel-gadolinium pin radial zones for burnup point 40 MWd/kgHM (^{235}U and ^{239}Pu) and for burnup point 2 MWd/kgHM (^{155}Gd and ^{157}Gd) are presented in Figs. 16-19. The radial distributions of the ^{235}U, ^{239}Pu and ^{155}Gd calculated by MCNP5-ORIGEN2 coupling scheme showed good agreement with the benchmark results. In detail, the deviation between MCNP5-ORIGEN2 coupling scheme and BM composition for ^{235}U, ^{239}Pu and ^{155}Gd

in outer zone are only -3.6%, -5.28% and 6.69% as shown in Table V, respectively. The ^{157}Gd concentration, however, had a huge deviation of nearly 50% in the outer zone as compared to the BM value. This is due to the fact that ^{157}Gd has neutron absorption cross-section larger than ^{155}Gd and therefore it burns most in the outer zone. Consequently, the concentration of ^{157}Gd at outer zone is small and leads to a large statistical error.

One can see from Fig. 17 that the gradient in ^{239}Pu concentration falls off nearly exponentially within the fuel volume. This is due to the spatial resonance self-shielding, there are more ^{238}U absorptions in the outer ring. More ^{239}Pu, therefore, is produced towards the surface of the fuel pellet. Such ^{239}Pu-formation by the neutron resonance absorption is well known via the so-called "rim effect". As the burnup increases, the local burnup in the fuel close to the surface is largely increased due to ^{239}Pu-formation and therefore the "rim effect" becomes more predominant at high burnup as can be seen in Fig. 20.

Figs. 18-19 show that gadolinium mostly burns in the outer rings due to the high absorption cross section of ^{155}Gd and ^{157}Gd. Gadolinium burning shifts toward the inner rings with fuel burnup until all gadolinium isotopes burn out such as the depletion of ^{157}Gd as shown in Fig. 21.

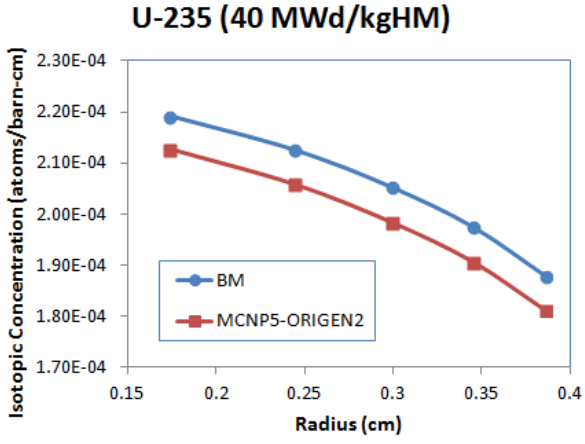

Fig. 16. ^{235}U isotopic composition versus radius

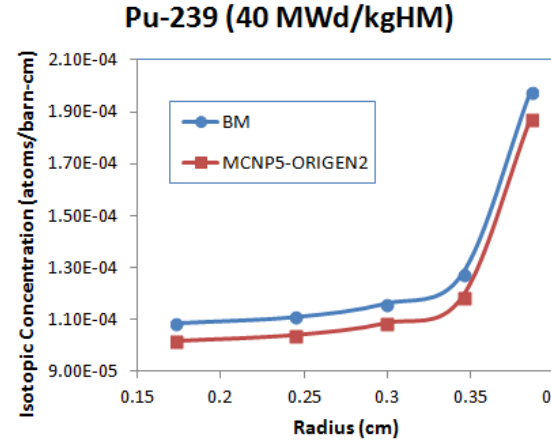

Fig. 17. ^{239}Pu isotopic composition versus radius

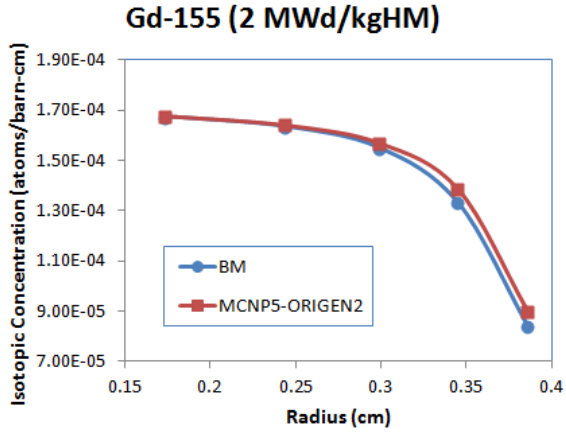

Fig. 18. ^{155}Gd isotopic composition versus radius

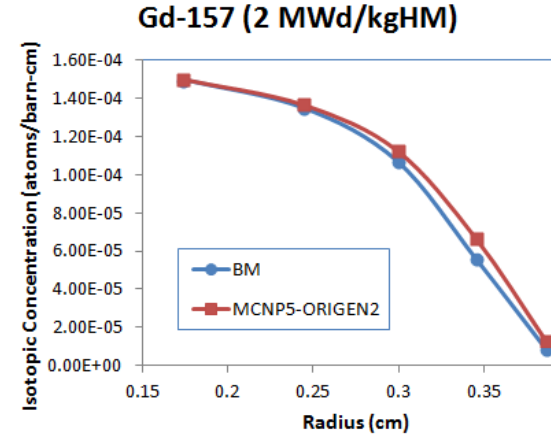

Fig. 19. ^{157}Gd isotopic composition versus radius

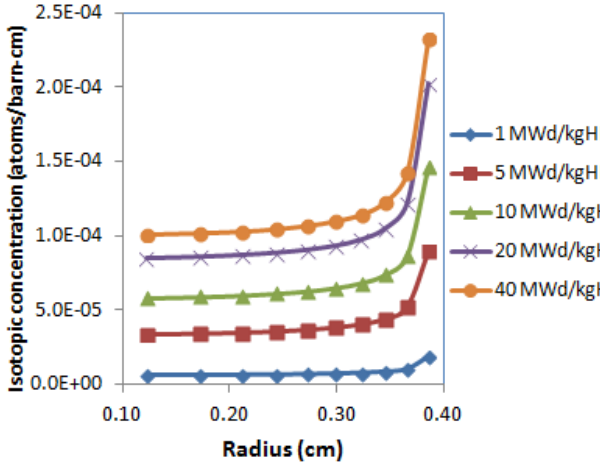

Fig. 20. Depletion of ^{239}Pu as a function of the radial position with burnup change

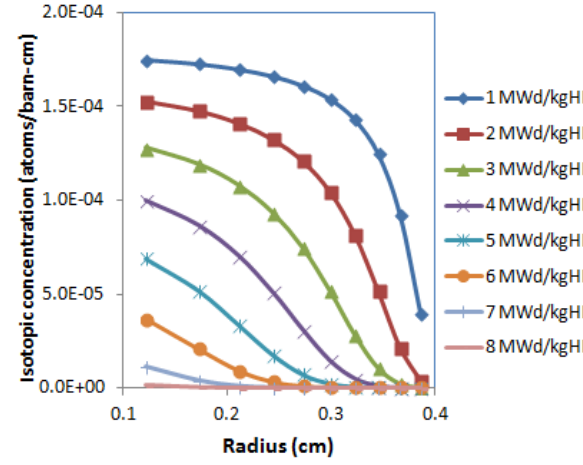

Fig. 21. Depletion of ^{157}Gd as a function of the radial position with burnup change

Table V. Error (%) of isotopic composition in cell-24 vs radius compared to BM values; Burnup=40 MWd/kgHM for ^{235}U, ^{239}Pu; Burnup=2 MWd/kgHM for ^{155}Gd, ^{157}Gd

Radius, cm		0.173	0.244	0.299	0.345	0.386	
Zone		1	2	3	4	5	average
Error (%)	^{235}U	-2.98	-3.20	-3.37	-3.48	-3.60	-3.30
	^{239}Pu	-6.41	-6.33	-6.57	-7.03	-5.28	-6.21
	^{155}Gd	0.14	0.32	1.21	4.00	6.69	1.96
	^{157}Gd	0.03	1.11	5.01	18.72	47.79	4.73

Table V shows the relative deviation from BM values of the isotopic composition in each zone of five annulars of equal area. The 'average' values are the comparison with BM values of the isotopic compositions of the entire fuel volume.

IV. CONCLUSIONS

In this paper, a burnup calculation for the VVER-1000 LEU benchmark assembly [14] through an MCNP5-ORIGEN2 coupling code has been performed. The coupling code was built based on the Monte Carlo neutron transport code MCNP5 and the versatile point depletion code ORIGEN2. The MCNP5-ORIGEN2 coupler can process the output files of MCNP5 and ORIGEN2 and then construct the input files automatically.

The calculation results of MCNP5-ORIGEN2 coupling scheme were compared with several other burnup codes and benchmark mean values from the benchmark document. The infinite multiplication factor (k_∞) and isotopic compositions of the important isotopes were compared and analyzed. The deviations between the obtained results and the BM values for the k_∞ were found within 600 pcm. At the end of burnup (40 MWd/kgHM) the differences of isotope compositions were generally within 6.5%. Moreover, the coupling scheme also reproduced well the isotopic composition behavior along the radius in the gadolinium bearing rods. This allowed us to conclude that the MCNP5-ORIGEN2 coupling scheme developed in this study can be applied for the burnup calculations of the VVER-1000 reactors.

However, potential errors can occur during the burnup calculation because of presence of the improper isotopic composition from strong absorbers like ^{157}Gd. Such errors can be reduced by using smaller time steps or integrate a predictor-corrector algorithm into the depletion calculation. Furthermore, all cross sections of the 1008 isotopes consisting of 129 actinides and 879 fission products should be updated through burnup time steps in order to avoid error accumulation. To do this, the cross section libraries, which are unavailable in MCNP5, should be created by using NJOY code [16]. Therefore, the future tasks needed are to (1) study the "modified predictor-corrector" method and integrate to the depletion calculation; (2) update one-group cross section libraries for more actinides and fission products; and (3) build up an MCNP5-ORIGEN2 coupling scheme for burnup calculation of VVER-1000 cores.

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