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.

1. Introduction

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 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 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.

2. Methodology

2.1. 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:

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

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.

2.2. Description of MCNP5-ORIGEN2 coupling procedure

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. The coupling procedure is illustrated in Fig. 1.

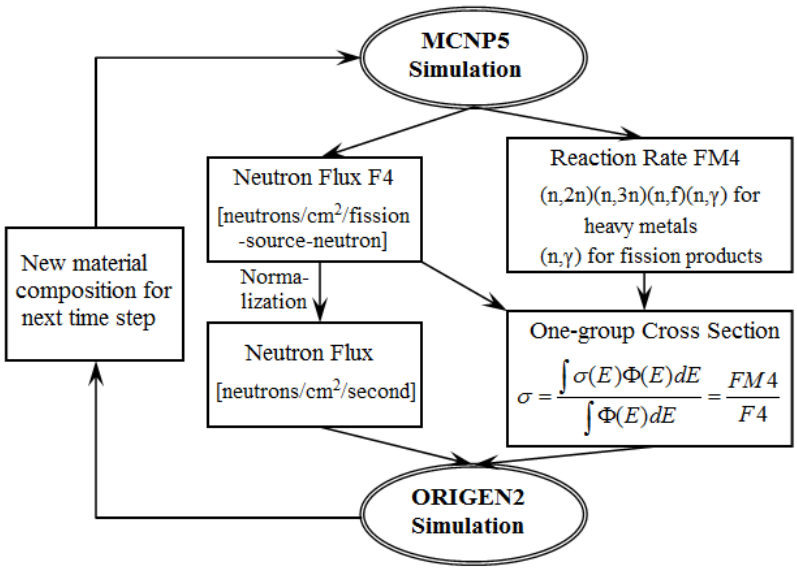

Fig. 1. MCNP5-ORIGEN coupling flow diagram

Since all tallies in MCNP5 are normalized as per fission source neutron, the flux values (Φ_{F4}) 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 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 is the actual total neutron flux in the system, P the power of the system, w_f the effective energy released per fission event, $\bar{\upsilon}$ the average number of neutrons released per fission.

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 ((n,γ), (n,f), (n,2n), and (n,3n)). The Eq. (3) shows how the above approach will be done.

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

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 1.

Table 1. 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 [16]) 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 [16]) 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.

3. 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).

3.1. 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.%.

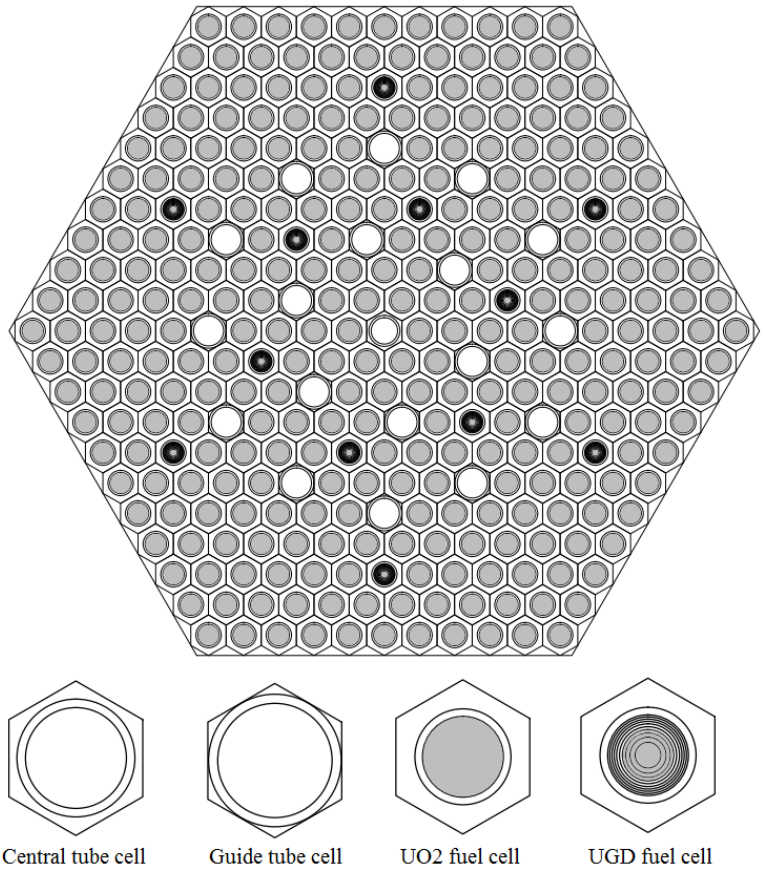

Fig. 2. MCNP5 model of the VVER-1000 LEU benchmark assembly

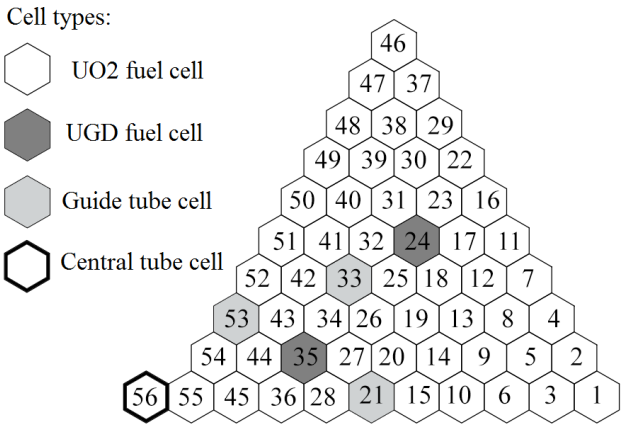

Fig. 3. Cell numeration in the 1/6 of the benchmark assembly

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]).

3.2. K-inf versus burnup

The infinite multiplication factors (*k-inf*) of the VVER-1000 LEU Benchmark Assembly were calculated with respect to burnup using MCNP5-ORIGEN2 coupling and compared to the *k-inf* values obtained by the aforementioned burnup codes as shown in Fig.4. As can be seen in Fig. 4, the results obtained using MCNP5-ORIGEN2 are in satisfactory agreement with the results estimated by the rest of burnup codes. At the beginning, the reactivity slightly increased with burnup with burnup due to the use of Gd_2O_3 in some fuel rods for core reactivity control. As the gadolinium isotopes burn out, the reactivity started 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 this MCNP5-ORIGEN2 coupling scheme. The deviation of MCNP5-ORIGEN2 calculations from BM values shown in Fig. 5 is within 600 pcm during entire 40 MWd/kgHM burnup time.

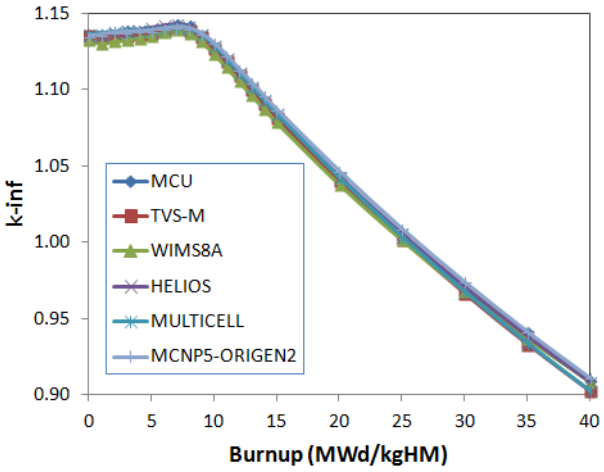

Fig. 4. Variation of k-inf with burnup for VVER-1000 LEU Benchmark Assembly

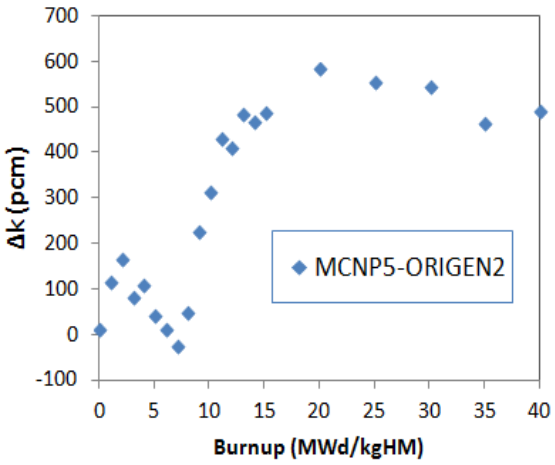

Fig. 5. Differences from BM values

3.3. Isotopic composition versus burnup

Figs. 6-11 display the MCNP5-ORIGEN2 calculations for the isotopic composition variation as a function of burnup of nuclides ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{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 2.

As can be seen in Figs. 10-11, 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.

Table 2. 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

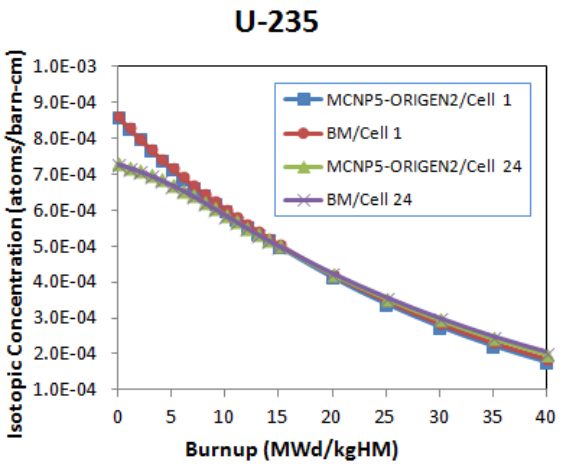

Fig. 6. ^{235}U isotopic composition as a function of burnup

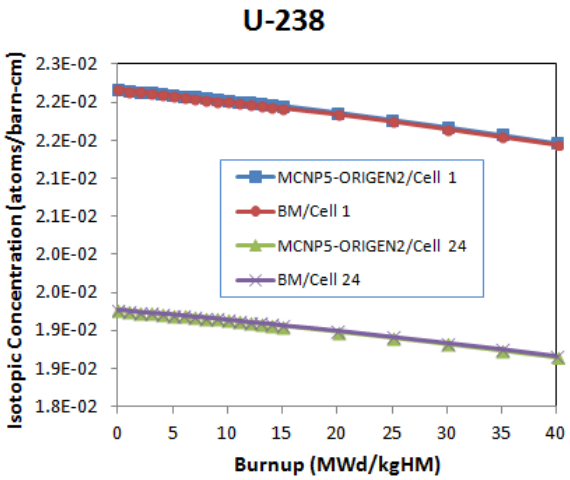

Fig. 7. ^{238}U isotopic composition as a function of burnup

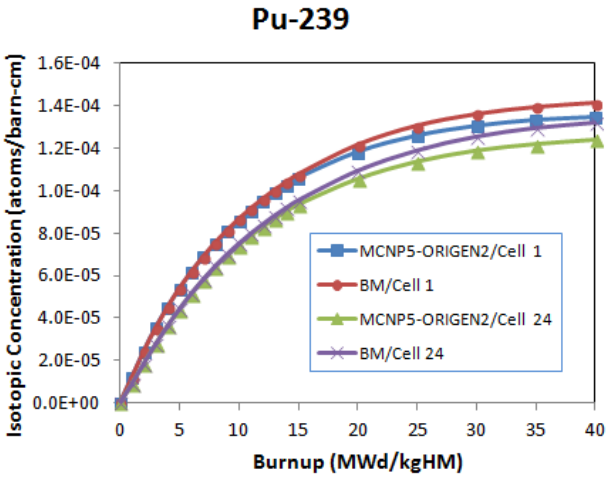

Fig. 8. ^{239}Pu isotopic composition as a function of burnup

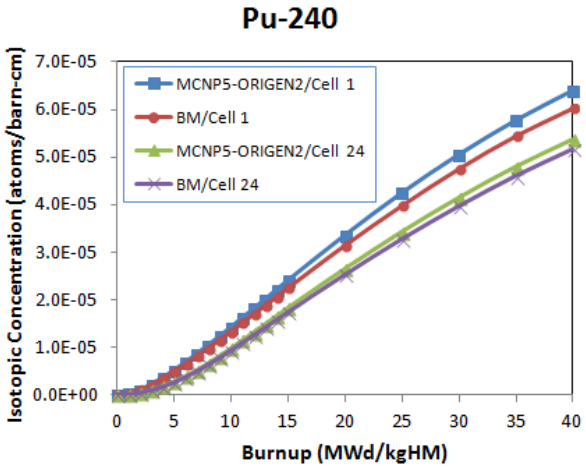

Fig. 9. ^{240}Pu isotopic composition as a function of burnup

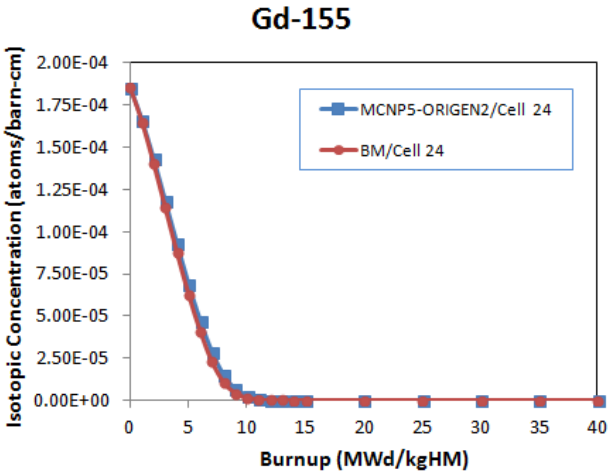

Fig. 10. ^{155}Gd isotopic composition as a function of burnup

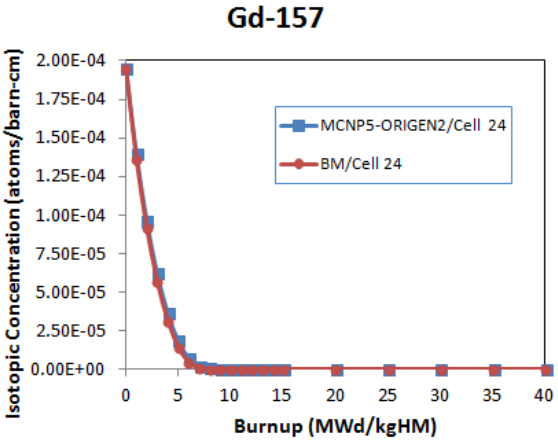

Fig. 11. ^{157}Gd isotopic composition as a function of burnup

3.4. 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 (^{239}Pu) and for burnup point 2 MWd/kgHM (^{157}Gd) are presented in Figs. 12-13 and showed good agreement with the benchmark results. In detail, the deviations between MCNP5-ORIGEN2 coupling scheme and BM compositions are shown in Table 3, 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. 12 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. 14.

Fig. 13 shows that gadolinium mostly burns in the outer rings due to the high absorption cross section of ^{157}Gd. Gadolinium burning shifts toward the inner rings with fuel burnup until all gadolinium isotopes burn out as shown in Fig. 15.

Table 3. Error (%) of isotopic composition in cell-24 vs radius compared to BM values; Burnup=40 MWd/kgHM for ^{239}Pu; Burnup=2 MWd/kgHM for ^{157}Gd

Radius, cm		0.173	0.244	0.299	0.345	0.386	
Zone		1	2	3	4	5	average
Error (%)	^{239}Pu	-6.41	-6.33	-6.57	-7.03	-5.28	-6.21
	^{157}Gd	0.03	1.11	5.01	18.72	47.79	4.73

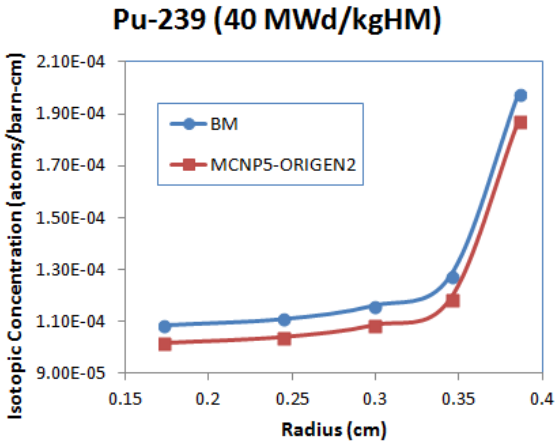

Fig. 12. ^{239}Pu isotopic composition versus radius

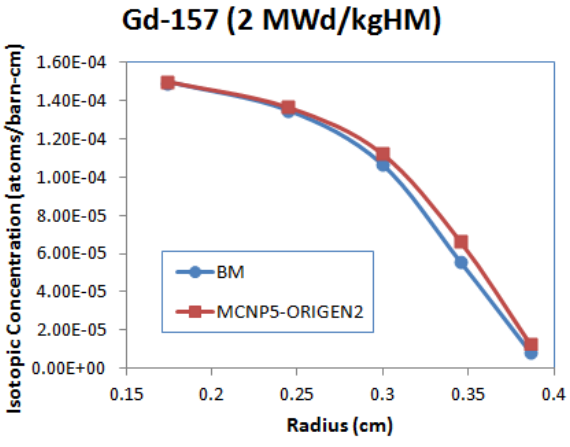

Fig. 13. ^{157}Gd isotopic composition versus radius

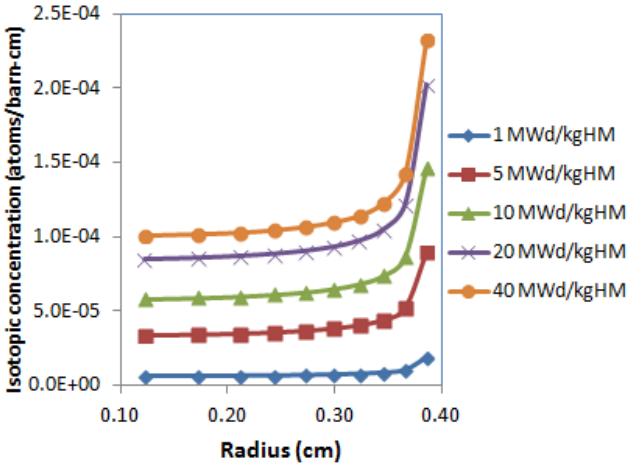

Fig. 14. Depletion of ^{239}Pu as a function of the radial position with burnup change

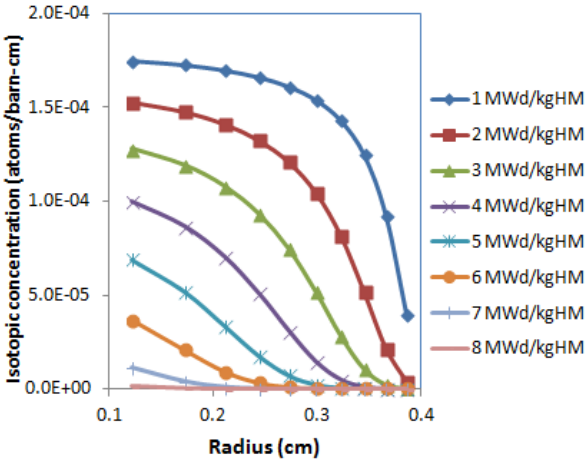

Fig. 15. Depletion of ^{157}Gd as a function of the radial position with burnup change

4. Conclusions

In this paper, a burnup calculation for the VVER-1000 LEU benchmark assembly [14] through an MCNP5-ORIGEN2 coupling program has been performed. 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 core.

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