Lumped pseudo fission products during burnup step in *MCNP5-ORIGEN* coupling system

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Abstract

Depletion calculation and accurate inventory of fission products in a nuclear system are required for criticality, safety and spent fuel management. Actual trend is to use Monte Carlo methods. It is well known that the fission process produces a large number of nuclides, some of which have a significant impact on the nuclear properties of the core and its behavior. In this study, we propose to determine the influence of fission products on the behavior of the IAEA 10 MW benchmark reactor. Even if nowadays we have powerful computing capability and we can solve the full system of fission products, such calculations are cumbersome and not needed because most of fission products have low absorption rates and therefore their precise concentrations calculation are not required. The practice is to identify and use only the nuclides which can have a significant absorption cross section.

From the entire fission products of the available fissionable actinides, 214 nuclides have been considered. Their selection was essentially based on their absorption rates. To carry out the calculation, 81 were treated explicitly and 133 were lumped into pseudo fission products.

A computational method has been developed for burnup and criticality calculations using *MCNP5-ORIGEN* coupling scheme. The *MIXE_ACE* program was developed and incorporated within this coupling scheme in order to mix and rewrite in *ACE* format the selected cross sections of the pseudo fission products for each burnup step. The mass weight of the constituent nuclides was used. The initial one group cross sections library for *ORIGEN* was generated using average flux spectrum in the core.

Using the above methodology, an estimation of k_{eff} and cross sections during depletion calculations has been carried out for the *IAEA 10 MW* reactor based on *UZrH1.6* fuel. The results are compared to those of *ANL (Argonne National Laboratory)*, *MCNP6* and other calculations by using selected fission products from *WIMS* library. Generally, the results are satisfactory but some discrepancies exist. The differences can be explained mainly by the nature of the fission products considered in the calculation and especially their cross sections.

Keywords: *MCNP5*, *ORIGEN*, *MCNP6*, Fission products, *UZrH1.6* fuel, End of cycle

1. Introduction

Nuclear systems require a reliable inventory of fission products for safety and waste management purposes. The fission process in the nuclear fuel causes the accumulation of fission products. Some of these products have a significant impact on the nuclear properties of the core and its criticality. The main objectives of the depletion calculations are to provide as much details as possible of the composition of the irradiated fuel and to quantify the radioactive inventory for potential source terms determination (D. Lopez Aldama et al).

Nowadays, several burnup calculation codes have been developed, such as the Multi-Step Monte Carlo Burnup Code System *MONTBURN* (RSICC PSR-455) and *MCNP-ORIGEN* burnup calculation system code *MCOR* (Meiyin Zheng et al). Along the same lines an *MCNP5-ORIGEN* coupling system was developed to study the absorption effect of the fission products in light water reactors.

In this paper we perform criticality calculation at different burnup steps by considering the fission products that have an important impact. One lumped pseudo fission product is generally used for burnup calculations. In our approach, the cross sections of the pseudo fission products are calculated in each burnup step to take into account the variation of the concentration of each nuclide during burnup step by the means of *MIXE_ACE* program, which can be used as a new module in *MCNP5-ORIGEN* coupled system. In this way, the inventory of fission products is established in each fuel assembly to get the end of cycle (EOC) with more precision. The developed scheme was applied to the initial fuel load (BOC, *Beginning of Cycle*) of IAEA 10 MW reactor which uses an *U_{Zr}H_{1.6}* fuel ($N_H/N_{Zr}=1.6$).

Since the *MCNP6* code (Denis B. Polowitz) allows burnup calculations, and in order to verify the obtained results and to validate the developed coupling scheme, burnup calculations have been carried out by *MCNP6* code using “burn” option with “tier3” fission products contents which have been treated explicitly.

2. Computational methods

2.1. Cross section processing

More than 450 fission products and the important fissionable nuclides were processed by using the comprehensive *NJOY* code system (RSICC PSR-480). *NJOY* is a modular computer code system used for processing and converting evaluated nuclear data in *ENDF* format into different types of data libraries that can be used in several applications, the 99+ version of the code was used. Evaluated nuclear data files for most nuclides are extracted from *ENDF/B-VII* (ENDF/B-VII.1) and from *TENDL2012* (Koning et al) for some nuclides. To produce point-wise data at 300 °K for the considered nuclides in *PENDF* files, the adapted sequence is the following: *MODER* (converts *ENDF* “tapes” back and forth between formatted and blocked binary modes), *RECONR*

(reconstructs energy-dependent pointwise cross sections), *BRODR* (Doppler-broadens), *HEATR* (heat production cross section), *GASPR* (gas production cross section), *THERMR* (scattering in the thermal energy range) and *PURR* (unresolved-region probability tables for the MCNP code) modules.

To produce *ACE* formatted files that are not available in *MCNP5* library, the *ACER* module has been used. For isotopes in isomeric states, the Zaid suffix has been changed (+50 to the ground state), ([Data Bank 2006](#))

2.2. Selection of the fission products

There are more than 1300 fission product yield data for each fissionable nuclide in the *ENDF/B-VII* fission product yield file ([Choong et al](#)). In this study, ~~from the fission products processed by *NJOY* code~~, only the nuclides that affect the criticality of the core during the fuel depletion have been taken into consideration, even if their radioactive decay constants are short. ~~In this way, the selection of the nuclides was essentially based on their absorption rates (fission yields and absorption cross sections). A total of 214 nuclides were identified, 81 nuclides were represented explicitly and 133 nuclides have been lumped into the pseudo fission product~~ ~~More precisely, only the highly absorbing fission products which satisfy $\gamma\sigma > 1.2 \times 10^{-8}$ barns, where γ and σ are the fission yield and the absorption cross section of the considered nuclides respectively ([A.Trkov](#)), have been selected. This assumption helps us to identify 214 fission products as important nuclides having significant effects on the criticality calculation.~~

In general, the fission products, which have large reactivity effects, are treated explicitly, and others are treated as a pseudo fission products.

Various fission product models were obtained by varying the above criterion and therefore the number of nuclides which must be treated explicitly. The models were carefully studied and tested. The condition is that the cross sections of the pseudo nuclide were calculated assuming infinite dilution but should provide the same criticality calculation if all fission products are treated explicitly. As a result of this study, our model was formed of 81 nuclides which were treated explicitly and 133 nuclides which were lumped into one pseudo nuclide as shown in ([Table1](#)).

[Insert Table 1.](#)

2.3. Lumped fission products cross sections

To generate cross sections for pseudo fission products used by *MCNP5* code, *MIXE_ACE* program was developed in order to mix and rewrite in *ACE* file cross sections for total, diffusion, (n,2n), (n,3n), (n,n'), (n, continuum), (n, γ), (n,p) and (n, α) reactions. Cross-sections of the pseudo fission products were calculated by adopting the mass weights of the constituent nuclides, linear-linear interpolation was applied. The mass weights were extracted from *ORIGEN* output for each burnup step. *MIXE_ACE* program uses, as input, the generated binary file, which contains the pertinent cross section for the all 214 selected fission product nuclides. This file was prepared from *PENDF* files

3. MCNP5- ORIGEN coupling system

A computational method has been developed for burnup calculation. The method uses the flux and reaction rates calculated by the General Monte Carlo N-Particle Transport Code *MCNP5* (Jeremy and al, 2003), developed by Los Alamos National Laboratory (*LANL*), and the *ORIGEN* computer code (M.J. Bell) intended to determine the fuel isotopic composition after irradiation. The *ORIGEN* code, developed for depletion calculation, uses zero-dimensional geometry and one group cross section. The code did not take account of spatial or resonance self-shielding effects or changes in neutron spectra other than embodied initially which is in accordance with our proposed scheme. For each burnup step in our coupling system six tasks are performed Fig 1:

- 1) Criticality calculation of the considered reactor core for initial concentrations by using *MCNP5* code. We obtain the multiplication factor, deposited power and one energy group average flux in each fuel assembly as well as the reaction rates for the considered nuclides of the fuel.
- 2) One group cross sections calculations using the average flux and reaction rates for each fuel assembly from the earlier *MCNP* output.
- 3) *ORIGEN* library updating by using the new obtained cross section sets.
- 4) New isotope concentrations calculations for burnup time-step, including a predictor-corrector scheme; hence a twice run of *ORIGEN* is performed for each fuel assembly.
- 5) Cross sections (*XS*) mixing for lumped fission product using the new concentrations.
- 6) *ACE* file updating for the pseudo fission product.

This sequence is repeated in an automatic way until the end of cycle (*EOC*, $K_{eff} \leq 1$), or until the number of prefixed burnup cycles is reached.

Insert Fig. 1.

4. Benchmark problem modeling

4.1. Core description

The *IAEA-10 MW* reactor is based on *UZrH1.6* fuel core. It consists of 6×6 grid core, containing 30 fuel cluster elements which have a 16 fuel rods in 4×4 square array, 4 control rods fully withdrawn from the core and two irradiation channels as shown in [Fig.2](#). In this study, we consider the case when the core is reflected by light water on the 4 sides. The cluster is contained within rectangular aluminum shroud with inner dimensions forming a 6.805 cm square and two different thicknesses of 0.384 cm and 0.579 cm. The fuel rod is 1.377 cm in diameter and active length of 55.88 cm, it is clad with 0.041 cm thickness of Incoloy 800. Detailed specifications of this benchmark are described in [Table 2 \(TECDOC 233\)](#).

[Insert Fig. 2.](#)

[Insert Table 2.](#)

4.2. *ORIGEN* library

For the *UZrH1.6* benchmark core, a specific *MCNP5* model is adopted considering only fresh fuel for all fuel assemblies and F4 tally in 450 energy intervals. This model is used to calculate average neutron energy spectrum. *MCNP5* provides the average flux between the two ends of each interval. To calculate the flux values in the considered points, we can suppose the flux as constant or linear between the two points. The results of the two assumptions are very close to each other and the curve of the average flux is presented in [Fig. 3](#).

[Insert Fig. 3.](#)

It is seen that the flux is nearly Maxwellian between 0 and 0.55 eV and is linear along the interval [0.55 eV, 100 keV].

One group average cross sections were calculated for more than 450 fission products and important fissionable nuclides. The calculations were carried out by averaging the desired cross sections in *PENDF* files produced by *NJOY* over the considered flux spectrum. The light water *ORIGEN* library was subsequently updated by the calculated one group cross sections.

4.3. MCNP Model for burnup calculation

A three dimensional model of the benchmark reactor was set up considering each fuel cluster separately Figs. 4 and 5. In total, 30 fuel regions were considered, each region and each nuclide have been treated explicitly, and pertinent tallies have been requested to calculate average flux, average deposited energy and reaction rates for (n,fission) and (n, γ) reactions from 0 to 20 MeV in concordance with the one group *ORIGEN* depletion calculations. Reactions of types (n,p), (n, α), (n,2n) and (n,3n) were not considered in *MCNP* calculation because their variation with fuel depletion are very small compared to the fission and capture cross sections. These reactions were supposed to be constant in *ORIGEN* calculations during burnup steps. *MCNP6* calculation is performed using the same model with burnup option and tier3 fission products contents.

Insert Fig. 4.

Insert Fig. 5.

5. Results and discussions

5.1. MCNP modeling Validation

In the *KCODE* calculations, a constant starting source was used. 300 inactive cycles were run, followed by 900 active cycles, each of 3,000 histories. The F7 tally was used to obtain average deposited energy in each fuel assembly and F4 tally for flux and reaction rates. The statistical error is less than 2% for flux, deposited energy, fission and capture rates.

To validate the *MCNP* model a comparison of the effective multiplication factor k_{eff} for initial core with *ANL* and *MCNP6* results was done. It should be noted that the k_{eff} for xenon equilibrium state in our calculation is estimated by considering the 214 fission products in the core after one hundred hours. The results are given in the following table 3:

Insert Table 3.

The results appear to be satisfactory for the beginning of cycle (*BOC*) and the reactor core model can be used to the study of the burnup for establishing the inventory of the fission products at the end of cycle. For Xenon equilibrium state, only the Xe-135 is considered in Argon National Laboratory results.

5.2. Burnup calculations:

Burnup calculations were performed using the *ORIGEN* code. The code was modified to allow automated calculation of each fuel assembly. *ORIGEN* uses the flux and cross sections such as calculated by *MCNP5*, and provides, as result, the inventory of the actinides and a very large number of fission products. The concentrations of the 214 selected nuclides with some other necessary actinides such as U-235, U-236, U-238, Pu-239, Pu-240, Pu-241 and Pu-242, have been extracted and employed to build the new input file for *MCNP5* code.

Considering the reactor core model, the *MCNP5-ORIGEN* coupling system was executed for *UZrH1.6* benchmark to calculate the effective multiplication factor as a function of burnup. The results are presented on [Figs. 6 and 7](#).

In a first calculation, all 214 fission products (FPs) were treated explicitly for our selection. The same work was carried out for the 135 fission products of the *WIMS* library ([D. Lopez Aldama et al](#)). These calculations were done to verify the results without considering the pseudo fission products. For *MCNP6* calculation, any pseudo fission product was considered [Fig.6](#)

[Insert Fig. 6.](#)

In this case, we note that a good agreement between our results (214 FPs) and those of *ANL*, the **differences** become significant when the concentrations of fission products become very important. Probably, some fission products and especially those in isomeric state are not considered by *ANL* calculation. These nuclides present substantial absorption cross sections and they are not considered in *WIMS* library and tier3 of *MCNP6*, which explains the large discrepancies in the results compared to our calculation.

Moreover, the obtained results with the nuclides of *WIMS* library are very close to those of *MCNP6*, even in “tier3” there are more fission products, but their cross sections are not very important and the variation of power with burnup is not considered in the calculation. Therefore, there is an important difference between *WIMS* fission products selection results and those of *ANL*. This difference can be explained by the absence of some fission products that affect the criticality calculation of the core in the *WIMS* library.

Repeating now the same calculation of k_{eff} with burnup using the pseudo fission products; in each burnup step, the 133 nuclides were lumped into a one pseudo fission product for our selection and 79 nuclides for *WIMS* library. The other nuclides were treated explicitly. The results are shown in [Fig. 7](#)

[Insert Fig. 7.](#)

When we consider a pseudo fission product in the calculation, we note a good agreement of the results compared to those when all fission products are treated explicitly as shown in [Fig. 7](#), particularly in the beginning of life. From 5000 *MWD*, the difference is small which can be neglected. This variation can be explained by the presence of some nuclides with absorption cross sections relatively important. On the other side, the results obtained when the pseudo fission product is introduced in the selected nuclides of *WIMS* library, coincides with those calculated without mixing.

The cross sections of the pseudo fission product were calculated assuming infinite dilution and adopting the mass weights of the nuclides without any self-shielding corrections in the pseudo composition. This assumption is used to identify the nuclides which compose the pseudo fission products. More than the highly absorbing nuclides are added to the pseudo fission product, more the results become unacceptable and the self-shielding correction will be necessary. Generally, the difference between the results of the criticality calculation is due essentially to the cross sections of the considered fission products, which should be carefully chosen.

In the following figure, we present (n,γ) one group absorption cross section as a function of burnup of the pseudo fission products calculated by *MCNP5* for 133 and 79 nuclides.

[Insert Fig. 8.](#)

To show the importance of the mixing cross sections of the lumped fission products in each burnup step, we present (n,γ) cross section of the pseudo fission products in the beginning and the end of load of the core for 133 nuclides and 79 fission products of *WIMS* library calculated by *MIXE_ACE* program in the following figures:

[Insert Fig. 9.](#)

[Insert Fig. 10.](#)

For *WIMS* library [Fig. 10](#), the difference between cross sections of the pseudo fission products is very small and can be neglected. In this case, we can consider only the cumulative yields data of the fission products for weighting cross-sections. But for our selection [Fig. 9](#), the difference is important, in particular in the thermal and epithermal regions, which can be easily explained by the significant change in the concentrations of different fission products during fuel depletion, and especially the nuclides representing important absorption cross section [Fig. 8](#).

6. Conclusion

The fission products are important for analyzing the core characteristics behavior with burnup and the determination of the end of cycle. The identification of the nuclides that affect the criticality of the core is very important, even if these nuclides have a short radioactive decay constant. It is customary to use pseudo fission products, their cross sections are calculated as weighted averages of the constituent's nuclides cross sections. The results obtained by the selection of 214 fission products are satisfactory and more realistic compared to other work (*ANL*). Also it is to be noted that the results with *WIMS* library nuclides are very close to those of *MCNP6*, which can be explained by assuming that the average absorption cross section of the fission products is in the same order of magnitude. In our opinion, the use of the *MCNP5-ORIGEN* coupled scheme and *MIXE_ACE* program for mixing cross section of the pseudo fission product in each burnup step gives more accurate results.

Acknowledgement

We thank the DOE for allowing the use of *MCNP* versions through the *GTRI* cluster.

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Table Captions

[Table 1:](#) Fission product nuclides, in bold those treated explicitly

[Table 2:](#) Benchmark specifications

[Table 3:](#) Eigenvalues for initial core

Figure Captions

[Fig.1.](#) Burnup calculation in *MCNP5-ORIGEN* computational method

[Fig.2.](#) XY Model for initial core, core burnup studies on 10 MW reactor using *UZrH1.6 LEU* Fuel

[Fig.3.](#) Average neutron flux spectrum in the fuel region

[Fig.4.](#) Radial Tally Cells

[Fig.5.](#) Axial Tally Cells

[Fig.6.](#) Variation of K_{eff} with burnup (All FPs treated explicitly)

[Fig.7.](#) Variation of K_{eff} with burnup considering the pseudo fission products

[Fig.8.](#) (n, γ) one group cross section of the pseudo fission products

[Fig.9.](#) (n, γ) cross section in the beginning and the end of cycle of the pseudo fission product (133 nuclides)

[Fig. 10.](#) (n, γ) cross section in the beginning and the end of cycle of the pseudo fission product (79 nuclides)

Fig. 3.

Fig. 4.

Fig. 5.

Fig. 6.

Fig. 7.

Fig. 8.

Fig. 9.

Fig. 10.

Table 1

No.Nuclide	No.Nuclide	No.Nuclide	No. Nuclide	No. Nuclide	No. Nuclide	No. Nuclide	No. Nuclide
1 Kr-83	28 Ag-109	55 Ce-142	82 Ga- 72	109 Sr-88	136 Cd-112	163 Sb-127	190 Pm-150
2 Kr-83M	29 Cd-113	56 Ce-143	83 Ge- 72	110 Sr-89	137 Cd-114	164 Sb-128	191 Sm-150
3 Y-89	30 Cd-113M	57 Ce-144	84 Ge- 73	111 Sr-90	138 Cd-115	165 Te-122	192 Sm-154
4 Y-90	31 In-115	58 Pr-141	85 Ge- 74	112 Zr-90	139 Cd-115M	166 Te-124	193 Sm-156
5 Y-91	32 Te-127	59 Pr-143	86 Ge- 76	113 Zr-92	140 Cd-116	167 Te-125	194 Eu-152M
6 Zr-91	33 Te-127M	60 Pr-145	87 As- 75	114 Zr-94	141 Cd-117M	168 Te-125M	195 Eu-154
7 Zr-93	34 Te-129M	61 Nd-143	88 As- 76	115 Zr-96	142 In-113	169 Te-126	196 Eu-157
8 Zr-95	35 I-129	62 Nd-144	89 As- 77	116 Nb-95M	143 In-115M	170 Te-128	197 Eu-158
9 Nb-93	36 I-131	63 Nd-145	90 Se- 76	117 Nb-96	144 Sn-117	171 Te-130	198 Gd-154
10 Nb-93M	37 I-133	64 Nd-146	91 Se-77	118 Mo-96	145 Sn-117M	172 Te-131M	199 Gd-156
11 Nb-95	38 I-135	65 Nd-147	92 Se-78	119 Mo-100	146 Sn-118	173 I-127	200 Gd-158
12 Mo-95	39 Xe-129	66 Nd-148	93 Se-79	120 Ru-100	147 Sn-119	174 I-130	201 Gd-159
13 Mo-97	40 Xe-131	67 Nd-149	94 Se-80	121 Ru-104	148 Sn-119M	175 Xe-128	202 Gd-160
14 Mo-98	41 Xe-131M	68 Pm-147	95 Se-82	122 Ru-106	149 Sn-120	176 Xe-130	203 Gd-161
15 Mo-99	42 Xe-132	69 Pm-149	96 Br-79	123 In-117M	150 Sn-121	177 Xe-134	204 Tb-159
16 T-99	43 Xe-133	70 Pm-151	97 Br-80M	124 Sn-115	151 Sn-121M	178 Xe-136	205 Tb-160
17 T-99M	44 Xe-133M	71 Sm-147	98 Br-81	125 Pd-106	152 Sn-122	179 Cs-134	206 Tb-161
18 Ru-99	45 Xe-135	72 Sm-149	99 Br-82	126 Pd-107	153 Sn-123	180 Cs-134M	207 Dy-160
19 Ru-101	46 Xe-135M	73 Sm-151	100 Kr-82	127 Pd-108	154 Sn-124	181 Cs-136	208 Dy-161
20 Ru-102	47 Cs-133	74 Sm-152	101 Kr-84	128 Pd-109	155 Sn-125	182 Cs-137	209 Dy-162
21 Ru-103	48 Cs-135	75 Sm-153	102 Kr-85	129 Pd-110	156 Sn-126	183 Ba-134	210 Dy-163
22 Rh-103M	49 Ba-135	76 Eu-151	103 Kr-86	130 Pd-111M	157 Sb-121	184 Ba-136	211 Dy-164
23 Rh-103	50 Ba-137	77 Eu-153	104 Rb-85	131 Pd-112	158 Sb-122	185 Ba-138	212 Dy-165
24 Rh-105M	51 Ba-140	78 Eu-155	105 Rb-86	132 Ag-111	159 Sb-123	186 Ce-140	213 Ho-165
25 Rh-105	52 La-139	79 Eu-156	106 Rb-87	133 Ag-112	160 Sb-124	187 Nd-150	214 Ho-166
26 Pd-105	53 La-140	80 Gd-155	107 Sr-86	134 Ag-113	161 Sb-125	188 Pm-148	
27 Ag-107	54 Ce-141	81 Gd-157	108 Sr-87	135 Cd-111	162 Sb-126	189 Pm-148M	

Table 2

Reactor design description	
Reactor type	Pool
Power level, MW	10
Number of standard fuel elements	30
Number of control fuel elements	0
Irradiation channels	1 at core center 1 at core edge
Lattice pitch, mm ²	77 × 81
Fuel rod loading, g	274
Moderator, coolant, reflectors	Water
Burnup status of core	Initial core
Fuel element description	
Fuel geometry	Rods
Fuel rods/standard Element	16
Fuel material	UZrH
Uranium enrichment, %	20
Uranium density, g/cm ³	3.72 (45 wt% U)
Fuel rod outer diameter, mm	12.95
Fuel rod active length, mm	558.8
Clad material	Incoloy 800
Clad outer diameter, mm	13.77
Clad thickness, mm	0.41
Shroud material	Aluminum
Shroud side dimensions, mm ²	75.72 × 79.63
Shroud thickness, mm	3.84 and 5.79
Rod center to center spacing, mm	16.33
Rod-rod clearance, mm	2.57
Rod-shroud clearance, mm	2.64
Clearance between shrouds, mm	1.37

Table 3

	<i>BOC</i>	<i>Xe Equilibrium</i>
Current calculation (<i>MCNP5</i>)	1.18624±0.0007	1.14974±0.00051
<i>MCNP6</i>	1.18838±0.0005	1.15319±0.00050
<i>ANL (REBUS-2)</i>	1.1864	1.1544