MCNP/WIMS MONTE CARLO BURNUP SIMULATIONS APPLIED TO TRIGA RESEARCH REACTOR

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ABSTRACT

Combination of the WIMSD5 and MCNP4B codes for criticality calculations of burned fuel cores in TRIGA research reactors was tested on a criticality experiment. Individual burnup of fuel elements was determined with the in-house code TRIGLAV. The WIMSD5 calculated burned fuel isotopic vector was compared to the isotopic vector calculated with the ORIGEN2.1 code in order to test accuracy of the WIMSD5/ORIGEN2.1 decay schemes. In addition, the differences between both codes were evaluated in terms of reactivity for different burnup levels. It was found out that both WIMSD5 and ORIGEN2.1 give similar isotopic vectors for burnups up to 20% burned ^{235}U, except of the larger differences in ^{95}Mo, ^{239}Pu and ^{236}U. In terms of the reactivity effect, larger differences between both codes were observed for ^{149}Sm, ^{151}Sm and ^{239}Pu. However, overall accuracy is still within 10% of the calculated burnup effect on the reactivity. The combined MCNP/WIMS code enables reliable criticality calculations of burned cores and well reproduces measurements on the TRIGA research reactor.

1. INTRODUCTION

Accurate criticality calculations of burned fuel systems have been gaining practical interest due to the problems related to reactor ageing, spent fuel management and reactor decommissioning. While the direct Monte Carlo depletion calculation is still too time-consuming, the more usual way is to link a deterministic depletion code with a Monte Carlo transport calculation code (e.g., Monteburns (1)). The main aim of this work was to test the application of WIMS burned fuel isotopic composition data in Monte Carlo criticality calculations with the MCNP code. Extensive sensitivity studies have been performed to test the accuracy of the WIMS calculated burned fuel isotopic composition and the results compared to the ORIGEN calculations. The combined MCNP/WIMS Monte Carlo burnup calculation approach has been tested on an experimental benchmark performed on the TRIGA Mark II research reactor in Ljubljana, Slovenia.

2. MATERIALS AND METHODS

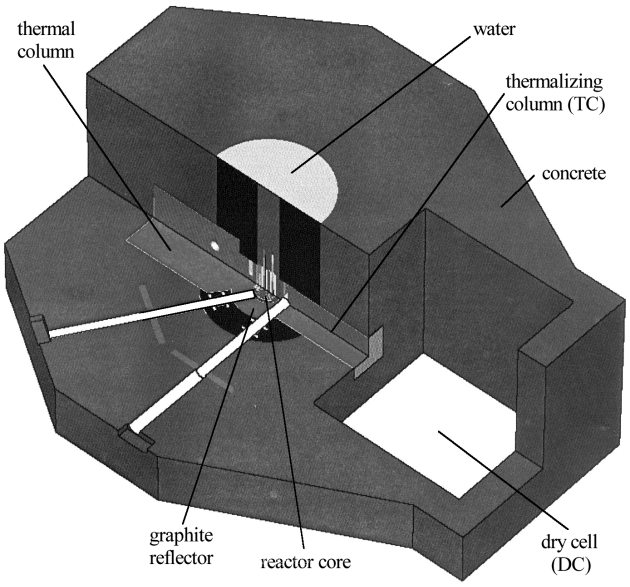
2.1 CALCULATIONS

The MCNP4B code (2) was used for Monte Carlo transport calculations. The cross section data for fresh cores were taken from the default MCNP cross section data libraries, which means that most of the used cross sections are from the continuous-energy ENDF/B-VI cross section libraries, except for the thermal cross sections, which are based on the ENDF/B-V evaluation. For burned fuel, the fission product cross sections are mostly from the KIDMAN library. Isotopic composition of the burned fuel was specified in MCNP based on the isotopic composition calculated by the WIMSD5 code (3) in a multigroup unit-cell approximation using data from WLUP project based on the ENDF/B-VI library (4, 5). The so-called pseudo fission product, as defined in the WIMSD5 library, was not included in the MCNP burned fuel material specification. However, its effect was determined to be negligible for the cases considered and thus no error was introduced to the model with this simplification (6). In order to simplify linking between WIMSD5 and MCNP, a script that automatically transcripts the WIMSD5 output into the material specification part of the MCNP input was written. Detailed discussion on the burned fuel material composition will be given in the following sections.

Extensive sensitivity studies have been performed to test WIMSD5 isotopic composition calculation. In order to estimate relative importance of different isotopes, the influence of each particular fission product on the WIMSD5 calculated unit-cell k_{eff} was investigated. Isotopic composition calculated with WIMSD5 was checked by comparing it to the ORIGEN2.1 results (7). In the WIMS unit-cell description the geometry model in the radial direction and material composition of the fresh fuel was realistic, and the geometry in the axial direction was assumed to be invariant. In ORIGEN calculation only one-group point reactor approximation is available. The structural materials were not taken into account since they have no influence on fuel depletion.

The linkage of WIMS and MCNP was tested on the TRIGA Mark II research reactor in Ljubljana, Slovenia. A very accurate MCNP model of the TRIGA reactor core has been developed (8, 9). The complete MCNP model of the reactor is shown in Figure 1.

Figure 1: Complete MCNP model of the TRIGA Mark II reactor.



The same MCNP geometry model of the TRIGA reactor was used for fresh and burned core configurations. All the details were modelled except of a few simplifications outside the core like irradiation channels, graphite of the thermalizing and thermal column and end caps of fuel elements and control/transient rods. Special care was put into modelling of the fuel elements and control rods. It has been shown (9)

that all the geometry simplifications increase k_{eff} for $+150 \pm 30$ pcm (0.15%), which is attributed mainly to the omitted void regions in the close vicinity of the core (irradiation channels). Based on the extensive sensitivity studies (6), it has been determined that uncertainties in fuel composition data represent approximately ±250 pcm uncertainty in the k_{eff} calculation. Effect of initial fuel composition uncertainty on burned fuel composition was found to be negligible. Other sources of uncertainty, among which stainless steel cladding dominates yield as much as ± 300 pcm uncertainty in total. Combining all uncertainties, the total uncertainty in the calculated k_{eff} for our model was estimated to be ± 560 pcm. It should be noted that even though the geometry and material composition uncertainties are relatively large, they affect only the absolute value of the calculated k_{eff} and only slightly the relative changes (e.g. when calculating effect of burnup).

In order to improve the accuracy of the Monte Carlo model the burnup of fuel elements used in the experiment was considered individually. The burnup of fuel elements used in WIMSD5 is calculated with the fuel management deterministic code TRIGLAV (10). Detailed description of the burnup calculation with TRIGLAV code is presented in (11). The code is based on a four-group diffusion equation for r-φ geometry, solved by finite differences method. The TRIGLAV program package consists of a four-group 2-D diffusion module and the WIMSD5 (3) code. WIMSD5 is linked automatically to the diffusion module to calculate unit-cell averaged effective group constants needed for diffusion calculation. All fuel elements in the reactor are treated in the unit-cell approximation. Unit-cell cross sections in the WIMSD5 program are calculated in a 32-group approximation and averaged to four-group structure for diffusion calculation. Use of different libraries showed no significant change in the calculated burnup indicating that the original 1986 WIMS library is suitable for burned fuel element composition calculations.

2.2. MEASUREMENTS

The measurements were performed on two core configurations labelled Core 133 and Core 134 (Figure 2).

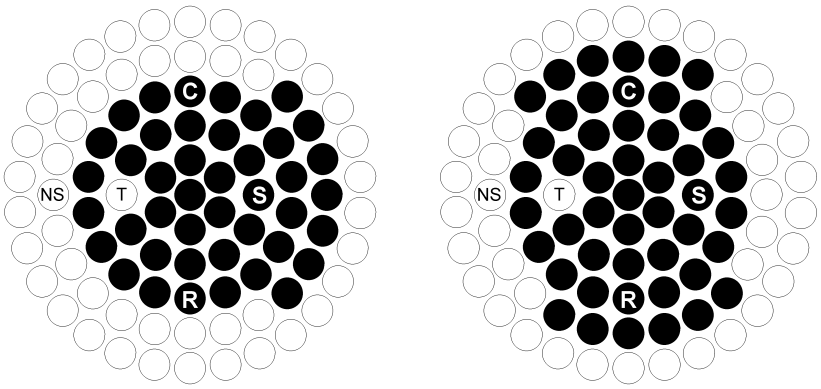


Figure 2. Schematic diagrams of the core 133 (left) and the core 134 (right). Black circles denote fuel element positions. S, C and R in black circles denote fuel-follower control rod positions (safety, compensating and regulating respectively). T indicates position of the transient control rod. NS is the neutron source position.

Experimental conditions in the criticality measurements (12) were equal in all experiments and carefully controlled. All the measurements were performed at negligible thermal power (<100W). The core excess reactivity was measured in three ways, depending on its range. In the range between 0 and 300 pcm (1 pcm ≡ 10^{-5} Δk/k) it was measured directly from the reactor period using an automatic digital reactivity meter (13). The error of this measurement was very small (+/-15 pcm). If the excess reactivity was higher than 300 pcm it was compensated by inserting a control rod and determined from its calibration curve, measured by the standard rod exchange method (14). Negative excess reactivity was determined by the negative reactivity insertion method. One control rod of known reactivity worth was inserted in to a subcritical reactor. Multiplication factor was determined from the relative change of the asymptotic flux signal. Error of this measurement was approximately similar to the case of large positive excess reactivity, i.e. 10% relative, since it originates from the same effects. Details of the measurements are given in (12).

3. RESULTS

3.1. SENSITIVITY STUDIES OF THE BURNED FUEL MATERIAL COMPOSITION

Results of the calculations of the isotope importance as functions of burn-up (Table 1) show that the largest influence on the burn-up slope of $k_{eff\ have}$ ^{135}Xe, ^{149}Sm, ^{151}Sm, ^{239}Pu and ^{143}Nd isotopes at low burn-up (less than 5%). Neglecting the rest of the fission products yields approximately ± 10% error in the slope of k_{eff} due to burn-up. For higher burn-up ^{240}Pu and some other isotopes (for 20% burn-up 12 isotopes in total) must be taken into account to achieve the same accuracy in the change of k_{eff}. In our MCNP calculations, however, all calculated isotopes were considered (except of the pseudo fission product) to avoid unnecessary systematic errors.

Nuclide	3% burnup [pcm]	10% burnup [pcm]	20% burnup [pcm]
54-Xe-135	**850**	**899**	**973**
62-Sm-149	**620**	**638**	**645**
62-Sm-151	**101**	**222**	**284**
94-Pu-239	**-95**	**-357**	**-840**
60-Nd-143	**51**	**178**	**384**
92-U -236	25	**84**	**168**
61-Pm-147	24	**65**	**102**
45-Rh-103	20	**82**	**179**
54-Xe-131	16	**56**	**118**
55-Cs-133	14	50	**105**
43-Tc- 99	11	38	**79**
94-Pu-240	5	**57**	**216**

Table 1. Results of the sensitivity studies of the effective multiplication factor for different burnup of fuel elements. Contributions to the total reactivity (Δk/k) are shown in relative values as calculated by the WIMSD5 program. Only the most important isotopes are shown. For complete table see (15). Bold numbers represent isotopes that contribute more than 90% of the total burnup reactivity change.

When comparing the WIMSD5 and ORIGEN2.1 results (see Table 2), it was observed that general agreement between the isotopic vectors is very good, however, larger differences in ^{95}Mo, ^{239}Pu and ^{236}U isotope concentrations were observed. Differences generally increase with burn-up. It should be emphasised that these differences have very little impact on criticality calculations.

	3 % burned fuel		10 % burned fuel		20 % burned fuel		20 % burned fuel + one year cooling time	
Nuclide	**WIMS [wt %]**	**ORIGEN [wt %]**	**WIMS [wt %]**	**ORIGEN [wt %]**	**WIMS [wt %]**	**ORIGEN [wt %]**	**WIMS [wt %]**	**ORIGEN [wt %]**
42-Mo-95	0.0016	0.0008	0.0057	0.0044	0.0113	0.0097	0.0114	0.0105
43-Tc-99	0.0015	0.0015	0.0056	0.0051	0.0110	0.0102	0.0112	0.0102
44-Ru-101	0.0013	0.0013	0.0048	0.0045	0.0096	0.0090	0.0097	0.0090
45-Rh-103	0.0006	0.0007	0.0027	0.0026	0.0054	0.0052	0.0057	0.0054
46-Pd-105	0.0003	0.0003	0.0010	0.0010	0.0020	0.0021	0.0021	0.0021
54-Xe-131	0.0010	0.0009	0.0035	0.0032	0.0067	0.0062	0.0068	0.0063
55-Cs-133	0.0023	0.0022	0.0082	0.0076	0.0161	0.0153	0.0164	0.0153
54-Xe-134	0.0027	0.0026	0.0097	0.0089	0.0193	0.0180	0.0196	0.0180
55-Cs-135	0.0018	0.0018	0.0063	0.0059	0.0124	0.0119	0.0126	0.0119
54-Xe-136	0.0026	0.0027	0.0095	0.0093	0.0191	0.0189	0.0194	0.0189
60-Nd-143	0.0022	0.0020	0.0076	0.0069	0.0147	0.0137	0.0149	0.0139
60-Nd-145	0.0014	0.0015	0.0052	0.0049	0.0103	0.0097	0.0105	0.0097
61-Pm-147	0.0008	0.0007	0.0021	0.0019	0.0030	0.0028	0.0023	0.0022
62-Sm-147	0.0001	0.0001	0.0008	0.0007	0.0026	0.0023	0.0034	0.0029
62-Sm-150	0.0003	0.0003	0.0014	0.0013	0.0029	0.0028	0.0029	0.0028
62-Sm-152	0.0001	0.0001	0.0007	0.0006	0.0016	0.0014	0.0016	0.0014
FP	0.0332		0.1202		0.2387		0.2423	
92-U-235	2.3050	2.3033	2.1201	2.1313	1.8721	1.8842	1.8645	1.8842
92-U-236	0.0117	0.0134	0.0418	0.0448	0.0817	0.0890	0.0829	0.0890
92-U-238	9.5564	9.5594	9.5381	9.5451	9.5107	9.5248	9.5100	9.5248
93-Np-237	0.0000	0.0001	0.0002	0.0004	0.0009	0.0016	0.0009	0.0016
94-Pu-239	0.0065	0.0045	0.0219	0.0140	0.0390	0.0252	0.0396	0.0253
94-Pu-240	0.0001	0.0001	0.0009	0.0008	0.0034	0.0030	0.0034	0.0030

Table 2. Isotopic composition of standard 20% enriched TRIGA fuel in wt % calculated for different burn-ups with WIMSD5 and ORIGEN2.1. Only actinides and fission products, which contribute more than 0.001 wt% to fuel composition are presented. Isotopes of H and Zr, which represent 88.0 wt% in UZrH TRIGA fuel meat, are not presented.

In terms of reactivity (see Table 3), the most important differences between both codes are observed for nuclides ^{149}Sm, ^{151}Sm and ^{239}Pu and for the pseudo fission product nuclide, which is present only in the WIMSD5 results.

Nuclide	3% burnup [pcm]	10% burnup [pcm]	20% burnup [pcm]
42-Mo- 95	2	4	5
43-Tc- 99	0	3	6
45-Rh-103	-1	3	7
54-Xe-131	1	5	9
55-Cs-133	1	4	5
55-Cs-134	0	0	-1
54-Xe-135	-2	-6	-10
60-Nd-143	5	16	26
61-Pm-147	2	6	7
62-Sm-149	**33**	19	1
62-Sm-151	-7	**-34**	**-87**
62-Sm-152	0	3	8
pseudo FP	6	21	**47**
92-U -236	-4	-6	-15
93-Np-237	0	-2	-10
94-Pu-239	-29	**-129**	**-297**
94-Pu-240	0	7	25

Table 3. Differences between WIMSD5 and ORIGEN2.1 calculated fission product nuclides concentrations expressed in terms of reactivity for different burnup of standard 20% enriched TRIGA fuel elements. Differences between both codes presented in this table are differences in concentrations from Table 3 multiplied by the reactivity of individual nuclides in Table 2. Significant reactivity differences are marked with bold numbers.

Because the peak concentration values are the same in WIMSD5 and ORIGEN2.1, the differences in Sm are attributed to decay constants in WIMSD5 and/or production schemes. The differences in ^{239}Pu are more likely due to ORIGEN2.1 in which the burnup is calculated in one group point reactor approximation. The spectrum and unit-cell effects are partly compensated by using appropriate one-group cross-section library provided with the code for various reactor types (7). In our case the PWR(LWR) library was used because of the lack of better options. Due to design differences between PWR and TRIGA reactor it can be expected that use of such library will underestimate resonance absorption in ^{238}U (and consequently production of ^{239}Pu) if applied for a homogeneous reactor like TRIGA. The total effect of all differences (all isotopes) on k_{eff} calculation is only 5, 80 and 270 pcm for 3, 10 and 20% burn-up, respectively. Agreement of WIMSD5 and ORIGEN2.1 results increases confidence in the calculated isotopic composition of the burned fuel.

3.2 COMPARISON TO THE EXPERIMENT

Results of the MCNP calculations for fresh and burned cores 133 and 134 are summarised in Table 4.

Core	Burnup [% ^{235}U]	k_{eff}		
		Experiment	**MCNP**	**MCNP - exp.**
133	0	1.00277 ± 0.00015	1.00420	$143 \cdot 10^{-5}$
	1	-	0.99602	-
	2	-	0.99114	-
	2.8	0.9842 ± 0.002	0.98844	424
	5	-	0.98226	-
	10	-	0.96763	-
134	0	1.0202 ± 0.0016	1.02293	273
	1	-	1.01465	-
	2	-	1.01018	-
	2.6	1.00460 ± 0.00015	1.00797	337
	5	-	1.00076	-
	10	-	0.98581	-

Table 4. Comparison of measured and calculated (MCNP4B) k_{eff} for cores 133 and 134 with fresh and burned fuel. The MCNP4B results have approximately 15 pcm statistical error.

Comparison of the calculations and measurements showed that the systematic discrepancy between the calculations and measurements is equal for fresh and burned core 134 and fresh core 133, but is slightly larger for the burned core 133. This indicates that the error of the subcritical k_{eff} core measurement of the core 133 might be larger than estimated in the measurement (10). The comparison of the calculated k_{eff} burn-up slopes also supports this hypothesis. While for the core 134, the calculated and measured burn-up slopes agree well, the measured slope is approximately 10% too steep for the core 133 compared to the calculated value.

4. CONCLUSIONS

The criticality experiments performed at the TRIGA research reactor in Ljubljana, Slovenia, were simulated with the MCNP4B Monte Carlo code. Because in the experiments the burned fuel was used as well, the suitability of MCNP4B for burnup calculations was tested. The material composition of the fuel elements was calculated with the WIMSD5 code and checked against the composition obtained with the ORIGEN2.1 calculations. The burnup of the fuel elements was determined with the fuel management diffusion code TRIGLAV, which was tested for criticality calculations as well.

It was determined that both WIMSD5 and ORIGEN2.1 give rather similar burned material compositions for burnups up to 20% burned ^{235}U. The effect of the pseudo fission product as defined in WIMSD5 was found to be negligible (below 10 pcm) for criticality calculations,

and therefore almost no systematic error was introduced, if it was not taken into account in our calculations. The remaining small differences were evaluated in terms of reactivity. WIMSD5 and ORIGEN2.1 gave very similar results (within 2% of the calculated reactivity change) for burnups up to 20% burned ^{235}U.

Importance of nuclides in burned fuel was examined by monitoring their worth compared to the total reactivity worth of fuel elements. It was found out that only ^{135}Xe, ^{149}Sm, ^{151}Sm ^{239}Pu and ^{143}Nd are important for criticality calculations if burnup of fuel is below 5%. In the case of higher burnups also other isotopes (for 20% burnup 12 isotopes in total) have to be taken into account to achieve 10% accuracy in determination of the burnup change of k_{eff}.

It was confirmed that MCNP4B successfully calculates k_{eff} for fresh fuel cores. In combination with the WIMSD5 code, used for the isotopic vector calculation of the burned fuel, the MCNP4B code can be successfully used for criticality calculations of burned fuel configurations as well. The results obtained for both, fresh and burned cores were well within the estimated systematic uncertainties of the Monte Carlo model. Small discrepancy between the measurements and calculations of $\Delta k/k$ was found for the core 133, which was attributed to the underestimation of the measured k_{eff} for the burned core. It can be concluded from our study that combination of MCNP/WIMS gives reliable results for criticality calculations with burned fuel and reproduces well criticality conditions in TRIGA research reactors.

5. REFERENCES

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