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EVALUATION OF TEMPERATURE DEPENDENCE ON CROSS SECTIONS FOR A (Th-U)O_2 FUEL PIN

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ABSTRACT

A (Th-U)O_2 fuel pin benchmark, consisting of 75w/o Th and 25w/o U, was used to analyze the effects of the temperature on the nuclear cross-sections obtained from the libraries on criticality calculations. In this case, the multiplication factor and the effective delayed neutron factor have been compared for different corrections, libraries and nuclear codes. The MCNP5 and SERPENT codes were used to criticality calculations and the NJOY99 code was used to obtain the cross-section at working temperature. The results demonstrated that the use of temperature correction on cross sections is fundamental to reach more precise neutronic calculations.

1. INTRODUCTION

There are many nuclear codes to evaluate the nuclear reactor physics. Some of them use continue nuclear data libraries, which contains important information about the cross section of each nuclide for few temperatures. Due to the temperature dependence effects, the use of an approximated temperature may cause differences in the criticality and depletion calculations. This effect is more important to absorbers nuclides in fuels that are composed by ^{238}U and ^{232}Th. To obtain nuclear data in the working temperature (WT), the NJOY99 [1] could be used. Another possibility is by interpolation using the temperature-dependent data available in the nuclear code data libraries.

In this work, the codes MCNP [2] and SERPENT [3] were used to the criticality calculations. Each one has its own cross-section data package. Most of the data libraries on MCNP5 are at room temperature and if not indicated the correction card, it assumes room temperature for the simulation. On the other hand, Serpent has data libraries at specific temperatures e.g. 300K, 600K, 900K, and 1200K. Also, in this case, if the specific temperature is not indicated, it uses in the simulation nuclear data at room temperature. So, there are many ways to model and simulate the temperature effects in a fuel pin, assembly or core and it can influence the results related to.

For the analysis, it was used a thorium unitary cell benchmark [4] to compare the criticality calculations using different temperatures modeled by MCNP5 and SERPENT codes. The first criticality evaluation is based on the utilization of the cross sections data package on the Serpent at specific temperatures (300K, 600K, 900K and 1200K) and the cross sections processed with NJOY99 at work temperature, both using the library ENDF/B-VII [5]. The second evaluation was done for both codes using the temperature correction leading to the working temperature (WT), which for the coolant material, the cladding and the fuel are 583K, 621K, and 900K, respectively.

2. METHODOLOGY

The methodology follows the benchmark calculations as a reference, using the same nuclear fuel based on thorium. The evaluation was performed using the codes temperature correction and the cross-section data at work temperature.

2.1. CRITICALITY EVALUATION BENCHMARK

Fig. 1. shows the fuel pin cell modeled on SERPENT and MCNP5 based on the benchmark [4]. Table 1 presents the parameters used in the benchmark and in the Table 2 it is shown the composition.

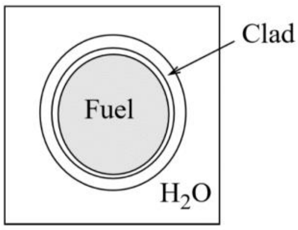

Figure 18. Thorium pin cell model extracted from benchmark [4]

Table 1. Full power operation parameters [4].

Parameters	Full Power
Fuel Density (g/cm³)	9.424
Fuel Temperature (K)	900
Cladding Density (g/cm³)	6.505
Cladding Temperature (K)	621.1
Coolant Density (g/cm³)	0.705
Coolant Temperature (K)	583.1
Fuel Pellet Radius (mm)	4.1274
Cladding Inner Radius (mm)	4.1896
Cladding Outer Radius (mm)	4.7609
Pin Pitch (mm)	12.626

Table 2. Nuclides Weight Percentage. [4]

	Nuclide	Weight Percent (%)
Fuel	Th-232	65.909
	U-234	0.034
	U-235	4.291
	U-238	17.740
	O-16	12.026
Cladding	Zr-4 (Zircaloy-4)	100
Coolant	H-1	11.19
	O-16	88.81

Table 3 shows nine different cases using the codes temperature correction and then the cross-section processed at work temperature (WT). In the first case, it was used the codes temperature correction, which uses the data package from the SERPENT ENDF/B-VII with cross-sections at 300K, 600K, 900K, and 1200K and room temperature for MCNP5. In the second case, it takes into consideration the cross-sections at working temperature (WT) using the library ENDF/B-VII, processed at 583K, 621K, and 900K.

In the SERPENT code, the temperature correction can only be used if the given temperature is above the original. Thus, to use the temperature correction on coolant and cladding, the 900K and 1200K datasets could not be used.

Table. 3. Data sets temperature definitions

Data Set	Material	Temperatures
Working Temperature (WT) ENDF/B-VII NJOY99	Fuel	900K
	Cladding	621K
	Coolant	583K
300K (03c) SERPENT ENDF/B-VII	Fuel	300K
	Cladding	300K
	Coolant	300K
600K (06c) SERPENT ENDF/B-VII	Fuel	600K
	Cladding	600K
	Coolant	600K
900K (09c) SERPENT ENDF/B-VII	Fuel	900K
	Cladding	900K
	Coolant	900K
1200K (12c) SERPENT ENDF/B-VII	Fuel	1200K
	Cladding	1200K
	Coolant	1200K
300K corrected to WT (03c→WT) SERPENT ENDF/B-VII	Fuel	300K→900K
	Cladding	300K→621K
	Coolant	300K→583K
600K corrected to WT (06c→WT) SERPENT ENDF/B-VII	Fuel	600K→900K
	Cladding	600K→621K
	Coolant	300K→583K
900K corrected to WT (09c→WT) SERPENT ENDF/B-VII	Fuel	900K→900K
	Cladding	600K→621K
	Coolant	300K→583K
1200K corrected to WT (12c→WT) SERPENT ENDF/B-VII	Fuel	1200K→1200K
	Cladding	600K→621K
	Coolant	300K→583K

→ it indicates the use of temperature correction.

3. RESULTS

The total number of neutrons used in each case was 100 million, 2000 generations with 50000 neutrons per generation. This large number of neutrons allowed the standard deviation of the codes to be around 6 pcm. The results present the differences in multiplication factor using a different type of correction, the SERPENT correction, the MCNP5 correction and both codes using working temperature data (WT) library processed with NJOY.

3.1. CRITICALITY

Table 4 shows the multiplication factor calculation for the SERPENT and MCNP5 using the codes correction (third and fourth column) at different temperature compared to the mean value (first column) obtained from the benchmark [4]. The last columns present the absolute differences of the multiplication factor between the codes used at DEN/UFMG and the MIT CASMO-4 case.

The case that presents the lowest absolute difference for SERPENT and MCNP5 was the (12c→WT). On the other hand, when the temperature corrections are not used, the results indicate that the MCNP5 using the 09c has a low absolute difference of the multiplication factor. Besides, the cases using the working temperature (WT) have the second lower absolute difference of the multiplication factor values for both codes.

Table 4. Multiplication factors and their respective maximum absolute difference. [4]

Reference Value	Cases	$k_{serpent}$	k_{MCNP5}	Absolute Differences (pcm)	SERPENT	MCNP5
1.23161 *	WT	1.23389	1.23517	MIT CASMO4 – WT	228	356
	03c	1.29379	1.24774	MIT CASMO4 - 03c	6218	1613
	06c	1.26342	1.23841	MIT CASMO4 - 06c	3181	680
	09c	1.24194	1.23009	MIT CASMO4 - 09c	1033	152
	12c	1.22506	1.22499	MIT CASMO4 - 12c	655	662
	03c→WT	1.24469	1.25153	MIT CASMO4 - (03c→WT)	1308	1992
	06c→WT	1.24475	1.24218	MIT CASMO4 - (06c→WT)	1314	1057
	09c→WT	1.24504	1.23476	MIT CASMO4 - (09c→WT)	1343	315
	12c→WT	1.22942	1.22857	MIT CASMO4 - (12c→WT)	219	304

→ it indicates the use of temperature correction.

To identify the impact of different nuclear data in the criticality calculations, the mean value, standard deviation and the relative standard deviations are applied to the multiplication factor values obtained with different codes/institutions. “Before” are the data just for the MIT case (benchmark) and “Updated” includes the MIT data and DEN/UFMG data.

Table 5. Statistics parameter for the chosen cases [4]

Country	Institute	Code	Library	k
USA	MIT[1]	CASMO-4	ENDF/B-VI	1.23782
USA	MIT	MOCUP	UTXS	1.23354
USA	INEEL[2]	MOCUP	UTXS	1.22347
BRAZIL	DEN[3]	MCNP5	ENDF/B-VII 09c	1.23009
BRAZIL	DEN	SERPENT	ENDF/B-VII 09c	1.24194
BRAZIL	DEN	MCNP5	ENDF/B-VII 12c→WT	1.22857
BRAZIL	DEN	SERPENT	ENDF/B-VII 12c→WT	1.22942
BRAZIL	DEN	MCNP5	ENDF/B-VII NJOY99	1.23517
BRAZIL	DEN	SERPENT	ENDF/B-VII NJOY99	1.23404
Multiplication Factor Mean Value			Before	1.23161
			Updated	1.23267
Multiplication Factor Standard Deviation			Before	0.00602
			Updated	0.00516
Multiplication Factor Relative Standard Deviation			Before	0.49%
			Updated	0.42%

→ it indicates the use of temperature correction.
1-Massachusetts Institute of Technology – MIT [4]
2-Idaho National Engineering and Environmental Laboratory – INEEL [4]
3-Departamento de Engenharia Nuclear – DEN - UFMG

3.2. DELAYED NEUTRON AND FUEL TEMPERATURE COEFFICIENT

The benchmark [4], uses the ^{235}U as a fissile material spiked with thorium as a nuclear fuel. Therefore, it is considered the delayed neutrons for the ^{235}U. According to the International Atomic Energy Agency (IAEA) publication [7], the delayed neutron data for ^{235}U is β_{235U} = 0.00665 ± 0.00021, which is like the ones obtained by MCNP5 and SERPENT for the three temperatures evaluated.

Table 6 provides the effective neutron delayed factor for the chosen cases in the analysis of Table 4 for MCNP5 and SERPENT codes. A similar statistics analysis is done for the effective delayed neutron factor, including the mean value, the standard deviation, and the relative standard deviation.

Table 6. Effective delayed neutron factors and statistics parameters.

$\beta_{235U(IAEA)}$	Cases	$\beta_{Serpent}$	β_{MCNP5}		$\beta_{Serpent}$	β_{MCNP5}
0.00665	WT	0.00669	0.00674	Relative differences	0.6%	1.33%
	09c	0.00668	0.00672		0.44%	1.04%
	12c→WT	0.00669	0.00677		0.6%	1.77%

→it indicates the use of temperature correction.

4. CONCLUSION

The k_{inf} absolute differences for SERPENT present six out of eight values above 1000 pcm in contrast to the MIT and INEEL mean value. Although, MCNP5 only has three out of eight results above 1000pcm.The optimal scenario for neutronic simulations involves the use of appropriate cross-section data. The corrections done by SERPENT and MCNP5 approximate the results to the MIT CASMO-4 reference case. Nevertheless, the results still varying with an average of 1046 pcm and 917 pcm from reference.

The results obtained at WT with cross sections processed using NJOY had an average absolute difference of 300 pcm in relation to reference case. Therefore, the results obtained depends strongly on cross-section processed temperatures. This observation is supported by the differences were lower at WT using NJOY. In fact, using the temperature correction without the corresponding cross-section, the results diverge from the expected value, contributing to the lack of accuracy.

The effective delayed neutron fraction obtained had very similar values when compared to theory. The maximum absolute difference from values obtained was 9pcm. The calculated fuel temperature coefficients values were -5.15492 and -0.08740 pcm/K for SERPENT and MCNP5, respectively. Therefore, the use of appropriate cross sections data was equally significant on all calculation performed.

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