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Analyses of the Doppler Coefficient of Reactivity Using Monte Carlo and Deterministic Codes

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ABSTRACT

Using the Mosteller [1] pin cell benchmark, the Doppler coefficient for UO_2 fuel was analysed using the Monte Carlo code Serpent [2] and the deterministic codes WIMS-D5 [3] and DRAGON. [4]. These coefficients were calculated using nuclear data from ENDF/B-VI.8, ENDF/B-VII.0, ENDF/B-VII.1 and ENDF/B-VIII.0. For the deterministic codes, the analysis was also performed with different energy structures. In this paper, the results of the listed codes are presented and compared.

1 INTRODUCTION

The interaction probability (cross sections) between neutrons and the target nuclei in a reactor depends on the temperature at which the system exists. The resonance behavior of the neutron interaction cross section can change due to the change in relative motion between the neutron and the fuel nuclei during thermal motion. The effect, known as Doppler broadening of the resonance peaks, is caused by an increase in material temperature. This increases neutron absorption in the fuel, which affects reactor stability. In reactor theory, the increased absorption is interpreted to result from the weakening of resonance self-shielding. However, self-shielding, is a macroscopic effect that is not present itself to individual neutrons. From the point of view of a single neutron, it is the random variation of the relative velocity between the neutron and the target nucleus that causes an increase in the interaction probability. When the neutron energy is near a high resonance peak, the energy dependence is strong, and the thermal motion of the target atom occasionally shifts the energy closer to the peak value.

The Doppler broadening of the resonances in the cross section of the fuel nuclei leads to a change in the neutron multiplication factor (k_{inf}). The Doppler coefficient is determined by studying the reactivity change as a function of fuel temperature. All other parameters such as the temperature of the moderator and the density are constant.

In this paper, the Doppler coefficient proposed as a benchmark is evaluated. Benchmark data for different fuel enrichments of a typical UO_2 lattice of a pressurized water reactor (PWR) are given. The aim of this work is to calculate the Doppler coefficient between the hot full power (900 K) and hot zero power (600 K) temperatures with different codes, different nuclear data and using different energy groups. The computational model and results are presented below.

2 TEST CASE MODEL OF THE BENCHMARK

The model used in the benchmark is an example of a PWR lattice shown in Figure 1. Model characteristics, material and geometry data are given in Table 1 and Table 2. Figure 1 shows a typical rectangular pin cell with reflecting boundary conditions with the following regions: fuel (green), clad (grey) and moderator (pink).

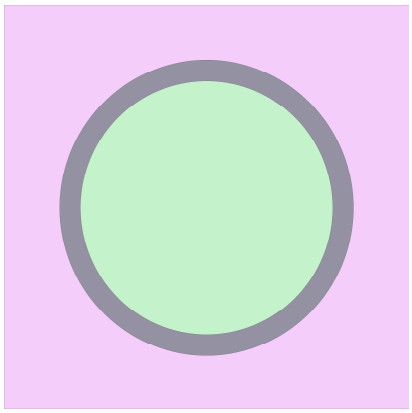

Figure 1: Schematic of the geometry for the benchmark

Table 1: Atomic densities [atoms/barn cm] of UO_2 fuel at 600 K and 900 K for different enrichments [wt.%].

T=600 K	**0.71**	**1.6**	**2.4**	**3.1**	**3.9**
^{235}U	1.66078E-04	3.73729E-04	5.60588E-04	7.24086E-04	9.10933E-04
^{238}U	2.28994E-02	2.26940E-02	2.25093E-02	2.23476E-02	2.21163E-02
^{16}O	4.61309E-02	4.61355E-02	4.61397E-02	4.61433E-02	4.61475E-02
TOTAL	6.91964E-02	6.92032E-02	6.92096E-02	6.92150E-02	6.91747E-02
T=900 K	**0.71**	**1.6**	**2.4**	**3.1**	**3.9**
^{235}U	1.64729E-04	3.70693E-04	5.56033E-04	7.18202E-04	9.03532E-04
^{238}U	2.27133E-02	2.25096E-02	2.23264E-02	2.21660E-02	2.19827E-02
^{16}O	4.57561E-02	4.57607E-02	4.57684E-02	4.57684E-02	4.57725E-02
TOTAL	6.86341E-02	6.86410E-02	6.86508E-02	6.86526E-02	6.86587E-02

Table 2: Pin cell dimensions

	Dimensions [cm]
Fuel radius	0.39306
Clad radius	0.45802
Pitch	1.26209

Our reference case for computing the Doppler coefficient calculation was performed using the Monte Carlo (MC) code Serpent. The basic principle of MC calculation in particle transport problems is very simple. The life of a single neutron or other particle type is simulated from its initial emission to its eventual death. Monte Carlo codes use continuous-energy cross sections, while deterministic codes use a group-wise format of energy dependent cross sections. The main difficulties in processing cross sections for use in these codes are the reconstruction of energy-dependent cross sections and Doppler broadening to account for temperature

dependent effects. These issues have already been explored in detail in the following articles [5], [6], [7] and [8].

One goal of this paper is to compare the deterministic lattice code DRAGON and WIMS-D5 and compare the results obtained with the Monte Carlo codes Serpent. Deterministic codes are generallyq much faster than MC codes. While MC codes use continuous-energy cross sections libraries the deterministic codes use few group energy structure for light water reactor analysis. The number of energy groups in a cross-section library significantly affects the lattice physics calculations in two ways, namely, accuracy and computation time. And as expected, there is a trade-off between these two parameters. Although the number of energy groups is very important, the structure of the energy groups is also crucial. Choosing an energy group structure is quite difficult, especially in the resonance energy domain. Since the resonance calculation is one of the most difficult and challenging parts of the reactor physics calculations, considerable efforts and studies have been directed to the development of various innovative calculation methods. In general, two different models are applied:

- Model based on equivalence in dilution: in its simplest form this technique reduces to the use of Bell and Dancoff factors. This type of model is implemented in the deterministic code WIMS-D5 [3].
- Model based on a subgroup approach: Here, the detailed energy dependent cross section behavior in each energy group is replaced by the probability density representation, resulting in so called probability tables. This type of model is implemented in the deterministic code DRAGON [4].

In addition, this paper analyzes the effect of energy structures.

3 NUCLEAR CODES AND LIBRARIES

Various methods can be used to solve transport equation. In this regard, there are two different classes of codes: stochastic and deterministic models. In this analysis, we used a stochastic MC code Serpent 2, which is the most accurate but also the most time consuming, and two deterministic codes WIMS-D5 and DRAGON. Each code uses specific library formats. Short overview of codes and libraries are given below.

- Serpent [2] is a MC code for calculating burnup, developed at the VTT Technical Research Centre in Finland and publicly available through the OECD/NEA Data Bank. The Serpent code uses a single unionized energy grid for all reaction cross sections, minimizing the number of time-consuming grid search iterations, allowing the transport simulation to run much faster, which is important in burnup calculations. Serpent uses a continuous energy data library in ACE (A Compact ENDF) format based on ENDF/B-VII.0 nuclear data. Serpent version 2.1.30 was used.
- The WIMS-D5 [3] code belongs to the family of lattice codes called WIMS. The original WIMS code, developed by AEE Winfrith, has been modified over the years to suit specific problem types. The WIMS-D5 version is available from the OECD/NEA Data Bank and has been used extensively in many laboratories. 69 group WIMS-D libraries format based on ENDF/B-VII.0, ENDF/B-VI.8 and ENDF/B-VII.1 evaluated nuclear data libraries have been used.
- DRAGON [4] is supported and developed by École Polytechnique de Montréal and provides 1D and 2D solutions with different modules. In our calculations, we used the collision probability method, using the EXCELL module. DRAGON is available from RSICC, NEA Data Bank or directly from École Polytechnique. 295 and 172 group Draglib library format based on ENDF/B-VII.0, ENDF/B-VIII.0 and ENDF/B-VI.8 evaluated nuclear data libraries were used. DRAGON version 5.0.5 was used.

4 RESULTS AND DISCUSSION

The results of multiplication factor (k_{inf}), reactivity (ρ), and Doppler coefficient (α) for different fuel enrichments (Enr.) of UO_2 are shown in Tables 3 to 12. The statistical uncertainty (σ_{kinf}), which is part of the MC calculation, was calculated for each MC calculation and is shown in Table 3. In the case of the deterministic calculation, three different data libraries were used. In addition, the DRAGON code was used to evaluate the effect of the energy structures by comparing the results of using 295 and 172 group energy structures. Equation (1) was used to calculate the reactivity from the multiplication factor (k_{inf}) at given fuel temperature:

$$\rho = \frac{k_{\text{inf}} - 1}{k_{\text{inf}}} \cdot 10^5 . \tag{1}$$

The Doppler coefficient (α) is then calculated using equation (2) as the change in reactivity per degree change in temperature of the fuel:

$$\alpha = \frac{\Delta\rho}{\Delta T} . \tag{2}$$

Table 3: Results of the multiplication factor, reactivity and Doppler coefficient at two fuel temperatures. In addition, the statistical uncertainties are given. The results are presented for five different fuel enrichments and ENDF/B-VII.0 library using the code Serpent 2.

Enr. [wt.%]	T [K]	k_{inf}	σ_{KINF}	ρ	σ_ρ	α	σ_α
0.71	600	6.6552E-01	1.2000E-04	-5.0259E+04	2.4000E-04	-5.5	0.2
	900	6.5832E-01	1.2000E-04	-5.1901E+04	2.4000E-04		
1.60	600	9.6181E-01	1.1000E-04	-3.9702E+03	2.2000E-04	-3.4	0.1
	900	9.5258E-01	1.0000E-04	-4.9782E+03	2.0000E-04		
2.40	600	1.1003E+00	1.0000E-04	9.1190E+03	2.0000E-04	-2.8	0.1
	900	1.0904E+00	7.2000E-05	8.2922E+03	1.4400E-04		
3.10	600	1.1789E+00	1.0000E-04	1.5178E+04	2.0000E-04	-2.5	0.1
	900	1.1685E+00	1.0000E-04	1.4417E+04	2.0000E-04		
3.90	600	1.2423E+00	9.4000E-05	1.9506E+04	1.8800E-04	-2.4	0.1
	900	1.2315E+00	9.9000E-05	1.8798E+04	1.9800E-04		

Table 4: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VII.0 library using the WIMS-D5 code.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.6476E-01	-5.0431E+04	-6.1
	900	6.5682E-01	-5.2249E+04	
1.60	600	9.5953E-01	-4.2173E+03	-3.8
	900	9.4923E-01	-5.3480E+03	
2.40	600	1.0972E+00	8.8607E+03	-3.1
	900	1.0862E+00	7.9337E+03	
3.10	600	1.1749E+00	1.4885E+04	-2.8
	900	1.1635E+00	1.4054E+04	
3.90	600	1.2377E+00	1.9203E+04	-2.6
	900	1.2257E+00	1.8411E+04	

Table 5: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VI.8 library using the WIMS-D5 code.

Enr. [wt.%]	**T [K]**	**k_{inf}**	**ρ**	**α**
0.71	600	6.6246E-01	-5.0952E+04	-6.0
	900	6.5461E-01	-5.2762E+04	
1.60	600	9.5627E-01	-4.5728E+03	-3.8
	900	9.4608E-01	-5.6991E+03	
2.40	600	1.0938E+00	8.5765E+03	-3.1
	900	1.0829E+00	7.6535E+03	
3.10	600	1.1715E+00	1.4638E+04	-2.8
	900	1.1602E+00	1.3811E+04	
3.90	600	1.2343E+00	1.8985E+04	-2.6
	900	1.2224E+00	1.8196E+04	

Table 6: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VII.1 library using the WIMS-D5 code.

Enr. [wt.%]	**T [K]**	**k_{inf}**	**ρ**	**α**
0.71	600	6.6482E-01	-5.0416E+04	-6.1
	900	6.5689E-01	-5.2233E+04	
1.60	600	9.5949E-01	-4.2215E+03	-3.8
	900	9.4920E-01	-5.3519E+03	
2.40	600	1.0972E+00	8.8553E+03	-3.1
	900	1.0861E+00	7.9286E+03	
3.10	600	1.1748E+00	1.4880E+04	-2.8
	900	1.1635E+00	1.4049E+04	
3.90	600	1.2376E+00	1.9198E+04	-2.6
	900	1.2256E+00	1.8406E+04	

Table 7: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VII.0 library using the DRAGON code with 295 energy groups.

Enr. [wt.%]	**T [K]**	**k_{inf}**	**ρ**	**α**
0.71	600	6.6661E-01	-5.0013E+04	-5.4
	900	6.5954E-01	-5.1620E+04	
1.60	600	9.6339E-01	-3.7996E+03	-3.3
	900	9.5440E-01	-4.7782E+03	
2.40	600	1.1022E+00	9.2751E+03	-2.6
	900	1.0927E+00	8.4813E+03	
3.10	600	1.1806E+00	1.5300E+04	-2.4
	900	1.1709E+00	1.4593E+04	
3.90	600	1.2441E+00	1.9621E+04	-2.2
	900	1.2338E+00	1.8949E+04	

Table 8: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VIII.0 library using the DRAGON code with 295 energy groups.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.7023E-01	-4.9203E+04	-5.4
	900	6.6298E-01	-5.0834E+04	
1.60	600	9.6583E-01	-3.5380E+03	-3.4
	900	9.5653E-01	-4.5442E+03	
2.40	600	1.1031E+00	9.3490E+03	-2.7
	900	1.0932E+00	8.5258E+03	
3.10	600	1.1803E+00	1.5278E+04	-2.5
	900	1.1701E+00	1.4539E+04	
3.90	600	1.2426E+00	1.9525E+04	-2.4
	900	1.2317E+00	1.8814E+04	

Table 9: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VI.8 library using the DRAGON code with 295 energy groups.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.6916E-01	-4.9442E+04	-4.9
	900	6.6259E-01	-5.0924E+04	
1.6	600	9.6406E-01	-3.7278E+03	-3.0
	900	9.5574E-01	-4.6308E+03	
2.4	600	1.1023E+00	9.2816E+03	-2.4
	900	1.0935E+00	8.5509E+03	
3.1	600	1.1805E+00	1.5289E+04	-2.2
	900	1.1715E+00	1.4640E+04	
3.9	600	1.2438E+00	1.9603E+04	-2.1
	900	1.2343E+00	1.8984E+04	

Table 10: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VII.0 library using the DRAGON code with 172 energy groups.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.6334E-01	-5.0753E+04	-5.9
	900	6.5569E-01	-5.2512E+04	
1.6	600	9.5822E-01	-4.3599E+03	-3.6
	900	9.4835E-01	-5.4466E+03	
2.4	600	1.0962E+00	8.7725E+03	-3.0
	900	1.0856E+00	7.8850E+03	
3.1	600	1.1741E+00	1.4826E+04	-2.6
	900	1.1632E+00	1.4032E+04	
3.9	600	1.2371E+00	1.9168E+04	-2.5
	900	1.2257E+00	1.8414E+04	

Table 11: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VIII.0 library using the DRAGON code with 172 energy groups.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.6714E-01	-4.9893E+04	-5.9
	900	6.5934E-01	-5.1666E+04	
1.6	600	9.6096E-01	-4.0628E+03	-3.7
	900	9.5088E-01	-5.1661E+03	
2.4	600	1.0974E+00	8.8773E+03	-3.0
	900	1.0866E+00	7.9731E+03	
3.1	600	1.1742E+00	1.4832E+04	-2.7
	900	1.1631E+00	1.4022E+04	
3.9	600	1.2361E+00	1.9099E+04	-2.6
	900	1.2244E+00	1.8328E+04	

Table 12: Multiplication factor results, calculated reactivity and calculated Doppler coefficient at two fuel temperatures. Results are presented for five different fuel enrichments and the ENDF/B-VI.8 library using the DRAGON code with 172 energy groups.

Enr. [wt.%]	T [K]	k_{inf}	ρ	α
0.71	600	6.6625E-01	-5.0094E+04	-5.8
	900	6.5861E-01	-5.1835E+04	
1.6	600	9.5941E-01	-4.2311E+03	-3.6
	900	9.4949E-01	-5.3201E+03	
2.4	600	1.0968E+00	8.8274E+03	-3.0
	900	1.0862E+00	7.9350E+03	
3.1	600	1.1745E+00	1.4859E+04	-2.7
	900	1.1636E+00	1.4060E+04	
3.9	600	1.2375E+00	1.9191E+04	-2.5
	900	1.2260E+00	1.8431E+04	

Table 3 shows that k_{inf} decreases with increasing fuel temperature. This is due to the increase in resonance absorption and fission capture. The Doppler reactivity coefficient can be calculated using equation (2). It can be seen that the reference results using the Serpent code for naturally enriched fuel give the Doppler coefficient -5.5 ± 0.2 pcm/°C. It can also be seen that the Doppler coefficient is less negative with increasing fuel enrichment as the ration absorption/fission is decreasing.

Comparing the Monte Carlo results with the deterministic WIMS-D5 results (Table 4), we find that the largest difference is for naturally enriched fuel. This difference decreases with increasing fuel enrichment as the content of ^{238}U decreases since it is a nuclide with a high number of resonances. A similar conclusion can be drawn from the results of using the code DRAGON.

In the case of the nuclear data, the comparison is made for the WIMS-D5 calculations. The comparison of the results of the Doppler coefficient with ENDF-B/VII.0 (Table 4), ENDF-B/VI.8 (Table 5) and ENDF-B/VII.1 (Table 6) shows that there are no differences. When comparing the nuclear data for the calculations of DRAGON using 295 energy groups, by comparing the results of the Doppler coefficient with ENDF-B/VII.0 (Table 7), ENDF-B/VIII.0 (Table 8Table 5) and ENDF-B/VI.8 (Table 9), it can be seen that there are some notable

differences, especially for the ENDF-B/VI.8 library, while the differences are smaller in the case of the calculations using 172 energy groups.

Comparing the results from Table 8 and Table 11, it is clear that the greatest difference is for naturally enriched fuel. In general, it can be seen that the results with 172 energy groups calculate more negative values for the Doppler coefficient.

Comparing the results of MC calculation (Table 3) with the deterministic results, it is found that the best results are obtained with DRAGON using 295 energy groups (Table 5). The deterministic results of the Doppler coefficient are within the uncertainty of the MC results.

5 CONCLUSION

This paper presents the analysis of the fuel Doppler coefficient. The reference calculations were performed with the Monte Carlo code Serpent using a library of continuous–energy nuclear data based on the ENDF-B/VII.0 data. The neutron multiplication factor (k_{inf}) is calculated for a typical UO_2 fuel pin cell at two different temperatures of 600K and 900K. The Doppler coefficient is calculated as the change in reactivity per unit fuel temperature.

It has been shown that the treatment of the resonance region is important, as shown by the comparison of deterministic and Monte Carlo calculations. The comparison of two deterministic results shows that the self-shielding models also affect temperature dependent problems such as the number and structure of energy groups.

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