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ENDF/B-V, ENDF/B-VI, AND ENDF/B-VII.0 RESULTS FOR THE DOPPLER-DEFECT BENCHMARK

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ABSTRACT

A set of computational benchmarks for the Doppler reactivity defect has been specified for an infinite array of identical fuel pin cells containing normal or enriched UO_2 fuel, reactor-recycle mixed-oxide (MOX) fuel, or weapons-grade MOX fuel. The Doppler coefficient of reactivity, as well as the Doppler defect, can be computed for each of the cells. The MCNP5 Monte Carlo code was used to perform calculations for these benchmarks using cross sections derived from the ENDF/B-V, ENDF/B-VI, and ENDF/B-VII.0 nuclear data sets. The Doppler coefficients obtained from the three data sets exhibit very similar behavior. The Doppler coefficient for UO_2 fuel becomes less negative with increasing enrichment, with a generally asymptotic shape. The Doppler coefficient for the reactor-recycle MOX becomes less negative with increasing PuO_2 content. The Doppler coefficient for weapons-grade MOX shows a pronounced shoulder btween 1 wt.% and 2 wt.% PuO_2, with a nearly constant value thereafter. The Doppler coefficients for the more heavily loaded MOX fuel, whether reactor-recycle or weapons-grade, are significantly more negative than those for the higher enrichments of UO_2 fuel considered in this study.

Key Words: Doppler, Benchmark, ENDF/B-V, ENDF/B-VI, ENDF/B-VII.0, UO_2, MOX

1. INTRODUCTION

A set of computational benchmarks [1] for the Doppler reactivity defect has been specified for an infinite array of identical fuel pin cells containing normal or enriched UO_2 fuel, reactor-recycle mixed-oxide (MOX) fuel, or weapons-grade MOX fuel. The pin cells are a simplified version of an “optimized” fuel assembly design that has been used in both initial and reload cycles of several pressurized water reactors [2]. There are corresponding pairs of pin cells for hot-zero-power (HZP) and hot-full-power (HFP) conditions. At HZP everything – fuel, cladding, and borated moderator – is at a uniform 600 K. At HFP, the fuel is at 900 K, while everything else still is at 600 K. The soluble boron concentration in the moderator is 1400 ppm for all cases. The Doppler defect can be calculated as the reactivity difference between HFP and HZP conditions, and the Doppler coefficient is simply the Doppler defect divided by the change in the fuel temperature. Specifically,

$$DC = \frac{\Delta \rho_{Dop}}{\Delta T_{Fuel}}$$

where DC is the Doppler coefficient of reactivity, ΔT_{Fuel} is 300 K, and the Doppler defect is

$$\Delta\rho_{Dop} = \frac{k_{HFP} - k_{HZP}}{k_{HFP} * k_{HZP}}$$

There are three subsets of benchmarks, but the pin cells for all three are identical except for the fuel they contain. The first subset contains UO_2 fuel, ranging from normal to 5.0 wt.% enriched uranium. The second subset contains reactor-recycle MOX, with 1 wt.% to 8 wt.% PuO_2. The third subset contains weapons-grade MOX, with 1 wt.% to 6 wt.% PuO_2. The plutonium isotopics for the two types of MOX cases are summarized in Table I.

Table I. Plutonium Isotopics (at.%)

Fuel	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
Reactor-Recycle MOX	45.0	30.0	15.0	10.0
Weapons-Grade MOX	93.6	5.9	0.4	0.1

2. CALCULATIONS

The calculations were performed with the MCNP5 Monte Carlo code [3], using cross sections based on ENDF/B-V [4], ENDF/B-VI [5], and ENDF/B-VII.0 [6]. The basic nuclear data for all three cross-section sets had been generated previously from the corresponding ENDF/B data files with the NJOY code [7]. However, many of the cross sections needed for the ENDF/B-VI and ENDF/B-VII.0 calculations were not readily available at 600 K and/or 900 K. Accordingly, the DOPPLER code [8,9] was employed to generate cross sections at those temperatures from the cross sections that were available.

The ENDF/B-V nuclear data were generated many years ago for two sets of benchmarks [2,10,11] that have been altered slightly and then subsumed into the current set. The basic ENDF/B-VI cross sections were taken from the ENDF66 [12] and ACTI [13] libraries that are included in the MCNP5 distribution. For the benchmark cases in this study, that combination of cross sections corresponds to the final release of ENDF/B-VI. The basic ENDF/B-VII.0 cross sections were processed directly from the initial release that occurred in December 2006.

Each MCNP5 calculation employed 550 generations of 10,000 neutrons each. The first 50 generations were excluded from the statistics. Consequently, the values of k_{eff} obtained from these calculations each are based on 5,000,000 active neutron histories. This number of histories is considered sufficient because it reduces the Monte Carlo standard deviation for the Doppler coefficient to 5% or less for all cases. In practical applications, uncertainties as high as 10% in the Doppler coefficients have been considered acceptable.

3. RESULTS

The value obtained for k_{eff} and for the Doppler coefficients for for the UO_2 cases are presented in Table II, and the resulting Doppler coefficients are plotted in Figure 1. ENDF/B-V and ENDF/B-VI produce very similar values for k_{eff}, with the difference between corresponding results usually less than 10 pcm. ENDF/B-VII.0 produces higher values for k_{eff} than either ENDF/B-V or ENDF/B-VI for every case. However, all three nuclear data sets produce very similar results for the Doppler coefficients. In fact, the Doppler coefficients from the three libraries are within a single standard deviation of each other at each enrichment except 5 wt.%. The Doppler coefficient becomes less negative with increasing enrichment, and the curve appears to take on an asymptotic shape.

Table II. Results for UO_2 Pin Cells

Nuclear Data Library	Enrichment (wt.%)	k_{eff}		Doppler Coefficient (pcm/K)
		HFP	HZP	
ENDF/B-V	0.711	0.65946 ± 0.00019	0.66481 ± 0.00019	-4.07 ± 0.20
	1.6	0.95155 ± 0.00026	0.95928 ± 0.00026	-2.82 ± 0.13
	2.4	1.08900 ± 0.00027	1.09750 ± 0.00026	-2.37 ± 0.10
	3.1	1.16636 ± 0.00027	1.17563 ± 0.00028	-2.25 ± 0.09
	3.9	1.22875 ± 0.00028	1.23877 ± 0.00029	-2.19 ± 0.09
	4.5	1.26448 ± 0.00028	1.27451 ± 0.00030	-2.07 ± 0.08
	5.0	1.28888 ± 0.00029	1.29885 ± 0.00030	-1.99 ± 0.08
ENDF/B-VI	0.711	0.65953 ± 0.00019	0.66500 ± 0.00020	-4.16 ± 0.21
	1.6	0.95107 ± 0.00025	0.95906 ± 0.00025	-2.92 ± 0.13
	2.4	1.08774 ± 0.00028	1.09638 ± 0.00027	-2.41 ± 0.11
	3.1	1.16542 ± 0.00027	1.17485 ± 0.00029	-2.30 ± 0.10
	3.9	1.22765 ± 0.00030	1.23733 ± 0.00027	-2.12 ± 0.09
	4.5	1.26240 ± 0.00027	1.27264 ± 0.00028	-2.12 ± 0.08
	5.0	1.28669 ± 0.00030	1.29690 ± 0.00030	-2.04 ± 0.08
ENDF/B-VII.0	0.711	0.66108 ± 0.00018	0.66661 ± 0.00019	-4.18 ± 0.20
	1.6	0.95411 ± 0.00026	0.96176 ± 0.00027	-2.78 ± 0.14
	2.4	1.09077 ± 0.00028	1.09955 ± 0.00027	-2.44 ± 0.11
	3.1	1.16794 ± 0.00028	1.17741 ± 0.00029	-2.30 ± 0.10
	3.9	1.23048 ± 0.00029	1.24054 ± 0.00032	-2.20 ± 0.09
	4.5	1.26598 ± 0.00029	1.27621 ± 0.00028	-2.11 ± 0.08
	5.0	1.28959 ± 0.00031	1.30027 ± 0.00029	-2.12 ± 0.08

The values obtained for k_{eff} and for the Doppler coefficients for the reactor-recycle MOX cases are given in Table III, and the resulting Doppler coefficients are plotted in Figure 2. The ENDF/B-V values for k_{eff} increase more slowly with plutonium content than do the

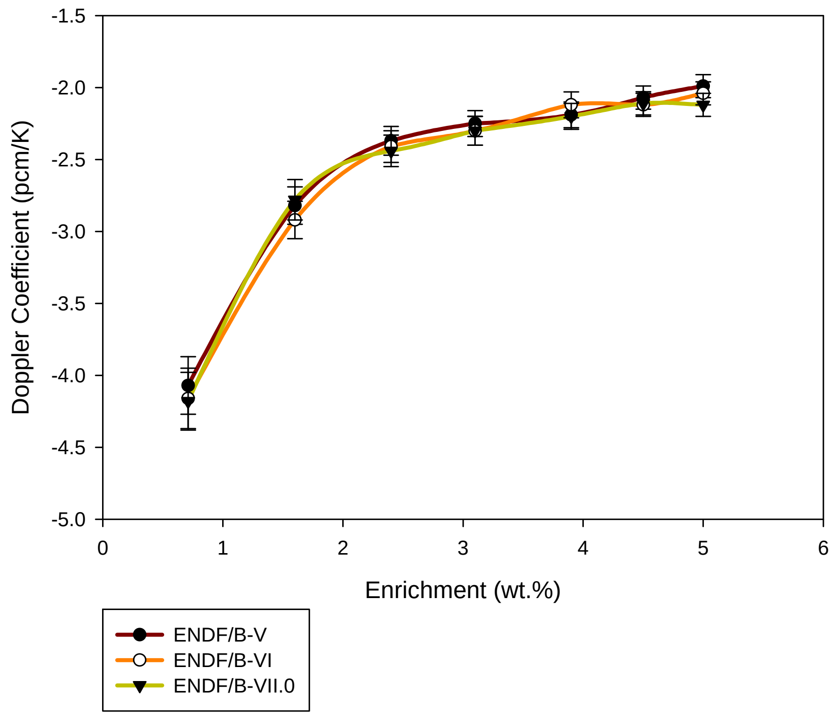

Figure 1. Doppler Coefficient for Normal and Enriched UO_2 Fuel.

corresponding values from ENDF/B-VI or ENDF/B-VII.0. In contrast to those obtained for UO_2 fuel, the ENDF/B-VI and ENDF/B-VII.0 values for k_{eff} are quite consistent with each other. Not surprisingly, the ENDF/B-VI and ENDF/B-VII.0 Doppler coefficients also are quite consistent with each other, showing a gentle but distinct shoulder between 1.0 and 2.0 wt.% PuO_2. Although the ENDF/B-V Doppler coefficients appear to produce a smoother slope, all three sets of results for the Doppler coefficient are within a single standard deviation of each other at each of the PuO_2 concentrations.

The values obtained for k_{eff} and for the Doppler coefficients obtained for the weapons-grade MOX cases are shown in Table IV, and the Doppler coefficients are plotted in Figure 3. The ENDF/B-V values for k_{eff} increase more slowly with plutonium content than do the corresponding values from ENDF/B-VI or ENDF/B-VII.0. However, in contrast with the reactor-recycle results, the ENDF/B-VI values for k_{eff} are consistently lower than those from ENDF/B-VII.0. Nonetheless, all three nuclear data sets once again produce very similar results for the Doppler coefficient. In fact, the Doppler coefficients from the three nuclear data libraries are within a single standard deviation for all but one of the PuO_2 concentrations (4.0 wt.%). The Doppler coefficients for the weapons-grade MOX from each of the three nuclear data libraries produce a pronounced shoulder at a PuO_2 content between 1 wt.% and 2 wt.%. Thereafter, ENDF/B-V produces a curve that is nearly flat, while both ENDF/B-VI and ENDF/B-VII.0 produce curves that become slightly less negative with increasing PuO_2 content.

Table III. Results for Reactor-Recycle MOX Pin Cells

Nuclear Data Library	MOX Content (wt.%)	k_{eff} HFP	k_{eff} HZP	Doppler Coefficient (pcm/K)
ENDF/B-V	1.0	0.93314 ± 0.00027	0.94342 ± 0.00026	-3.89 ± 0.14
	2.0	1.00753 ± 0.00030	1.01884 ± 0.00030	-3.67 ± 0.14
	4. 0	1.06157 ± 0.00030	1.07329 ± 0.00029	-3.43 ± 0.12
	6.0	1.08988 ± 0.00031	1.10180 ± 0.00032	-3.31 ± 0.12
	8.0	1.11360 ± 0.00032	1.12534 ± 0.00030	-3.12 ± 0.12
ENDF/B-VI	1.0	0.93347 ± 0.00027	0.94334 ± 0.00029	-3.74 ± 0.15
	2.0	1.00925 ± 0.00028	1.02025 ± 0.00029	-3.56 ± 0.13
	4. 0	1.06440 ± 0.00031	1.07616 ± 0.00031	-3.42 ± 0.13
	6.0	1.09340 ± 0.00031	1.10532 ± 0.00032	-3.29 ± 0.12
	8.0	1.11705± 0.00030	1.12879 ± 0.00032	-3.10 ± 0.12
ENDF/B-VII.0	1.0	0.93451 ± 0.00027	0.94448 ± 0.00028	-3.77 ± 0.15
	2.0	1.00987 ± 0.00029	1.02081 ± 0.00030	-3.54 ± 0.13
	4. 0	1.06481 ± 0.00032	1.07643 ± 0.00032	-3.38 ± 0.13
	6.0	1.09385 ± 0.00032	1.10568 ± 0.00032	-3.26 ± 0.12
	8.0	1.11694 ± 0.00032	1.12880 ± 0.00031	-3.14 ± 0.12

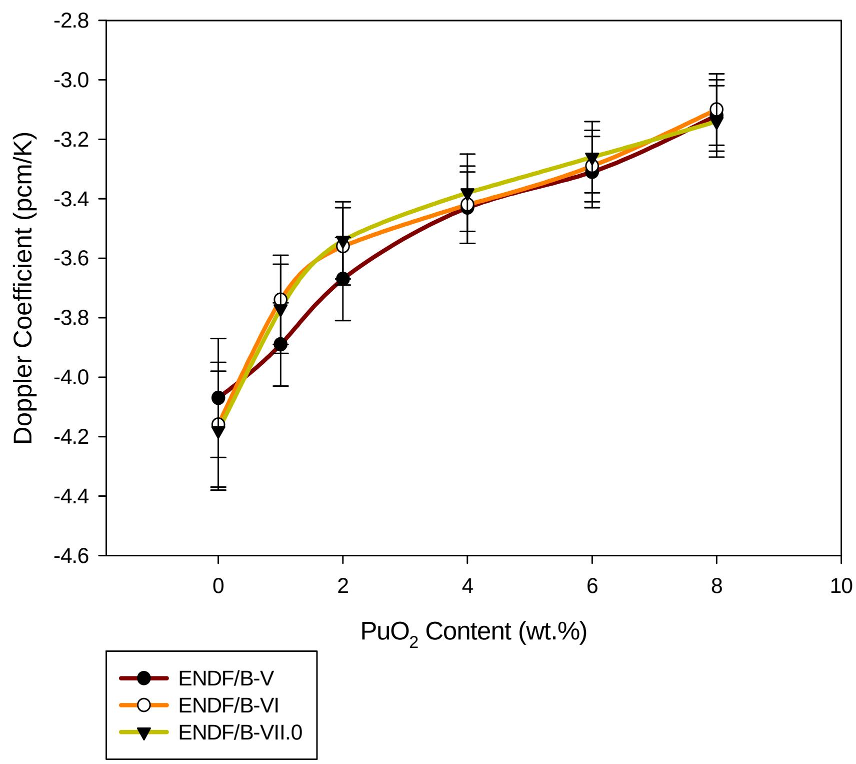

Figure 2. Doppler Coefficient for Reactor-Recycle MOX Fuel.

Table IV. Results for Weapons-Grade MOX Pin Cells

Nuclear Data Library	MOX Content (wt.%)	k_{eff}		Doppler Coefficient (pcm/K)
		HFP	HZP	
ENDF/B-V	1.0	1.07945 ± 0.00029	1.08911 ± 0.00026	-2.74 ± 0.11
	2.0	1.16785 ± 0.00029	1.17847 ± 0.00028	-2.57 ± 0.10
	4.0	1.23410 ± 0.00029	1.24574 ± 0.00029	-2.52 ± 0.09
	6.0	1.26905 ± 0.00029	1.28160 ± 0.00029	-2.57 ± 0.08
ENDF/B-VI	1.0	1.07812 ± 0.00027	1.08821 ± 0.00027	-2.87 ± 0.11
	2.0	1.16813 ± 0.00028	1.17920 ± 0.00029	-2.68 ± 0.10
	4. 0	1.23620 ± 0.00029	1.24839 ± 0.00030	-2.63 ± 0.09
	6.0	1.27284 ± 0.00030	1.28493 ± 0.00031	-2.46 ± 0.09
ENDF/B-VII.0	1.0	1.08002 ± 0.00027	1.09000 ± 0.00027	-2.83 ± 0.11
	2.0	1.17055 ± 0.00029	1.18180 ± 0.00029	-2.71 ± 0.10
	4. 0	1.23823 ± 0.00030	1.25067 ± 0.00029	-2.68 ± 0.09
	6.0	1.27495 ± 0.00030	1.28722 ± 0.00031	-2.49 ± 0.09

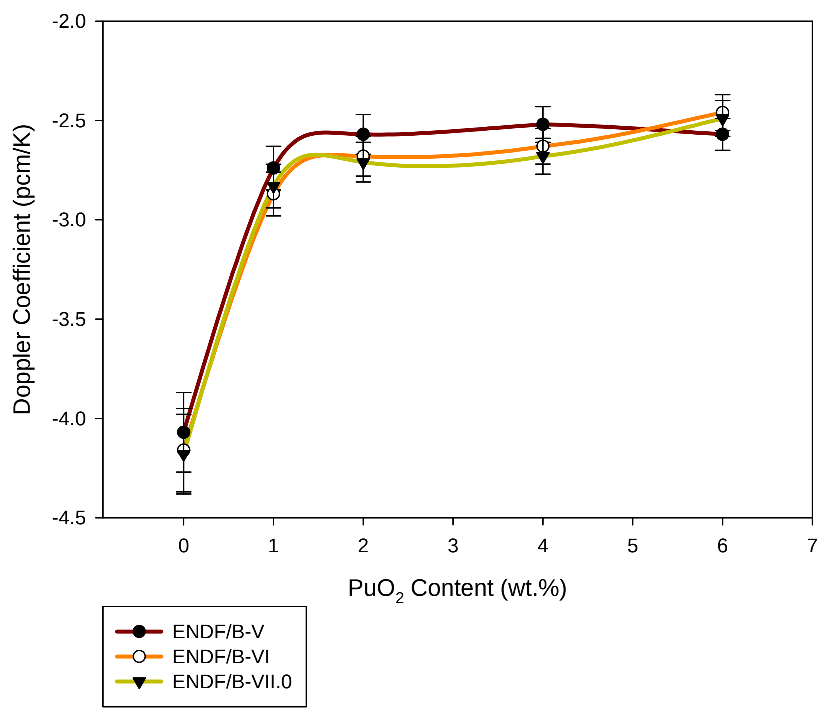

Figure 3. Doppler Coefficient for Weapons-Grade MOX Fuel.

The Doppler coefficients for both reactor-recycle and weapons-grade MOX fuel show considerably less variation with PuO_2 content than the Doppler coefficient for UO_2 fuel shows with enrichment. Furthermore, for the loadings in this study, the Doppler coefficients for the higher PuO_2 concentrations in MOX fuel are significantly more negative than those for the higher enrichments in UO_2 fuel.

4. SUMMARY AND CONCLUSIONS

Calculations with cross sections derived from ENDF/B-V, ENDF/B-VI, and ENDF/B-VII.0 have been performed for all of the cases in the benchmark specifications for the Doppler defect. All three data sets produce very similar results, so similar in fact that for nearly all of the cases the Doppler coefficients from the three nuclear data libraries are statistically indistinguishable. Consequently, even though differences can be observed in the values for k_{eff}, in practical terms it doesn't much matter which of the three nuclear data libraries is used to calculate the Doppler coefficient.

The behavior of the Doppler coefficients for the UO_2, reactor-recycle MOX, and weapons-grade MOX fuels are significantly different, however. The Doppler coefficient for UO_2 fuel follows an approximately asymptotic curve that becomes less negative with increasing enrichment. The Doppler coefficient for reactor-recycle MOX fuel becomes less negative as a function of increasing plutonium content, with a gentle shoulder between 1.0 and 2.0 wt.% PuO_2. The Doppler coefficient for the weapons-grade MOX cases also initially becomes less negative with increasing plutonium content, but it has a pronounced shoulder between 1.0 and 2.0 wt.% PuO_2 and thereafter either becomes less negative much more slowly or remains essentially constant.

The Doppler coefficients for both reactor-recycle and weapons-grade MOX fuel show considerably less variation with PuO_2 content than the Doppler coefficient for UO_2 fuel shows with enrichment. Furthermore, for the loadings in this study, the Doppler coefficients for the higher PuO_2 concentrations in MOX fuel are significantly more negative than those for the higher enrichments in UO_2 fuel.

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