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COMPUTATIONAL BENCHMARK OF THE DOPPLER REACTIVITY DEFECT

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ABSTRACT

A series of MCNP calculations has been performed as a benchmark for the Doppler reactivity defect and Doppler coefficient of reactivity. The geometry is a semi-infinite array of identical fuel pins of infinite length. This geometry was used to calculate the effective multiplication factor at hot zero power and hot full power. Small changes in the dimensions of the fuel pins and cladding were made to account for thermal expansion. Three fuel types were studied: enriched uranium, Reactor-Recycle MOX, and Weapons-Grade MOX with varying enrichments or plutonium concentrations. The Doppler coefficient of reactivity was calculated from the hot zero power and hot full power multiplication factors for each case.

Key Words: MCNP, Doppler Coefficient of Reactivity, Benchmark.

1. INTRODUCTION

The calculation of the Doppler coefficient of reactivity is important for the evaluation of light water reactors. The Doppler reactivity defect—the decrease in reactivity due to the increase in temperature—is of the order of 1% from hot zero power (HZP) to hot full power (HFP) in a light water reactor. The Doppler defect cannot be directly measured in a reactor, but must be calculated from several other parameters. Uncertainties in the Doppler coefficient of reactivity as high as 10% have traditionally been considered acceptable.

A set of benchmark calculations has been constructed for the Doppler reactivity defect and the Doppler coefficient of reactivity. They are based upon previous benchmark studies[1, 2]. This report extends the benchmark calculations to higher uranium enrichments and higher concentrations of plutonium oxide in Reactor-Grade MOX fuels. This report also extends the benchmark by including calculations for Weapons-Grade MOX fuels. This paper presents one set of results for these benchmarks and is included in a summary of similar benchmark calculations[3].

2. BENCHMARK SPECIFICATIONS

The geometry for the benchmark calculations is an infinite array of identical pin cells, infinite in length. The pin cell consists of a cylindrical fuel pin surrounded by a gap, zirconium cladding and borated water. All structural materials were ignored. In this set of results the gap was homogenized with the cladding.

The benchmark is a pair of calculations for hot zero power (HZP) and hot full power (HFP) for the infinite array of pin cells. At HZP the temperature for the fuel, clad, and moderator is uniform at 600 K. At HFP the clad and moderator temperature remains at 600 K and the temperature of the fuel is increased to 900 K. The Doppler defect is the calculated change in the reactivity between HFP and HZP.

The dimensions of the pin cell increased slightly for the HFP to account for thermal expansion. The dimensions of the pin cell is shown in Table I.

Table I. Pin cell dimensions [cm]

Parameter	HZP	HFP
Outer Radius of Fuel	0.39398	0.39433
Outer Radius of Cladding	0.45972	0.45972
Pin to Pin Pitch	1.26678	1.26678

Three different types of fuel are considered in this benchmark; enriched uranium, Reactor-Recycle MOX, and Weapons-Grade MOX. The uranium enrichments range from 0.7 weight percent to 5.0 weight percent. The PuO_2 concentration in the Reactor-Recycle fuels range from 1.0 to 8.0 weight percent and in the Weapons-Grade fuels range from 1.0 to 6.0 weight percent.

The fuel is assumed to be pure UO_2 or MOX with no impurities. The MOX fuel contains natural uranium and PuO_2 with only the four major plutonium isotopes. The plutonium isotopics are taken from previous studies[2, 4] and are given in Table II.

Table II. Plutonium Isotopics [atom %]

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

MCNP was run in criticality mode for these calculations. The number of histories and generations were chosen to reduce the uncertainty in the k-effective calculation to $\sim$0.02 %. For the uranium fuel, 1020 generations were run with the first 20 generations discarded. Each generation had 20,000 histories for a total of 20,000,000 active histories. In the MOX fuel types, 520 generations were run, again discarding the first 20 generations. Each generation had 20,000 histories for a total of 10,000,000 active histories.

3. DESCRIPTION AND ORIGIN OF CROSS SECTIONS

The ENDF66[5] library was used for cross sections for this benchmark. Libraries included in the standard MCNP5 distribution were evaluated at 300K (and 3000K for select uranium and plutonium isotopes). The correct temperature was achieved by Doppler broadening the cross sections using the DOPPLER code[6]. In regions of unresolved resonances, the DOPPLER code interpolated the cross sections between two given libraries. The treatment of thermal scattering off hydrogen in water was treated using original MCNP S(α, β) data libraries without modification.

Figure 1. An example of the `doplr` data card.

```
doplr path=/Volumes/Vol2/sources/mcnpdata
      1001.66c              5.1702E-8   1001.00c
      5010.66c              5.1702E-8   5010.00c
      5011.66c              5.1702E-8   5011.00c
      8016.66c              5.1702E-8   8016.00c
      40000.66c             5.1702E-8   40000.00c
      92234.66c  92234.65c  5.1702E-8   92234.99c
      92235.66c  92235.65c  5.1702E-8   92235.99c
      92238.66c  92238.65c  5.1702E-8   92238.99c
```

To facilitate the use of th DOPPLER code, an unofficial MCNP data card was introduced, `doplr`. A pre-MCNP processing script[7] was created to read an MCNP input file. This script reads the `doplr` data card, prepares an input file for and runs DOPPLER for those cross sections which need Doppler broadening.

An example of the `doplr` card is shown in Fig. 1. In the example, eight libraries are created at 600K for the isotopes: ^{1}H, ^{10}B, ^{11}B, ^{16}O, Zr, ^{234}U, ^{235}U, and ^{238}U. The new libraries are Doppler broadened from existing MCNP libraries specified in the first column. The uranium libraries are created by an interpolation between two given libraries.

Including the `doplr` card and using the pre-MCNP processing script makes creating new cross section libraries simple. The script includes the capability of creating Pseudo Materials[8] as an alternative to generating new libraries, but this feature was not utilized for these benchmark calculations.

4. RESULTS

The data obtained from MCNP are found in Tables III-V and corresponding plots are shown in Figures 2-4. There are a few notable trends worth mentioning. First the Doppler coefficient of reactivity is negative—as we expect it to be—and increases with uranium enrichment or MOX concentration. The uranium fuel shows an increasing function to an asymptotic value. A straight line can be drawn through the data points of the MOX fuel indicating a linear response. For the Weapons-Grade MOX fuel, that line is nearly flat—a constant value for the Doppler coefficient would be within a single standard deviation for all the Weapons-Grade fuel results.

Natural uranium has been included in all three fuel types. In the MOX fuel, this is just a MOX concentration of zero percent and is used as a reference. In all the plots, the error bars indicate one standard deviation.

Table III. UO_2 fuel

Enrichment (wt %)	Hot Zero Power k_{eff}	Hot Full Power k_{eff}	Doppler Defect $(\Delta\rho)$	Doppler Coefficient $(\Delta\rho/\Delta T)$ [pcm/K]
0.711	0.6619 ± 0.00019	0.6562 ± 0.00009	-0.01322 ± 0.00019	-4.4052 ± 0.064
1.600	0.9559 ± 0.00013	0.9476 ± 0.00012	-0.00915 ± 0.00019	-3.0506 ± 0.061
2.400	1.0937 ± 0.00014	1.0845 ± 0.00013	-0.00774 ± 0.00018	-2.5797 ± 0.058
3.100	1.1715 ± 0.00014	1.1620 ± 0.00014	-0.00699 ± 0.00017	-2.3312 ± 0.056
3.900	1.2341 ± 0.00014	1.2245 ± 0.00015	-0.00638 ± 0.00017	-2.1264 ± 0.055
4.500	1.2695 ± 0.00025	1.2598 ± 0.00014	-0.00610 ± 0.00016	-2.0343 ± 0.054
5.000	1.2939 ± 0.00025	1.2840 ± 0.00014	-0.00592 ± 0.00016	-1.9742 ± 0.053

Table IV. Reactor-Recycle MOX Fuel

Concentration (wt %)	Hot Zero Power k_{eff}	Hot Full Power k_{eff}	Doppler Defect $(\Delta\rho)$	Doppler Coefficient $(\Delta\rho/\Delta T)$ [pcm/K]
0.000	0.6619 ± 0.00019	0.6562 ± 0.00009	-0.01322 ± 0.00019	-4.4052 ± 0.064
1.000	0.9441 ± 0.00018	0.9323 ± 0.00020	-0.01338 ± 0.00029	-3.5838 ± 0.095
2.000	1.0177 ± 0.00022	1.0070 ± 0.00020	-0.01047 ± 0.00029	-3.4901 ± 0.097
4.000	1.0732 ± 0.00022	1.0614 ± 0.00022	-0.01032 ± 0.00029	-3.4413 ± 0.097
6.000	1.1020 ± 0.00023	1.0902 ± 0.00023	-0.00988 ± 0.00030	-3.2934 ± 0.098
8.000	1.1257 ± 0.00023	1.1136 ± 0.00022	-0.00966 ± 0.00028	-3.2200 ± 0.094

Table V. Weapons-Grade MOX Fuel

Concentration (wt %)	Hot Zero Power k_{eff}	Hot Full Power k_{eff}	Doppler Defect $(\Delta\rho)$	Doppler Coefficient $(\Delta\rho/\Delta T)$ [pcm/K]
0.000	0.6619 ± 0.00019	0.6562 ± 0.00009	-0.01322 ± 0.00019	-4.4052 ± 0.064
1.000	1.0858 ± 0.00018	1.0769 ± 0.00020	-0.007619 ± 0.00025	-2.5398 ± 0.082
2.000	1.1761 ± 0.00022	1.1651 ± 0.00019	-0.008064 ± 0.00025	-2.6880 ± 0.082
4.000	1.2450 ± 0.00021	1.2329 ± 0.00021	-0.007902 ± 0.00024	-2.6341 ± 0.079
6.000	1.2818 ± 0.00022	1.2693 ± 0.00021	-0.007689 ± 0.00024	-2.5630 ± 0.079

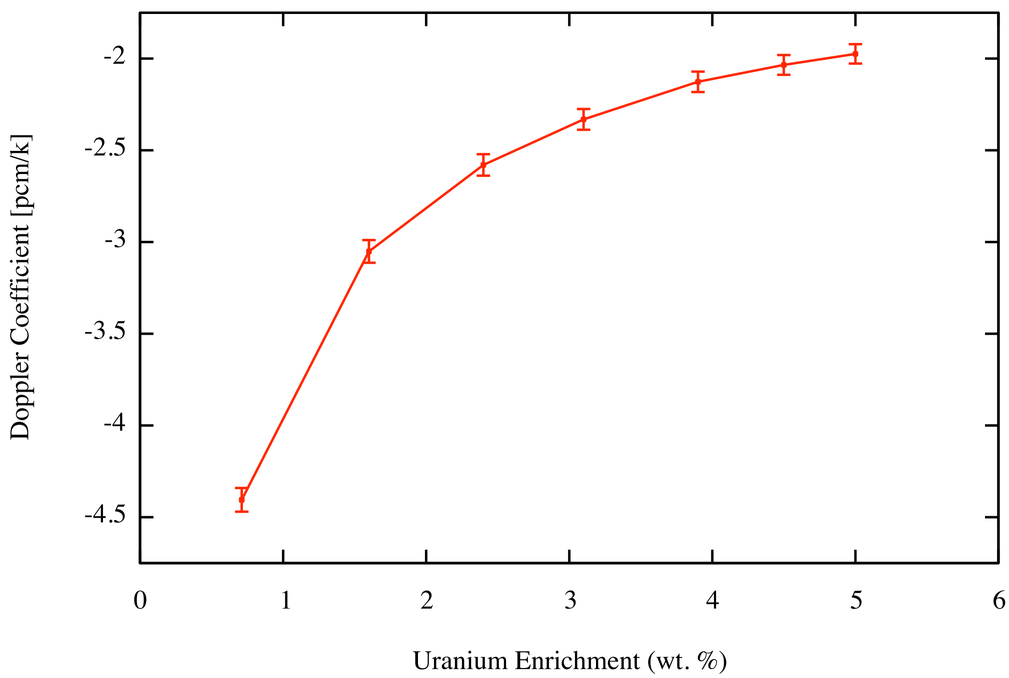

Figure 2. Doppler Coefficient for UO_2 Fuel

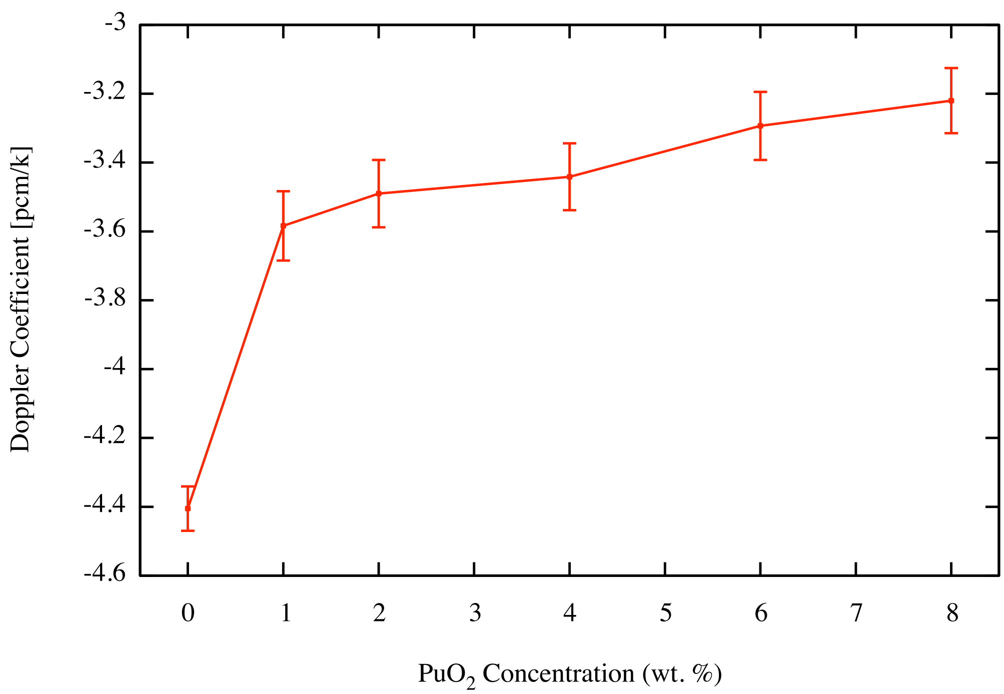

Figure 3. Doppler Coefficient for Reactor-Recycle MOX Fuel

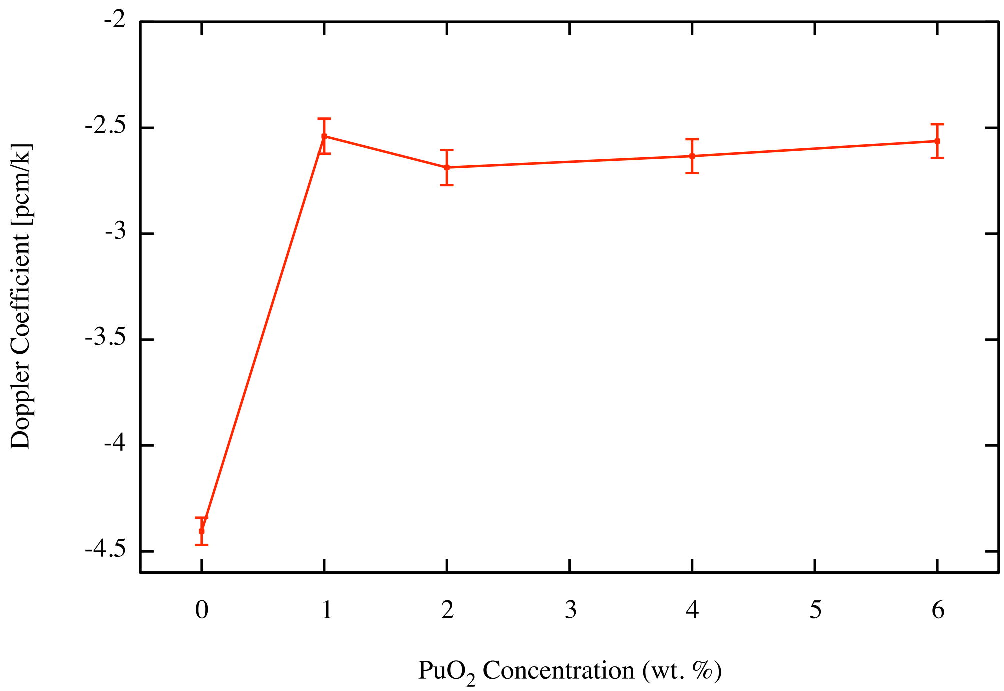

Figure 4. Doppler Coefficient for Weapons-Grade MOX Fuel

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