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**Benchmark Calculations of Lattice Codes for the Doppler  
Coefficient of MOX Fuel**

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**Abstract**

In this study we calculate the infinite multiplication factors ( $k_{inf}$ ) and the Doppler temperature coefficients (DTC) of two mixed-oxide (MOX) fuel rods with different plutonium contents by using PHOENIX-P, HELIOS and CASMO-3 codes. The results were compared against the reference values obtained by MCNP-3A continuous-energy Monte Carlo code. The purpose of this study is to benchmark the accuracy of these lattice codes. The PHOENIX-P's Doppler coefficients calculated were in good agreement with the MCNP results within the Monte-Carlo uncertainty band which is in the order of  $\pm 10\%$  for the Doppler coefficients.

**1. Introduction**

Many countries, which have chosen the nuclear power development, have been vigorously driving the policy to reprocess the plutonium from spent fuels and use it in the form of mixed-oxide(MOX) fuel. It is not only for securing long term economy of nuclear fuel cycle but also for constructing extensive technology in preparation for the era of fast reactors[1]. The neutronic properties of MOX fuel are different from those of UO<sub>2</sub> fuel in view of the thermal cross section, depletion property and delayed neutron fraction, etc. Especially, the self shielding effect of Pu-240, and the larger neutron capture cross sections of Pu-239 and Pu-241 than those of uranium isotopes induce a neutron spectrum hardening, which reduces the neutron flux level in thermal energy range. Therefore, it is important to make further investigations on MOX fuel to improve the accuracy of the current commercial lattice codes. This study calculates the k-infinities and the Doppler coefficients of two MOX fuel pins with different plutonium contents by using PHOENIX-P, HELIOS and CASMO-3 codes. The Doppler coefficient is a significant factor in the evaluation of transient from hot zero power (HZP) to hot full power

(HFP) in LWRs. It is relatively small in magnitude and cannot be measured directly in operating reactors. The purpose of this study is to benchmark and to compare the accuracy of these lattice codes against the reference solution given by MCNP-3A continuous-energy Monte Carlo code. MCNP-3A code uses data taken directly from the ENDF/B-V nuclear data library.

## 2. Lattice Code Descriptions

PHOENIX-P is a two-dimensional transport code that calculates lattice physics parameters for the Westinghouse's Advanced Nodal Code(ANC) core models. PHOENIX-P uses a 42-energy group library which has been generated mainly from ENDF/B-V files. The FIGHTH module automatically generates the effective resonance temperatures(U-238 and Pu-240) for PHOENIX-P as a function of rod burnup. The burnup chains include 22 separate fission products, 2 pseudo fission products and 15 heavy nuclides.

HELIOS code was developed by Scandpower(Norway and USA) with ABB Atom. The unique characteristics of HELIOS is to handle almost any shape of two dimensional geometry and use many nuclides (29 heavy-metals and 114 fission products) to calculate the burnup chain. This study used a 39-group library which has been derived from ENDF/B-VI.

STUDSVIK's CASMO3 is a multigroup two-dimensional transport code for burnup calculations on BWR and PWR pin cells and/or assemblies. The neutron data library is based on data from ENDF/B-IV. A 40-group library has been used in this study. The resonance region is defined to lie between 4 eV and 9,118 eV. Four nuclides (U-235, U-236, U-238 and Pu-239) are treated as resonance absorbers. The burnup chains include 24 separate fission products, 2 pseudo fission products and 17 heavy nuclides.

## 3. Benchmark Case Descriptions

The geometry and material data of pin-cell are directly taken from the Mosteller's Doppler benchmark problem[2]. The dimensions of that pin-cell are presented in Table 1, and a schematic of the cell is given in Fig.1. It is assumed to be at a pressure of 2,250 psia and a soluble boron concentration of 1,400 ppm. The fuel is assumed to be at a temperature of 600°K at HZP and 900°K at HFP. The cladding and moderator are assumed to remain at 600°K for both conditions.

To simplify problem without significant change the characteristics of Doppler feedback, we idealize the pin cell in some respects : (i) the cladding is taken to be

natural zirconium, (ii) the cladding gap is homogenized with the cladding to form a single region, and (iii) structural components, fission products, and actinides have been omitted. Because MCNP can not treat the burnup calculation, the results of PHOENIX-P, HELIOS and CASMO-3 codes are obtained only at BOL.

The calculations are separately performed for the three cases. The first case includes UO<sub>2</sub> fuel pins with five different enrichments ranging from 0.711 w/o to 3.9 w/o at conditions which correspond to HZP and HFP, respectively. The purpose of UO<sub>2</sub> pin calculations is to preliminarily figure out the trend and accuracy of the lattice codes used in this study. The second case includes the plutonium contents of 1 w/o and 2 w/o at the same conditions[3]. The pin with 1 w/o plutonium represents a typical pin at its discharge exposure, while the pin with 2 w/o plutonium is a uncommon pin experienced extremely high exposure. These plutoniums are consisted of 45 a/o Pu-239, 30 a/o Pu-240, 15 a/o Pu-241, and 10 a/o Pu-242. This isotopic composition is a characteristic of LWR fuel pins at high exposures. Because the neutron cross section library for CASMO-3 contains only data of Zr-2 and Zr-4, the cladding could not be specified as natural Zirconium[4]. In the third case, natural Zirconium was replaced by Zircaloy-2 as the cladding material. Then the benchmark calculations were performed in the same way adopted by the first two cases.

Finally, the Doppler coefficients are obtained from k-infinities calculated at HZP and HFP. The Doppler coefficient, C<sub>D</sub>, was defined as

$$C_D = \frac{k_{\infty}^{HFP} - k_{\infty}^{HZP}}{k_{\infty}^{HFP} k_{\infty}^{HZP}} \frac{1.0E05}{T^{HFP} - T^{HZP}} \quad (\text{pcm} / ^\circ\text{K})$$

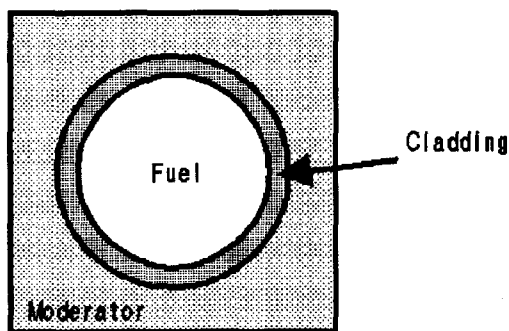


Fig.1. Pin-cell geometry

Outer radius of fuel pellet	0.39306
Outer radius of cladding	0.45802
Pin cell pitch	1.26209
Equivalent pin cell radius	0.71206

Table 1. Dimensions for calculations (cm)

## 4. Results and Conclusions

The Doppler coefficient of 5 different enriched UO<sub>2</sub> rods and 2 MOX fuel rods with different contents are calculated as the function of the enrichment and the fuel temperature using PHOENIX-P, HELIOS and CASMO-3. The calculated k-infinities and the Doppler coefficients are given in Table 2 through Table 5. As shown in Table 3 and Table 5, the replacement of Zircaloy-2 as the cladding material affected only the values of k-infinities but did not have much effect on the Doppler coefficients. Therefore, the comparison of the Doppler coefficient is based on the Zircaloy-2 cladding.

For the UO<sub>2</sub> rods, Fig. 2 shows that the Doppler coefficients of PHOENIX-P and HELIOS are in good agreement with that of MCNP within the Monte-Carlo uncertainty band which is in the order of  $\pm 10\%$  for the Doppler coefficients. On the other hand, CASMO-3 code slightly overestimates the Doppler coefficients.

For MOX fuel rods, Fig. 3 shows that only PHOENIX-P predicted the Doppler coefficients within the MCNP uncertainty band, whereas both HELIOS and CASMO-3 codes overestimate the Doppler coefficients.

The lattice code PHOENIX-P is assured to be valid for MOX fuel with up to 2 w/o Pu contents without changing its methodology and the neutron cross section library. We plan to calculate the MOX rods with higher Pu contents, the unit assembly and guard assembly to ensure the accuracy of PHOENIX-P code.

## REFERENCES

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3. R.D. Mosteller, J.T. Holly and L.A. Mott, "Benchmark Calculations for the Doppler Coefficient of Reactivity in the Mixed-oxide Fuel", ANS International Topical Mtg., Apr., 1991, Vol.2.
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Table 2. The K-inf of UO<sub>2</sub> fuel pin with natural Zr cladding as a function of fuel enrichment

Fuel Enrichment	Fuel Temp. (K)	MCNP	PHOENIX-P	HELIOS
0.711	600	0.6638 ± 0.0006	0.66877	0.66651
	900	0.6567 ± 0.0008	0.66177	0.65845
1.6	600	0.9581 ± 0.0006	0.96474	0.96309
	900	0.9484 ± 0.0006	0.95550	0.95275
2.4	600	1.0961 ± 0.0007	1.10267	1.10198
	900	1.0864 ± 0.0007	1.09264	1.09097
3.1	600	1.1747 ± 0.0007	1.18022	1.18059
	900	1.1641 ± 0.0006	1.16979	1.16932
3.9	600	1.2379 ± 0.0006	1.24273	1.24435
	900	1.2271 ± 0.0006	1.23155	1.23251

Table 3. The Doppler coefficients (pcm/K) of UO<sub>2</sub> fuel Pin Vs. Fuel enrichments

Fuel Enrichment (wt%)	MCNP	PHOENIX-P		HELIOS		CASMO-3
	Nat. Zr	Nat. Zr	Zr-2	Nat. Zr	Zr-2	Zr-2
0.711	-5.4 ± 0.8	-5.27	-5.30	-6.12	-6.10	-6.24
1.6	-3.6 ± 0.3	-3.34	-3.37	-3.76	-3.76	-3.91
2.4	-2.7 ± 0.3	-2.77	-2.78	-3.05	-3.04	-3.21
3.1	-2.6 ± 0.2	-2.52	-2.53	-2.72	-2.71	-2.88
3.9	-2.4 ± 0.2	-2.43	-2.44	-2.57	-2.57	-2.74

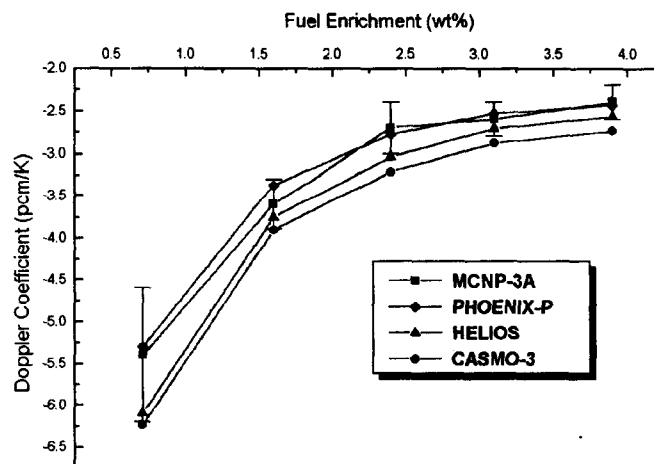


Fig. 2. Doppler coefficient of UO<sub>2</sub> as a function of fuel enrichment

Table 4. The K-inf of MOX fuel pin with natural Zr cladding as a function of fuel enrichment

Fuel Enrichment (a/o)	Fuel Temp. (K)	MCNP	PHOENIX-P	HELIOS
1.0	600	0.9445 ± .0007	0.94682	0.94378
	900	0.9347 ± .0007	0.93624	0.93216
2.0	600	1.0182 ± .0007	1.01845	1.01430
	900	1.0077 ± .0007	1.00750	1.00141

Table 5. The Doppler coefficients (pcm/K) of MOX fuel Pin Vs. Fuel enrichments

Fuel Enrichment (a/o)	MCNP	PHOENIX-P		HELIOS		CASMO-3
	Nat. Zr	Nat. Zr	Zr-2	Nat. Zr	Zr-2	Zr-2
1	-3.7 ± 0.4	-3.98	-3.99	-4.40	-4.39	-4.20
2	-3.4 ± 0.3	-3.56	-3.57	-4.23	-4.22	-3.78

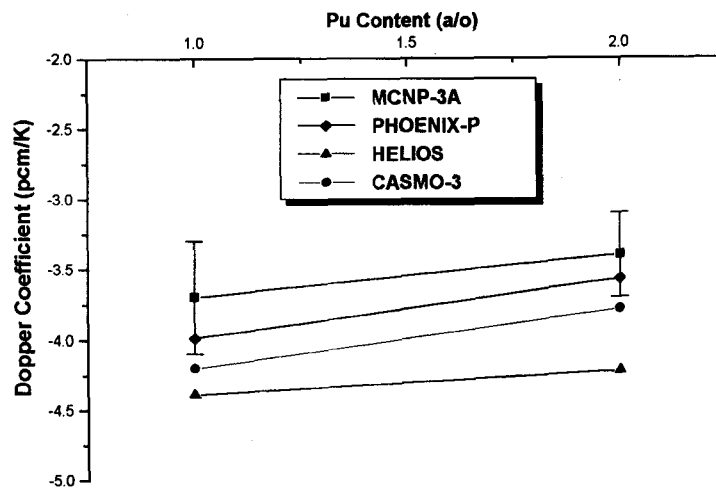


Fig. 3. Doppler coefficient of MOX fuel as a function of fuel enrichment