# Comparison of Fuel Temperature Coefficients of PWR $UO_2$ Fuel from Monte Carlo Codes (MCNP6.1 and KENO6)

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## 1. Introduction

The interaction probability of incident neutron with nuclear fuel is depended on the relative velocity between the neutron and the target nuclei. However, since the nucleus are in continual thermal motion, this relative velocity can be changed to be faster or slower than the neutron speed, and their thermal motion is mainly influenced by the change of fuel temperature. Especially, the resonance in neutron absorption cross-section is broadened with increasing fuel temperature, while its peak magnitude is decreased. This phenomenon is called as Doppler effect of cross section, which leads the change of the neutron multiplication factor ($k_{eff}$) in nuclear core. The Fuel Temperature Coefficient (FTC) is defined as the change of Doppler effect with respect to the change in fuel temperature without any other change such as moderator temperature, moderator density, etc.

In this study, the FTCs for $UO_2$ fuel were evaluated by using MCNP6.1 [1] and KENO6 [2] codes based on a Monte Carlo method. In addition, the latest neutron cross-sections (ENDF/B-VI and VII) were applied to analyze the effect of these data on the evaluation of FTC, and nuclear data used in MCNP calculations were generated from the makxsf code [3].

## 2. Methods and Materials

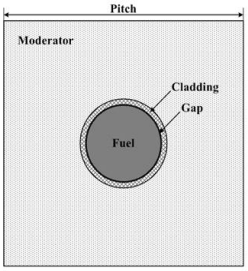
The Doppler effect ($\Delta\rho_{DD}$) can be simply evaluated from the reactivity difference between the Hot Full Power (HFP) and Hot Zero Power (HZP) conditions, which is mathematically presented as follows;

$$\Delta\rho_{DD} = \frac{k_{eff}^{HFP} - k_{eff}^{HZP}}{k_{eff}^{HFP} \times k_{eff}^{HZP}} \quad (1)$$

The FTC ($D_c$) is defined as the change of Doppler effect with respect to the change in fuel temperature ($\Delta T_{Fuel}$) without any other change such as moderator temperature, moderator density, etc., and it can be denoted as follows;

$$D_c = \frac{\Delta\rho_{DD}}{\Delta T_{Fuel}} \quad (2)$$

The nuclear fuels used in PWR are arranged in lumps of rods separated by borated water, in which neutrons are moderated to thermal energy with a minimum of capture. Also, the $UO_2$ material is surrounded by a cladding separating the fission products from the cooling water, and the circular horizontal intersection of these fuel elements is arranged in squares. Hence, a typical unit cell of PWR $UO_2$ fuel can be assumed to be a square with a cylindrical fuel rod in a center, and its specification applied in this study is presented in **Figure 1**.




| Parameter | Value |
|---|---|
| Pitch [cm] | 1.26678 |
| Fuel Diameter [cm] | 0.78796 (HZP)<br>0.78866 (HPF) |
| Fuel Material | $UO_2$ |
| Fuel Density [g/cm³] | 10.339 (HZP)<br>10.312 (HFP) |
| Cladding Outside Diameter [cm] | 0.91944 |
| Cladding Thickness [cm] | 0.05746 |
| Cladding Material | Zirconium |
| Cladding Density [g/cm³] | 6.3902 |
| Moderator Material | Borated Water<br>(Boron 1400ppm) |
| Moderator Density [g/cm³] | 0.66163 |

**Figure 1.** Unit Cell Model of PWR $UO_2$ Fuel

The unit cell model was composed of $UO_2$ fuel, cladding, and moderator regions and was on the basis of Mosteller pin-cell benchmark [4]. The fuel, cladding, and moderator were pure $UO_2$ with no $^{236}U$ concentration, natural zirconium, and borated water respectively, and the gap was modeled as a void. Since the unit cell model was established to evaluate the FTCs, the moderator and cladding temperatures were assumed to remain at 600K for the HZP and HFP conditions. On the other hand, the fuel temperature was assumed to be changed from 600K at the HZP to 900K at the HFP, and there were some differences in fuel diameter and density at those temperatures. The uranium enrichments with the range of natural to 5% were also considered in the evaluations of the neutron multiplication factor and FTC.

A series of evaluations were performed by using MCNP6.1 and KENO6 codes with the latest neutron cross-sections (ENDF/B-VI and VII). Although the basic cross-sections generated from the NJOY code with ENDF/B data files are already included in MCNP code package, specific cross-sections adequate to the HZP and HFP conditions cannot be readily available for these evaluations. Accordingly, the makxsf code was introduced to generate the cross-sections at the desired temperatures, and new data were created from the existing library files (ENDF66a, ENDF66e, and ENDF71x) in MCNP code. Each evaluation was performed with 10,000 neutrons per cycle and an initial guess for $k_{eff}$ of 1.0. The first 500 cycles were skipped before $k_{eff}$ data accumulation, and a total of 3,500 cycles were run.

## 3. Results and Discussions

For seven different uranium enrichments (0.711 wt% – 5.0 wt% $^{235}$U), $k_{eff}$ values calculated from two Monte Carlo codes were tabulated in **Table 1**. The relative error, corresponding to one standard deviation (σ), for each calculation was less than 15 pcm. As expected, $k_{eff}$ values were slowly increased with the increase of uranium enrichment, and $k_{eff}$ values at HZP condition were higher than those values at HFP condition. Particularly, MCNP code produced $k_{eff}$ values higher than those calculated from KENO code, and the result using the ENDF/B-VII cross-section presented approximately 300 to 400 pcm higher $k_{eff}$ values compared to the other cases.

**Table 1.** Calculation Results for the Unit Cell Model of PWR $UO_2$ Fuel

| Code | $^{235}$U wt% | $k_{eff}$ at HFP (Rel. Error) | | $k_{eff}$ at HZP (Rel. Error) | |
|---|---|---|---|---|---|
| | | ENDF/B-VI | ENDF/B-VII | ENDF/B-VI | ENDF/B-VII |
| MCNP | 0.711 | 0.65918 (0.00007) | 0.66192 (0.00008) | 0.66465 (0.00008) | 0.66752 (0.00008) |
| | 1.6 | 0.95052 (0.00010) | 0.95458 (0.00010) | 0.95876 (0.00010) | 0.96236 (0.00010) |
| | 2.4 | 1.08755 (0.00011) | 1.09147 (0.00011) | 1.09643 (0.00011) | 1.10049 (0.00011) |
| | 3.1 | 1.16489 (0.00012) | 1.16873 (0.00011) | 1.17402 (0.00011) | 1.17850 (0.00012) |
| | 3.9 | 1.22696 (0.00012) | 1.23084 (0.00012) | 1.23685 (0.00012) | 1.24080 (0.00012) |
| | 4.5 | 1.26195 (0.00012) | 1.26615 (0.00012) | 1.27209 (0.00012) | 1.27648 (0.00012) |
| | 5.0 | 1.28623 (0.00012) | 1.29018 (0.00012) | 1.29649 (0.00012) | 1.30079 (0.00012) |
| KENO | 0.711 | 0.65752 (0.00013) | 0.65946 (0.00013) | 0.66359 (0.00013) | 0.66568 (0.00013) |
| | 1.6 | 0.94901 (0.00014) | 0.95233 (0.00014) | 0.95726 (0.00014) | 0.96051 (0.00015) |
| | 2.4 | 1.08599 (0.00014) | 1.08905 (0.00015) | 1.09534 (0.00014) | 1.09879 (0.00014) |
| | 3.1 | 1.16340 (0.00014) | 1.16648 (0.00014) | 1.17333 (0.00015) | 1.17637 (0.00014) |
| | 3.9 | 1.22551 (0.00014) | 1.22874 (0.00014) | 1.23562 (0.00014) | 1.23905 (0.00014) |
| | 4.5 | 1.26076 (0.00014) | 1.26413 (0.00014) | 1.27098 (0.00014) | 1.27441 (0.00014) |
| | 5.0 | 1.28502 (0.00014) | 1.28822 (0.00014) | 1.29544 (0.00014) | 1.29885 (0.00014) |

Based on these results, the FTCs were derived by Eq. (1) and (2), and they were plotted in **Figure 2**. In this figure, every symbol indicated the results at seven uranium enrichments considered in this study, and colored-lines were made with fitting these results by a 4$^{th}$ order polynomial equation. As a result, the FTC was changed to be less negative with increasing uranium enrichment, and the fitted curves appeared to take on an asymptotic shape. In the case of MCNP calculations with the ENDF/B-VI and VII, there was a difference more than two standard deviation (2σ) between the FTCs at specific uranium enrichments (1.6 wt% and 3.1 wt% $^{235}$U). On the other hand, KENO calculation produced very similar results, regardless of the applied cross-section data. The largest difference of these results was observed at natural uranium enrichment, and this phenomenon might be due to the highest $^{238}$U concentration and the difference in Doppler broadening models employed in two codes. In the case of MCNP codes, the standard Sampling of Velocity of Target nucleus (SVT) method was used to determine the energy and angle of a scattered neutron. Whereas, in the other code, the cross-sections for the scattering kernel were obtained by solving the slowing-down equation with the continuous energy cross sections and integrating the continuous energy flux and cross section over each group.

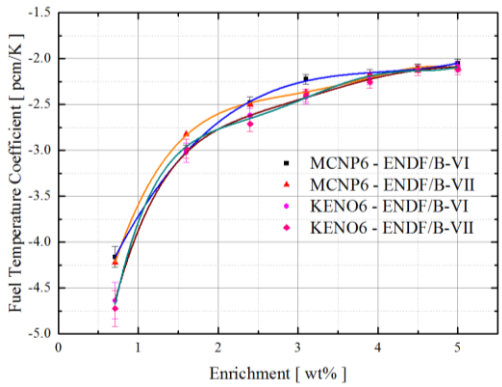



**Figure 2.** Fuel Temperature Coefficients for PWR $UO_2$ Fuel

## 4. Conclusions

An evaluation of the Doppler effect and FTC for $UO_2$ fuel widely used in PWR was conducted using MCNP6.1 and KENO6 codes. The ENDF/B-VI and VII were also applied to analyze what effect these data has on those evaluations. All cross-sections needed for MCNP calculation were produced using makxsf code. The calculation models used in the evaluations were based on the typical PWR $UO_2$ lattice. As a result, there was a difference within about 300–400 pcm between $k_{eff}$ values at each enrichment due to the difference of codes and nuclear data used in the evaluations. The FTC was changed to be less negative with the increase of uranium enrichment, and it followed the form of asymptotic curve. However, it is necessary to perform additional study for investigating what factor causes the differences more than two standard deviation (2σ) among the FTCs at partial enrichment region.

## REFERENCES

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