# Verification of MC<sup>2</sup>-3 Doppler Sample Models in ZPPR-15D Experiments

Min Jae Lee<sup>\*</sup>, Donny Hartanto and Sang Ji Kim Korea Atomic Energy Research Institute (KAERI) 989-111 Daedeok-daero, Yuseong-gu, Daejeon, Korea, 305-353 *\*Corresponding author: lmj@kaeri.re.kr* 

### 1. Introduction

The Doppler broadening is an instant feedback mechanism that improves safety and stability for both thermal and fast reactors. Therefore, the accuracy of Doppler coefficient becomes an important parameter in reactor design as well as in the safety analysis. The capability of the Doppler worth calculation by a modern computer code suites such as MC<sup>2</sup>-3 [1] and DIF3D-VARIANT [2], has been validated against the Zero Power Physics Reactor-15 (ZPPR-15) Doppler worth measurement experiments [3,4]. For the same experiments, our previous work suggested four different MC<sup>2</sup>-3 Doppler sample models for enhanced accuracy, which are combinations of heterogeneous models and the super cell approach [5]. In this paper, the change of reaction rate and broadened cross section were estimated by as-built MCNP models for metallic uranium sample in ZPPR-15D using ENDF/B-VII.0 library, and the results were compared with deterministic calculations provided in previous work.

## 2. Estimation of reaction density by MCNP

A Monte Carlo Doppler worth calculation for a small sample is considered to be unrealistic because the Doppler worth is normally extremely small compared to the typical uncertainty of criticality. However, Monte Carlo method can estimate the cross section and the neutron spectrum of a Doppler sample with reasonable accuracy. From the broadened cross sections and neutron spectrum, the change of reaction density  $\Delta(\sigma\phi)$  by Doppler broadening can be evaluated with simple arithmetic. As the Doppler effects are mostly controlled by the broadened cross section of U-238, the total reaction and flux of a Doppler sample are tallied. Among four ZPPR-15 Doppler samples as tabulated in Table I, N-11 sample was chosen for the analysis since it has relatively large Doppler worth than others and the worth was measured for ZPPR-15A, -15B and -15D.

Table I: Doppler Samples in ZPPR-15

Name	Description	А	В	D
N-3	UO2 natural	0	0	0
N-11	Uranium metal depleted	0	0	0
N-24	U-Zr metal depleted	-	0	0
E-33-A	UO <sub>2</sub> 33% enriched	-	-	0

The measurements in ZPPR-15D, which is uranium fueled core, were examined in this paper, since the

calculated Doppler worth from MC<sup>2</sup>-3/DIF3D showed a relatively large underestimation in this phase.

The total reaction rate of U-238 and the neutron spectrum of the Doppler Sample are obtained from MCNP6 [6], and they are plotted in Figs. 1 and 2 respectively based on the 33 energy group structure in  $MC^{2}$ -3. The total reaction of U-238 slightly increases in  $10keV \sim 100keV$  as temperature increases, while the neutron spectrum does not change meaningfully at 1011K.



Fig. 1. U-238 Total reaction rate of N-11 in ZPPR-15D



From Figs.1 and 2, the microscopic total cross section of U-238 can be estimated as plotted in Fig. 3. The uncertainty of the cross sections is obtained using the typical error propagation formula below:

$$\sigma_{\sigma_{T}}^{2} = \sigma_{T}^{2} \left[ \left( \frac{\sigma_{R}}{R} \right)^{2} + \left( \frac{\sigma_{\phi}}{\phi} \right)^{2} - 2 \frac{\sigma_{R\phi}}{R \cdot \phi} \right]$$

$$\approx \sigma_{T}^{2} \left[ \left( \frac{\sigma_{R}}{R} \right)^{2} + \left( \frac{\sigma_{\phi}}{\phi} \right)^{2} \right]$$
(1)

where  $\sigma$  stands for standard deviation while  $\sigma_T$ , R,  $\phi$  are microscopic cross section of total reaction, reaction rate and flux respectively.

Note that the covariance term in Eq. (1) is omitted since the covariance between flux and reaction tallies is unknown. However, the correlation of those two tallies must be very strong, which implies that the real uncertainty of the estimated cross section might be much smaller than appeared in Fig. 3.



Fig. 3. Estimated U-238 total cross section of sample N-11

From the above cross section and neutron spectrum, the transition of U-238 reaction density can be easily obtained as:

$$\Delta(\sigma\phi) = (\sigma\phi)_{101\,\text{IK}} - (\sigma\phi)_{300\text{K}} \tag{2}$$

Most of the neutrons measured in Doppler sample are coming from neighbor fuel cells, and the portion of fission neutron in the Doppler sample is negligible. Therefore the difference in neutron spectrum between 300K and 1011K is negligible as plotted in Fig. 4, so Eq. (2) can be simplified further as:

$$\Delta(\sigma\phi) \cong (\sigma_{101\,\text{IK}} - \sigma_{300\text{K}})\phi_{300\text{K}}$$

$$\cong (\sigma_{101\,\text{IK}} - \sigma_{300\text{K}})\phi_{101\,\text{IK}}$$
(3)



Fig. 4. Difference of neutron spectrum between 300K and 1011K

Fig. 5 shows the transition of reaction density  $\Delta(\sigma\phi)$  obtained from Eq. (2) and (3), and the two plots show different behavior. The one by Eq. (2) has negative values above 20keV, which is caused by the uncertainty of neutron spectrum. However, the blue one by Eq. (3) has much improved shape above 20keV. The error bars are greater for the blue one because of the exaggerated cross section uncertainty, but the real uncertainty of the blue one is expected to be smaller. Since the neutron spectrum plays a role of weighting function, the local fluctuation of flux is not important to estimate the transition of reaction density. Therefore more reliable results could be obtained from Eq. (3) by ignoring the errors coming from the flux uncertainty.



#### 3. Analysis on MC<sup>2</sup>-3 Doppler sample models

The four Doppler sample models of  $MC^{2}$ -3 are as follows; 1) Homogeneous Model (HOM), 2) Homogeneous Model with Super Cell (SPC), 3) 2D MOC model and 4) 2D MOC with Super Cell model (MOC-SPC). In the super cell models, the Doppler samples are surrounded by fuel cells. The 2D heterogeneous geometry of the Doppler sample is explicitly modeled in 2D MOC models as plotted in Fig. 6.



U-238 total cross sections from MC<sup>2</sup>-3 calculations were obtained for four different models, and compared with MCNP6 for 300K and 1011K as plotted in Fig. 7 and Fig. 8. The error of MOC and MOC-SPC models show smaller error than HOM and SPC models for both 300K and 1011K. This implies that the local heterogeneous effects cannot be ignored even in the small Doppler sample although the effects are known to be minor for fast reactor problems.





Fig. 8. Error of U-238 total cross section at 1011K

Since the cross section change  $(\Delta \sigma)$  directly shows the effects of Doppler broadening, it is compared as plotted in Fig. 9 and Fig. 10. The error of  $\Delta \sigma$  is generally smaller with MOC models. The error of MOC models becomes greater for lower energy ranges below 1keV, but the effects on Doppler worth is minor since the neutron population is low.



Fig. 9 Broadened cross section ( $\Delta \sigma$ ) for different models



The broadened cross section in the energy range of high neutron population becomes more important, and vice versa. Therefore the broadened cross section should be considered together with neutron spectrum as plotted in Fig. 11. Note that the calculated Doppler worth will be almost linearly proportional to the summation of the area under each line in Fig. 11.



Fig. 12 shows the error of  $\Delta(\sigma\phi)$ , and relatively small error of broadened cross section in higher energy range in Fig. 10 becomes magnified by high neutron population, and vice versa. The MOC and MOC-SPC models showed much smaller error compared to other two models. However, the positive error can be canceled out by the negative error when Doppler worth is considered, so the calculated Doppler worth can be expected to be similar for four different models, and our previous work has proved this as given in Table II. The effects of super cell approach seems minor compared to the local heterogeneity effects since the results do not change much after applying super cell approach.

Table II: Error of calculated Doppler worth

C/E-1 [%]					
HOM	SPC	MOC	MOC-SPC		
-17.05	-17.05	-14.47	-15.86		



#### 4. Conclusions

Finding reference Monte Carlo solution of Doppler sample's worth calculation is unfeasible because of the small magnitude of Doppler worth. Instead of the worth itself, the transition of reaction density was accurately estimated by Monte Carlo method, and it is utilized to analyze the performance of MC<sup>2</sup>-3 Doppler sample models.

The MOC and MOC-SPC models showed the smallest error in estimating the U-238 total cross section of Doppler sample N-11, and the Doppler broadening effects are well applied to the cross section compared to other two models, HOM and SPC. The effects of the super cell approach can be hardly seen, since the broadened cross section is almost the same with and without the super cell approach. Comparing the transition of reaction density, MOC and MOC-SPC models also show similar behavior as MCNP's with minor errors. As a conclusion, we could obtain more consistent broadened cross section as well as reaction density transition by providing heterogeneous models from MC<sup>2</sup>-3's MOC module.

#### ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP). (No. NRF-2013M2A8A2078239)

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