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Analysis on Modeling Effects of Doppler Samples in ZPPR-15 Experiments

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1. Introduction

The Korea Atomic Energy Research Institute (KAERI) and Argonne National Laboratory are jointly carrying out a broad R&D program in support of the 150 MWe Prototype Generation-IV Sodium-cooled Fast Reactor (PGSFR) to demonstrate the performance of metallic fuel containing SFRs. Currently, validation database of metallic-fueled fast reactors using the Zero Power Physics Reactor-15 (ZPPR-15) [1] are being generated for validation of modern code suites for PGSFR design analysis including Doppler worth measurements. Doppler broadening is one of the most important feedback mechanisms in safety analysis of PGSFR, so the accuracy of Doppler coefficient calculated from current design procedure becomes a main concern. The validation calculation was performed for ZPPR-15 Doppler measurements and showed a good agreement between measured and calculated results [2], but only homogenous Doppler sample model was examined.

In this study, Doppler reactivity worth calculations were performed for ZPPR-15 Doppler measurement experiment using MC^2-3 [3] based on ENDF/B-VII and DIF3D-VARIANT [4]. Four different Doppler sample models are suggested for the homogenized cross section generation stage in MC^2-3 calculations, and their effects on Doppler worth calculation are analyzed. The details of each model will be described in Section 2, and the calculated Doppler worth and its analysis will be discussed in Section 3.

2. Four Different Doppler Sample Models

The calculated Doppler worth is highly dependent on the homogenized cross sections at each temperature step. Since explicit geometry as well as core configurations are not considered in the cross section generation step, several models of Doppler sample can be considered with proper approximations. One of the simplest model is homogeneous 0D, which neglects local heterogeneity since high energy neutrons are dominant in fast reactor problems. However, this model has one drawback such that the ultra-fine group spectrum, which is used for group collapsing to generate broad-group cross sections, is obtained only from the internal fissions of Doppler samples. The actual spectrum of a Doppler sample will be determined by other fuel drawers, because the k-inf of Doppler sample drawer is only around 0.2 and most of neutrons are coming from surrounding fuel drawers.

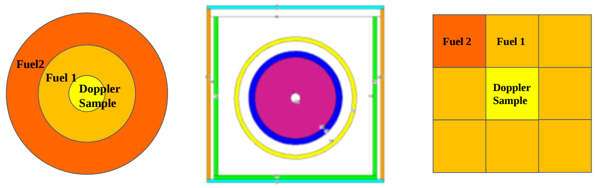
In order to overcome this drawback, a simple super cell model is suggested as plotted in Fig. 1 (a). Note that the fuels surrounding Doppler sample are indicated as fuel 1, and fuel 2 is the most frequently used fuel in a core. 1D Collision Probability Method (CPM) based on cylinder geometry was employed for a transport calculation.

On the other hand, the effects of local heterogeneity can be taken into account by providing 2D Method of Characteristic (MOC) with reflective boundary conditions. The 2D MOC solver was developed in Purdue University, and utilized for cross section generation coupled with other subroutines in the MC^2-3 code. The 2D cross sectional view of Doppler sample model is plotted in Fig. 1 (b). Two types of 2D MOC models can be suggested here; one is an equivalent 2D model that preserve the mass of 3D Doppler sample in 2D model by smearing axial structures into radial meshes, and the other one is the sliced model that is obtained from center-cut of Doppler sample axially. The calculation results of Doppler worth from those two models are almost the same, so we adopted the sliced 2D model for investigation to avoid complicated procedures for generating an equivalent 2D model.

The combined effects of neutron spectrum and local heterogeneity were also examined by providing 2D MOC with super cell calculation. The 3x3 model plotted in Fig. 1 (c) is actual 3x3 drawer configurations around the Doppler sample.

Note that the axial regions of the drawer containing Doppler sample is divided according to the axial boundaries of Doppler sample, and they are homogenized separately since the axial regions beyond Doppler sample is almost void.

As a summary, a) homogeneous single cell model (Hom.), b) homogeneous model with super cell (S. C), c) MOC single cell (MOC), d) MOC with super cell (M.S.C) are four types of Doppler sample models to be investigated in this work. 'Single cell' will be omitted afterward for briefness.



(a) Hom. w/ Super Cell (b) 2D MOC (c) MOC w/ Super Cell

Fig. 1 Three types of Doppler sample models

3. Modeling Effects of ZPPR-15 Doppler Samples

The homogenized cross sections were generated from MC[2]-3 at each measurement temperature, and the difference in k eigenvalues according to Doppler sample's temperature was converted to Doppler worth. For a full core transport calculation, a DIF3D-VARIANT calculation was employed. The convergence criteria for eigenvalue was set to 1×10^{-9}. The order of source and flux approximation were 4 and 6 respectively with a P_3 flux and P_3 scattering kernel. Note that the MOC options for an MC[2]-3 calculation were selected as 0.05 cm of ray spacing, 4 axial angles and 24 azimuthal angles. The number of energy group was set to 33 for all the cases to be consistent with PGSFR design procedure.
Four different types of Doppler samples were measured in ZPPR-15 and they are summarized in Table I. Note that the capital alphabet A, B and D indicates the phase of ZPPR-15 experiments. ZPPR-15A contains plutonium fuels without Zr alloy, while ZPPR-15B represents plutonium fueled cores with Zr alloy. ZPPR-15D contains enriched Uranium cores.

Table I. List of Doppler Samples in ZPPR-15

Name	Description	A	B	D
N-3	UO_2 natural	O	O	O
N-11	Uranium metal depleted	O	O	O
N-24	U-Zr metal depleted	-	O	O
E-33-A	UO_2 33% enriched	-	-	O

3.1 Calculated Doppler Worth from MC[2]-3/DIF3D

From Table II to Table IV summarize the Doppler worth calculated by MC[2]-3/DIF3D-VARIANT with various Doppler Sample models.

Table II. Doppler Worth Results from ZPPR-15A

	Temp.	Exp. [¢/kgU]	C/E-1 [%]			
			Hom.	S.C.	MOC	M.S.C.
N-3	543 K	-0.035	-1.39	4.88	-6.08	-3.73
	685 K	-0.049	-1.25	4.88	-2.37	-0.14
	800 K	-0.057	1.88	8.13	1.88	3.80
	954 K	-0.069	0.04	6.00	-1.15	1.23
	1100 K	-0.078	-0.77	5.52	-1.82	0.63
N-11	503 K	-0.025	8.42	9.90	2.51	0.54
	640 K	-0.037	8.68	10.35	4.68	2.68
	784 K	-0.048	7.65	9.20	1.45	-0.10
	892 K	-0.056	6.14	7.93	-0.79	-2.57
	1023 K	-0.062	7.50	9.30	0.91	-0.69

The calculated results of Doppler worth in ZPPR-15A are summarized in Table II. For the N-3 sample, the homogeneous model showed a good agreement with measured values, while the C/E-1 values become slightly worse with the MOC as well as super cell models. On the other hand, the calculated worth was improved by the MOC models for the sample N-11. MOC with super cell models showed the best performance in terms of average error and errors' deviations, but others are also good enough since C/E-1 values are within 10%.

Table III. Doppler Worth Results from ZPPR-15B

	Temp.	Exp. [¢/kgU]	C/E-1 [%]			
			Hom.	S.C.	MOC	M.S.C.
N-3	490 K	-0.026	9.94	8.90	8.89	9.94
	642 K	-0.041	5.87	9.20	5.87	7.20
	777 K	-0.053	1.70	7.44	4.31	5.87
	914 K	-0.061	2.09	9.28	4.34	5.68
	1013 K	-0.071	-2.90	2.88	-2.13	-0.59
N-11	490 K	-0.028	-3.87	-2.98	-7.47	-10.16
	659 K	-0.044	-6.99	-6.13	-11.25	-12.96
	802 K	-0.055	-4.80	-4.12	-8.92	-10.74
	913 K	-0.061	-4.24	-3.22	-8.14	-9.78
	1016 K	-0.067	-2.73	-1.79	-6.11	-9.49
N-24	505 K	-0.027	-7.09	-6.62	-12.28	-13.22
	655 K	-0.040	-7.32	-6.07	-11.37	-12.62
	806 K	-0.050	-5.72	-4.23	-8.97	-9.97
	904 K	-0.055	-3.52	-1.92	-6.25	-7.17
	1047 K	-0.064	-5.07	-3.50	-9.61	-10.59

It is also difficult to find the best model in ZPPR-15B calculation given in Table III. Super cell calculation slightly improves the accuracy of Doppler worth, and can be considered the best. However, the improvement is very minor compared to homogeneous model results. The calculated worth becomes worse for the samples N-11 and N-24 when MOC models are adopted.

Table IV. Doppler Worth Results from ZPPR-15D

	Temp.	Exp. [¢/kgU]	C/E-1 [%]			
			Hom.	S.C.	MOC	M.S.C.
N-3	531 K	-0.015	-17.79	-12.18	-6.58	-6.58
	651 K	-0.020	-17.33	-11.08	-9.69	-6.22
	790 K	-0.025	-16.85	-11.89	-10.79	-6.94
	936 K	-0.030	-20.53	-14.66	-13.30	-10.14
	1081 K	-0.033	-18.47	-12.30	-10.65	-7.77
N-11	503 K	-0.013	-16.04	-16.99	-11.78	-13.67
	650 K	-0.020	-19.50	-19.50	-15.86	-17.38
	797 K	-0.025	-18.35	-19.08	-15.92	-17.38
	896 K	-0.028	-17.49	-17.71	-15.30	-16.61
	1011 K	-0.031	-17.05	-17.05	-14.47	-15.86
N-24	532 K	-0.015	-24.90	-24.90	-23.20	-23.20
	656 K	-0.020	-25.91	-24.98	-23.11	-23.73
	809 K	-0.025	-26.59	-24.88	-22.93	-23.42
	904 K	-0.029	-26.75	-26.10	-24.58	-25.01
	1032 K	-0.032	-25.97	-25.19	-23.44	-23.83
E-33-A	500 K	-0.008	-29.41	-16.41	-27.56	-21.98
	649 K	-0.013	-34.84	-21.13	-31.42	-25.70
	786 K	-0.017	-37.79	-25.70	-35.20	-30.02
	940 K	-0.019	-35.66	-21.87	-31.83	-26.47
	1083 K	-0.024	-39.93	-27.91	-36.13	-31.07

Unlike ZPPR-15A or ZPPR-15B, relatively large calculation errors were observed for calculated Doppler worth of ZPPR-15D as given in Table IV. Super cell model improves the accuracy of calculated worth for the samples N-3 and E-33-A, its effect is marginal for other samples. For the samples N-11 and N-24, the accuracy is improved as well by MOC models so that the best results could be obtained from MOC. Regarding the errors of all the calculated samples, MOC with super cell model can be considered the best even though the improvement is minor.

From the summarized results given in Table II to Table IV, both super cell and MOC models are not remarkably effective to enhance the accuracy of Doppler worth calculation. However, the effects of each model on Doppler worth calculation can be found by observing broadened cross sections and neutron spectra of Doppler samples.

3.2. Variations of Cross Section and Reaction Density according to temperature

The neutron spectra of the Doppler sample N-3 in ZPPR-15D is plotted Fig. 2, which are obtained in the super cell calculation. The neutron spectrum in the Doppler sample is very similar to those in fuels, while the spectrum without fuel shows noticeably different shape compared to a fuel spectrum. The neutron spectra of the sample N-24 in ZPPR-15D are plotted in Fig. 3. With super cell calculation, the neutron spectrum becomes almost identical regardless of model's transport solver (0D homogeneous or 2D MOC), and we can refer that the spectrum will be very close to that of fuels. Note that slightly different spectrum transition was observed between N-3(oxide) and N-24(metal) Doppler samples.

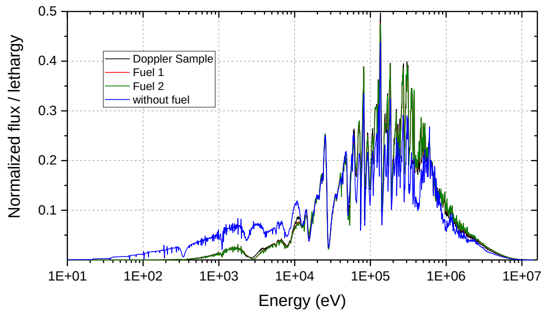


Fig. 2 Neutron spectra of N-3 in super cell calculation

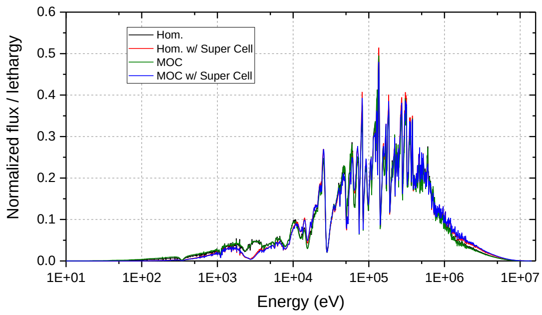


Fig. 3. Neutron spectra of N-24 w/ various models

The variation of U-238 total cross section (Δσ) in the sample N-3 between the initial temperature and the highest temperature is plotted in Fig. 4. With super cell calculation, Δσ was observed slightly increased globally. And Δσ in homogeneous models are significantly greater than MOC models in lower energy regions below 500 eV, while Δσ in MOC models are greater in higher energy regions beyond 5 keV.

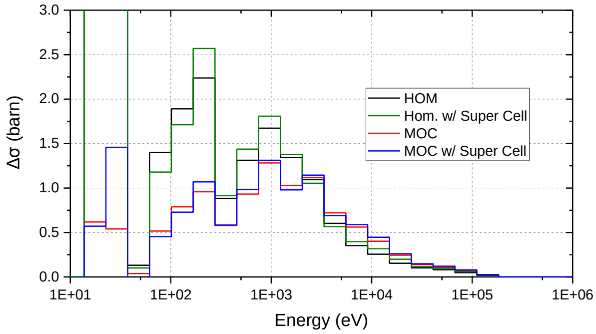


Fig. 4. U-238 total cross section changes in the Doppler sample N-3 (ZPPR-15D)

The contribution of cross section change on the calculated Doppler worth can be assessed by monitoring the reaction density change, which can be defined as:

$$reaction\ density\ change = \Delta(\sigma_g \phi_g) \qquad (1)$$

where

σ_g = total cross section of energy group g and

ϕ_g = neutron flux in a Doppler sample.

The reaction density changes, $\Delta(\sigma_g \phi_g)$, of the Doppler sample N-3 in ZPPR-15D are plotted in Fig. 5. Note that the neutron flux in the Doppler sample is obtained from the homogeneous super cell model at each temperature. Even though Δσ is greater in lower energy regions below 5 keV, its contribution is dominated by the reactions beyond 10 keV because of higher neutron flux. The total reaction density change, which is represented by the area of each line, becomes greater as adopting super cell as well as MOC, so the magnitude of Doppler worth was increased and C/E-1 values are reduced in Table IV.

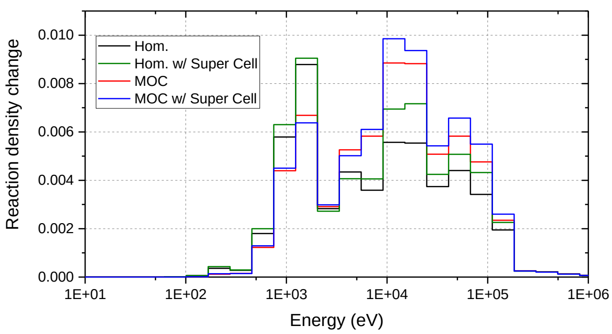


Fig. 5. U-238 total reaction density changes of the Doppler sample N-3 (ZPPR-15D)

Fig. 6 shows Δσ of the Doppler sample N-24 in ZPPR-15D, and similar behavior of Δσ can be observed as Fig. 4, while $\Delta(\sigma_g \phi_g)$ in Fig. 7 appeared differently compared to Fig. 5. Despite outstanding difference Δσ between the homogeneous model and the homogeneous super cell model, $\Delta(\sigma_g \phi_g)$ values are almost the same. For MOC models, Δσ as well as $\Delta(\sigma_g \phi_g)$ values are very similar regardless of the super cell calculation. Additionally, when the homogenous models and MOC models are compared in terms of total reaction density change (the area of plot), they are also almost the same because of increased reactions in higher energy are canceled out by reduced reactions in lower energy. In this manner, the modeling effects were not appeared in the calculated Doppler worth of N-24 in ZPPR-15D, even though the broadened cross sections and the neutron spectra are different for each model.

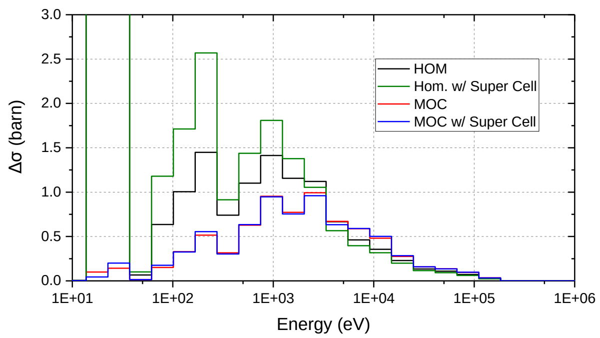


Fig. 6. U-238 total cross section changes in the Doppler sample N-24 (ZPPR-15D)

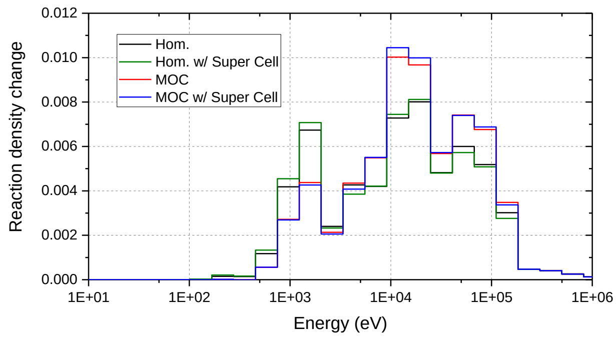


Fig. 7. U-238 total reaction density changes of the Doppler sample N-24 (ZPPR-15D)

Applying similar analysis to other Doppler samples, the modeling effects on Doppler samples can be summarized as follows. a) Super cell calculation lead to increased Doppler worth for samples N-3 and E-33-A while the worth is not changed significantly for the samples N-11 and N-24. That is because the samples N-3 and E-33-A are oxide Doppler samples and the number density of U-238 is lower than others. Okajima [5] observed similar results such that Doppler sample has larger radius and/or higher density, the interaction between Doppler sample and core becomes smaller. b) When a 2D MOC model is applied, Δσ lower than 5 keV becomes decreased while Δσ greater than 5 keV becomes increased compared to a homogeneous model. The contribution by changed cross sections on the Doppler worth calculation should be assessed with the neutron spectrum in a Doppler sample. The effect of MOC models in the ZPPR-15 Doppler worth calculations was observed minor since the increased reactions in higher energy are canceled out by the decreased reactions.

4. Conclusions

In this work, modeling effects of Doppler sample were analyzed for ZPPR-15 experiments. Four different Doppler sample models, combinations of MOC and super cell, were suggested in the stage of cross section generation in MC^2-3, in order to take into account the local heterogeneity and the core spectrum effects respectively. The MOC and super cell models were expected to improve the accuracy of the calculated Doppler worth, but their performance were turned out to be marginal. The reasons were investigated in terms of broadened cross section of U-238 and changed reaction densities. The Doppler worth of oxide samples were increased when a core spectrum is applied to cross section generation, while the effect was observed minor for metallic Doppler samples. The effects of local heterogeneity were observed as broadened cross section and shifted reaction density, and the increased reactions in higher energy tends to be canceled out by reduced reactions in lower energy.

Acknowledgements

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