Benchmarks on the Doppler Reactivity Coefficients for the Library Generation Procedure by Conserving Self-shielded Cross Sections

Aung Tharn Daing[(1)], Myung-Hyun Kim[(1)] and Han-Gyu Joo[(2)]

(1) Department of Nuclear Engineering, Kyung Hee University, Yongin-si, Gyeonggi-do, 446-701, Rep. of Korea
(2) Department of Nuclear Engineering, Seoul National University, Gwanak-gu, Seoul, 151-742, Rep. of Korea
mhkim@khu.ac.kr

1. Introduction

A new procedure for generation of multi-group cross section data for nTRACER by conserving a resonance shielded cross section for a reference fuel pin had already been proposed [1,2]. In this work, the new library setup procedure was verified through the comparison of the calculation results of the multiplication factors and the Doppler reactivity coefficients of UO_2 pins between nTRACER and the previous data. The same Mosteller benchmark problem [3] by using same library was assigned into both nTRACER and Monte Carlo calculations. Comparison was also performed with the ones from multi-group 2D transport theory codes such as CASMO-5, APOLLO2-A, and DRAGON.

As a preliminary study, the safety relevant negative Doppler coefficients are analyzed to investigate whether the asymptotic elastic scattering model brings under-prediction of the Doppler coefficients of LWR lattices by nTRACER or negligible effect. The Doppler reactivity defects evaluated by nTRACER are compared with the results of other different transport theory code, CASMO-5 which uses cross sections generated through the Monte Carlo Slowing Down Code (MCSD) [4] that Lee, Smith and Rhodes implemented an exact scattering kernel with upscattering.

2. Subgroup Weight Generation and Verification

In this library processing procedure, the pointwise cross sections of the isotopes of interest are firstly generated by NJOY runs [5]. By using the RMET21 code which solves a neutron slowing down equation in a heterogeneous 1D cylindrical geometry on an ultra-fine energy grid provided by execution of GEXSCO [5], the groupwise effective cross sections which are averaged over the fuel region for each resonance group are calculated. Since the self-shielding that determines the groupwise effective cross section is strongly dependent on the material compositions as well as the geometrical configurations, 10 different dilution cases (geometry and density variation) for 69 resonance groups at 5 temperatures are considered. Again, the shielded subgroup level dependent background cross sections are produced through the standalone mode in nTRACER which solves a subgroup fixed source problem (SGFSP) given an effective cross section. The subgroup parameters can be determined by the utility program called, GENOME which implements the method of Lagrange multiplier by solving a constrained minimization problem. The resulting subgroup weights reproduce the reference shielded cross sections. The relative errors in the reconstructed groupwise shielded absorption cross sections of U-238 and U-235 for a reference fuel pin at 700 K are verified as illustrated in Fig. 1, through the results from the error estimation routine written at the end of GENOME code. As the maximum errors for both U-238 and U-235 are merely 0.17% and 0.13%, the energy groups do not encounter unacceptable errors.

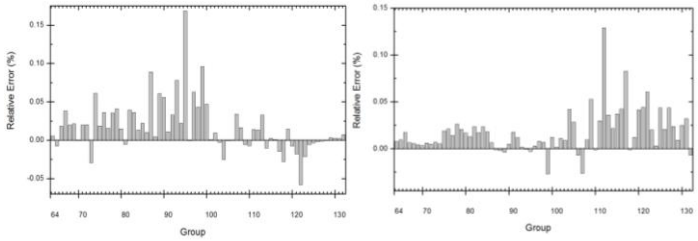
By using the same library such as ENDF/B-VII, the continuous cross section libraries at various temperatures are also processed with mainly NJOY for the calculations of the pointwise cross sections of isotopes composed in the fuel pin model of interest by the Monte Carlo code, MCNPX [6]. When compared to the MCNPX results, the maximum relative error of shielded cross section of resonant, U-238 by the RMET21 code package for the Mosteller benchmark problem is observed 12% at 0.3 keV. The rest two resonant isotopes; U-234 and U-235 present better agreement as the maximum errors of observations for those are 6% at 6.1 eV, and 5.5% at 0.2 keV correspondingly. Finally, the groupwise cross section is processed by using NJOY, and the post processing program namely, LIBDEC was used to organize and integrate the subgroup parameters and all other nuclide-wise data for use in the nTRACER simulation.

3. Analysis of Benchmarks on the Reactivity and the Doppler Reactivity Defect

The effective multiplication factor, k_{eff} and the reactivity differences, $\Delta\rho$ are summarized in Table I, as a comparative analysis between MCNPX and nTRACER using the same basic JEFF-3.1 library. Except natural enrichment level of U-235 case, both results are very close to each other. The Doppler reactivity defects arising from the change of temperature in the fuel between the hot zero power state (HZP) and the hot full power state (HFP) are investigated among different transport theory codes with the same library despite different group structures.

As seen in Fig. 2, the fuel temperature coefficients (FTCs) evaluated by the deterministic codes such as nTRACER and APPOLO2-A [7] using same JEFF-3.1

library could be kept below 10% of FTC maximum relative error by comparing with Monte Carlo calculation results except DRAGON code [8] which reached about 16.5% of the FTC maximum relative error. Although we utilized different slowing down code with same and/or different scattering kernel but starting with same cross section library (ENDF/B-VII), the comparison was performed to roughly analyze the results of FTC differences from CASMO-5 which used the resonance integral data generated by MCSD employing the fast effective scattering kernel (FESK).



*Relative Error = (1-(SG XS)/(REMT21 XS)),%

Fig. 1. Relative errors in the reconstructed groupwise shielded cross sections of U-238 (left) and U-235 (right).

Table II shows slightly increase of the negative FTCs of 0.04~0.13% by nTRACER from those by CASMO in the case of the same asymptotic elastic scattering model. The nTRACER in that case brings more positive FTC in the range of 0.17~0.3% from higher to lower U-235 enrichment level when compared to the results of CASMO-5 in the different case of FESK.

Table I. The Comparison of Reactivity Difference

Enrich-ment (wt.%)	HZP k_{eff} (MCNP)	HZP k_{eff} (nTRACE)	Δρ (pcm)	HFP k_{eff} (MCNPX)	HFP k_{eff} (nTRACER)	Δρ (pcm)
0.711	0.66596	0.66483	256	0.66005	0.65847	364
1.6	0.96117	0.96015	110	0.95284	0.95123	178
2.4	1.09913	1.09856	48	1.08998	1.08863	114
3.1	1.17740	1.17670	51	1.16772	1.16629	105
3.9	1.23964	1.23948	10	1.23027	1.22874	101
4.5	1.27543	1.27499	27	1.26512	1.26409	64
5	1.29962	1.29937	15	1.28932	1.28838	57

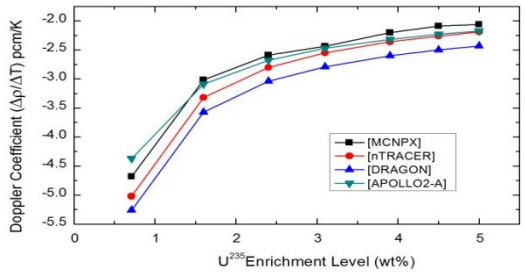


Fig. 2.Fuel temperature coefficients of UO_2 pin.

Table II. The Comparison of FTC Difference

Enrichment (wt.%)	FTC* (Asymptotic Kernel)		FTC Diff.	FTC (FESK)	FTC Diff.
	nTRACER	CASMO-5		CASMO-5	
0.711	-4.84	-4.71	-0.13	-5.14	0.30
1.6	-3.26	-3.17	-0.09	-3.47	0.21
2.4	-2.77	-2.70	-0.06	-2.96	0.19
3.1	-2.53	-2.47	-0.06	-2.71	0.18
3.9	-2.35	-2.30	-0.05	-2.53	0.18
4.5	-2.25	-2.21	-0.04	-2.43	0.18
5	-2.19	-2.15	-0.04	-2.36	0.17

* FTC = $[1/k_{eff}(HZP)- 1/k_{eff}(HFP)]$*1E+5/300 (pcm/K)

3. Conclusion

There is a profound difference in the temperature treatment of the thermal motion of the targeted nucleus with consideration of the upscattering kernel between nTRACER with REMT21 code package and the CASMO-5 with MCSD involving different FESK. It may lead to larger discrepancies of FTCs by reaching 0.3%. Since the large systematic errors in nTRACER as well as in CASMO-5 with both scattering kernels are observed at lower enriched fuel when compared to MCNPX, it should be also noticed that that Monte Carlo code has also similar inadequate approximation for heavy nuclide resonance scattering when using for low-enriched uranium [4].

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