

## Validation Tests of the Multigroup Cross Section Libraries for Fast Reactors

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### Abstract

The MATXS-format 150-group neutron libraries for fast reactors were generated based on the ENDF/B-VII beta 0, JEFF-3.1, and JENDL-3.3. The libraries have been validated through the 18 fast benchmark experiments from the CSEWG benchmark specifications and BFS critical assemblies. The  $k_{\text{eff}}$ 's and several central spectral indices obtained by the DANTSYS code have been compared with the results of the experiments and MCNPX.

**KEYWORDS:** *MATXS-format library, CSEWG fast benchmark, BFS critical assembly, DANTSYS, MCNPX, central spectral index*

### 1. Introduction

In Korea, a design study for a fast breeder reactor named Korea Advanced LIquid METal Reactor (KALIMER) has been carried out. So far, the simulations of the KALIMER core have been performed with the JEF-2.2-based 80-group neutron library KAFAX-F22 or the ENDF/B-VI.6-based 150-group neutron library KAFAX-E66. [1] Recently, newly evaluated nuclear data files such as ENDF/B-VII (beta 0 and 1), JEFF-3.1, and JENDL-3.3 have been released. And thus there is a need to update the libraries for the KALIMER by using the new data files.

In this study, the fast cross section sets with 150 groups were prepared based on ENDF/B-VII beta 0, JEFF-3.1, and JENDL-3.3. The validation tests of the libraries have been carried out for 14 Cross Section Evaluation Working Group (CSEWG) fast benchmark problems [2] and 4 BFS critical assemblies [1] through the 1-D and/or 2-D DANTSYS [3] calculations. The effective multiplication factors ( $k_{\text{eff}}$ 's) and some central spectral indices have been compared with the experimental values and the results by the MCNPX [4] calculations.

### 2. Data Processing

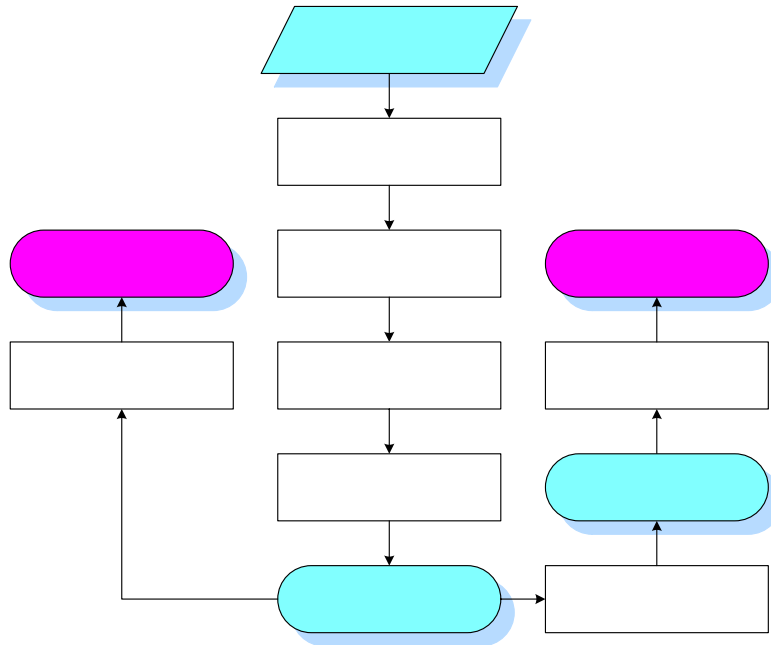
The MATXS-format 150-group neutron libraries have been produced through the nuclear data processing by the patched version of NJOY99.90 code [5]. The neutron group structure uses one-eighth lethargy widths in almost all the energy range, except between 1 and 10 keV in which one-sixteenth lethargy widths are used. In the NJOY processing, an equilibrium core flux of the KALIMER was used as a weighting function. Background cross sections for a self-shielding were also selected from those of the calculations. The libraries for MCNP code have also been generated

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based on the same data files. Figure 1 shows the flow diagram of NJOY for generating the neutron libraries for DANTSYS and MCNP. They are going through the same procedures up to the PURR module for considering the self-shielding effect in the unresolved-resonance energy region.

**Figure 1:** Flow diagram of NJOY99.90 data processing for neutron library generation.



### 3. Benchmark Calculations and Results

#### 3.1 Benchmark Problems

The 14 fast benchmark problems have been chosen from the CSEWG benchmark specifications [2], which are shown in Tab. 1 along with their core characteristics. In this study, the problems were classified into two categories such as the plutonium (Pu)-dominant and uranium (U)-dominant cores corresponding to the major fissile materials.

For the development of the KALIMER, some experimental studies on the fast critical assemblies loaded with U metal fuel were carried out under the contract between Korea Atomic Energy Research Institute (KAERI) and Institute of Physics and Power Engineering (IPPE) in Russia. The BFS-73-1 is composed of the U metal fuelled core of 18.5% enrichment, which is a homogeneous system without control rods in the core. The BFS-75-1 consists of two core zones with zirconium (Zr) added U metal fuel of different enrichment (~15% and ~20%). The BFS-55-1 is a one-zone simple core loaded with metallic U-10% enriched Pu fuel. Finally, the BFS-55-2 consists of two core zones with Zr added U-14% enriched Pu metal fuel and U-10% enriched Pu metal fuel, respectively.

**Table 1:** Descriptions of the CSEWG benchmark problems.

Major fissile material	Benchmark core	Fertile-to-fissile ratio	Approx. core vol. (liter)	Comments
Pu	VERA-11A	0.05	12	No U in the core, diluted with graphite
	ZEBRA-3	8.60	60	Hard spectrum (80% above 100 keV)
	SNEAK-7A	3.00*	110	
	SNEAK-7B	7.00	310	
	ZPR-3-48	4.50	410	Graphite added to soften spectrum
	ZPR-3-56B	4.60	610	PuO <sub>2</sub> -UO <sub>2</sub> , predominant Ni reflector
	ZPPR-2	6.50*	2400	Equal volume 2-zone core, L/D≈0.5
	ZPR-6-7	6.60	3100	PuO <sub>2</sub> , LMFBR design, L/D≈0.9
U	VERA-1B	0.08	30	Enriched U, diluted with graphite
	ZPR-3-6F	1.10	50	About 1:1 fertile-to-fissile
	ZPR-3-12	3.80	100	4:1 U-C system, soft spectrum
	ZPR-3-11	7.50	140	U metal
	ZEBRA-2	6.20	430	6:1 U-C system
	ZPR-6-6A	5.00	4000	UO <sub>2</sub> , LMFBR design, L/D≈0.8

\* Fertile-to-fissile ratio in the inner core zone.

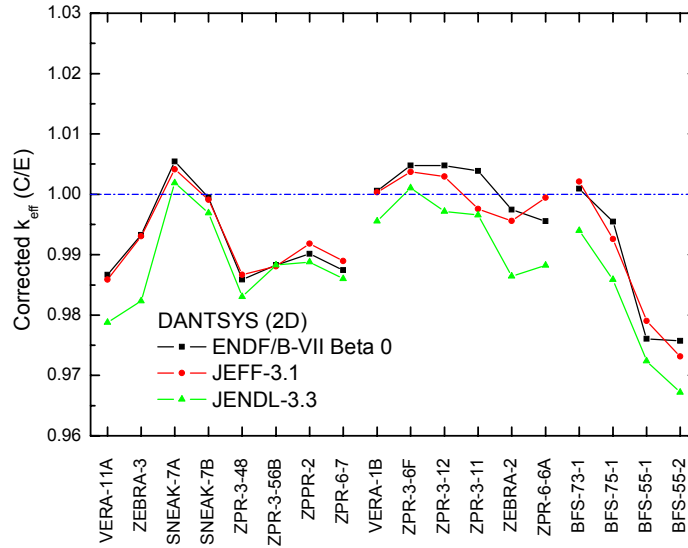
### 3.2 Results

For the benchmark problems, the  $k_{eff}$ 's and several central spectral indices have been estimated. The spectral indices are defined as the ratios of average reaction rates of fission and/or capture, which can characterize the neutron spectrum of the benchmark core. Usually, the measurements are carried out at the core center where the neutron flux anisotropy can be practically ignored. In this study, the followings are taken into account:

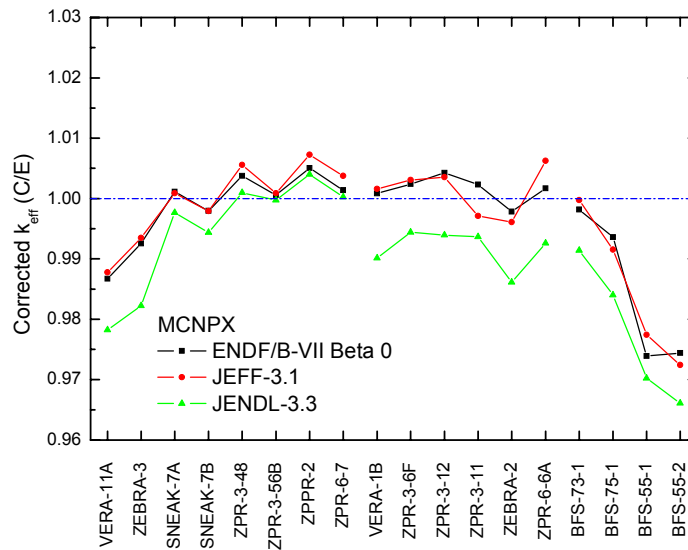
- F28/F25: the fission reaction rates ratio of U-238 to U-235,
- F49/F25: the fission reaction rates ratio of Pu-239 to U-235,
- F40/F25: the fission reaction rates ratio of Pu-240 to U-235,
- C28/F25: the ratio of U-238 capture to U-235 fission reaction rates, and
- C28/F49: the ratio of U-238 capture to Pu-239 fission reaction rates.

Figures 2 and 3 show the comparisons of the ratios of calculated-to-experimental values (C/E's) of  $k_{eff}$ 's obtained by the 2-D DANTSYS and MCNPX calculations using the libraries based on ENDF/B-VII beta 0, JEFF-3.1, and JENDL-3.3. Note that the results of the BFS-55-1 and BFS-55-2 are the  $k_{eff}$ 's itself, which require to be corrected by considering the core heterogeneity effects. The  $k_{eff}$ 's agree well with the experiments except for some large size benchmark problems loaded with Pu-dominant MOX fuels and the VERA-11A core. The JENDL-3.3 results are underestimated when compared with the ENDF/B-VII beta 0 and JEFF-3.1. For the large size Pu-dominant MOX cores, as shown in Fig. 4, the  $k_{eff}$ 's by the 2-D DANTSYS are largely underestimated compared with the experiments and MCNPX results. The 1-D and 2-D results by the DANTSYS show good agreements except ZPR-3-56B and ZPPR-2.

**Figure 2:** C/E values of  $k_{eff}$ 's by 2-D DANTSYS calculation.



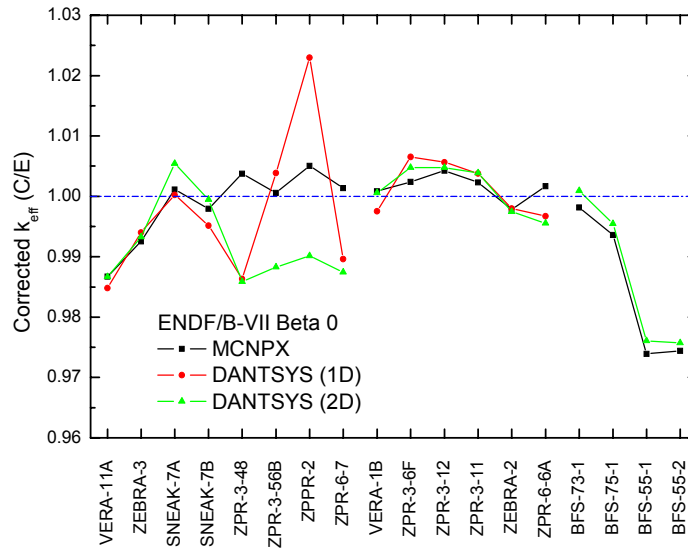
**Figure 3:** C/E values of  $k_{eff}$ 's by MCNPX calculation.



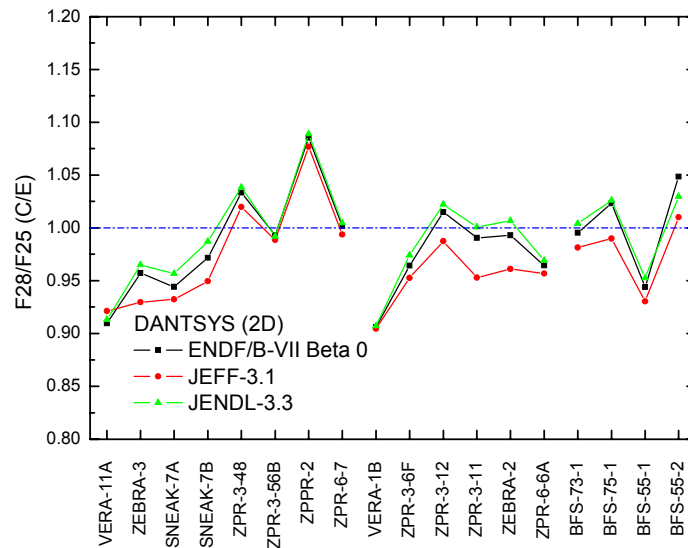
Figures 5 and 6 show the comparisons of the C/E values of F28/F25 obtained by the 2-D DANTSYS and MCNPX calculations using the libraries. For the DANTSYS, the F28/F25 values agree well with the experiments to within ~10% when considering the uncertainties of the

experiments. For the MCNPX, however, somewhat large discrepancies among the three libraries are shown in the ZPR-3-56B, ZPPR-2, ZEBRA-2, ZPR-6-6A, and all BFS benchmarks. These seem to be caused by the large uncertainties in the U-238 fission reaction rate resulting from the relatively large size of the problems.

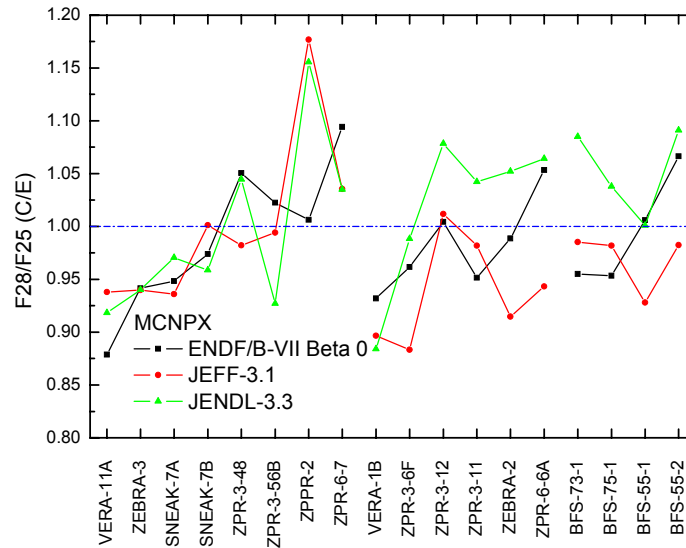
**Figure 4:** C/E values of  $k_{eff}$ 's by MCNPX, 2-D and 1-D DANTSYS based on ENDF/B-VII beta 0.



**Figure 5:** C/E values of F28/F25 by 2-D DANTSYS calculation.



**Figure 6:** C/E values of F28/F25 by MCNPX calculation.



For all the libraries, the F49/F25 values are very close to the experimental results, while the F40/F25 values show more than 10% differences in the VERA-11A, ZPR-3-56B, and VERA-1B. The F49/F25 and F40/F25 show small discrepancies between the DANTSYS and MCNPX. The C28/F25 and C28/F49 by the DANTSYS generally agree well with the experiments within the differences of ~10% except BFS-55-1. The results by the MCNPX show good agreements with the experiments except ZPR-6-7 using JEFF-3.1. For the BFS-55-1 and BFS-55-2, the C28/F25 and C28/F49 show relatively large differences between the DANTSYS and MCNPX.

**Table 2:** Average values of  $|(C/E - 1)|$  in percent for whole benchmark problems.

Calculation	Source	$k_{eff}$	F28/F25	F49/F25	F40/F25	C28/F25	C28/F49
DANTSYS-2D	ENDF/B-VII.0	0.63	3.74	1.95	7.56	6.00	5.61
	JEFF-3.1	0.59	4.31	1.98	8.40	5.85	5.20
	JENDL-3.3	0.97	3.35	1.75	7.31	6.28	6.49
DANTSYS-1D	ENDF/B-VII.0	0.72	3.80	2.23	7.59	6.00	4.50
	JEFF-3.1	0.69	4.71	2.31	8.45	6.00	4.48
	JENDL-3.3	1.03	3.40	1.91	7.33	6.45	5.74
MCNPX	ENDF/B-VII.0	0.35	4.55	2.11	7.92	5.63	4.35
	JEFF-3.1	0.43	5.21	2.29	8.78	5.90	4.96
	JENDL-3.3	0.79	6.11	2.08	7.90	5.24	3.30

The overall performances of the three libraries can be evaluated by averaging the absolute values of relative error to the experimental value, as shown in Tab. 2. The  $k_{eff}$ 's by MCNPX show

good agreements comparing with DANTSYS, while the 2-D DANTSYS calculations produce better results for the most of spectral indices than MCNPX. For all the DANTSYS and MCNPX calculations, the  $k_{\text{eff}}$ 's by ENDF/B-VII beta 0 and JEFF-3.1 show better agreements with the experiments comparing with those by JENDL-3.3.

#### 4. Summary

The 150-group neutron libraries for fast reactors have been generated based on the ENDF/B-VII beta 0, JEFF-3.1 and JENDL-3.3, and validated through the 1-D and/or 2-D DANTSYS calculations for the CSEWG fast benchmark problems and BFS critical assemblies. The  $k_{\text{eff}}$ 's by DANTSYS calculations generally agree well with the experiments and MCNPX results except for a few large assemblies loaded with Pu-dominant MOX fuels. The C/E values of central spectral indices by the DANTSYS code show reasonably good agreements with the experiments. The best fast cross section set for the KALIMER will be chosen after further investigations.

#### Acknowledgements

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