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Comparison of Cross Section Data Library for High Temperature using MCNPX

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I. Introduction.

MCNPX is a common computer code that applies Monte Carlo method and uses pointwise cross section data in term of ACE format processed from Evaluated Nuclear Data File (ENDF) library to simulate nuclear-related problems. ENDF library was released by the U.S. Cross Section Evaluation Working Group (CSEWG), contains nuclear reaction data of almost 400 isotopes obtaining from experimental data and theoretical predictions [1]. However, the ENDF/ B-VI library basically provides neutron cross section at temperature 0K. To simulate a system at a higher temperature, the TMP card in MCNPX must be used to adjust the temperature of the system. According to MCNPX manual, the TMP card is only applied to neutron elastic and total cross section [5], then there is a significant error in calculated results caused by the Doppler-broadening effect on absorption cross section. To eliminating the error, a new cross section data for MCNPX is processed from ENDF library at specifying temperature by users.

This study describes the procedure to process neutron cross-section data from ENDF/ B-VI for MCNPX using NJOY-99 computer code. In NJOY, the BROADR module is used to generate Doppler-broadened cross sections. The new generated cross section data for MCNPX (ENDF/B-VI-NJOY) was generated to compare with cross section data of endf60, endf66b, and endf70e package derived from ENDF/B-VI through calculating the multiplication factor (k_∞) of the *leu-sol-therm-001*, a benchmark problem from the International Handbook of Evaluated Criticality Safety Benchmark Experiments at room temperature [2]. After the comparison, ENDF/B-VI-NJOY cross section was applied to calculate k_∞ values at various burnups of 17×17 fuel assembly types of a Small Module Reactor (SMR) at operating temperature. The library *lwtr.62t* of SAB2002 was applied for H_2O cross section in MCNPX calculations. There are two types of fuel assembly model were used for calculation, one without Burnable Absorber (BA) and other having 8% enrichment of BA (Gd_2O_3). The results calculated by MCNPX using ENDF/B-VI-NJOY cross section were compared with the results calculated by cross section library from endf60, endf66b, and endf70e package (ENDF/B-VI) applying TMP card to adjust cross section temperature. In addition, the results from ENDF/B-VI-NJOY calculation were also compared with the results of the same fuel assembly models calculated by two-dimensional transport code CASMO-4 [4], which uses 70 energy groups cross section data processed from ENDF/ B-VI library.

II. Processing cross section by NJOY code

The code NJOY-99 is used to process pointwise cross section from ENDF/ B-VI library to ACE format that is used for MCNPX [3]. There are total 9 modules were used for processing cross section. The processing sequence starts from MODER module for converting ENDF, PNDF from binary format to ASCII format, and vice versa. After that, resonance cross section of the data converted by MODER module is reconstructed by RECONR module with reconstruction tolerance of 0.1% at 960K, 612K, and 585K for fuel, cladding, and moderator respectively. The output tape of RECONR module is written as pointwise ENDF (PENDF) and imported to BROADR module for generating Doppler-broadened cross section with thinning tolerance of 0.1%. Next step, heating cross sections and radiation damage energy production is added by HEATR module, charged particle production is added by GASPR module, and unresolved resonance self-shielding are treated by PURR module. Finally, ACER modules generated the cross section as an ACE format for MCNPX with extension file .00c. The whole processing procedure for NJOY-99 is shown in Figure 1.

For fuel assembly calculation, cross sections of 40 isotopes were generated at a different temperature as shown in Table 1. These library files are imported to MCNPX library by xsdir file for calculating the k_∞ at various burnup.

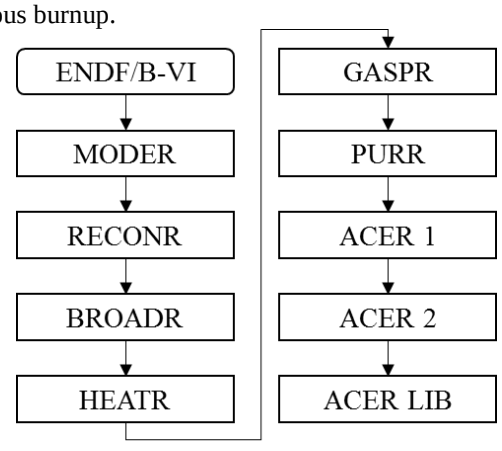

Figure 1. NJOY processing procedure

Table 1. List of isotopes was processed

ISOTOPE	T (K)	ACE LIB NAME	ENDF/B-VI-NJOY
^{1}H	585	aceH2585	1001.00c
^{16}O	585	aceO16585	8016.01c
^{16}O	960	aceO16960	8016.00c
^{235}U	960	aceU235960	92235.00c
^{238}U	960	aceU238960	92238.00c
^{156}Gd	960	aceGD152960	64152.00c
^{154}Gd	960	aceGD154960	64154.00c
^{155}Gd	960	aceGD155960	64155.00c
^{156}Gd	960	aceGD156960	64156.00c
^{157}Gd	960	aceGD157960	64157.00c
^{158}Gd	960	aceGD158960	64158.00c
^{160}Gd	960	aceGD160960	64160.00c
^{50}Cr	612	aceCr50612	24050.00c
^{52}Cr	612	aceCr52612	24052.00c
^{53}Cr	612	aceCr53612	24053.00c
^{54}Cr	612	aceCr54612	24054.00c
^{54}Fe	612	aceFe54612	26054.00c
^{56}Fe	612	aceFe56612	26056.00c
^{57}Fe	612	aceFe57612	26057.00c
^{58}Fe	612	aceFe58612	26058.00c
^{58}Ni	612	aceNi58612	28058.00c
^{60}Ni	612	aceNi60612	28060.00c
^{61}Ni	612	aceNi61612	28061.00c
^{62}Ni	612	aceNi62612	28062.00c
^{64}Ni	612	aceNi64612	28064.01c
^{90}Zr	612	aceZr90612	40090.00c
^{91}Zr	612	aceZr91612	40091.00c
^{92}Zr	612	aceZr92612	40092.00c
^{94}Zr	612	aceZr94612	40094.00c
^{96}Zr	612	aceZr96612	40096.00c
^{112}Sn	612	aceSn112612	50112.00c
^{114}Sn	612	aceSn114612	50114.00c
^{115}Sn	612	aceSn115612	50115.00c
^{116}Sn	612	aceSn116612	50116.00c
^{117}Sn	612	aceSn117612	50117.00c
^{118}Sn	612	aceSn118612	50118.00c
^{119}Sn	612	aceSn119612	50119.00c
^{120}Sn	612	aceSn120612	50120.00c
^{122}Sn	612	aceSn122612	50122.00c
^{124}Sn	612	aceSn124612	50124.00c

III. Application of generated library for MCNPX

1. Comparison of Cross section Library

The ENDF/B-VI-NJOY cross sections were applied to calculate the multiplication factor of the benchmark problem *leu-sol-therm-001* at room temperature (293K) [2] for checking the usability of the generated cross sections. This benchmark problem is an unreflected UO_2F_2+H_2O cylindrical assembly SHEBA-II having geometry as shown in Figure 2. The results were compared between two calculations using different cross section library, one uses ENDF/B-VI cross section and the other uses ENDF/B-VI-NJOY cross section. Table 2 shows the result of k_∞ calculated using ENDF/B-VI cross section and ENDF/B-VI-NJOY cross section at room temperature. From the results, it is observed about 200 pcm difference between two libraries.

Table 2. k_∞ results from benchmark calculation

LIBRARY	k_∞ (293K)	SD
ORIGIN MCNPX LIBRARY .60c	1.00706	0.00048
GENERATED LIBRARY .00c	**1.00912**	**0.00048**
ERROR (pcm)	**202.707**	-

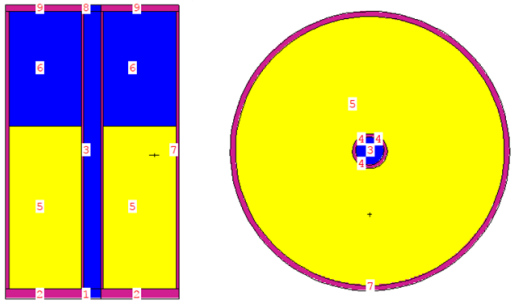

Figure 2. Geometry of Benchmark problem

2. Application Cross section data for MCNPX

After verification by calculation of benchmark problem, ENDF/B-VI-NJOY cross section of all isotope shown in Table.1 was applied to calculate the k_∞ at different burnup of a fuel assembly of Smart Module Reactor (SMR). As mentioned before, there are two models of fuel assemblies were used for this calculation, the first one has no BA rod and the second one has 24 BA rods containing 8w/o of Gd_2O_3 located octant-symmetry in a fuel assembly. These fuel assemblies have 17x17 fuel rod, 24 guide tubes, and one instrumentation tube at the center. The fuel assembly specification is shown in Table 2 and the layout of fuel assemblies is shown in Figure 3.

Table 3. Fuel assembly specification

Assembly type	17x17
Fuel material	UO_2
Enrichment of fuel	4.95 %
Cladding material	ZR-2
Coolant/Moderator material	H_2O
Burnable absorber material	Gd_2O_3
Number of BA	24
Fuel rod diameter	0.819 cm
Fuel rod pitch	1.254 cm
Assembly pitch	21.50 cm
Fuel pellet density	10.176 g/cm^3
Cladding inner diameter	0.819 cm
Cladding outer diameter	0.950 cm
Guide tube inner diameter	1.140 cm
Guide tube outer diameter	1.220 cm
Active length	200.0 cm
Fuel temperature	960.95 K
Moderator temperature	585.35 K
Cladding temperature	612.00 K

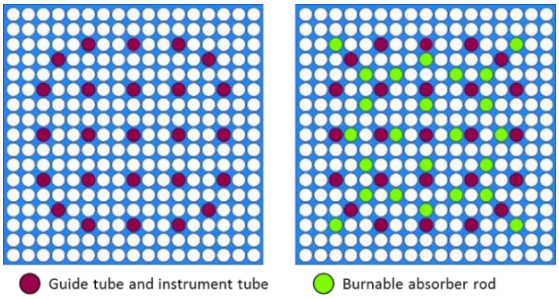

Figure 3. Fuel assembly layout

3. Evaluation of cross section data

To evaluate the ENDF/B-VI-NJOY cross section, the k_∞ values at different burn up of fuel assemblies having BA and without BA calculated by MCNPX and CASMO-4 were compared. The kcode in MCNPX used 100000 of neutron population with 300 cycles for these calculations. The Figure 4 shows the k_∞ at different burnup of the fuel assembly have no BA. For the results calculated by CASMO-4, the k_∞ values are lower than others. The k_∞ values obtained by MCNPX using ENDF/B-VI cross section are higher at low burnup and lower at high burnup compare with ENDF/B-VI-NJOY cross section. At high burnup, the results of ENDF/B-VI-NJOY cross section is higher than results of ENDF/B-VI cross section because of Doppler broadening effect at high temperature.

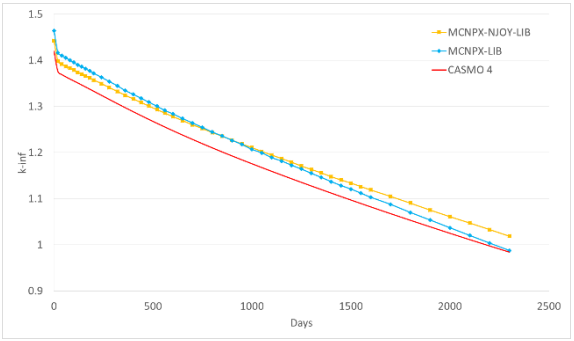

Figure 4. Changing of k_∞ of no BA assembly

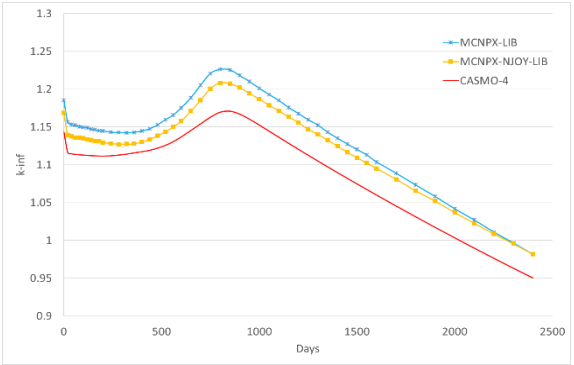

Figure 5. Changing of k_∞ of having BA assembly

For the fuel assembly having BA, the k_∞ at different burn up is shown in Figure 5. The k_∞ values calculated by CASMO-4 are also lower than others. The k_∞ values obtained by ENDF/B-VI cross section are higher than results of ENDF/B-VI-NJOY cross section.

IV. Conclusions

In summary, this study shows the method of customizing the cross section library for MCNPX matching with a special condition of a simulation model. The result from the benchmark problem calculation shown the usability of ENDF/B-VI-NJOY cross section. Compared with the ENDF/B-VI cross section, ENDF/B-VI-NJOY cross section reflects the effect of Doppler Broadening more than ENDF/B-VI. However, there is a noticeable error between MCNPX results and CASMO-4 results. This error may come from different parameters used for cross section processing by NJOY and CASMO4 library which is a university version of e60200 [6]. Furthermore, MCNPX applied Monte Carlo method and used pointwise cross section library, while CASMO-4 applied multi-group two-dimensional transport theory and used multi-group cross section library.

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