Assessment of the Influence of Thermal Scattering Library on Monte-Carlo Calculation

Gwanyoung Kim * and Swengwoong Woo
Korea Institute of Nuclear Safety, 62 Gwahak-ro, Yuseong-gu, Daejeon, Republic of Korea
**Corresponding author:k722kgy@kins.re.kr*

1. Introduction

Monte-Carlo Neutron Transport Code uses continuous energy neutron libraries generally. Also thermal scattering libraries are used to represent a thermal neutron scattering by molecules and crystalline solids completely. Both neutron libraries and thermal scattering libraries are generated by NJOY[1,2] based on ENDF data. While a neutron library can be generated for any specific temperature, a thermal scattering library can be generated for restricted temperatures when using ENDF data. However it is able to generate a thermal scattering for any specific temperature by using the LEAPR module in NJOY instead of using ENDF data.

In this study, thermal scattering libraries of hydrogen bound in light water and carbon bound in graphite are generated by using the LEAPR module and ENDF data, and it is assessed the influence of each libraries on Monte-Carlo calculations. In addition, it is assessed the influence of a library temperature on Monte-Carlo calculations.

2. Methods

2.1 Procedure of Thermal Scattering Library Generation

Usually thermal scattering libraries are generated following a procedure as shown in fig. 1. ENDF thermal scattering data contain the scattering law S(α,β) and related quantities, which describe thermal neutron scattering from bound moderators. And it is used in THERMR module in NJOY. However, it is offered the ENDF thermal scattering data with specific temperatures only. So it is unable to generate a library with any temperature, which is not offered in ENDF data.

Another procedure to generating a thermal scattering library is shown in fig. 2. The scattering law S(α,β) and related quantities are prepared by using the LEAPR module of NJOY. While it is able to generate a library with any temperature, it is re required input parameters such as α,β–grid in LEAPR module. That is to say, the choice of input parameters has an influence on libraries.

In this study, thermal scattering libraries are generated targeting hydrogen bound in light water and carbon bound in graphite. And it is referred to write a LEAPR input including α and β values from some references, which are NJOY manual[3], LANL report[4] and INDC report[5,6]. The α values, β values and maximum energy transfer in each references are list in Table I and II.

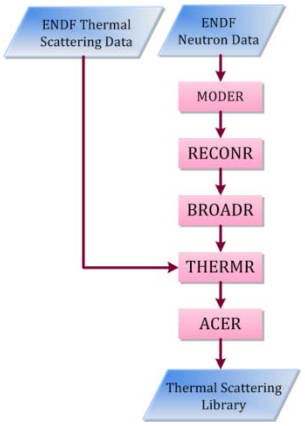

Fig. 1. Thermal scattering library generation by using ENDF data

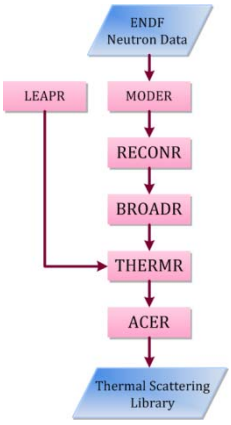

Fig. 2. Thermal scattering library generation by using LEAPR module in NJOY

Table I: Comparison of LEAPR input data for H in H_2O

	Number of α values	Number of β values	Maximum Energy Transfer, eV
NJOY manual	187	274	4
LANL report	97	95	4.048
INDC 0470	182	259	4

Table II: Comparison of LEAPR input data for C in Graphite

	Number of α values	Number of β values	Maximum Energy Transfer, eV
NJOY manual, LANL report (ENDF/B-VI)	72	96	2.204
INDC 0475 (GA)	126	185	1.86

2.2 Development of NIM program for Automatic Library Generation

NIM (NJOY Input Maker) program is developed to generate libraries as mentioned earlier automatically. The overall procedure of the program is shown in Fig. 3. Thermal scattering library as well as neutron library is generated by using NIM.

NIM makes batch files and NJOY input files following user-input data. User can select an option for procedure of generating a thermal scattering library. Thus thermal scattering libraries can be generated by using ENDF data or by using LEARP module with input data in NJOY manual, LANL report, INDC reports in NIM program.

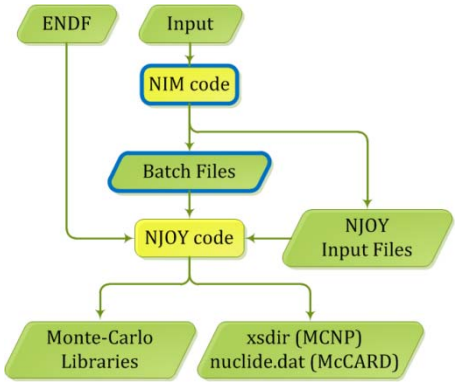

Fig. 3. Flow chart of NIM program

2.3 Assessment Model and McCARD Calculation

McCARD[7] is used for assessing the influence of library generation procedures and the influence of library temperature. McCARD calculations are carried out for a pin cell problem and an assembly problem. And they carried out with enough histories and so the standard deviation is enough small about 10 pcm.

In order to assess the influence of library generation procedures, McCARD calculations carried out with various libraries generated from NIM program. And the influences are assessed for H in H_2O and C in graphite.

Also McCARD calculations carried out with a thermal scattering library, which is generated for a temperature different from a problem temperature

3. Results and Conclusions

3.1 Influence of Library Generation Procedures

The k-inf calculated by McCARD with various thermal scattering libraries for H in H_2O list in Table III. It is set up the k-inf calculated with ENDF VII.0 library as reference, and it is compared with the others. The k-inf calculated with library generated following NJOY manual is same with reference for pin cell problems and assembly problems. The maximum difference is shown at library generated with input data in LANL report. And it is about 43 pcm($\Delta\rho$).

Table III: Comparisons of k-inf for H in H_2O

Problem	Temp. (K)	ENDF VII.0 (Ref.)	NJOY manual	LANL Report	INDC 0470
Pin	293.6	1.34372	0.0 [a]	**-43.2**	-22.7
	400	1.33699	0.0	-30.2	**-22.9**
	600	1.32442	0.0	-27.9	-11.4
	800	1.31390	0.0	-13.9	-8.7
Assembly	293.6	1.37363	0.0	-38.2	-9.5
	400	1.36586	0.0	-16.1	-16.1
	600	1.35214	0.0	-6.6	-2.2
	800	1.34098	0.0	-8.9	2.8

a) $\left(\frac{1}{\text{k-inf}_{ref}}-\frac{1}{\text{k-inf}_i}\right)\times 1.e^5$

The k-inf calculated by McCARD with various thermal scattering libraries for C in graphite list in Table IV. Just same with previous results, it is set up the k-inf calculated with ENDF VII.0 library as reference, and it is compared with the others. The maximum difference is shown at library generated with input data in INDC report. And it is about 34 pcm($\Delta\rho$).

Table IV: Comparisons of k-inf for C in graphite

Problem	Temp. (K)	ENDF VII.0 (Ref.)	NJOY manual	INDC 0475
Pin	296	1.36192	-4.9 [a]	-4.3
	400	1.33942	-4.5	**-34.0**
	600	1.30207	0.6	2.4
	1000	1.24853	-7.7	-17.3
Block	296	1.47289	-7.4	-6.5
	400	1.45302	-4.3	-7.1
	600	1.41973	-3.5	-4.5
	1000	1.37135	**11.2**	1.1

a) $\left(\frac{1}{\text{k-inf}_{ref}}-\frac{1}{\text{k-inf}_i}\right)\times 1.e^5$

3.2 Influence of Temperature

The results for assessing the influence of temperature in thermal scattering library list in Table V.

The case of an identical temperature between a problem and a thermal scattering temperature is set to reference. As a temperature of a thermal scattering library alter comparing to a temperature of problem, a difference of k-inf increases. And it is about 1 pcm ($\Delta\rho$) / K.

Table V: Comparisons of k-inf according to Temperature of Problem and Thermal Scattering Library

Temp. of Library (K) / Temp. of Problem (K)	293.6	400	600	800
293.6	1.37363 (Ref.)	-94 [a]	-291	-488
400	84	1.36586 (Ref.)	-196	-403
600	301	214	1.35214 (Ref.)	-190
800	466	403	183	1.34098 (Ref.)

a) $\left(\frac{1}{\text{k-inf}_{ref}}-\frac{1}{\text{k-inf}_i}\right)\times 1.e^5$

3.3 Conclusions

In this study, thermal scattering libraries are generated by using LEAPR module in NJOY, and it is developed NIM program to do this work. It is compared above libraries with libraries generated from ENDF thermal scattering data. And the comparison carried out for H in H_2O and C in graphite.

As a result, similar results came out between libraries generated from LEAPR module and that generated from ENDF thermal scattering data. Hereby, it is conclude that the generation of thermal scattering libraries with LEAPR module is appropriate to use and it is able to generate a library with user-specific temperature. Also it is assessed how much a temperature in a thermal scattering library influences on Monte-Carlo calculations.

REFERENCES

[1] R. E. MacFarlane and R. M. Boicourt, "NJOY: A Neutron and Photon Processing System," Trans. Am. Nucl. Soc. 22, 720 (1975).
[2] R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91," Los Alamos National Laboratory report LA-12740-M(1994).
[3] R. E. MacFarlane, et al., "The NJOY Nuclear Data Processing System, Version 2012", LA-UR-12-27079, December 20, 2012.
[4] R.E. MacFarlane, "New thermal neutron scattering Files for ENDF/B-VI release 2", LANL Report, LA-12639-MS, August 1994.
[5] M. Mattes and J. Keinert, "Thermal Neutron Scattering Data for the Moderator Materials H2O, D2O and ZrHx in ENDF-6 Format and as ACE Library for MCNP(X) Codes," INDC(NDS)-0470, IAEA (2005).
[6] M. Mattes and J. Keinert, "Status of Thermal Neutron Scattering Data for Graphite," INDC(NDS)-0475, IAEA (2005).
[7] Hyung Jin Shim, Beom Seok Han, Jong Sung Jung, Ho Jin Park, Chang Hyo Kim, "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," Nucl. Eng. Technol., 44[2], 161~176 (2012).