A Sensitivity Study on Nuclear Criticality According to NJOY Processing Options for Thermal Neutron Scattering Data of H-in-ZrH

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1. Introduction

The MCNP team of Los Alamos National Laboratory (LANL) has re-released the ACE-format thermal neutron scattering library based on the ENDF/B-VIII.0 processed by NJOY2016. [1,2,3] They made some big changes there, one of which is to adopt a different value for IWT (weighting option) of the NJOY/ACER module instead of the existing default value.

The IAEA Nuclear Data Section (NDS) has been organizing the Technical Meeting (TM) every year for the purpose of encouraging the development of globally available nuclear data processing codes and advancing and standardizing the processing techniques of those codes. Recently they proposed a sensitivity study of nuclear data processing options for production of ACE-format thermal neutron scattering libraries, including IFENG of ACEMAKER code [4] (equivalent to IWT of NJOY code).

In this study, the H-in-ZrH data of ENDF/B-VIII.0 was processed by changing some options related to thermal neutron scattering data in the ACER and/or THERMR modules of NJOY code, and the resulting inelastic scattering cross sections were compared with each other. In addition, the criticality benchmark calculations were performed for some benchmark problems including ZrH taken from the ICSBEP [5] using the MCNP6.2 code [6], and the influence of the NJOY processing options on the criticality calculation was examined.

2. NJOY Processing Options and Criticality Benchmark Problems

As NJOY processing options for this study, the four options presented in Table I were considered.

The IWT option of the ACER module specifies the weighting pattern for the energy distribution of the emitted thermal neutrons after inelastic scattering reactions. Although the NJOY code recommends IWT=0 (discrete variable weighting) as the default value, it is known that this can cause some artificial peaks in the typical thermal neutron spectra. Therefore, the NJOY code provides a preferred option (IWT=2) for using the continuous distribution in outgoing energy to solve this problem, which is valid for MCNP 5.1.50 and later. The IWT option is equivalent to the IFENG option of the ACEMAKER code developed based on the PREPRO 2019 code [7] under the auspices of the IAEA NDS.

The NBIN option of the THERMR module specifies the number of equi-probable angles of the emitted thermal neutrons, and values of 16, 32, 48, and 64 were considered. The EMAX option of the THERMR and ACER modules specifies the maximum energy for thermal treatment, and values from 5eV to 10eV in 1eV intervals were considered. The TOL option of the RECONR, BROADR, and THERMR modules specifies the tolerance for linear interpolation. The values in red in Table I indicate the reference values for each option.

Table I: NJOY Processing Options (Reference Values in Red)

NJOY Option	Value					
Weighting option (IWT; IFENG/ ACEMAKER)	0 (1)	2 (2)				
No. of equi-probable angles (NBIN)	16	32	48	64		
Max. energy for thermal treatment (EMAX, eV)	5	6	7	8	9	10
Tolerance (TOL, %)	1.0	0.5	0.3	0.2	0.1	

Table II shows the list of 10 criticality benchmark problems including ZrH taken from the ICSBEP. These problems require thermal neutron scattering data for various materials other than ZrH, for which the reference options presented in Table I were applied to the NJOY processing. Exceptionally, for al27 and fe56, ENDF71SAB library in the MCNP6.2 code package was used.

3. Benchmark Calculation Results

Even if the IWT option is changed, the inelastic scattering cross section of H-in-ZrH does not change. However, this option was found to significantly change the energy-angle distribution of the inelastic scattering cross section. As a result, this caused differences in k-eff values between the IWT options for each benchmark problem, as shown in Fig. 1. As shown in Fig. 2, the k-eff differences compared to the reference option of IWT are 296pcm for hcm003-001, -62pcm and -72pcm for ict003-001 and ict003-002, respectively, and less than 40pcm for the other problems.

Table II: List of Criticality Benchmark Problems Including ZrH

no.	ICSBEP (short name)	Common Name	TSL Data (used)
1	hcm003-001	Narcis-M-1	hzrh, zrzrh, be, bebeo, obeo, hh2o
2	hct007-004	RRCt-1	hzrh, zrzrh, hh2o
3	hct007-005	RRCt-2	hzrh, zrzrh, hh2o
4	hct007-006	RRCt-3	hzrh, zrzrh, hh2o
5	ict003-001	TRIGA	hzrh, zrzrh, grph1, hh2o
6	ict003-002	TRIGA	hzrh, zrzrh, grph1, hh2o
7	ict013-001	NRAD-TRIGA-56	hzrh, zrzrh, hh2o, dd2o, grph1, fe56, al27
8	ict013-002	NRAD-TRIGA-60	hzrh, zrzrh, hh2o, dd2o, grph1, fe56, al27
9	ict013-003	NRAD-TRIGA-62	hzrh, zrzrh, hh2o, dd2o, grph1, fe56, al27
10	ict013-004	NRAD-TRIGA-64	hzrh, zrzrh, hh2o, dd2o, grph1, fe56, al27

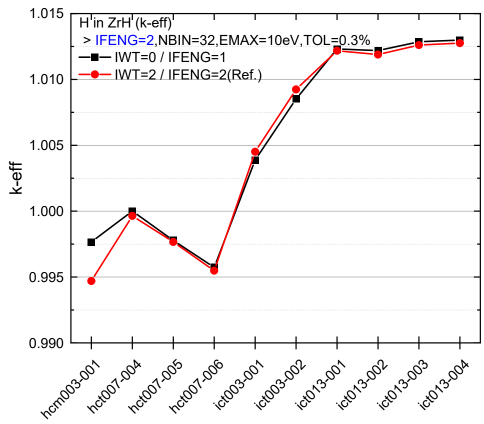

Fig. 1. Comparison of k-eff calculation results according to IWT option changes.

For the NBINs, the relative differences of inelastic scattering cross sections are very small, less than 0.003%. As shown in Fig. 3, the differences of k-eff values with NBIN option changes are less than 40pcm for all benchmark problems. But, the differences tend to be slightly larger at NBIN of 64 for some benchmark problems.

For the EMAXs, the relative differences of inelastic scattering cross sections are less than about 0.003% even near the EMAX boundaries. As shown in Fig. 4, the differences of k-eff values with EMAX option changes tend to increase for smaller EMAXs. Considering ict013-002, the EMAX of at least 8eV seems to be required.

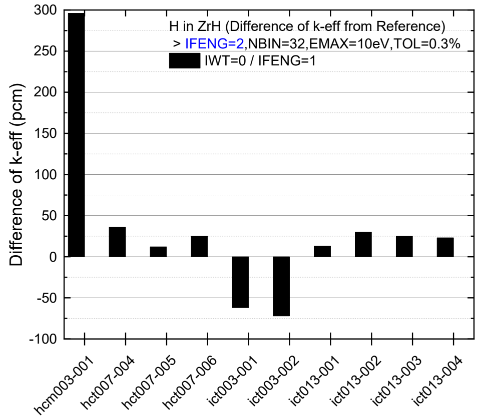

Fig. 2. Difference of k-eff calculation results according to IWT change compared to reference NJOY option.

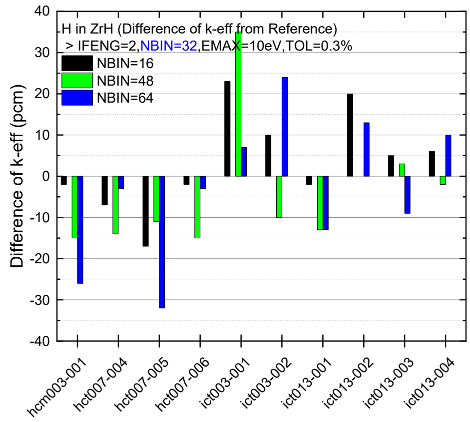

Fig. 3. Difference of k-eff calculation results according to NBIN changes compared to reference NJOY option.

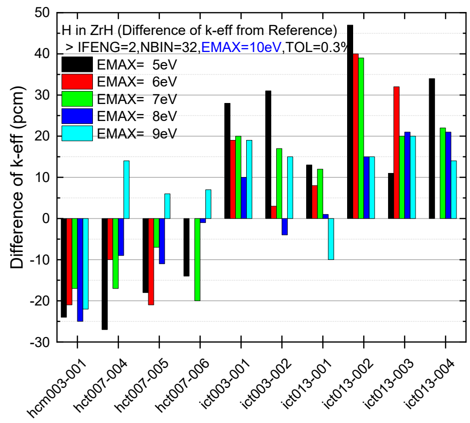

Fig. 4. Difference of k-eff calculation results according to EMAX changes compared to reference NJOY option.

For the TOLs, the relative differences of inelastic scattering cross sections are increasing up to about 4% at some energies. As shown in Fig. 5, the differences of k-eff values tend to be large for TOL options of 0.2% and 0.1%. Considering this trend, it seems necessary to check the TOL options below 0.1%.

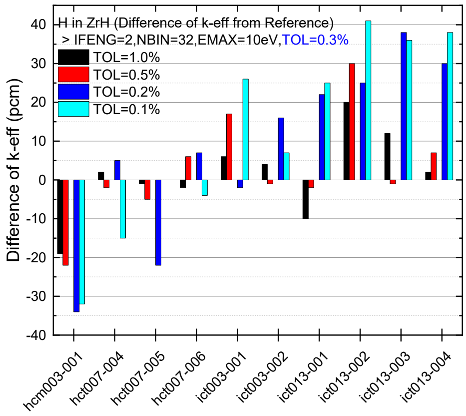

Fig. 5. Difference of k-eff calculation results according to TOL changes compared to reference NJOY option.

4. Summary

For the H-in-ZrH thermal neutron scattering data of ENDF/B-VIII.0, the inelastic scattering cross sections were compared by varying the processing options such as IWT, NBIN, EMAX, and TOL of the NJOY code. In addition, the influence on the criticality calculation due to the NJOY option changes was investigated. In conclusion, it is expected that the IWT option of the ACER module may have a significant impact on the criticality calculation depending on the thermal neutron scattering data and benchmark problems used. Therefore, it is thought that additional studies using other thermal neutron scattering data are needed.

ACKNOWLEDGMENT

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