Transactions of the Korean Nuclear Society Autumn Meeting
Gyeongju, Korea, October 26-27, 2023

Criticality Validation of Thermal Neutron Scattering Data of Light and Heavy Water Produced Based on Molecular Dynamics Simulation

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***Keywords :** thermal neutron scattering data, H_2O, D_2O, molecular dynamics simulation, criticality benchmark

1. Introduction

In the 2010s, research on the production of thermal neutron scattering data using molecular dynamics (MD) code simulation has been actively conducted. Furthermore, the latest nuclear data files of the US and Europe, ENDF/B-VIII.0 and JEFF-3.3, adopted the thermal scattering law (TSL) data of heavy and/or light water evaluated by J.I. Marquez Damian, et al.[1] Korea Atomic Energy Research Institute (KAERI) is conducting research on establishing a thermal neutron scattering data production system for future advanced nuclear reactors based on MD codes. As preliminary results, KAERI produced TSL data for light and heavy water through GROMACS simulation with the TIP4P/2005f water model and LAMMPS simulation with the SPC/E water model.[2,3]

In this study, benchmark problems including light and heavy water as moderator or coolant materials were selected from the expanded criticality validation suite in the MCNP6.2 code package[4], and comparative criticality calculations were performed for these problems according to TSL libraries. As TSL data for light and heavy water for comparison, ENDF/B-VII.1, ENDF/B-VIII.0, and two new preliminary TSL data from KAERI were used. Except for ENDF71SAB from the MCNP code package, other TSL data were processed in ACE-format using the same options of NJOY2016 code[5].

2. NJOY Processing and Criticality Benchmark Problems

As an NJOY processing option for this study, the influence of the IWT options in the ACER module on the k-eff calculation was examined. The IWT option 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.

MD-based TSL data of heavy water from ENDF/B-VIII.0 and new KAERI evaluations include not only D-in-D_2O but also O-in-D_2O, which represent the thermal neutron scattering effects of deuteron and oxygen molecules bound to heavy water, respectively. In this study, the effect of k-eff calculation according to the additional use of O-in-D_2O data was also investigated.

As shown in Table I, the criticality benchmark problems selected from the expanded criticality validation suite in the MCNP6.2 package consist of 41 problems with light water and 11 problems with heavy water. In MCNP6.2 calculation, the KNE80 library generated based on ENDF/B-VIII.0 by KAERI was used as neutron-induced nuclear reaction data other than TSL data.

Table I: List of Criticality Benchmark Problems Including Light and Heavy Water

TSL Material	Benchmark Problem
Light Water (41)	heu-met-fast-004-case-1
	heu-sol-therm-013-case-1
	heu-sol-therm-013-case-2
	heu-sol-therm-013-case-3
	heu-sol-therm-013-case-4
	heu-sol-therm-032
	ieu-comp-therm-002-case-3
	leu-comp-therm-008-case-1
	leu-comp-therm-008-case-2
	leu-comp-therm-008-case-5
	leu-comp-therm-008-case-7
	leu-comp-therm-008-case-8
	leu-comp-therm-008-case-11
	leu-sol-therm-002-case-1
	leu-sol-therm-002-case-2
	leu-sol-therm-007-case-14
	leu-sol-therm-007-case-30
	leu-sol-therm-007-case-32
	leu-sol-therm-007-case-36
	leu-sol-therm-007-case-49
	pu-met-fast-011
	pu-sol-therm-009-case-3a
	pu-sol-therm-011-case-16-5
	pu-sol-therm-011-case-18-1
	pu-sol-therm-011-case-18-6
	pu-sol-therm-018-case-9
	pu-sol-therm-021-case-1
	pu-sol-therm-021-case-3
	pu-sol-therm-034-case-1
	u233-sol-therm-001-case-1
	u233-sol-therm-001-case-2

	u233-sol-therm-001-case-3
	u233-sol-therm-001-case-4
	u233-sol-therm-001-case-5
	u233-sol-therm-008
	mix-comp-therm-002-case-pnl30
	mix-comp-therm-002-case-pnl31
	mix-comp-therm-002-case-pnl32
	mix-comp-therm-002-case-pnl33
	mix-comp-therm-002-case-pnl34
	mix-comp-therm-002-case-pnl35
Heavy Water (11)	heu-sol-therm-004-case-1
	heu-sol-therm-004-case-2
	heu-sol-therm-004-case-3
	heu-sol-therm-004-case-4
	heu-sol-therm-004-case-5
	heu-sol-therm-004-case-6
	heu-sol-therm-020-case-1
	heu-sol-therm-020-case-2
	heu-sol-therm-020-case-3
	heu-sol-therm-020-case-4
	heu-sol-therm-020-case-5

3. Benchmark Calculation Results

For the TSL data of light water of ENDF/B-VIII.0, compared to the TSL library processed with IWT=0, the library processed with IWT=2 shows k-eff effects within about 100 pcm except for some problems (132 pcm for leu-sol-therm-007-case-30, 106 pcm for leu-sol-therm-007-case-36, and -115 pcm for mix-comp-therm-002-case-pnl32). For the TSL data of heavy water, the effect of IWT=2 was less than 100 pcm when O-in-D_2O data was not used, but the effect was slightly increased when O-in-D_2O data was used. For heu-sol-therm-020-case-3 using O-in-D_2O data, in particular, the effect was the largest with -148 pcm. In terms of the effect of IWT=2, the TSL data from KAERI showed similar tendencies to that of ENDF/B-VIII.0 for both light and heavy water, but for the LAMMPS-based TSL data of heavy water, the effect tended to decrease slightly when using O-in-D_2O data.

Figures 1 and 2 show the differences of the MCNP6.2 calculation results from the reference experimental k-eff values for the light water and heavy water criticality benchmark problems, respectively. Note that these figures are for calculation results using the TSL libraries processed with IWT=2.

For the TSL data of light water, it was found that the TSL libraries used in this study showed k-eff differences within about 200 pcm, except for some problems. The ieu-comp-therm-002-case-3 showed differences of 245 pcm between ENDF/B-VIII.0 and LAMMPS and 409 pcm between GROMACS and LAMMPS. Also, the mix-comp-therm-002-case-pnl30 showed a difference of 201 pcm between GROMACS and LAMMPS. The TSL data of light water evaluated by KAERI showed reasonably good agreements with that of ENDF/B-VIII.0 with differences of about 200 pcm in k-eff values calculated for almost all benchmark problems.

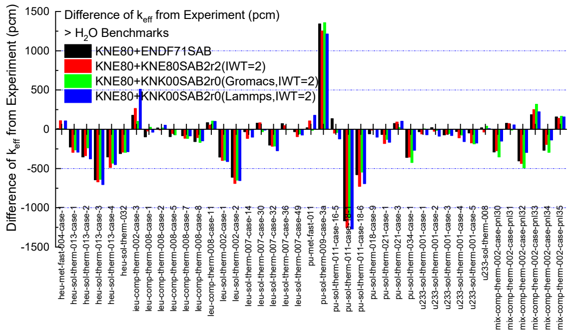

Fig. 1. Differences of k-eff calculation results from reference experimental values according to light water TSL libraries used. (IWT=2)

For the TSL data of heavy water, the TSL libraries used in this study showed small k-eff differences of less than about 200 pcm for all calculations with and without O-in-D_2O data. In particular, excellent agreement was found within 100 pcm between ENDF/B-VIII.0 and GROMACS-based TSL data of heavy water. The effect of O-in-D_2O data on k-eff calculation becomes significant in some benchmark problems. The ENDF/B-VIII.0 showed effects of O-in-D_2O greater than about 100 pcm for heu-sol-therm-004-case-3 (114 pcm), heu-sol-therm-020-case-3 (-219 pcm), heu-sol-therm-020-case-4 (-140 pcm), and heu-sol-therm-020-case-5 (-206 pcm). The GROMACS-based TSL data showed effects of O-in-D_2O greater than about 100 pcm for heu-sol-therm-020-case-2 (-108 pcm) and heu-sol-therm-020-case-3 (-150 pcm). Finally, the LAMMPS-based TSL data showed effects of O-in-D_2O greater than about 100 pcm for heu-sol-therm-004-case-5 (-134 pcm), heu-sol-therm-020-case-1 (-110 pcm), and heu-sol-therm-020-case-5 (-158 pcm).

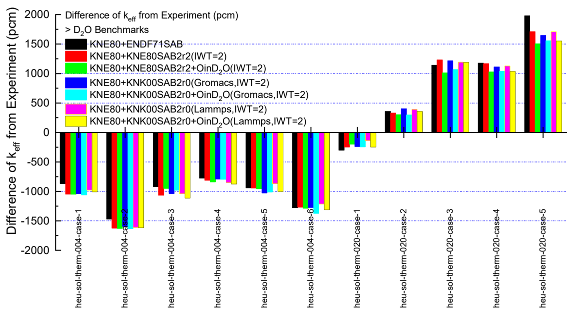

Fig. 2. Differences of k-eff calculation results from reference experimental values according to heavy water TSL libraries used. (IWT=2)

4. Summary

Criticality benchmark calculations were performed on TSL data of light and heavy water from ENDF/B-VIII.0 and two new preliminary KAERI evaluations based on GROMACS and LAMMPS MD simulations. For each TSL data, the effect of NJOY2016/ACER processing option, IWT, on k-eff calculation was examined. In addition, the effects of O-in-D_2O data on k-eff calculation were investigated.

ACKNOWLEDGMENT

The work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. NRF-2022M2D2A1A020552 22).

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