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EVALUATION OF THERMAL SCATTERING LAW FOR LIGHT WATER BASED ON NEW TIME-OF-FLIGHT MEASUREMENTS AT THE INSTITUT LAUE-LANGEVIN (ILL)

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ABSTRACT

The Institut de Radioprotection et de Sûreté Nucléaire (IRSN) carried out time-of-flight experiments for light water at several temperatures and pressures aiming at developing new evaluations of thermal scattering law based on experimental data. Measurement of dynamic structure factor $S(q, \omega)$ for light water has been carried out at the Institut Laue-Langevin (ILL), Grenoble. The $S(q, \omega)$ has then been transformed to density of states/frequency spectrum and utilized to generate the thermal scattering law using the LEAPR module of the NJOY nuclear data processing code. The thermal scattering law has been evaluated for the experimental temperatures varying from room temperature up to 500K. The impact of the newly developed thermal scattering law data on criticality safety benchmarks is investigated and compared with the existing thermal scattering law evaluations available in the JEFF-3.3 and ENDF/B-VIII.0 nuclear data library.

Key Words: Cross-sections, Thermal scattering law, Time-of-flight experiments, Evaluations

1. INTRODUCTION

Accurate determination of the Thermal Scattering Law (TSL) for light water is of interest to IRSN for reactor physics and criticality safety applications. While recent advancements in the experimental measurements of the dynamic structure factor $S(q, \omega)$ and molecular dynamics (MD) simulations of light water have been made, one still observes some discrepancies in the existing TSL libraries presently available to users in the nuclear data community. Currently, available TSLs for light water in the JEFF-3.3 and ENDF/B-VIII.0 differ due to the fact that both libraries are generated using frequency spectrum of light water obtained from different methods. The former is based on experimental frequency spectrum whereas the latter is based on the frequency spectrum obtained by performing MD simulations. Consequently an effort has been made to generate new frequency spectrum of light water by performing time-of-flight (TOF) experiments at the Institute Laue-Langevin (ILL). This paper demonstrates the ability to use the frequency spectrum obtained experimentally and generate TSL using the LEAPR module of the NJOY code system.

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2. THERMAL SCATTERING LAW

The double-differential scattering cross-section (DDXS) for neutrons with an incident energy E , scattering angle θ , final energy E' and at temperature T can be expressed as a function of $S(\alpha, \beta)$, the thermal scattering law by:

$$\frac{d^2\sigma_T}{d\Omega dE'}(E \rightarrow E', \mu) = \frac{\sigma_b}{4\pi k_B T} \sqrt{\frac{E'}{E}} S(\alpha, \beta) \quad (1)$$

where α and β are, unit-less quantities, related to the change in momentum and energy transfers represented, respectively, by:

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{Ak_B T} \quad \beta = \frac{E' - E}{k_B T} \quad (2)$$

where σ_b is the bound atom scattering cross-section, μ is the neutron scattering cosine ($\mu = \cos\theta$), A is the ratio of the scatterer mass to that of the neutron mass and k_B is the Boltzmann constant. A great deal of information can be found at references [1–3] which provide a complete description of the thermal scattering process. Presently, all the existing evaluations of TSL for light water is developed based upon an analytical function of frequency spectrum $\rho(\beta)$. This information is included in the LEAPR code to generate TSL as follows:

$$S(\alpha, \beta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i\beta\hat{t}} e^{-\gamma(\hat{t})} d\hat{t} \quad (3)$$

where \hat{t} is the time measured in the units of $\hbar/(k_B T)$ seconds. $\gamma(\hat{t})$ is given by:

$$\gamma(\hat{t}) = \alpha \int_{-\infty}^{+\infty} P(\beta)(1 - e^{-i\beta\hat{t}}) e^{-\beta/2} d\beta \quad (4)$$

and

$$P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)} \quad (5)$$

An accurate estimation of the frequency spectrum is needed to correctly evaluate the TSL for a required temperature. Frequency spectrum can be measured experimentally by performing TOF measurements of light water to have a proper estimation of the structural properties of light water.

3. EVALUATION PROCEDURE

Inelastic neutron scattering (INS) spectra of light water were measured on two time-of-flight spectrometers, IN4c and IN6, at the Institut Laue-Langevin (ILL), Grenoble. The incident neutron energy for IN4c and IN6 were 14.2 meV and 3.15 meV respectively. These two spectrometers provide high resolution spectroscopy, allowing a flexible energy and momentum transfer range. Measurements were carried out in the temperature range of 300-517 K and pressure range of 1-470 bar matching the normal operating conditions of nuclear power reactors. The dynamic structure

factor $S(q, \omega)$ was obtained after the necessary data reduction of the experimental data. A careful data reduction and analysis of the experimental data were carried out using the LAMP code [4] and an in-house data analysis tool developed at IRSN. More information can be obtained in [5]. $S(q, \omega)$ was finally transformed to the frequency spectrum $\rho(\omega)$ based on equation:

$$\rho(\omega) \simeq \lim_{q \rightarrow 0} S(q, \omega) \frac{\omega^2}{q^2} \quad (6)$$

The frequency spectrum is then used as an input to generate TSL for light water at the experimental temperatures.

4. BENCHMARKING NEW TSL DATA

The impact of the newly generated TSL evaluation will be studied using ICSBEP benchmarks. Careful selection of thermal benchmarks sensitive to the TSL for light water will be used for this purpose. Presently, TSL testing will be carried out only for room temperature benchmarks as high temperature benchmarks close to reactor operating temperature are limited. However, the effect of temperature on TSL, beyond room temperature, will be investigated. It should be noted that the effect of pressure on the TSL is negligible [5, 6].

5. RESULTS AND CONCLUSIONS

IRSN carried out new TOF experiments for light water at the ILL for several temperatures and pressures. The measured structure factor of light water was transformed to the frequency spectrum to develop new TSL evaluations for light water for temperature varying from room temperature up to 500K. Details on the TSL evaluation methodology will be presented in the full paper. This paper will highlight the differences in the existing TSL evaluations of light water and compliment it with a new evaluation fully based on experimental data. The impact of the newly developed thermal scattering law on criticality safety benchmarks will be investigated and the results will be compared with the existing TSL evaluations in the JEFF-3.3 and ENDF/B-VIII.0 data libraries. Thermal benchmarks close to reactor operating temperatures are very scarce. One of the objective of this work is to verify and validate the room temperature TSL evaluation based upon ILL experimental data with a series of thermal benchmarks and then investigate the high temperature evaluations.

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