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NEUTRON THERMAL SCATTERING LAWS FOR LIGHT AND HEAVY WATER FOR MODELING CRITICAL ASSEMBLIES AND TOF EXPERIMENTAL SET-UPS WITH NEUTRON TRANSPORT CODES

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Seven years have passed since the seminal work, "*How Accurately Can We Calculate Thermal Systems?*" by D.E. Cullen et al. was issued [1]. Meanwhile, the new Thermal Scattering Laws (TSL) for H_2O and D_2O have been available in the evaluated nuclear data libraries, such as JEFF 3.1 (2005, [2]) and ENDF/B-VII.0 (2006, [3]); see also multi-group libraries developed by Kyoto University group [4]. Consequently one can ask whether we can now do a better (more accurate) modeling of the thermal systems with the new TSL.

To address this question, we will discuss the theoretical models and methods used to produce the neutron TSL for H_2O and D_2O that are accepted in the modern evaluated nuclear data libraries, such as, JEFF 3.1, ENDF/B-VII.0, and JENDL 4.0. These TSL are usually used to produce the thermal scattering data files for Monte Carlo transport codes, such as MCNP(X), and multi-group deterministic transport codes, such as, WIMS, HELIOS, etc. The standard way to produce a TSL in the ENDF format is to use LEAPR module of the nuclear data processing code NJOY developed at LANL, USA [5]. As with any computer code designed to model physical phenomena, LEAPR has some limitations from both the theory and computational standpoints [6, 7]. For example, it is generally assumed that the self-diffusion, librations (hindered translations and hindered rotations), and intra-molecular vibrations in liquids are independent [8]. It is also assumed that one can disregard coherence effects in neutron scattering on H_2O and use Vineyard's or Sköld's approximation for the coherent scattering component of the thermal scattering kernel of D_2O [2]. Nevertheless, within the current LEAPR capabilities and NJOY structure, there is a way to improve the accuracy of TSL for H_2O and D_2O by using, for example, the temperature dependent libration spectra and static structure factors based on recent advances in simulations and experiments on liquids.

Then, can we distinguish different models of neutron scattering on light/heavy water in reactor physics applications and in modeling neutron scattering set-ups using standard neutron transport codes and the nuclear data libraries? In addressing this question, we will discuss how the results of simulations of the ZED-2 reactor at the Chalk River Laboratories (CRL) are sensitive to the different TSL's of H_2O and D_2O in terms of k_{eff} bias. For this study, we use MCNP5 [9] and a multi-temperature ENDF/B-VII.0-based MCNP library generated at CRL [10]. In the ZED-2 reactor, one can assemble different critical cores by using different types of coolant (light water/heavy water/air), different lattice pitch, etc.; the cores are always moderated by heavy water. As there is a large amount of heavy water moderator and reflector in the ZED-2 cores, the neutron spectrum in such a moderator is always dominated by its Maxwellian component; see Figure 1. We found that the TSL reactivity worth of D-in-D_2O is not very large,

$$k_{\mathrm{eff}}(\text{D-in-D}_2\text{O } \sigma_{\mathrm{s}}(E,T)) - k_{\mathrm{eff}}(\text{Free-Gas-H } \sigma_{\mathrm{s}}(E,T)) \sim 1 \text{ mk } (= 100 \text{ pcm}),$$

and so the sensitivity of k_{eff} to the details of D-in-D_2O scattering data is small. Here, the TSL reactivity worth for a nuclide A is

$$\rho_{\mathrm{eff}}(\text{TSL } A) - \rho_{\mathrm{eff}}(\text{Free-Gas-Model } A) \approx k_{\mathrm{eff}}(\text{TSL } A) - k_{\mathrm{eff}}(\text{Free-Gas-Model } A)$$

for modeling the critical cores ($k_{\mathrm{eff}} \approx 1.0$). For the coolant, on the other hand, the situation is different and, for example, for H_2O-cooled cases, the TSL reactivity worth of H-in-H_2O is significant,

$$k_{\mathrm{eff}}(\text{H-in-H}_2\text{O } \sigma_{\mathrm{s}}(E,T)) - k_{\mathrm{eff}}(\text{Free-Gas-H } \sigma_{\mathrm{s}}(E,T)) \sim 10 \text{ mk } (= 1000 \text{ pcm}),$$

and k_{eff} is sensitive enough to H-in-H_2O scattering data (see Figure 2), such as the position of the hindered rotation peak in the libration spectrum of H_2O. Then we will discuss whether one can obtain significant deviations from the Maxwellian asymptotic behavior of the neutron fluxes $\phi(\mathbf{r}, E)$ at low energies ($E < 0.1$ eV).

For testing of TSL's and transport calculations, we discuss the MCNP simulation of time-of-flight (TOF) measurement set-up, in which thermal neutrons are incident on a thick slab of water and the thermal neutron leakage is measured; see Figure 3. Although it is more an integral-type of experiment, experiments with water slabs could be performed to address the question of how accurately can we predict the responses of simple thermal systems using the available TSL's and Monte Carlo neutron transport codes.

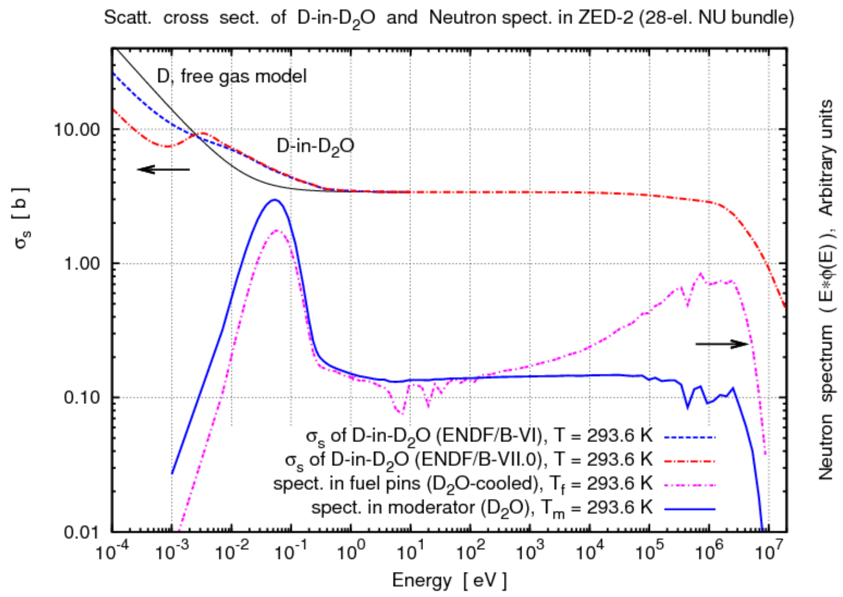

Figure 1. Thermal scattering cross sections for D-in-D$_2$O at T= 293.6 K and a typical neutron spectrum in ZED-2 (D$_2$O-cooled and D$_2$O-moderated reactor lattice)

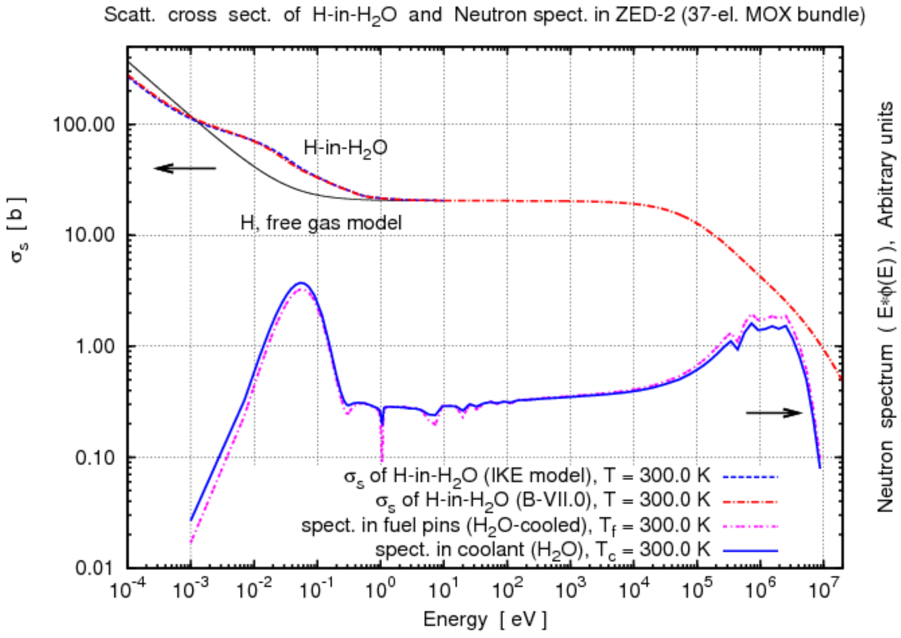

Figure 2. Thermal scattering cross sections for H-in-H$_2$O at T= 300.0 K and a typical neutron spectrum in ZED-2 (H$_2$O-cooled and D$_2$O-moderated reactor lattice)

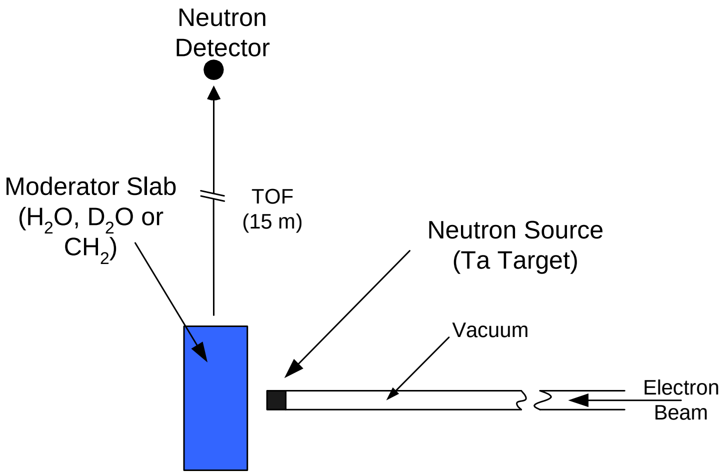

Figure 3. Neutron leakage experiment (neutron beam is slowed down in a slab of water)

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