

Thermal Scattering Law Comparison of Experimental Ice and Concrete Data

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INTRODUCTION

One of the most important materials for structural integrity, radiation shielding, and moderation of nuclear radiation systems is concrete. Every laboratory, reactor, and storage facility utilizes concrete in one form or another and in large amounts. Effects of radiation in the fast neutron regime have been explored for concrete in many situations; radiation effects of thermal neutrons for concrete have not been explored thoroughly. Quartz (SiO₂) and light water (H₂O) have been used to approximate the scattering and crystalline properties of concrete for decades in the whole nuclear related studies and quantifications [1].

SiO₂ crystals have coherent elastic scattering as the bulk of the scattering probability. Though coherent elastic scattering is important in concrete, concrete also has bound hydrogen from the cured water and other hydrogenous materials which scatter incoherently. The effects of the addition of bound hydrogen in the scattering kernel are currently unknown which may lead significant error in the current practice of using SiO₂ or H₂O to substitute concrete in studies such as radiation shielding.

Recent developments in thermal scattering law (TSL) data files at places like the National Nuclear Data Center, with the evaluated nuclear data files (ENDF), allow for new theories to be tested. The novel idea presented below is the use of bound hydrogen materials, such as ice (solid H₂O) or potentially polyethylene (CH₂), to simulate the thermal neutron scattering effects of concrete.

To test this theory, experimental data was collected and the effects on criticality benchmarks were explored.

Thermal Neutron Scattering Theory

The thermal scattering law, or $S(\alpha, \beta)$, is the common approximation for inelastic scattering in thermal neutron systems. It is related to the underlying double differential scattering cross section (DDSCS) of the material [2] by,

$$\frac{\partial^2 \sigma}{\partial E' \partial \Omega}(E \rightarrow E', \Omega) = \frac{\sigma_b}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S(\alpha, \beta). \quad (1)$$

Where σ_b is the bound cross section, k is the Boltzmann constant, and T is the temperature of the material. E and E' are the incident and scattered energy, respectively. $S(\alpha, \beta)$ is defined as the structure factor. It is a function of α and β , which are the unit-less momentum and energy transfer variables defined as [2],

$$\alpha = \frac{E'+E - 2\mu\sqrt{EE'}}{AkT} \text{ and} \quad (2)$$

$$\beta = \frac{E'-E}{kT}. \quad (3)$$

Where A is the mass ratio of the scatter mass to the neutron mass and is μ the cosine of the neutron scattering angle. $S(\alpha, \beta)$ is a special case of the dynamic structure factor, $S(q, \omega)$. The relationship between them can be represented by [2],

$$S(\alpha, \beta) = kTe^{\frac{-\hbar\omega}{2kT}} S(q, \omega) \cong kTS(q, \omega). \quad (4)$$

Where q and ω are defined by,

$$\alpha = \frac{-q^2 \hbar^2}{2MkT} \text{ and} \quad (5)$$

$$\beta = \frac{-\hbar\omega}{kT}. \quad (6)$$

Where q and ω are momentum and energy transfer, respectively.

Elastic scattering at thermal neutron energies is split between incoherent and coherent processes. For more crystalline structures, like SiO₂, coherent scattering is more prevalent. The coherent elastic scattering is defined as [3],

$$\begin{aligned} & \frac{\partial^2 \sigma_c}{\partial E' \partial \Omega}(E \rightarrow E', \Omega) \\ &= \frac{\sigma_b}{E} \sum_{E_i < E} f_i e^{-4WE_i/A} \delta(\mu - \mu_i) \delta(E - E_i). \end{aligned} \quad (7)$$

Where f_i are lattice constants, E_i are the Bragg edge energies, and W is the De Bye-Waller factor.

Incoherent elastic scattering is the more prevalent factor in hydrogenous and amorphous material such as CH₂. It is defined as [3],

$$\frac{\partial \sigma_{in}}{\partial E' \partial \Omega}(E \rightarrow E', \Omega) = \frac{\sigma_b}{2} e^{-2WE(1-\mu)} \delta(E - E'). \quad (8)$$

Details of the Experiment

The experiments were completed by two separate groups. Both of the experiments were done at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory. The experiments were done using 2 time-of-flight spectrometers which allows for straight-forward comparisons using above theory.

The first experiment was done in 2010 by Senesi [4]. Using the Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) an experimental $S(Q,\omega)$ was gathered for ice. The sample had an in-beam thickness of 0.25 mm to limit multiple scattering events [4].

The second experiment was done at the Wide-Angular Range Chopper Spectrometer (ARCS) by the authors of this summary. A concrete sample with 1 mm cylindrical shell and an internal diameter of 2.5 cm was completed in 2017.

RESULTS

To simulate the experiments a model was created in MCNP 6.1 [5] using the physical dimensions of the two instruments [6, 7]. A two-step resolution function was used as was described by Wendorff [8].

There has been very little work done to validate the ENDF/B-VIII.b4 ice thermal scattering library at the $S(\alpha,\beta)$ level. A comparison between the experimental ice data and the ENDF/B-VIII.b4 library was done. As seen in Fig. 1 multiple simulated angular data was used to compare the experimental ice $S(Q,\omega)$ to the simulation. MCNP 6.1 [5] allows for multiple thermal neutron libraries to be attached to a single material. The simulation shows a much wider peak and is missing some of the Bragg edges at higher energy transfer. The library leaves plenty of room for improvement, but the couple major underlying structural peaks are represented to varying degrees of success.

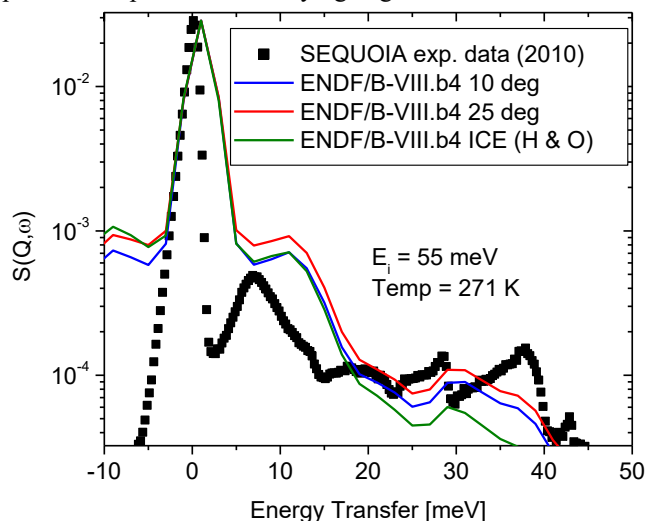


Fig. 1. Comparison between experimental $S(Q,\omega)$ and simulation for ice

Now that there is a basis for the use of the ENDF/B-VIII.b4 ice thermal scattering library, we can look at the use for the approximation of concrete. The second experiment done at ARCS on concrete can now be used to study the validity of the approximations.

For the simulation of concrete in the ARCS instrument, the only change between the separate tests was that the thermal scattering material card was changed for concrete.

For the H_2O and ice library, the file was used to expand the scattering effects on hydrogen atoms only. When the SiO_2 library is used it only changes the scattering on the silicon atoms in the concrete. As seen in Fig. 2, the ice file shows the best representation of the elastic scattering peak. Liquid H_2O shows best at inelastic scattering.

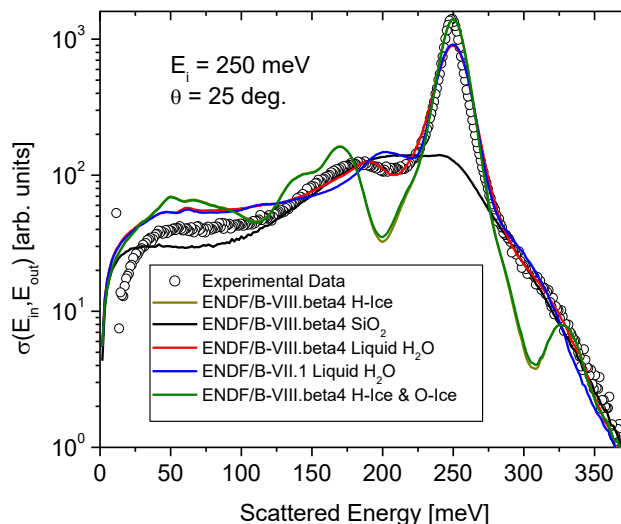


Fig. 2. Comparison of DDSCS and multiple libraries

Fig. 2 compares derivative data. To test the effect on integral systems, comparisons using criticality benchmarks was done. The criticality benchmark was found using the International Handbook of Evaluated Criticality Safety Benchmark Experiments (DICE) [9]. The benchmark shown is a test of the PLANET assembly at Los Alamos National Laboratory [10]. The experimental k -effective for the system is 1.0001 ± 0.0041 [10].

As shown in Table I, the best representation of the experimental k -effective in this case is the ENDF/B-VIII.b4.

TABLE I. Concrete Criticality Benchmark (HEU-MET-THERM-018)

$S(\alpha,\beta)$ Library	K -effective	Standard Deviation
ENDF/B-VII.1 H_2O	1.00048	0.00035
ENDF/B-VIII.beta4 H_2O	1.00041	0.00037
ENDF/B-VIII.beta2 SiO_2	1.00073	0.00036
ENDF/B-VIII.beta4 ICE	0.99998	0.00035
None	1.00110	0.00035

Therefore, with the fact that the ice thermal scattering file shows the best representation of the derivative and integral tests, it should be considered for the approximation of concrete in simulations. Since the validation is not complete for the ice file, other bound hydrogen files like CH_2 could be used also as an approximation with further study.

ENDNOTES

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