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Title: Verification of the Re-Released ENDF/B VIII.0 Based Thermal Scattering Libraries

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Verification of the Re-Released ENDF/B VIII.0 Based Thermal Scattering Libraries

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Talk Outline

- Thermal Scattering Law (TSL) data for neutrons
- Previous Production of S(α,β) Libraries
- Verification of new S(α,β) Libraries
- Release of the new S(α,β) Libraries

Thermal Scattering Law (TSL) Effects for Neutrons

- At low incident energy, neutrons are sensitive to molecular effects, crystalline structures, and other such thermal phenomena
- The evaluation of low energy cross sections requires advanced models in regards to the “free gas” traditional model
- Practically, low energy cross section are given through Thermal Scattering Law also called $S(\alpha,\beta)$
- $S(\alpha,\beta)$ are processed into NJOY to produce continuous or multigroup cross section at various temperatures

Recent Previous S(α,β) Libraries

- ENDF/B VII.0 (2008)
  - 20 tsl materials and 111 evaluations
- ENDF/B VII.1 (2014)
  - 21 tsl materials and 149 evaluations
- ENDF/B VIII.0 (2018, 2020)
  - 34 tsl materials and 253 evaluations
  - Significant expansion of tsl data !!

What Went Wrong in 2018?

- 10 materials had incorrect ACER inputs for elastic incoherent scattering
- 2 materials (SiO_2 in alpha and beta phases) had bad processing
- 2 materials (rgraphite10 and rgraphite30) were reversed
- A few bookkeeping errors

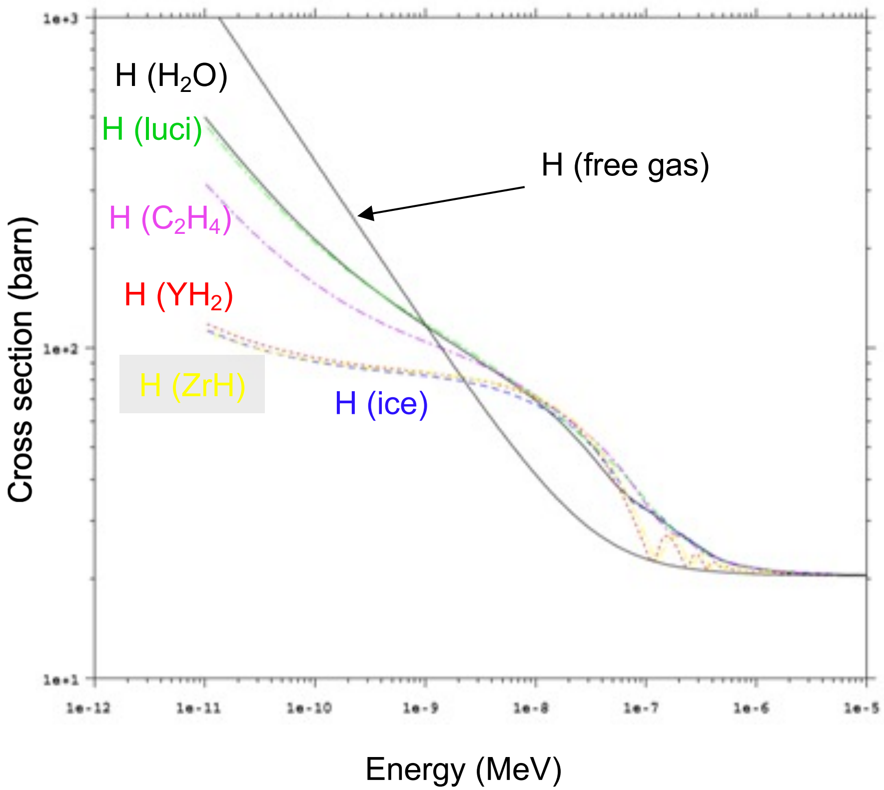
lucite ($C_5O_2H_8$), poly-methylene (CH_2), ice, YH_2, ZrH, UN, SiO2, graphite, solid methane

How Did We Verify the Data? *(this time, as opposed to last time)*

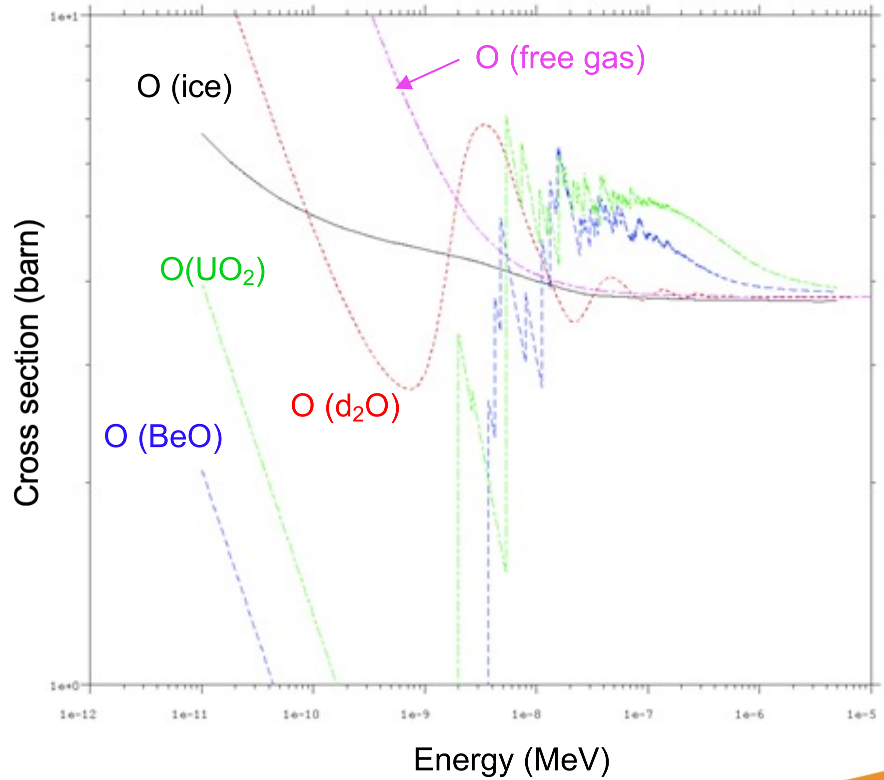
- (1) Verification by continuity at E_{max} between S(α,β) and free gas
- (2) Verification by tabular results across all temperatures for all materials (506 sample problems = 253 * 2)
  - Comparisons between S(α,β) and free gas cross sections
  - Consistency checks as the temperature changes
  - Also did some plots of S(α,β) with respect to temperature
- (3) Verification by comparison plots with GROUPR data

(1) Continuity at E_{max} (for Hydrogen and Oxygen)

Low energy cross section for Hydrogen



Low energy cross section for Oxygen



(2) 506 Sample Problems

all matls, all temps, with and without S(α,β)

- Infinite Media of Thermal Scattering Law Material at nominal density
- Fixed Source of Thermal Neutrons in a Maxwellian Spectrum corresponding to the material temperature
- TMP cards for the non-S(α,β) materials to set the material temperature
- Tallies for the volumetric flux (F4), the average neutron velocity, and flux-weighted cross sections for total, scattering, and capture
- NO IMPLICIT CAPTURE (see the PHYS:n card)
  - Number of Collisions will be actual physical collisions
- Lots of particle histories (10 million) – expect numerical precision to 3 or 4 significant digits – and except for deuterium and graphite, MCNP runs quickly

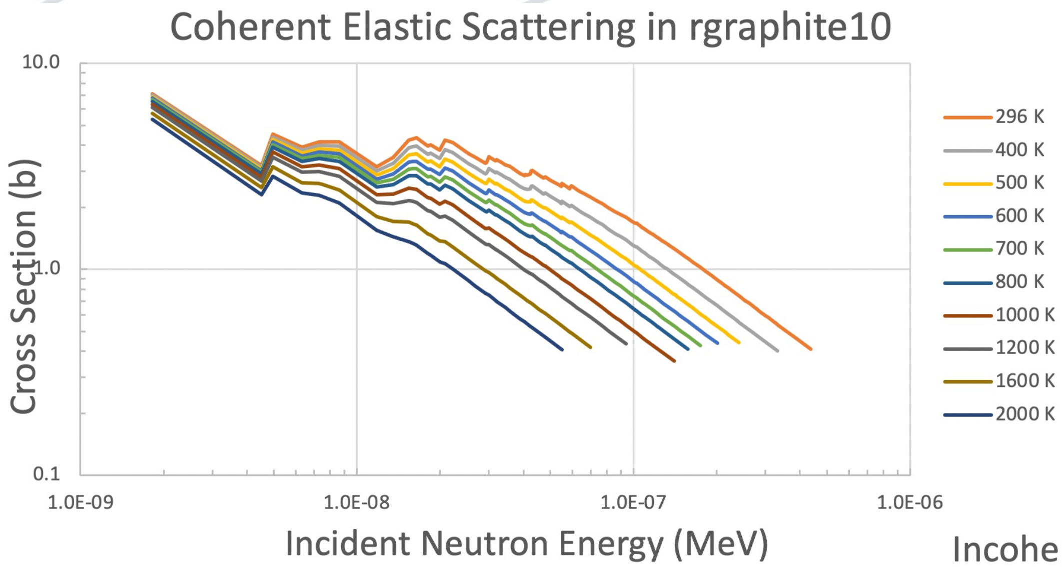
(2) A Sample Table of Results part of H_2O with $S(\alpha,\beta)$ Scattering

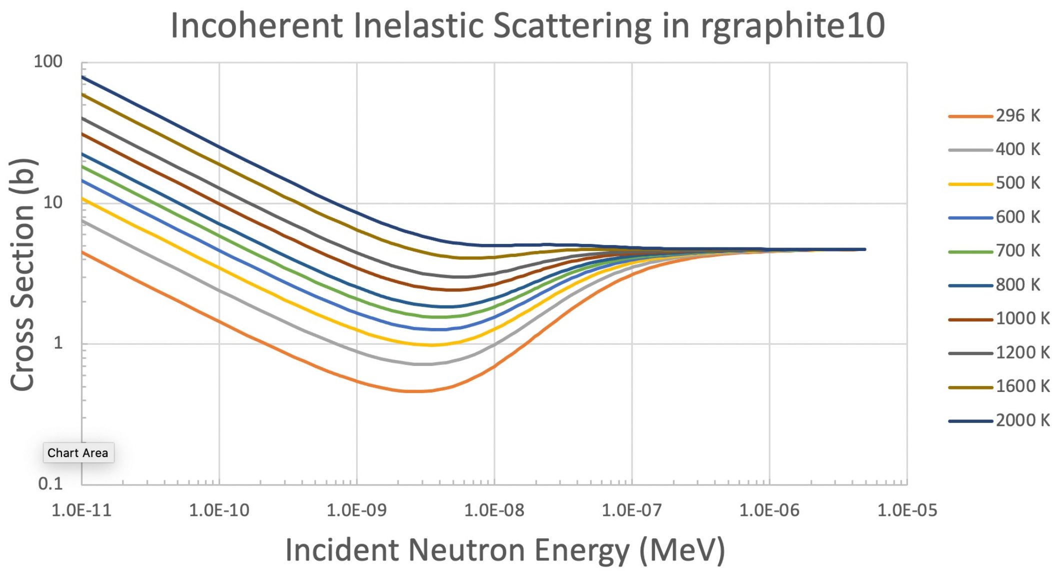
H_2O $S(\alpha,\beta)$	temp (MeV)	temp (K)	avg. no. collisions	lifetime (sh)	mfp (cm)	avg n vel (m/sec)
	2.444E-08	283.6	161.37	2.0435E+04	0.3294	2440
	2.530E-08	293.6	162.54	2.0435E+04	0.3329	2483
	2.585E-08	300.0	163.22	2.0432E+04	0.3351	2510
	2.789E-08	323.7	165.81	2.0432E+04	0.3427	2607
	3.016E-08	350.0	168.66	2.0431E+04	0.3504	2711
	3.219E-08	373.5	171.09	2.0432E+04	0.3569	2801
	3.447E-08	400.0	173.72	2.0431E+04	0.3636	2899
	3.650E-08	423.6	176.08	2.0430E+04	0.3690	2983
	3.878E-08	450.0	178.66	2.0433E+04	0.3747	3074
	4.081E-08	473.6	180.97	2.0431E+04	0.3793	3154
	4.309E-08	500.0	183.59	2.0431E+04	0.3841	3241
	4.512E-08	523.6	185.81	2.0432E+04	0.3882	3316

(2) Consistencies in the Tables

- The average neutron velocity should be invariant with respect to scattering. It is only dependent on the material temperature.
  - Good diagnostic for finding inconsistent data or inconsistent input decks
- At higher temperatures, the S(α,β) results and the free gas results for the same material should begin to approach each other (i.e., getting closer to E_{max})
- As the temperature increases, the number of collisions and the velocities should increase. The mfp should be (relatively) constant for free gas materials, but increase with temperature for S(α,β) materials

(2) Consistency plots with temperature



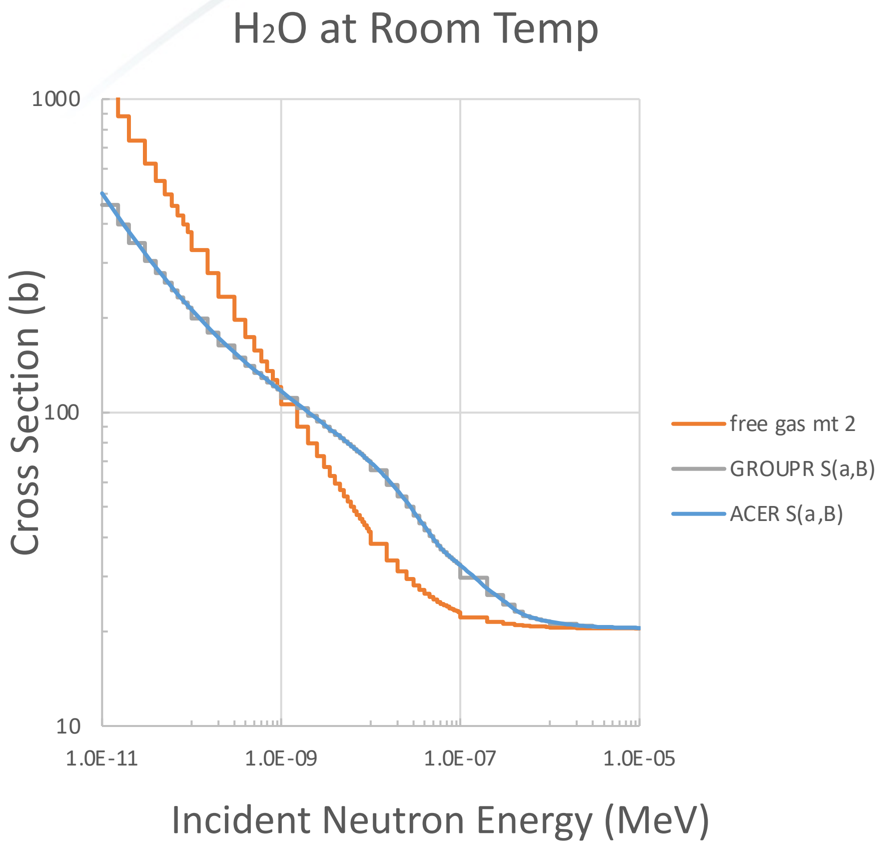


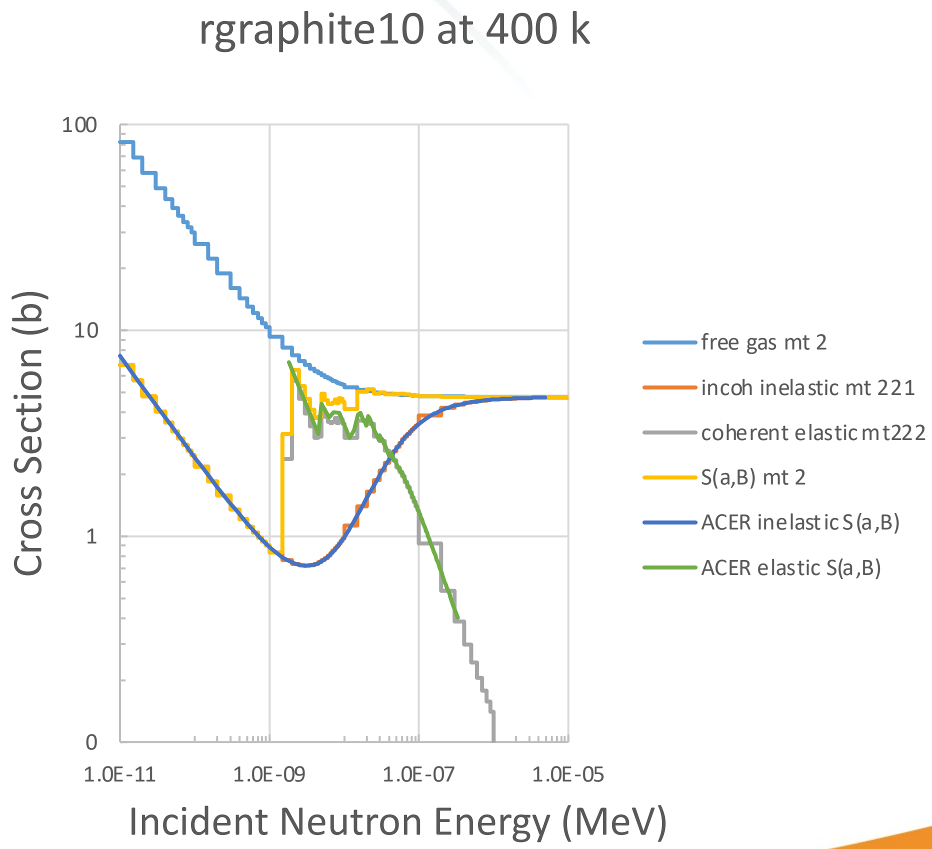
(3) Comparisons between ACER and GROUPR (multi-group)

- Same NJOY processing for both through the THERMR routine
- Independent processing and input decks for ACER / GROUPR
- Comparisons can be made by plots of the cross section data
- GROUPR used an arbitrary group structure and no weight function
- One example from each of the 3 kinds of TSL data
(all TSL materials have Incoherent Inelastic)
  - No elastic scattering (light water)
  - Coherent Elastic Scattering (graphite) → Bragg Edges
  - Incoherent Elastic Scattering (ZrH)

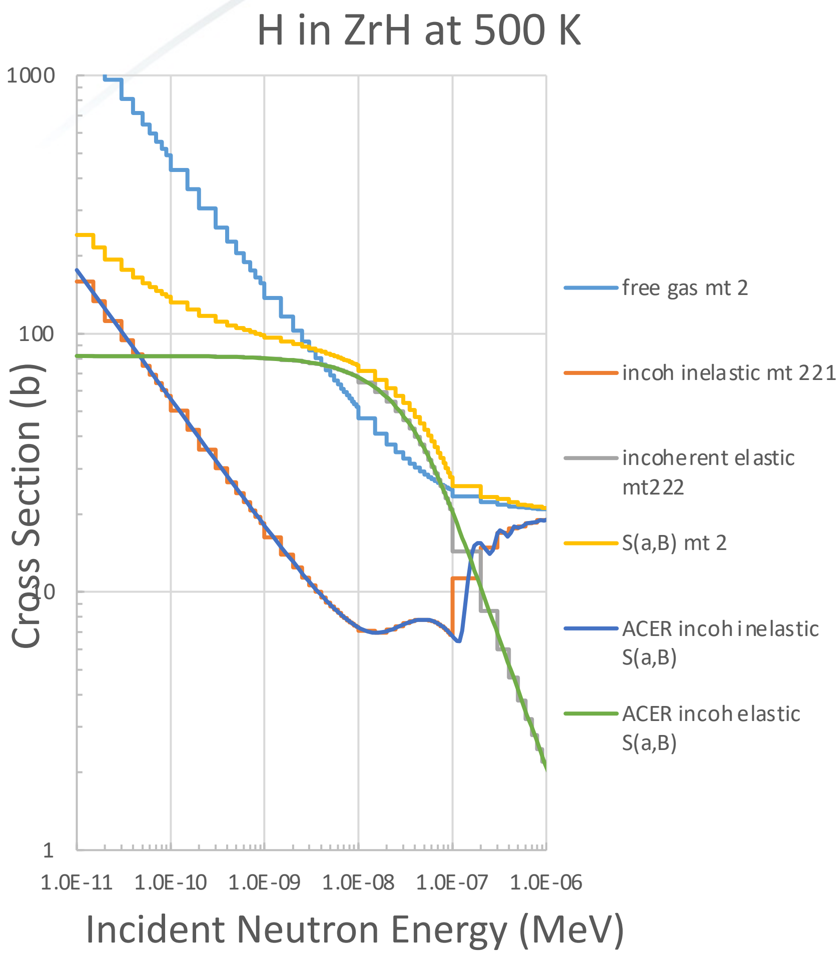
- *CSEWG proposal last November to allow combinations of elastic scattering data …*

ACER / GROUPR Comparison for water and graphite (10% porosity)

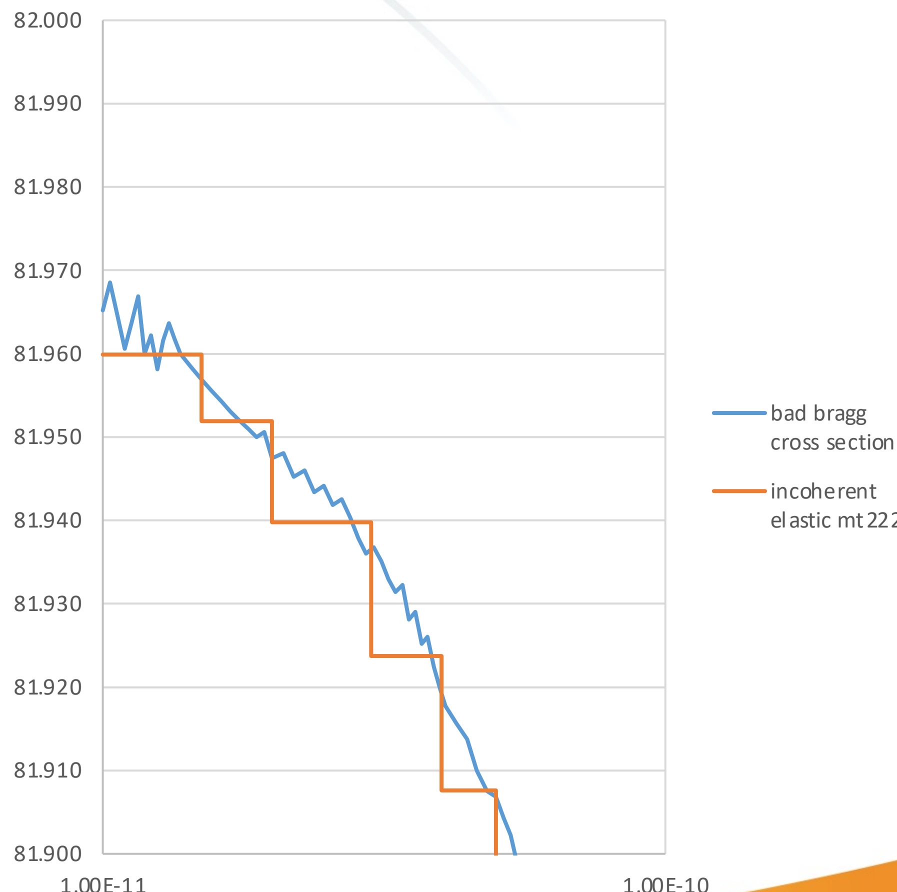




ACER / GROUPR Comparison for ZrH



What I should have noticed in 2018!



Summary

- Re-Processed ENDF/B VIII.0 S(α,β) Data has been Released by the Nuclear Data Team at Los Alamos. Available at:

  https://nucleardata.lanl.gov

- Comprehensive and Systematic Verification has been carried out

- 64 page release document with **excruciating** detail is also available with the data at nucleardata.lanl.gov

Final Word

- The issues in the first release of the ENDF/B VIII.0 S(α,β) were pointed out by users

  → Thanks to Dimitris kontogeorgakos, Paul Romano, Lei Zheng, and Alyssa Kersting

- Your feedback is extremely valuable to us and contributes to the entire community

  → Please contact us for any concern you may have

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