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On integral benchmarks for resolving TSL conflicts for ENDF/B-VIII.1 release

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Conflicting Reviews: Polyethylene and Lucite

- 2 research groups evaluating and reviewing each others work
  -ORNL
  -NCSU
- NCSU review of ORNL ENDF/B-VIII.1.b2 PE candidate:
  > From the above, and consistent with CSEWG's "do no harm" policy, I recommend (1) maintaining the ENDF/B-VIII.0 evaluation of HinCH2 for ENDF/B-VIII.1, and (2) rejecting this polyethylene evaluation.
- However, we believe that:
  - ORNL ENDF/B-VIII.1.b2 candidates "do no harm" to integral benchmarks
  - ORNL ENDF/B-VIII.1.b2 candidates candidates perform better on semi-differential & differential validation (transmission & inelastic scattering exp.)
  - **ENDF should match the differential data, not be adjusted to integral!**
    + Analogous to decision made at mini-CSEWG 2021

Neutron scattering sampling in neutronics codes

- How do CE Monte Carlo neutronics codes use TSLs for scattering?
  - Sampling the distance to next collision (transmission!)
  - Sampling the reaction ratio probability
  - Sampling the exit energy and angle distributions (TSL!)
- We test these with:
  - Experimental transmission
  - Experimental inelastic scattering ($S(\alpha, \beta)$)

Scattering cross sections are based on phonon spectrum

- Inelastic scattering (coherent plus incoherent):

In the incoherent and Gaussian approximation, the $S(\alpha, \beta)$, as expressed in NJOY LEAPR module, in terms of phonon expansion can be written as:

$$S(\alpha, \beta) = e^{-\alpha\lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \alpha^n \frac{1}{2\pi} \times \int_{-\infty}^{\infty} e^{i\beta\hat{t}} \left[\int_{-\infty}^{\infty} P(\beta') e^{i\beta'\hat{t}} e^{-\beta'/2} d\beta' \right] \quad (1)$$

where:

$$P(\beta) = \frac{\rho(\beta)}{2\beta \sinh(\beta/2)} \quad \text{and} \quad W = \frac{\int_{-\infty}^{\infty} P(\beta) e^{-\beta/2} d\beta}{AkT} \quad (2)$$

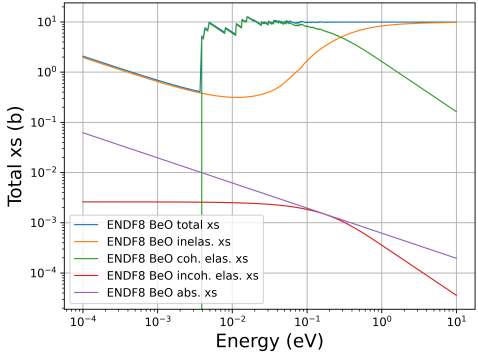
with $\rho(\beta)$ as the phonon spectrum.

- Coherent elastic scattering:

$$\sigma^{coh} = \frac{\sigma_c}{E} \sum_{E_i > E} f_i e^{-2WE_i} \quad (3)$$

- Incoherent elastic scattering:

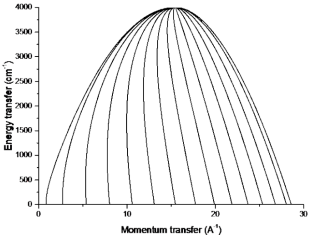
$$\sigma^{incoh} = \frac{\sigma_b}{2} \left(\frac{1 - e^{-4WE}}{2WE} \right) \quad (4)$$



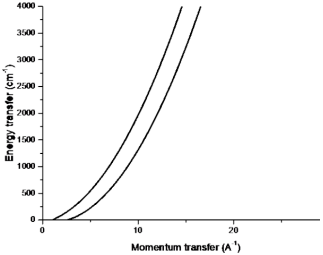
- **As we can see all the scattering components are dependent on the inelastic physics through $\rho(\beta)$ and W (Debye-Waller factor)**

INS measurements can validate $S(\alpha, \beta)$

- Direct geometry spectrometers (ARCS and SEQUOIA):



- Indirect geometry spectrometers (VISON):



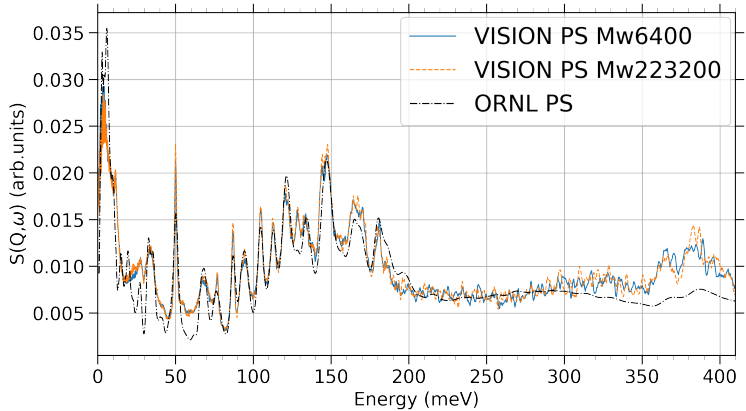
+ Measured quantity $S(Q, \omega)$ is directly related to $S(\alpha, \beta)$:

$$S(\alpha, \beta) = k_B T \; exp\left(\frac{-\hbar\omega}{2k_B T}\right) S(Q, \omega) \tag{5}$$

where T is the temperature, and k_B is the Boltzmann constant.

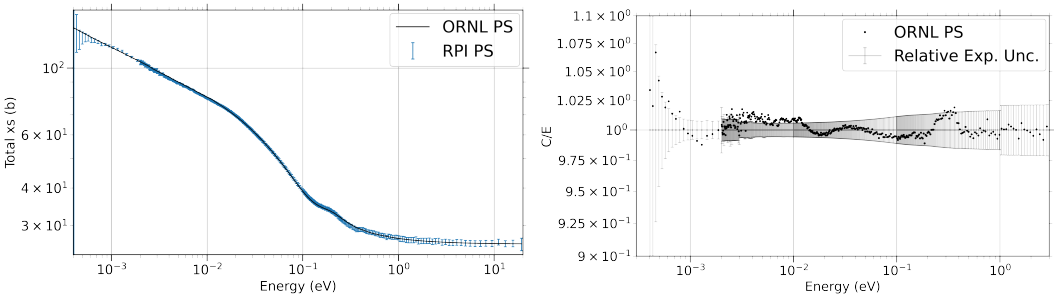
+ **This means that we can directly measure what we store in ENDF TSL files.**

Integral Performance ≠ Differential Performance
Example: Polystyrene & Polyethylene



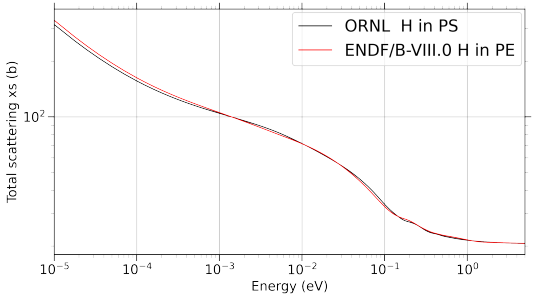
- Structurally different polystyrene (different molecular weights, Mw) have almost identical inelastic spectra.

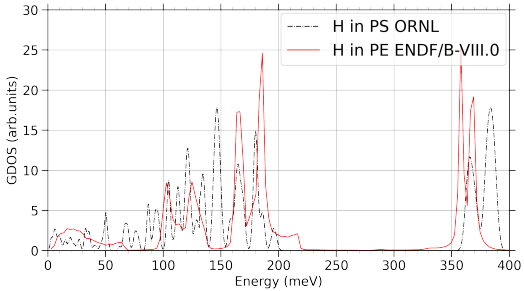
Integral Performance $\neq$ Differential Performance
Example: Polystyrene & Polyethylene



- Excellent agreement with RPI transmission measurement. Ideally for validation purposes multiple transmission measurements should be used.

Integral Performance $\neq$ Differential Performance
Example: Polystyrene & Polyethylene

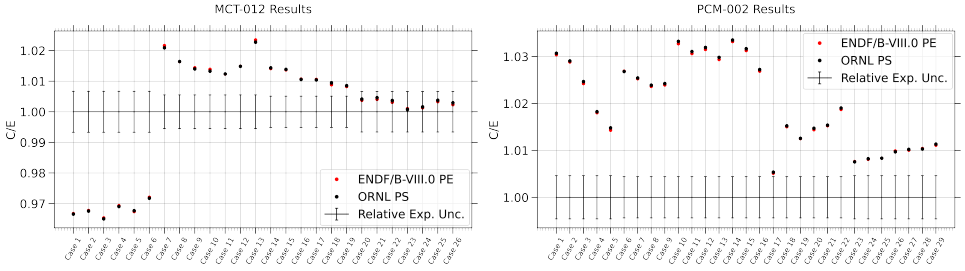




- PS and PE have almost identical total cross section for hydrogen.
- PS and PE have significantly different phonon spectrum.

Integral Performance $\neq$ Differential Performance

Example: Polystyrene & Polyethylene

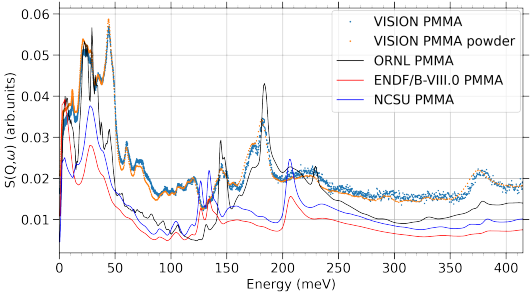


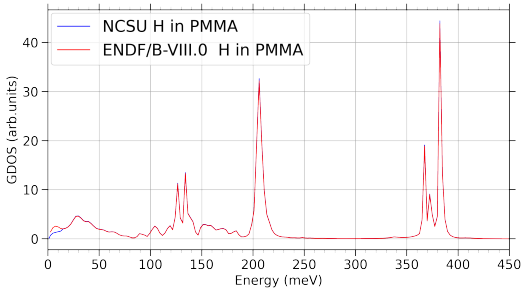
	MCT-012 χ^2	PCM-002 χ^2
Polyethylene	9.12	24.12
Polystyrene	9.13	24.7

Table 1: Calculated χ^2 value using PS and PE TSLs for MCT-012 and PCM-002 benchmarks.

- **This demonstrates importance of INS and transmission measurements, because with different phonon spectra we can calculate total cross section nearly identically, as well as critical benchmarks.**

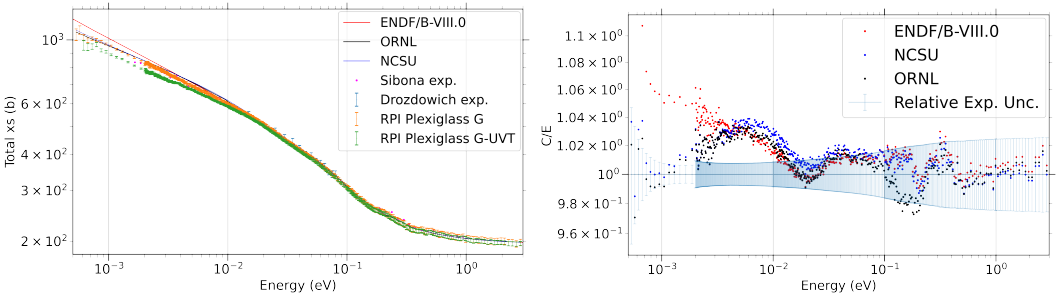
Lucite evaluation - INS validation





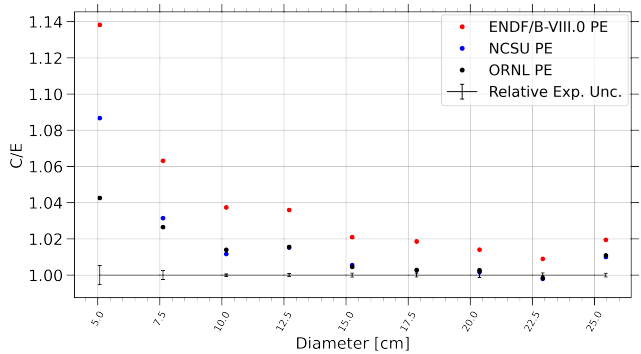
- Different PMMA samples, powder and sheet (with additives) have almost identical INS spectra.
- ORNL has a better agreement with INS measurement.
- NCSU updated the phonon spectrum yet agreement with INS measurements was not improved.

Lucite evaluation - Transmission validation



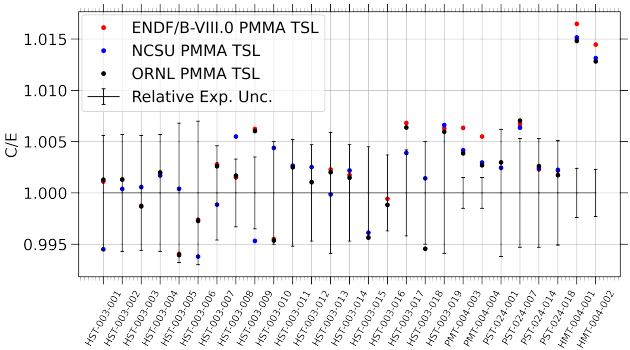
- Plexiglass G and G-UVT samples have different total cross section due to additives.
- ORNL TSL has an overall better agreement with Plexiglass G (common form) than both updated NCSU and ENDF/B-VIII.0 evaluations.

Lucite - Pulsed neutron die-away validation



- ORNL TSL performs significantly better than ENDF/B-VIII.0 evaluation.
- ORNL and NCSU perform similarly due to their similar total cross sections.
- Similar to critical benchmarks there is a high sensitivity in changes to the total cross section, which may not be justifiable in comparison with inelastic measurements.

Lucite - Critical benchmarks validation



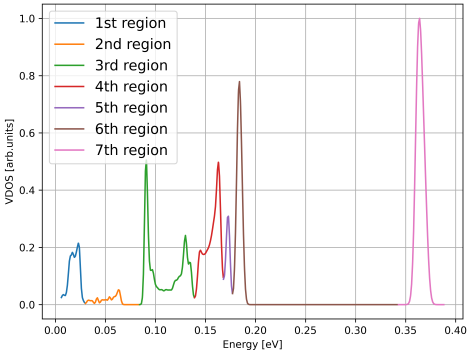
TSL	χ^2
ENDF/B-VIII.0	0.899
NCSU	0.784
ORNL	0.75

- ORNL TSL performs better including new HMT-004 benchmarks from LLNL
- **This demonstrates importance of INS and transmission measurements, because with different phonon spectra we can calculate total cross section similarly, as well as critical benchmarks.**

Polyethylene (PE) evaluation

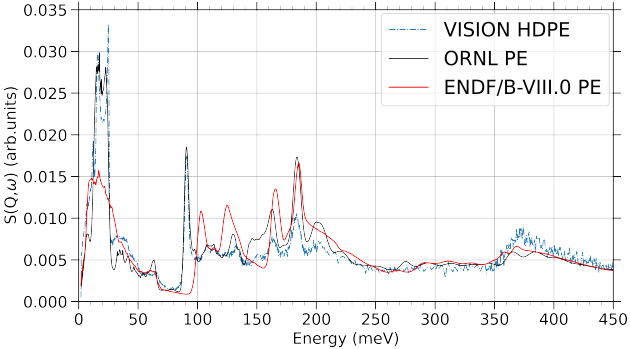
- Motivation:
  - New transmission measurements at RPI, as well as criticality benchmarks from LLNL and LANL.
  - ORNL PE evaluation was optimized with respect to differential measurement at VISION spectrometer at SNS, as well as transmission measurement from RPI.

- Optimization summary:
  - assign weights for each distinct region of GDOS and vary them by Dakota
  - calculate χ^2 with respect to VISION INS measurement. ENDF files can be directly compared to the VISION data by extracting $S(\alpha, \beta)$ at specific (α, β) values measured in VISION experiment and applying well-know VISION experimental resolution.
  - calculate χ^2 with respect to RPI transmission measurement
  - repeat the process until combined χ^2 is minimized

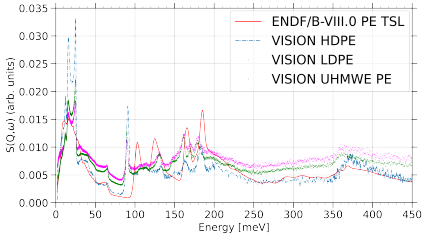


Polyethylene validation- INS measurements at ORNL

- VISION HDPE comparison:



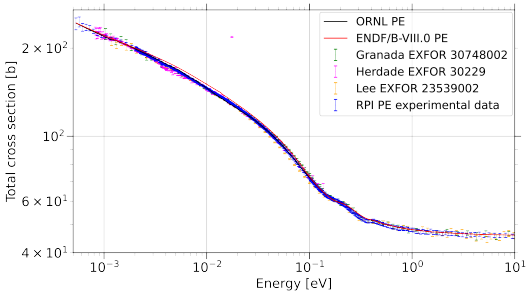
- VISION HDPE, LDPE, and UHMW comparison:



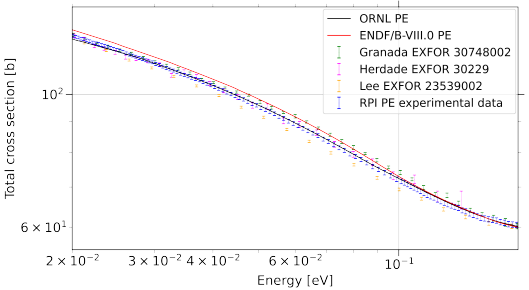
* **ORNL PE has better agreement with the shape of all different PEs!**

Polyethylene validation- Transmission measurements at RPI

- Total xs comparison (5e-4 to 10 eV):

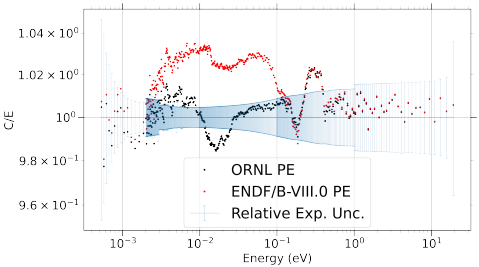


- Total xs comparison (2e-2 to 2e-1 eV):

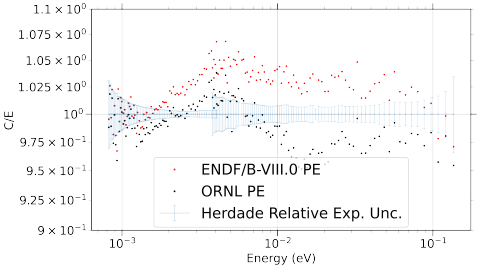


Polyethylene validation- Transmission measurements at RPI

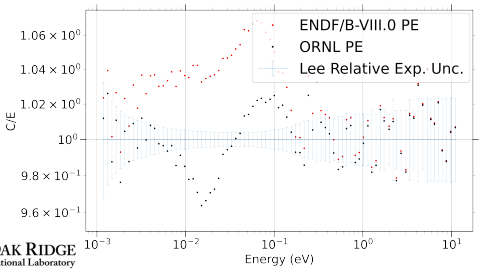
- C/E comparison to new RPI data:



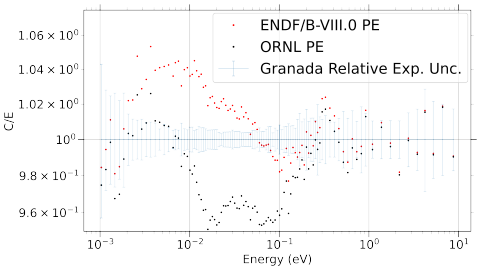
- C/E comparison to Herdade data:



- C/E comparison to Lee data:

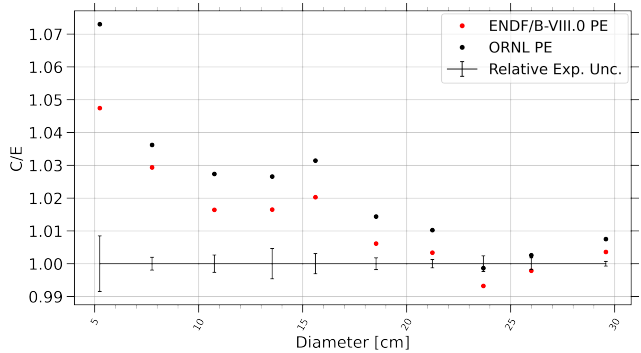


- C/E comparison to Granada data:



Polyethylene validation- Pulsed neutron die-away measurements

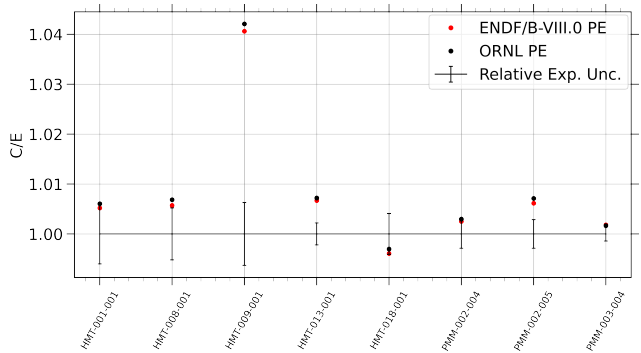
- New pulsed neutron die-away measurements at LLNL.



- New ORNL evaluation reduces, compared to ENDF/B-VIII.0, total neutron scattering cross section resulting in an increase in PNDA α compared to ENDF/B-VIII.0. ENDF/B-VIII.0 and ORNL calculated α values are within 1-2% of each other.

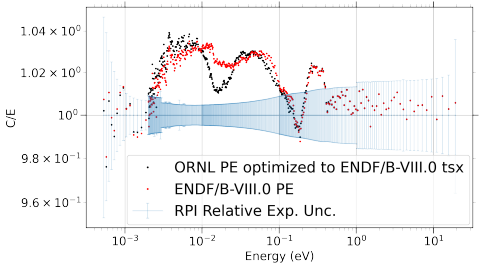
Polyethylene validation- Integral criticality benchmarks

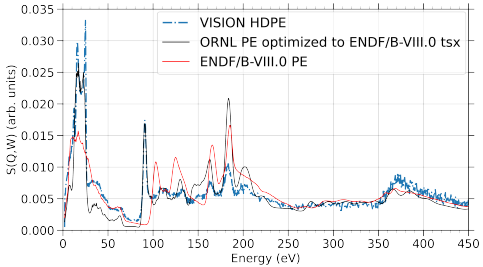
- We have tried to identify all relevant thermal benchmarks that contain Polyethylene in International Handbook of Evaluated Criticality Safety Benchmark Experiments 2021.

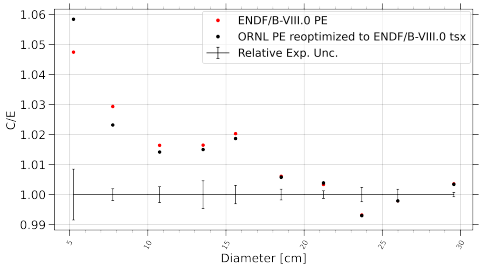


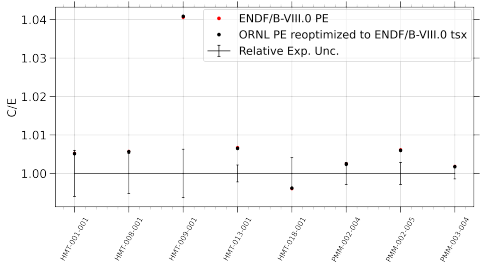
- ORNL evaluation reduces, compared to ENDF/B-VIII.0, total neutron scattering cross section resulting in an increase in neutron multiplication factor k_{eff}.
- For most benchmarks k_{eff} for calculated values is anywhere from 200- 4000 pcm away from experimental values, which is indicative of possible issues with nuclear data besides TSL.

- Optimizing the cross section with respect to ENDF:



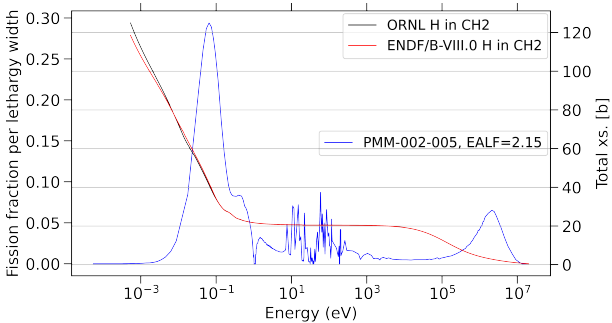






Fission density spectra in benchmarks

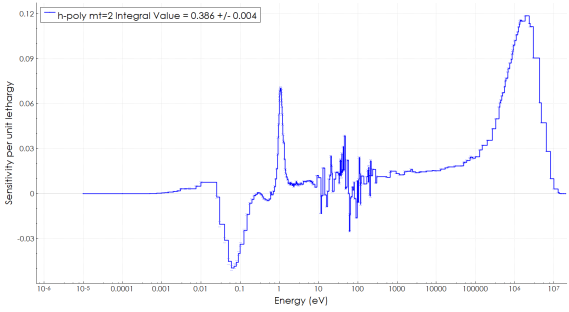
- Three bin spectral definition from ICSBEP Handbook provides a rough quantification of the neutron energy spectrum
- TEX thermal cases are not very thermal
- PU-MET-THERM-002-005 has about 66% fissions induced by thermal neutrons, corresponding to an EALF of 2.15 eV



- **How effective are these benchmarks at differentiating among different 1H-poly TSL evaluations?**

Sensitivity data confirm lack of sensitivity

- Majority of sensitivity is above 10 eV
  - TSL not even being used
- Misprediction of k_{eff} for this benchmark is unlikely to be driven by TSL
  - CAUTION: This is based on the integrated 1D scattering sensitivity



+ **Good news:** new experiments with thicker moderator plates have been performed and evaluated
  - PMT-004 evaluations approved at April TRG meeting for inclusion in 2023 ICSBEP Handbook
  - Two cases include polyethylene
  - Thermal fission fraction of these two cases is 72.9% and 74.6%
  - Patience: these two cases will likely be useful and available within the next year
+ **Less good news:** Only two points, both with Pu, and likely highly correlated

Summary & Conclusions

- Polystyrene:
  - ORNL evaluation in TSL review process for ENDF/B-VIII.1
  - Excellent agreement with INS and transmission measurements
  - **PS and PE evaluations with different phonon spectra, similar total xs., calculate k_{eff} similarly**

	Polyethylene		**Lucite**	
	ORNL	ENDF/B-VIII.0	ORNL	NCSU
Crit. bench.	slightly worse	slightly better	same	same
PNDA	slightly worse	slightly better	same	same
Quasi-differential	better	worse	better	worse
Differential	better	worse	better	worse

- Crit. benchmarks:
  - While extremely useful for validation of nuclear data at all energies, critical benchmarks are not the best tool to provide a definitive answer on conflicting TSLs
  - *INS and transmission measurements need to be the basis of validation of TSLs*

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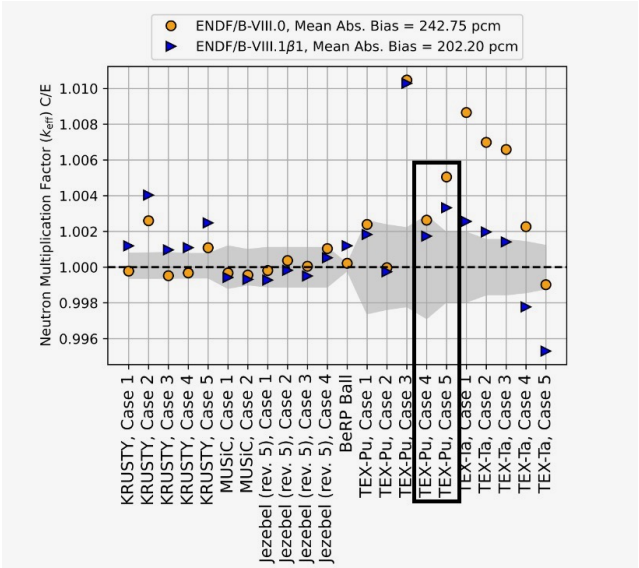
LANL ENDF/B-VIII.1.b1 testing



Backup slides