AMPX and ENDF/B-VIII.1 Thermal Scattering Library

AMPX Team

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U.S. DEPARTMENT OF
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DISCUSSION OF AMPX and ENDF/B-VIII.1

- General ENDF issues encountered
- Issues particular to thermal scattering library:
  - Clear communication of the intended use for the file – "Which graphite should I use in model?"
  - TSL files with many Bragg peaks are driving a change in SCALE CE library format and transport codes
  - Usage of thermal kernels with sharp peaks – issue encountered using ENDF/B-VIII.0 data, and resolved

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GENERAL ENDF ISSUES ENCOUNTERED

Resonances with total widths greater than sum of partial widths ($\Gamma > \sum \Gamma_c$):

- Hg-203 (1500% relative change)
- Pm-144, Pm-145, Pm-146
- Tb-158, Tb-161
- V-49 (20,000% relative change)
- Yb-175

Note: AMPX (polident) uses the widths specified in the ENDF file, whereas NJOY resums. This is still in violation of the ENDF format.

Likely common ground: Files were produced by TALYS

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GENERAL ENDF ISSUES ENCOUNTERED

Negative cross sections at 0 K:

- Fe-57, MT=2
- Cu-65, MT=3

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GENERAL ENDF ISSUES ENCOUNTERED

Incorrect `NVER`:

- Cr-50, Cr-52, Cr-53, Cr-54
- Fe-54. Fe-56 also has bad `NLIB`
- Se-78
- U-235 (also bad `NLIB`)
- Ta-181
- Te-122

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GENERAL ENDF ISSUES ENCOUNTERED

In order to process TSL files with the new mixed-elastic scattering format, AMPX and SCALE need development effort.

- Processing in AMPX is under development and subsequent code review.
- Inclusion in SCALE has required discussion of how to do so – strategy will involve a new (internal to SCALE) MT number, propagating the change into the transport codes.

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TSL FILES: WHICH FILE?

Case: I was running an ICSBEP ZEUS case which contains graphite.

Questions that arose:

- Which of the ENDF/B-VIII.1 graphite files most accurately represents the graphite used in that experiment? Should I simply use the crystalline graphite file? Choose a porosity…?
- Do I have enough information (i.e., from the ICSBEP Handbook) to determine which file most accurately represents the real material?
- Within SCALE, what can we do in the Standard Composition Library to continue making "correct" material specification easy for users?

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TSL FILES: MANY TEMPERATURES…

Some of the TSL files have many temperature points (90).

Is this necessary?

Some of the temperature differences are under 5 K. Note that SCALE codes do not expect a granularity smaller than 5 K for the sake of Doppler broadening.

For the SCALE CE library: We will offer a subset of the temperatures specified in such files.

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TSL FILES: SCALE CE LIBRARY FORMAT

- Size of ENDF/B-VIII.0 CE library: 46 GB
- Size of ENDF/B-VIII.1 CE library: 155 GB

Main contributor: The many Bragg edges in TSL files, which are represented in the SCALE CE library format in lab frame, double differential form.

Proposal within SCALE team: New CE library format that stores Bragg edges as a simple table, then samples "on-the-fly" during transport.

Note: More than a change in CE data format, this imposes a change in the philosophy for SCALE transport codes. Up to now, the philosophy has been to represent reaction data as uniformly as possible (all lab frame, double differential, without needing special treatment for specific reactions)

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THERMAL KERNELS WITH SHARP PEAKS – ENDF/B-VIII.0
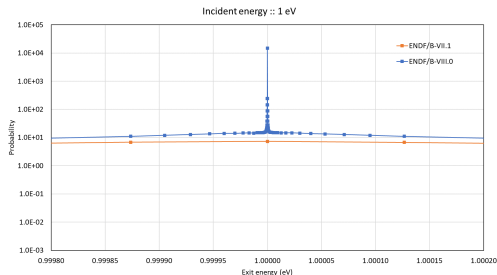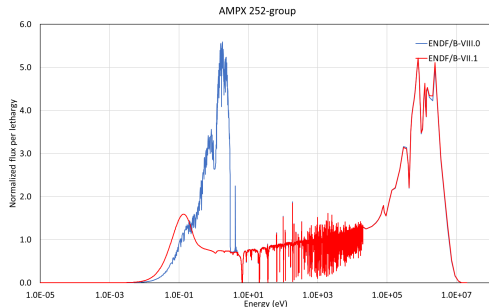
- Using the ENDF/B-VIII.0 library to calculate self-shielding factors for a uranium pincell encountered unexpected PW fluxes.
- A long investigation traced this to the CENTRM handling of interpolation when encountering the sharp peaks in the h_in_h2o thermal kernel! This has been resolved by using an interpolation algorithm similar to corresponding points in CENTRM.

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CONCLUSIONS

- AMPX processing has identified ENDF issues to correct for some files
  - See `git.nndc.bnl.gov` Issue #470
- Guidance for users to use the correct TSL file for a given material will be crucial
- Inclusion of these materials requires commitment from user codes
- Sharp peaks in thermal kernels can lead to surprising effects in user codes

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