OAK RIDGE National Laboratory

# Validating TSLs for ENDF/B-VIII.1

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# Validation Goal

- Given an ENDF file, how do I determine whether it is a faithful representation of the real world?
  - Compare with and determine agreement with measured data
- What is measured data?
  - Neutron-induced reactions and integral quantities based on those reactions

**Purpose of this talk is to determine whether there is *well-defined, publicly available* data to validate TSL files**

# Validation Goal

- TSLs are a bit different compared to other forms of nuclear data
- Inputs for TSLs can also be used as inputs for calculation of other thermophysical properties:
  - Density, specific heat capacity, diffusion coefficient, mean square displacement, etc.
- These properties can't be directly computed from information provided in an ENDF file, so won't be included here

# Validation Hierarchy

- Cross section measurements
  1. Double differential scattering cross section
  2. Total cross section
- Benchmarks
  3. Quasi-integral (e.g., pulsed neutron die away)
  4. Integral (e.g., ICSBEP, IRPhEP, etc.)

# List of ENDF/B-VIII.1 TSL Materials

- Graphite
  - 3 different porosities, 2 different crystalline
- Fuels
  - $UO_2$, UC, UN, & U-metal
    - (6 enrichments each)
  - $PuO_2$
- Liquids
  - $H_2O$, $D_2O$, HF
- Advanced Moderators
  - SiC, FLiBe, $CaH_2$, $Be_2C$, $^{7}$Li{H,D}, BeO, ZrC, $UH_3$
- Metal Hydrides
  - $YH_2$, $ZrH_{1,2,x}$
- Accelerator/Cryogenic Applications
  - {para,ortho}-{H,D}, Mesitylene-Phase 2, Toluene, $Al_2O_3$, Be-metal (2 types), Ice, Mg, Si, $SiO_2$ (2 types)
- Polymers
  - Polyethylene, Lucite, Polystyrene, Teflon, Paraffinic Oil
- Historic
  - $^{27}$Al, $^{56}$Fe, {l,s}-$CH_4$, Benzene

# List of ENDF/B-VIII.1 **New** or *Updated* Materials

- Graphite
  - **20% porous, crystalline+SD**
- Fuels
  - *$UO_2$ (natural), UN (natural)*
  - **$UO_2$, UN (5 new enrichments)**
  - **UC, & U-metal (6 enrichments)**
  - **$PuO_2$**
- Liquids
  - *$H_2O$*, **HF**
- Advanced Moderators
  - **SiC, FLiBe, $CaH_2$, $Be_2C$, $^7$Li{H,D}, BeO, ZrC, $UH_3$**
- Metal Hydrides
  - **$ZrH_2$, $ZrH_x$**
- Accelerator/Cryogenic Applications
  - *{para,ortho}-{H,D}*, **Mesitylene-Phase 2, Toluene, $Al_2O_3$**, *Be-metal*, **Be-metal+SD**, **Mg, Si**, *$SiO_2$ alpha*
- Polymers
  - *Polyethylene, Lucite*, **Polystyrene, Teflon, Paraffinic Oil**
- Historic
  - N/A

# List of Materials

- A total of **70** materials* across 112 different ENDF files
  - Including **57** new or updated materials across 97 different ENDF files for ENDF/B-VIII.1

- How many of these 57 new or updated materials can we validate?

# Least challenging to validate

- Multiple benchmarks and cross section measurements
  - Light water, polyethylene, Lucite, polystyrene, graphite
  - Be-metal, BeO, paraffinic oil, Teflon, $SiO_2$
  - $ZrH_2$, $ZrH_x$
  - $UO_2$ & U-metal (kind of)

# Slightly challenging to validate

- Cross section measurements, but no integral benchmarks (or benchmarks are poorly defined)
  - $Al_2O_3$, $CaH_2$
  - UC, UN (kind of)
  - Mesitylene – Phase II, Toluene, Si, Mg, {para,ortho}-{H,D}

- Integral benchmarks, but no cross section measurements
  - HF, $UH_3$
  - $PuO_2$ (kind of)

# Impossible to Validate

- No cross section measurements or well-defined public benchmarks
  - FLiBe
  - $^{7}$LiD, $^{7}$LiH
  - $Be_2C$
  - SiC
  - ZrC

# Fuel TSLs – A Quandary

- Fuel TSLs pose a unique problem:
  - Which to use in the thermal energy range: TSL or resonances?
  - Does choosing one over the other have any unintended side effects (e.g., lack of resonance interference) that are not physical?
- Additionally, uranium fuels have multiple enrichments
  - Natural (0.72%), 5%, 10%, HALEU (19.75%) HEU (93%), 100%
  - Magnitude of the cross section will be different, but will the inelastic spectra be noticeably different?
    - If not, is this the best way to represent this data?
- Underlying theory needs to be carefully scrutinized

# Path Forward

- Of the 57 new or updated TSL files:
  - 14 are easy to validate
  - 12 are either lacking cross section or benchmarks
  - 6 have **neither** cross section nor benchmarks
  - 25 are fuel materials that require thorough investigation

- What can be done?
  - Provide DFT/MD input files for extra validation of material properties?
  - Require corresponding measurement (benchmark or cross section) for all materials?
  - Look towards other ENDF sub-library standards for validation?

# Conclusions

| | Cross Section Measurement | No Cross Section Measurement |
|---|---|---|
| **Benchmark** | UO2 & U-metal | $PuO_2$ |
| | Light water, $ZrH_2$, $ZrH_x$, graphite, BeO, polyethylene | |
| | Lucite, polystyrene, Be-metal, paraffinic oil, Teflon, $SiO_2$ | HF, $UH_3$ |
| **No Benchmark** | UC, UN | |
| | $CaH_2$ | FLiBe, $Be_2C$, SiC, ZrC |
| | Mesitylene – Phase II, Toluene, Si, Mg, {para,ortho}-{H,D}, $Al_2O_3$ | $^7LiD$, $^7LiH$ |

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# Questions?