See PowerPoint *notes* for discussion of content

# Where will we go in ENDF/B-IX – Thermal Neuron Scattering

**Michael L. Zerkle (NNL)**

Ayman I. Hawari (NCSU)

Mini-CSEWG Meeting, August 13-15, 2024
Los Alamos National Laboratory

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# Guided Discussion Topics

- New/revised TSL evaluations
- Areas ripe for targeted strategic investment to prepare for ENDF/B-IX
  - TSL Validation
  - Relaxing of physics approximations
  - Alternate enrichment treatment for fuel compounds
  - TSL Covariance Data
  - Machine Learned TSL Kernels

# New/Revised TSL Evaluations from NCSU (NCSP Appendix B)

- Polyethylene ($(C_2H_4)_n$)
  - Additional temperatures to support TEX-low temp
  - Transportation analyses
- Uranium silicide ($U_3Si_2$)
- Paraffin (Wax)
- Light Paraffinic Oil (Mineral Oil)
- HEU/HALEU fuel materials
  - $U_3O_8$
  - U-Mo
- Fissile Solutions
  - Uranyl Fluoride ($UO_2F_2$)
  - Uranyl Nitrate ($UO_2(NO_3)_2$)
  - Plutonium Nitrate ($Pu(NO_3)_4$)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Light Paraffinic Oil (Mineral Oil) | NCSU | NCSU | NCSU | | | | |
| Basis | TSL evaluation. Mineral oil and other light paraffinic oils are moderators often found in fissile handling areas (FHAs). A thermal scattering law for light paraffinic oils would reduce excessing margins in nuclear criticality safety evaluations for fissile handling areas containing this class of moderator. TSL requested by NNL. | | | | | | |
| Triuranium Octoxide ($U_3O_8$) | | NCSU | NCSU | NCSU | | | |
| Basis | TSL evaluation. A common fissile compound for which there are numerous critical experiments in the ICSBEP Handbook. A thermal scattering law for $U_3O_8$ will improve Doppler broadening using advanced methods currently under development as LLNL ND12. | | | | | | |
| U-Mo | | | NCSU | NCSU | NCSU | | |
| Basis | TSL evaluation. HALEU U-Mo is one of the fuel systems being developed for use in research and test reactors. A thermal scattering law for the HALEU U-Mo fuel system will improve simulations through higher fidelity and reduced uncertainty. Supports design studies related to the conversion of high-performance research and test reactors from HEU to HALEU, fuel cycle facilities producing this fuel system, and transportation analyses. | | | | | | |
| Uranyl Fluoride ($UO_2F_2$) | | | NCSU | NCSU | NCSU | | |
| Basis | TSL evaluation. A common fissile compound for which there are numerous critical experiments in the ICSBEP Handbook. A thermal scattering law for $UO_2F_2$ solutions will improve modeling and simulation of fissile solution systems. | | | | | | |
| Uranyl Nitrate ($UO_2(NO_3)_2$) | | | | NCSU | NCSU | NCSU | |
| Basis | TSL evaluation. A common fissile compound for which there are numerous critical experiments in the ICSBEP Handbook. A thermal scattering law for $UO_2(NO_3)_2$ will improve modeling and simulation of fissile solution systems. | | | | | | |
| Plutonium Nitrate ($Pu(NO_3)_4$) | | | | | NCSU | NCSU | NCSU |
| Basis | TSL evaluation. A common fissile compound for which there are numerous critical experiments in the ICSBEP Handbook. A thermal scattering law $Pu(NO_3)_4$ will improve modeling and simulation of fissile solution systems. | | | | | | |

# TSL Validation

- Subthermal neutron transmission measurements
- Add capability to heat/cool samples
- PNDA measurements
  - Add capability to heat/cool samples
  - Develop pre-moderated capability for non-hydrogenous moderators
- More critical experiments
  - TEX series of experiments useful framework
- New benchmarks from startups

# Relaxing Physics Approximations

- Accounting for effect of thermal expansion on coherent elastic scattering
  - Could be useful for some advanced high temperature reactor applications
  - Currently assume Bragg edge energies are temperature independent
  - One of last remaining TSL physics approximations in ENDF-6 format
    - Supported in GNDS
  - Bragg edge energies become temperature dependent in MF7/MT2
  - Will need to develop implementation guidance for evaluators, nuclear data processing codes, and application codes
    - Temperature dependent interpolation
    - Logically rectangular data structure for Sd factors
- Ripe for targeted strategic programmatic investment

# Alt. Enrichment Representation for Fuel Compounds

- Current treatment NCSU uses for enrichment in fuel compounds is rigorous
  - Enrichment effects on scattering are real
  - Fission dominates
- May be useful to explore approximations that could be easier to implement in reactor depletion calculations
  - Different partitioning of isotopic contributions
  - Assess impact of approximation
- Options for alternate organization of TSL information for enriched fuel compounds
  - C(UC)
  - $^{234}$U(UC)
  - $^{235}$U(UC)
  - $^{236}$U(UC)
  - $^{238}$U(UC)

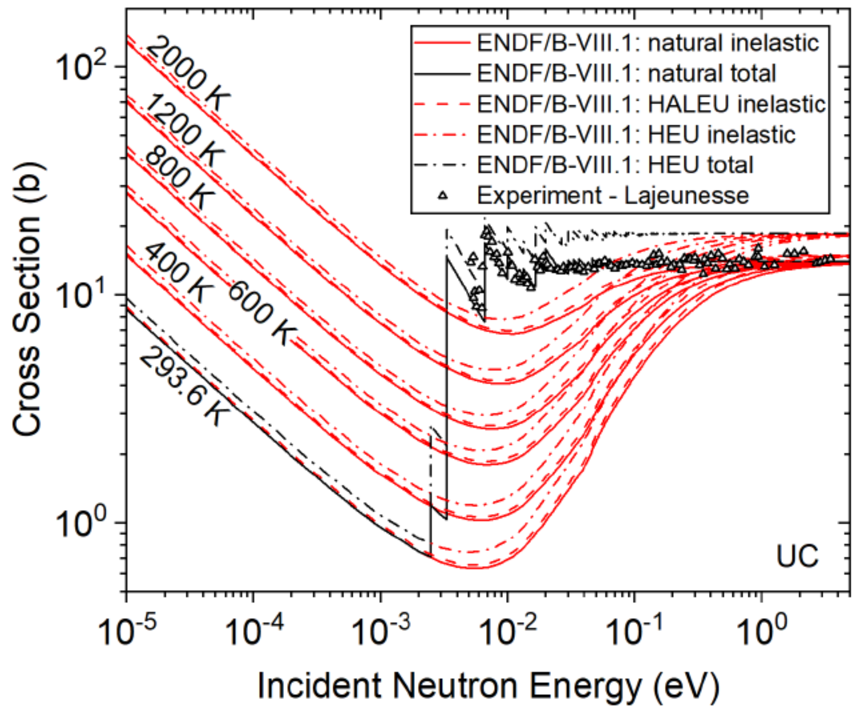


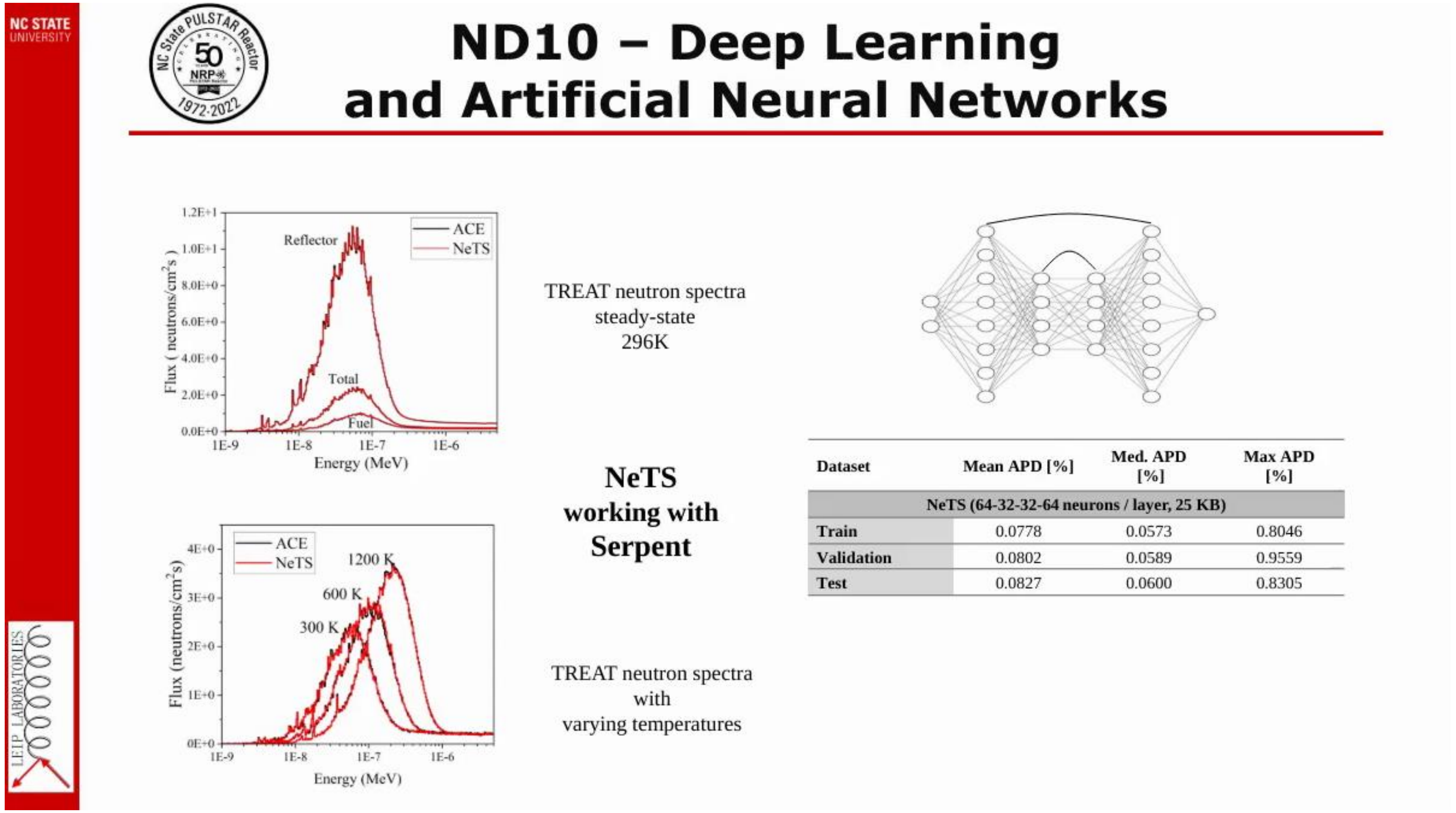

FIG. 15. (Color online) The inelastic scattering cross section of UC shown at selected temperatures and enrichments. The natural total scattering cross sections of UC at 293.6 K and measurement [40] are also shown.

# TSL Covariance Data

- While some work has been done on covariance data evaluation frameworks
  - Holmes for AILD
  - Chapman for MD
- Additional R&D needs to be done to complete development needed to deliver production quality covariance data
  - Complete development of evaluation methodology
  - Evaluator/User guidance
  - Format
  - Implementation in TSL evaluation codes
- Focused community effort will be needed to prepare for ENDF/B-IX

# Machine Learned TSL Kernels

- Recent R&D has shown potential
  - Smaller memory footprint
  - Higher temperature fidelity
  - Well suited for reactor engineering and Multiphysics simulations
- Potential disruptive technology
- Different format/data structure
  - Neural network
  - GNDS can likely be adapted to accommodate
- Not clear if should be included in ENDF or code system implementation
  - On-the-fly analysis may require code system implementation




| Dataset | Mean APD [%] | Med. APD [%] | Max APD [%] |
|---|---|---|---|
| NeTS (64-32-32-64 neurons / layer, 25 KB) | | | |
| Train | 0.0778 | 0.0573 | 0.8046 |
| Validation | 0.0802 | 0.0589 | 0.9559 |
| Test | 0.0827 | 0.0600 | 0.8305 |

# Other Areas for Strategic Investment

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