ORNL Nuclear Data Evaluation Accomplishments for FY2013

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Nuclear Data & Criticality Safety Group

NCSP Technical Program Review
Los Alamos National Laboratory
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Outline

• ORNL nuclear data evaluation work to address NCS nuclear data needs
• Data analysis and evaluation effort with SAMMY
• ORNL collaboration efforts with IRSN and CEA/Cadarache
• Collaborative International Evaluated Library Organization (CIELO) Project
• Summary of Evaluation Accomplishments
<table>
<thead>
<tr>
<th>Isotope</th>
<th>Energy Range</th>
<th>Resonance Covariance Evaluation</th>
<th>Target date to deliver the evaluation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{63,65}\text{Cu}$</td>
<td>Thermal to 300 keV</td>
<td>Yes</td>
<td>Completed</td>
</tr>
<tr>
<td>$^{182}\text{W}$</td>
<td>Thermal to 10 keV</td>
<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>$^{183}\text{W}$</td>
<td>Thermal to 5 keV</td>
<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>$^{184}\text{W}$</td>
<td>Thermal to 10 keV</td>
<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>$^{186}\text{W}$</td>
<td>Thermal to 10 keV</td>
<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>$^{56}\text{Fe}$</td>
<td>Thermal to 2 MeV</td>
<td>Yes</td>
<td>FY2014—new angular data &amp; testing may delay to FY15 CIELO</td>
</tr>
<tr>
<td>$^{239}\text{Pu}$</td>
<td>Thermal to 2.5 keV</td>
<td>Use ENDF/B-VII.1 (FILE33)</td>
<td>Completed</td>
</tr>
<tr>
<td>$^{235}\text{U}$</td>
<td>Thermal to 2.25 keV</td>
<td>Use ENDF/B-VII.1 (FILE33)</td>
<td>FY2014 CIELO</td>
</tr>
<tr>
<td>Element</td>
<td>Energy Range</td>
<td>Resonance Covariance Evaluation</td>
<td>Target date for delivery the evaluation</td>
</tr>
<tr>
<td>---------</td>
<td>--------------</td>
<td>---------------------------------</td>
<td>----------------------------------------</td>
</tr>
</tbody>
</table>
| Ca      | $^{40}$Ca (96.95 %)  
$^{44}$Ca (2.086 %) | Yes | FY2015 |
| Ce      | $^{140}$Ce (88.450 %)  
$^{142}$Ce (11.114 %) | Yes | FY2015 |
| Dy      | $^{161}$Dy (18.889 %)  
$^{162}$Dy (25.475 %)  
$^{163}$Dy (24.896 %)  
$^{164}$Dy (28.260 %) | Yes | FY2015 |
| Gd      | $^{155}$Gd (14.80 %)  
$^{156}$Gd (20.47 %)  
$^{157}$Gd (15.65 %)  
$^{158}$Gd (24.84 %)  
$^{160}$Gd (21.86 %) | Yes | FY2015 |
| CH$_2$ | Thermal Scattering $S(\alpha,\beta)$ | - | FY2015 |
Copper Evaluation (Vladimir Sobes Ph.D. Thesis – completed September 2013)

• Vladimir Ph.D. thesis work for the NCSP
  – Performed thermal $^{63,65}$Cu cross-section measurements at MITR
  – Completed $^{63,65}$Cu resonance evaluations (with covariance data) through analysis of measured data from ORELA, GELINA (IRMM) and MITR
  – Development of analysis capability that couples TSUNAMI sensitivity/uncertainty tool with SAMMY resonance analysis tool – couples integral with differential data analysis

• Transmission and capture data:
  – ORELA: 32 eV – 185 keV
  – ORELA: 1 keV – 1.4 MeV
  – MITR: 0.01 eV – 0.1 eV
  – GELINA: Capture Cross-section 1 keV – 200 keV
SAMMY fit at low energy (MIT data)
Resolved Resonance Region for $^{63}\text{Cu}$
Resolved Resonance Region for $^{65}$Cu
## Tungsten Resolved Resonance

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Energy Range (old)</th>
<th>Energy Range (new)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{182}\text{W}$</td>
<td>$10^{-5} \text{ eV} – 5 \text{ keV}$</td>
<td>$10^{-5} \text{ eV} – 10 \text{ keV}$</td>
</tr>
<tr>
<td>$^{183}\text{W}$</td>
<td>$10^{-5} \text{ eV} – 2.2 \text{ keV}$</td>
<td>$10^{-5} \text{ eV} – 5 \text{ keV}$</td>
</tr>
<tr>
<td>$^{184}\text{W}$</td>
<td>$10^{-5} \text{ eV} – 4 \text{ keV}$</td>
<td>$10^{-5} \text{ eV} – 10 \text{ keV}$</td>
</tr>
<tr>
<td>$^{186}\text{W}$</td>
<td>$10^{-5} \text{ eV} – 8 \text{ keV}$</td>
<td>$10^{-5} \text{ eV} – 10 \text{ keV}$</td>
</tr>
</tbody>
</table>
SAMMY fit of W-182 transmission and capture (GELINA)
SAMMY fit of W-183 transmission and capture (GELINA)
SAMMY fit of W-184 transmission and capture (GELINA)
SAMMY fit of W-186 transmission and capture (GELINA)
56Fe Resonance Evaluation up to 2.0 MeV

• Motivation for evaluating 56Fe in the resolved resonance Region

• Evaluation description

• Use RML option of the SAMMY code (R-matrix Limited Format)

• Experimental Data

• Preliminary results
Motivation for evaluating $^{56}$Fe in the Resolved Resonance Region

• New high resolution transmission measurements done at the RPI extending the resonance region up to 5 MeV (Yaron Danon)

• New inelastic cross-section measurements done at IRMM (Arjan Plompen)

• Use the SAMMY/RML feature to include inelastic channel in the R-matrix analysis

• Improve the results of benchmark systems calculations
Evaluation Features

• Extend the resolved resonance region from 850 keV to 2.0 MeV

• Include new transmission measurements and inelastic cross section data

• Use the extended R-matrix formalism in the SAMMY code for fitting the experimental data

• Compare the cross section processed with SAMMY, NJOY, AMPX and PREPRO using the evaluated iron resonance parameters
## Experimental Data for the $n^{+56}$Fe Interaction

<table>
<thead>
<tr>
<th>Reference</th>
<th>Energy Range</th>
<th>Facility</th>
<th>TOF (meters)</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harvey (1987)</td>
<td>20 keV – 2 MeV</td>
<td>ORELA</td>
<td>201.575</td>
<td>Transmission</td>
</tr>
<tr>
<td>Perey (1990)</td>
<td>120 keV – 850 keV</td>
<td>ORELA</td>
<td>201.575</td>
<td>Transmission</td>
</tr>
<tr>
<td>Danon (2012) (three thicknesses)</td>
<td>500 keV – 2 MeV</td>
<td>RPI</td>
<td>249.740</td>
<td>Transmission</td>
</tr>
<tr>
<td>Perey (1990)</td>
<td>850 keV – 1.5 MeV</td>
<td>ORELA</td>
<td>201.575</td>
<td>Inelastic</td>
</tr>
<tr>
<td>Plompen (2011)</td>
<td>850 keV – 2 MeV</td>
<td>GELINA</td>
<td>198.686</td>
<td>Inelastic</td>
</tr>
<tr>
<td>Spencer (1994) (two thicknesses)</td>
<td>10 eV – 650 KeV</td>
<td>ORELA</td>
<td>40.0</td>
<td>Capture</td>
</tr>
<tr>
<td>Perey (1990)</td>
<td>850 keV – 1.5 MeV</td>
<td>ORELA</td>
<td>200.191</td>
<td>elastic</td>
</tr>
<tr>
<td>Cabé (1967)</td>
<td>500 keV – 1.2 MeV</td>
<td>Université de Louvain (Van de Graaff)</td>
<td>~ 1</td>
<td>elastic</td>
</tr>
<tr>
<td>O.A.Shcherbakov (1977)</td>
<td>0.001 eV – 10 eV</td>
<td>TOF/Russia</td>
<td>9.5</td>
<td>Total</td>
</tr>
<tr>
<td>O.A.Shcherbakov (1977)</td>
<td>0.001 eV – 10 eV</td>
<td>TOF/Russia</td>
<td>9.5</td>
<td>Capture</td>
</tr>
</tbody>
</table>
Comparison of SAMMY Fits for Total and Inelastic $^{56}$Fe data.
Comparison of SAMMY Fits to Perey Differential Elastic $^{56}$Fe data
Comparison of SAMMY Fit of $^{56}$Fe differential elastic data of Cabé.
Comparison of SAMMY Predictions of $^{56}$Fe differential inelastic with ENDF
Issues with Fe-56 capture cross-section data identified through collaboration working visit at IRSN
Fe-56 Benchmark Calculations Performed at IRSN

Case: 70 cm
$^{239}$Pu Resonance Evaluation—Task Completed

- $^{239}$Pu evaluation details presented at previous NCSP TPR
- Resonance parameters evaluation done with SAMMY
- Work performed in collaboration with CEA/Cadarache and as part of WPEC Subgroup 34
- Evaluation testing collaboration with Skip Kahler (LANL)
- Final data library submitted to BNL
- Library being tested for further improvements—will likely require updates to fission spectrum and $^{240}$Pu to improve results further for thermal solution systems

![ICSBEP Pu benchmarks](image)
235U Evaluation

• Working Party on International Nuclear Data Evaluation Co-operation (WPEC) subgroup 29 (SG 29)

• Problem Description: 235U data issue in the energy range 0.1 to 2.25 keV

• Issues and Resolutions

• Method of Evaluation: SAMMY code

• ZEUS Benchmark Results

• Conclusions
WPEC subgroup 29: “Uranium-235 Capture Cross-section in the keV to MeV Energy Region”

Mission:

• Investigate C/E discrepancies in uranium-core integral parameters observed with all major evaluated libraries (ENDF, JENDL, JEFF)

• Perform sensitivity analyses of integral parameters with respect to differential data

• Review the $^{235}$U capture cross-section to determine recommended values in the energy region from 100 eV to 1 MeV

• Perform Benchmark calculations for the FCA-IX-1, -2 and -3 cores and the ZEUS-1, -2, -3, and -4
235U Issues and Resolutions:

Issues:

Overestimation of 235U capture cross-section in the resonance region range (0.1 to 2.5 keV).

Recommend:

1. New measurements of capture and fission cross-section in the keV region
2. Perform new resonance analysis in the 0.1 to 2.5 keV region
3. Investigate the reason for the overestimation of criticalities for some benchmarks
235U Issues and Resolutions:

Resolution:

- New data measurements from RPI (capture and fission yields) (kind of alpha measurements)
- New capture data from LANL
- Use SAMMY code for fitting the new data
- Test the new evaluation in benchmark calculations:
  - ZEUS benchmarks (FCA not available)
- Use JENDL4 as the template
- Benchmark Calculations done with MCNP with everything else from ENDF/B-VII.0
RPI capture data and ENDF evaluation (SG29 prediction confirmed)
ORNL, RPI and LANL Capture Data

- ORELA (Perey): 39.70 m, 20 ns
- RPI: 25.56 m, 15 ns
- LANL: 25.45 m, 125 ns
RPI and LANL Capture Data

Capture Yield

Energy (eV)

σγ (b)

25.56 m
15 ns

25.45 m
125 ns
<table>
<thead>
<tr>
<th>Author</th>
<th>Energy (eV)</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>De Saussure (RPI/1967)</td>
<td>0.01 - 2250.0</td>
<td>Fission and Capture at 25.2 meters</td>
</tr>
<tr>
<td>Perez (ORNL/1972)</td>
<td>0.01 - 200.0</td>
<td>Fission and Capture at 39.7 meters</td>
</tr>
<tr>
<td>Weston (ORNL/1984)</td>
<td>14.0 - 2250.0</td>
<td>Fission at 18.9 meters</td>
</tr>
<tr>
<td>Gwin (ORNL/1984)</td>
<td>0.01 - 20.0</td>
<td>Fission at 25.6 meters</td>
</tr>
<tr>
<td>Spencer (ORNL/1984)</td>
<td>0.01 - 1.0</td>
<td>Transmission at 18 meters and sample thickness of 0.001468 atom/barn</td>
</tr>
<tr>
<td>Harvey (ORNL/1986)</td>
<td>0.4 - 68.0</td>
<td>Transmission at 18 meters and sample thickness of 0.03269 atom/barn</td>
</tr>
</tbody>
</table>
### Selected Measurements

<table>
<thead>
<tr>
<th>Author</th>
<th>Energy (eV)</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harvey (ORNL/1986)</td>
<td>4.0 - 2250.0</td>
<td>Transmission at 80 meters and sample thickness of 0.00233 atom/barn cooled to 77 K</td>
</tr>
<tr>
<td>Harvey (ORNL/1986)</td>
<td>4.0 - 2250.0</td>
<td>Transmission at 80 meters and sample thickness of 0.03269 atom/barn cooled to 77 K</td>
</tr>
<tr>
<td>Wartena (Geel/1987)</td>
<td>0.0018 - 1.0</td>
<td>Eta at 8 meters</td>
</tr>
<tr>
<td>Wagemans (Geel/1988)</td>
<td>0.001 – 0.4</td>
<td>Fission at 18 meters</td>
</tr>
<tr>
<td>Schrack (RPI/1988)</td>
<td>0.02 - 20.0</td>
<td>Fission at 8.4 meters</td>
</tr>
<tr>
<td>Weigman (ILL/1990)</td>
<td>0.0015 – 0.15</td>
<td>Eta (Chopper)</td>
</tr>
</tbody>
</table>
## Selected Measurements

<table>
<thead>
<tr>
<th>Author</th>
<th>Energy (eV)</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weston (ORNL/1992)</td>
<td>100.0 - 2000.0</td>
<td>Fission at 86.5 meters</td>
</tr>
<tr>
<td>Moxon (ORNL/1992)</td>
<td>0.01 - 50.0</td>
<td>Fission Yield</td>
</tr>
<tr>
<td>Gwin (ORNL/1996)</td>
<td>0.01 - 4.0</td>
<td>Absorption and fission at 21.68 meters</td>
</tr>
<tr>
<td>Danon (RPI/2012)</td>
<td>100.0 – 5000</td>
<td>Fission and capture yield at 25.56 meters (burst 15 ns)</td>
</tr>
<tr>
<td>Jandel (LANL/2012)</td>
<td>100.0 - 5000</td>
<td>Capture at 25.45 meters (burst 125 ns)</td>
</tr>
</tbody>
</table>
Fit of the RPI Capture Data

![Graph showing fit of RPI Capture Data](image-url)
Fit of the RPI Fission data
Intermediate Energy Benchmark:
Designed to test the $^{235}\text{U}$ cross sections in the intermediate energy range.

ISCEB description:
- heu-met-inter-006-1 (ZEUS1)
- heu-met-inter-006-2 (ZEUS2)
- heu-met-inter-006-3 (ZEUS3)
- heu-met-inter-006-4 (ZEUS4)
### The HEU-MET-INTER-006 cases (ZEUS)

<table>
<thead>
<tr>
<th>Case Number</th>
<th>k(_{\text{eff}})</th>
<th>EALF (keV)</th>
<th>Intermediate-Energy Fission Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (ZEUS1)</td>
<td>0.9977 ± 0.0008</td>
<td>4.44</td>
<td>0.730</td>
</tr>
<tr>
<td>2 (ZEUS2)</td>
<td>1.0001 ± 0.0008</td>
<td>9.45</td>
<td>0.698</td>
</tr>
<tr>
<td>3 (ZEUS3)</td>
<td>1.0015 ± 0.0008</td>
<td>22.80</td>
<td>0.636</td>
</tr>
<tr>
<td>4 (ZEUS4)</td>
<td>1.0016 ± 0.0008</td>
<td>80.80</td>
<td>0.503</td>
</tr>
</tbody>
</table>

EALF: Energy Average Lethargy Causing Fission
# The HEU-MET-INTER-006 cases (ZEUS)

<table>
<thead>
<tr>
<th>Case Number</th>
<th>Benchmark $k_{\text{eff}}$</th>
<th>Calculated $k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>ENDF/B-VII.0</td>
</tr>
<tr>
<td>1 (ZEUS1)</td>
<td>0.9977 ± 0.0008</td>
<td>0.9977 ± 0.0008</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.99304 ± 0.00035</td>
</tr>
<tr>
<td>2 (ZEUS2)</td>
<td>1.0001 ± 0.0008</td>
<td>1.0001 ± 0.0008</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.99603 ± 0.00035</td>
</tr>
<tr>
<td>3 (ZEUS3)</td>
<td>1.0015 ± 0.0008</td>
<td>1.0015 ± 0.0008</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.00065 ± 0.00035</td>
</tr>
<tr>
<td>4 (ZEUS4)</td>
<td>1.0016 ± 0.0008</td>
<td>1.0016 ± 0.0008</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.00750 ± 0.00031</td>
</tr>
</tbody>
</table>
The HEU-MET-INTER-006 cases (ZEUS)

- 4.45 keV
- 9.45 keV
- 22.8 keV
- 80.8 keV

**Graph Details:**
- **Y-axis:** C/E
- **X-axis:** Benchmark (ZEUS-1, ZEUS-2, ZEUS-3, ZEUS-4)
- **Data Points:**
  - ENDF/B-VII.0
  - JENDL 4.0
  - ORNL/RPI

**Energy Levels:**
- EALF
- 4.45 keV
- 9.45 keV
- 22.8 keV
- 80.8 keV
Summary of Evaluation Accomplishments

• ORNL resonance evaluations on schedule per the NCSP Five Year Plan

• $^{63,65}\text{Cu}$ evaluations completed and delivered to NNDC—Vladimir Sobes completed Ph.D. dissertation

• Completed measurement and resonance analysis work for 4 tungsten isotopes ($^{182,183,184,186}\text{W}$)—finalization of evaluations in progress and on schedule to submit to NNDC in FY14

• Completed novel work on $^{56}\text{Fe}$ resonance evaluation to produce angular distributions from resonance parameters
  – Initiated work with processing code developers to add new processing capabilities to provide detailed angular distributions
  – Benchmark testing with LANL and IRSN in progress—providing much needed feedback to finalize and improve the evaluation

• $^{239}\text{Pu}$ resonance evaluation completed and submitted to NNDC

• Completed preliminary $^{235}\text{U}$ evaluation
  – Includes new measured data from RPI and LANSCE in the low keV region
  – Testing in progress to finalize the evaluation for submittal in FY14