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LLNL Evaluations for ENDF/B-VII.1

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CSEWG Actions

- 257: Zn
  - BROND elemental Zn-0 evaluation replaced with JENDL-4 isotopic evaluations Zn-64,65,66,67,68,70
- 258: $^{74,75}$As
  - $^{73-75}$As will resubmit LLNL evaluations
- 267: W-isotopes: finalize these evaluations, and merge EGAF data if possible
  - Aaron Hurst (moved from LLNL to LBL) still working on level scheme evaluations (see Aaron Hurst talk in USNDP Wed morning)
262: $^{123,124}$Xe submitted (open)

- LLNL evaluations were used in ENDF/B-VII.1beta0
- $^{123}$Xe (unstable): resonances missing – will add and resubmit
- $^{124}$Xe: is new LLNL improvement over ENDF/B-VII.0?
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269: $^{185,187}$Re submitted

- LLNL Re evaluations used in ENDF/B-VII.1beta0, but Tracker comments say not using it
- LLNL currently performing testing on these evaluations and will present results at next CSEWG
New LLNL evaluations for Ta-181 and T-180 submitted (too late for ENDF/B-VII.1beta0)
- Pulse sphere testing shows improvement over ENDF/B-VII.0
- Activation foil tests of \((n,\gamma)\) agree w/ exp.
Agenda

- Won’t discuss planned activities that we still want to carry out:
  - Add MT458 data to all minor actinides
  - Update minor actinides from JENDL/AC with those from JENDL-4 to get JAEA covariance data
- Outstanding CSEWG Action Items
- Proposed new 239-Pu PFNS and nubar evaluation
CSEWG Action Items

- **231-Pa:** Please check whether overwriting the IAEA file with the JENDL Actinoid evaluation was justified. Note the sibling IAEA evaluation is retained for 233Pa.
  - BNL Reverted to the VII.0 Version: Capote noted we should be sure we prefer the fission in JENDL cf his 231 fission- he thinks there are good arguments why 231 in his file (in VII.0) is more reliable.

- **6-Li:** D. Brown reformat these data into more standard format
  - Need ENDF file to begin work. *Has it been posted?*

- **Cm:** review KAERI's new Cm isotope evaluations
  - KAERI made new evaluations of Cm isotopes using EMPIRE calculations. The covariance data are given.
  - As of ND2010, files were not ready for review. *Are they now?*

- **240-Am:** see next slides

- **239-U:** see next slides
240-Am from LLNL adopted 11/2009, but there were problems...

- Issues:
  - Replace resonances in LLNL evaluation with JENDL/AC
  - Angular distributions missing for fission neutrons
- Solution: Take JENDL-4 evaluation
  - Clearly has resonances from JENDL/AC
  - Has missing distributions
  - Matches \((n,f)\) surrogate reaction “data”
  - Even has covariance data

JENDL-4 240Am evaluation committed to ENDF/B-VII svn trunk
Burke et al. performed surrogate measurement of $^{239}$U(n,f), so we re-evaluated $^{239}$U, folding in Younes & Britt (n,f) evaluation.

Fit folds in uncertainties from three classes of surrogate measurements: (t, pf), ($^3$He, xf) and ($^{18}$O, $^{17}$O).
The original $^{239}\text{U}$ resonances required several fixes since they were a copy of the $^{237}\text{U}$ resonances

- RRR was “picket fence”
- URR average parameters matched to “picket fence”
- $J^\Pi$ set to $^{237}\text{U}$ values g.s. of $^{237}\text{U}$ is $\frac{1}{2}^+$
- Changing to $^{239}\text{U}$ $J^\Pi$ made things worse (g.s. of $^{239}\text{U}$ is $5/2^+$)
- Matching onto high energy (n,f) looks scary

Use URR for all resonances, match averages to high energy cross-sections and thermal $\sigma$ values from Mughabghab

<table>
<thead>
<tr>
<th>Channel</th>
<th>Therm. $\sigma$ (barns)</th>
<th>Therm. $\sigma$ (barns) Mughabghab</th>
<th>Res. Int. (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n,el)</td>
<td>21.32</td>
<td>199.9</td>
<td></td>
</tr>
<tr>
<td>(n,γ)</td>
<td>22.16</td>
<td>22 ± 5</td>
<td>50.5</td>
</tr>
<tr>
<td>(n,f)</td>
<td>13.97</td>
<td>14 ± 3</td>
<td>19.0</td>
</tr>
</tbody>
</table>
As Andrej Trkov points out in this comment, this scheme has practical problems

- What is the meaning of "average resonance parameters" at thermal energies (down to 1e-5 eV!) and how would one interpret the "average self-shielded" cross sections at these energies?

- Processing:
  - The Pre-Pro codes swallow the file and produce cross sections, but NJOY does not. It does not crash (not on Windows with Lahey compiler, anyway), but the total and elastic cross-sections are set to 1e-8 barns over the entire resonance region.

- ENDF/B-VII.0
  - The main problem with the resonance part of ENDF/B-VII.0 was the coarse energy mesh and lin-lin interpolation in the pointwise background in MF3.

- Solution: None at present! A resonance specialist should look at the problem and propose something reasonable.
To re-evaluate 239Pu PFNS, we require the improved fission modeling in FREYA

- PFNS data not good enough
  - PFNS for thermal neutrons (right) inconsistent with each other and have large uncertainties
  - Published data at higher energies limited, poor statistics
  - Spectral data do not extend to low energy
  - More differential measurements of other quantities e.g. total fragment kinetic energy (TKE) and neutron multiplicity per fragment only exist for low incident energies

- Note, FREYA produces:
  \[
  \frac{d\tilde{\nu}(E)}{dE'} = \tilde{\nu}(E)P(E|E')
  \]
  - So, we get PFNS for free by fitting nubar

Can’t fit PFNS data, but have shown fit to nubar is good enough
World’s collection of 239Pu nubar was evaluated for ENDF/B-VII.0
Talou (LANL).
This may(?) end up in the ENDF/B-VII.1 evaluation

**nubar uncertainty**

"Spikes" caused by regions of missing data => 100% uncertainty

**nubar covariance**

Some (but not many) off-diagonal elements
Fit introduction

- Did Monte-Carlo sampling to fit nubar data using PSUADE, optimize chi2:

\[ \chi^2 = \left( \bar{\nu}_{exp}(E) - \bar{\nu}_{fit}(E) \right)^T \cdot \left( \Delta^2 \bar{\nu}_{exp} \right)^{-1} \cdot \left( \bar{\nu}_{exp}(E) - \bar{\nu}_{fit}(E) \right) \]

- Varied following:
  - alevel: level density parameter in decaying fragments
  - xexcit: balance between excitation of heavy & light fragment
  - dTKE: energy dependent shift in total kinetic energy from thermal data

- Did 3.5 fits:
  - Using uncertainty alone, energy dependent xexcit, alevel, dTKE
  - Using full nubar covariance, const xexcit, alevel, energy dependent dTKE
  - Using full nubar covariance, same as previous, but biasing xexcit & alevel
  - (Also experimented with full energy dependent xexcit, alevel, dTKE using full covariance, but will never sample parameter space well enough to work)
Best fit parameters

Energy-independent parameters:

\[ e_0 = 8.542 \pm 0.5449 \text{ MeV}^{-1} \]
\[ \chi = 1.139 \pm 0.0616 \]
We match nubar by eye, to see differences, must look deeper
Fit residual of nubar: here only uncertainties can be shown
New PFNS & nubar perform at least as good as ENDF/BVII.0 in critical assemblies and outperforms it at 14 MeV

- Using best-fit values, generated modifications to ENDF/B-VII.0 239Pu evaluation with new PFNS and our revised, best fit, nubar
- Tested in various Pu-rich critical assemblies and in LLNL Pulsed Sphere

To do: generate ENDF files with new data & covariances

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But corners were cut..

4. $n+^{239}$Pu prompt fission neutron multiplicity

In the incident neutron energy range $10^{-5}$ eV-1.0 keV, the evaluation is taken directly from ENDF/B-VI.8 without change. The ENDF/B-VI.8 evaluation in this energy range is based on an evaluation by Fort et al. [235], after a small renormalization for consistency with the CSEWG thermal nubar value from the ENDF/B-VI standards analysis.

In the energy region 1 keV-20 MeV, minor modifications were made to the ENDF/B-VI.8 evaluation to improve agreement with the results of the covariance analysis of experimental data that was used for that evaluation and with integral experimental results. Also, the ENDF/B-VI.8 data were adjusted above 6-8 MeV for consistency with the ENDF/B-VII standard $^{252}$Cf nubar value.

The results of our evaluation are compared to experimental data and to other evaluation between $E_n$ 0.001-2.0 MeV in Fig. 99. A similar comparison is given for neutron energies between 2 and 18 MeV in Fig. 100. The experimental data in Figs. 99 and 100 are from the measurements of Frehaut et al. [224], Gwin et al. [113], Zhang et al. [236], Hopkins and Diven [237], Conde et al. [238], and Savin et al. [239].

We attempted to follow the covariance data as well as possible but mainly to stay within uncertainties in the data and at the same time to keep good agreement with fast critical benchmarks. In order to get good agreement with the JEZEBEL fast critical assembly, however, the evaluated curve is slightly higher than the uncertainty limit in the covariance analysis around 1 MeV, although it remains well within the scatter in the experimental data (see Fig. 99). At all other energies the evaluated nubar curve is within uncertainties in the covariance analysis and agrees well with that analysis (Figs. 99 and 100).

5. $n+^{239}$Pu total cross section

The $n+^{239}$Pu total cross section above the resonance region (0.03-20 MeV) was taken from ENDF/B-VI.8, which is based on coupled-channel optical calculations combined with a covariance analysis of the experimental database available circa 1990. The covariance analysis was performed using the GLUCS code system [97], as described earlier (Sec. IV.B.1). The experimental data of Pienitz et al. [18], [118], Shamu [21], Schwartz et al. [151], Foster and Glasgow [116], Smith et al. [240], Nadolny et al. [241], Peterson et al. [152], Cabe and Cance [154], and Lisowski [31] were included in the co-