OVERVIEW OF THE 2009 RELEASE OF THE EVALUATED NUCLEAR DATA LIBRARY (ENDL2009)


May 6, 2010

International Conference on Nuclear Data for Science and Technology (ND2010)
Seogwipo, Jeju, South Korea
April 26, 2010 through April 30, 2010
Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.
OVERVIEW OF THE 2009 RELEASE OF THE EVALUATED NUCLEAR DATA LIBRARY (ENDL2009)

Lawrence Livermore National Laboratory, Box 808, Livermore CA, 94550, USA
1Nuclear Engineering and Radiological Sciences Department, University of Michigan, Ann Arbor MI, 48109-2104 USA
*Corresponding author. E-mail : brown170@llnl.gov

Received
Accepted for Publication

The Lawrence Livermore National Laboratory (LLNL) Physics Division has produced the next iteration of LLNL's evaluated nuclear database, ENDL2009. ENDL2009 is the second in a series of major ENDL library releases designed to support LLNL's current and future nuclear data needs. This library includes 585 distinct transport-ready evaluations in the neutron sub-library and many physics improvements for stockpile stewardship, attribution signatures, key radiochemical diagnostics and performance of conventional and hybrid fission/fusion reactors. In building this library, we adopted the best of the world's nuclear data efforts: 46% of the library is from the ENDF/B-VII.0 library, 10% is from the JENDL libraries and 8% from other libraries. The remaining 36% of the neutron sub-library and all of the charged-particle sub-libraries consist of new evaluations developed at LLNL for the ENDL2009 library. In addition, ENDL2009 supports new features such as energy-dependent Q values from fission, support for unresolved resonances and average momentum deposition. Finally, this release is our most highly tested release as we have strengthened our already rigorous testing regime by adding tests against LANL Activation Ratio Measurements and more than 1200 new critical assemblies. Our testing is now being incorporated into our development process and is serving to guide database improvements.

KEYWORDS : ND2010, Nuclear Data, ENDF

1. GENERAL INFORMATION

The Lawrence Livermore National Laboratory (LLNL) Physics Division has created the 2009 release of the Evaluated Nuclear Data Library (ENDL2009). ENDL2009 is designed to support LLNL's current and future nuclear data needs and will be used for use in nuclear reactor, nuclear security and stockpile stewardship applications. This database is currently the most complete nuclear database for Monte Carlo and deterministic transport of neutrons and charged particles. This library was assembled with strong support from the US Department of Energy’s National Nuclear Security Administration and the US Department of Energy’s Office of Science/Nuclear Data Program.

ENDL2009 includes 585 distinct transport-ready evaluations in the neutron sub-library and another 35 evaluations in the charged-particle sub-libraries. ENDL2009 contains many physics improvements for stockpile stewardship, attribution signatures, key radiochemical diagnostics and performance of conventional and hybrid fission/fusion reactors. In building this library, the best output from the world's nuclear data efforts were adopted: 46% of the library is from the ENDF/B-VII.0 library, 10% is from the JENDL libraries and 8% from other libraries. The remaining 36% of the neutron sub-library and most of the charged-particle sub-libraries consist of new evaluations developed at LLNL for the ENDL2009 library. In addition, ENDL2009 supports new features such as energy-dependent Q values from fission, average momentum deposition, large-angle Coulomb scattering for all charged particles, support for unresolved resonances and cross-section covariance data. Finally, this library is LLNL's most highly tested nuclear data release as LLNL's already rigorous testing regime has been strengthened by adding tests against activation ratio measurements and approximately 1200 new critical assemblies.

In these proceedings, we provide an overview of some of the evaluations, specifically those submitted to the development library for the ENDF/B library, ENDF/B-VII.B1.

2. EVALUATIONS

All of the new evaluations discussed here were created using Hauser-Feshbach calculations with code talys [1]. In general we tuned our calculations to all available EXFOR cross section data. For the structural materials, this was simple hand-tuning. However for the fission fragments, we made a Monte-Carlo sampling of talys inputs to make estimates of theoretical uncertainties as well as to match EXFOR data.
The talys calculations mainly model the fast neutron region, but can be extrapolated to thermal energies for the average cross-sections. For stable nuclei, where resonance data are available, we reviewed and adopted the best resonance regions available, otherwise we used the talys average cross sections. As the ENDF format is a purely point-wise, the resonances are most efficiently stored in the ENDF format. We used the codes endl2endf [2] and geft [3] to first build the evaluations in ENDF format and merge them with selected resonance regions. Then we use the code fete [4] to convert the ENDF formatted evaluation into the ENDF format. This method allows us to keep the unresolved resonance region intact and store the discrete γ’s in parameterized form until the final translation step. Also, this allows us to use Kalbach systematics along with the pre-equilibrium fraction which is modeled by talys.

2.1 Aluminum

For aluminum, only $^{27}$Al is stable but we wanted $^{25-29}$Al. Our calculations were tuned for $^{27}$Al and talys was used for the unstables. For $^{27}$Al, resonance parameters extend only to 1 MeV (from ENDF/B-VII.0), but the cross section still fluctuates up 10 MeV. We note that there are large ($n,γ$) data disagreements above 1 MeV. The apparent disagreements in the $(n,2n)$ cross section is due to the presence of an isomer in $^{26}$Al. Cross sections are plotted in Fig. 1 and test results are given in Fig. 2 and Table 1.

![Fig. 1. Cross-section data from the new ENDL2009 evaluation of $^{27}$Al compared to all available EXFOR data. Also plotted are the ENDF/B-VII.0 and JENDL-3.3 evaluations.](image1)

![Fig. 2. LLNL Pulsed Sphere neutron time-of-flight results for $^{23}$Al. Both the new ENDL2009 and the ENDF/B-VII.0 evaluation behave similarly.](image2)

**Table 1.** Benchmark results for $^{23}$Al in various fast critical assemblies. The ENDL2009 evaluation performs well in these tests.

<table>
<thead>
<tr>
<th>Case</th>
<th>Reflector</th>
<th>Exp. $k_{\text{eff}}$</th>
<th>Calc. $k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF084_1</td>
<td>$^{27}$Al</td>
<td>0.9994 ± 0.0019</td>
<td>0.9994 ± 0.0001</td>
</tr>
<tr>
<td>HMF084_2</td>
<td>Al$_2$O$_3$</td>
<td>0.9994 ± 0.0021</td>
<td>0.9997 ± 0.0001</td>
</tr>
<tr>
<td>HMF084_15</td>
<td>Al$_2$O$_3$</td>
<td>0.9995 ± 0.0021</td>
<td>0.9982 ± 0.0001</td>
</tr>
<tr>
<td>PMF_009</td>
<td>$^{27}$Al</td>
<td>1.0000 ± 0.0027</td>
<td>1.0066 ± 0.0001</td>
</tr>
</tbody>
</table>

2.2 Tantalum

Only $^{181}$Ta is stable, but we evaluated $^{178-183}$Ta. The $^{181}$Ta resonances extend to 2 keV. The apparent disagreements in the $(n,2n)$ cross section is due to the presence of an isomer in $^{186}$Ta. Cross sections are plotted in Fig. 3 and test results are given in Fig. 4 and Table 2.

2.3 Rhenium

While $^{183,187}$Re are stable, we evaluated $^{183-189}$Re. Cross sections for $^{187}$Re are plotted in Fig. 5 and test results are given in Table 2. Due to space limitations, the $^{185}$Re cross-sections are not shown.

2.4 Fission Fragments Kr and Xe

Evaluations for $^{76-78}$Kr and $^{122-124}$Xe were generated, taking resonances from ENDF/B-VII.0 when available. In both cases, the charged-particle channels were small, making the neutron channels reliable. $^{78}$Kr($n,γ$) is essentially unchanged from the WPEC-23 evaluation used in ENDF/B-VII.0. We computed cross section uncertainties, but did not
Fig. 3. Cross-section data from the new ENDL2009 evaluation of \(^{181}\)Ta compared to all available EXFOR data. Also plotted are the ENDF/B-VII.0 and JENDL-3.3 evaluations.

Fig. 4. LLNL Pulsed Sphere time-of-flight results for \(^{181}\)Ta. The new ENDL2009 performs significantly better than the ENDF/B-VII.0 evaluation, however both evaluations appear to poorly match the 150-200 nsec data, presumably due to deficiencies in pre-equilibrium modeling.

Table 2. \((n,\gamma)\) activation foil results. All new tantalum and rhenium evaluations perform well in this tests.

<table>
<thead>
<tr>
<th>Assembly</th>
<th>Foil</th>
<th>Calc./Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Godiva</td>
<td>(^{181})Ta</td>
<td>98.60 ± 9.62%</td>
</tr>
<tr>
<td>Godiva</td>
<td>(^{187})Re</td>
<td>110.12 ± 4.75%</td>
</tr>
<tr>
<td>Godiva</td>
<td>(^{187})Re</td>
<td>102.57 ± 8.60%</td>
</tr>
<tr>
<td>Big Ten</td>
<td>(^{181})Ta</td>
<td>92.20%</td>
</tr>
</tbody>
</table>

in Fig. 7.

3. REVIEW OF THE JENDL/ACTINOID-2008 LIBRARY

In 2008, the JENDL Actinoid library was released to the larger nuclear data community. As part of our annual library review process, we reviewed this library for isotopes to include in ENDL2009. Our procedure for this review was simple: we make cross section plots of all the major reactions, including EXFOR data. In addition, we compute the \(\chi^2\), comparing data to evaluation: \(\chi^2 = \sum_i (\sigma_i - \sigma_{\text{eval}}(E_i))^2 / (\sigma_i)^2\). Here the sum runs over all data points for a given reaction. We use the \(\chi^2\) as a crude measure of evaluation quality when we can not determine the best by eye. We also take into consideration the scope and
quality of systematics used in the evaluations when no data exists. The result of this review was a large report [6] and recommendations for evaluations to use in ENDL2009 and ENDF/B-VII.β1.

4. LIBRARY AVAILABILITY

The ENDF files for the stable isotope evaluations described in these proceedings as well as a few others (237U, 239U, 240Am) are available in the ENDF/B-VII.β1 library. Other ENDF files are in preparation, namely 62−73Zn, 57−61Co and several unstable Al, Ta, W, Re, Au isotopes. While these proceedings focused on the neutron sublibrary, ENDL2009 also contains a sizable charged-particle sublibrary updating the Evaluated Charged Particle Library (ECPL) [7]. These data may also be made available if there is sufficient interest.

This new library can be found on LLNL’s Open and Secure Computing facilities. In addition, the data may be viewed in the Nuclear and Atomic Data System data viewer at http://nuclear.llnl.gov/NADS. The ENDF formatted library and specific ENDF formatted evaluations are also available from the authors. A detailed LLNL laboratory report is in preparation and should be available by May 2010.

ACKNOWLEDGMENTS

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

REFERENCES