LA-UR-12-20003

LANL Data Evaluation Support for ENDF/B-VII.1

M. B. Chadwick, P. Talou, T. Kawano, G. Hale, J. Lestone, M. MacInnes, D. K. Parsons, J. L. Conlin, A. C. Kahler

Los Alamos National Laboratory

Presented at the NCSP Technical Symposium held at Oak Ridge National Laboratory

March 13 – 14, 2012

Abstract

We review the results of NCSP sponsored data evaluation work performed to support development and release of the ENDF/B-VII.1 Neutron Library during FY11.

Introduction - I

- **The ENDF/B-VII.1 General Purpose Nuclear Data File was released in December, 2011.**
  - Followed data testing and analyses of several “beta” files during 2011.
- **In parallel, the December, 2011 issue of the Nuclear Data Sheets contained a number of peer-reviewed technical papers documenting much of the underlying work performed to develop these data files.**
  - This report summarizes LANL’s contribution to the data evaluation effort of the ENDF/B-VII.1 Library.

Introduction - II

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 2887–2996
ELSEVIER
Nuclear Data Sheets
www.elsevier.com/locate/nds

ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data

M.B. Chadwick,[1,*] M. Herman,[2] P. Obložinský,[2] M.E. Dunn,[3] Y. Danon,[4] A.C. Kahler,[1] D.L. Smith,[5] B. Pritychenko,[2] G. Arbanas,[3] R. Arcilla,[2] R. Brewer,[1] D.A. Brown,[2,6] R. Capote,[7] A.D. Carlson,[8] Y.S. Cho,[13] H. Derrien,[3] K. Guber,[3] G.M. Hale,[1] S. Hoblit,[2] S. Holloway,[1] T.D. Johnson,[2] T. Kawano,[1] B.C. Kiedrowski,[1] H. Kim,[13] S. Kunieda,[1,15] N.M. Larson,[3] L. Leal,[3] J.P. Lestone,[1] R.C. Little,[1] E.A. McCutchan,[2] R.E. MacFarlane,[1] M. MacInnes,[1] C.M. Mattoon,[6] R.D. McKnight,[5] S.F. Mughabghab,[2] G.P.A. Nobre,[2] G. Palmiotti,[14] A. Palumbo,[2] M.T. Pigni,[3] V.G. Pronyaev,[9] R.O. Sayer,[3] A.A. Sonzogni,[2] N.C. Summers,[6] P. Talou,[1] I.J. Thompson,[6] A. Trkov,[10] R.L. Vogt,[6] S.C. van der Marck,[11] A. Wallner, [12] M.C. White,[1] D. Wiarda,[3] P.G. Young[1]

[1] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2] *Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[3] *Oak Ridge National Laboratory, Oak Ridge, TN 37831-6171, USA*
[4] *Rensselaer Polytechnic Institute, Troy, NY 12180, USA*
[5] *Argonne National Laboratory, Argonne, IL 60439-4842 USA*
[6] *Lawrence Livermore National Laboratory, Livermore, CA 94551-0808, USA*
[7] *International Atomic Energy Agency, Vienna-A-1400, PO Box 100, Austria*
[8] *National Institute of Standards and Technology, Gaithersburg, MD 20899-8463, USA*
[9] *Institute of Physics and Power Engineering, Obninsk, Russian Federation*
[10] *Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[11] *Nuclear Research and Consultancy Group, P.O. Box 25, NL-1755, ZG Petten, The Netherlands*
[12] *Faculty of Physics, University of Vienna, Waehringer Strasse 17, A-1090 Vienna, Austria*
[13] *Korea Atomic Energy Research Institute, Daejeon, Korea*
[14] *Idaho National Laboratory, Idaho Falls, ID 83415, USA and*
[15] *Japan Atomic Energy Agency, Tokai-mura Naka-gun, Ibaraki 319-1195, Japan*

(Received 12 July 2011; revised received 22 September 2011; accepted 17 October 2011)

The ENDF/B-VII.1 library is our latest recommended evaluated nuclear data file for use in nuclear science and technology applications, and incorporates advances made in the five years since the release of ENDF/B-VII.0. These advances focus on neutron cross sections, covariances, fission product yields and decay data, and represent work by the US Cross Section Evaluation Working Group (CSEWG) in nuclear data evaluation that utilizes developments in nuclear theory, modeling, simulation, and experiment.

The principal advances in the new library are: (1) An increase in the breadth of neutron reaction cross section coverage, extending from 393 nuclides to 423 nuclides; (2) Covariance uncertainty data for 190 of the most important nuclides, as documented in companion papers in this edition; (3) R-matrix analyses of neutron reactions on light nuclei, including isotopes of He, Li, and Be; (4) Resonance parameter analyses at lower energies and statistical high energy reactions for isotopes of Cl, K, Ti, V, Mn, Cr, Ni, Zr and W; (5) Modifications to thermal neutron reactions on fission products (isotopes of Mo, Tc, Rh, Ag, Cs, Nd, Sm, Eu) and neutron absorber materials (Cd, Gd); (6) Improved minor actinide evaluations for isotopes of U, Np, Pu, and Am (we are not making changes to the major actinides ^{235,238}U and ^{239}Pu at this point, except for delayed neutron data and covariances, and instead we intend to update them after a further period of research in experiment and theory), and our adoption of JENDL-4.0 evaluations for isotopes of Cm, Bk, Cf, Es, Fm, and some other minor actinides; (7) Fission energy release evaluations; (8) Fission product yield advances for fission-spectrum neutrons and 14 MeV neutrons incident on ^{239}Pu; and (9) A new decay data sublibrary.

Integral validation testing of the ENDF/B-VII.1 library is provided for a variety of quantities: For nuclear criticality, the VII.1 library maintains the generally-good performance seen for VII.0 for a wide range of MCNP simulations of criticality benchmarks, with improved performance coming from new structural material evaluations, especially for Ti, Mn, Cr, Zr and W. For Be we see some improvements although the fast assembly data appear to be mutually inconsistent. Actinide cross section updates are also assessed through comparisons of fission and capture reaction rate measurements in critical assemblies and fast reactors, and improvements are evident. Maxwellian-averaged capture cross sections at 30 keV are also provided for astrophysics applications.

We describe the cross section evaluations that have been updated for ENDF/B-VII.1 and the measured data and calculations that motivated the changes, and therefore this paper augments the ENDF/B-VII.0 publication [1].

*) Electronic address: mbchadwick@lanl.gov

Nuclear Data Sheets, **112**, 2888 (2011).

We focus on LANL work below, but the complete evaluation effort was a multi-lab (and multi-country!) effort.

Introduction - III

Quantification of Uncertainties
for Evaluated Neutron-Induced Reactions on Actinides
in the Fast Energy Range

P. Talou*, P.G. Young, and T. Kawano
T-2, Nuclear Physics Group, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

M. Rising
Department of Nuclear Engineering, University of New Mexico, Albuquerque, NM

M.B. Chadwick
X-CP, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
(Received 12 July 2011; revised received 4 October 2011; accepted 7 October 2011)

Covariance matrix evaluations in the fast energy range were performed for a large number of actinides, either using low-fidelity techniques or more sophisticated methods that rely on both experimental data as well as model calculations. The latter covariance evaluations included in the ENDF/B-VII.1 library are discussed for each actinide separately.

Nuclear Data Sheets, **<u>112</u>**, 3054 (2011)

Nuclear Data Sheets, **<u>112</u>**, 3120 (2011)

Nuclear Data Sheets, **<u>112</u>**, 3135 (2011)

The NCSP Program benefitted from an overlap in interest from the Advanced Simulation and Computing (ASC), Physics and Engineering Models Program (PEM).

Energy Dependence of Plutonium Fission-Product Yields

J.P. Lestone*[1]
[1]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
(Received 1 August 2011; revised received 21 September 2011; accepted 8 October 2011)

A method is developed for interpolating between and/or extrapolating from two pre-neutron-emission first-chance mass-asymmetric fission-product yield curves. Measured ^{240}Pu spontaneous fission and thermal-neutron-induced fission of ^{239}Pu fission-product yields (FPY) are extrapolated to give predictions for the energy dependence of the n + ^{239}Pu FPY for incident neutron energies from 0 to 16 MeV. After the inclusion of corrections associated with mass-symmetric fission, prompt-neutron emission, and multi-chance fission, model calculated FPY are compared to data and the ENDF/B-VII.1 evaluation. The ability of the model to reproduce the energy dependence of the ENDF/B-VII.1 evaluation suggests that plutonium fission mass distributions are not locked in near the fission barrier region, but are instead determined by the temperature and nuclear potential-energy surface at larger deformation.

Fission Product Yields for 14 MeV Neutrons on ^{235}U, ^{238}U and ^{239}Pu

M. Mac Innes*, M.B. Chadwick, and T. Kawano[1]
[1]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
(Received 24 June 2011, revised received 22 September 2011; accepted 14 October 2011)

We report cumulative fission product yields (FPY) measured at Los Alamos for 14 MeV neutrons on ^{235}U, ^{238}U and ^{239}Pu. The results are from historical measurements made in the 1950s-1970s, not previously available in the peer reviewed literature, although an early version of the data was reported in the Ford and Norris review. The results are compared with other measurements and with the ENDF/B-VI England and Rider evaluation. Compared to the Laurec (CEA) data and to ENDF/B-VI evaluation, good agreement is seen for ^{235}U and ^{238}U, but our FPYs are generally higher for ^{239}Pu. The reason for the higher plutonium FPYs compared to earlier Los Alamos assessments reported by Ford and Norris is that we update the measured values to use modern nuclear data, and in particular the 14 MeV ^{239}Pu fission cross section is now known to be 15-20% lower than the value assumed in the 1950s, and therefore our assessed number of fissions in the plutonium sample is correspondingly lower. Our results are in excellent agreement with absolute FPY measurements by Nethaway (1971), although Nethaway later renormalized his data down by 9% having hypothesized that he had a normalization error. The new ENDF/B-VII.1 14 MeV FPY evaluation is in good agreement with our data.

ENDF/B-VII.0 Deficiencies Addressed

- ^{238,240}Pu
- Minor actinides (^{236,237,239}U, ^{237}Np, ^{242}Pu, ^{241,243}Am)
- Minor actinides (Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm)
- Light Elements (Astrophysics, Capture Cross Sections)
- Structural materials (Ti, V, Mn, Cr, Ni, W)
- Fission Product Thermal Capture
- Fission Product Yields (FPY)
- Delayed Neutron (DN) Data
- Covariances (Fast Energy Range, Actinides)
- Thermal Kernel Processing for MCNP
- NOTE: Major actinide (^{235,238}U, ^{239}Pu) evaluations are unchanged (except for reverting to ENDF/B-VI.8 DN data)

^{238,240}Pu

- Updated old (1978, 1986 respectively) evaluations previously carried forward from ENDF/B-V or -VI
- Mix of modern GNASH calculations and recent experimental data
- This work performed prior to 2011 and has been discussed previously.

Minor actinides (^{236,237,239}U, ^{237}Np, ^{242}Pu, ^{241,243}Am)

- Revised fission and capture cross section evaluations based upon integral data testing feedback.
- LLNL surrogate data used to update the ^{239}U evaluation.
- Much of the basic re-evaluation work pre-dates 2011; integral data testing has occurred in 2010 & 2011 …

^{236,237}U – LANL Integral Reaction Rate Data

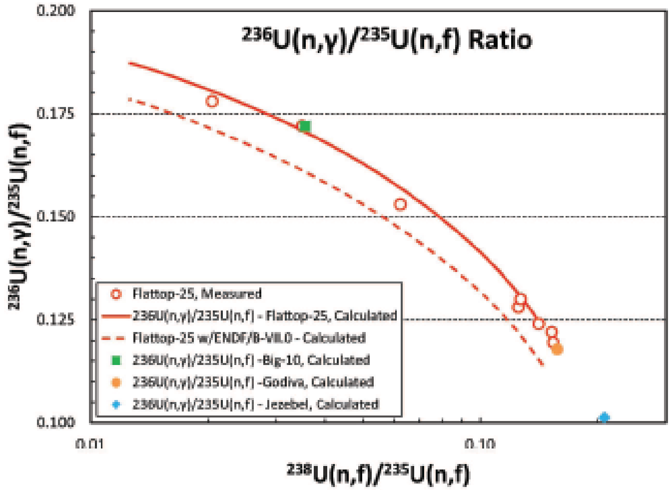


FIG. 52: ^{236}U(n, γ) comparison of experimental radiochemical data with an MCNP simulation using ENDF/B-VII.1 and ENDF/B-VII.0 data. The spectral index, a measure of the hardness of the neutron spectrum, is given on the x-axis.

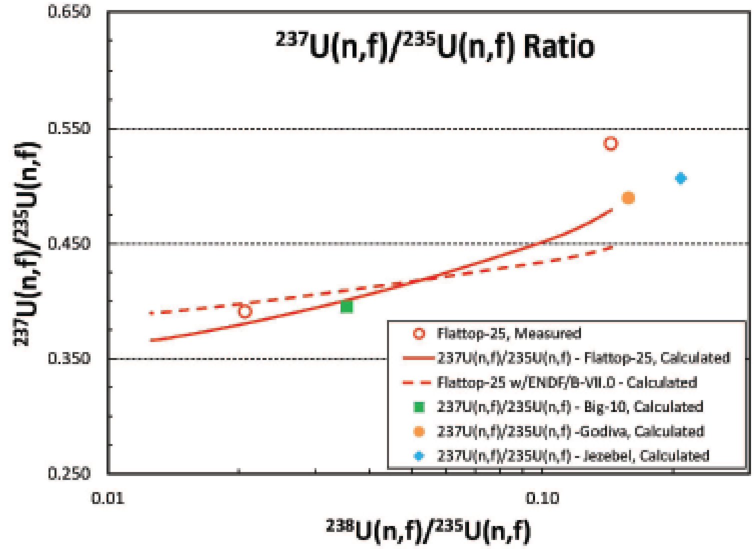


FIG. 56: MCNP calculated ^{237}U fission reaction rate (in ratio to the well known ^{235}U fission rate) compared with measurements, for samples placed in the Flattop-25 fast critical assembly at LANL. Two measurements were made by Barr, one in the (hot) center, and one in the (softer) tamper region.

^{238}U – LANL Integral Reaction Rate Data

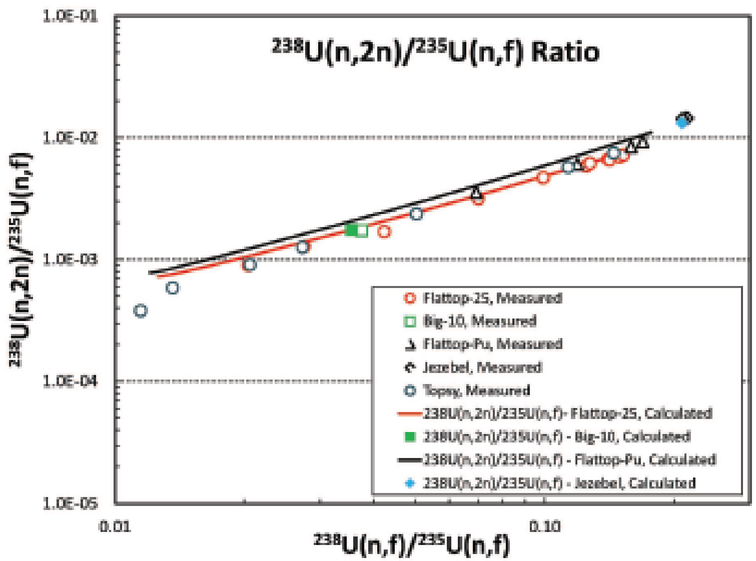


FIG. 57: The ratio of the ^{238}U(n,2n) reaction rate to the ^{235}U fission rate is plotted against the ratio of the ^{238}U fission rate to the ^{235}U fission rate (spectral index) for different positions (with central positions to the right and positions in the reflector to the left).

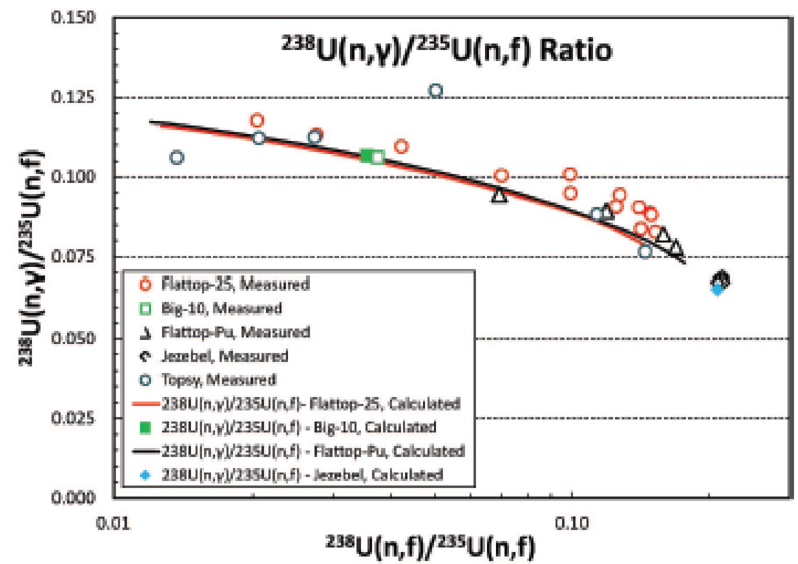


FIG. 58: The integral ^{238}U neutron capture rate (divided by the ^{235}U fission rate) as a function of spectral index for different critical assembly locations.

^{241,243}Am – LANL Integral Reaction Rate Data

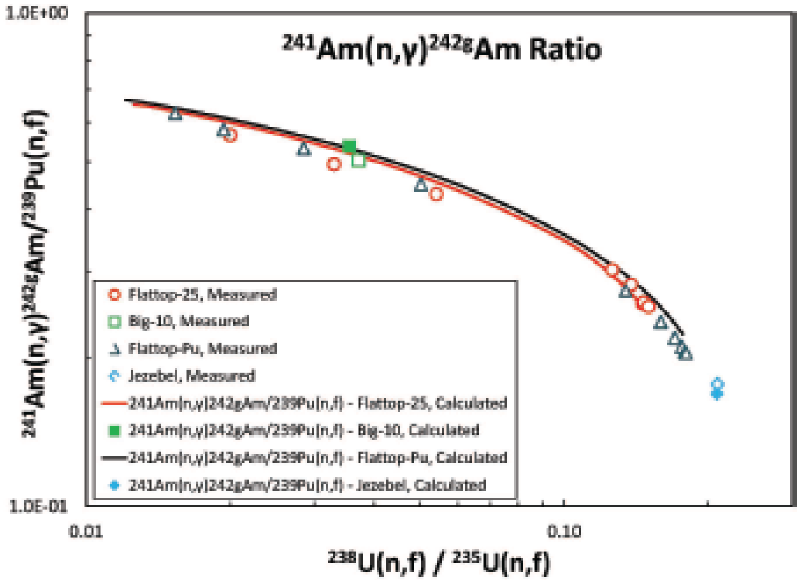


FIG. 93: The integral ^{241}Am neutron capture rate (divided by the ^{239}Pu fission rate) as a function of spectral index for different critical assembly locations. In this case the measurements, which detect the ^{242}Cm are divided by 0.827 to account for the fraction of ^{242g}Am that beta decays to ^{242}Cm.

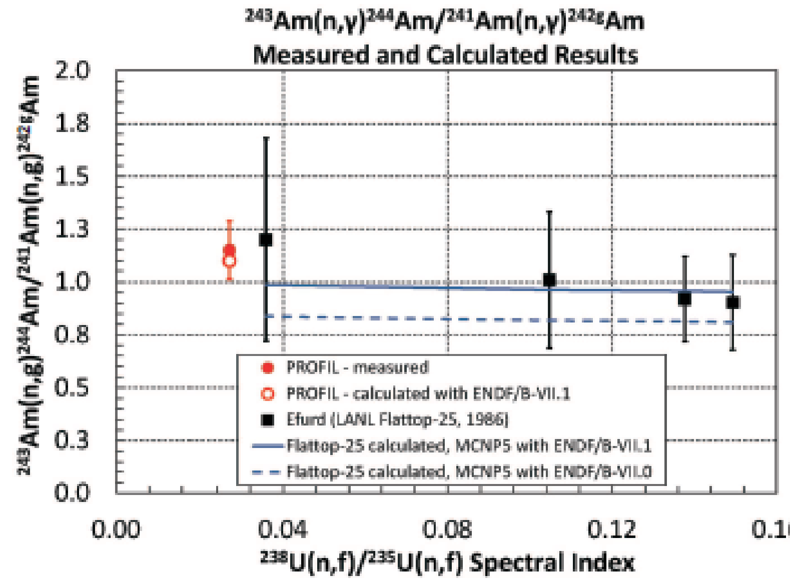


FIG. 97: Measured reaction rate ratios for ^{243}Am(n,γ)/^{241}Am(n,γ)^{242g}Am compared to LANL radiochemistry critical assembly data [162] and to PROFIL reactor data. The LANL measurements are in Flattop-25, located at 1,4, 6 and 11 cm from the center, where ratio values were measured to be 0.90, 0.92, 1.0, and 1.2 with uncertainties of about 25%.

Minor actinides (Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm)

- **Replace many (59) minor actinide evaluations with JENDL-4.0 data**
  - Include missing MT=458 (components of energy release due to fission) data with LLNL / Ramona Vogt evaluation.

Light Elements – ^{3}He, ^{9}Be, ^{nat}C, ^{16}O

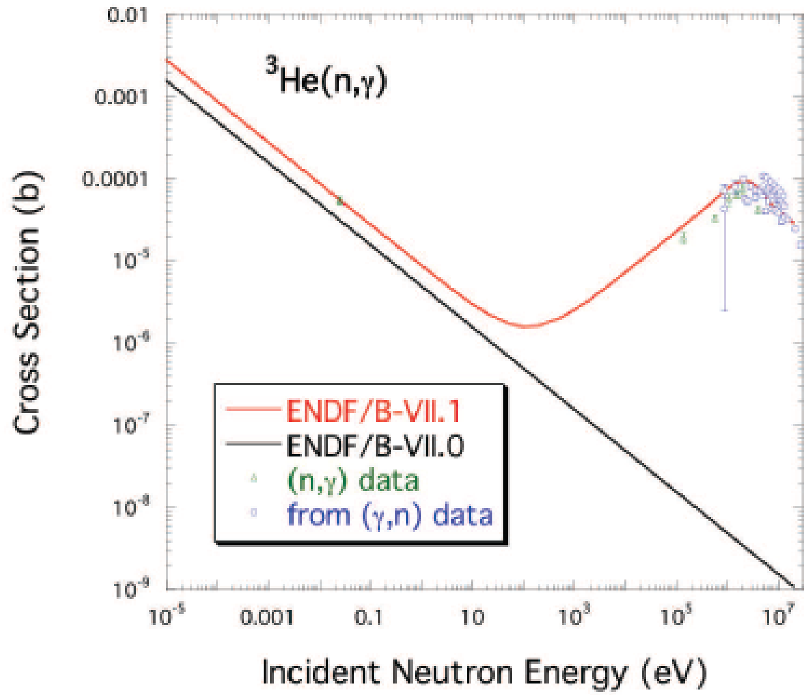


FIG. 4: Neutron capture on ^{3}He. Compared are cross sections in ENDF/B-VII.1 (red curve) with those in ENDF/B-VII.0 (black line), and with experimental data from $n+^3$He capture (green triangles) and inverted $\gamma+^4$He photodisintegration (blue circles).

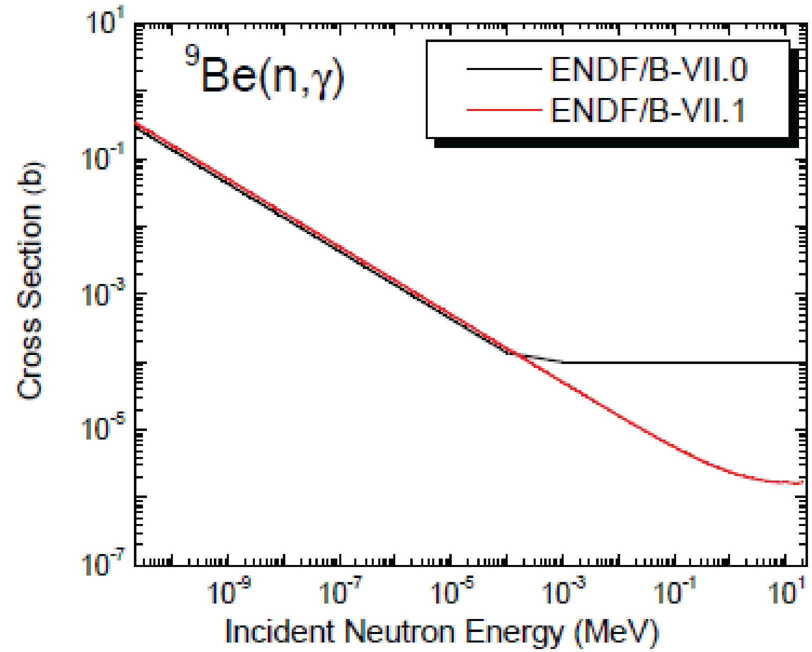


FIG. 10: Neutron capture on ^{9}Be. The red curve is ENDF/B-VII.1, the black curve is ENDF/B-VII.0, and the circles are measured values.

This work initiated after deficiencies were noted by NNDC staff for 30 keV Maxwellian average capture data.

Light Elements – ^{3}He, ^{9}Be, ^{nat}C, ^{16}O

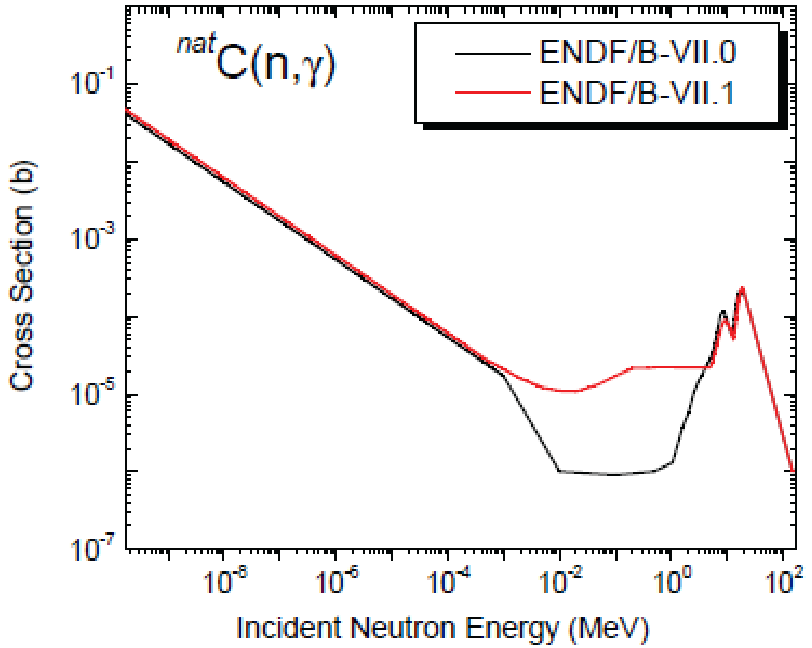


FIG. 11: Neutron capture on ^{nat}C. Compared are cross sections in ENDF/B-VII.1 with ENDF/B-VII.0.

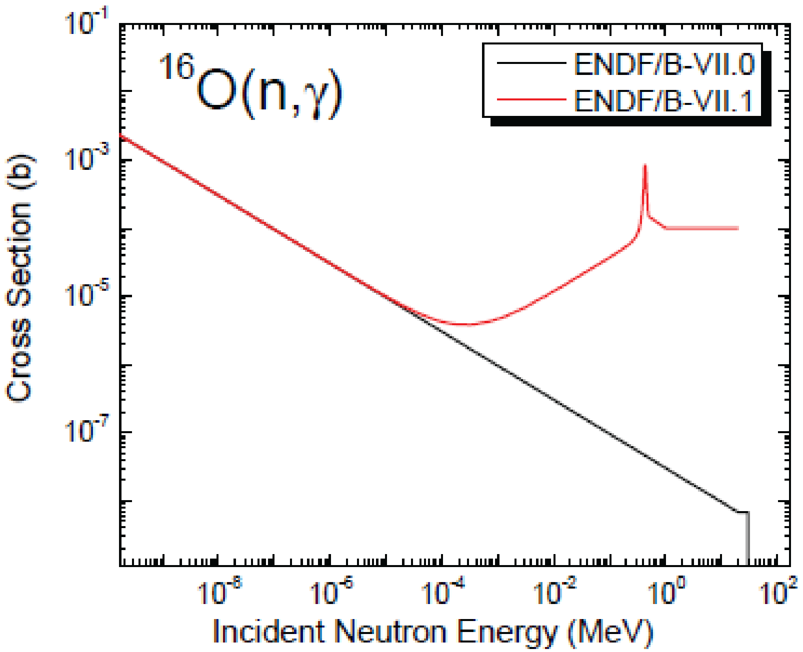


FIG. 12: Neutron capture on ^{16}O. Compared are cross sections in ENDF/B-VII.1 with ENDF/B-VII.0.

Structural materials (Ti, V, Mn, Cr, Ni, W)

- Ti – Revised ^{48}Ti evaluation (ORNL and LANL), based upon reported k_{eff} bias in critical assembly testing (next presentation), new ORNL RR evaluation and new LANSCE data.
- V – Replace an elemental evaluation with isotopic evaluations (use JENDL-4.0 for the minor isotope, ^{50}V). ^{51}V updated to account for new gas-production data and modern reaction code calculations.
- Mn – Update the 1988 evaluation (ORNL and LANL) to account for new (n,2n) and (n,γ) data and advanced reaction codes.
- ^{50,52,53,54}Cr, ^{58,60}Ni – ORNL revisions in the resolved resonance region; LANL revisions to high energy α production.
- W – Update old (~1980 for ENDF/B-V) isotopic evaluations accounting for new data, advanced reaction models and integral data testing feedback; include missing ^{180}W.

^{48}Ti Angular Distributions; Cr, Ni Alpha Production

LA-UR-12-20003

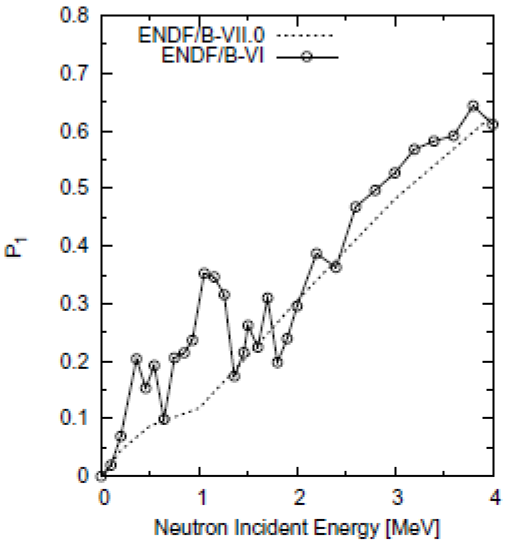


FIG. 15: The $L = 1$ component of the Legendre expansion coefficients for the differential elastic scattering from ^{48}Ti, as a function of neutron incident energy.

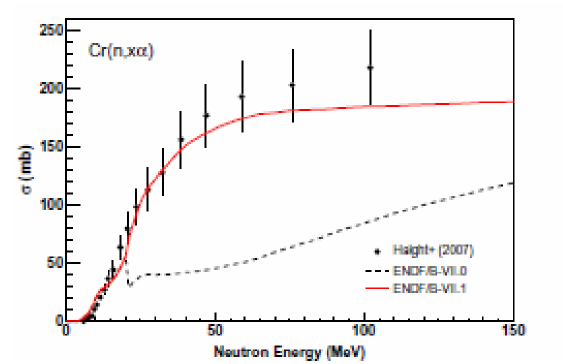


FIG. 35: Calculated alpha production cross section for neutrons on chromium, compared to Haight's data from LANSCE.

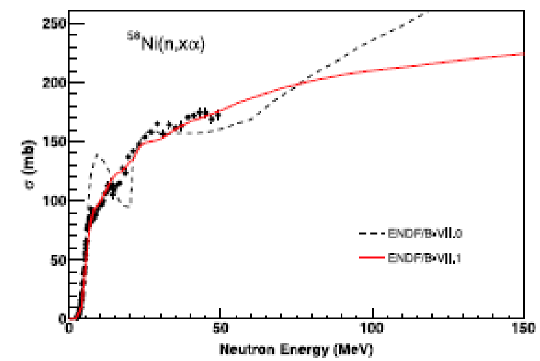


FIG. 36: Calculated alpha production cross section for neutrons on ^{58}Ni, compared to Haight's data from LANSCE.

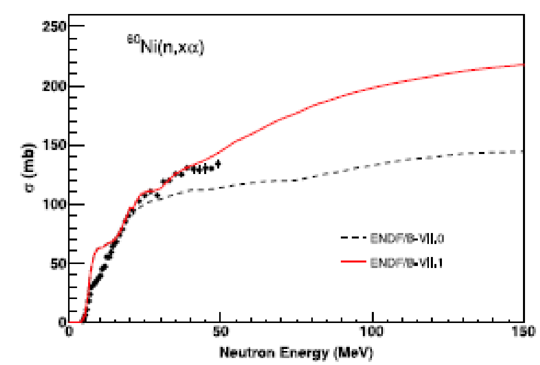


FIG. 37: Calculated alpha production cross section for neutrons on ^{60}Ni, compared to Haight's data from LANSCE.

^{48}Ti - Revert to more forward peaked elastic scattering angular distributions, as in older evaluations.

Fission Product Thermal Capture

- **Revisions performed at BNL by Said Mughabghab**

Fission Product Yields (FPY)

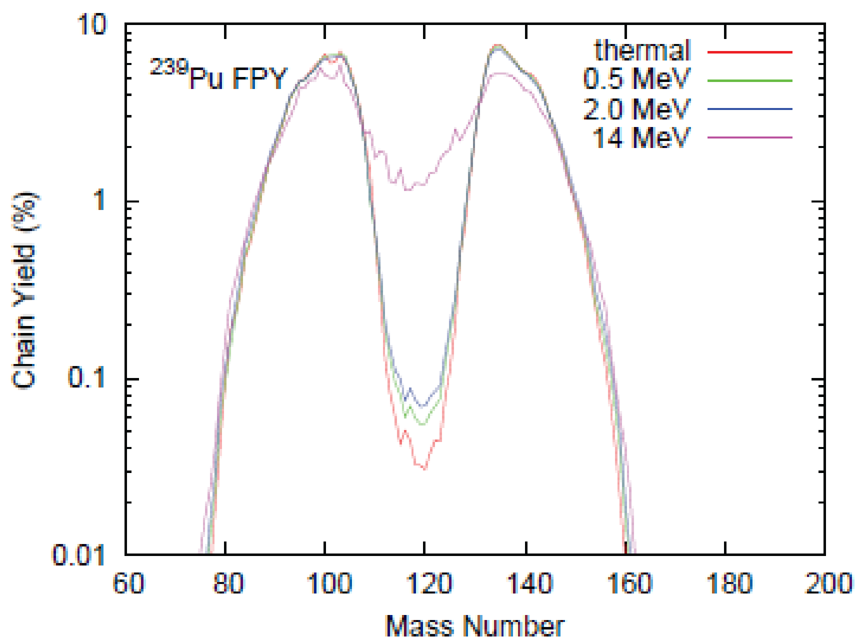


FIG. 101: A-Chain yields for n+^{239}Pu in ENDF/B-VII.1. Thermal yields are unchanged from ENDF/B-VI.

- **^{239}Pu**
  - Thermal FPY data are unchanged
  - Fission and 14 MeV energy FPY's are revised
    - Fission energy includes 0.5 MeV and 2.0 MeV incident neutron energy
      - Documented in Chadwick *et al*, *Nuclear Data Sheets*, **111**, 2923 (2010).
    - 14 MeV results documented in MacInnes *et al*, *Nuclear Data Sheets*, **112**, 3135 (2011).

Delayed Neutron (DN) Data

- **"Based upon unfavorable feedback there is evidence to suggest that the ENDF/B-VII.0 delayed neutron data are not as reflective of physical reality as the earlier ENDF/B-VI.8 delayed data".**

From ENDF/B-VII.0 to ENDF/B-VII.1
Quantify Uncertainties with Evaluated Data

- **LANL, T-2 work on major actinides in the fast energy range**
- **Included:**
  - Cross-sections for most important reactions; e.g., (n,capture), (n,fission), (n,2n), etc
  - Prompt fission neutron spectra and multiplicities for ^{239}Pu, ^{235}U and ^{238}U thermal
- **Model calculations using T-2 nuclear reaction codes (e.g., CoH, GNASH, PFNS, …) + covariance analyses of experimental data + Bayesian statistics to combine both experiments and theory into evaluated files.**
- **Full documentation in**
  "Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Energy Range", P.Talou, P.G.Young, T.Kawano, M.Rising, and M.B.Chadwick, *Nuclear Data Sheets* **112**, 3054 (2011).

Some examples

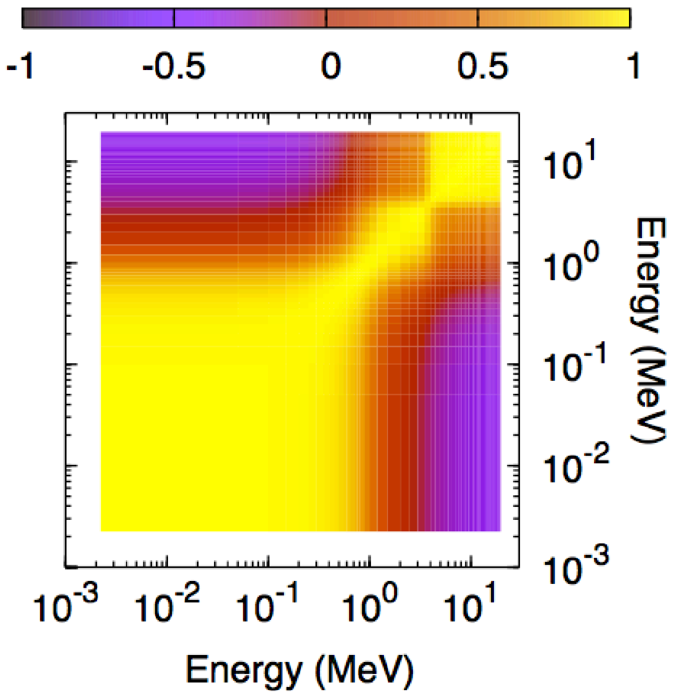


FIG. 6: Correlation matrix for the capture cross section of n+^{235}U.

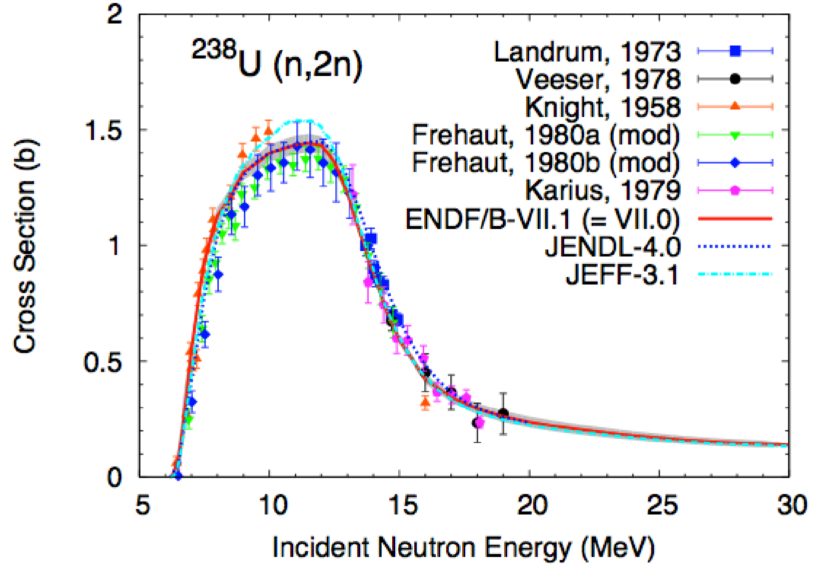


FIG. 16: Evaluated and experimental cross sections for the ^{238}U (n,2n) reaction from threshold to 20 MeV.

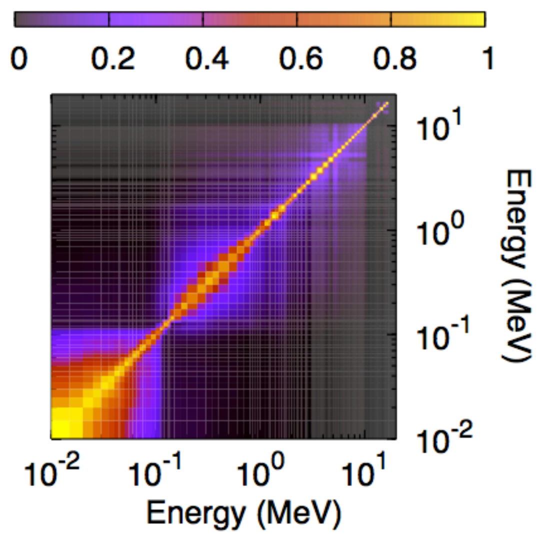
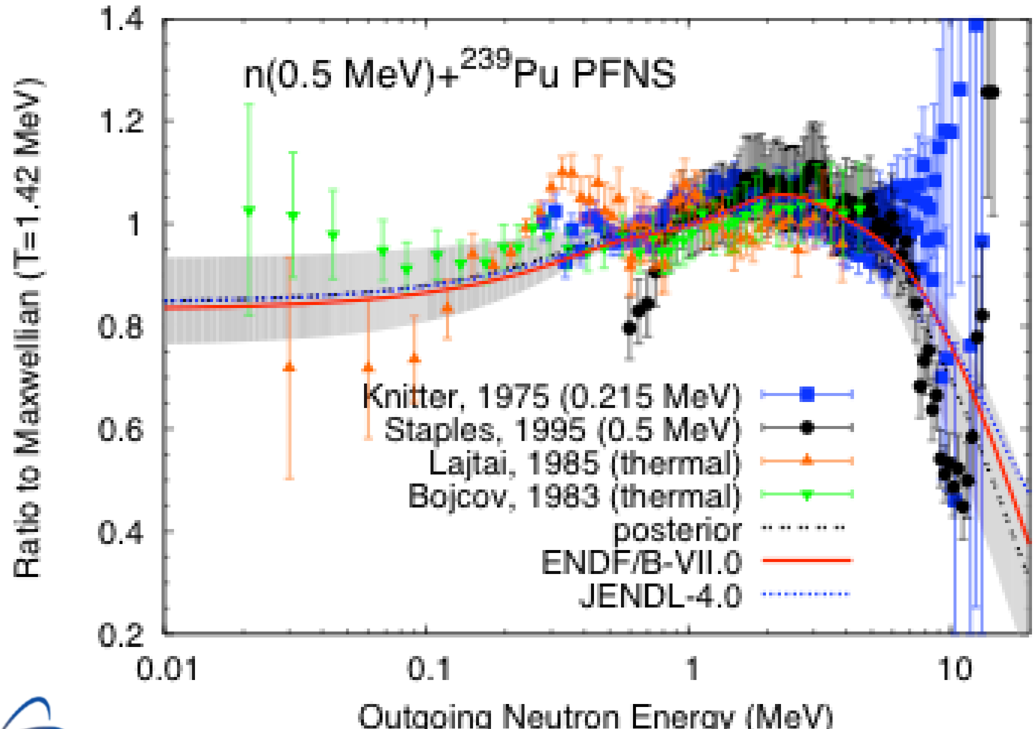
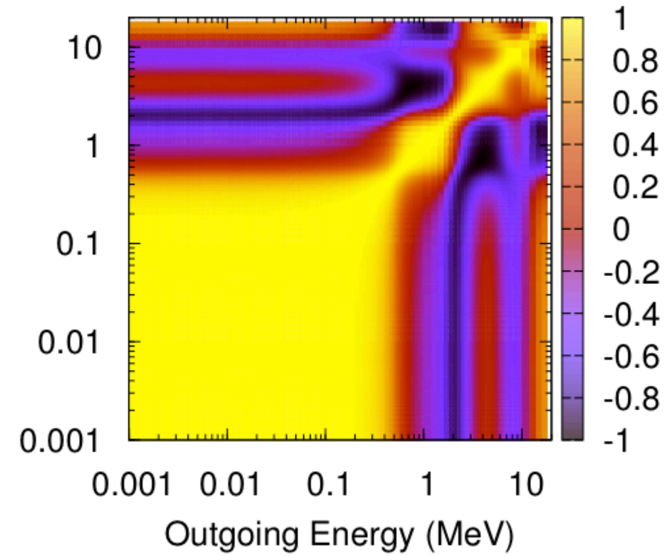


FIG. 25: Correlation matrix evaluated for the ^{238}Pu (n,fission) cross section.

Prompt Fission Neutron Spectrum, n_{th}+^{239}Pu

- "Uncertainty Quantification of Prompt Fission Neutron Spectrum for n(0.5 MeV)+239Pu", P.Talou, T.Kawano, D.G.Madland, A.C.Kahler, D.K.Parsons, M.C.White, R.C.Little and M.B.Chadwick, Nucl. Sci. Eng. **166**, 254 (2010).





Thermal Kernel Processing for MCNP

- **Processed all thermal kernel data files in the ENDF/B-VII.1 library; documented in LA-UR-12-00800.**
  - Use NJOY and create "continuous" kernel files.
  - Requires use of MCNP5.1.50 or later.
    - File format is unchanged, ☹, and so older versions of MCNP will execute but yield incorrect results.
    - "Continuous" files are significantly larger than previous "discrete" files but have little impact on k_{crit} runtime calculations.
- **New thermal data for ENDF/B-VII.1 is Si in SiO_2.**
- **Will be part of the nuclear data library included with the next MCNP release.**

Acknowledgements

- **While this report has highlighted evaluation work performed at LANL, mostly during FY11, significant contributions to the overall ENDF/B-VII.1 General Purpose File development effort have been made by colleagues worldwide; many whom appear as co-authors on the various papers cited previously, or have contributed via feedback from Benchmark Data Testing.**
  - AECL, ANL, Bettis, BNL, KAPL, INL, ORNL
  - Overseas colleagues (IAEA, JEFF, JENDL, KAERI, NRG/Petten, UK, Slovenia)