LA-UR-12-26077

Data Testing at LANL

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presented at the

Fall 2012 CSEWG Meeting

held at

Brookhaven National Laboratory

November 7 - 9, 2012

Abstract

We review recent data testing efforts at LANL with the ENDF/B-VII.1 neutron cross section file and note areas of weakness that should be investigated in coming years as work proceeds for the next generation ENDF/B release.

ENDF/B-VII.1

- **Released last December …**
  - Documented in the December, 2011 issue of Nuclear Data Sheets
  - Neutron library continues to grow …
    - 424 evaluated files (up from 393 in ENDF/B-VII.0);
      - All evaluations except carbon are now isotopic.
    - Much new covariance data;
      - 190 of 424 files contain covariance data.
    - Many minor actinides were upgraded to JENDL-4.0;
      - If not J40, delayed neutron data were reverted to ENDF/B-VI.8;
      - "Big-3" PFNS energy grid improved above 10 MeV.
  - Decay library was re-evaluated by BNL;
  - ^{239}Pu fast and 14 MeV fission yields were re-evaluated;
  - See Chadwick *et al* 2011 NDS paper for more …

ENDF/B-VII.1

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Nuclear Data Sheets 112 (2011) 2887–2996

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

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(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].

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

ENDF/B-VII.1

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Available online at www.sciencedirect.com
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Nuclear Data Sheets 112 (2011) 2997–3036

Nuclear Data Sheets

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Nuclear Data Sheets, **<u>112</u>**, 2997 (2011).

ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks and Reactor Experiments

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(Received 9 August 2011; revised received 21 September 2011; accepted 17 October 2011)

The ENDF/B-VII.1 library is the latest revision to the United States' Evaluated Nuclear Data File (ENDF). The ENDF library is currently in its seventh generation, with ENDF/B-VII.0 being released in 2006. This revision expands upon that library, including the addition of new evaluated files (was 393 neutron files previously, now 423 including replacement of elemental vanadium and zinc evaluations with isotopic evaluations) and extension or updating of many existing neutron data files. Complete details are provided in the companion paper [1]. This paper focuses on how accurately application libraries may be expected to perform in criticality calculations with these data. Continuous energy cross section libraries, suitable for use with the MCNP Monte Carlo transport code, have been generated and applied to a suite of nearly one thousand critical benchmark assemblies defined in the International Criticality Safety Benchmark Evaluation Project's International Handbook of Evaluated Criticality Safety Benchmark Experiments. This suite covers uranium and plutonium fuel systems in a variety of forms such as metallic, oxide or solution, and under a variety of spectral conditions, including unmoderated (i.e., bare), metal reflected and water or other light element reflected. Assembly eigenvalues that were accurately predicted with ENDF/B-VII.0 cross sections such as unmoderated and uranium reflected ^{235}U and ^{239}Pu assemblies, HEU solution systems and LEU oxide lattice systems that mimic commercial PWR configurations continue to be accurately calculated with ENDF/B-VII.1 cross sections, and deficiencies in predicted eigenvalues for assemblies containing selected materials, including titanium, manganese, cadmium and tungsten are greatly reduced. Improvements are also confirmed for selected actinide reaction rates such as ^{236}U, ^{238,242}Pu and ^{241,243}Am capture in fast systems. Other deficiencies, such as the overprediction of Pu solution system critical eigenvalues and a decreasing trend in calculated eigenvalue for ^{233}U fueled systems as a function of Above-Thermal Fission Fraction remain. The comprehensive nature of this critical benchmark suite and the generally accurate calculated eigenvalues obtained with ENDF/B-VII.1 neutron cross sections support the conclusion that this is the most accurate general purpose ENDF/B cross section library yet released to the technical community.

ENDF/B-VII.1

Nuclear Data Sheets, **112**, 3054 (2011);
Nuclear Data Sheets, **112**, 3120 (2011);
Nuclear Data Sheets, **112**, 3135 (2011).

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

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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.

Energy Dependence of Plutonium Fission-Product Yields

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(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

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(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.

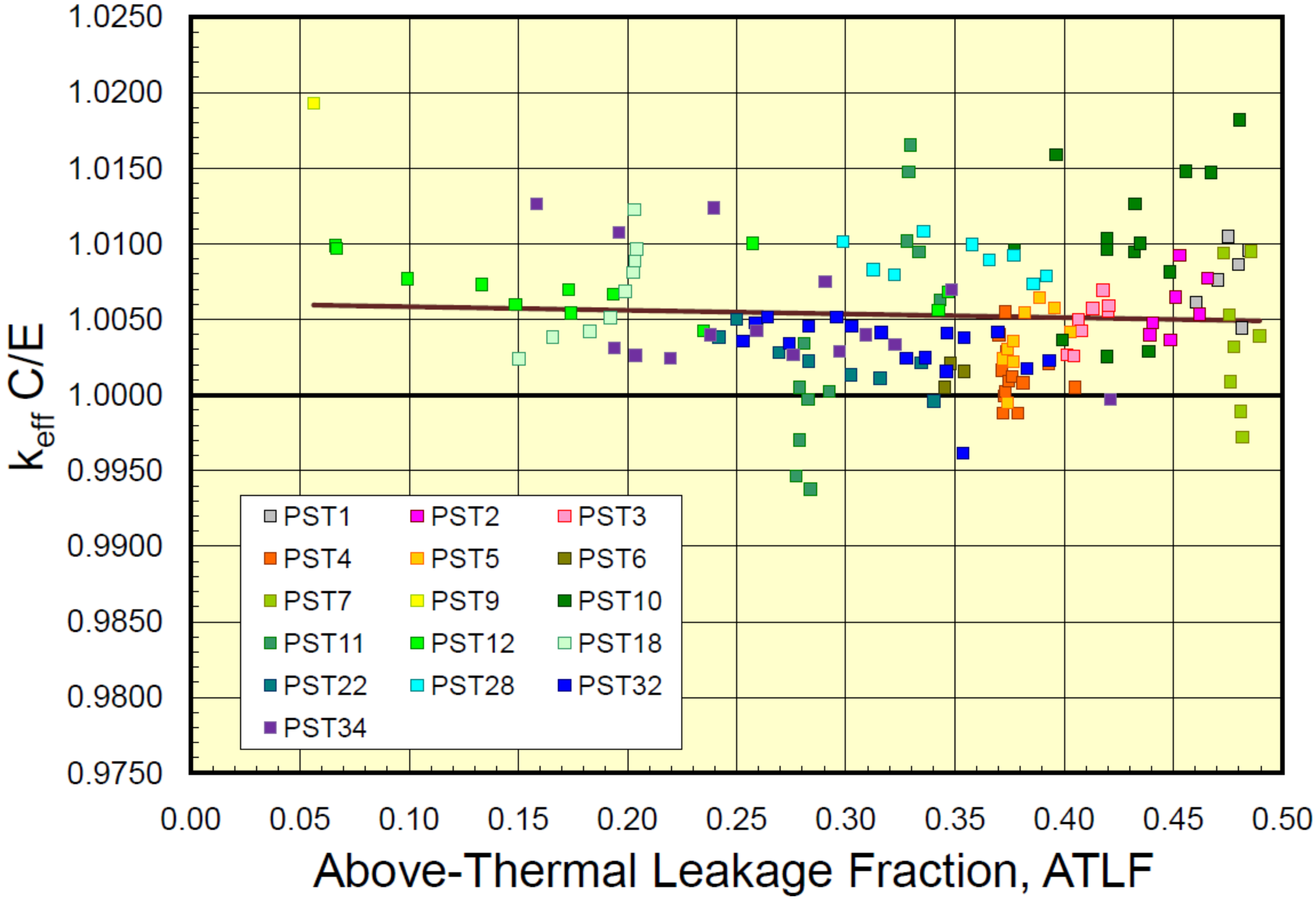
ENDF/B-VII.1

- **LANL Data Testing has focused on ICSBEP Benchmarks and Actinide Reaction Rate Testing**
  - Calculated k_{eff} is accurate for a wide range of ICSBEP Benchmarks
    - The previous (ENDF/B-VI.8 and ENDF/B-VII.0), accurate results have been retained;
      - Many FAST (HEU, Pu) systems
        - … but not all, ☹.
      - HST's
      - LEU's
    - Some deficiencies have been reduced or eliminated;
    - Previously ignored issues have not gone away!

ENDF/B-VII.1 – Areas to Improve

- Pu-SOL-THERM;
- Pu-MET-FAST versus Energy;
- HEU-MET-FAST or LEU-COMP-THERM with Pb reflector;
- HEU-MET-FAST with V reflector;
- HEU-MET-FAST with Ni reflector;
- Fast Be reflected systems;
- ^{233}U Intermediate and Thermal systems;
- See 2011 ENDF/B-VII.1 NDS papers for more …

ENDF/B-VII.1 – Pu-SOL-THERM (I)



ENDF/B-VII.1 – Pu-SOL-THERM (II)

- **Pu-SOL-THERM k_{calc} can be correlated against a number of parameters, including**
  - Above-Thermal Leakage Fraction (ATLF);
  - ^{239}Pu atom-percent in Pu;
  - Above-Thermal Fission Fraction (ATFF);
  - H/Pu Number Density;
  - … more … see Validation Paper.
  - Can pick a small sub-set of the 150+ Pu-SOL-THERM benchmarks for cross section data testing.
  - Luiz Leal (ORNL) is leading a WPEC Sub-Group tasked with resolving this issue.

ENDF/B-VII.1 – Pu-SOL-THERM (III)

- **A set of seven Pu-SOL-THERM benchmarks have been extracted from the larger set.**
  - PST1.4 & PST12.13 span the ATLF space;
  - PST12.10 & PST34.15 span the ATFF space;
  - PST4.1 & PST18.6 span the ^{239}Pu atom percent space;
  - PST12.10 & PST34.4 span the g Pu per liter space.

- **All benchmark experiments are performed in simple geometry**
  - PST1.4 & PST4.1 are a water-reflected spheres;
  - PST18.6, PST34.4 & PST34.15 are water-reflected cylinders;
  - PST12.10 & PST12.13 are a water-reflected slabs;

ENDF/B-VII.1 – Pu-SOL-THERM (IV)

Calculated Eigenvalues[a] for a Selection of PST Assemblies Using Various ^{239}Pu Cross Sections

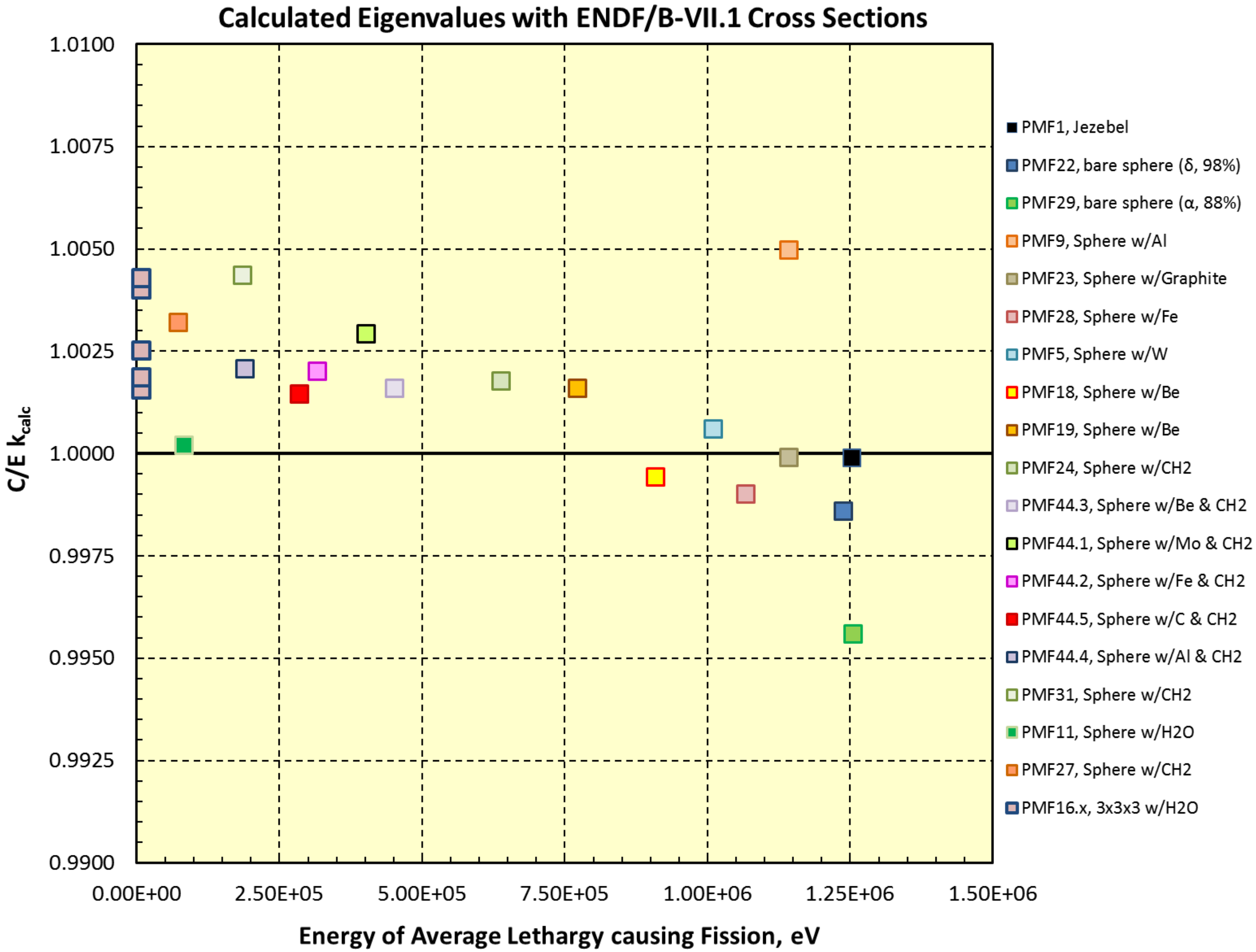
Assembly	ENDF/B-VII.1	JEFF-3.1.2 [b]	JENDL-4.0 [b]	Leal7a [c] + e71	Leal7a (RR, nu, pfns only) + e71
PST1.4	1.00448	1.00127	1.00588	1.00199	1.00202
PST4.1	1.00383	0.99907	1.00482	1.00044	1.00044
PST9	1.01939	1.01367	1.02510	1.01543	1.01546
PST12.10	1.00412	0.99973	1.00498	1.00083	1.00080
PST12.13	1.00955	1.00468	1.01069	1.00611	1.00620
PST18.6	1.00472	1.00153	1.00557	1.00202	1.00208
PST34.4	1.00258	0.99999	1.00417	0.99922	0.99937
PST34.15	0.99742	0.99563	0.99844	0.99679	0.99707
Average	**1.00576**	**1.00195**	**1.00746**	**1.00285**	**1.00293**

a) MCNP calculations are for 250M histories; stochastic uncertainty is ~5 pcm.

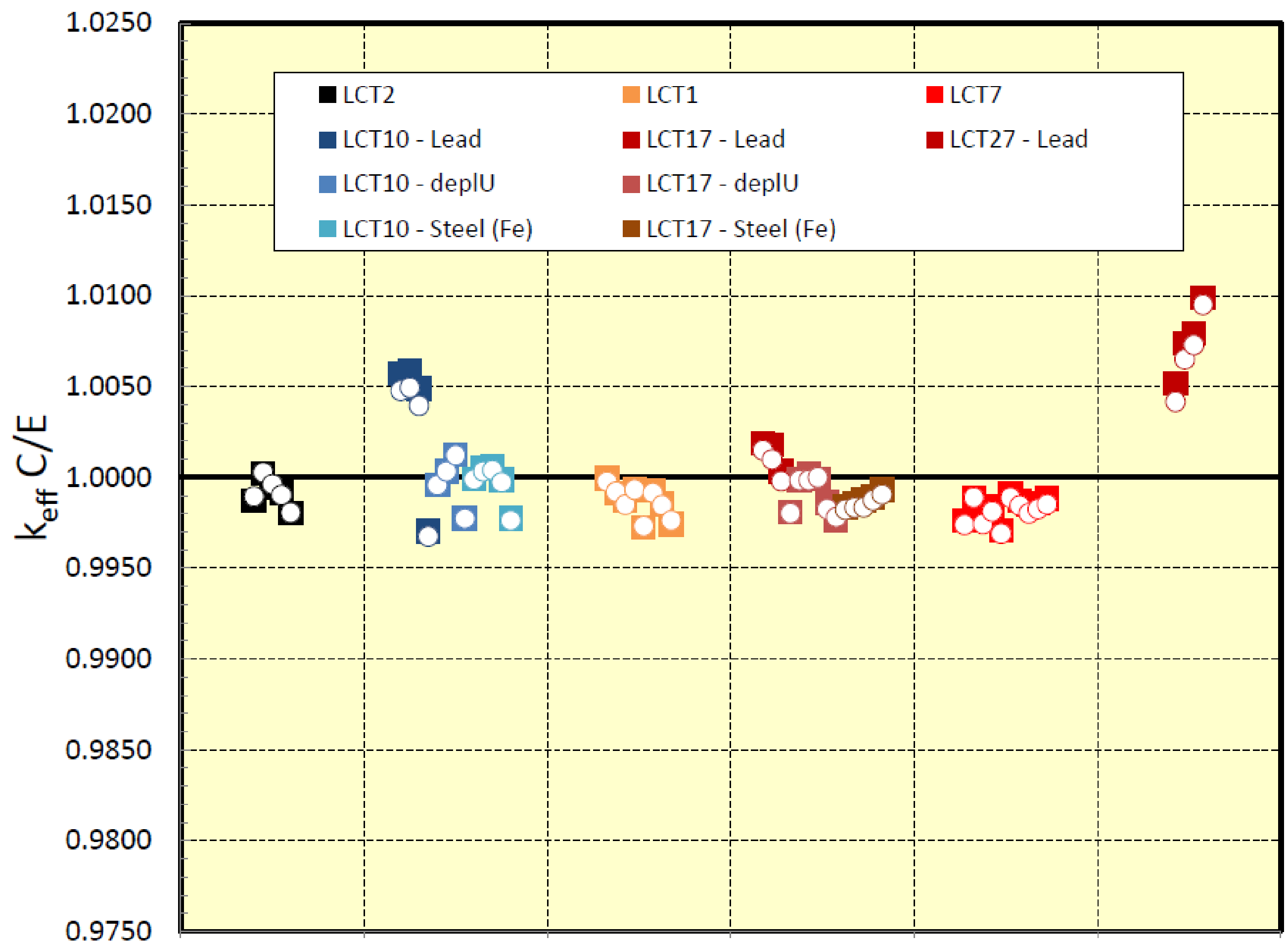
b) JEFF-3.1.2 and JENDL-4.0 ^{239}Pu only; remaining nuclides are ENDF/B-VII.1

c) "LEAL7a" evaluation provides revised resolved resonance parameters coupled to a joint ORNL/CEA evaluated ^{239}Pu file; the "LEAL7a (RR,nu,pfns)" file couples just these data to the existing ENDF/B-VII.1 ^{239}Pu file.

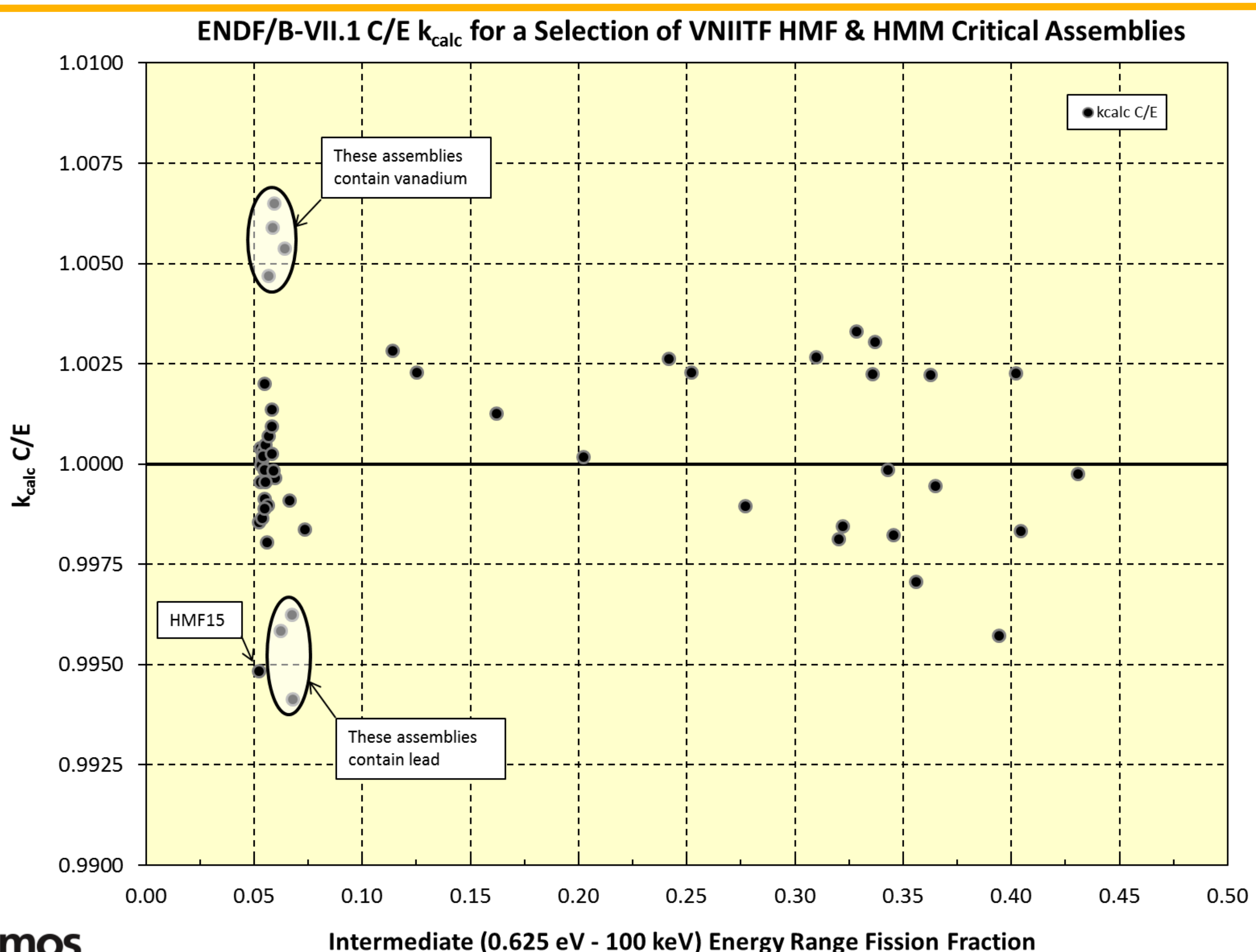
ENDF/B-VII.1 – Pu-MET-FAST



ENDF/B-VII.1 – LCT w/Pb Reflectors



ENDF/B-VII.1 – HMF w/Pb or V Reflectors

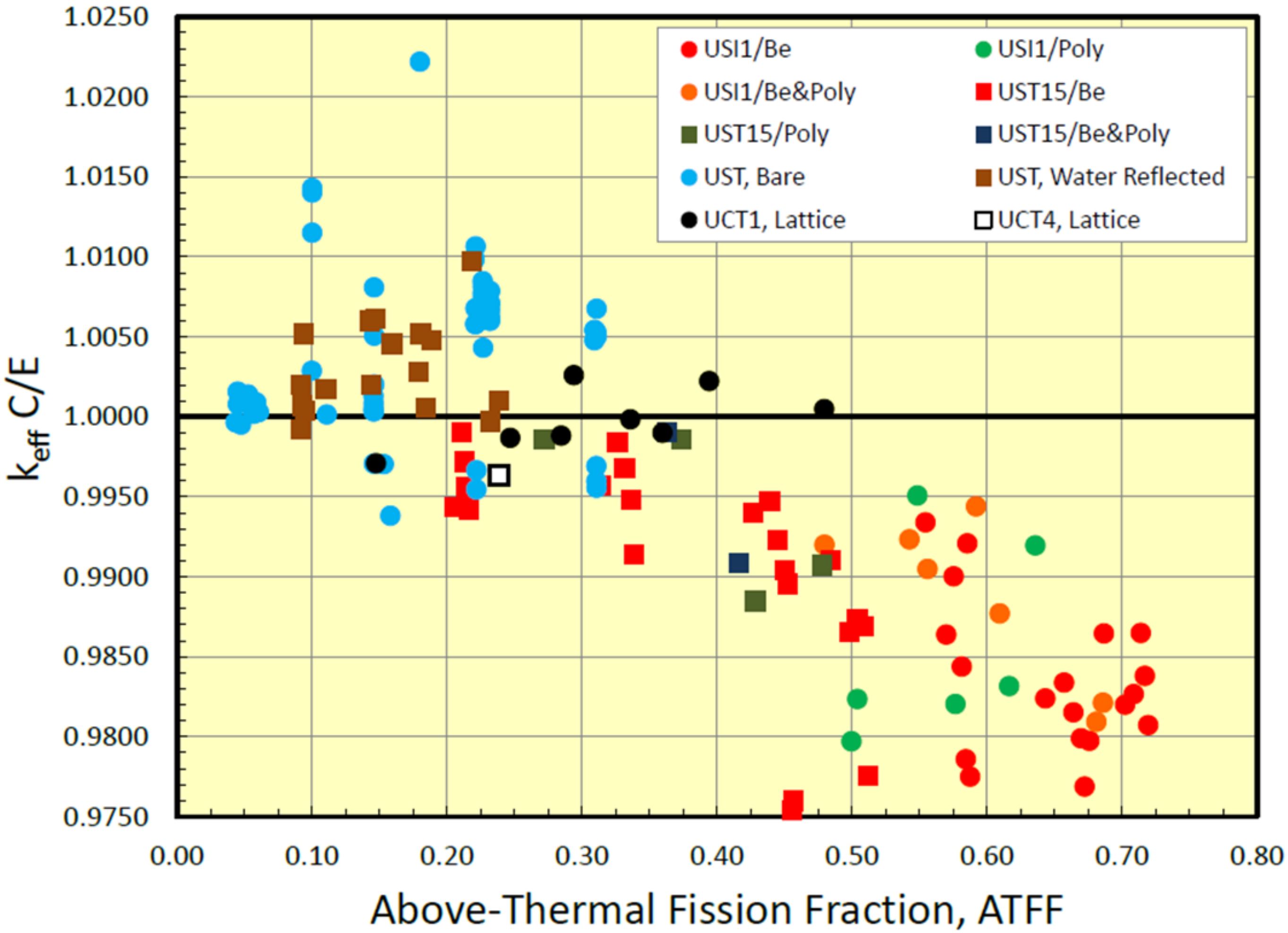


ENDF/B-VII.1 – Ni and Be Reflectors

- **HMF3.12 – Ni reflected HEU "sphere"**
  - Historical k_{calc} is ~1.009;
  - Latest (Kawano) ^{iso}Ni evaluated file with revised high energy scattering distributions yields k_{calc} of ~0.998.

- **Be Reflected Systems**
  - Inconsistent k_{calc} values for a wide range of HMF and PMF reflected systems;
    - ENDF/B-VI.8 is best for some; ENDF/B-VII.0 is best for others
      - Difference in k_{calc} is several hundred pcm.
  - Expect new scattering angular distributions in the next Be file;
  - New experiments are scheduled for NCERC …

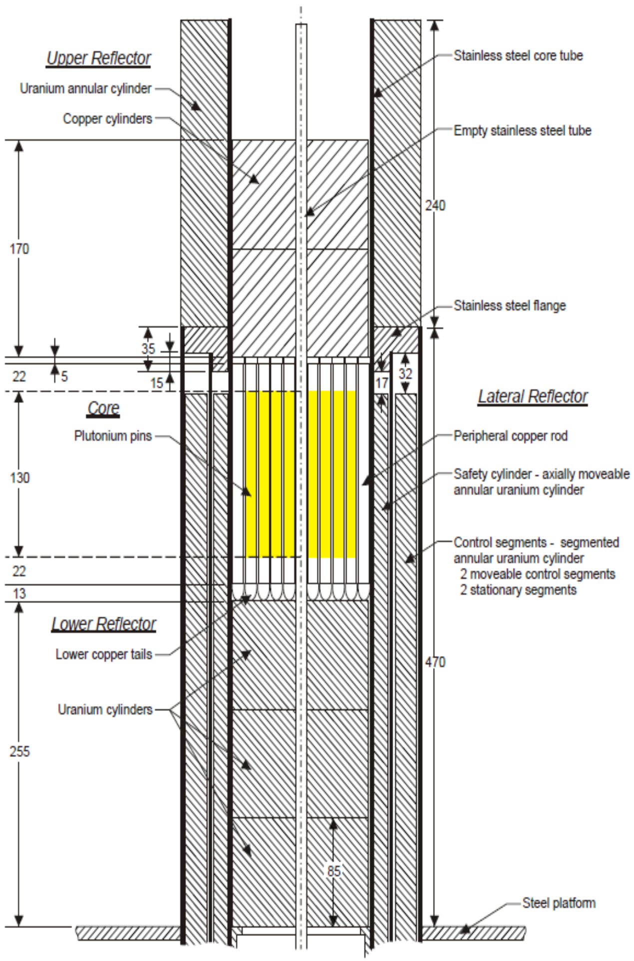
ENDF/B-VII.1 – ^{233}U Systems

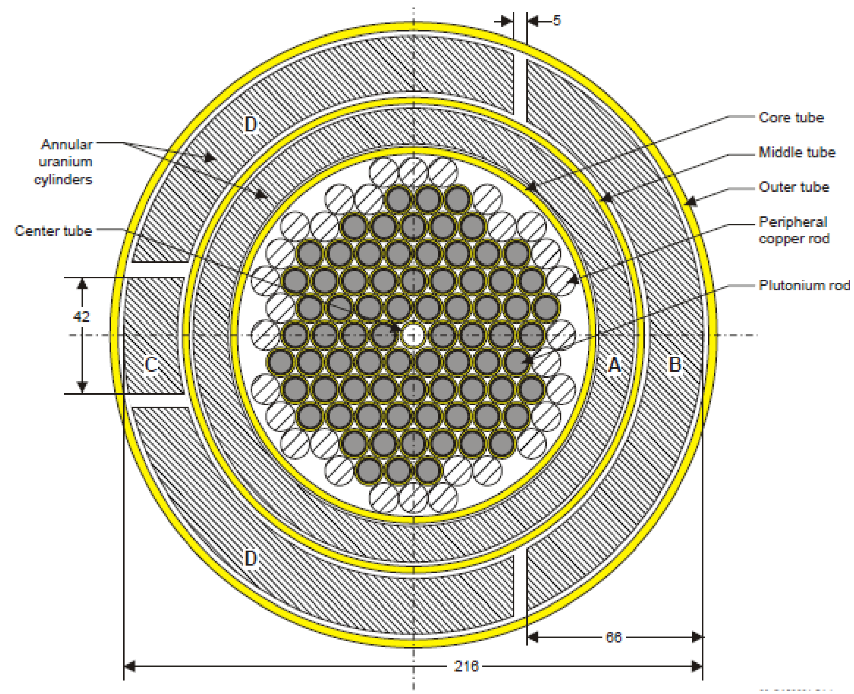


ENDF/B-VII.1

- **LANL Data Testing has focused on ICSBEP Bench-marks and Actinide Reaction Rate Testing (con't)**
  - The FUND-IPPE-FR-MULT-RRR-001 benchmark provides much reaction rate data
    - Need to compare selected ENDF/B-VII.1 cross sections with new IRDFF evaluations.
  - In-house reaction rate data from historical LANL assemblies (Godiva, Flattop-28, Jezebel, Flattop-Pu) are being reviewed and *small* revisions to previous experimental values are likely.

ICSBEP - FUND-IPPE-FR-MULT-RRR-001





Dimensions are in mm.

ICSBEP - FUND-IPPE-FR-MULT-RRR-001

Selected actinide reaction rate ratio C/E results for ENDF/B-VII.1 …

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{232}Th(n,f) / ^{235}U(n,f)	0.0398	0.0000	0.0430	0.0013	0.927	0.028
^{233}U(n,f) / ^{235}U(n,f)	1.5545	0.0002	1.54	0.03	1.009	0.020
^{234}U(n,f) / ^{235}U(n,f)	0.7293	0.0002	0.790	0.024	0.923	0.028
^{236}U(n,f) / ^{235}U(n,f)	0.3216	0.0001	0.333	0.010	0.966	0.029
^{238}U(n,f) / ^{235}U(n,f)	0.1622	0.0001	0.165	0.005	0.983	0.030
^{237}Np(n,f) / ^{235}U(n,f)	0.8134	0.0002	0.771	0.023	1.055	0.031
^{239}Pu(n,f) / ^{235}U(n,f)	1.3603	0.0002	1.33	0.04	1.023	0.031
^{240}Pu(n,f) / ^{235}U(n,f)	0.8110	0.0002	0.877	0.026	0.925	0.027
^{241}Pu(n,f) / ^{235}U(n,f)	1.3219	0.0002	1.29	0.04	1.025	0.032
^{242}Pu(n,f) / ^{235}U(n,f)	0.6859	0.0002	0.658	0.020	1.042	0.032
^{241}Am(n,f) / ^{235}U(n,f)	0.7782	0.0003	0.825	0.025	0.943	0.029
^{232}Th(n,g) / ^{235}U(n,f)	0.1029	0.0000	0.109	0.004	0.944	0.035
^{236}U(n,g) / ^{235}U(n,f)	0.1201	0.0000	0.123	0.006	0.977	0.048
^{238}U(n,g) / ^{235}U(n,f)	0.0777	0.0000	0.077	0.003	1.010	0.039
^{237}Np(n,g) / ^{235}U(n,f)	0.3006	0.0001	0.240	0.012	1.253	0.063
^{232}Th(n,2n) / ^{235}U(n,f)	0.01070	0.00003	0.00924	0.00050	1.158	0.063
^{238}U(n,2n) / ^{235}U(n,f)	0.00948	0.00002	0.00916	0.00050	1.035	0.057

ICSBEP - FUND-IPPE-FR-MULT-RRR-001

Selected reaction rate ratio C/E results for ENDF/B-VII.1 …

Can the new IRDFF files do better???

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{50}Cr(n,g) / ^{235}U(n,f)	0.005200	0.000015	0.0057	0.0005	0.912	0.080
^{55}Mn(n,g) / ^{235}U(n,f)	0.003906	0.000005	0.00297	0.00015	1.315	0.066
^{58}Fe(n,g) / ^{235}U(n,f)	0.003004	0.000008	0.00228	0.00009	1.317	0.052
^{59}Co(n,g) / ^{235}U(n,f)	0.005860	0.000005	0.0064	0.0003	0.916	0.043
^{64}Ni(n,g) / ^{235}U(n,f)	0.003525	0.000013	0.00185	0.00008	1.906	0.083
^{63}Cu(n,g) / ^{235}U(n,f)	0.012032	0.000006	0.0114	0.0005	1.055	0.046
^{65}Cu(n,g) / ^{235}U(n,f)	0.007472	0.000003	0.0076	0.0006	0.983	0.078
^{94}Zr(n,g) / ^{235}U(n,f)	0.009761	0.000010	0.0064	0.0004	1.525	0.095
^{96}Zr(n,g) / ^{235}U(n,f)	0.006169	0.000004	0.00306	0.00015	2.016	0.099
^{98}Mo(n,g) / ^{235}U(n,f)	0.027135	0.000023	0.0193	0.0008	1.406	0.058
^{197}Au(n,g) / ^{235}U(n,f)	0.100919	0.000029	0.105	0.005	0.961	0.046
^{24}Mg(n,p) / ^{235}U(n,f)	0.001006	0.000002	0.00090	0.00004	1.118	0.050
^{27}Al(n,p) / ^{235}U(n,f)	0.002149	0.000002	0.00221	0.00015	0.972	0.066
^{46}Ti(n,p) / ^{235}U(n,f)	0.005814	0.000006	0.0066	0.0003	0.881	0.040
^{47}Ti(n,p) / ^{235}U(n,f)	0.010160	0.000008	0.0097	0.0005	1.047	0.054
^{48}Ti(n,p) / ^{235}U(n,f)	0.000219	0.000000	0.000180	0.000008	1.214	0.054
^{54}Fe(n,p) / ^{235}U(n,f)	0.041835	0.000035	0.0447	0.0015	0.936	0.031
^{56}Fe(n,p) / ^{235}U(n,f)	0.000612	0.000001	0.00061	0.00002	1.003	0.033
^{59}Co(n,p) / ^{235}U(n,f)	0.000776	0.000001	0.00084	0.00004	0.924	0.044
^{58}Ni(n,p) / ^{235}U(n,f)	0.055264	0.000044	0.055	0.003	1.005	0.055
^{27}Al(n,a) / ^{235}U(n,f)	0.00045	0.00000	0.00043	0.0000	1.055	0.049
^{54}Fe(n,a) / ^{235}U(n,f)	0.00053	0.00000	0.00050	0.0000	1.059	0.042
^{59}Co(n,a) / ^{235}U(n,f)	0.000095	0.000000	0.000095	0.00000	1.001	0.042
^{92}Mo(n,a) / ^{235}U(n,f)	0.000085	0.000000	0.000055	0.00001	1.548	0.141

Closing Observations

- **There are many strengths and success stories associated with ENDF/B-VII.1.**

- **There are also a number of remaining deficiencies that should guide future efforts as we begin the next upgrade cycle for ENDF/B.**