LA-UR-12-26244

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

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Abstract

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

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 and data validation effort of the ENDF/B-VII.1 Library.

Introduction - II

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Nuclear Data Sheets

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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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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).

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

Introduction - III

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Nuclear Data Sheets 112 (2011) 2997–3036

Nuclear Data Sheets

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

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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.

Nuclear Data Sheets, **112**, 2997 (2011).

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

Introduction - IV

Nuclear Data Sheets, **112**, 3054 (2011)

Nuclear Data Sheets, **112**, 3120 (2011)

Nuclear Data Sheets, **112**, 3135 (2011)

The NCSP Program benefitted from an overlap in interest with the Physics and Engineering Models (PEM) element of DOE's Advanced Simulation and Computing (ASC) Program.

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

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(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.

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.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)

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 …**

^{238}U – LANL Integral Reaction Rate Data

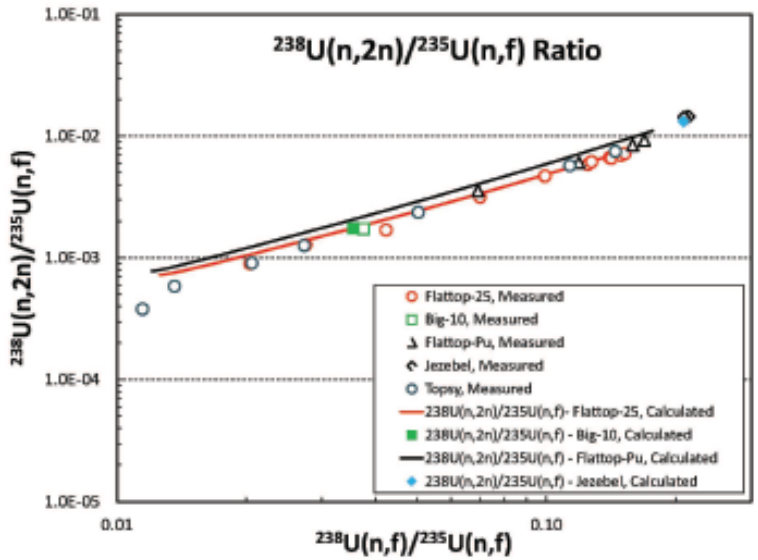

FIG. 57: The ratio of the ^{238}U(n,2n) reaction rate to the ^{235}U fission rate is plotted against the ratio of the ^{238}U fission rate to the ^{235}U fission rate (spectral index) for different positions (with central positions to the right and positions in the reflector to the left).

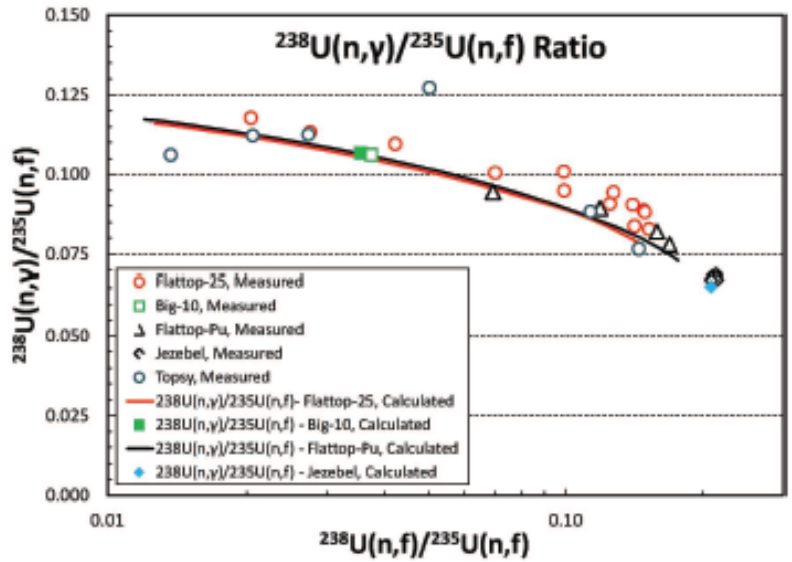

FIG. 58: The integral ^{238}U neutron capture rate (divided by the ^{235}U fission rate) as a function of spectral index for different critical assembly locations.

^{241}Am – LANL Integral Reaction Rate Data

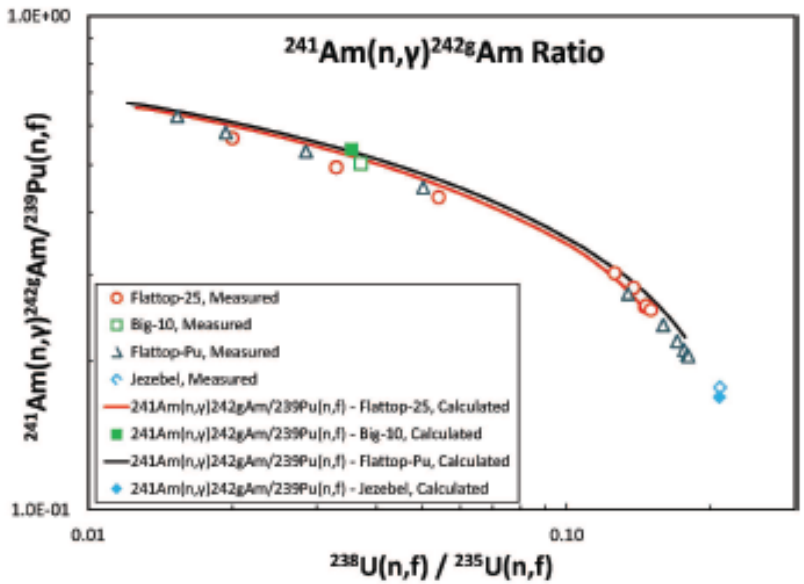

FIG. 93: The integral ^{241}Am neutron capture rate (divided by the ^{239}Pu fission rate) as a function of spectral index for different critical assembly locations. In this case the measurements, which detect the ^{242}Cm are divided by 0.827 to account for the fraction of ^{242g}Am that beta decays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

- See Chadwick *et al* paper for additional results …

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

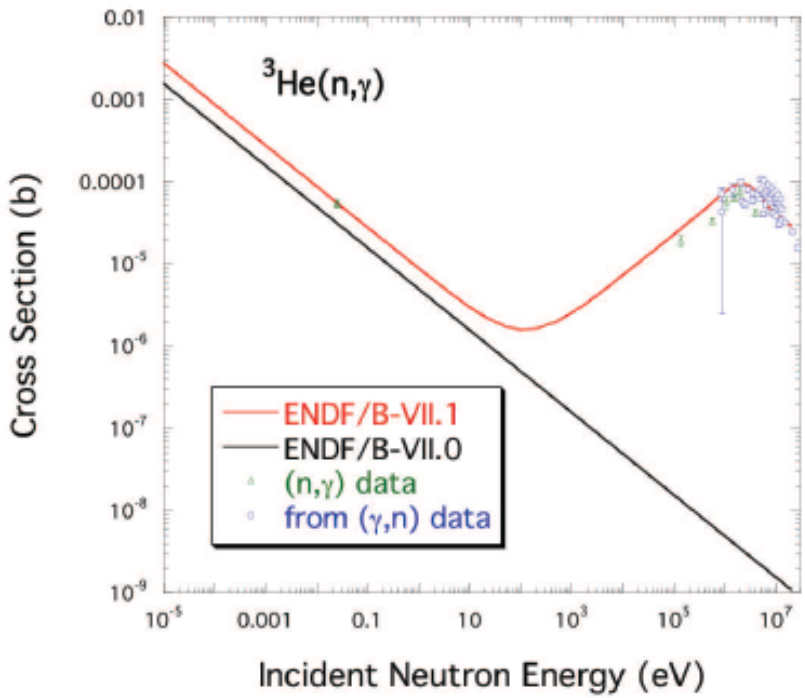

FIG. 4: Neutron capture on ^{3}He. Compared are cross sections in ENDF/B-VII.1 (red curve) with those in ENDF/B-VII.0 (black line), and with experimental data from $n+^{3}$He capture (green triangles) and inverted $\gamma+^{4}$He photodisintegration (blue circles).

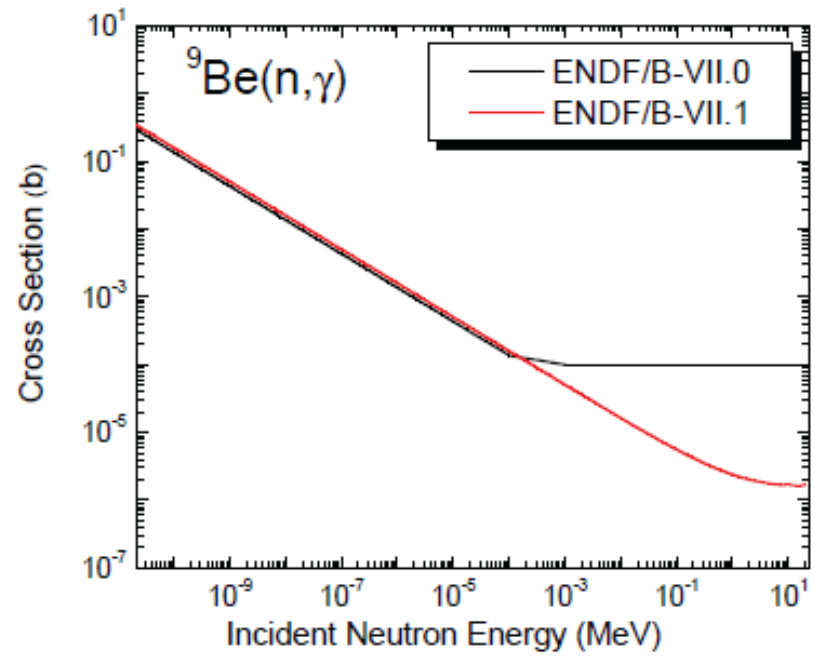

FIG. 10: Neutron capture on ^{9}Be. The red curve is ENDF/B-VII.1, the black curve is ENDF/B-VII.0, and the circles are measured values.

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

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

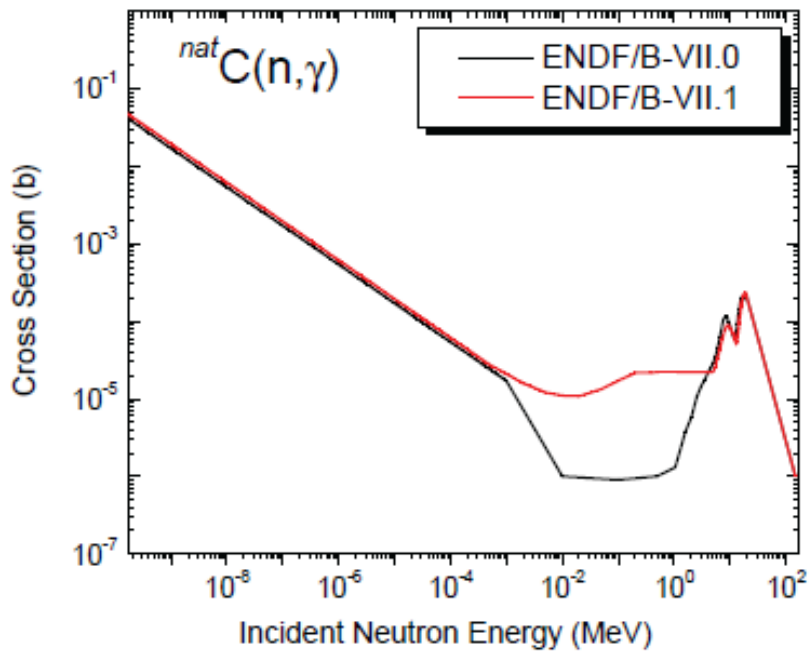

FIG. 11: Neutron capture on ^{nat}C. Compared are cross sections in ENDF/B-VII.1 with ENDF/B-VII.0.

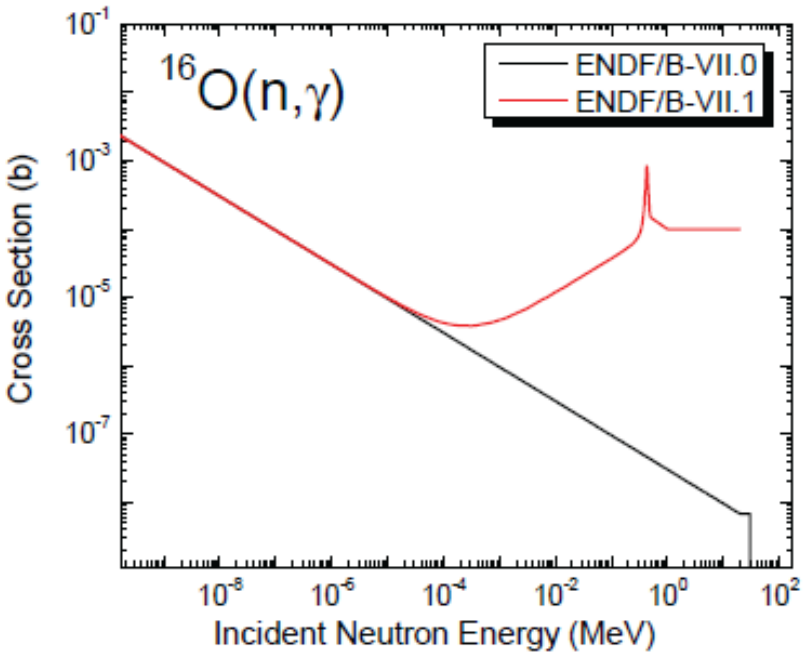

FIG. 12: Neutron capture on ^{16}O. Compared are cross sections in ENDF/B-VII.1 with ENDF/B-VII.0.

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

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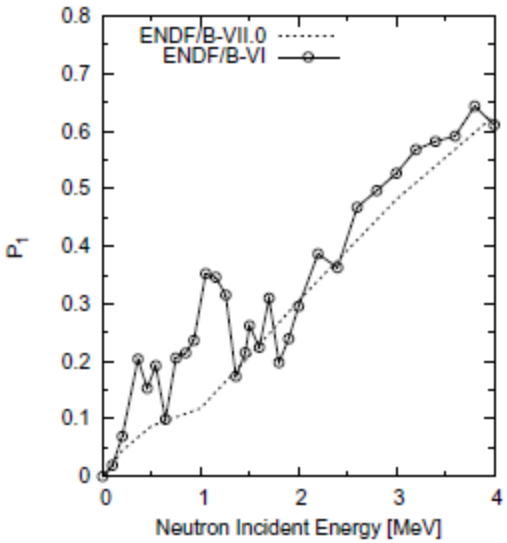


FIG. 15: The $L = 1$ component of the Legendre expansion coefficients for the differential elastic scattering from ^{48}Ti, as a function of neutron incident energy.

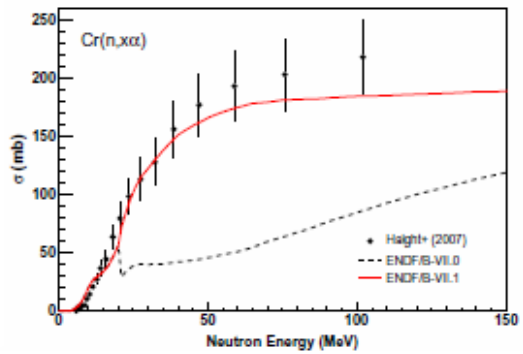


FIG. 35: Calculated alpha production cross section for neutrons on chromium, compared to Haight's data from LANSCE.

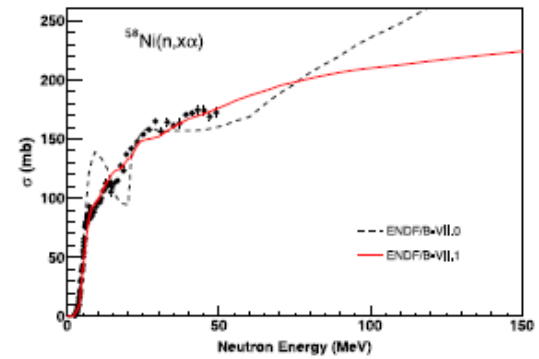


FIG. 36: Calculated alpha production cross section for neutrons on ^{58}Ni, compared to Haight's data from LANSCE.

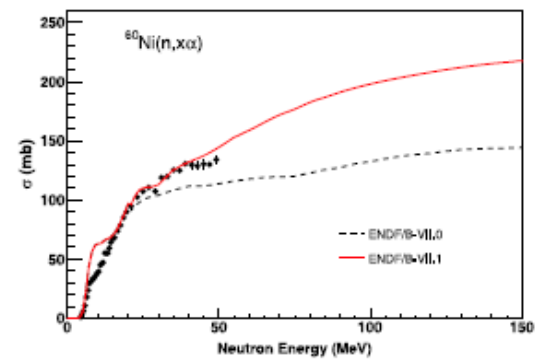


FIG. 37: Calculated alpha production cross section for neutrons on ^{60}Ni, compared to Haight's data from LANSCE.

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

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).

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.**

LANL Data Validation Work

- **Mostly ICSBEP Benchmark Eigenvalue Calculations using MCNP5**
  - All data files were processed into ACE format using NJOY.
  - Linear-linear interpolation tolerance set to 0.1%.
  - Only room temperature (INL used 900K & 1500K data).

- **ICSBEP Nomenclature Reminder – XXX-YYY-ZZZ-###**
  - XXX = Fuel (HEU, IEU, LEU, Pu, MIX(U/Pu), U233, SPEC).
  - YYY = Fuel Form (MET (metal), COMP (compound), SOL (solution)).
  - ZZZ = Spectrum (FAST, INTER, THERM).
  - ### = sequential index.

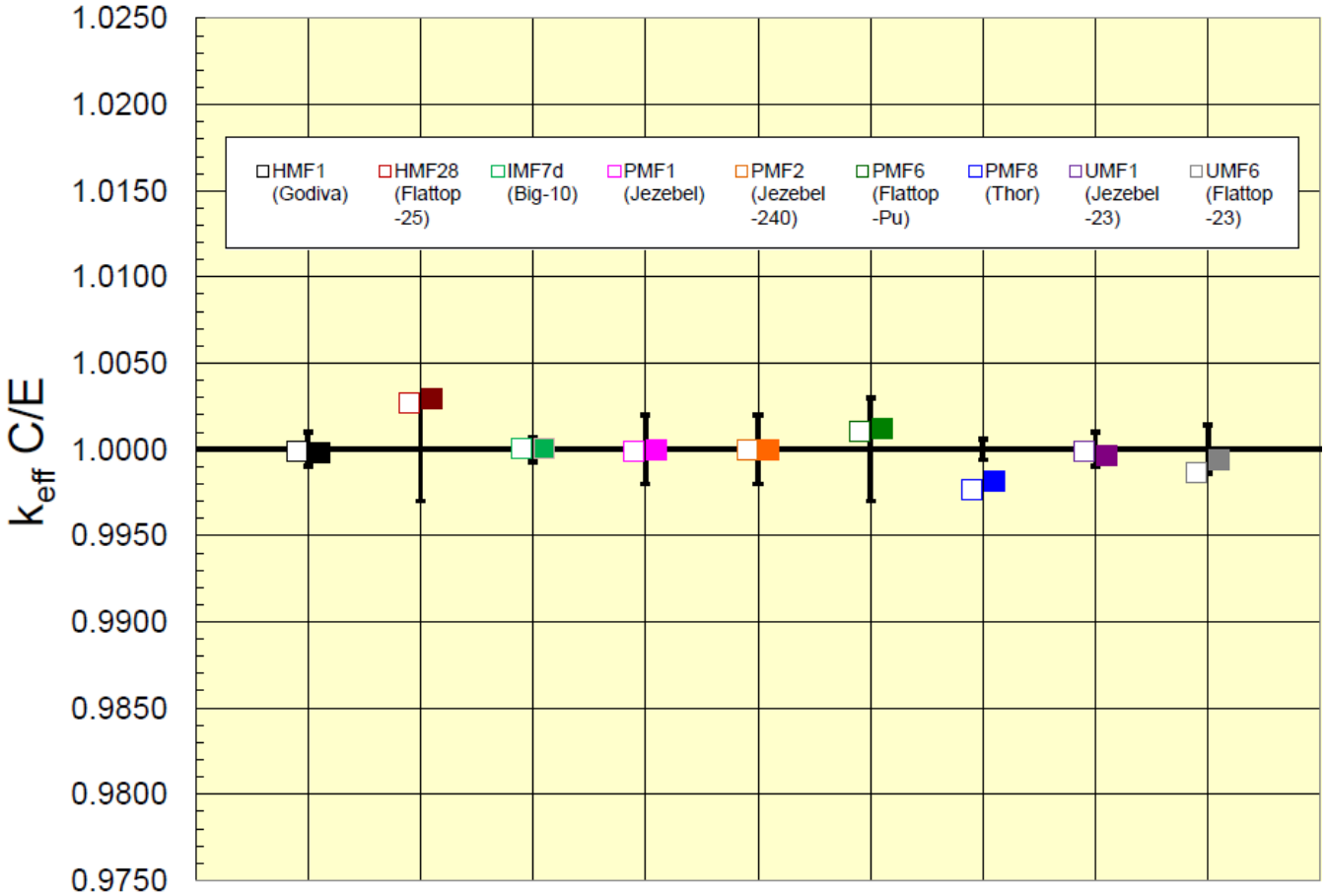
LANL Data Validation Work

- **ICSBEP usefulness is extended by using multiple benchmarks where an easily measured attribute varies**
  - HMF7 – ORNL experiment with HEU plates and polyethylene.
    - Multiple cases with varying polyethylene causes systematic change in average fission energy
  - HMF66 or HMF77 – LLNL experiments with varying amounts of Be
  - HMF34, HMF79, HMM15 – Russian experiments with Titanium and polyethylene
    - Ti is axial reflector (variable thickness) or diluent with varying polyethylene
    - Other HEU/HMM or other fuel systems with varying structural materials and polyethylene (Al, V, Fe, W)

LANL Data Validation Work

- **Three Types of Results**
  - "Do No Harm" – If we had accurate eigenvalue predictions with previous cross section files, are we still accurate?
    - Maybe no change to the important data files, or have eliminated cancelling errors.
  - If we had poor results before, have we made changes (**consistent with the underlying microscopic data!**) that lead to improved eigenvalue predictions?
  - If we had poor results before, and have made no changes in the important cross sections, are the previous results confirmed?
    - At least we have processed the basic nuclear data files in a consistent manner.

A “Do No Harm” Example - FAST

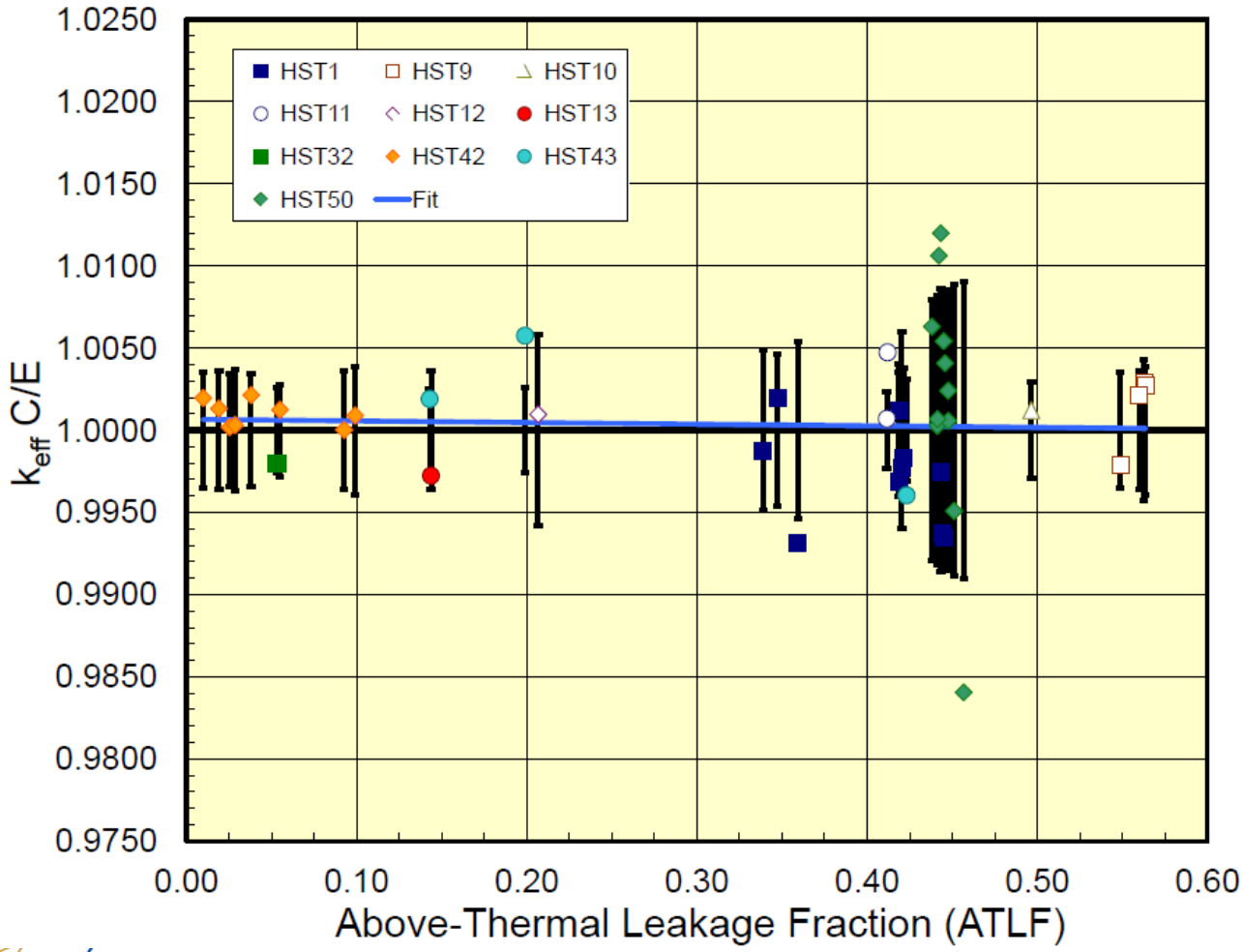


“Open” squares are E71; “Solid” squares are E70.

LANL Historical Critical Assemblies

Previous good results are retained (as expected).

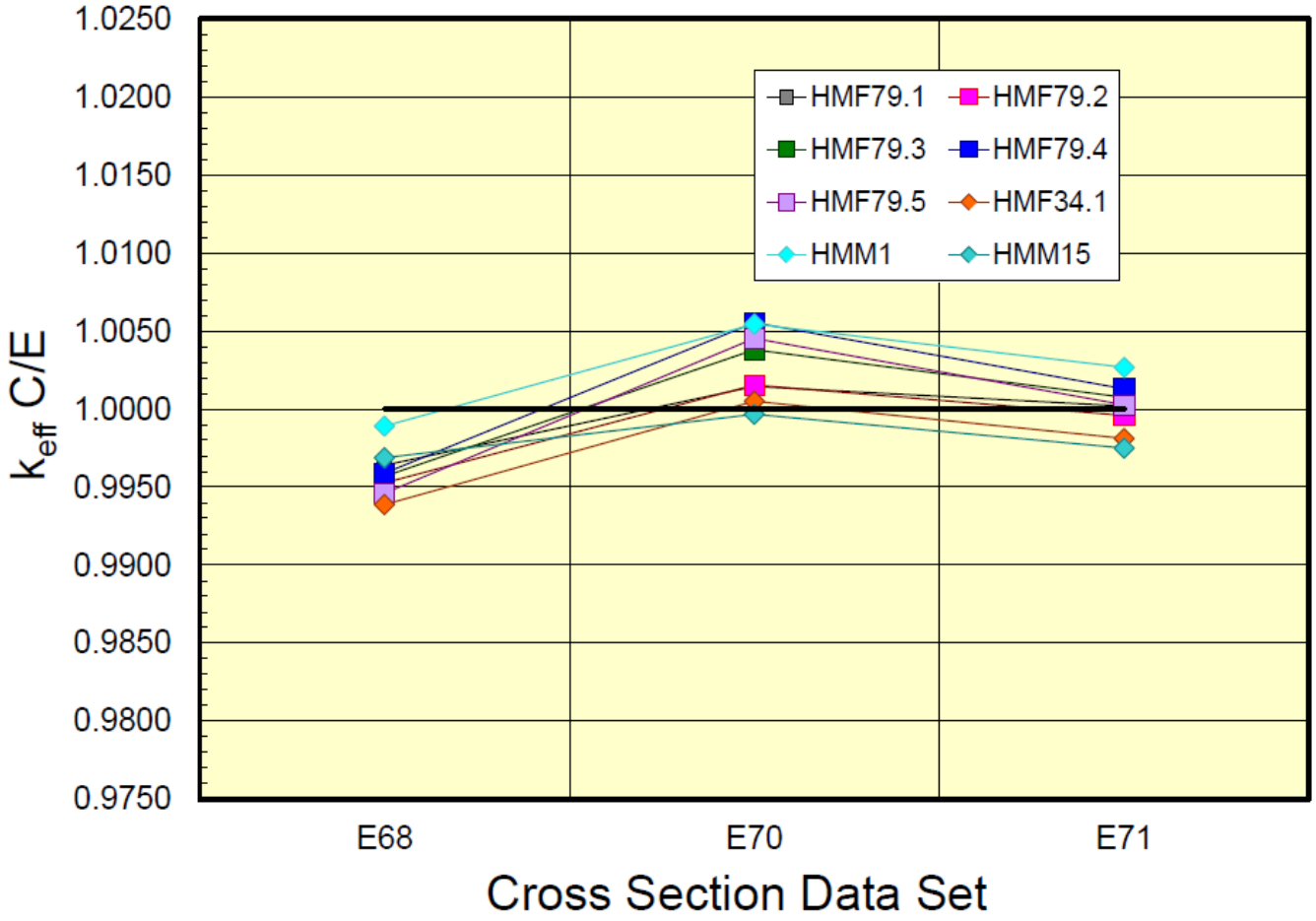
A "Do No Harm" Example - THERMAL



E71 Regression Coefficients are identical to those obtained with E70 Cross Sections.

Previous good results are retained (as expected).

Improved ("Goldilocks") Example



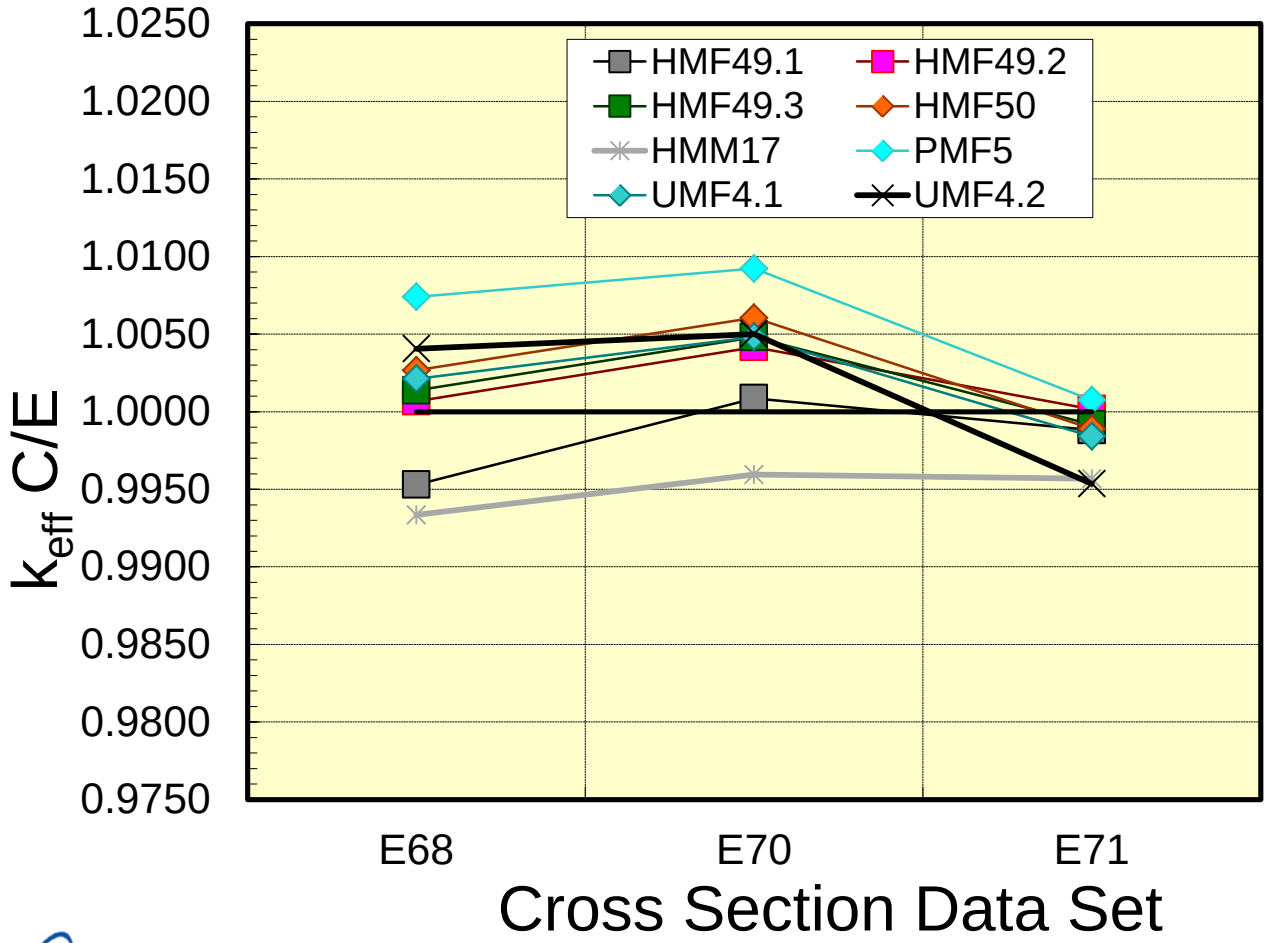
Ti bearing assemblies

ENDF/B-VI.8 is "too cold"

ENDF/B-VII.0 is "too hot"

ENDF/B-VII.1 is "just right"!

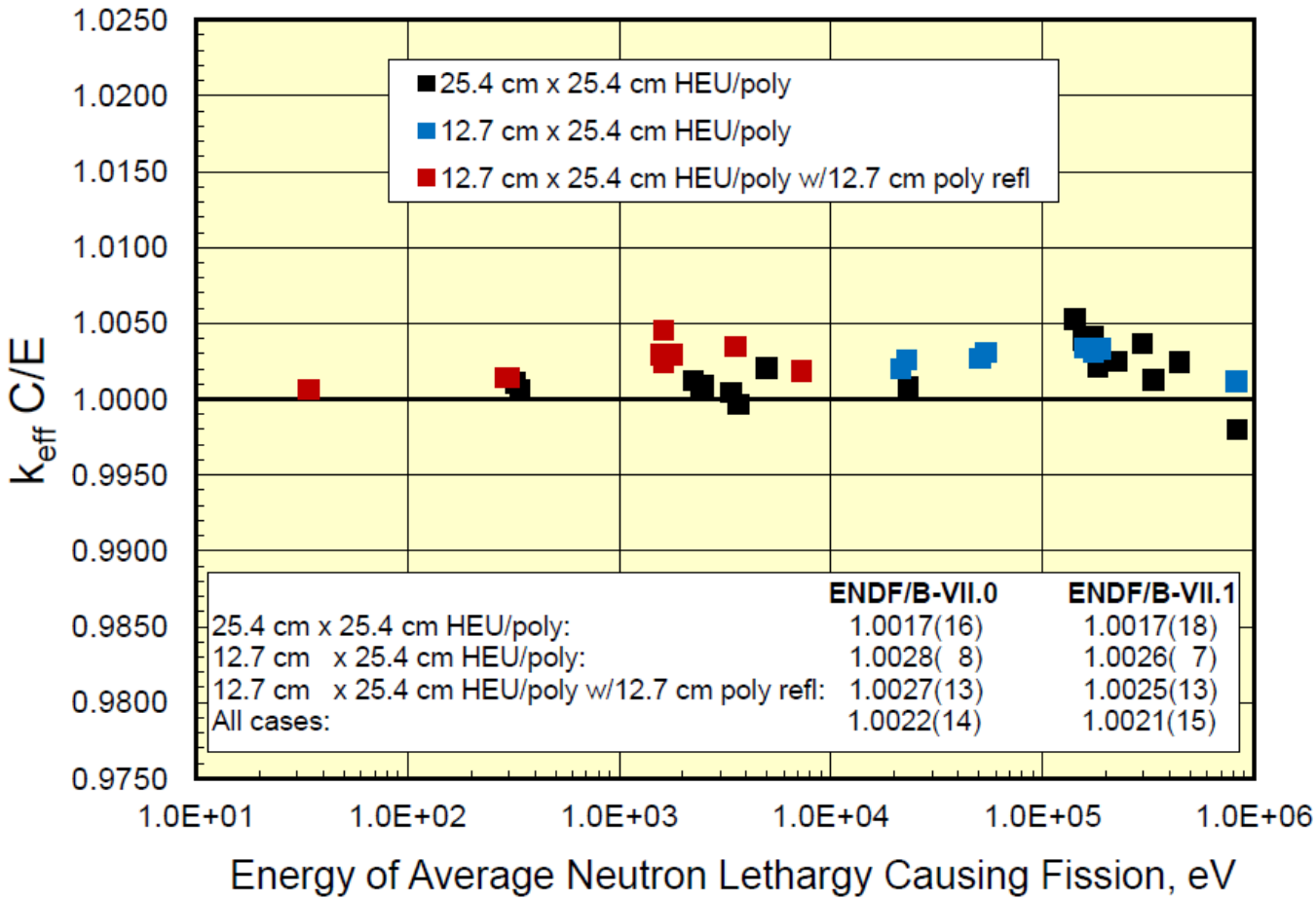
W Bearing Assemblies – Another Success



E71 Calculated Eigenvalue Spread is significantly reduced compared to E70 or E68.

Revised W evaluations were contributed to the ENDF/B community by the IAEA.

A Large Variation in Energy

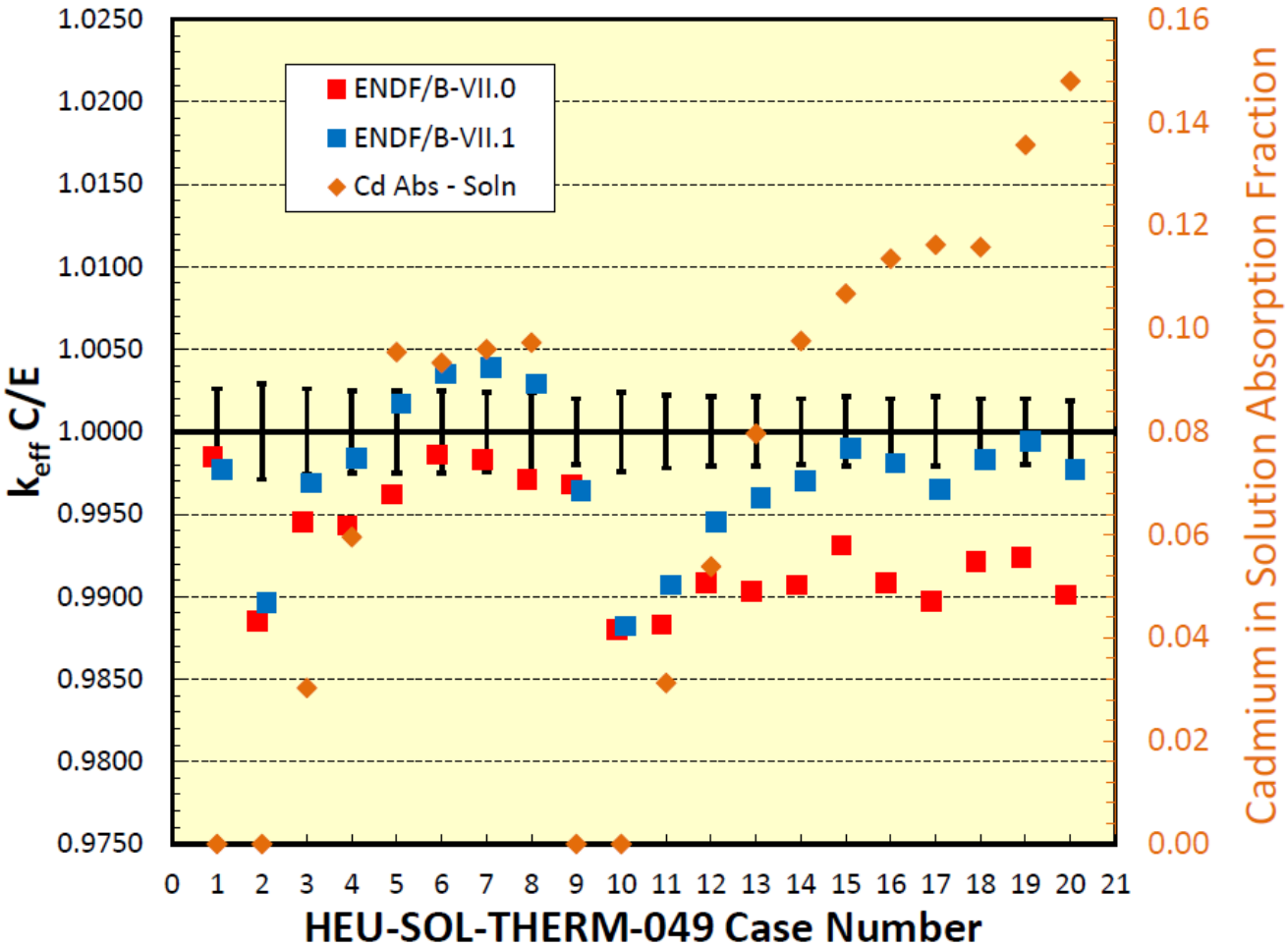


HMF7 (ORNL)

Moderation via varying amounts of CH_2 placed between and surrounding a set of HEU plates.

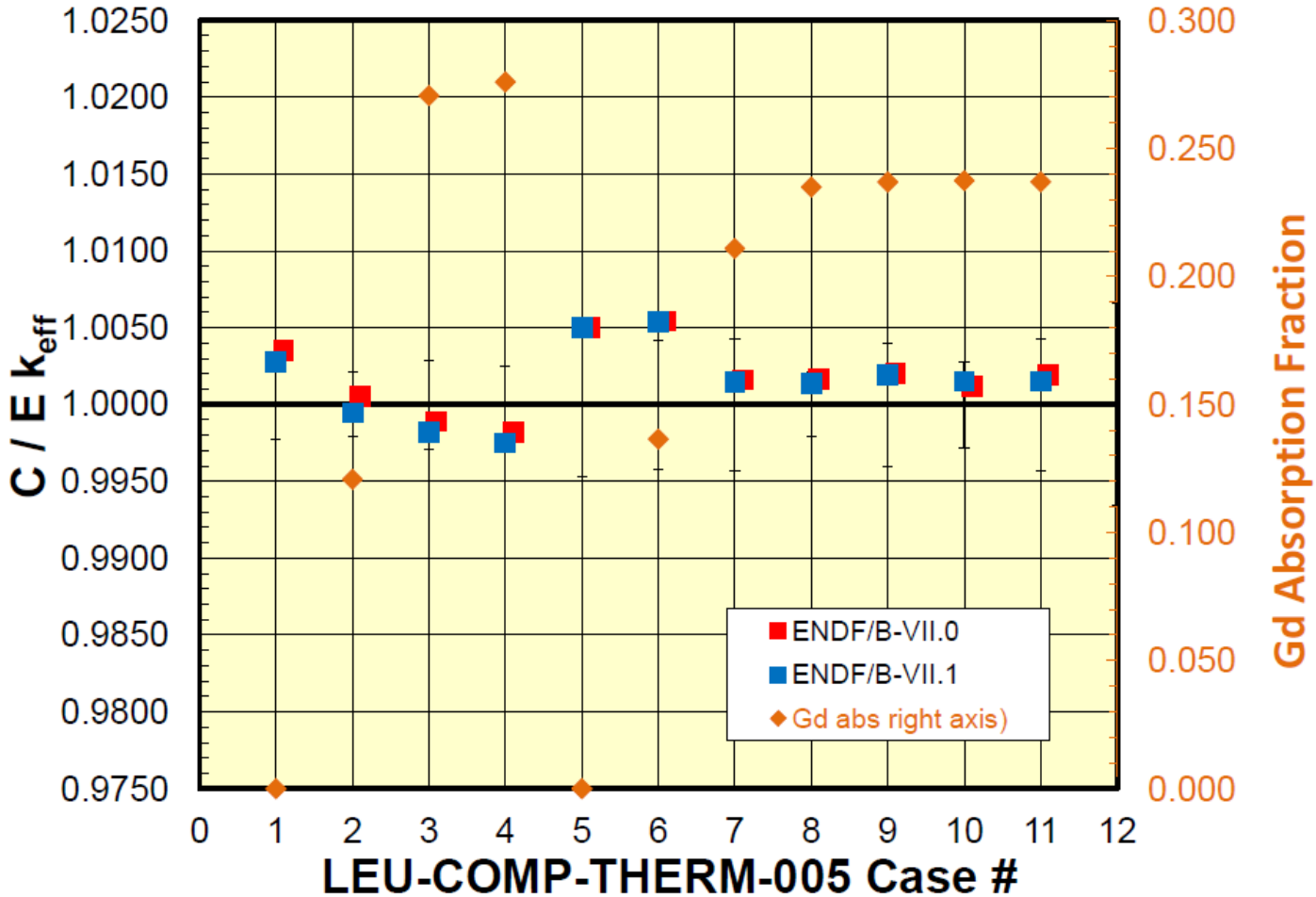
E71 (or E70) eigenvalues are about 300 pcm larger than E68.

Poisoned Solution and Lattice Systems - I



Large variation in calculated eigenvalues, but in general E71 based results are superior to E70.

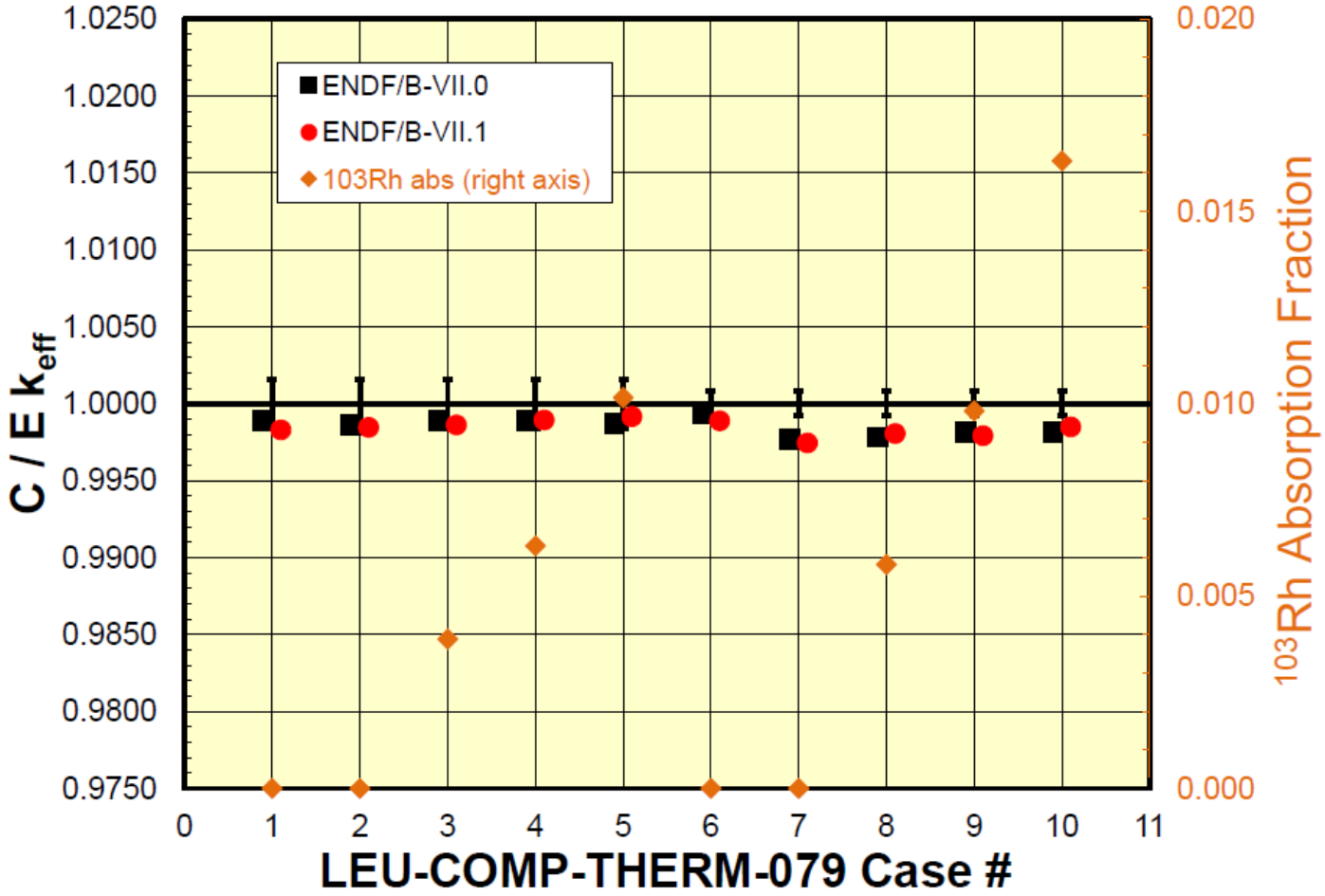
Poisoned Solution and Lattice Systems - II



"Base Case" (LCT2) calculated eigenvalue is about 200 pcm less.

Potential decrease in Gd absorption would make this comparison even worse.

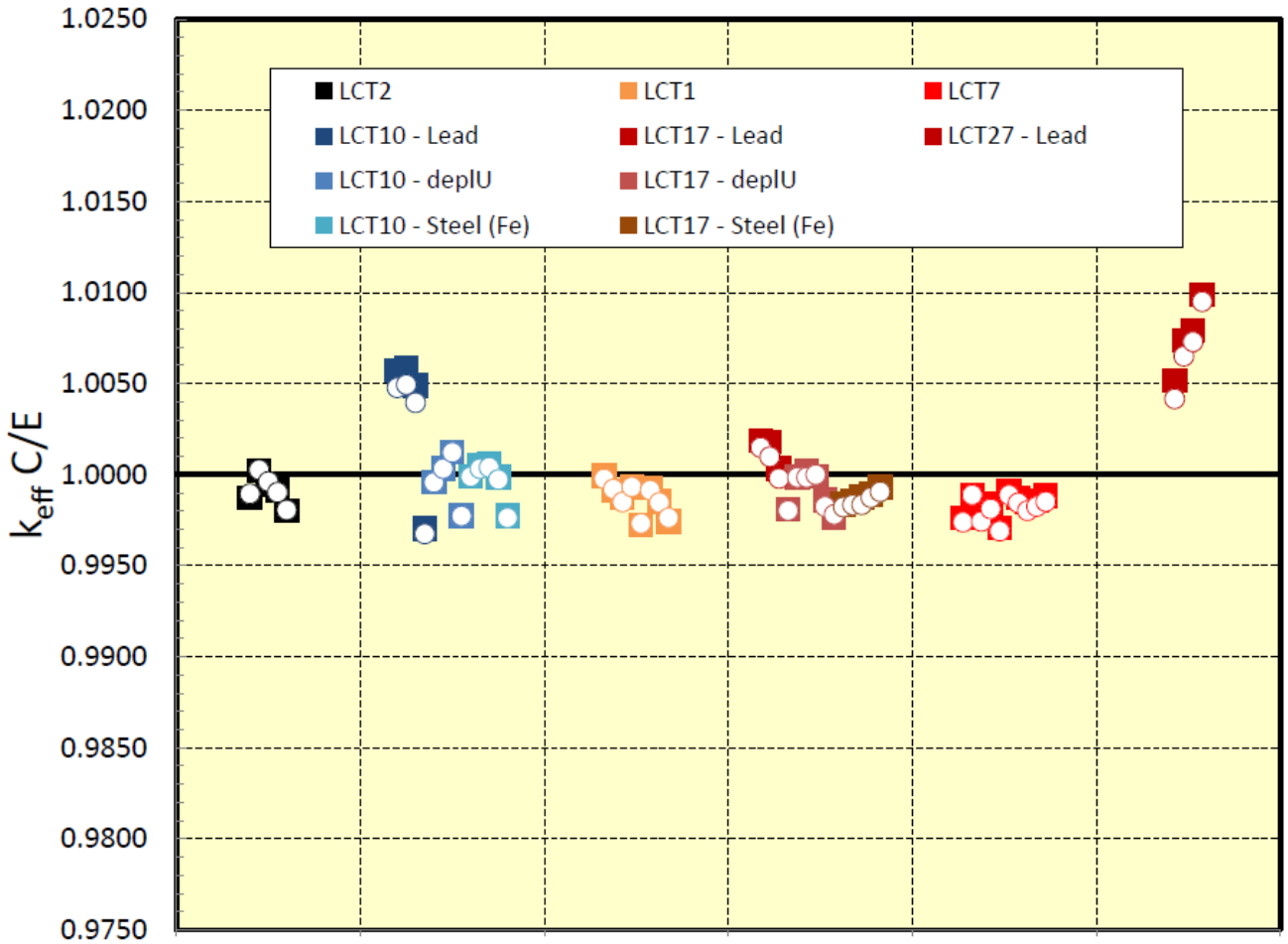
Poisoned Solution and Lattice Systems - III



LCT79 Calculated Eigenvalues

UO_2 lattice assembly with varying amounts of ^{103}Rh (a fission product poison).

Where We Need More Work - Lead

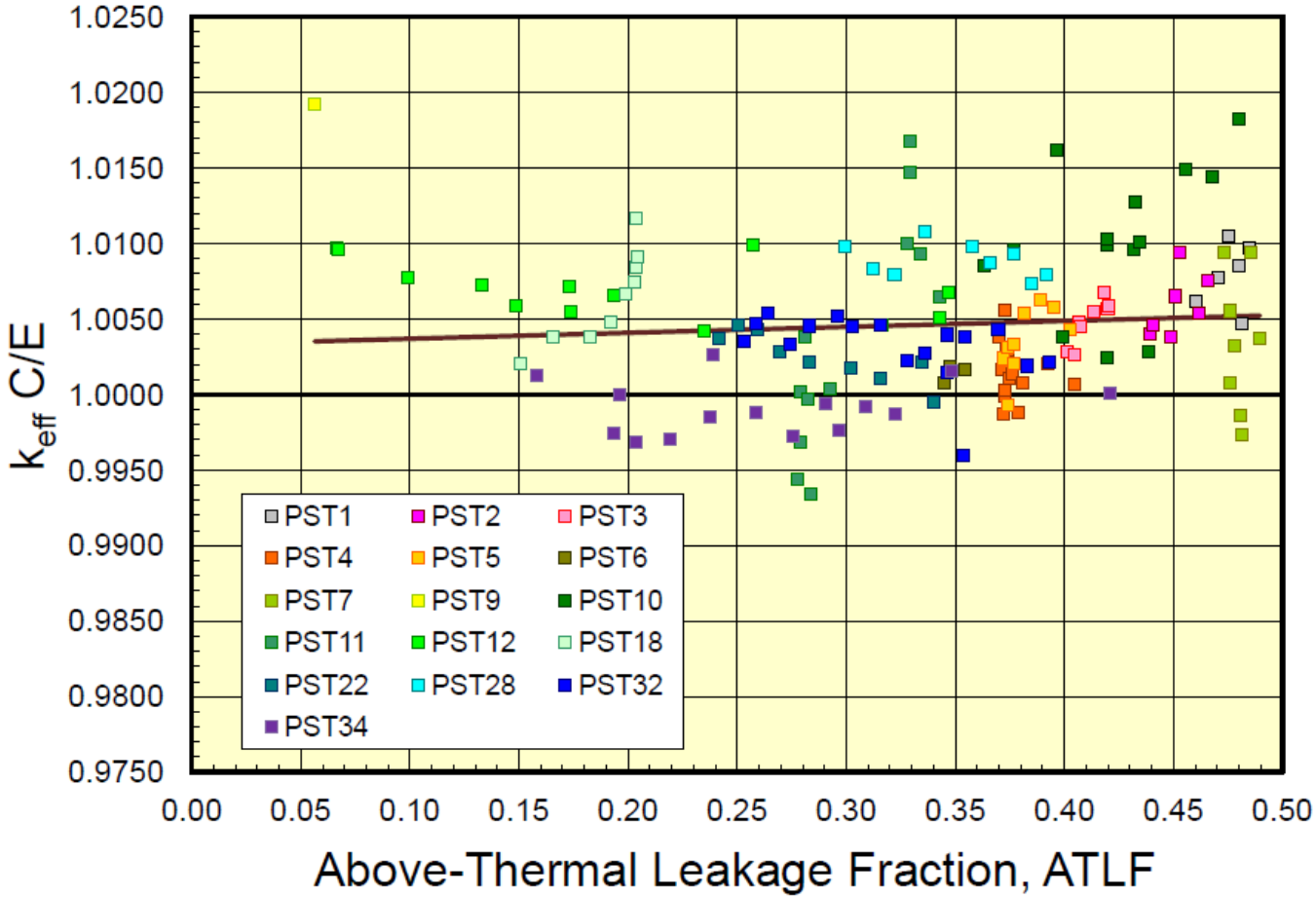


Water moderated attice systems with and without metal reflectors.

Steel (Fe) and ^{depl}U results are good; Pb results are poor.

HMF with Pb is also poorly predicted.

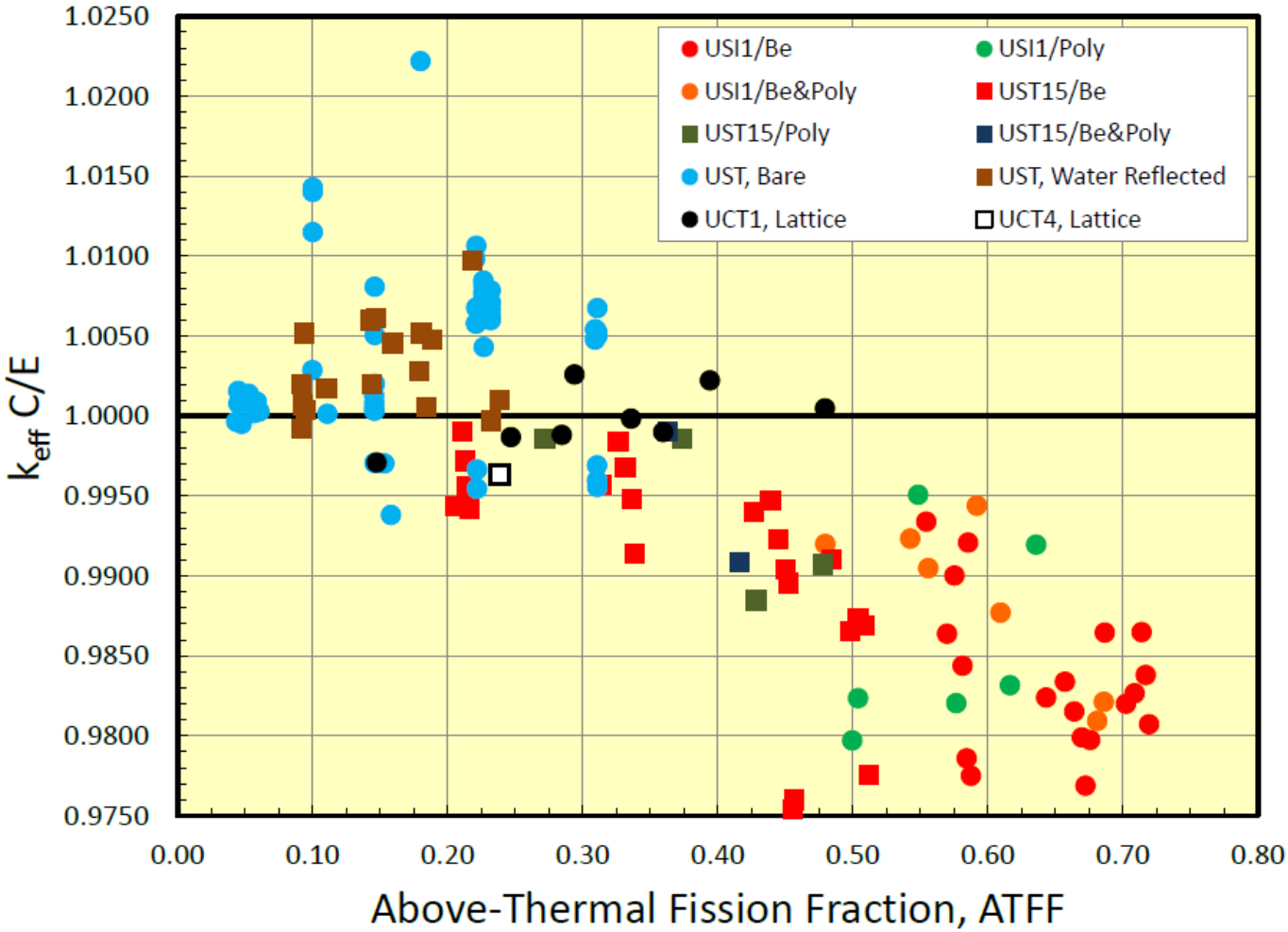
Pu Solution Systems



Calculated Eigenvalues are historically biased high by 500 pcm or so; no change, as expected, in the current results.

This is the subject of a WPEC Sub-Group (ORNL/LANL/ ANL/Europe).

^{233}U Intermediate and Thermal Systems



A long-standing bias in calculated eigenvalues; little change in E71 results.

Black circles are UCT (LWBR) related; a successful though little publicized NR program); were we lucky?

LANL Data Testing Conclusions

- **Good E71 Calculated Eigenvalues for FAST (HEU, Pu, ^{233}U; Bare and natU Reflected) Systems (as expected)**
- **Good E71 Calculated Eigenvalues for HST Systems (as expected)**
- **Good E71 Calculated Results for Uranium Systems from FAST to THERMAL**
  - Accurate CH_2 and Ti/CH_2 results.
- **Good E71 Calculated Eigenvalues for LCT Systems**
  - Accurate Steel (Fe) and ^{depl}U reflected system calculated eigenvalues.

LANL Data Testing Conclusions

- **But we're not done yet!**
  - FAST and THERMAL Pb reflected system calculated eigenvalues exhibit large scatter (biased both high and low).
  - Pu solution system calculated eigenvalues are biased high.
    - A long-standing unresolved issue.
  - ^{233}U thermal and intermediate spectrum calculated eigenvalues exhibit a significant trend with Above-Thermal Fission Fraction.
  - Unresolved questions remain with respect to the true thermal absorption cross section for ^{155}Gd.
    - Microscopic data from RPI supports a decreased value; integral data testing supports the current value or a small increase.
  - Variation in Be reflected system's k_{calc} is large and not fully understood.
  - Differences among ENDF/B, JEFF and JENDL even though all libraries yield generally accurate k_{calc} values.

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 to CSEWG through the Evaluation, Data Validation and Covariance Committees**
  - AECL, ANL, Bettis, BNL, KAPL, INL, ORNL
  - Overseas colleagues (IAEA, JEFF, JENDL, KAERI, NRG/Petten, UK, Slovenia)