

LA-UR-12-22550

Approved for public release; distribution is unlimited.

Title: ICSBEP Criticality Benchmark Eigenvalues with ENDF/B-VII.1 Cross Sections

Author(s): Kahler, Albert C. III
MacFarlane, Robert

Intended for: ANS 2012 Annual Meeting, 2012-06-24/2012-06-28 (Chicago, Illinois, United States)



Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

ICSBEP Criticality Benchmark Eigenvalues with ENDF/B-VII.1 Cross Sections

ANS 2012 Annual Meeting
June, 2012

A. C. (Skip) Kahler & R. E. MacFarlane
Theoretical Division
Los Alamos National Laboratory

Abstract

We review MCNP eigenvalue calculations from a suite of International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook evaluations with the recently distributed ENDF/B-VII.1 cross section library.

ENDF/B-VII.1

ENDF/B-VII.1 was released through the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory in December, 2011.

Was accompanied by a series of peer-reviewed technical papers in the December 2011 issue of Nuclear Data Sheets.

The validation related paper is shown. LANL's contribution to this effort focused on critical eigenvalue calculations, primarily using ICSBEP benchmarks.



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

A. C. Kahler,^{1,*} R. E. MacFarlane,¹ R. D. Mosteller,¹ B. C. Kiedrowski,¹ S. C. Frankle,¹ M. B. Chadwick,¹ R. D. McKnight,² R. M. Lell,² G. Palmiotti,³ H. Hiruta,³ M. Herman,⁴ R. Arcilla,⁴ S. F. Mughabghab,⁴ J. C. Sublet,⁵ A. Trikov,⁶ T. H. Trumbull,⁷ and M. Dunn⁸

¹*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

²*Argonne National Laboratory, Argonne, IL 60349, USA*

³*Idaho National Laboratory, Idaho Falls, ID 83415, USA*

⁴*Brookhaven National Laboratory, Upton, NY 11973, USA*

⁵*Culham Center for Fusion Energy, Abingdon, OX14 3DB, UK*

⁶*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*

⁷*Knolls Atomic Power Laboratory, Schenectady, NY 12309, USA*

⁸*Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

(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 , $^{238,242}\text{Pu}$ and $^{241,243}\text{Am}$ 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.

ICSBEP Introduction

- **The International Criticality Safety Benchmark Evaluation Project**
 - Started as a DOE activity in the early 1990s
 - First edition of the Handbook was seven bound volumes, published in ~1995.
 - An ongoing DOE/OECD NEA Activity
 - Technical contributions from ~20 countries
 - The Handbook is revised and updated annually
 - Technical review group annual meeting typically reviews 15 to 20 new evaluations each year
 - 2011 Edition contains ...
>60,000 pages; 532 evaluations; >4500 configurations
 - Distributed on DVD through the OECD/NEA Data Bank

<http://icsbep.inel.gov/>

ICSBEP Introduction

- The basic organization of the Handbook is by Fuel type:
 - HEU, IEU, LEU (uranium) systems ...
 - > 90 w/o, 10 w/o to 90 w/o, < 10 w/o ^{235}U
 - Pu systems
 - Mixed (U-Pu) systems
 - ^{233}U systems
 - SPEC (Special Isotope Systems)
- For each Fuel type there is a further breakdown:
 - Composition
 - Metal, Oxide, Solution, Misc (miscellaneous)
 - Spectrum
 - Fast, Intermediate, Thermal (or Mix) energy ranges
 - Defined by having at least 50% of the flux above 100 keV, between 0.625 eV and 100 keV, below 0.625 eV

ICSBEP Introduction

- **ICSBEP Nomenclature – 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.
- **Can get by with XYZ#**
 - e.g. ... HEU-MET-FAST-001 → HMF1

ICSBEP Introduction

- **LANL has created MCNP models for ~1000 ICSBEP configurations**
 - Focus on Pu, HEU & LEU and ^{233}U fuel systems
- **Reflector Materials include**
 - H_2O , D_2O , Polyethylene, Be, graphite, Ti, V, Fe (steel), Ni, Cu, Pb
- **“Poison” Materials include**
 - ^{10}B , ^{iso}Cd , ^{iso}Gd
- **FUND-xxx for reaction rate tallies in an unmoderated Pu metal system**
 - Historical LANL reaction rate tallies
 - Sometimes tabulated in the CSEWG Benchmark book.

ENDF/B-VII.1 & NJOY Summary

- **423 neutron evaluations in ENDF/B-VII.1**
 - Use NJOY to create ACE formatted .c files
 - RECONR/BROADR/PURR/ACER
 - Resonance reconstruction (0.1%), Doppler broadening (293.6K), Unresolved resonance probability tables, create continuous energy ACE file for MCNP
 - Not all ENDF/B-VII.1 evaluations appear in the Benchmark suite.
 - Execute a fictitious Godiva-like MCNP job
 - Thermal kernel data from ENDF/B-VII.0 carried forward
 - A new kernel, Si-SiO₂ is available
 - Not used in LANL benchmark testing (yet)
 - A new, continuous representation of the S(a,b) data was described by Conlin *et al* in this morning's "Advancing Criticality Safety Capabilities in a Growing Nuclear World" Session

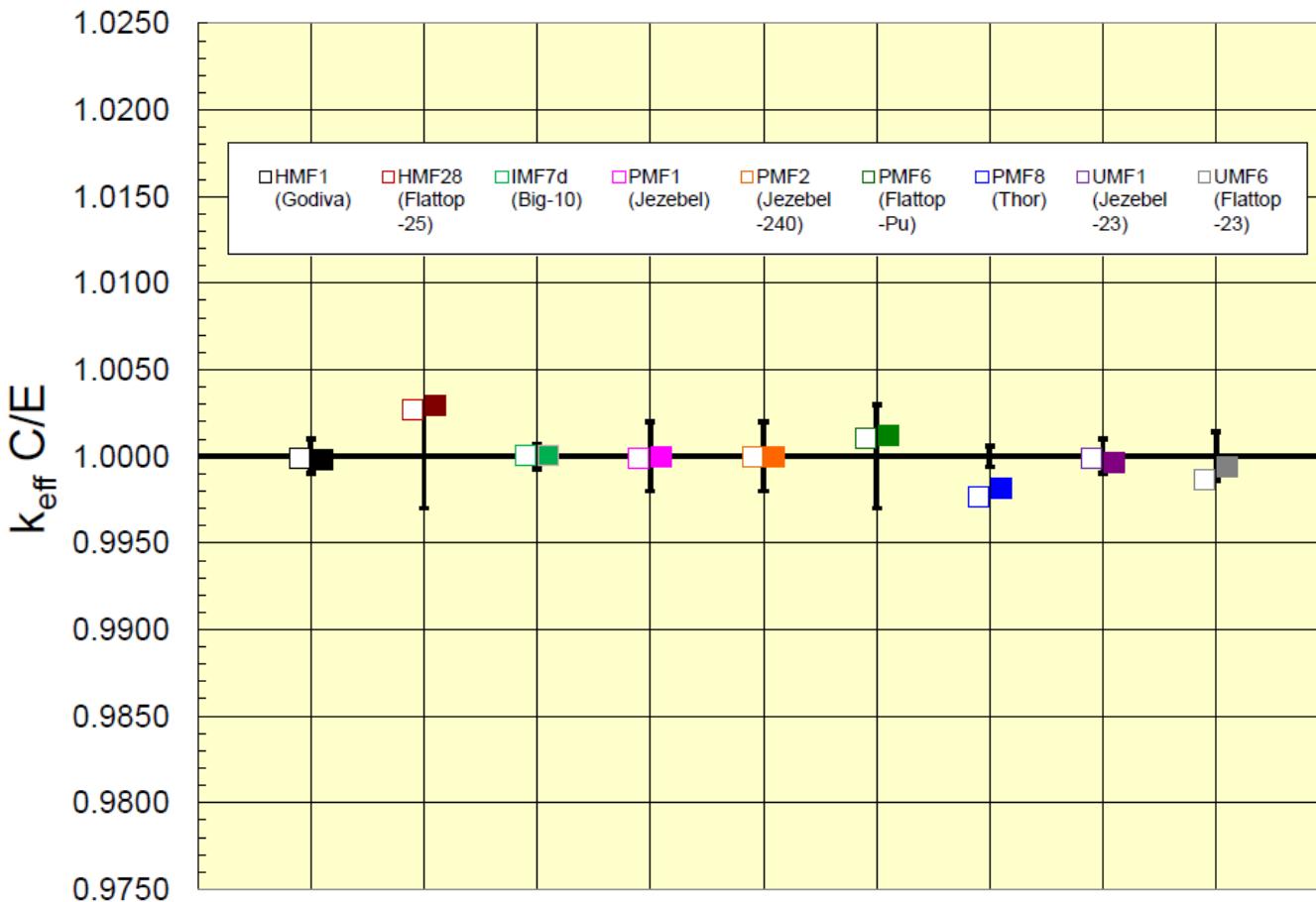
ENDF/B-VII.1 & NJOY Summary

- **Significant changes from ENDF/B-VII.0 to VII.1:**
 - “Significant” in the sense that ICSBEP benchmarks containing these materials are available.
 - ^9Be , $^{50,51}\text{V}$, $^{46,47,48,49,50}\text{Ti}$, ^{113}Cd , $^{180,182,183,184,186}\text{W}$
 - New R-Matrix analysis for ^9Be
 - ENDF/B-VII.0 has $^{\text{nat}}\text{V}$.
 - ENDF/B-VII.0 omits ^{180}W ; other isotopes revised per IAEA
 - Many other changes; see Chadwick et al paper in the December 2011 issue of Nuclear Data Sheets.
- **Significant lack of change ... the “Big 3”, namely $^{235,238}\text{U}$ and ^{239}Pu are virtually unchanged.**
 - pfns and intermediate energy cross section revisions (e.g. ^{235}U capture) will likely occur for the next release.
 - Resolve differences between ENDF/B, JEFF and JENDL

ENDF/B-VII.1 Criticality Testing

- **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.
- **Examples of all three conditions follow**

A “Do No Harm” Example - FAST

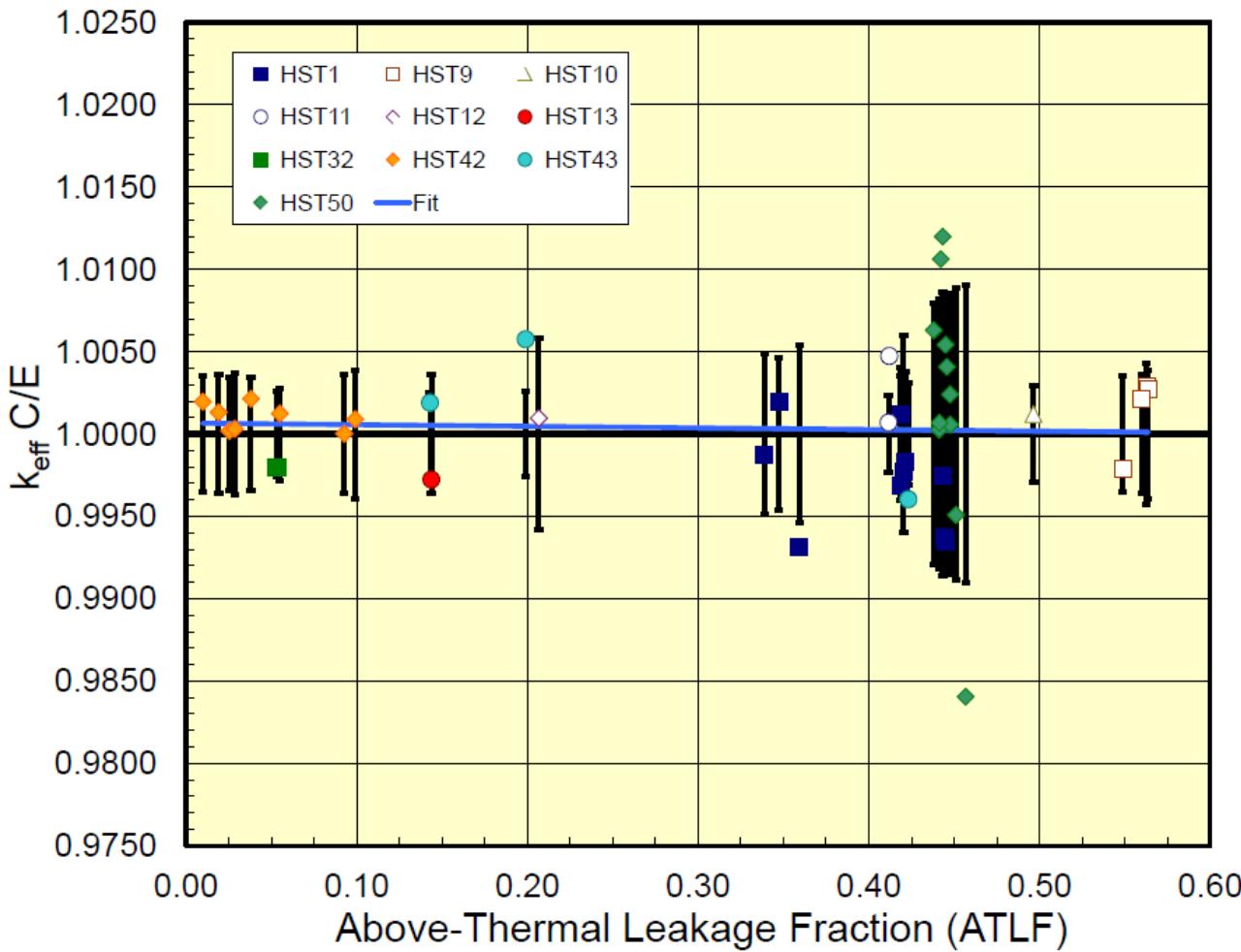


“Open” squares are E71;

“Solid” squares are E70.

LANL historical critical assembly's previous good results are retained (as expected).

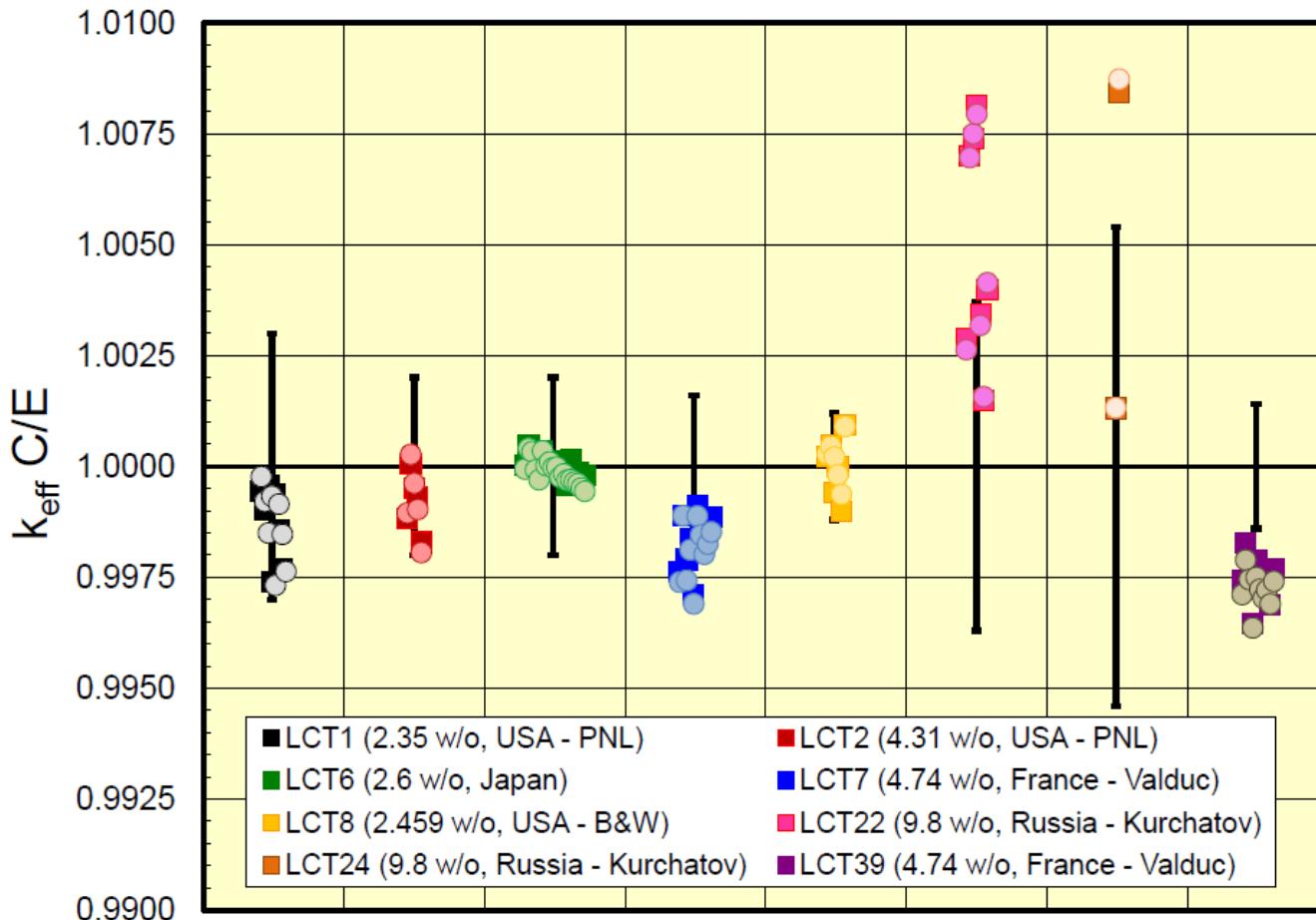
A “Do No Harm” Example - THERMAL



E71 regression coefficients are identical to those obtained with E70 Cross Sections.

Previous good results are retained (as expected).

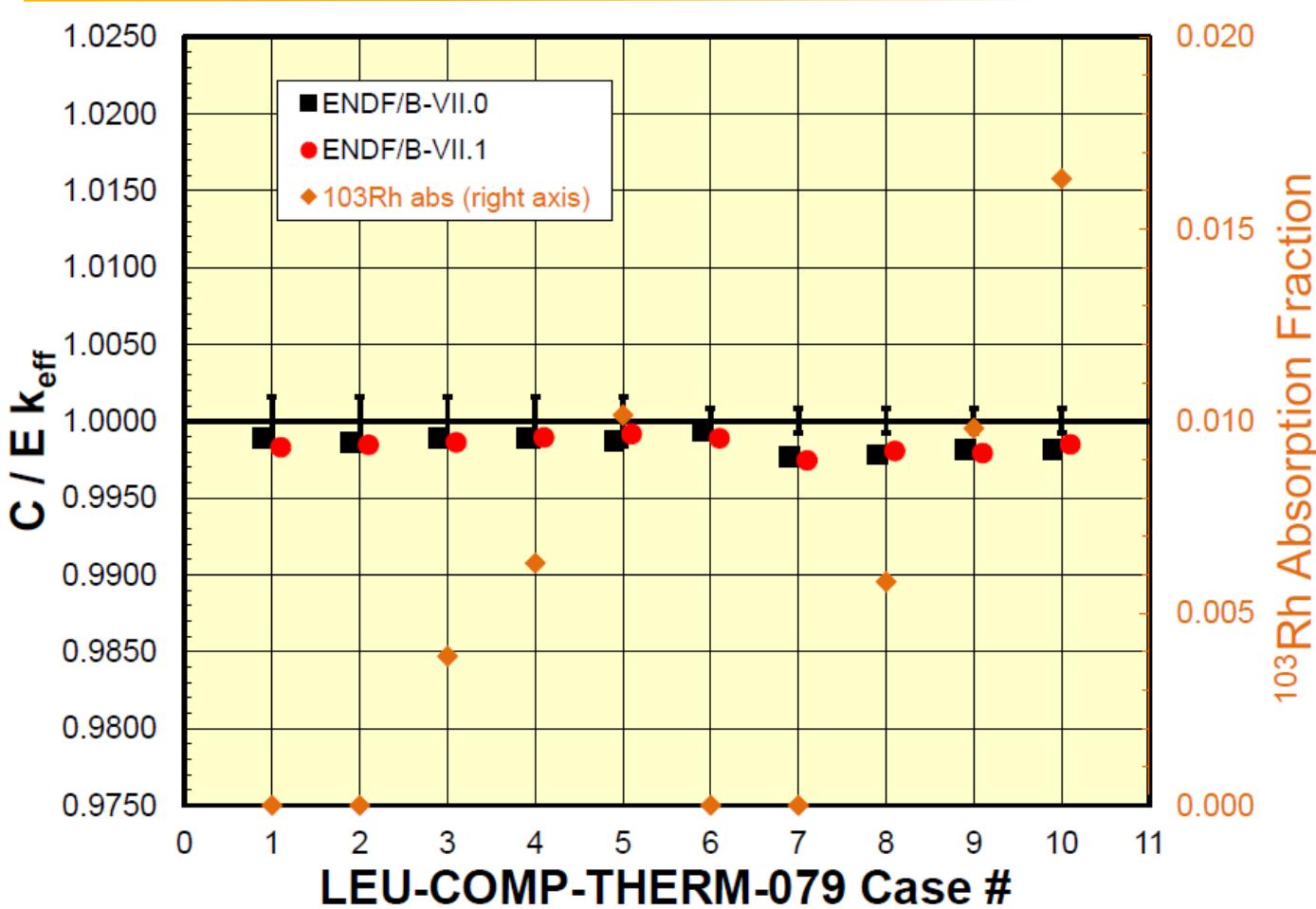
A “Do No Harm” Example - LCT



Benchmark calculated eigenvalues (circle=E71, square=E70) for a selection of water reflected LCT assemblies.

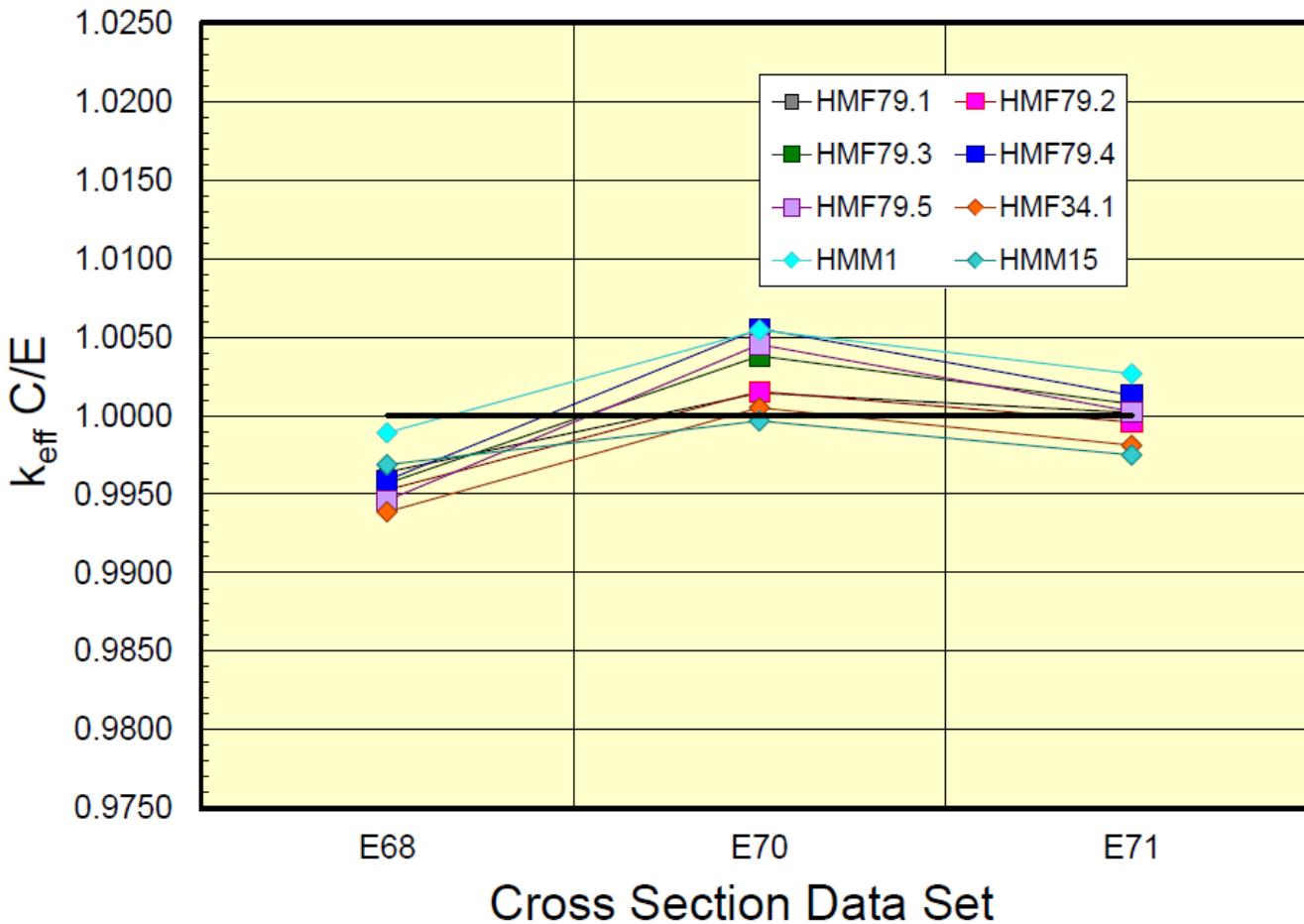
LCT w/ ^{103}Rh Poison

A New Benchmark for ENDF/B-VII.1



UO_2 lattice assembly with varying amounts of ^{103}Rh (a fission product poison). Under-moderated (cases 1 – 5) and optimally moderated (cases 6 - 11).

Ti Bearing Assemblies – A Success Story



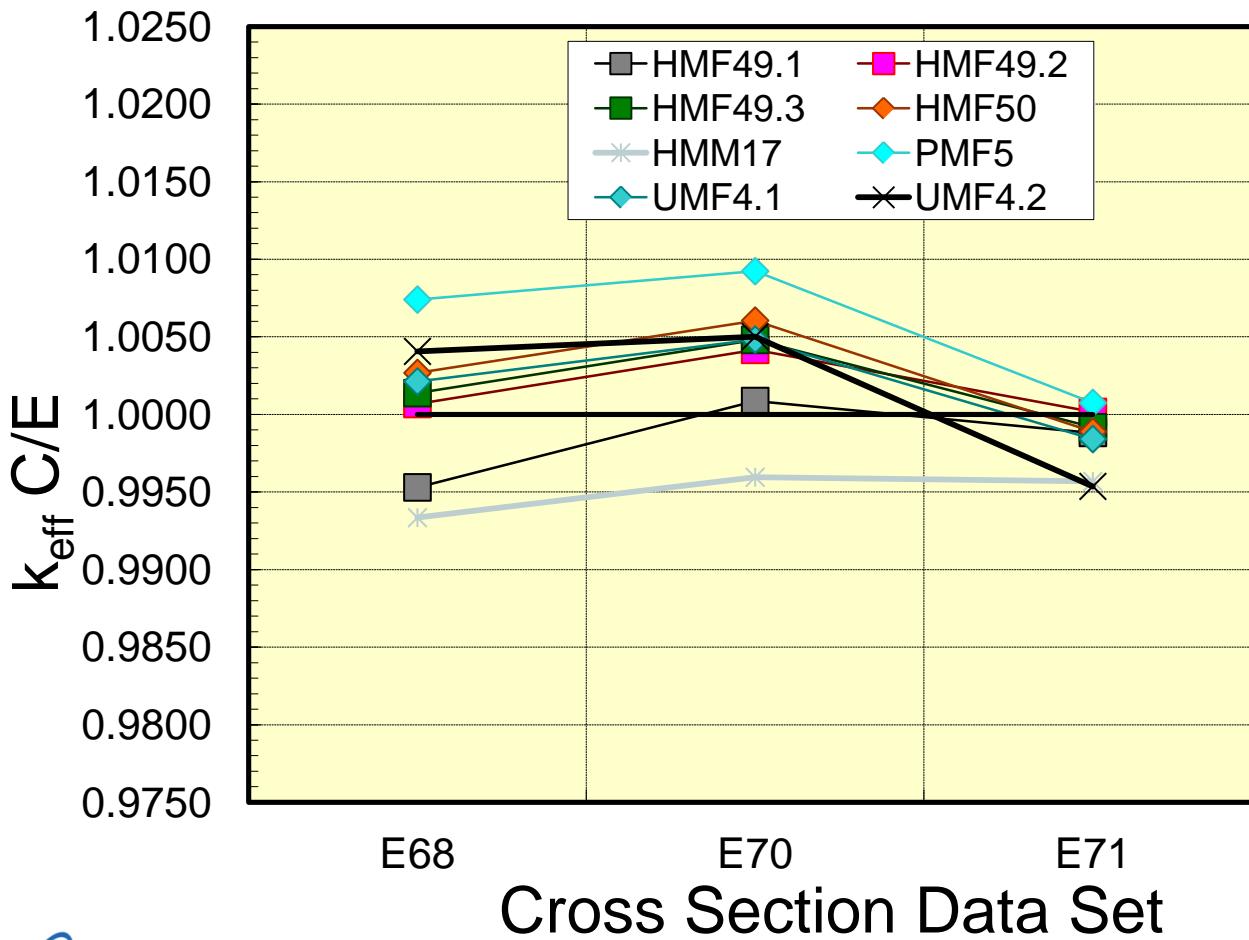
Ti bearing assemblies.

ENDF/B-VI.8
is “too cold”

ENDF/B-VII.0
is “too hot”

ENDF/B-VII.1
is “just right”!

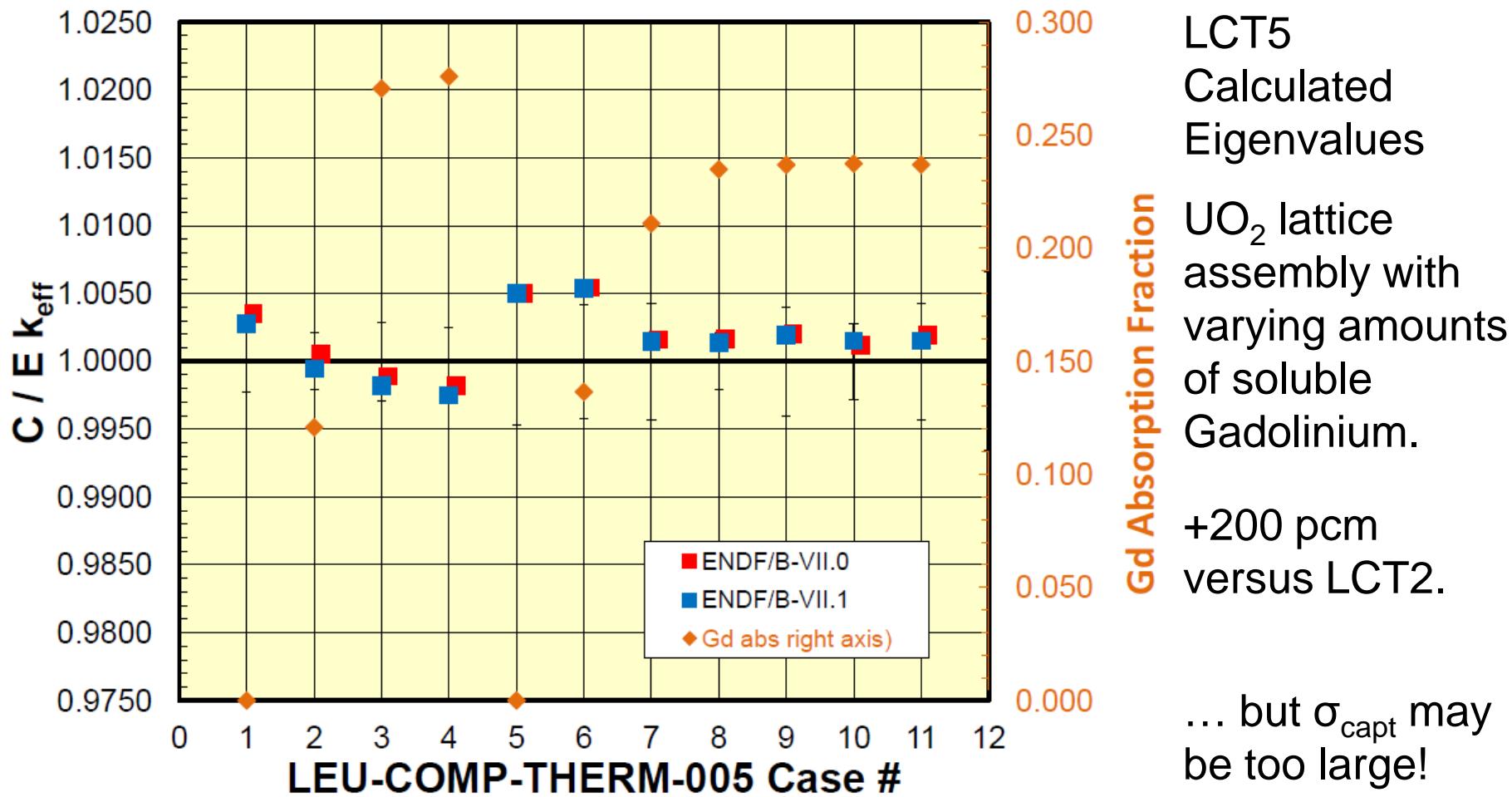
W Bearing Assemblies – Another Success



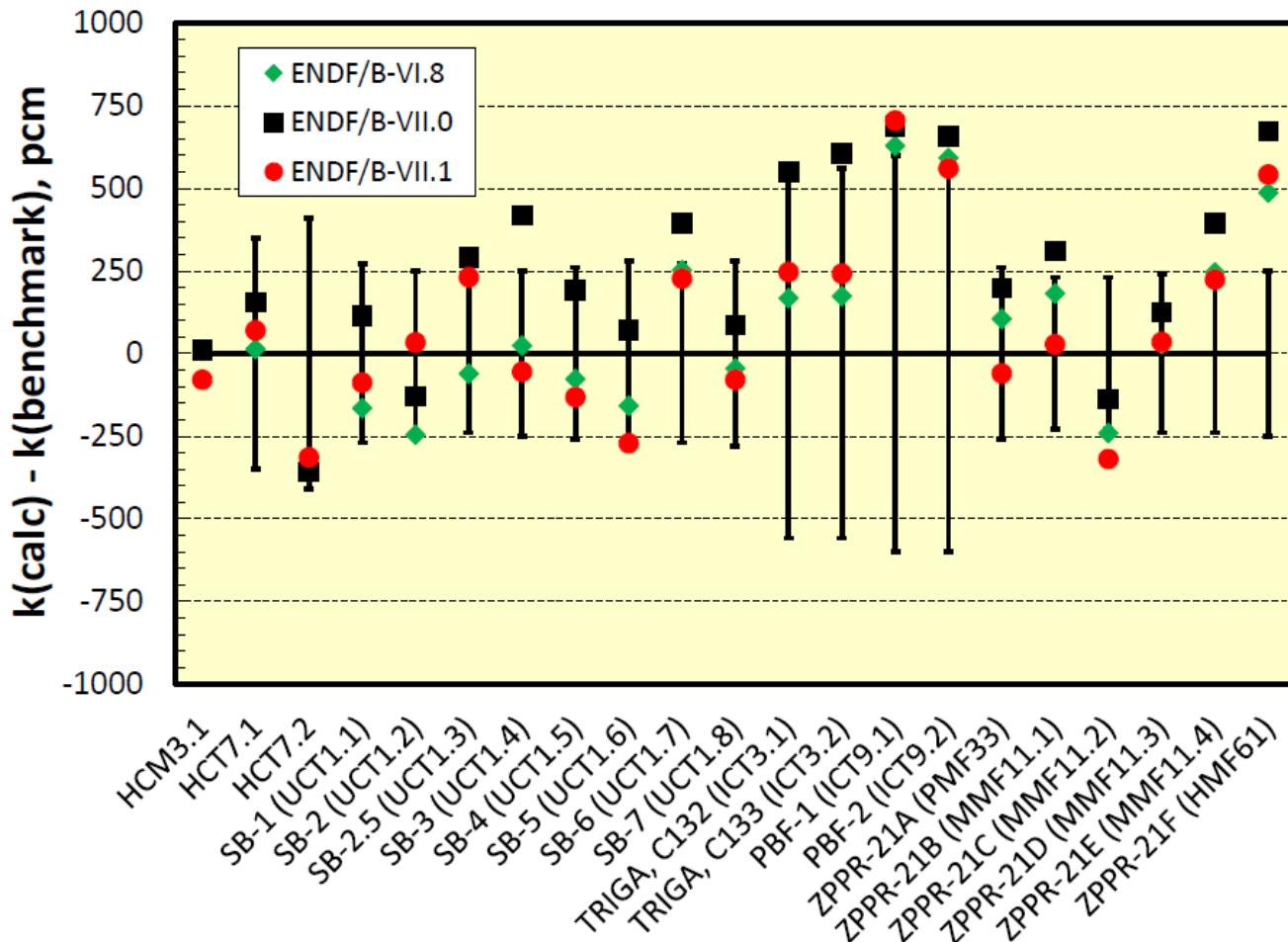
E71 calculated eigenvalue spread is significantly reduced compared to E70 or E68.

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

Gd Poisoned LCT – Good or Lucky?



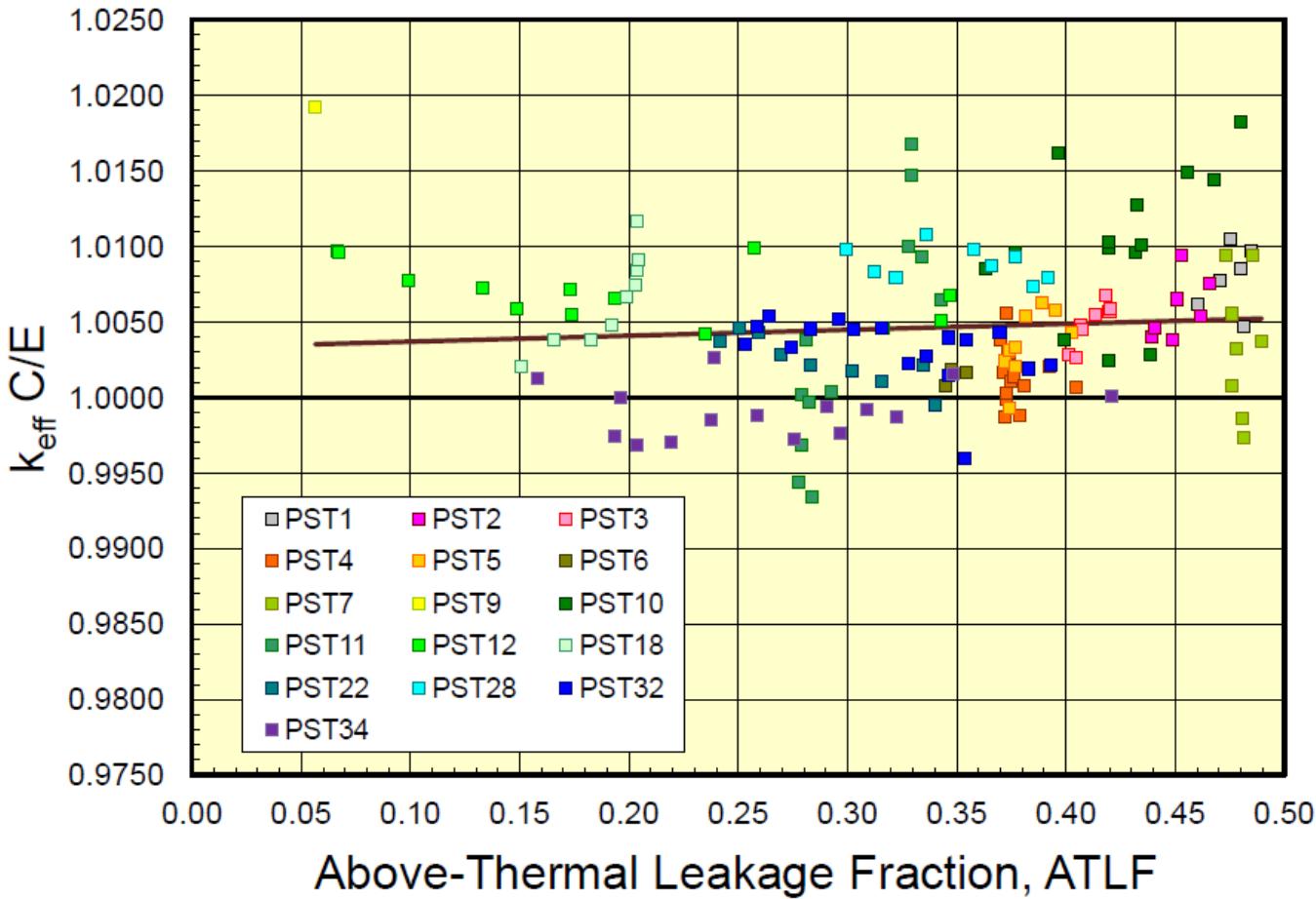
Zr Bearing Assemblies – A Continuing Story



Various benchmarks with Zr.

E71 (red) results are closer to the superior E68 (green) results than E70 (black).

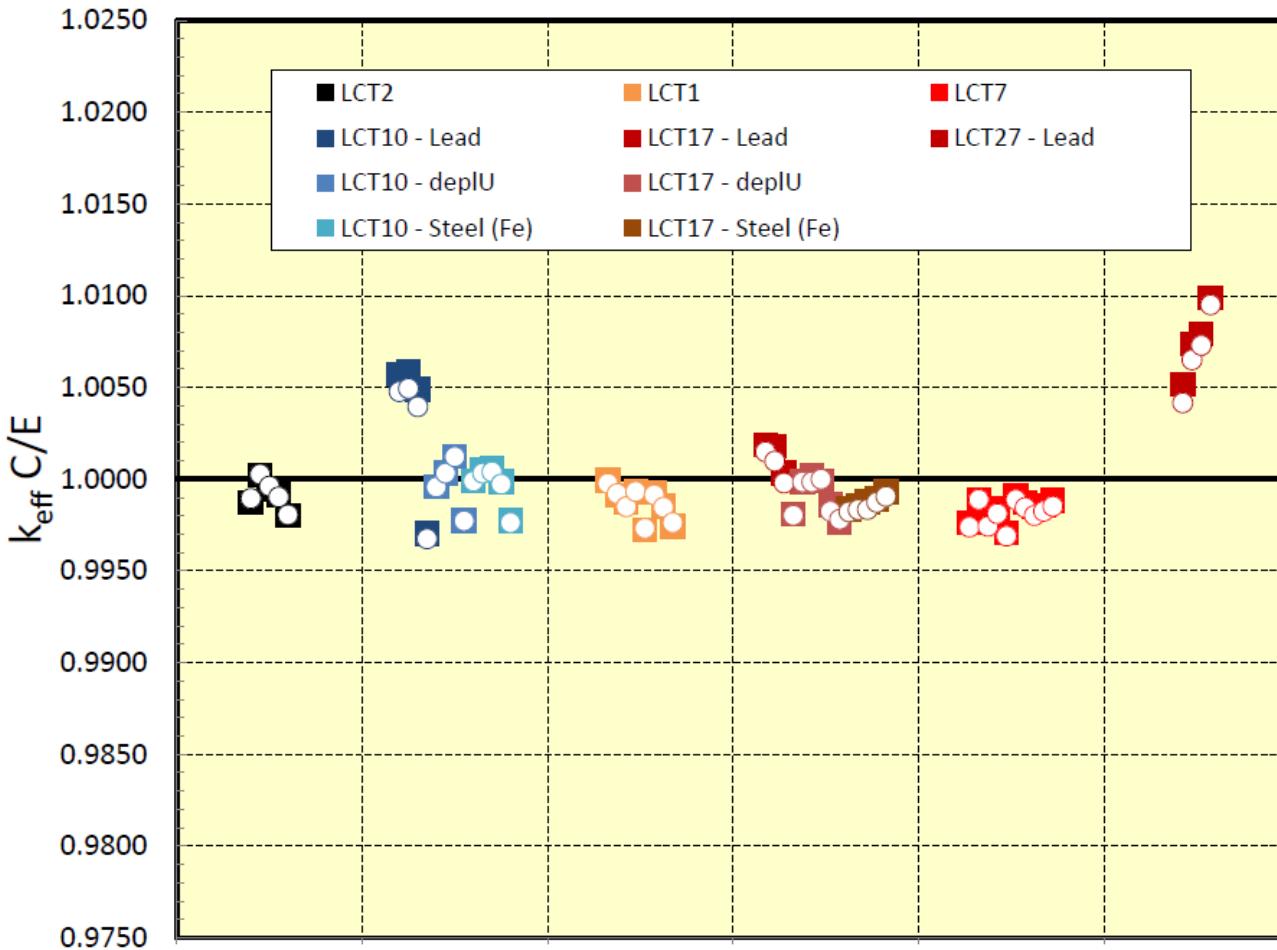
Where We Need More Work - Pu



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).

Where We Need More Work - Lead

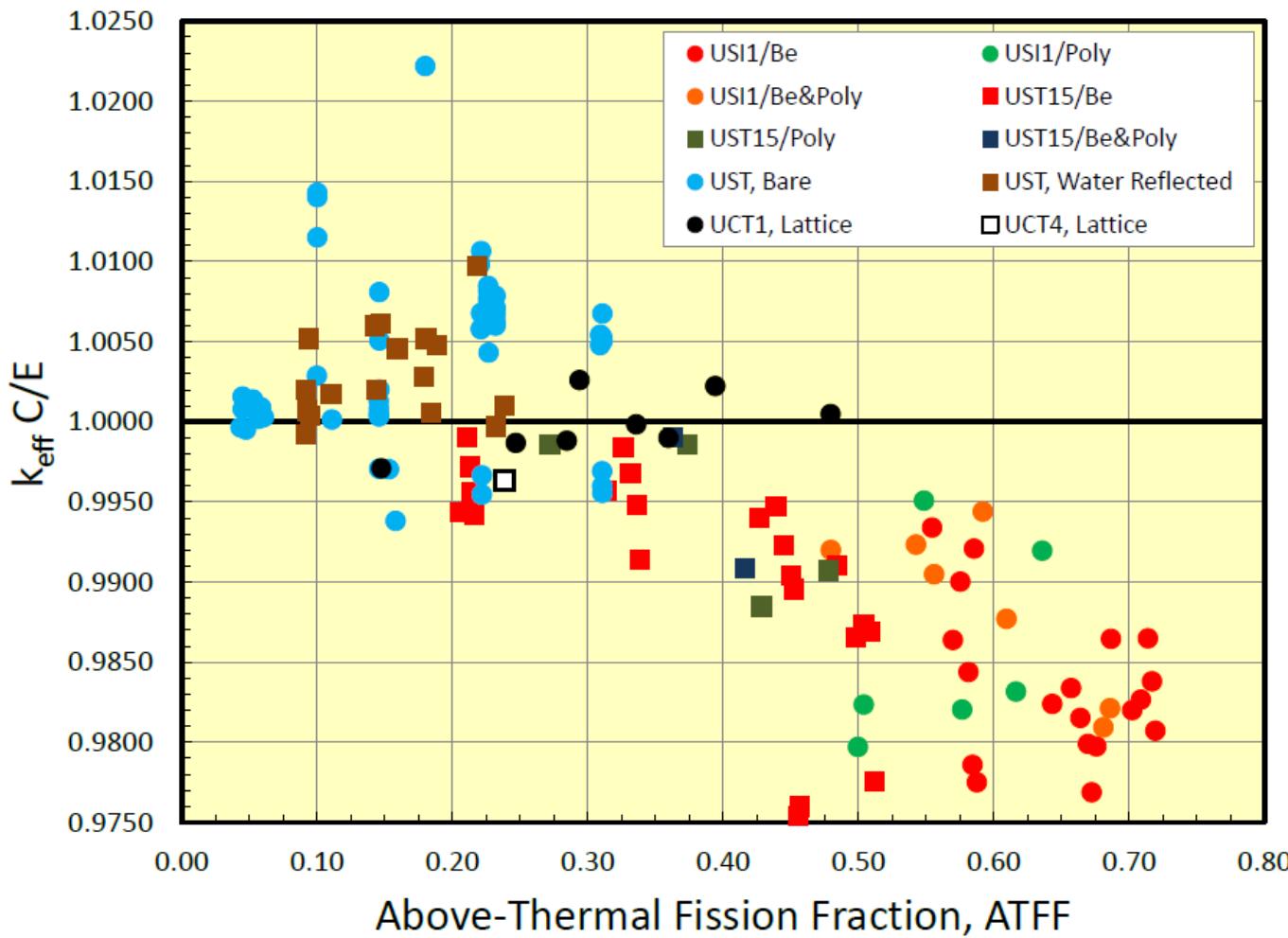


Water moderated lattice systems with and without metal reflectors.

Steel (Fe) and deplU results are good; Pb results are poor.

HMF with Pb is also poorly predicted.

Where We Need More Work - ^{233}U



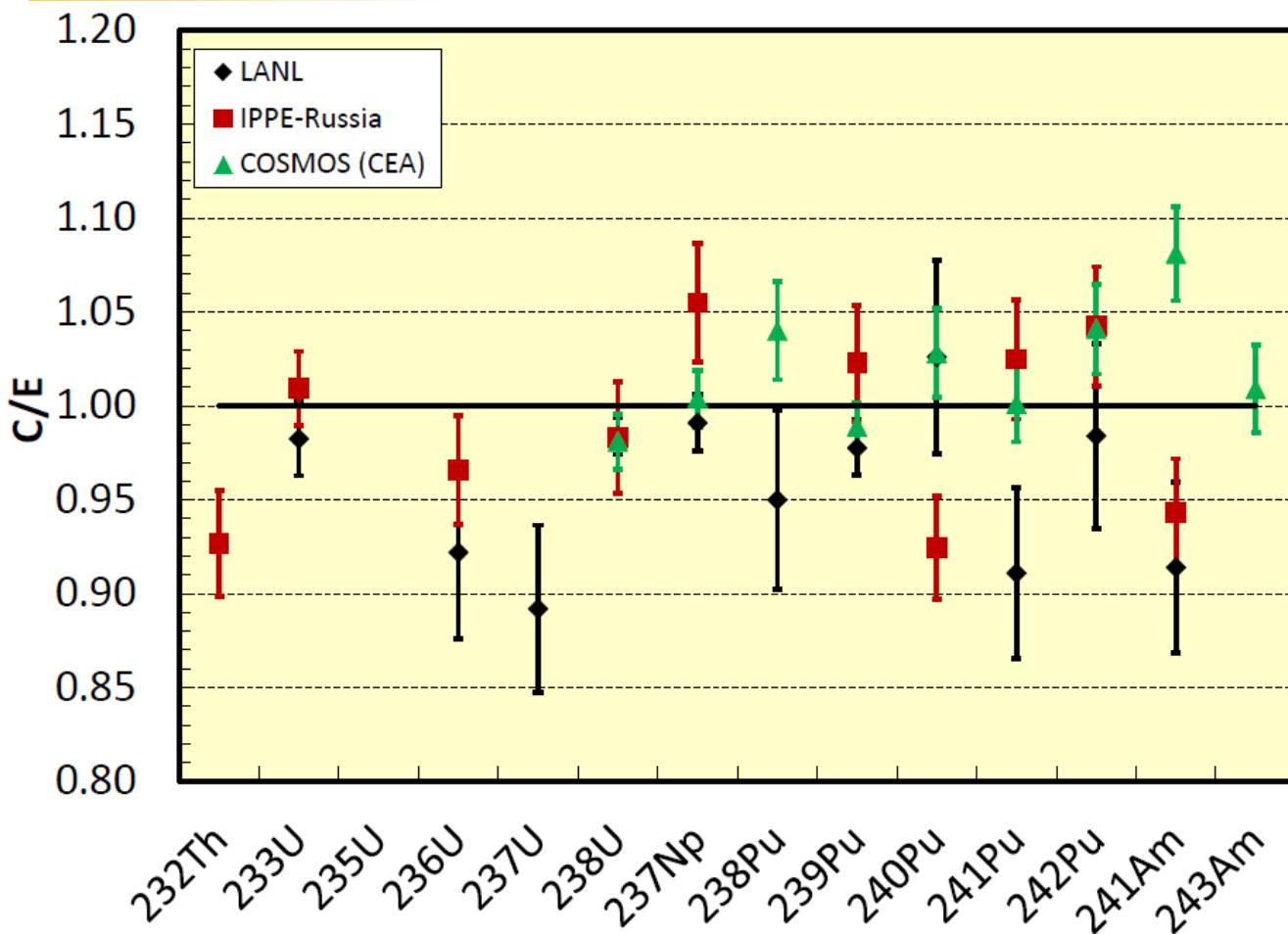
A long-standing bias in calculated eigenvalues; little change in E71 results.

Black circles are UCT (LWBR) related; a successful though little publicized Naval Reactors Program experiment); were we lucky?

Where We Need More Work

- There are significant differences between ENDF/B, JEFF (Europe) and JENDL (Japan) for the “Big 3”
 - ENDF/B and JEFF calculate Jezebel (Pu-MET-FAST-001; a bare Pu sphere) very well but the respective ^{239}Pu evaluated data files differ in σ_{inel} , σ_{fiss} , $\nu(E)$ and pfns.
 - Someone, probably both of us, is getting the right answer for the wrong reason!
 - There are significant differences between ^{235}U capture in the keV region.
 - Feedback from some at JAEA is that the ENDF/B-VII.1 Ti changes are not needed if ENDF/B had adopted the JENDL-4.0 evaluation

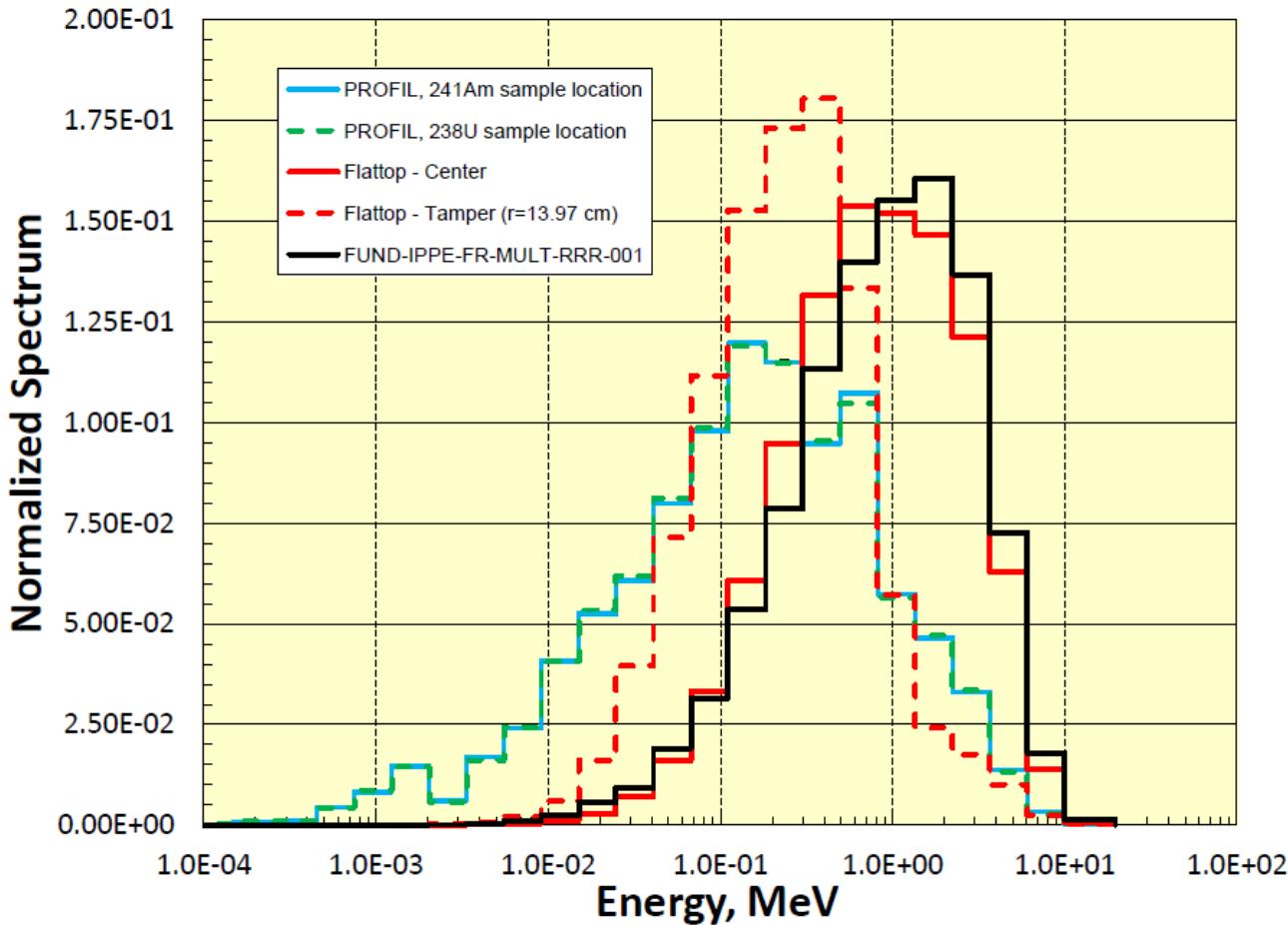
It's Not Always Criticality!



Fission Cross Section spectral index (i.e., ratio of $\sigma_f X / \sigma_f^{235}\text{U}$)
C/E results in selected "FAST" systems.

Also have capture and (n,2n) data

Not All “FAST” Spectra are the Same



Calculated Flux Spectra at the Sample Location for Selected “FAST” Reactor Systems.

Final Observations

- Not Conclusions, because we're clearly not done!
- The Cross Section Evaluation Working Group is justifiably proud of the ENDF/B-VII.1 library
- ... but the European community can say the same for JEFF-3.1.2
- ... and the Japanese community can say the same for JENDL-4.0 ... and China ... and Russia ... and
- ... and the benchmark testing examples clearly show that some materials have clear deficiencies.
 - **Stay tuned ... ENDF/B-VII.2 (or maybe ENDF/B-VIII.0) is only ~5 years away!**