LA-UR-12-20002

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

A. C. Kahler, R. E. MacFarlane, R. D. Mosteller,
B. C. Kiedrowski, M. B. Chadwick

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 testing for the ENDF/B-VII.1 Neutron Library during FY11.

Introduction

- **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 validation effort of the ENDF/B-VII.1 Neutron Sub-Library.

Introduction

ELSEVIER

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Nuclear Data Sheets 112 (2011) 2997–3036

Nuclear Data Sheets

www.elsevier.com/locate/nds

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. Trkov,[6] T. H. Trumbull,[7] and M. Dunn[8]

[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}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.

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

TABLE II: Summary list of fast ICSBEP benchmarks with common fuel plates and varying reflector and/or diluent materials.

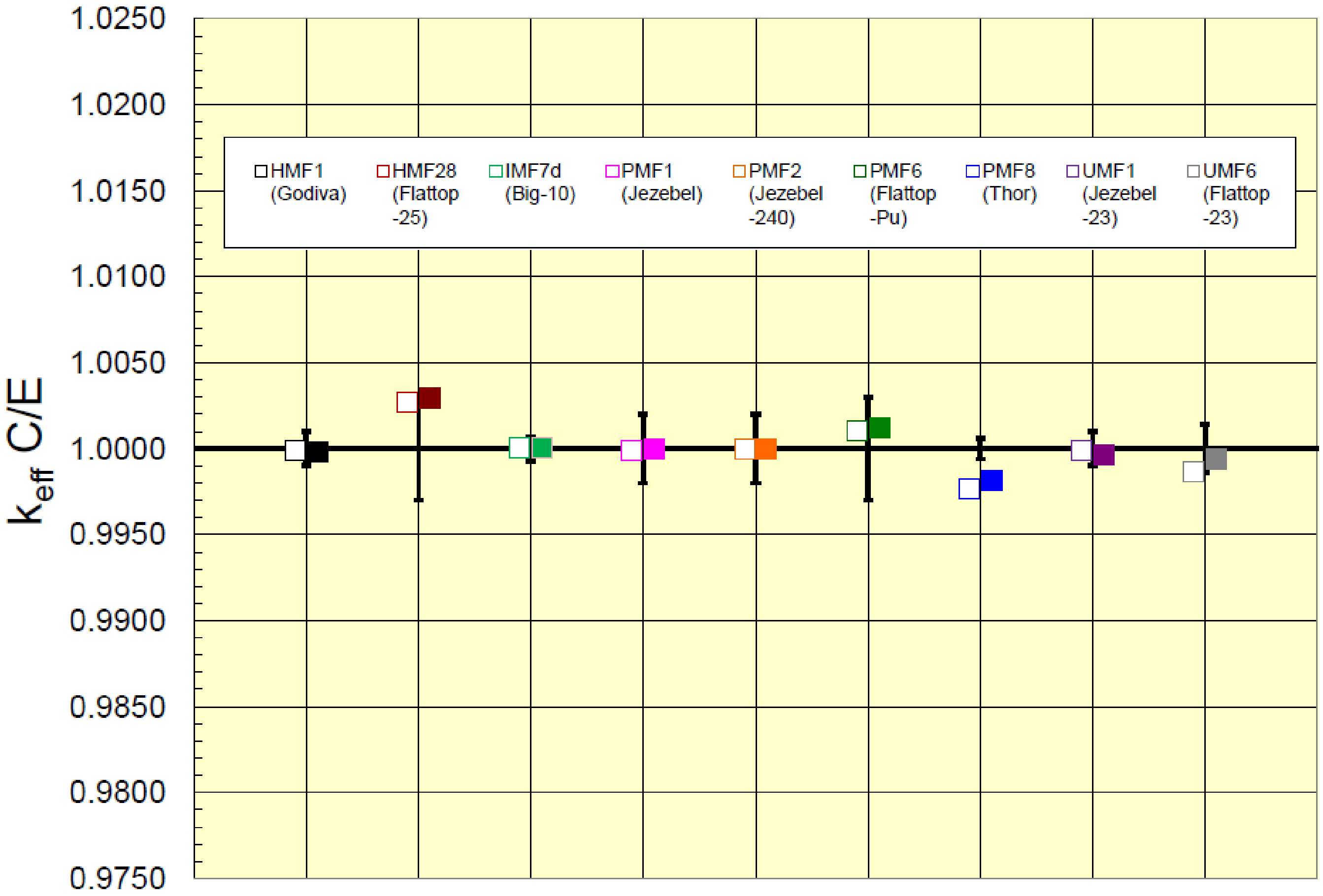
Benchmark	Axial Reflector	Diluent	Radial Reflector
HMF15	—	—	—
HMF65	—	—	—
HMF82	CH_2 (top)	—	—
HMF91	CH_2	—	—
HMF44	Al	—	—
HMF89	—	Al	—
HMF34.2	—	Al/CH_2	CH_2
HMF79	Ti	—	—
HMF34.1	—	Ti/CH_2	Ti/CH_2
HMM1	—	Ti/CH_2	Ti/CH_2
HMM15	—	Ti/CH_2	Ti/CH_2
HMF25	V	—	—
HMF40	—	V	—
HMM16	CH_2	V/CH_2	CH_2
HMF43	Fe (steel)	—	—
HMF87	—	Fe (steel)	—
HMF33	—	Fe (steel)/CH_2	—
HMF34.3	—	Fe (steel)/CH_2	—
HMF49	W	—	—
HMF50	—	W	—
HMM17	CH_2	W/CH_2	CH_2

Summary of Related VNIITF Experiments currently in the ICSBEP Handbook

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

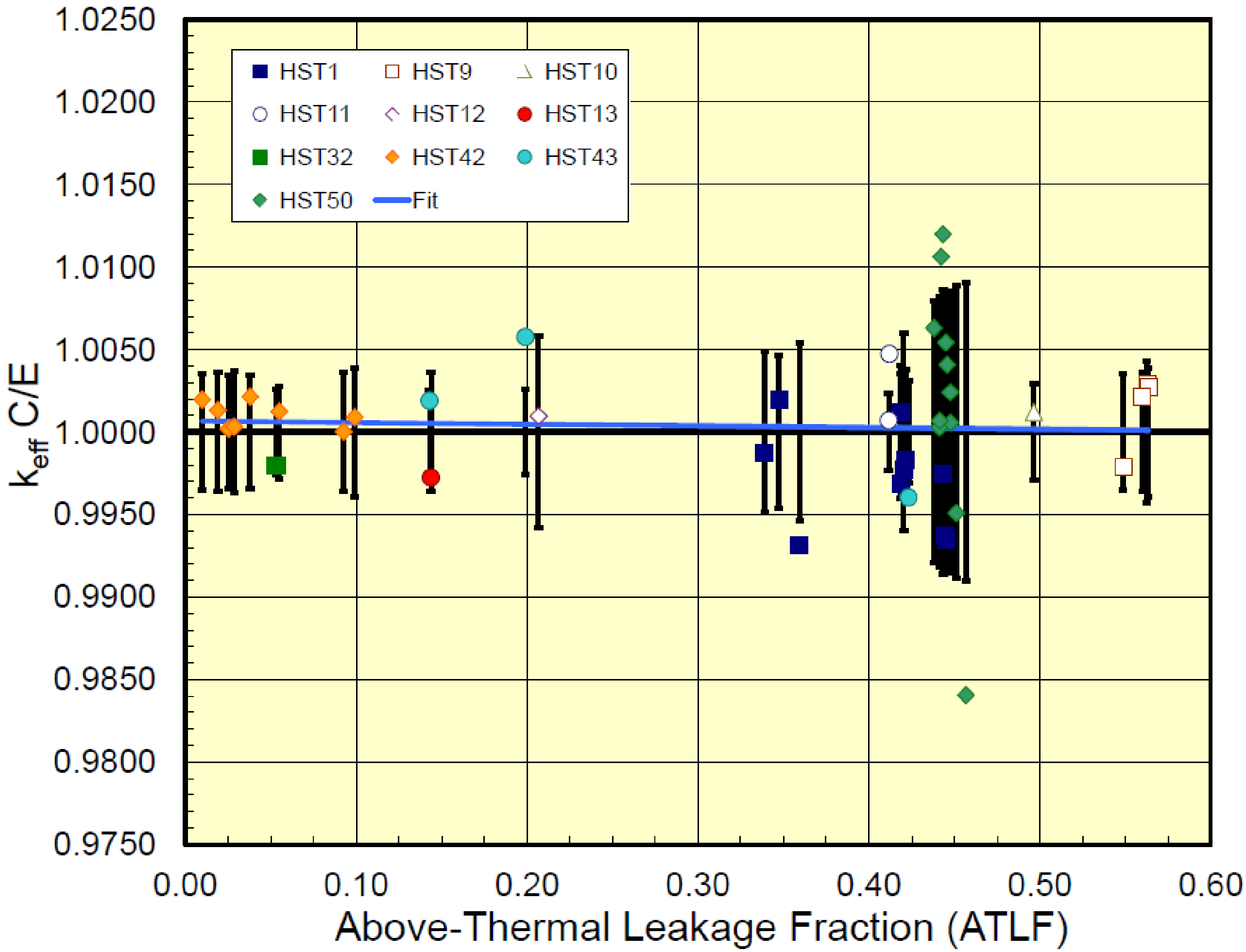


"Open" squares are E71; "Solid" squares are E70.

LANL Historical Critical Assemblies

Previous good results are retained (as expected).

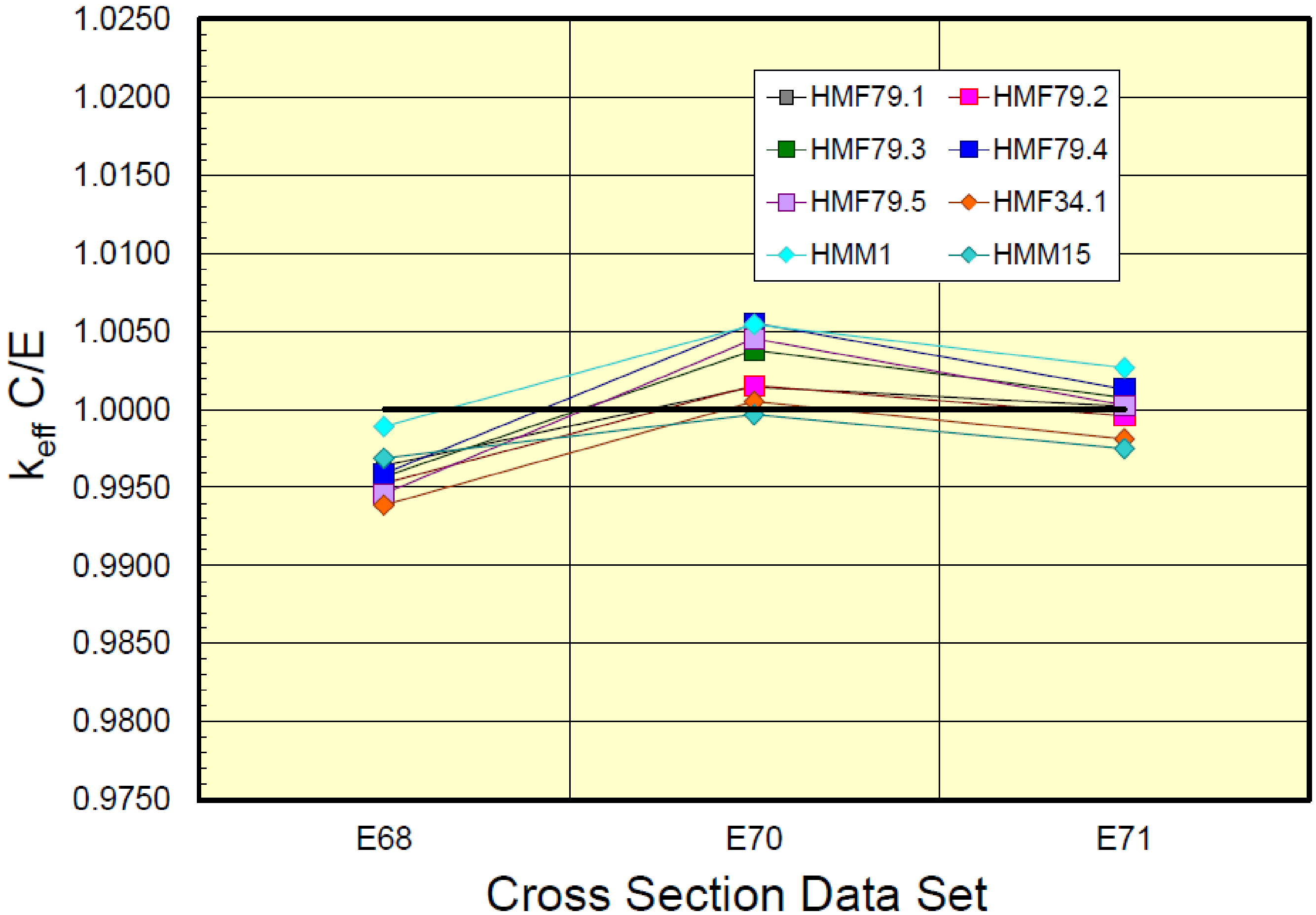
A “Do No Harm” Example - THERMAL



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

Previous good results are retained (as expected).

Improved ("Goldilocks") Example



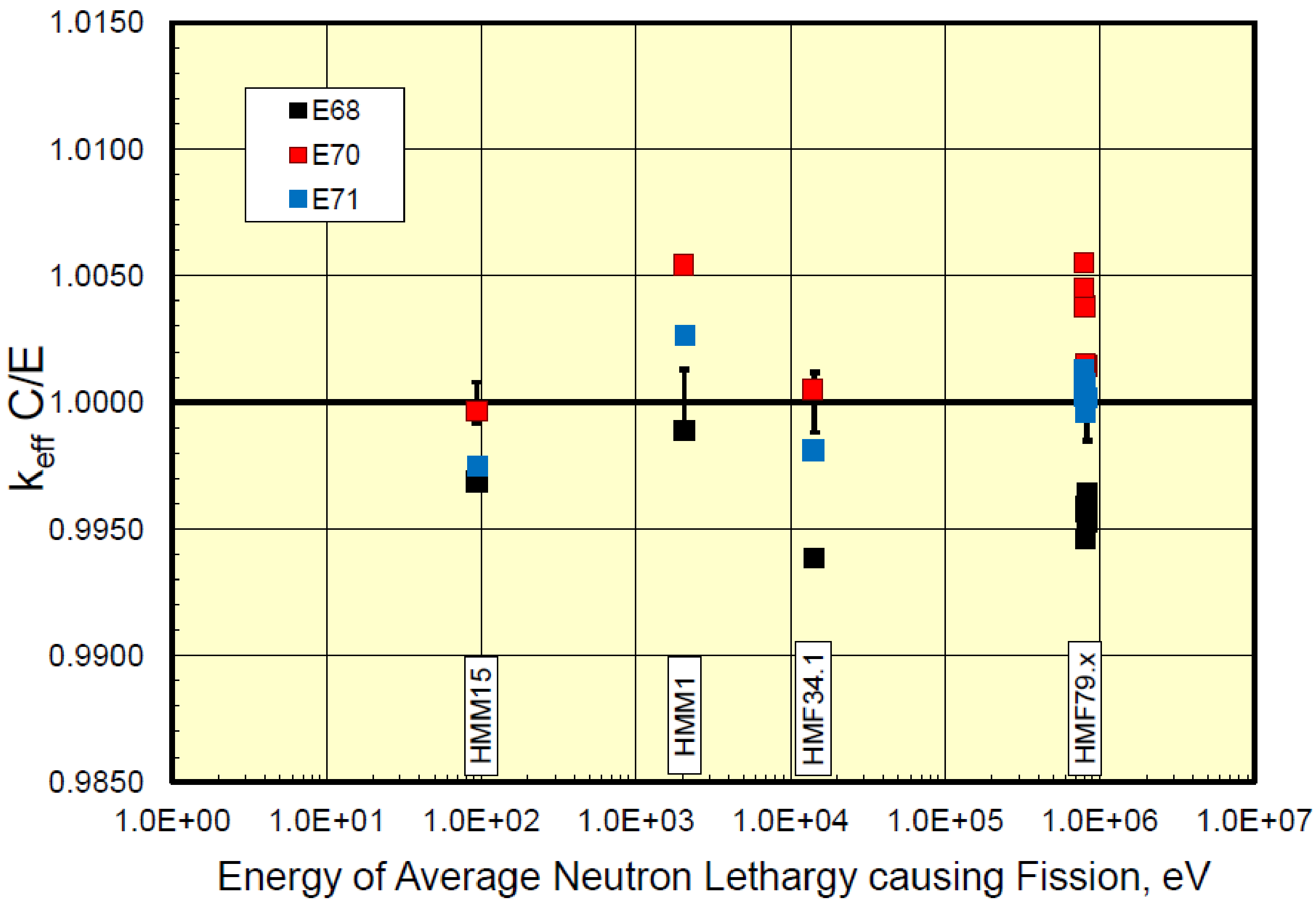
Ti bearing assemblies

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

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

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

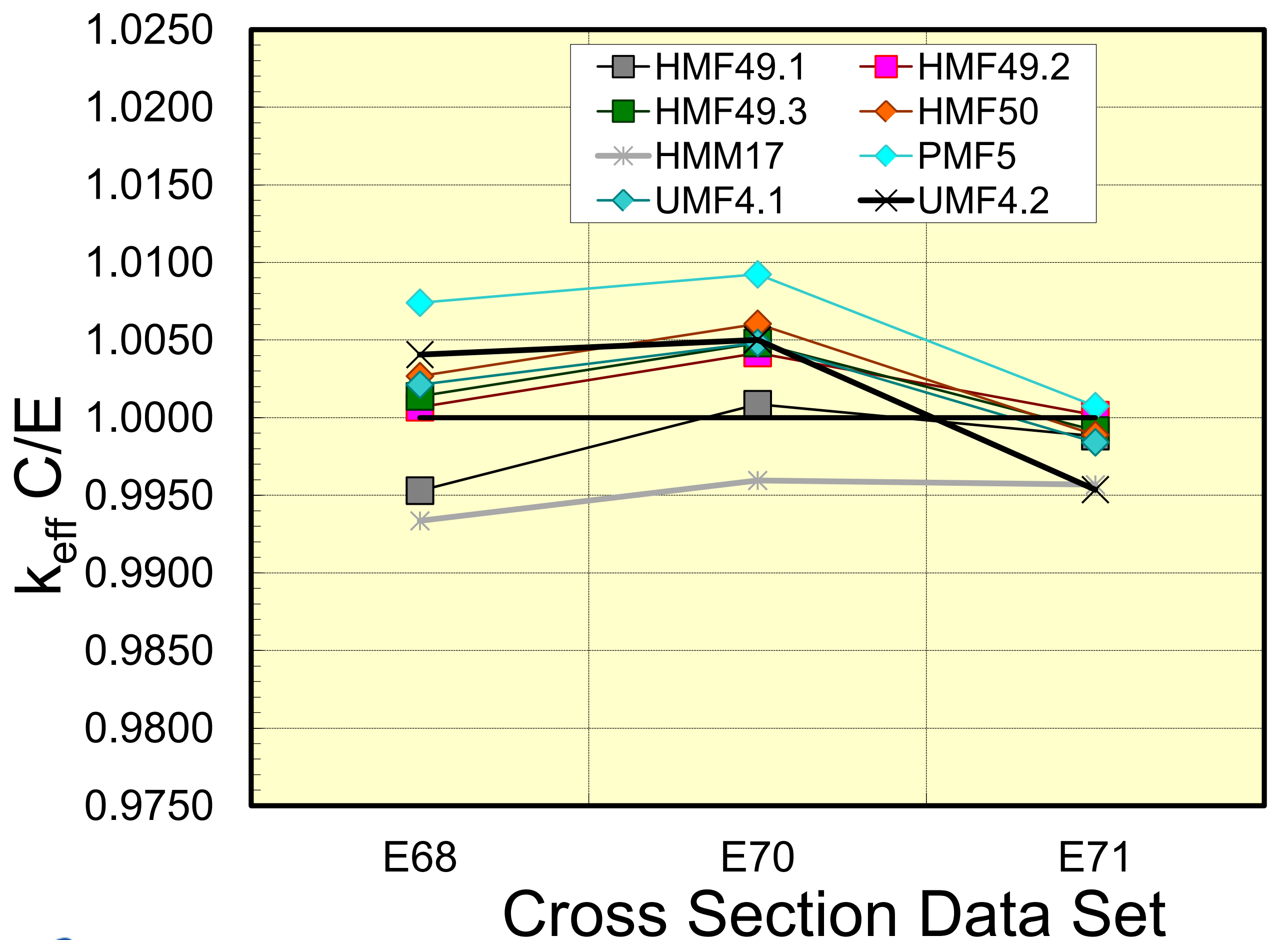
Ti Bearing Assemblies – Another View



Calculated Eigenvalues versus Fission Energy.

No trend observed over a four decade variation in energy.

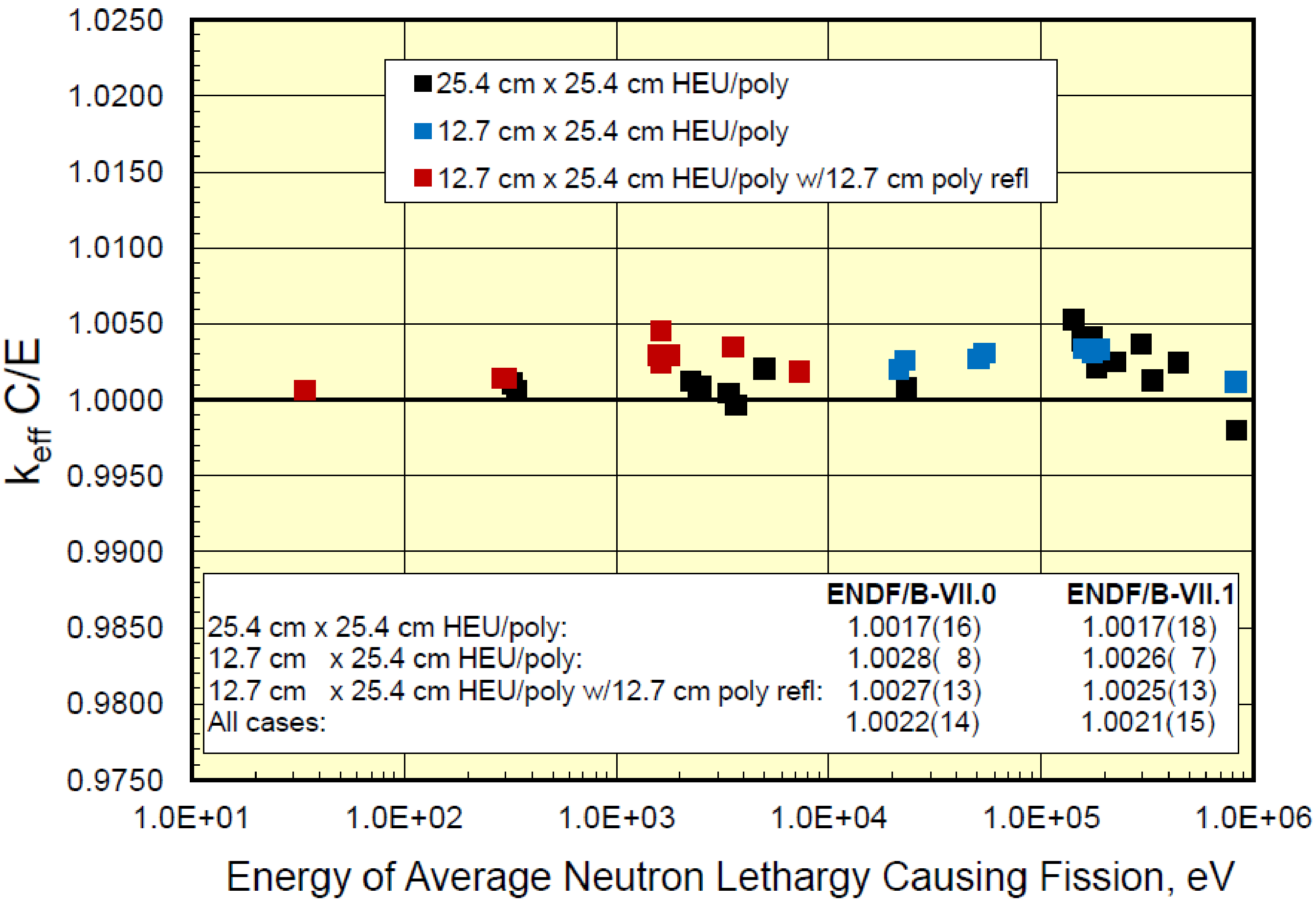
W Bearing Assemblies – Another Success



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.

Another Large Variation in Energy



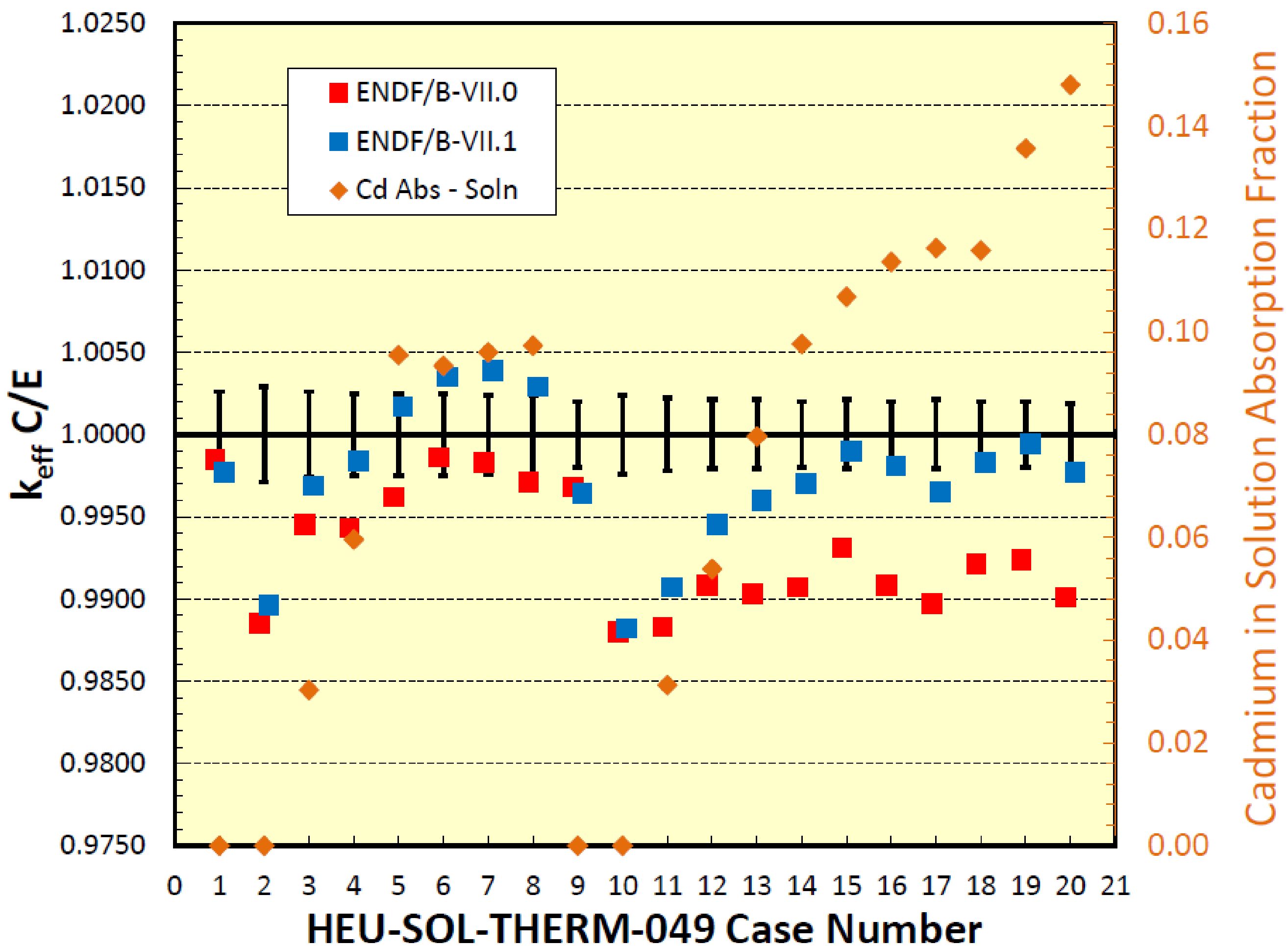
	ENDF/B-VII.0	ENDF/B-VII.1
25.4 cm x 25.4 cm HEU/poly:	1.0017(16)	1.0017(18)
12.7 cm x 25.4 cm HEU/poly:	1.0028(8)	1.0026(7)
12.7 cm x 25.4 cm HEU/poly w/12.7 cm poly refl:	1.0027(13)	1.0025(13)
All cases:	1.0022(14)	1.0021(15)

HMF7 (ORNL)

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

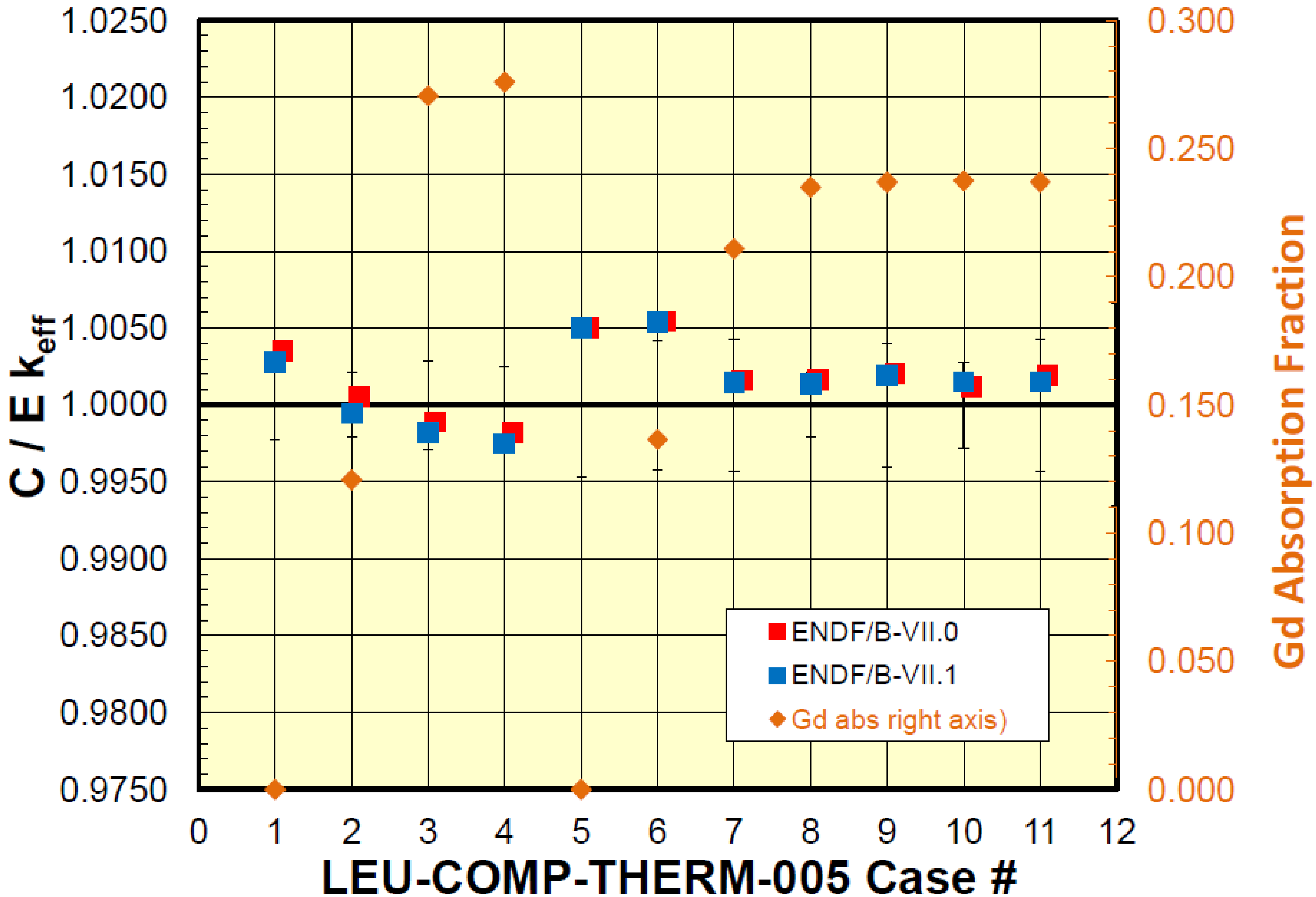
E71 (or E70) eigenvalues are about 300 pcm larger than E68.

Poisoned Solution and Lattice Systems - I



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

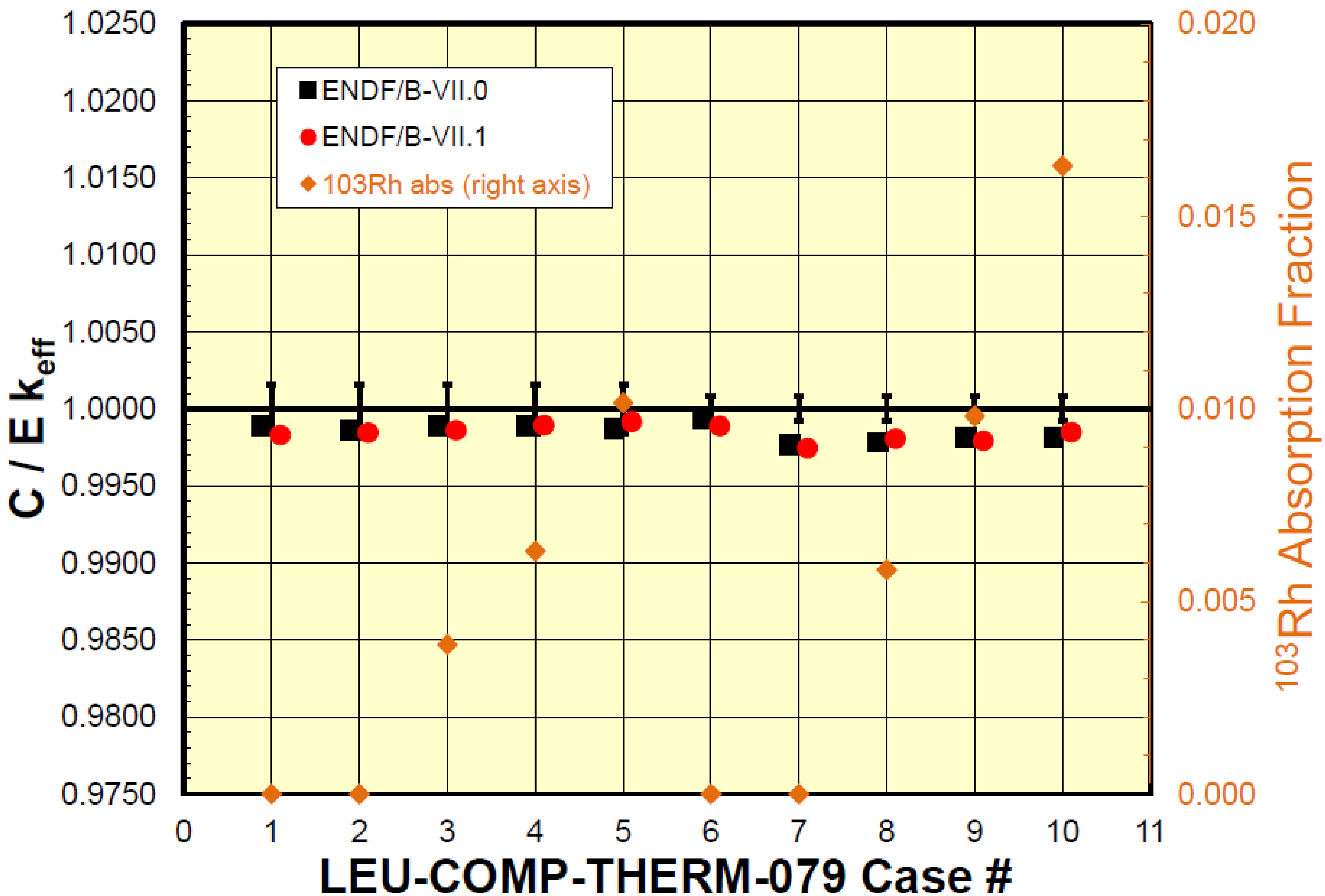
Poisoned Solution and Lattice Systems - II



"Base Case" (LCT2) calc-ulated eigen-value is about 200 pcm less.

Potential decrease in Gd absorp-tion would make this comparison even worse.

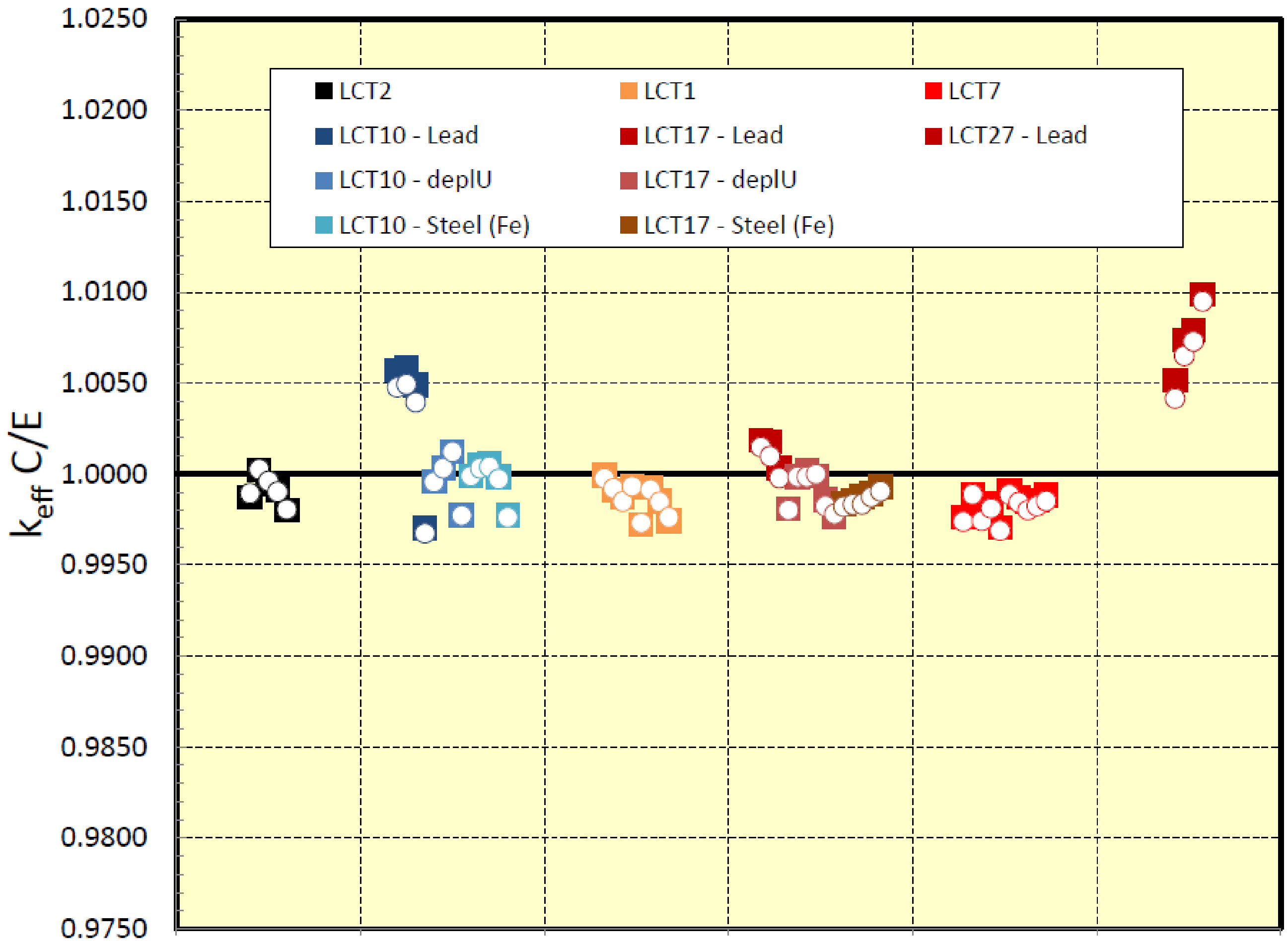
Poisoned Solution and Lattice Systems - III



LCT79 Calculated Eigenvalues

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

Where We Need More Work - Lead

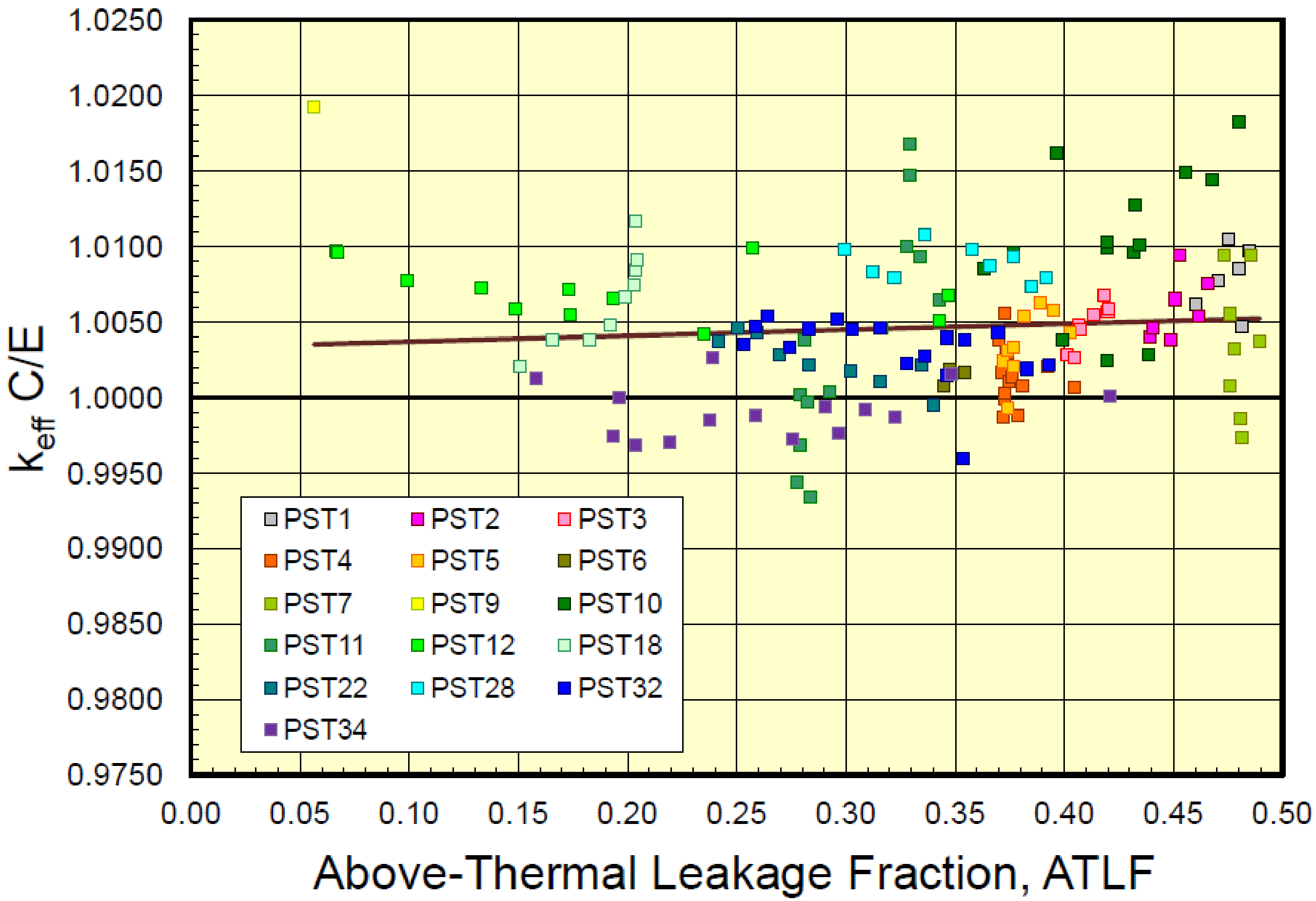


Water moderated attice systems with and without metal reflectors.

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

HMF with Pb is also poorly predicted.

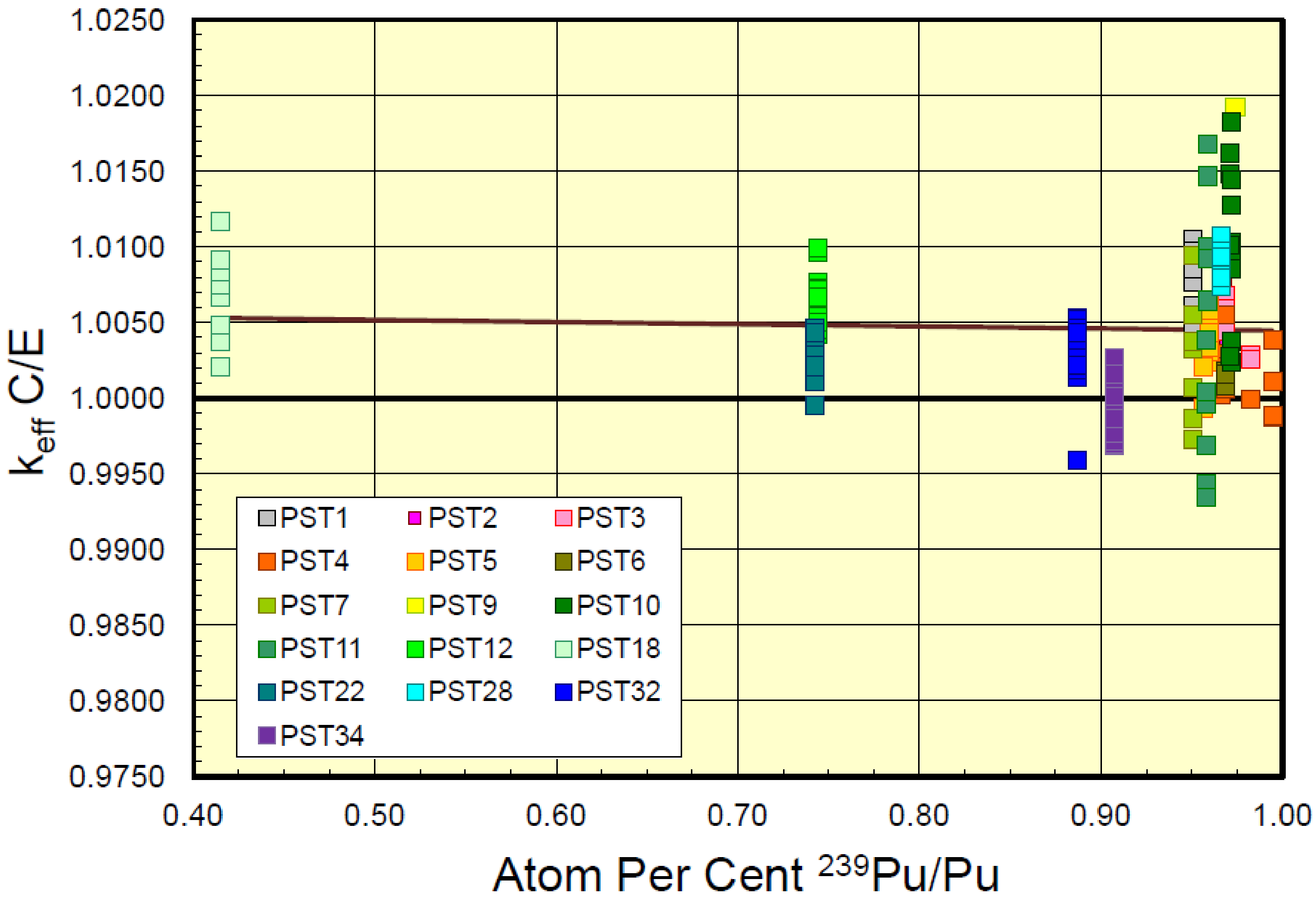
Pu Solution Systems



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

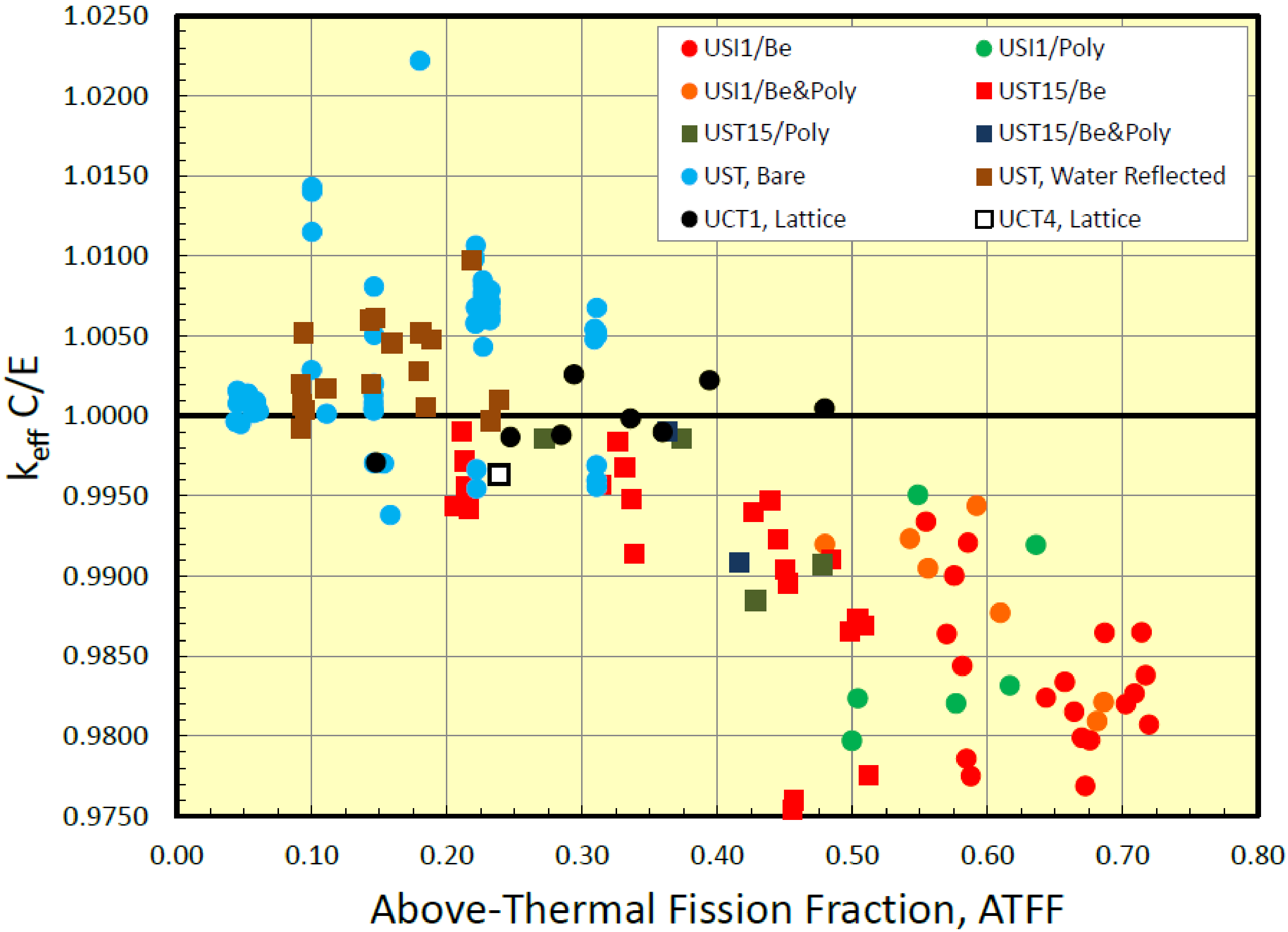
This is the subject of a WPEC Sub-Group (ORNL/LANL/ANL/Europe).

Pu Solution Systems – Another View



Even when focus on a single PST Series no obvious trend that relates back to the fundamental nuclear data has been observed.

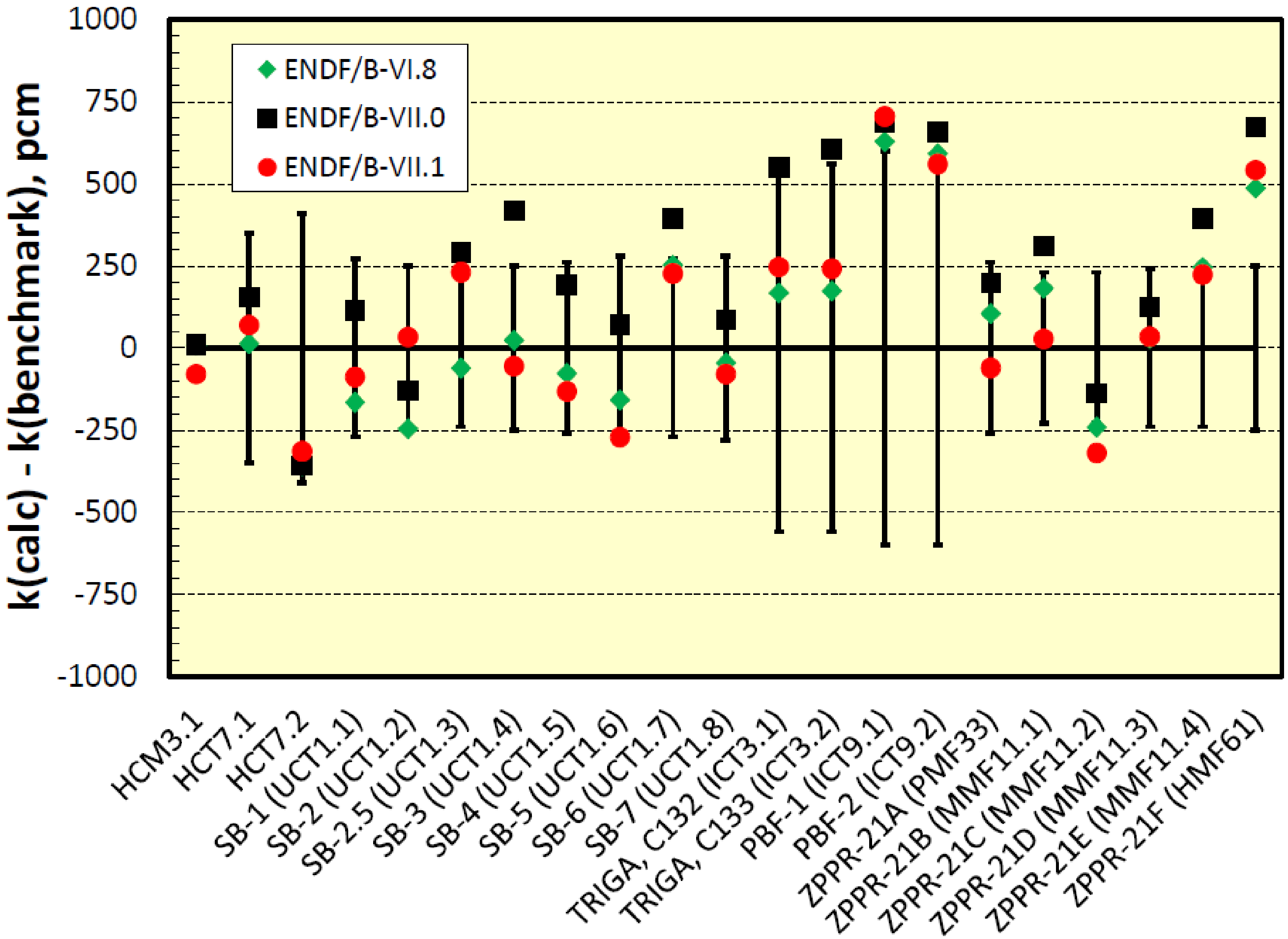
^{233}U Intermediate and Thermal Systems



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?

Benchmarks with Zr



Cross Section revisions by BNL have moved E71 based C/E results closer to unity.

TRIGA change from E68 to E70 was particularly worrisome.

Delayed Critical Rossi-α Validation

- **Delayed Critical Rossi-α measures the decay rate of prompt neutrons in a system at delayed criticality**

- **MCNP assumes point-kinetics model**

$$\alpha_R = -\frac{\beta}{\Lambda}$$

  - **β = effective delayed neutron fraction**
  - **Λ = neutron generation time**

- **Calculations have units (10^4 gens/second)**

Delayed Critical Rossi-α Validation

Benchmark	Measured	MCNP5-1.60	
		ENDF/B-VII.0	ENDF/B-VII.1
Jezebel-23	-100(1)	-108(1)	-104(1)
Flattop-23	-26.7(5)	-30.2(4)	-28.6(4)
Godiva	-111(2)	-113(2)	-113(2)
Flattop-25	-38.2(2)	-39.7(2)	-39.6(0.2)
Zeus-1	-0.338(8)	-0.363(2)	-0.360(2)
Zeus-5	-7.96(8)	-10.8(1)	-10.8(1)
Zeus-6	-3.73(5)	-4.14(3)	-4.19(3)
Big-Ten	-11.7(1)	-11.8(1)	-11.8(1)
STACY-30	-0.0127(3)	-0.0133(3)	-0.0127(3)
STACY-46	-0.0106(4)	-0.0104(2)	-0.0109(3)
Jezebel	-64(1)	-65(1)	-64(1)
Flattop-Pu	-21.4(5)	-21.0(3)	-20.8(3)
THOR	-19(1)	-20(1)	-21(1)

Delayed Critical Rossi-α Validation

- ^{233}U results are in better agreement with experiment for ENDF/B-VII.1 (compared to ENDF/B-VII.0).
  - Possibly because of improvements to ^{233}U inelastic cross section.

- Otherwise, results generally consistent with those obtained with ENDF/B-VII.0 data.

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 are biased high.
  - 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.
  - Further data (both microscopic and integral) are needed to better understand the calculated eigenvalues for Be reflected systems
    - Discussed last year; nothing new to report this year.

Acknowledgements

- **While this report has highlighted data testing work performed at LANL during FY11, significant contributions to the overall ENDF/B-VII.1 Data Validation effort have been made by colleagues worldwide; many whom appear as co-authors on the Validation Paper or have participated in CSEWG Validation Committee meetings in recent years.**
  - AECL, ANL, Bettis, BNL, KAPL, INL, ORNL
  - European colleagues (IAEA, UK, NRG/Petten, Slovenia)