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ICSBEP Benchmark Testing of CIELO Nuclides at LANL

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UNCLASSIFIED

Abstract

We review criticality data testing performed at Los Alamos with a combination of ENDF/B-VII.1 + potential CIELO nuclear data evaluations.

Outline

- CIELO Overview
- Criticality Data Testing
  - ICSBEP HMF, HST, IMF, LCT, PMF, PST benchmarks
- Summary

CIELO Overview

- CIELO = **C**oordinated **I**nternational **E**valuated **L**ibrary **O**rganization (WPEC Subgroup 40).
- Goal: To develop updated, best available evaluated nuclear data files for a select group of nuclides … ^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U and ^{239}Pu.
  - *"… The goal is to provide evaluations that perform in integral simulations (k_{eff}, spectral indices, etc.) as well as, or better, compared to existing evaluations, whilst using more accurate fundamental cross sections and spectra data. CIELO data will not be adjusted in the formal sense, but we recognize that some aspects of CIELO will include evaluation choices based upon feedback from simulations of integral experiments. …"*
- Why: The major international evaluated nuclear data libraries don't agree on the internal cross section details of these most important nuclides!

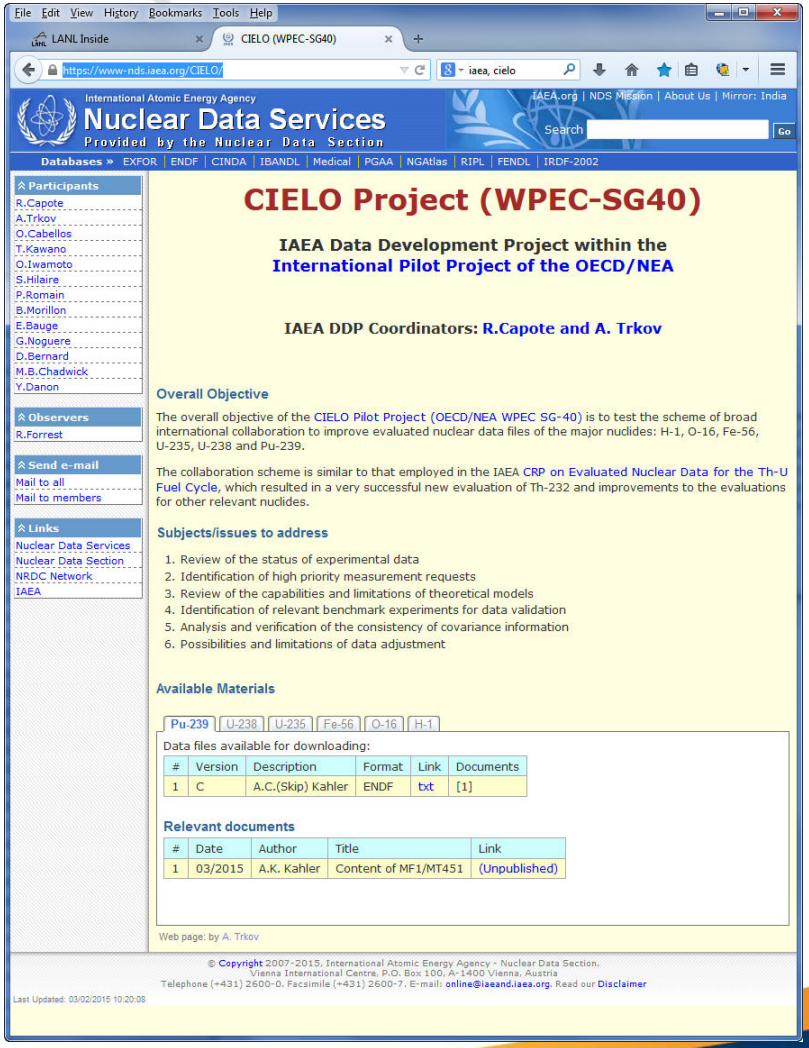
CIELO Nuclides

- ^{1}H –
- ^{16}O – (05c), Hale 7/2014 evaluation (mf3/mt2, mf3/mt800 and mf4/mt2) spliced to existing ENDF/B-VII.1 (IAEA 16O_halead).
- ^{56}Fe – (02c), BNL GForge v88.
- ^{235}U – (19c), ENDF/B-VII.1 plus (i) Leal “isrn_v2” RR; (ii) IAEA low energy ν(E) + IAEA & LANL pfns revisions.
  - *Now available from the IAEA CIELO web site.*
- ^{238}U – (04c), IAEA “ib44”.
- ^{239}Pu – (23c), ENDF/B-VII.1 plus SG34 plus recent Romano & LANL pfns revisions and LANL high energy ν(E) tweak .
  - *Now available from the IAEA web site.*

CIELO Overview

- The IAEA Nuclear Data Section has created a web page … https://www-nds.iaea.org/CIELO/ … with links to candidate evaluated data files.

- CIELO candidate ^{56}Fe files are also available from the "CIELO-Iron" project from the BNL NNDC GForge server.



^{235,238}U, ^{239}Pu – HMF & PMF Benchmarks

Benchmark	Benchmark keff	endf/b-vii.1 (e71)	e71 + ^{235}U_19c + ^{238}U_04c	"new" - e71, pcm
HMF1 (Godiva)	1.0000	0.99989	1.00010	21
HMF28 (Flattop-25)	1.0000	1.00284	1.00380	96
IMF7 (Big-10)	1.0045	1.00448	1.00329	-119
			e71 + ^{239}Pu_23c + ^{238}U_04c	"new" - e71, pcm
PMF1, rev3 (Jezebel)	1.0000	1.00061	1.00024	-37
PMF6 (Flattop-Pu)	1.0000	1.00111	1.00164	53

Fast, bare (Godiva and Jezebel) system calculated eigenvalues remain near unity.

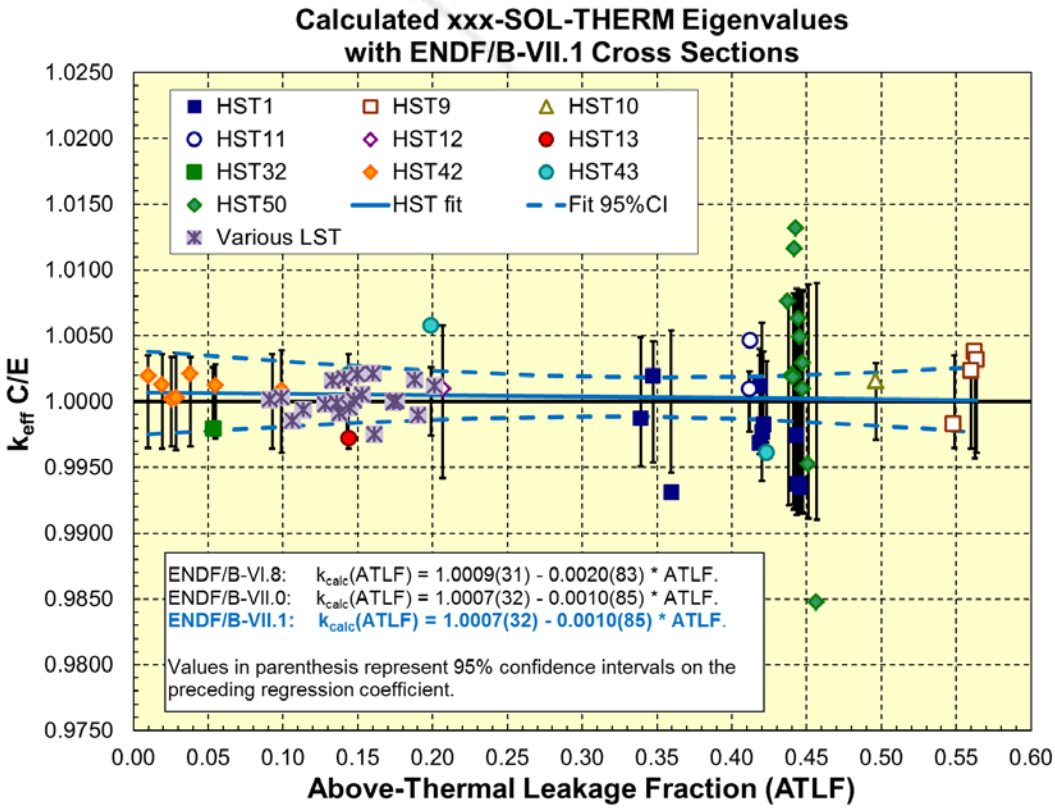
Fast, reflected (Flattops, Big-10) system calculated eigenvalues aren't as good, ☹.

^{235}U (& ^{1}H, ^{16}O) – HST Benchmarks

- A suite of 45 HEU-SOL-THERM benchmark critical configurations has been used for many years.
  - Accurate calculated eigenvalues, correlated against Above-Thermal Leakage Fraction (ATLF), have been obtained since ENDF/B-VI.3 in the early 1990s.
    - No trends observed for other regression analyses such as k_{calc} versus Above-Thermal Fission Fraction (ATFF); versus Average Energy of a Neutron causing Fission (EAF); versus Energy of Average Lethargy of a Neutron causing Fission (EALF) or versus solution H/U ratio.
  - Tests of revised data sets must answer the question … “are we still ok or did we break something?”.

^{235}U (& ^{1}H, ^{16}O) – HST Benchmarks

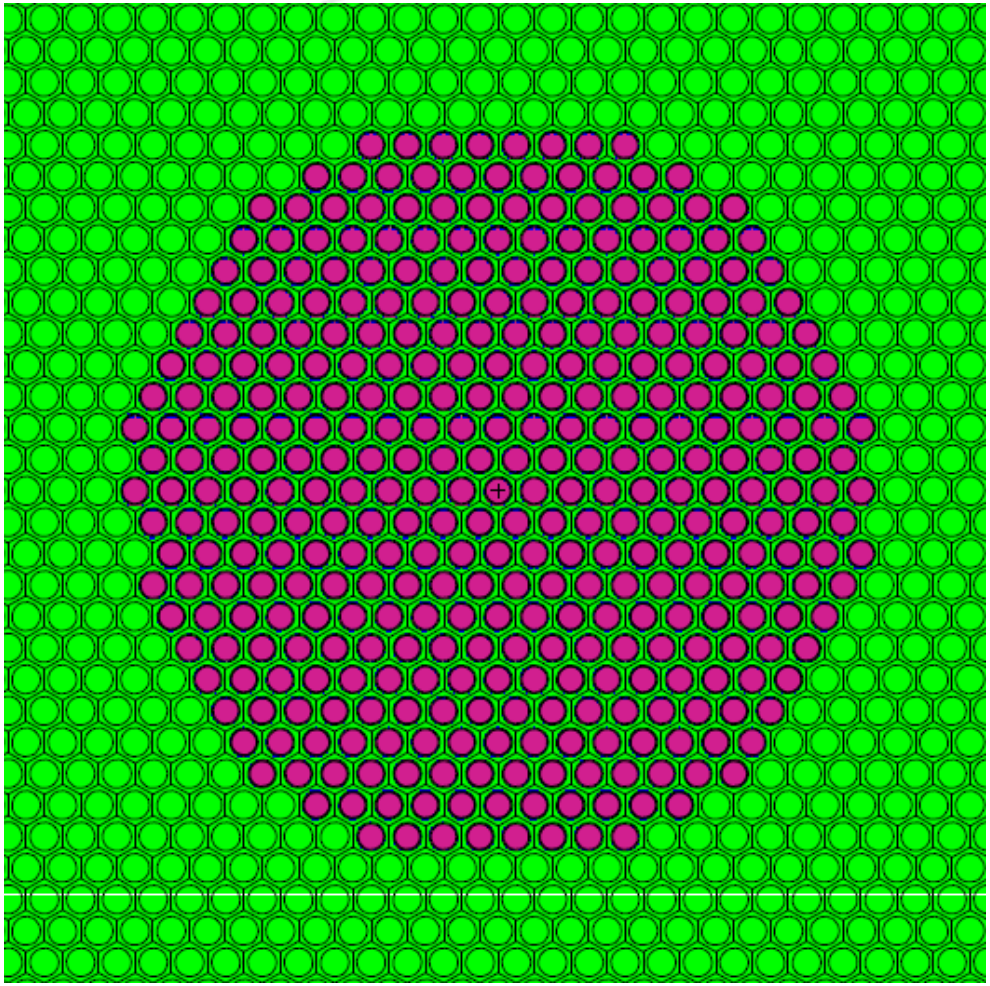
- Near unity intercept and near zero slope indicate no bias in calculated eigenvalues for the HST benchmark class (with e71).
  - e71 + ^{235}U_19c + ^{238}U_04c + ^{16}O_05c:
    - b = 1.0002(31)
    - m = +0.0019(83)
  - e71 + CAB h-h_2o kernel:
    - b = 1.0003(33)
    - m = -0.0005(87)



^{235}U (& ^{1}H, ^{16}O, ^{238}U) – LCT Benchmarks

- Use a subset of LEU-COMP-THERM (LCT) benchmarks
  - LCT5 cases 1, 5 and 12 have water-to-fuel volume ratio of 2.7, 1.0 and 0.5, respectively.
  - The variable rod pitch in LCT7 allows testing of under-moderated (1.26 cm rod pitch), near optimally moderated (1.6 cm and 2.1 cm rod pitch) and over-moderated (2.52 cm rod pitch) conditions.
  - LCT10 and LCT17 consist of several clusters plus one of (i) Lead; (ii) ^{nat}U; or (iii) Steel reflectors.
    - Can use LCT2 and LCT1, respectively, for unreflected “base case” comparison.
  - LCT8 are B&W lattices with varying amounts of soluble boron.
  - LCT42 is similar to LCT10 and LCT17 but also includes metal plates between the clusters.
- As with HST, we’re in pretty good shape for this benchmark class, so “… if it isn’t broke, don’t fix it!”.

^{235}U (& ^{1}H, ^{16}O, ^{238}U) – LCT Benchmarks

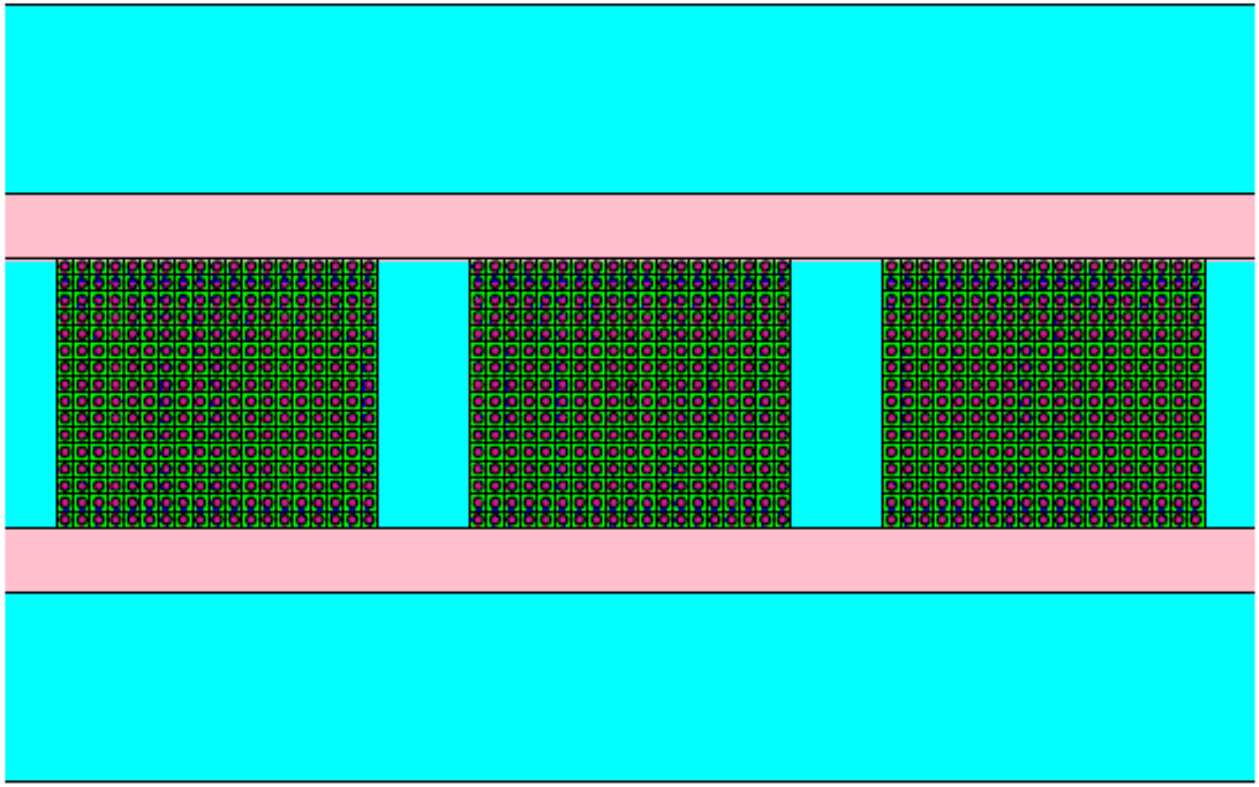


LEU-COMP-THERM-005, case 5 is shown
- 378 rods, 1.801 cm pitch.

Other LCT5 cases include:
- case 1: 132 rods, 2.398 cm pitch;
- case 12: 1185 rods, 1.598 cm pitch.

These three configurations do not contain soluble Gd poison, but other LCT5 cases do.

^{235}U (& ^{1}H, ^{16}O, ^{238}U) – LCT Benchmarks



LEU-COMP-THERM-017 geometry (three 19x16 clusters on a 2.032 cm rod pitch).

- LEU-COMP-THERM-001 uses the same fuel without walls.

LEU-COMP-THERM-010 employs smaller clusters (mostly 13x8 on a 2.54 cm rod pitch).

- LEU-COMP-THERM-002 uses the same fuel without walls.

LEU-COMP-THERM-042 employs 20x18 and 25x18 clusters on a 1.684 cm rod pitch with steel reflecting walls and various intracluster absorber plates.

^{235}U (& ^{1}H, ^{16}O, ^{238}U) – LCT Benchmarks

Benchmark	Benchmark keff	endf/b-vii.1 (e71)	e71 + 235U_19c + 238U_04c + 16O_05c + 56Fe_02c	"new" - e71, pcm
LCT1.1	0.9998	0.99955	0.99871	-84
LCT1.2	0.9998	0.99906	0.99786	-120
LCT1.3	0.9998	0.99850	0.99762	-88
LCT1.4	0.9998	0.99908	0.99813	-95
LCT1.5	0.9998	0.99695	0.99604	-91
LCT1.6	0.9998	0.99890	0.99784	-106
LCT1.7	0.9998	0.99829	0.99726	-103
LCT1.8	0.9998	0.99732	0.99641	-91
				-97
LCT2.1	0.9997	0.99845	0.99805	-40
LCT2.2	0.9997	0.99978	0.99941	-37
LCT2.3	0.9997	0.99914	0.99877	-37
LCT2.4	0.9997	0.99870	0.99847	-23
LCT2.5	0.9997	0.99772	0.99712	-60
				-39
LCT5.1	1.0000	1.00265	1.00197	-68
LCT5.5	1.0000	1.00504	1.00137	-367
LCT5.12	1.0000	1.00645	1.00062	-583
				-339

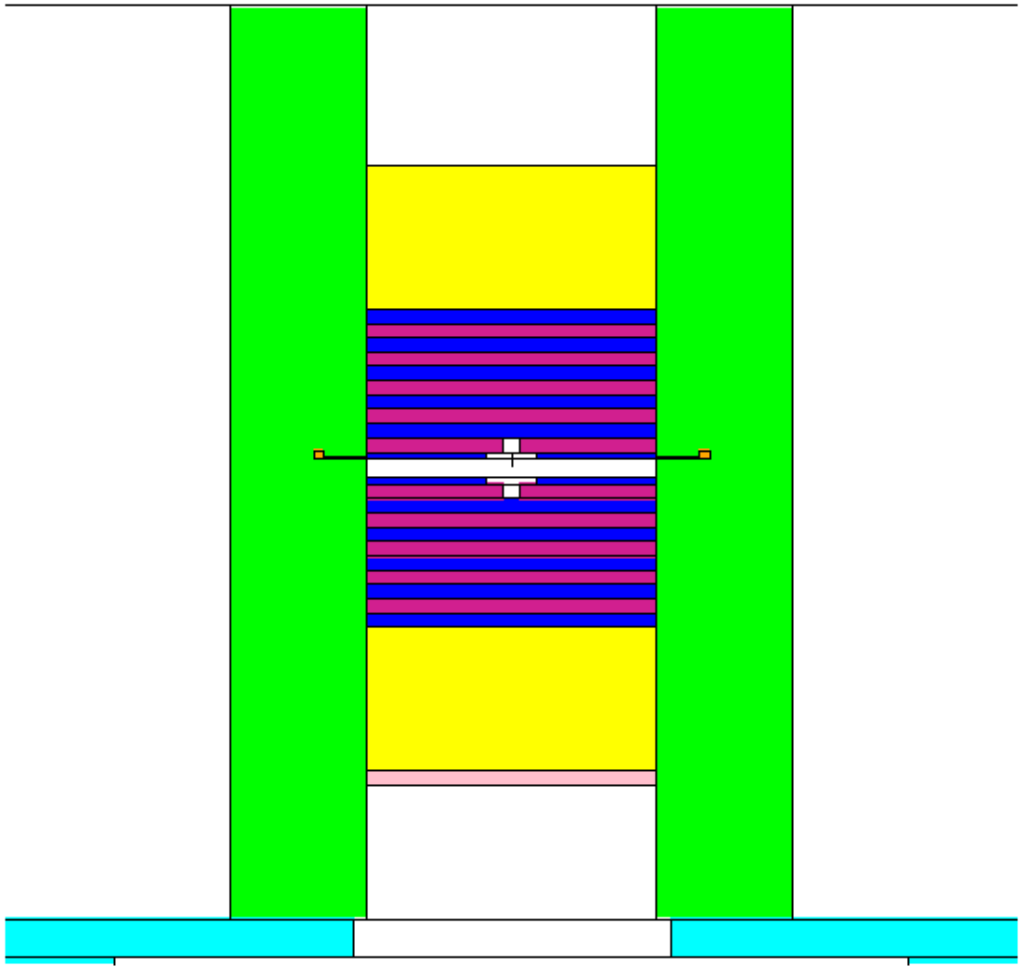
Benchmark	Benchmark keff	endf/b-vii.1 (e71)	e71 + 235U_19c + 238U_04c + 16O_05c + 56Fe_02c	"new" - e71, pcm
LCT7.1	1.0000	0.99759	0.99574	-185
LCT7.2	1.0000	0.99884	0.99852	-32
LCT7.3	1.0000	0.99750	0.99786	36
LCT7.4	1.0000	0.99810	0.99784	-26
				-52
LCT8.1	1.0007	1.00060	0.99677	-383
LCT8.2	1.0007	1.00087	0.99724	-363
LCT8.5	1.0007	1.00042	0.99665	-377
LCT8.7	1.0007	1.00017	0.99665	-352
LCT8.8	1.0007	0.99981	0.99624	-357
LCT8.11	1.0007	1.00135	0.99747	-388
				-370
LCT10.5	1.0000	0.99950	0.99812	-138
LCT10.6	1.0000	1.00008	0.99910	-98
LCT10.7	1.0000	1.00122	1.00071	-51
LCT10.8	1.0000	0.99788	0.99747	-41
				-82
LCT17.4	1.0000	0.99803	0.99660	-143
LCT17.5	1.0000	0.99989	0.99846	-143
LCT17.6	1.0000	1.00002	0.99882	-120
LCT17.7	1.0000	0.99986	0.99880	-106
LCT17.8	1.0000	0.99822	0.99721	-101
LCT17.9	1.0000	0.99770	0.99670	-100
				-119

MCNP stochastic uncertainty is typically 10 pcm, or less.

(Some) ICSBEP Benchmarks with Iron

- HMF13 – Spherical HEU assembly with 3.65 cm thick steel.
- HMF21 – Spherical HEU assembly with 9.7 cm thick steel.
- HMF24 – Spherical HEU assembly with 0.8 cm thick steel & 9.65 cm thick polyethylene.
- HMF87 – HEU cylindrical assembly with interstitial steel.
- HMF88 – HEU cylindrical assembly with interstitial steel or steel & polyethylene plus a polyethylene radial/axial reflector.
- LCT10, 17 & 42 – multiple UO_2 rod clusters with steel reflecting walls (LCT42 also has absorber plates between clusters).
- PMF25 – Spherical ^{239}Pu assembly with 1.55 cm thick steel.
- PMF26 – Spherical ^{239}Pu assembly with 11.9 cm thick steel.
- PMF28 – Spherical ^{239}Pu assembly with 19.65 cm thick steel.
- PMF32 – Spherical ^{239}Pu assembly with 4.49 cm thick steel.

ICSBEP's HMF88.1 Geometry



HEU-MET-FAST-088, case 1 (interstitial steel with radial and axial CH_2 reflectors).

Similar benchmarks, such as HEU-MET-FAST-087, do not have axial or radial reflectors.

^{235}U, ^{239}Pu & ^{56}Fe – HMF & PMF assemblies

Benchmark	Benchmark keff	endf/b-vii.1 (e71) kcalc C/E	e71 + ^{235}U (19c) + ^{238}U (04c) + ^{16}O (05c)	e71 + ^{235}U (19c) + ^{238}U (04c) + ^{16}O (05c) + ^{56}Fe (02c)	"new" - e71, pcm
HMF13	0.9990	0.99834	0.99843	0.99817	-17
HMF21	1.0000	0.99730	0.99732	0.99651	-79
HMF24	0.9990	0.99939	0.99986	0.99944	5
HMF87	0.9987	0.99970	1.00001	1.00040	70
HMF88.1	0.9993	0.99745	0.99872	0.99862	117
HMF88.2	0.9993	0.99734	0.99858	0.99782	48
Benchmark	Benchmark keff	endf/b-vii.1 (e71) kcalc	e71 + ^{239}Pu (23c)	e71 + ^{239}Pu (23c) + ^{56}Fe (02c)	"new" - e71, pcm
PMF25	1.0000	0.99880	0.99821	0.99857	-23
PMF26	1.0000	0.99845	0.99786	0.99725	-120
PMF28	1.0000	0.99896	0.99830	0.99743	-153
PMF32	1.0000	0.99862	0.99780	0.99790	-72

$^{235,238}U$, ^{16}O & ^{56}Fe – LCT assemblies

Benchmark	Benchmark keff	endf/b-vii.1 (e71) kcalc	e71 + ^{235}U (19c) + ^{238}U (04c) + ^{16}O (05c)	e71 + ^{235}U (19c) + ^{238}U (04c) + ^{16}O (05c) + ^{56}Fe (02c)	"new" - e71, pcm
LCT10.9	1.0000	0.99994	0.99874	1.00001	7
LCT10.10	1.0000	1.00024	0.99920	1.00025	1
LCT10.11	1.0000	1.00062	0.99940	1.00037	-25
LCT10.12	1.0000	0.99975	0.99873	0.99939	-36
LCT10.13	1.0000	0.99758	0.99706	0.99696	-62
LCT17.10	1.0000	0.99809	0.99692	0.99742	-67
LCT17.11	1.0000	0.99842	0.99731	0.99771	-71
LCT17.12	1.0000	0.99860	0.99735	0.99731	-129
LCT17.13	1.0000	0.99881	0.99775	0.99772	-109
LCT17.14	1.0000	0.99915	0.99777	0.99810	-105
LCT42.1	1.0000	0.99816	0.99592	0.99658	-158
LCT42.2	1.0000	0.99804	0.99563	0.99608	-196
LCT42.3	1.0000	0.99897	0.99652	0.99690	-207
LCT42.4	1.0000	0.99838	0.99615	0.99622	-216
LCT42.5	1.0000	0.99930	0.99712	0.99756	-174
LCT42.6	1.0000	0.99937	0.99727	0.99780	-157
LCT42.7	1.0000	0.99776	0.99538	0.99588	-188

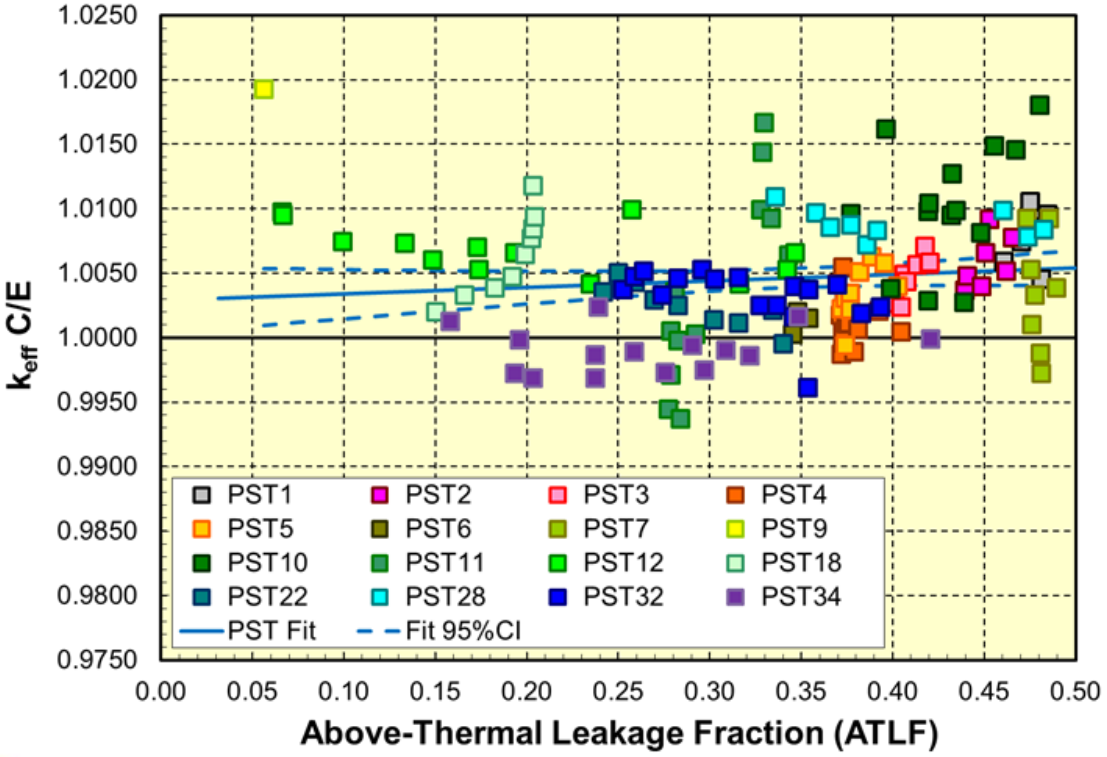
LCT10 has the largest rod pitch (2.54 cm).

LCT17 is smaller (2.032 cm).

LCT42 is smallest (1.684 cm).

^{239}Pu (& ^{1}H, ^{16}O) – PST Benchmarks

- The average calculated eigenvalue for the Pu-SOL-THERM benchmark class has been biased high by about 500 pcm for many years (ENDF/B-VII.1 results shown).



We use a small subset of the Pu-SOL-THERM benchmark population to assess candidate files.

- 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.

^{239}Pu (& ^{1}H, ^{16}O) – PST Benchmarks

- k_{eff} C/E results with various SG34 and CIELO candidate files …

Benchmark	Benchmark keff	e71 (with mf3/mt18 background fix)	e71 + SG34 ^{239}Pu	e71 + ^{239}Pu (23c) + ^{16}O (05c)
PST1.4	1.0000	1.00451	1.00209	0.99969
PST4.1	1.0000	1.00411	1.00052	0.99870
PST12.10	1.0000	1.00417	1.00078	0.99931
PST12.13	1.0000	1.00974	1.00623	1.00503
PST18.6	1.0000	1.00484	1.00195	1.00082
PST34.4	1.0000	1.00248	0.99933	0.99767
PST34.15	1.0000	0.99733	0.99719	0.99590
PST average:		***1.00388***	***1.00116***	***0.99959***

For ENDF, WPEC Subgroup 34 efforts eliminated ~75% of the historical *average* k_{calc} bias.

On average, the latest ^{239}Pu and ^{16}O files eliminate the remaining bias.

PFNS Uncertainty (^{239}Pu)

- Impact of pfns uncertainty on k_{calc} and reaction rates …
  - Use the LANL Pu-MET-FAST-001 (Jezebel) critical assembly
    - ENDF/B-VII.1 cross sections plus a recent Neudecker ^{239}Pu pfns yields a calculated eigenvalue of 0.99797(3).
    - Generate a suite of 1000 pfns data sets, based upon evaluated uncertainty
      - Average k_{calc} is 0.99798, *population* standard deviation is 107 pcm.
      - The standard deviation in calculated spectral indices varies from a fraction of a per cent to almost 10%, depending upon the reaction rate average energy …
        - e.g., ^{239}Pu(n,f)/^{235}U(n,f) = 1.4203 ± 0.0017; ^{238}U(n,f)/^{235}U(n,f) = 0.2031 ± 0.0022
        - e.g., ^{238}U(n,2n)/^{235}U(n,f) = 0.0119 ± 0.0007; ^{169}Tm(n,2n)/^{235}U(n,f) = 0.00307 ± 0.00029.
  - For the Pu-SOL-THERM-001.4 critical assembly …
    - ENDF/B-VII.1 cross sections plus a recent Neudecker ^{239}Pu pfns yielded a calculated eigenvalue of 1.00948(6).
    - 1000 sample average is 1.01042 with a *population* standard deviation of 283 pcm (wow!).

Summary

- Work to revise the evaluated data files for ^{1}H, ^{16}O, ^{56}Fe, $^{235,238}U$ and ^{239}Pu continues …
- LANL testing to date has concentrated on ICSBEP benchmark eigenvalues. Reaction rate (spectral indices) data, pulsed sphere spectra, shielding (SINBAD) and reactor physics (IRPhEP) benchmarks are also important resources to be utilized in a comprehensive data testing regimen (and are being utilized by our international colleagues).
- New tools are becoming available to assist data testing.
  - See https://www-nds.iaea.org/index-meeting-crp/CM_Compensating_Effects_2015/, and in particular the contribution by Oscar Cabellos, OECD/NEA.
    - DICE = Database for ICSBEP & NDaST = Nuclear Data Sensitivity Tool.
- The CIELO evaluated data files are expected to be an important component in the next ENDF/B release.