^{235}U and ^{1}H Data Set Testing with (mostly) ICSBEP Benchmarks

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- Bettis has performed continuous energy Monte Carlo (RCP01 and MCNP5) eigenvalue calculations for a variety of ICSBEP uranium fueled benchmarks with ENDF/B-VI.8 cross sections, with the "pre-VIIβ0" cross sections released by BNL in March 2005, with LANL's "1p3326x.txt" ^{1}h data set and with the new JEFF-3.1 (Mattes) h-h_2o scattering kernel data.

- RCP01 eigenvalues presented on subsequent slides are calculated from tracking 50 million neutron histories in ten independent 5 million history jobs.
  - For RCP01, the 95% eigenvalue confidence interval is determined from the variance in the ten independent eigenvalue estimates and is typically less than 0.0005 Δk (i.e., roughly the size of the plot symbol in subsequent graphs).

- MCNP5 eigenvalues are based upon single 100 million history jobs for each benchmark configuration.

- Calculated eigenvalues and subsequent correlations are based upon RCP01 results unless explicitly labeled otherwise.

- A majority of these calculations use models derived from the ICSBEP Handbook:
  - xxx-SOL-THERM
    - 9 HEU evaluations, 31 critical configurations plus two ORNL experiments (L5, L6) that will appear in the 2005 edition of the Handbook.
      - 4 evaluations (8 critical configurations) include a H_2O reflector.
    - 9 LEU evaluations, 39 critical configurations
      - 4 evaluations (19 critical configurations) include a H_2O reflector.
  - HEU-MET-FAST-007 (2005 version)
    - 26 polyethylene moderated, but bare, rectangular slab assemblies.
    - 9 polyethylene moderated and reflected rectangular slab assemblies.
  - LEU-COMP-THERM-006
    - 18 configurations, 15 by 15 to 21 by 21 rod arrays with rectangular pitch.
    - multiple configurations with one of four rod pitches, ranging from 1.85 cm to 2.30 cm.
  - LEU-COMP-THERM-002 & LEU-COMP-THERM-010
    - 2 configurations, three sets of 13 x 8 or 15 x 8 rod arrays, water reflector.
    - 13 configurations, three sets of 13 x 8 rod arrays with Pb, ^{depl}U, or Steel (Fe) reflectors.

HEU- and LEU-SOL-THERM Benchmark Characteristics

- Geometrically simple systems – spheres, cylinders or slabs with and without water reflection.
- Only a few nuclides – $^{235,238}U$, hydrogen, oxygen plus small amounts of fluorine or nitrogen.
  - Thin walled aluminum or stainless steel container is neutronically unimportant (but is still incorporated in modern models).
  - ^{235}U accounts for > 99% of fission.
  - ^{238}U absorption ranges from a fraction of a per cent in HEU solutions to several per cent in LEU STACY solutions.

Selected HEU-SOL-THERM ICSBEP Benchmarks

Benchmark	Description
HEU-SOL-THERM-001 (encompass “RF#”)	Unreflected cylinders (~28cm, ~33cm and ~51cm diameter) containing uranyl nitrate.
HEU-SOL-THERM-009 (Case 3 = ORNL L7)	Water reflected spheres (6.4-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-010	Water reflected sphere (9.7-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-011	Water reflected spheres (17-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-012 (ORNL L10)	Water reflected sphere (91-liter) containing uranium oxyfluoride.
HEU-SOL-THERM-013 (ORNL1)	Unreflected sphere (174-liter) containing uranium nitrate.
HEU-SOL-THERM-032 (ORNL10)	Unreflected sphere (48-inch diameter) containing uranyl nitrate.
HEU-SOL-THERM-042 (encompass ORNL12 through ORNL23)	Unreflected cylinders (~77cm and ~137cm diameter) containing uranium nitrate.
HEU-SOL-THERM-043 (Cases 2 and 3 are ORNL L8 and ORNL L9)	Unreflected spheres (17-liter, 91-liter and 174-liter) containing uranium oxyfluoride solution.
ORNL L5, L6 will appear as cases 3 & 4 of HEU-SOL-THERM-050 in the 2005 Edition of the ICSBEP Handbook)	Unreflected cylinders (13cm diameter) of uranium oxyfluoride. Low $H/^{235}U$ ratios of 27 and 44 lead to large leakage.

Selected LEU-SOL-THERM ICSBEP Benchmarks

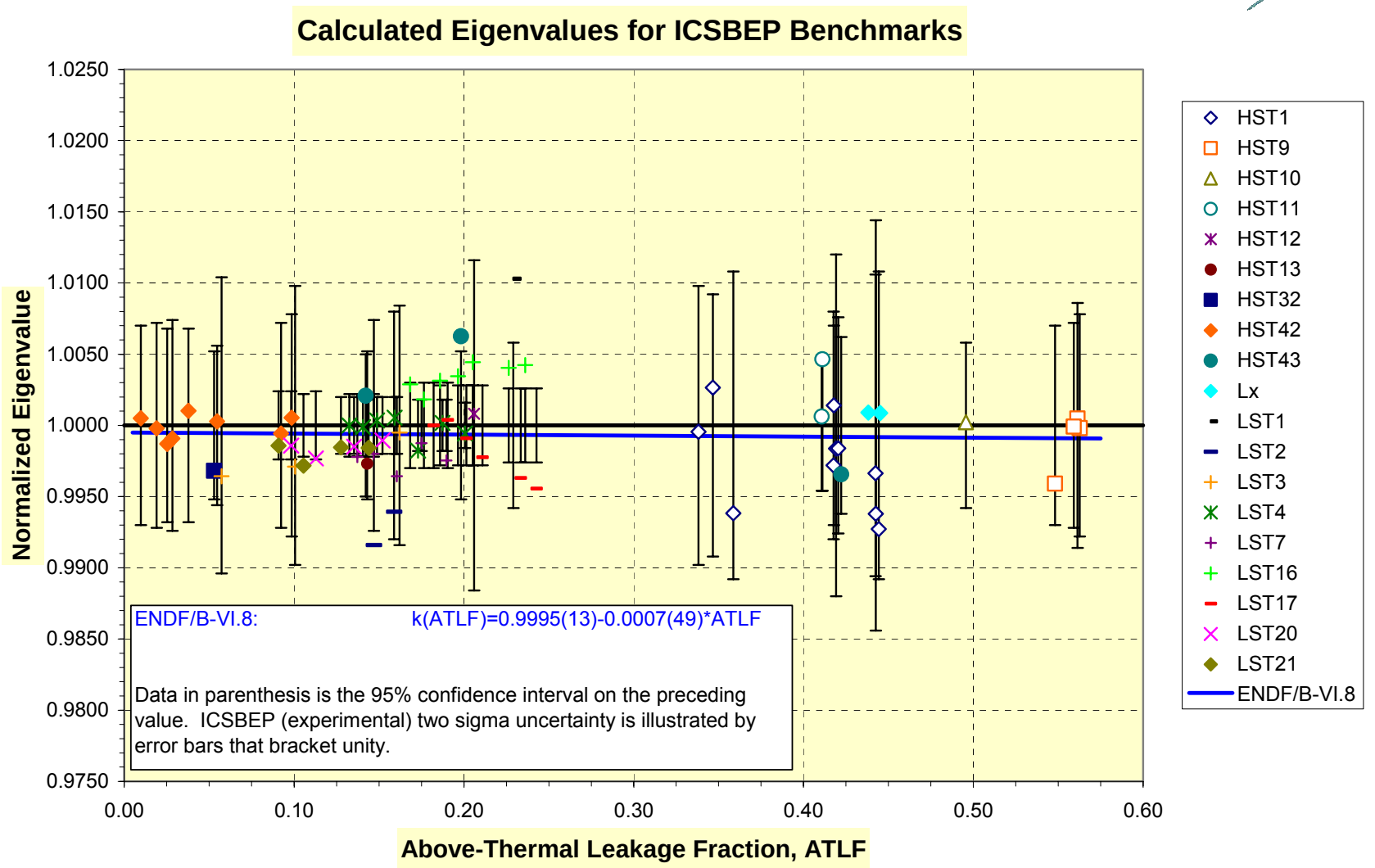
Benchmark	Description
LEU-SOL-THERM-001	"SHEBA-II". An unreflected UO_2F_2 + H_2O cylindrical (~20 inch diameter) assembly.
LEU-SOL-THERM-002	174-liter spheres of low enriched (4.9%) uranium oxyfluoride solutions. Case 1 is a water reflected solution, case 2 is unreflected.
LEU-SOL-THERM-003	Bare spheres of 10% enriched uranyl nitrate water solutions. Cases 3, 6 and 9 are full spheres with increasing H-to-^{235}U ratio.
LEU-SOL-THERM-004	STACY; Water reflected, 10% enriched uranyl nitrate solution in a 60cm diameter cylindrical tank. Seven cases with varying gU/liter.
LEU-SOL-THERM-007	STACY; Unreflected, 10% enriched uranyl nitrate solution in a 60cm diameter cylindrical tank. Five cases with varying gU/liter.
LEU-SOL-THERM-016	STACY; Water reflected, 10% enriched uranyl nitrate solution in a rectangular (slab, ~28cm x ~69cm) tank. Seven cases with varying gU/liter.
LEU-SOL-THERM-017	STACY; Unreflected, 10% enriched uranyl nitrate solution in a rectangular (slab, ~28cm x ~69cm) tank. Six cases with varying gU/liter.
LEU-SOL-THERM-020	STACY; Water reflected, 10% enriched uranyl nitrate solution in an 80cm diameter cylindrical tank. Four cases with varying gU/liter.
LEU-SOL-THERM-021	STACY; Unreflected, 10% enriched uranyl nitrate solution in an 80cm diameter cylindrical tank. Four cases with varying gU/liter.

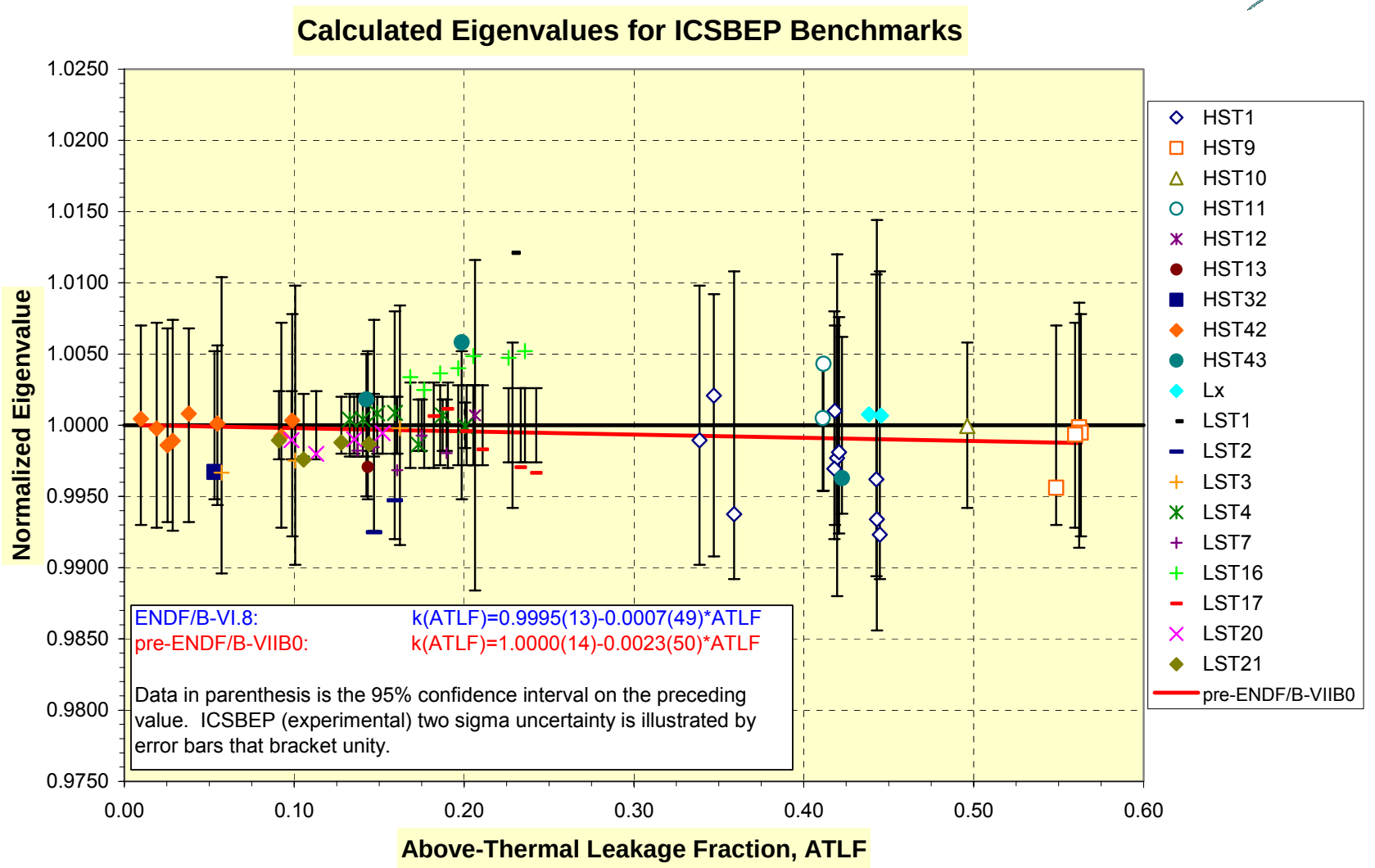
Regression Analysis – HST & LST Benchmarks

- Correlate calculated eigenvalue, k_{calc}, against various parameters such as Above-Thermal Leakage Fraction (ATLF) or hydrogen in solution absorption (H_{abs}).
  - k_{calc}(parameter) = intercept + slope * parameter
  - Looking for an intercept whose magnitude is statistically equivalent to unity and whose slope is statistically equivalent to zero.

- ATLF regression for HST benchmarks with ENDF/B-VI.8 is:
  - k_{calc}(ATLF) = 1.0002(19) – 0.0028(54) * ATLF: RCP01
  - k_{calc}(ATLF) = 1.0010(19) – 0.0035(54) * ATLF: MCNP5

- Hydrogen absorption regression for ENDF/B-VI.8 is:
  - $k_{calc}(H_{abs})$ = 0.9993(13) + 0.0003(56) * H_{abs}: RCP01
  - $k_{calc}(H_{abs})$ = 1.0005(13) – 0.0005(57) * H_{abs}: MCNP5


Calculated Eigenvalues for ICSBEP Benchmarks
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
0.00
0.10
0.20
0.30
0.40
0.50
0.60
Above-Thermal Leakage Fraction, ATLF
ENDF/B-VI.8:
k(ATLF)=0.9995(13)-0.0007(49)*ATLF
Data in parenthesis is the 95% confidence interval on the preceding value. ICSBEP (experimental) two sigma uncertainty is illustrated by error bars that bracket unity.
HST1
HST9
HST10
HST11
HST12
HST13
HST32
HST42
HST43
Lx
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
ENDF/B-VI.8

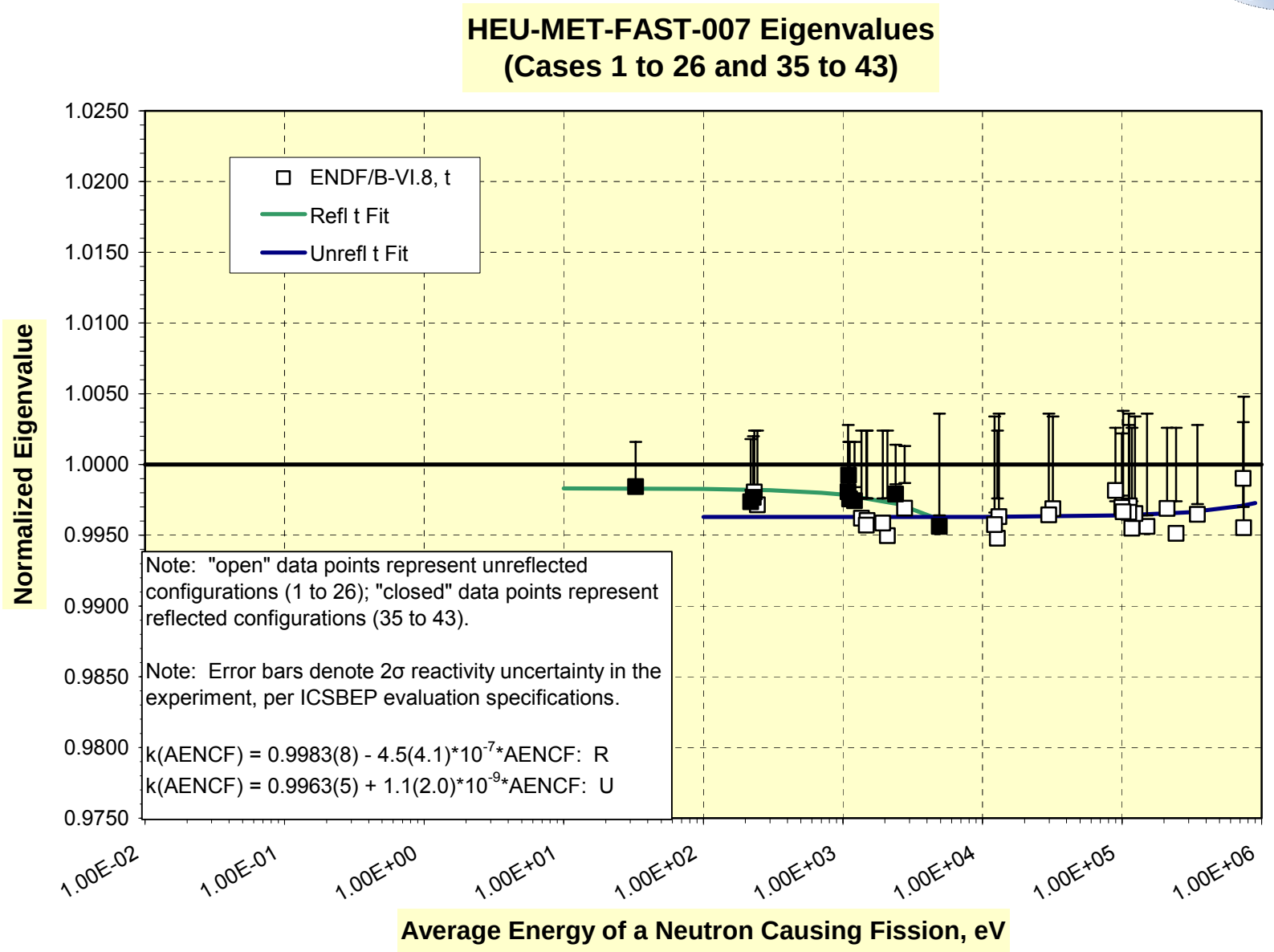

Calculated Eigenvalues for ICSBEP Benchmarks
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
0.00
0.10
0.20
0.30
0.40
0.50
0.60
Above-Thermal Leakage Fraction, ATLF
ENDF/B-VI.8: k(ATLF)=0.9995(13)-0.0007(49)*ATLF
pre-ENDF/B-VIIB0: k(ATLF)=1.0000(14)-0.0023(50)*ATLF
Data in parenthesis is the 95% confidence interval on the preceding value. ICSBEP (experimental) two sigma uncertainty is illustrated by error bars that bracket unity.
HST1
HST9
HST10
HST11
HST12
HST13
HST32
HST42
HST43
Lx
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
pre-ENDF/B-VIIB0

Regression Analysis – HST & LST Benchmarks

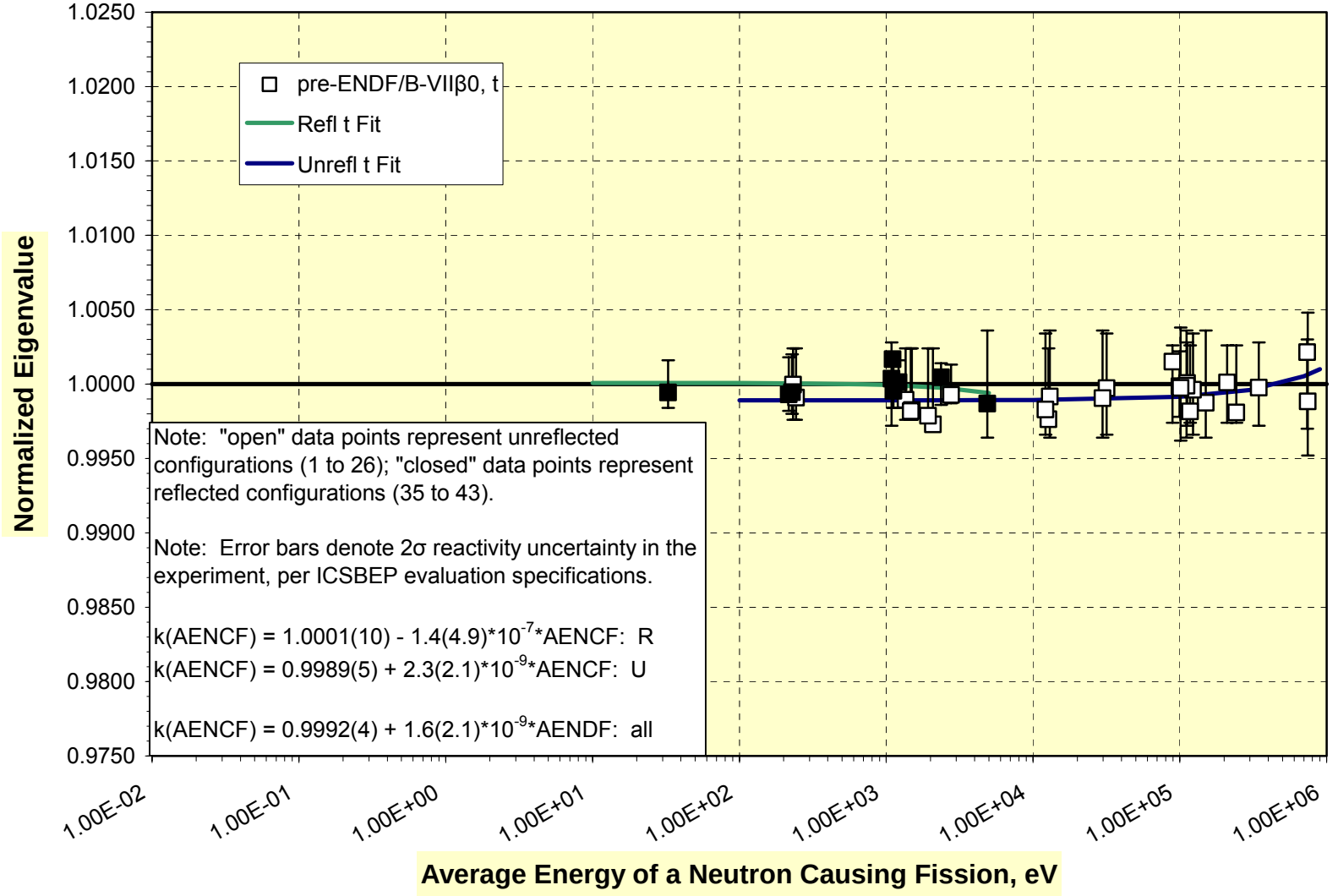
- ATLF Regression:
  - ENDF/B-VI.8: k(ATLF) = 0.9995(13) – 0.0007(49)*ATLF
  - Pre-ENDF/B-VIIβ0: k(ATLF) = 1.0000(13) – 0.0023(50)*ATLF
    - The "improved" intercept (1.0000 versus 0.9995) in the pre-ENDF/B-VIIβ0 regression is an artifact of the larger negative ATLF slope and an increase in the average LST eigenvalue. The average eigenvalue for the eight low ATLF HST42 benchmarks is virtually unchanged; 0.99992 with ENDF/B-VI.8 cross sections and 0.99978 with pre-ENDF/B-VIIβ0.
    - The average eigenvalue for the 33 HST benchmarks decreases from 0.99930 with ENDF/B-VI.8 cross sections to 0.99902 with pre-ENDF/B-VIIβ0.
    - The average eigenvalue for the 39 LST benchmarks increases from 0.99937 with ENDF/B-VI.8 cross sections to 0.99992 with pre-ENDF/B-VIIβ0

HEU-MET-FAST-007 Benchmark Description

- HEU-MET-FAST-007 (using specifications approved for publication in the Fall 2005 version of the ICSBEP Handbook)
  - 18 unreflected 10” x 10” and 8 unreflected 5” x 10” HEU slab configurations with interleaved sheets of polyethylene.
    - Average energy of a neutron causing fission is ~1.5 keV to ~750 keV.
  - 9 reflected 5” x 10” HEU slab configurations with interleaved polyethylene plus a 6” thick polyethylene reflector on six sides.
    - Average energy of a neutron causing fission is ~30 eV to ~4.5 keV.


HEU-MET-FAST-007 Eigenvalues
(Cases 1 to 26 and 35 to 43)
ENDF/B-VI.8, t
Refl t Fit
Unrefl t Fit
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
Note: "open" data points represent unreflected configurations (1 to 26); "closed" data points represent reflected configurations (35 to 43).
Note: Error bars denote 2σ reactivity uncertainty in the experiment, per ICSBEP evaluation specifications.
k(AENCF) = 0.9983(8) - 4.5(4.1)*10^-7*AENCF: R
k(AENCF) = 0.9963(5) + 1.1(2.0)*10^-9*AENCF: U
1.00E-02
1.00E-01
1.00E+00
1.00E+01
1.00E+02
1.00E+03
1.00E+04
1.00E+05
1.00E+06
Average Energy of a Neutron Causing Fission, eV

HEU-MET-FAST-007 Eigenvalues
(Cases 1 to 26 and 35 to 43)



Note: "open" data points represent unreflected configurations (1 to 26); "closed" data points represent reflected configurations (35 to 43).

Note: Error bars denote 2σ reactivity uncertainty in the experiment, per ICSBEP evaluation specifications.

k(AENCF) = 1.0001(10) - 1.4(4.9)*10^{-7}*AENCF: R

k(AENCF) = 0.9989(5) + 2.3(2.1)*10^{-9}*AENCF: U

k(AENCF) = 0.9992(4) + 1.6(2.1)*10^{-9}*AENDF: all

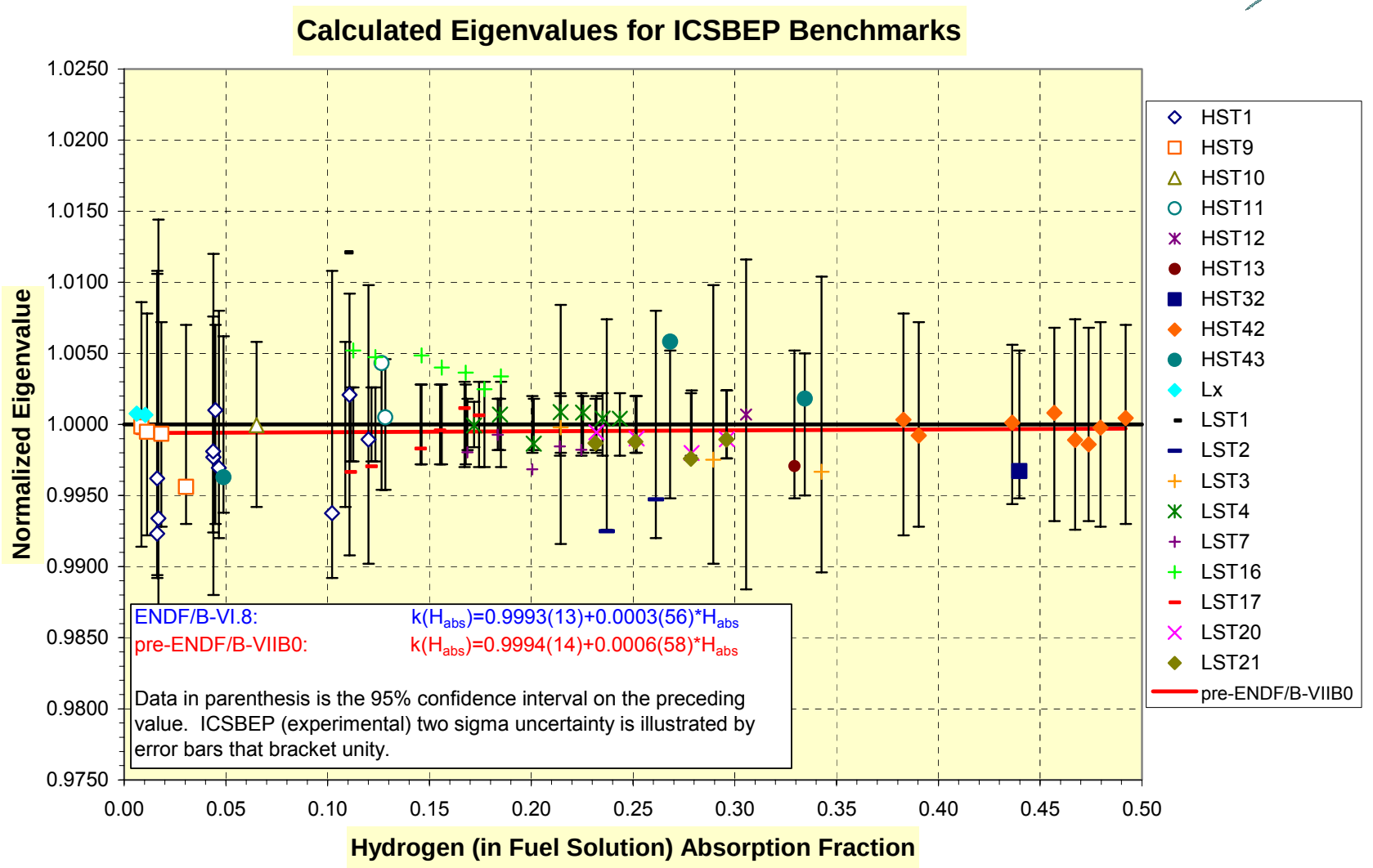
HEU-MET-FAST-007 Observations

- HEU-MET-FAST-007 (ORNL)
  - With ENDF/B-VI.8 there is a ~0.2% bias in calculated eigenvalues between reflected and unreflected configurations. Furthermore, all calculated eigenvalues were biased low.
  - With ENDF/B-VIIβ0 this bias is substantially reduced (to ~0.1%) and individual eigenvalues are more likely to be distributed about unity, although a small (< 0.1%) below unity bias remains.
  - With the ENDF/B-VIIβ0 data set and for the combined suite of 26 critical configurations there is no trend in calculated eigenvalue as a function of the Average Energy of a Neutron Causing Fission, AENCF.

HST Results for Hydrogen Capture Perturbation

- ^{1}H in ENDF/B-VI.8 and pre-ENDF/B-VIIβ0 has a thermal capture cross section of 0.3320 barns.
  - The HST42.1 to 42.8 ENDF/B-VI.8 average eigenvalue = 0.99992.
  - The HST42.1 to 42.8 pre-VIIβ0 average eigenvalue = 0.99978.
  - The HST9.1 to 9.4 ENDF/B-VI.8 average eigenvalue = 0.99903.
  - The HST9.1 to 9.4 pre-VIIβ0 average eigenvalue = 0.99857.

- LANL's "1p3326.txt" ^{1}H has a thermal capture cross section of 0.3326 barns. Remaining nuclides are pre-ENDF/B-VIIβ0.
  - The HST42.1 to 42.8 average eigenvalue = 0.99897.
  - The HST9.1 to 9.4 average eigenvalue = 0.99844.


Calculated Eigenvalues for ICSBEP Benchmarks
Normalized Eigenvalue
1.0250
1.0200
1.0150
1.0100
1.0050
1.0000
0.9950
0.9900
0.9850
0.9800
0.9750
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50
Hydrogen (in Fuel Solution) Absorption Fraction
HST1
HST9
HST10
HST11
HST12
HST13
HST32
HST42
HST43
Lx
LST1
LST2
LST3
LST4
LST7
LST16
LST17
LST20
LST21
pre-ENDF/B-VIIB0
ENDF/B-VI.8: k(H_abs)=0.9993(13)+0.0003(56)*H_abs
pre-ENDF/B-VIIB0: k(H_abs)=0.9994(14)+0.0006(58)*H_abs
Data in parenthesis is the 95% confidence interval on the preceding value. ICSBEP (experimental) two sigma uncertainty is illustrated by error bars that bracket unity.

HST & LST Results with the Standard ENDF/B-VI.2 and the New JEFF-3.1 h-h_2o Kernel

- Regression fit versus ATLF for ENDF/B-VI.8 with the standard h-h_2o kernel and the JEFF-3.1 h-h_2o kernel (Note: RCP01 only uses kernel data below 0.625 eV):
  - k_{calc}(ATLF) = 0.9995(13) – 0.0007(49) * ATLF: ENDF/B-VI.8
  - k_{calc}(ATLF) = 0.9990(13) – 0.0008(49) * ATLF: JEFF-3.1
  - Bare solution assemblies see an eigenvalue decrease of ~0.0005Δk. These assemblies typically have small ATLF values, hence they influence the intercept value in the regression analysis.
  - Reflected solution benchmarks see a slightly larger eigenvalue decrease. Since these assemblies typically have large ATLF values, this results in a slightly larger negative slope.

Final xxx-SOL-THERM Observations

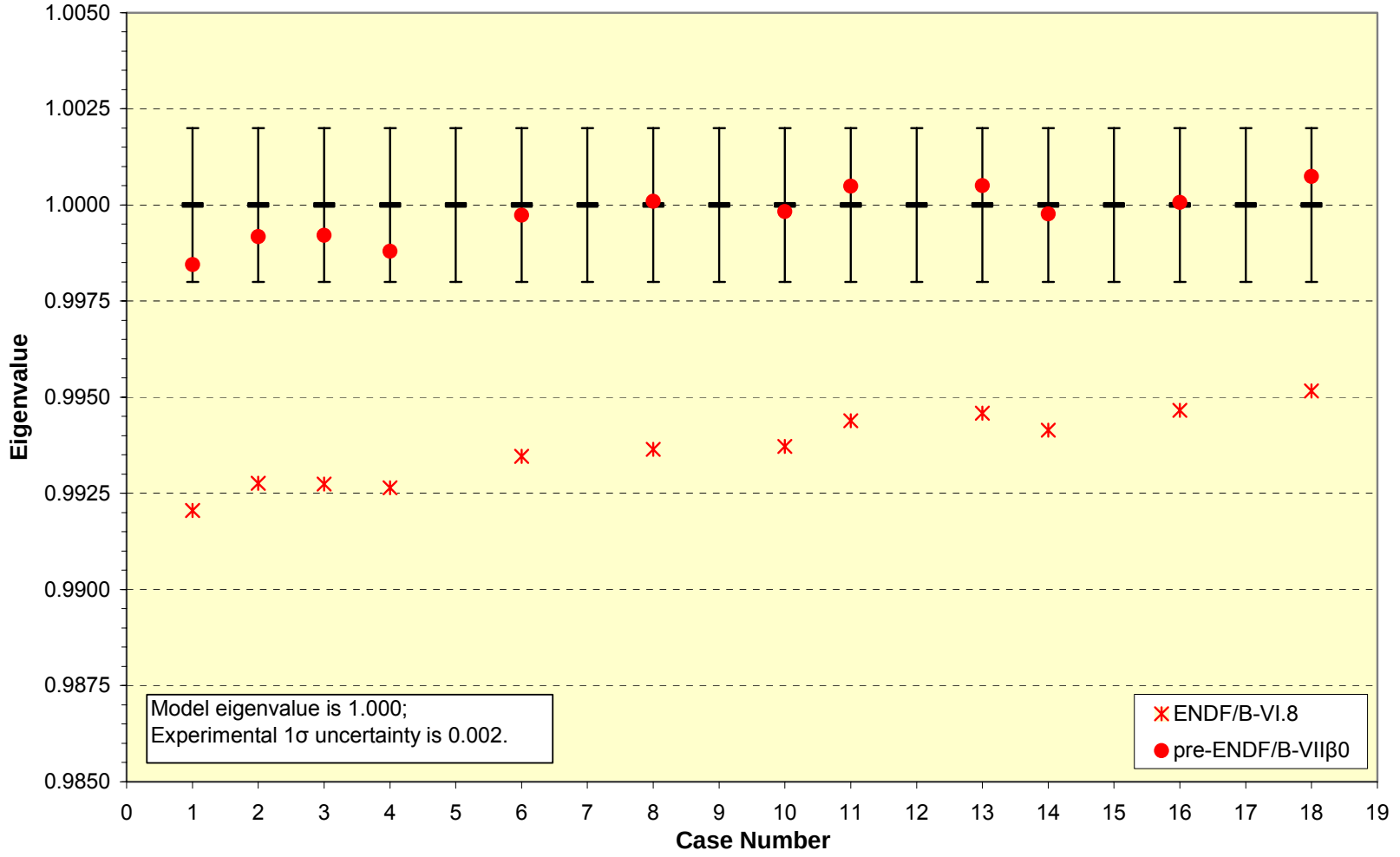
- The ENDF/B-VI.8 library yields accurate eigenvalues for HEU-SOL-THERM and LEU-SOL-THERM solution benchmarks.
  - Average eigenvalues are close to unity with no underlying eigenvalue trend as a function of Above-Thermal Leakage Fraction (ATLF).
- Similar eigenvalues are calculated with the Pre-ENDF/B-VIIβ0 data set, however
  - Changes in the magnitude of the regression fitting parameters suggest that small trends and/or biases not present in ENDB/B-VI.8 may exist in Pre-ENDF/B-VIIβ0.
  - Increasing the thermal hydrogen capture cross section will likely reduce the ATLF correlation intercept by 0.0005Δk to 0.0010Δk while simultaneously reducing the regression trend.
  - Use of the JEFF-3.1 (Mattes) h-h2o kernel data may further reduce the ATLF correlation intercept while slightly increasing the regression trend.

LEU-COMP-THERM-006 Benchmark Description

- Eighteen configurations of 2.6 w/o UO_2 fuel rods set on a square pitch. Water height used for reactivity control.
  - Fuel pellet stack is ~1.44 meters long
  - Four basic pitch settings:
    - 19 x 19, 20 x 20 and 21 x 21 rod arrays on a 1.849 cm pitch.
      - Water height varied from ~60 cm to ~99 cm.
    - 17 x 17, …, 21 x 21 rod arrays on a 1.956 cm pitch.
      - Water height varied from ~46 cm to ~116 cm.
    - 16 x 16, …, 20 x 20 rod arrays on a 2.150 cm pitch.
      - Water height varied from ~40 cm to ~79 cm.
    - 15 x 15, …, 19 x 19 rod arrays on a 2.293 cm pitch.
      - Water height varied from ~41 cm to ~90 cm.
  - Reflector is h_2o.

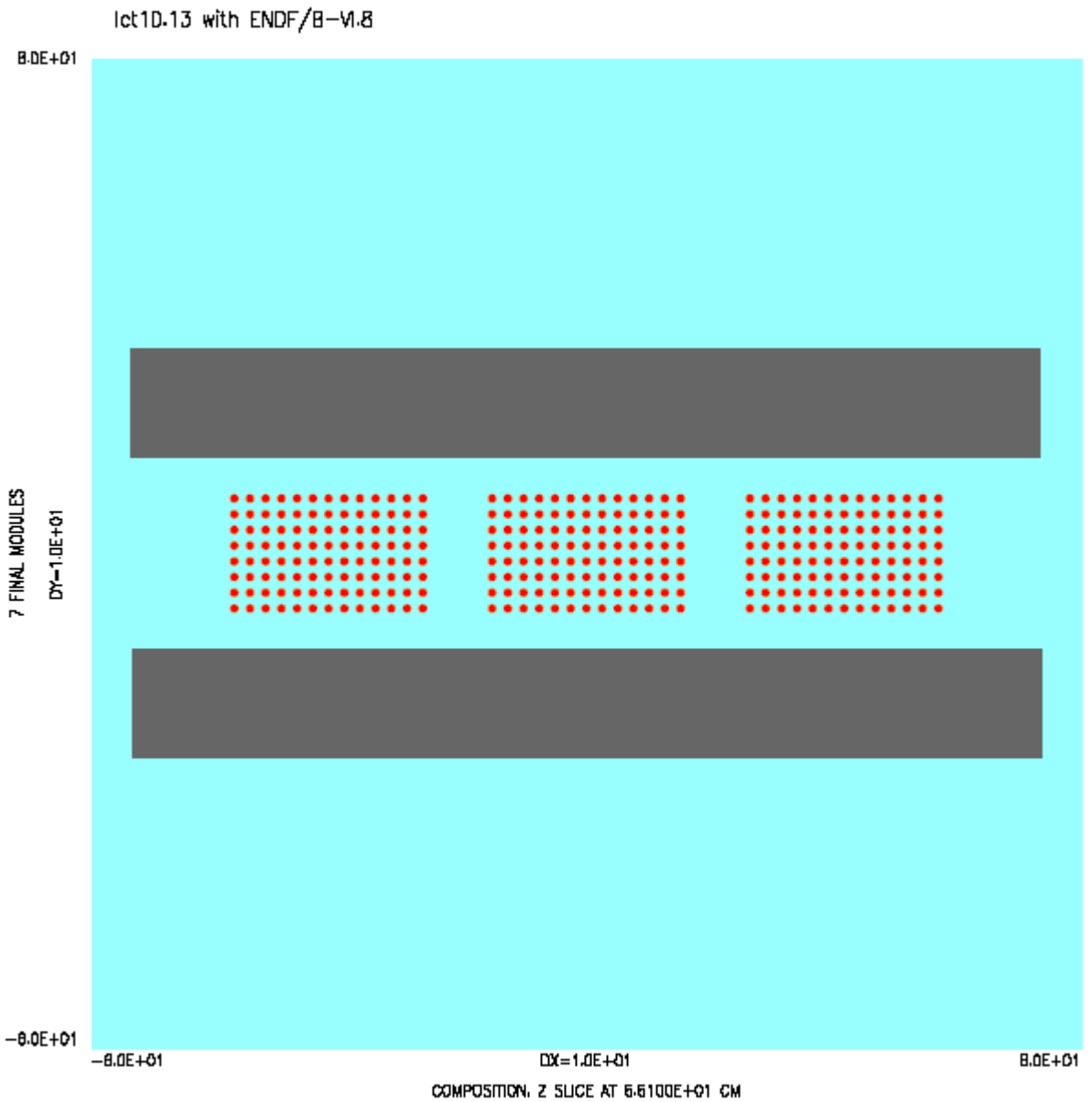
LEU-COMP-THERM-006 Eigenvalues with Various Cross Section Data Sets				
Case	Lattice Data		ENDF/B-VI.8	Pre-ENDF/B-VIIβ0
1	19 x 19	1.849 cm pitch	0.99205(23)	**0.99845(42)**
2	20 x 20		0.99276(20)	**0.99918(19)**
3	21 x 21		0.99274(24)	**0.99921(20)**
4	17 x 17	1.956 cm pitch	0.99264(20)	**0.99879(29)**
5	18 x 18		---	**---**
6	19 x 19		0.99346(23)	**0.99974(27)**
7	20 x 20		---	**---**
8	21 x 21		0.99365(31)	**1.00009(30)**
9	16 x 16	2.150 cm pitch	0.99372(23)	**0.99983(24)**
10	17 x 17		---	**---**
11	18 x 18		0.99438(20)	**1.00049(21)**
12	19 x 19		---	**---**
13	20 x 20		0.99458(26)	**1.00050(47)**
14	15 x 15	2.293 cm pitch	0.99414(23)	**0.99977(30)**
15	16 x 16		---	**---**
16	17 x 17		0.99466(46)	**1.00007(36)**
17	18 x 18		---	**---**
18	19 x 19		0.99517(34)	**1.00074(28)**

LEU-COMP-THERM-006 Eigenvalues with Selected Cross Section Data Sets



LEU-COMP-THERM-002 & -010 Benchmark Description

- Multiple clusters of 4.31 w/o UO_2 rods set on a 2.54 cm square pitch.
  - Generally three sets of 13 x 8 or three sets of 15 x 8 fuel rods.
  - 92 cm tall fuel stack is totally immersed in water.
    - Reactivity controlled by the inter-cluster gap.
- LEU-COMP-THERM-002 configurations are water reflected.
- LEU-COMP-THERM-010 configurations are water plus one of lead, ^{depl}U or steel (mostly iron) reflected.
  - Reflecting wall positioned along the long axis of the rod clusters.
  - Wall-to-unit cell separation varied from ~0.0 cm to ~5.4 cm.

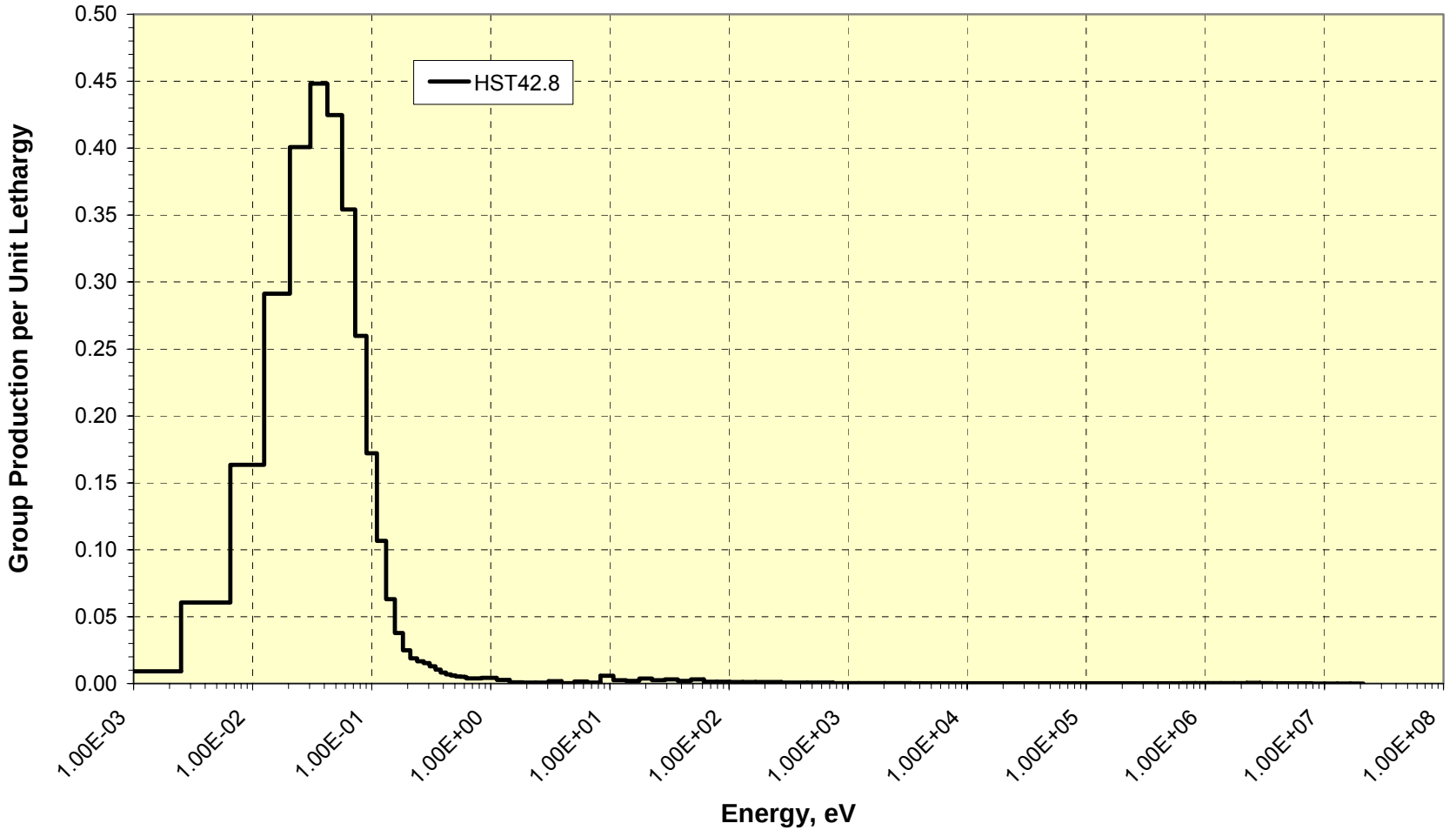

lct1D.13 with ENDF/B-VI.8
8.0E+01
7 FINAL MODULES
DY=1.0E+01
-8.0E+01
-8.0E+01
DX=1.0E+01
8.0E+01
COMPOSITION, Z SLICE AT 6.6100E+01 CM

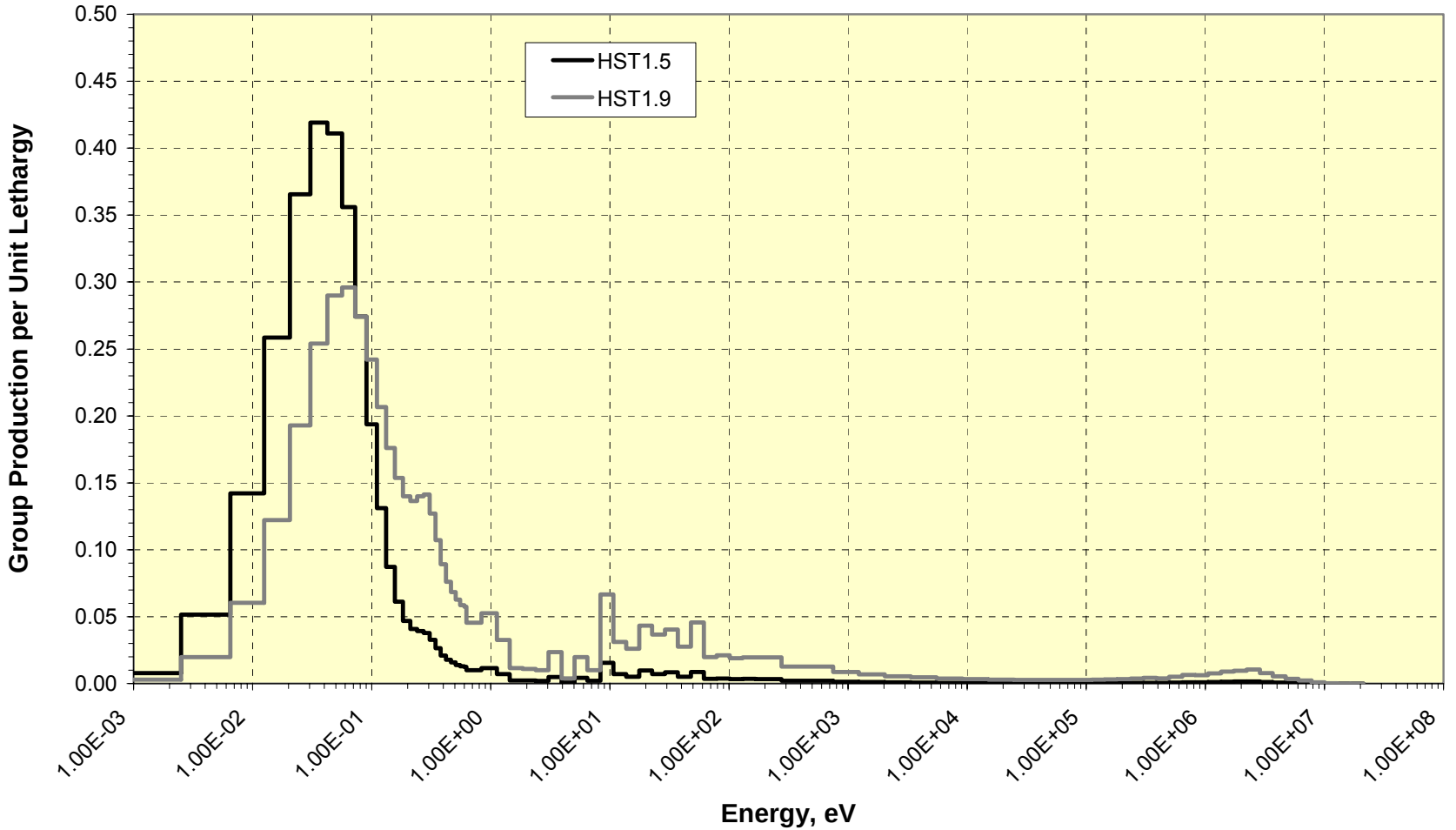
LEU-COMP-THERM-002 & LEU-COMP-THERM-010 Normalized Eigenvalues with Various Cross Section Data Sets				
Case	Lattice Data		ENDF/B-VI.8	Pre-ENDF/B-VIIβ0
LCT2.4	3 sets of 15 x 8 rods, 2.540 cm pitch	H_2O reflector	0.99350(41)	**0.99763(32)**
LCT2.5	3 sets of 13 x 8 rods, 2.540 cm pitch		0.99219(31)	**0.99591(26)**
LCT10.1	3 sets of 13 x 8 rods, 2.540 cm pitch	Pb, 0.0 cm	1.00493(30)	**1.00862(22)**
LCT10.2		Pb, 0.660 cm	1.00462(35)	**1.00812(29)**
LCT10.3		Pb, 1.321 cm	1.00259(36)	**1.00659(24)**
LCT10.4		Pb, 5.405 cm	0.99203(26)	**0.99583(38)**
LCT10.5	3 sets of 13 x 8 rods or 12 x 8 rods, 2.540 cm pitch	^{depl}U, 0.0 cm	0.99697(27)	**0.99943(35)**
LCT10.6		^{depl}U, 1.956 cm	0.99683(14)	**---**
LCT10.7		^{depl}U, 3.912 cm	0.99741(17)	**1.00039(25)**
LCT10.8		^{depl}U, 5.405 cm	0.99344(24)	**0.99656(32)**
LCT10.9	3 sets of 13 x 8 rods, 2.540 cm pitch	Steel, 0.0 cm	0.99622(31)	**1.00016(20)**
LCT10.10		Steel, 0.660 cm	0.99620(36)	**---**
LCT10.11		Steel, 1.321 cm	0.99661(27)	**---**
LCT10.12		Steel, 2.616 cm	0.99575(43)	**---**
LCT10.13		Steel, 5.405 cm	0.99221(41)	**0.99600(16)**
Note: Steel is ~97 w/o iron.				

Final LEU-COMP-THERM Observations

- Historically low LEU-COMP-THERM benchmark eigenvalues are significantly improved.
  - LEU-COMP-THERM-006 ENDF/B-VI.8 average = 0.99366;
  - Pre-ENDF/B-VIIβ0 ave = 0.99974.
  - LEU-COMP-THERM-002 ENDF/B-VI.8 average = 0.99285.
  - Pre-ENDF/B-VIIβ0 ave = 0.99677.
  - The trend of increasing eigenvalue as non-hydrogenous reflectors approach the fuel lattice remains (Pb, ^{depl}U, steel (Fe)).

BETTIS LABORATORY


HST42.8
Group Production per Unit Lethargy
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1.00E-03
1.00E-02
1.00E-01
1.00E+00
1.00E+01
1.00E+02
1.00E+03
1.00E+04
1.00E+05
1.00E+06
1.00E+07
1.00E+08
Energy, eV


HST1.5
HST1.9
Group Production per Unit Lethargy
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1.00E-03
1.00E-02
1.00E-01
1.00E+00
1.00E+01
1.00E+02
1.00E+03
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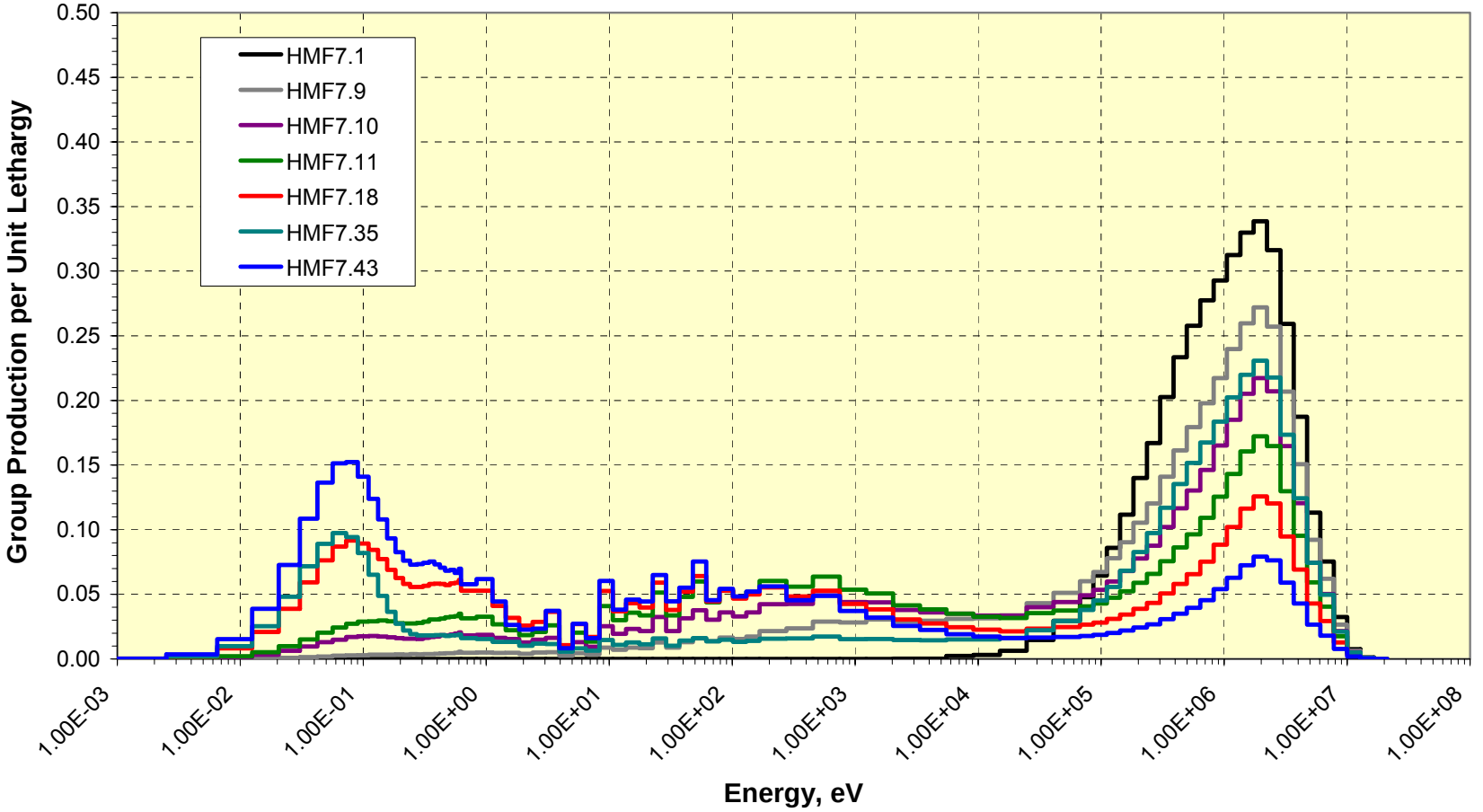
1.00E+07
1.00E+08
Energy, eV


HMF7.1
HMF7.9
HMF7.10
HMF7.11
HMF7.18
HMF7.35
HMF7.43
Group Production per Unit Lethargy
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1.00E-03
1.00E-02
1.00E-01
1.00E+00
1.00E+01
1.00E+02
1.00E+03
1.00E+04
1.00E+05
1.00E+06
1.00E+07
1.00E+08
Energy, eV