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International Atomic Energy Agency
Atoms for Peace and Development

CSEWG Validation – Contribution from the IAEA
- Code validation for ACE
- Analysis of LCT benchmarks
- Temperature coefficient
- Iron evaluations
- Chromium evaluations
- ICSBEP/SINBAD

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Scope

- Report from the code-validation exercise for ACE libraries
- Analysis of ICSBEP LEU-COMP-THERM benchmarks
- Impact of U-235 on the temperature coefficient.
- Iron evaluations
- Chromium evaluations
- News from ICSBEP/SINBAD

Code validation for generating ACE files

Background:

- IAEA Member States expressed desire to have a processing code independent of NJOY
- IAEA initiated an activity to develop a module for generating ACE files as a supplement to PREPRO → ACEMAKER
- Other codes with ACE capability were developed/announced
- In the meantime, NJOY became “open source”

Code validation for generating ACE files

Nine (9) codes have the capability to generate ACE files for neutrons above the thermal energy range

- NJOY – USA
- FUDGE - USA
- GRUCON – Russia
- FRENDY – Japan
- ACEMAKER/PREPRO – IAEA
- NECP-Atlas – China
- RULER – China
- GAIA – France
- GALILEE- France

No.	ICSBEP Label	Short name	Common name
1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-002	hmf002-002	Topsy-002
3	HEU-MET-FAST-003	hmf003-001	Topsy-U_2.0in
4	HEU-MET-FAST-003	hmf003-002	Topsy-U_3.0in
5	HEU-MET-FAST-003	hmf003-003	Topsy-U_4.0in
6	HEU-MET-FAST-003	hmf003-010	Topsy-W_4.5in
7	HEU-MET-FAST-003	hmf003-011	Topsy-W_6.5in
8	HEU-MET-FAST-014	hmf014	VNIIEF-CTF-DU
9	HEU-MET-FAST-032	hmf032-001	COMET-TU1_3.93in
10	HEU-MET-FAST-032	hmf032-002	COMET-TU1_3.52in
11	HEU-MET-FAST-032	hmf032-003	COMET-TU1_1.742in
12	HEU-MET-FAST-032	hmf032-004	COMET-TU1-0.683in
13	IEU-COMP-FAST-004	icf004	ZPR-3/12
14	IEU-MET-FAST-007	imf007	Big_Ten(s)
15	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
16	IEU-MET-FAST-010	imf010	ZPR-6/9(U9)
17	IEU-MET-FAST-012	imf012	ZPR-3/41
18	IEU-MET-FAST-013	imf013	ZPR-9/1
19	IEU-MET-FAST-014	imf014-002	ZPR-9/2
20	IEU-MET-FAST-022	imf022-001	FR0_3X-S
21	IEU-MET-FAST-022	imf022-002	FR0_5-S
22	IEU-MET-FAST-022	imf022-003	FR0_6A-S
23	IEU-MET-FAST-022	imf022-004	FR0_7-S
24	IEU-MET-FAST-022	imf022-005	FR0_8-S
25	IEU-MET-FAST-022	imf022-006	FR0_9-S
26	IEU-MET-FAST-022	imf022-007	FR0_10-S
27	MIX-MISC-FAST-001	mif001-001	BFS-35-1
28	MIX-MISC-FAST-001	mif001-002	BFS-35-2
29	MIX-MISC-FAST-001	mif001-003	BFS-35-3
30	MIX-MISC-FAST-001	mif001-009	BFS-31-4
31	MIX-MISC-FAST-001	mif001-010	BFS-31-5
32	MIX-MISC-FAST-001	mif001-011	BFS-42

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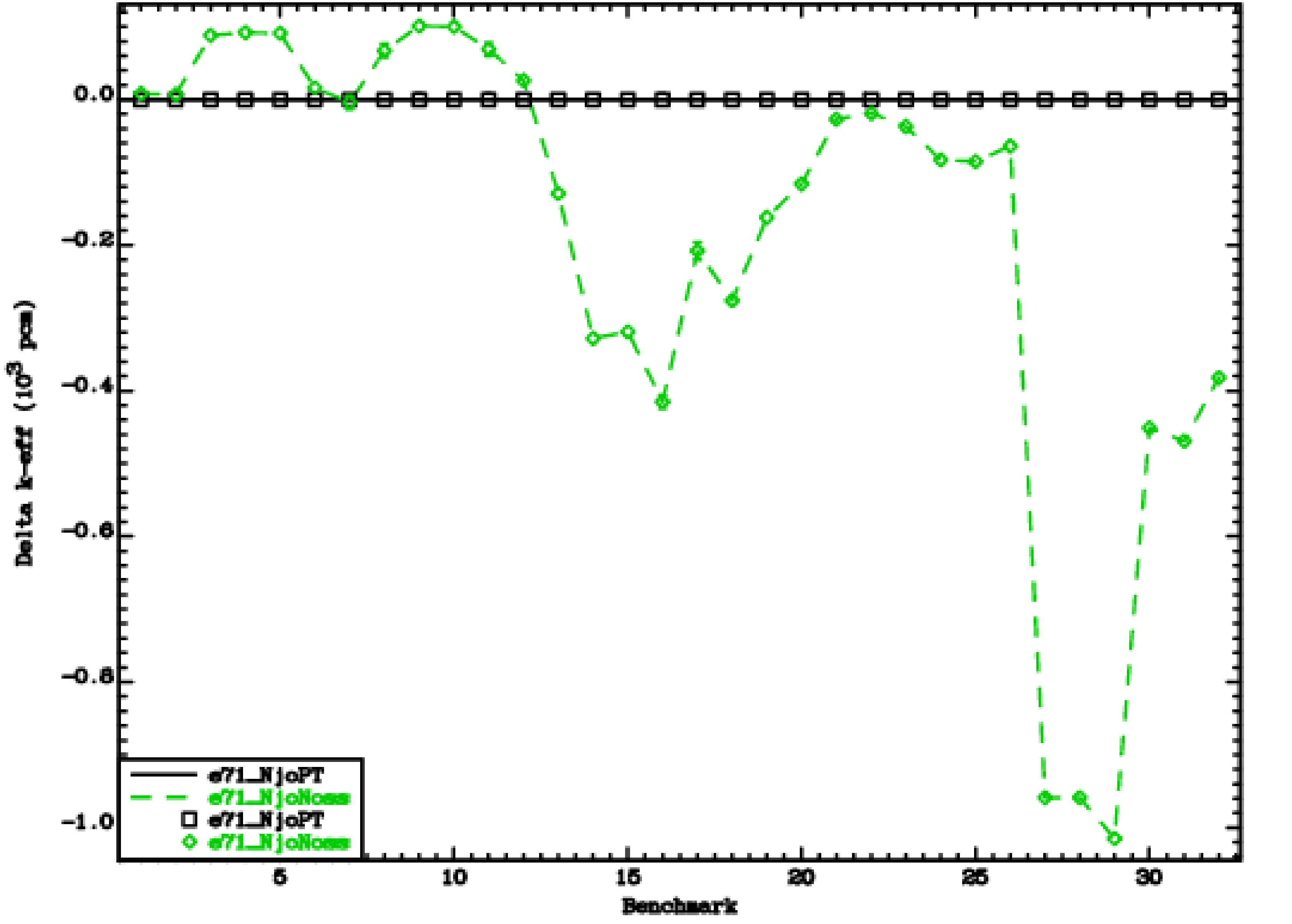
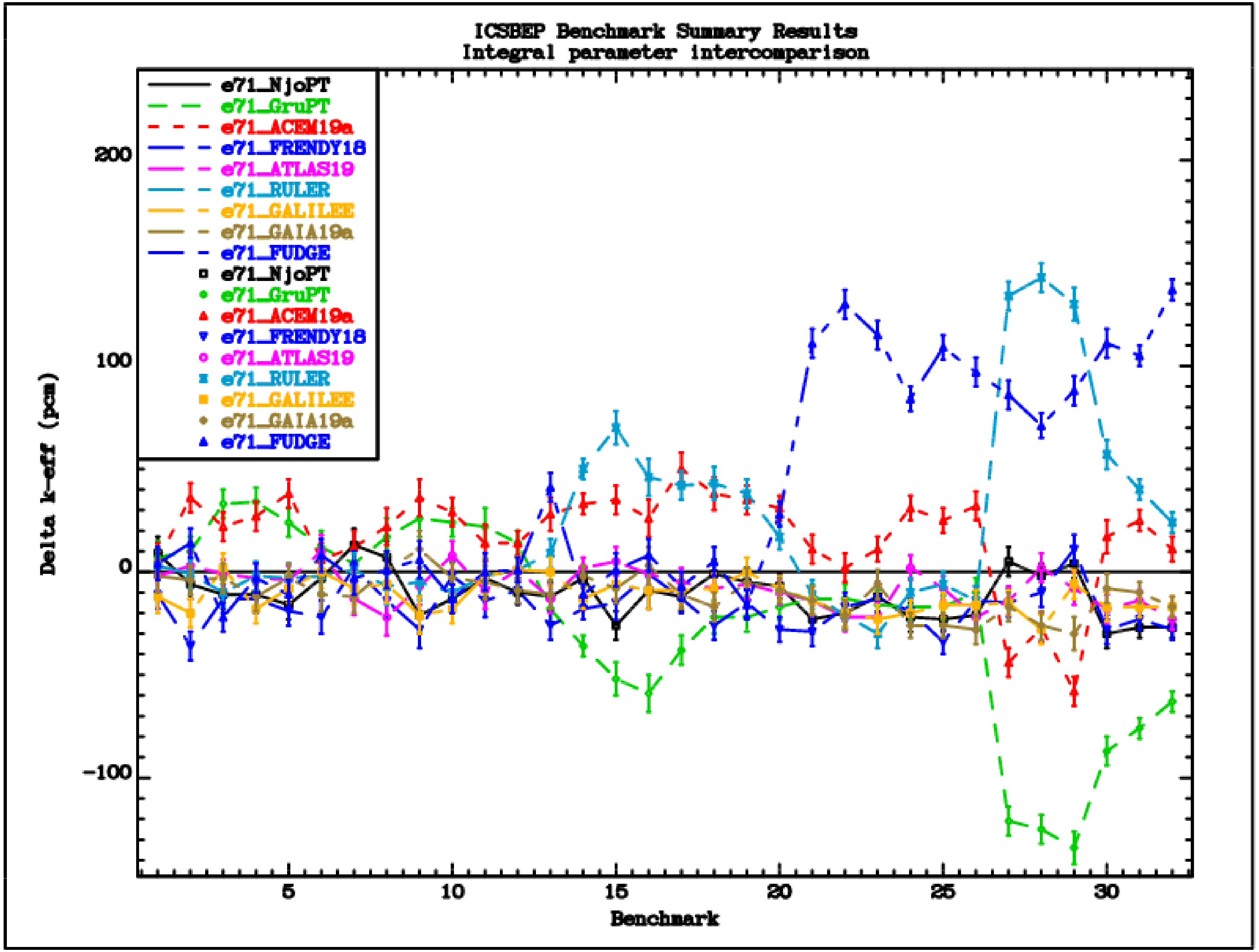
Importance of Self-Shielding



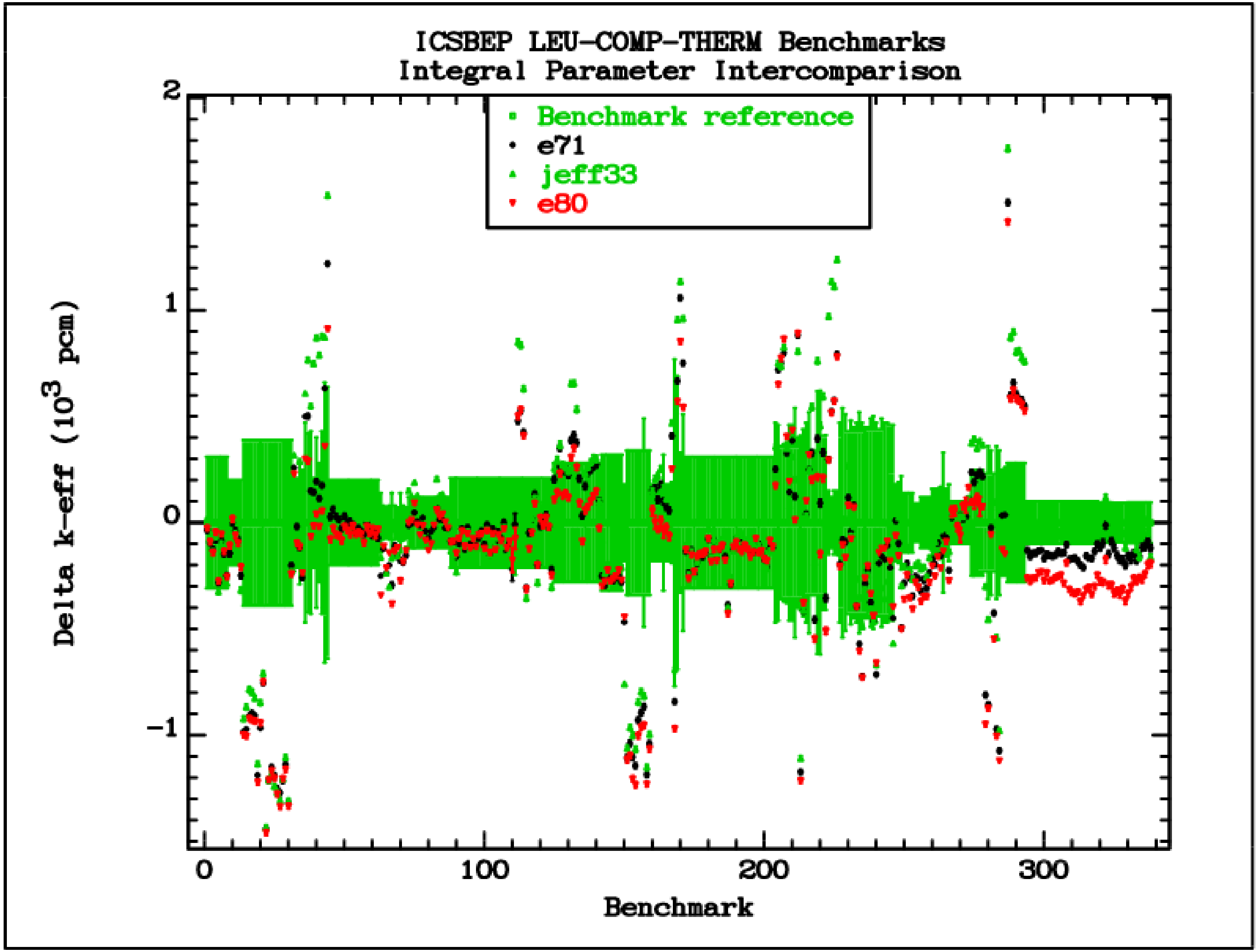

ICSBEP Benchmark Summary Results
Integral parameter intercomparison
e71_NjoPT
e71_GruPT
e71_ACEM19a
e71_FRENDY18
e71_ATLAS19
e71_RULER
e71_GALILEE
e71_GAIA19a
e71_FUDGE
e71_NjoPT
e71_GruPT
e71_ACEM19a
e71_FRENDY18
e71_ATLAS19
e71_RULER
e71_GALILEE
e71_GAIA19a
e71_FUDGE
Delta k-eff (pcm)
200
100
0
−100
5
10
15
20
25
30
Benchmark

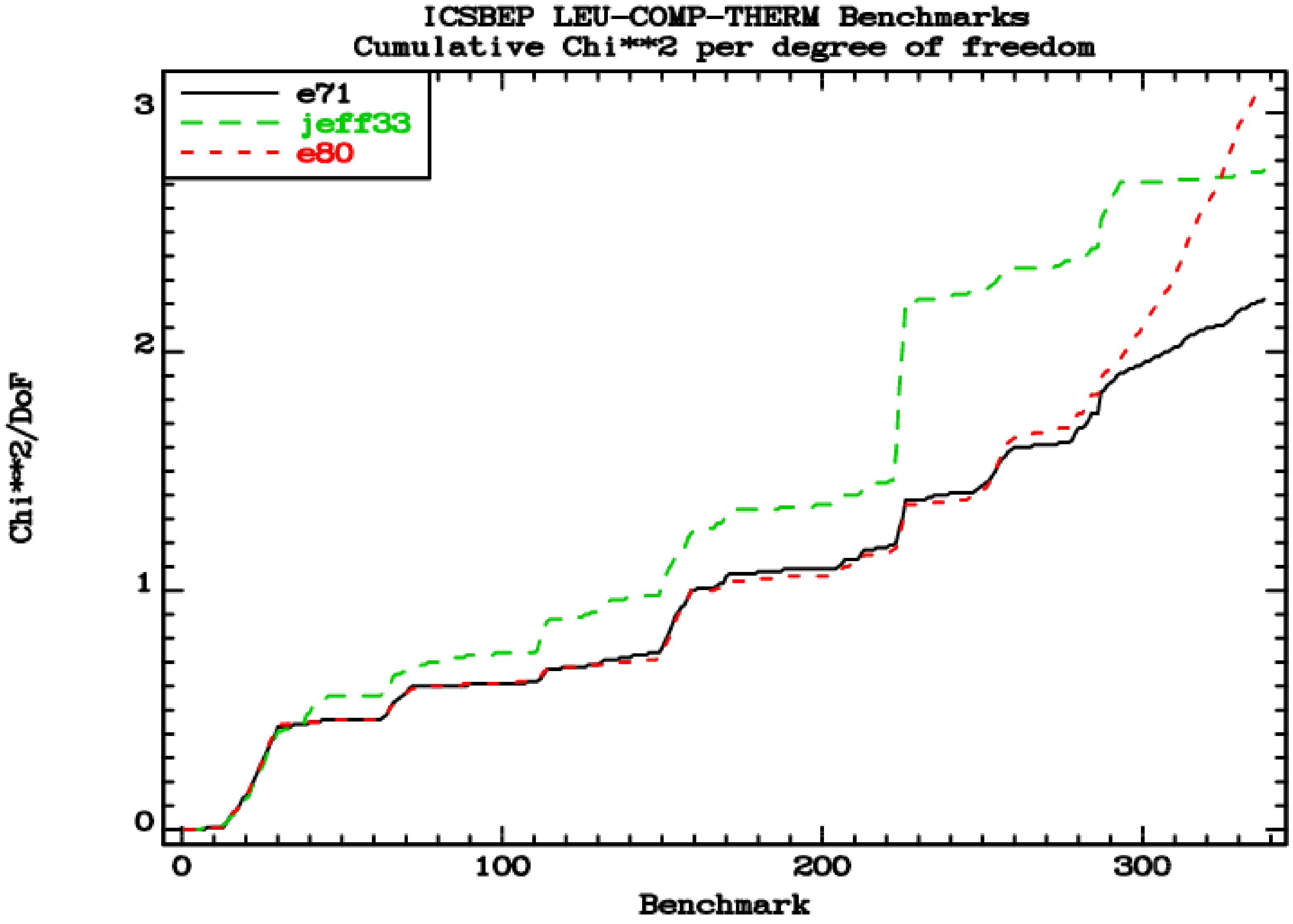
Conclusions on ACE Library Validation

- Without self-shielding, all codes are capable of generating ACE files that produce results within 20 pcm (~10 pcm convergence criterion in MCNP)
- With self-shielding included in the calculations, the preliminary results are within 100 pcm

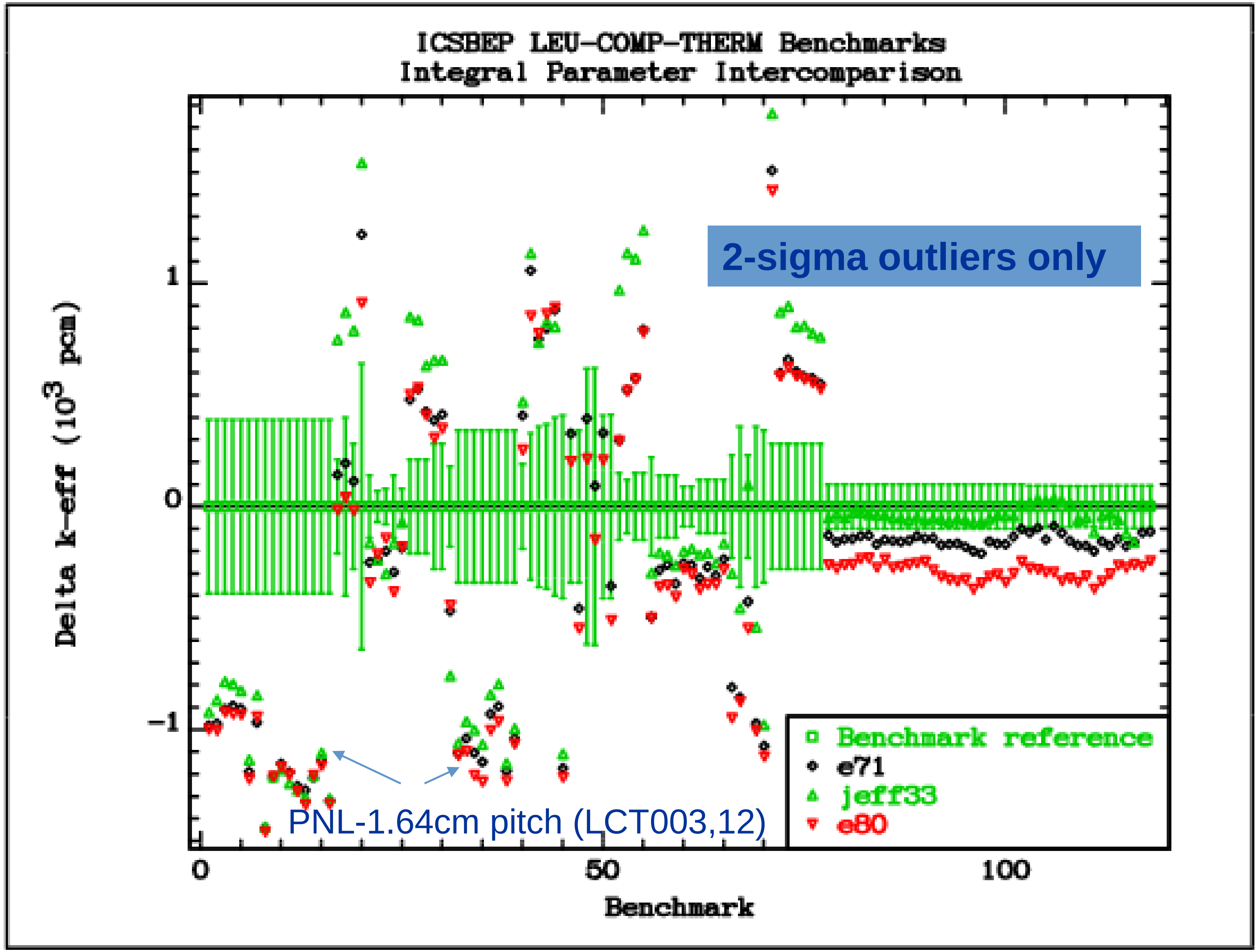
ICSBEP LEU-COMP-THERM

- ICSBEP-2018 contains 97 benchmarks, most of them include several cases
- At the IAEA, the computational models are available for **338 cases** (input models obtained from the Handbook, Skip Kahler or otherwise)
- Some of the benchmarks show huge discrepancies, which can hardly be attributed to nuclear data
- "e80" performance is similar to "e71", except for LCT078, LCT080 and LCT096, where "e80" is distinctly worse (see cumulative χ^2/DoF plot)

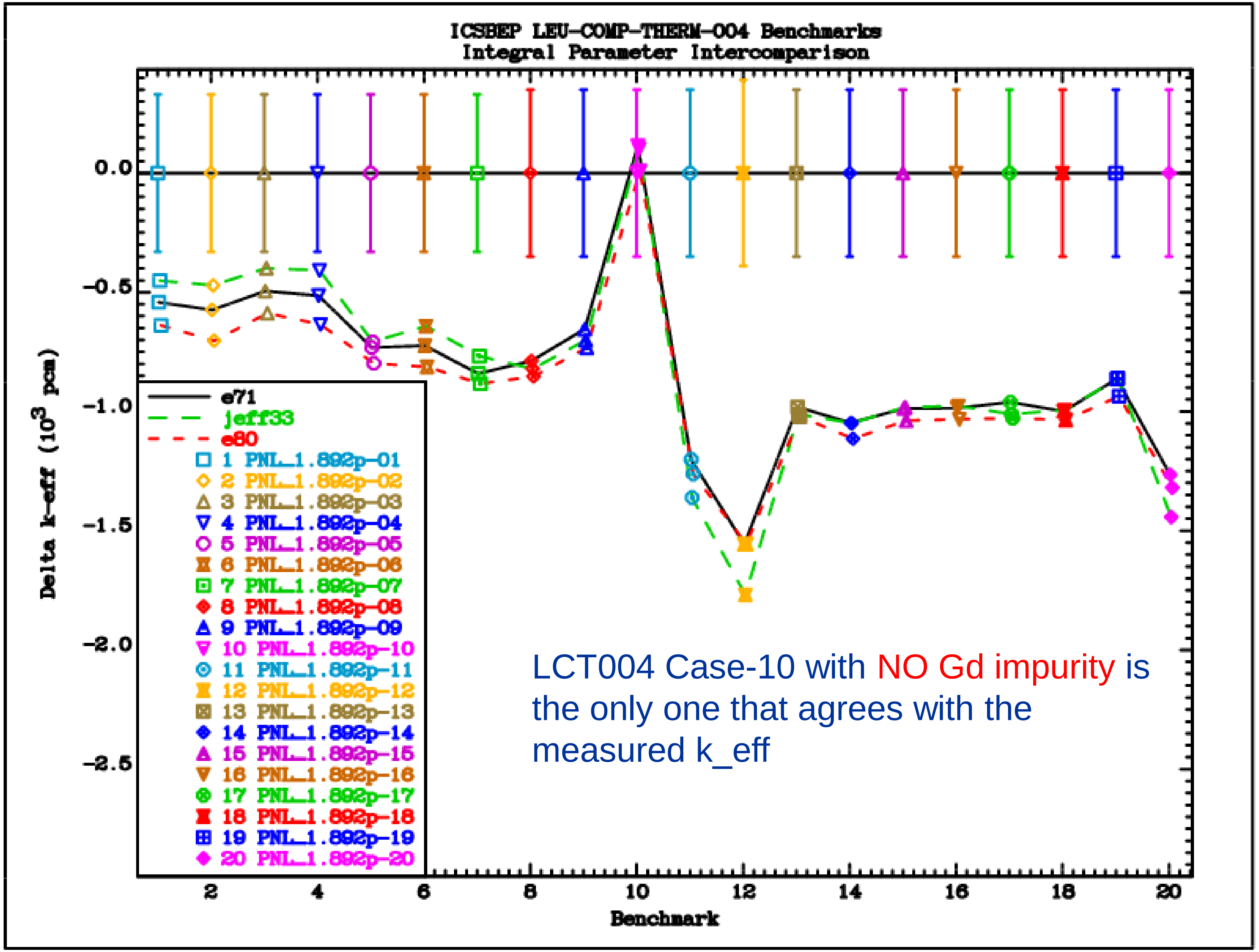

ICSBEP LEU-COMP-THERM Benchmarks
Integral Parameter Intercomparison
Benchmark reference
e71
jeff33
e80
Delta k-eff (10^3 pcm)
Benchmark
2
1
0
−1
0
100
200
300



ICSBEP LEU-COMP-THERM Benchmarks
Cumulative Chi**2 per degree of freedom
e71
jeff33
e80
Chi**2/DoF
Benchmark
0
1
2
3
0
100
200
300



ICSBEP LEU-COMP-THERM Benchmarks
Integral Parameter Intercomparison
Delta k-eff (10^3 pcm)
Benchmark
2-sigma outliers only
PNL-1.64cm pitch (LCT003,12)
Benchmark reference
e71
jeff33
e80



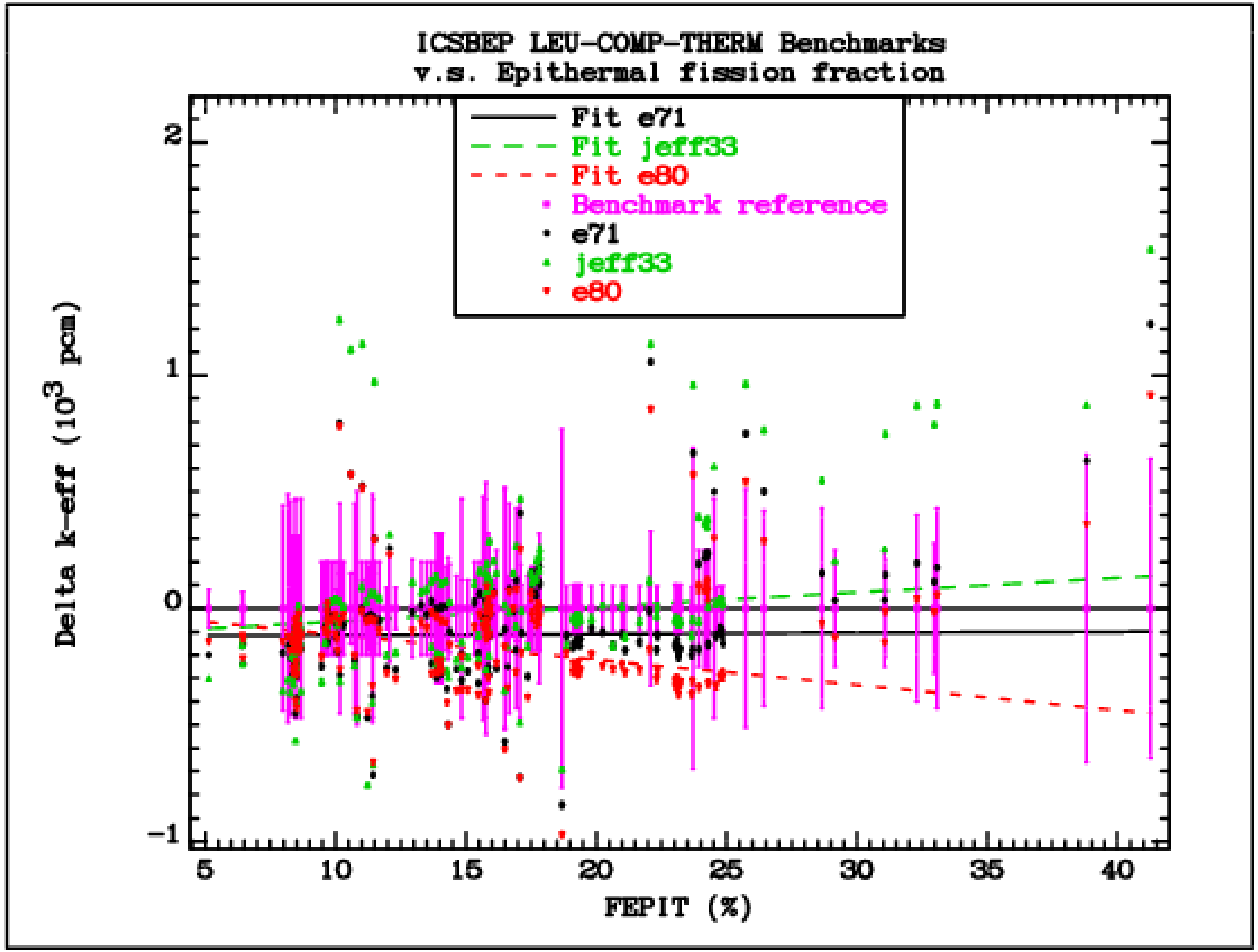
LCT004 Case-10 with NO Gd impurity is the only one that agrees with the measured k_eff

ICSBEP LEU-COMP-THERM - Rejected

- LEU-COMP-THERM-003 (PNL_1.64p) (*)
- LEU-COMP-THERM-004 (PNL_1.89p) (*)
- LEU-COMP-THERM-009 (PNL_2.54p not an outlier - correlated with LCT010)
- LEU-COMP-THERM-010 (PNL_2.54p_Pb-1)
- LEU-COMP-THERM-012 (PNL_1.64p, correlation with LCT003?) (*)
- LEU-COMP-THERM-022 (RRC-KI-0.70p_hx)
- LEU-COMP-THERM-024 (RRC-KI-0.62p_hx)
- LEU-COMP-THERM-025 (RRC-KI-0.80p_sq)
- LEU-COMP-THERM-027 (Valduc-Pb)
- LEU-COMP-THERM-042 (Fuel clusters, SS reflector, not an outlier)
- LEU-COMP-THERM-052 (Valduc hx Gd)
- LEU-COMP-THERM-064 (VVER_1.27p)
- Temperature-dependent cases

The remainder comprises **207 cases**

(*) Gd impurity is mentioned, which might not be there?



ICSBEP LEU-COMP-THERM Benchmarks
v.s. Epithermal fission fraction
Fit e71
Fit jeff33
Fit e80
Benchmark reference
e71
jeff33
e80
Delta k-eff (10^3 pcm)
FEPIT (%)

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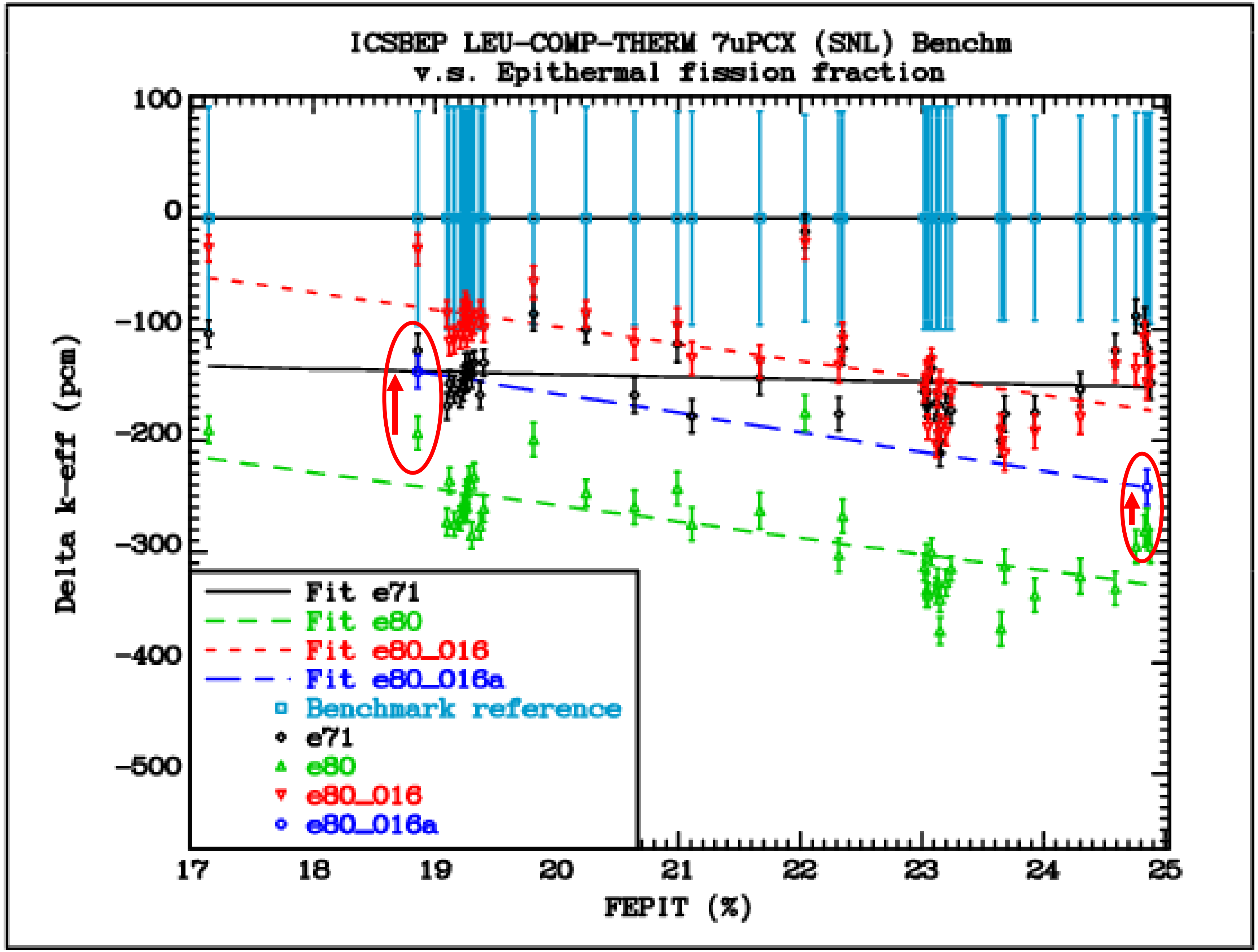
ICSBEP LEU-COMP-THERM-078, 080, 096

- Why are "**e80**" results lower than "**e71**"?
  - Processing: swap U-235,238 in "e71" with "e80b4" processed with ACEMAKER → no effect → neither processing nor U data are responsible for the difference
  - TSL at room temperature: Swap "e80" tsl into "e71" library → slight increase in reactivity → TSL is not responsible for the large difference
  - O-16:
    - Swap O-16 from "e80" into "e71" → performance is degraded
    - Swap O-16 from "e71" into "e80" → performance is restored (see "**e80_O16**")
    - Swapping O-16 from JEFF-3.3 instead of "e71" makes no difference.
    - Swap elastic cross section below 0.3 MeV from "e71" into "e80" helps only in cases with softer spectra (see "**e80_O16a**" on next slide)

Proof that O-16 is the reason for the degraded performance!

The problem is not limited to the cross sections in the low-energy range, although soft-spectrum assemblies are affected slightly more

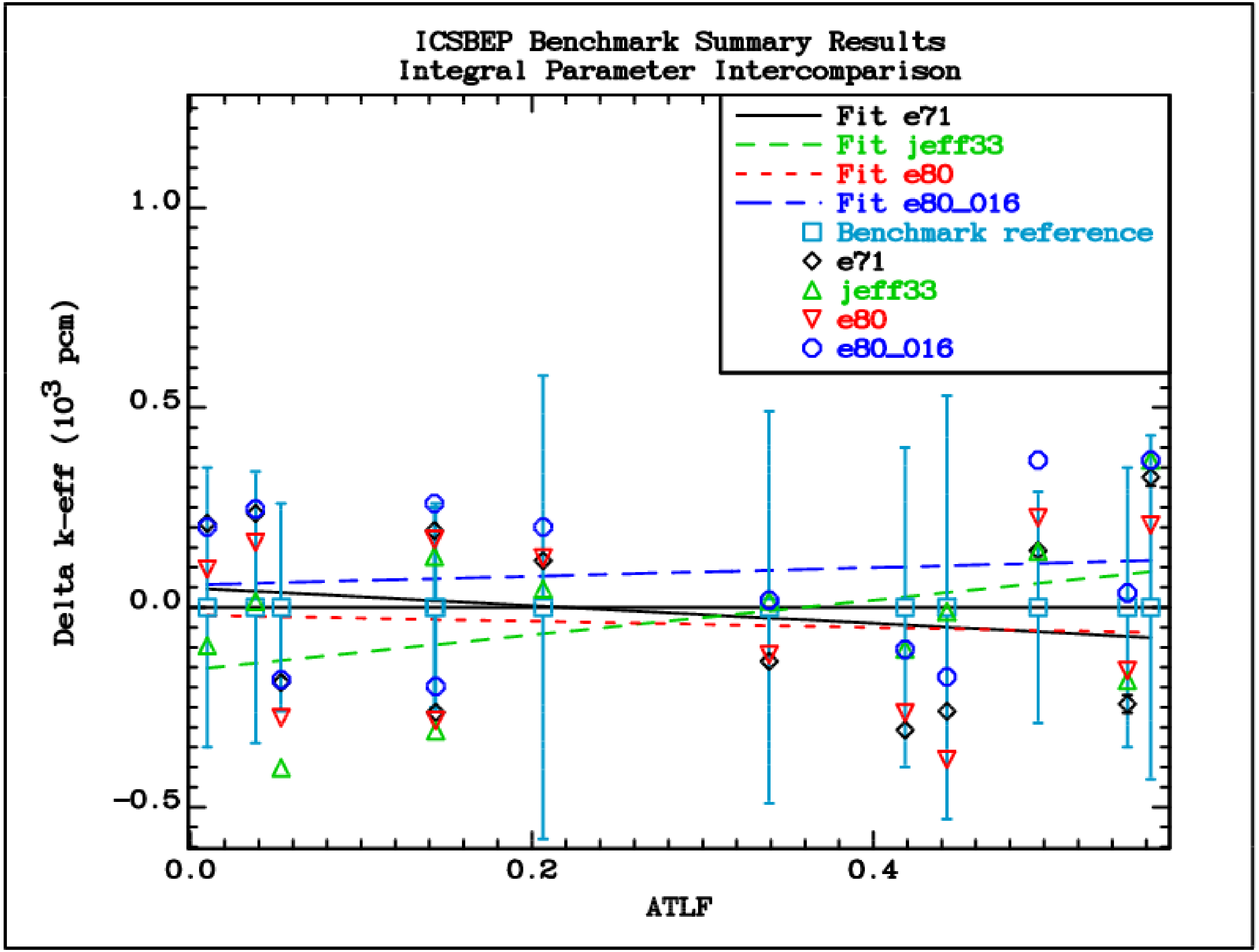

ICSBEP LEU-COMP-THERM 7uPCX (SNL) Benchm
v.s. Epithermal fission fraction
Delta k-eff (pcm)
FEPIT (%)
100
0
-100
-200
-300
-400
-500
17
18
19
20
21
22
23
24
25
Fit e71
Fit e80
Fit e80_016
Fit e80_016a
Benchmark reference
e71
e80
e80_016
e80_016a

DICE sensitivities on k_eff for LCT096 cases 1, 19

Case	Nuclide	Reaction	Thermal	Epithermal	Fast	Total
LEU-COMP-THERM-096-019	H1	capture	-0.1369	-0.0054	0.0000	-0.1423
LEU-COMP-THERM-096-001	H1	capture	-0.0744	-0.0048	0.0000	-0.0792
LEU-COMP-THERM-096-001	O16	elastic	-0.0014	0.0206	0.0734	0.0926
LEU-COMP-THERM-096-001	H1	elastic	-0.0199	0.2774	0.2018	0.4593
LEU-COMP-THERM-096-019	H1	elastic	-0.0610	0.2199	0.2065	0.3654
LEU-COMP-THERM-096-019	O16	elastic	-0.0036	0.0192	0.0692	0.0848
LEU-COMP-THERM-096-001	Al27	elastic	-0.0005	0.0035	0.0140	0.0170
LEU-COMP-THERM-096-019	Al27	elastic	-0.0003	0.0027	0.0111	0.0135

HEU-SOL-THERM O-16 impact on ATLF

- Flat dependence on ATLF of HST was one of the constraints for ENDF/B-VIII.0
- Swapping O-16 from ENDF/B-VII.1 increases the reactivity bias and increases the gradient slightly, but not excessively

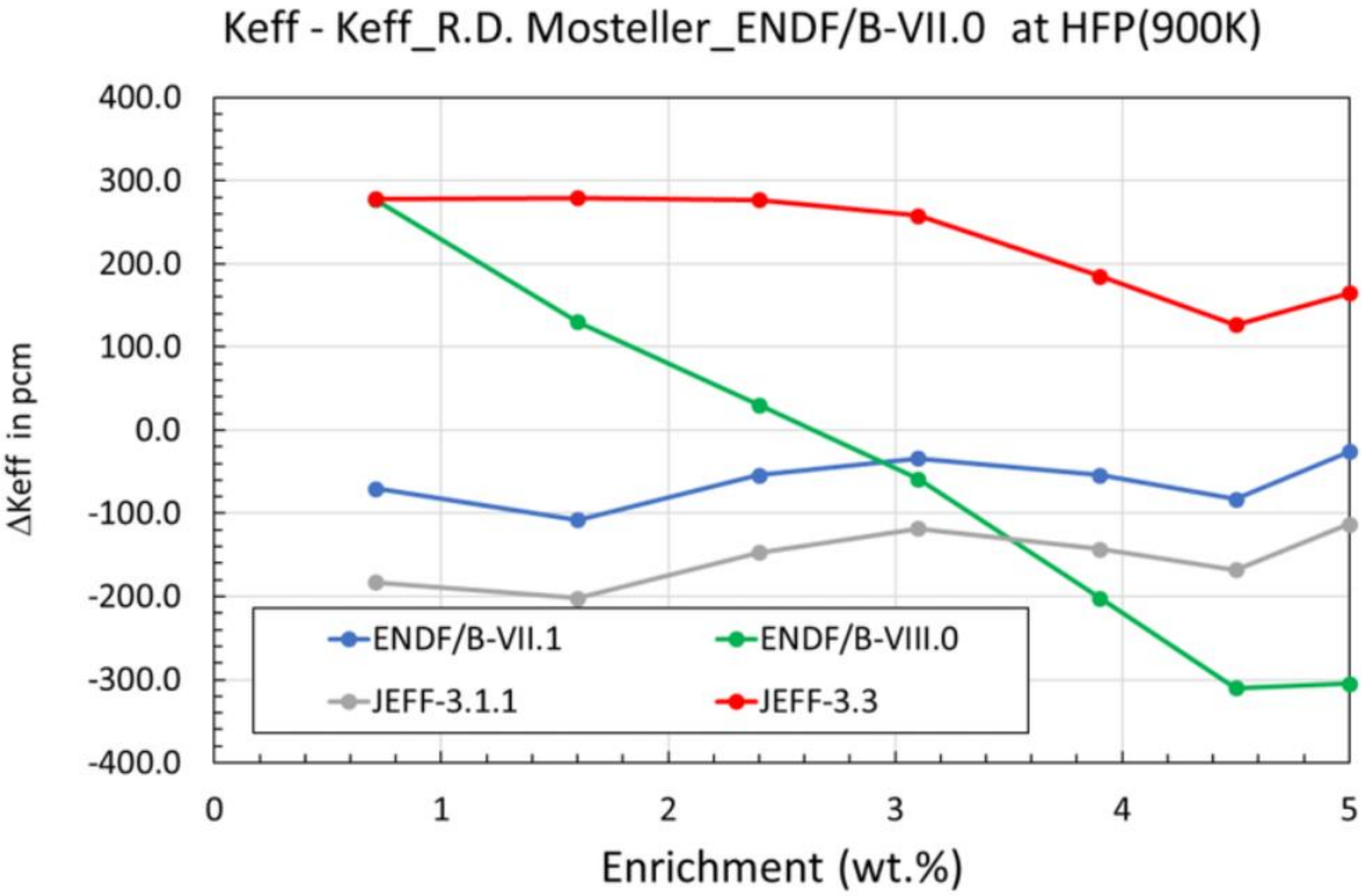

ICSBEP Benchmark Summary Results
Integral Parameter Intercomparison
Fit e71
Fit jeff33
Fit e80
Fit e80_016
Benchmark reference
e71
jeff33
e80
e80_016
1.0
0.5
0.0
−0.5
Delta k-eff (10³ pcm)
0.0
0.2
0.4
ATLF

Coefficients of the polynomial fit

Parameter	Library	Coefficients	
k-eff	e71	4.83E+1	-2.21E+2
k-eff	jeff33	-1.56E+2	4.35E+2
k-eff	e80	-1.95E+1	-7.68E+1
k-eff	e80_O16	5.59E+1	1.09E+2

Temperature Coefficient due to U-235

- Oscar Cabellos showed a potentially alarming plot of a reactivity decrease with increasing enrichment using ENDF/B-VIII.0 data for the Mosteller pin-cell benchmark (~600 pcm at 5% enr.)
- The plot shows there is a difference between “e80” and “e71”, but it does not say which one is less wrong.
- Candidate benchmarks for temperature coefficient:
  - HCT016: IGR-graphite up to T=600 deg.C
  - LCT026: IPPE-MATR (water) up to T=~231 deg.C
  - There are more benchmarks in ICSBEP with lower span of T
  - KRITZ (KRITZ-1 = LEU-COMP-THERM-104, to be included in the next release of ICSBEP)


Keff - Keff_R.D. Mosteller_ENDF/B-VII.0 at HFP(900K)
400.0
300.0
200.0
100.0
0.0
-100.0
-200.0
-300.0
-400.0
ΔKeff in pcm
0
1
2
3
4
5
Enrichment (wt.%)
ENDF/B-VII.1
ENDF/B-VIII.0
JEFF-3.1.1
JEFF-3.3

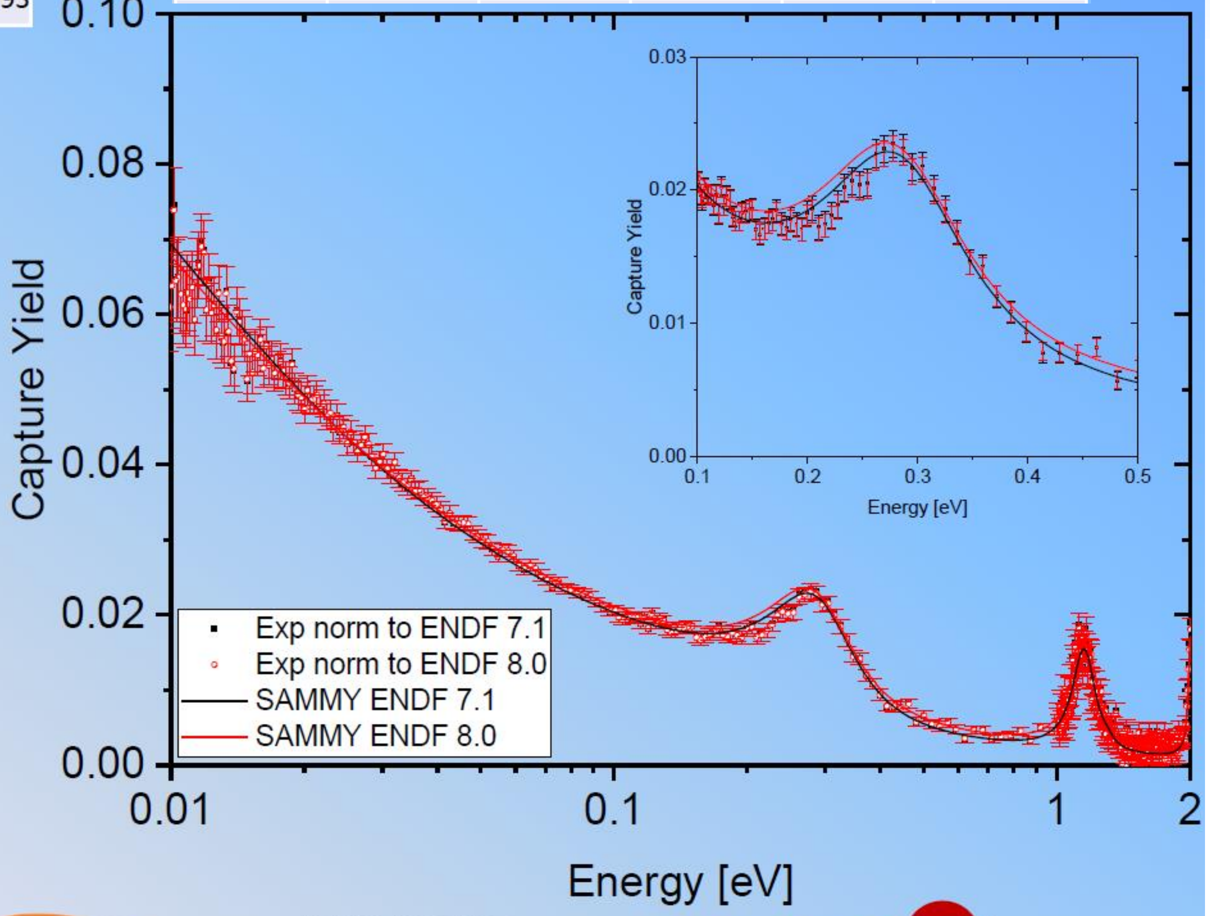
Slide by Y. Danon at the 2018 INDEN Meeting

Thermal Capture

Evaluation	E_0 [eV]	Γ_n [eV]	Γ_γ [eV]	Γ_f [eV]
ENDF 7.1	0.2738	4.249E-06	0.0462	0.1181
ENDF 8.0	0.2684	4.271E-06	0.0473	0.1193

Energy [eV]		Fission C/E		Capture C/E	
From	To	ENDF 7.1	ENDF 8.0	ENDF 7.1	ENDF 8.0
0.0253	9.4	0.98	0.99	0.99	1.06
7.8	11	0.97	0.97	0.97	1.07

- The experiment was normalized using the thermal value and the 11.7 eV resonance
- In the energy range from 0.15 to 0.3 eV the evaluations are higher than the data. ENDF 8.0 is not an improvement here.
- Might need to adjust bound levels instead of the 0.27 eV resonance
  - Suggest to compare with other experimental data



Rensselaer NCSP NUCLEAR CRITICALITY SAFETY PROGRAM NAVAL NUCLEAR LABORATORY linac The Gaertner LINAC Center

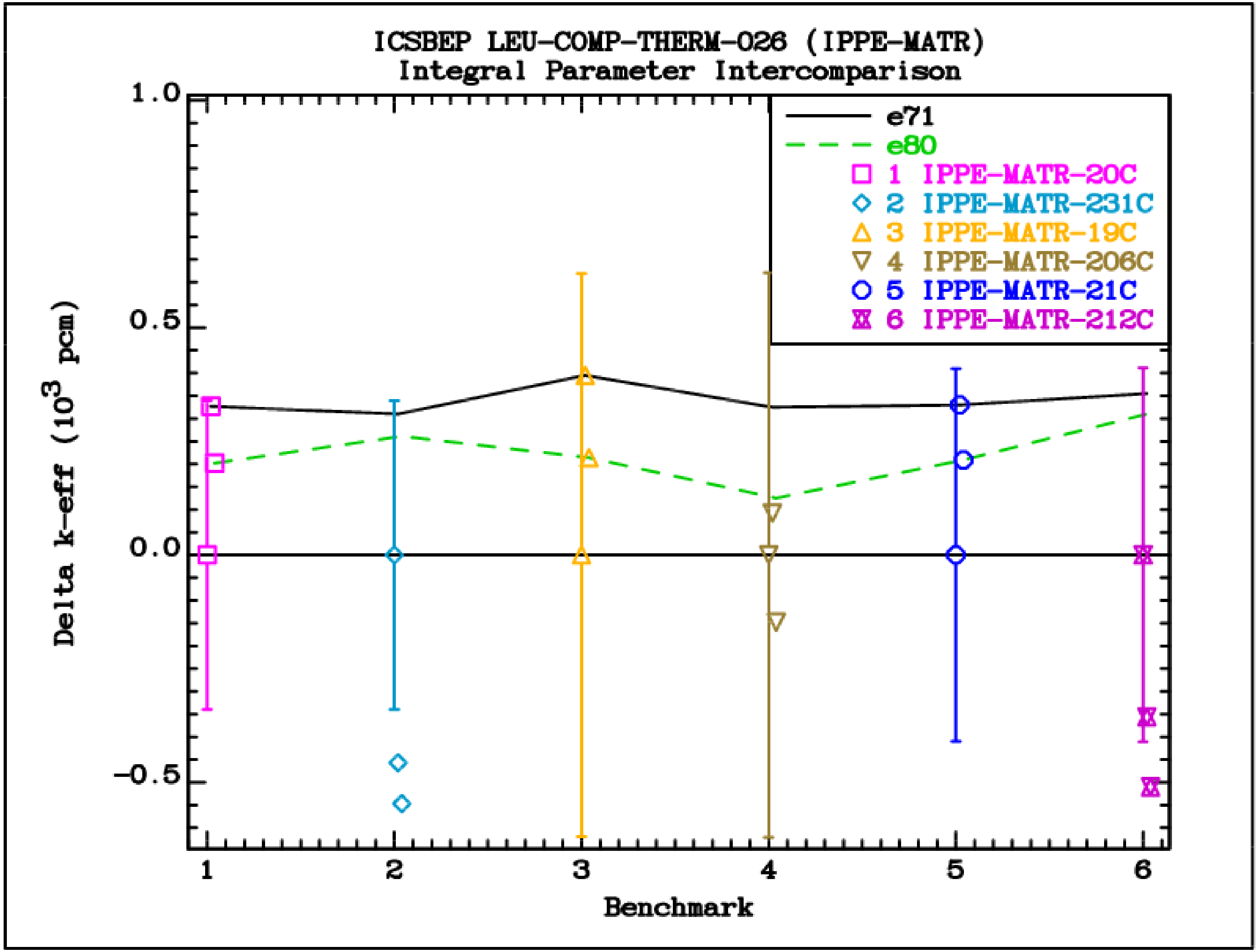
Temperature coefficient (Cont.)

- HCT016:
  - Need ACE files at high temperature, ACE Fast and TSL have different temperature grids
  - Ambiguity about which graphite TSL to use
- KRITZ:
  - WIMS-D (1D/buckling) quick test (contributed by O. Cabellos) does not show any degraded performance of ENDF/B-VIII.0
  - KRITZ-1 will be in ICSBEP LEU-COMP-THERM-104, but not in 2019 edition (private communication with **Dennis Mennerdahl** shows no clear indication of ENDF/B-VIII.0 deficiency).

Temperature coefficient (Cont.)

- LCT026:
  - Light water array up to ~200 deg.C (=~480 K)
  - “e80” calculation done at 293.6K and 600 K
  - K_eff interpolated as 1/sqrt(T)
  - Flat prediction of reactivity with “e71” and “e80”

There is no observable difference with respect to temperature effects between “e71” and “e80” in this benchmark

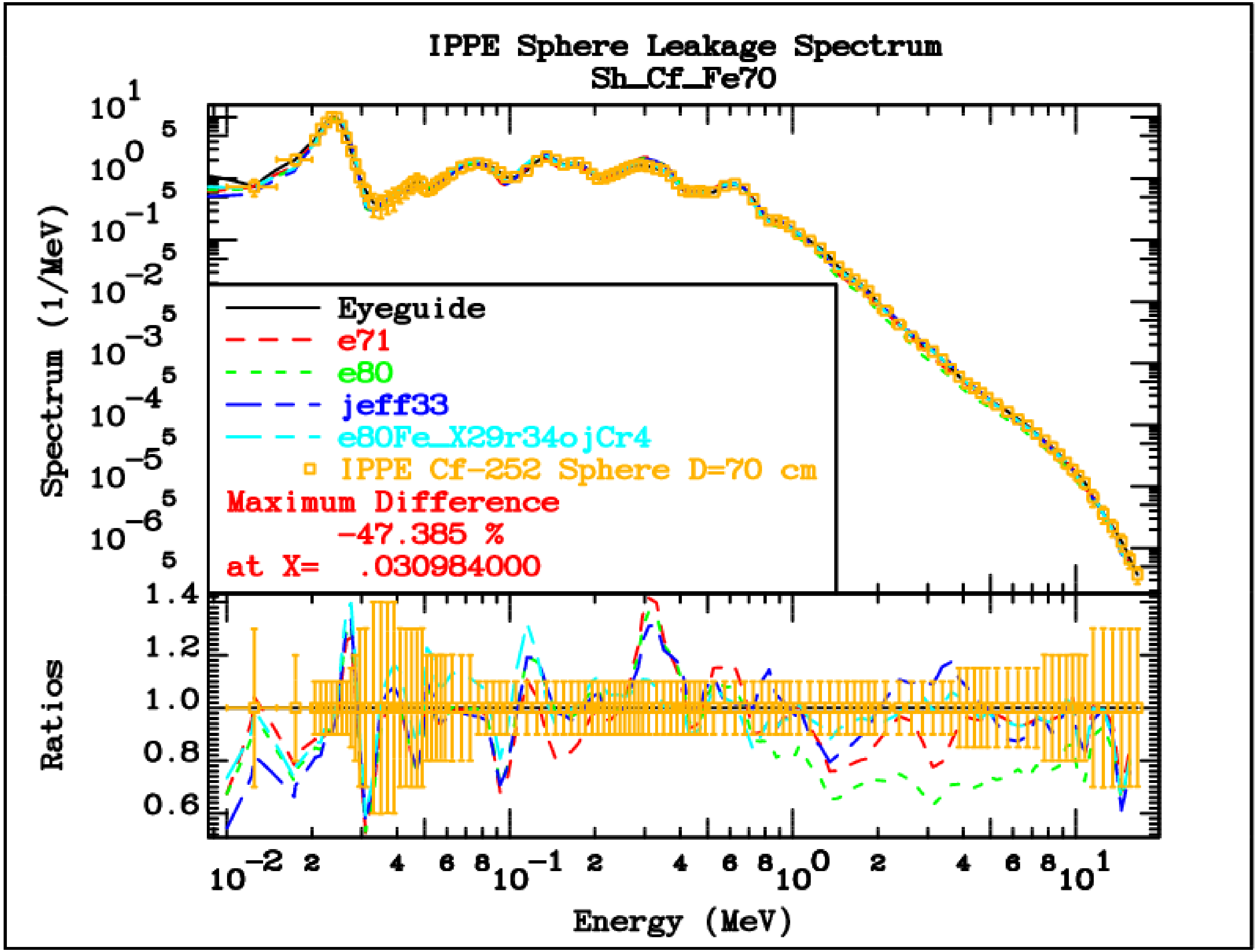


ICSBEP LEU-COMP-THERM-026 (IPPE-MATR)
Integral Parameter Intercomparison
e71
e80
1 IPPE-MATR-20C
2 IPPE-MATR-231C
3 IPPE-MATR-19C
4 IPPE-MATR-206C
5 IPPE-MATR-21C
6 IPPE-MATR-212C
1.0
0.5
0.0
−0.5
Delta k-eff (10^3 pcm)
1
2
3
4
5
6
Benchmark

Iron cross sections

- CIELO=ENDF/B-VIII.0 evaluation
- Inelastic cross sections from Geel by Negret
- Leakage spectra from thick spheres with ^{252}Cf source are under-predicted by up to 40% from 2 MeV to 6 MeV (shown by Simakov just before the release of ENDF/B-VIII.0)
- Patch to the Fe-56 is available that
  - Shows good performance in leakage spectra from thick spheres
  - Removes some deficiencies (e.g. near 300 keV)

New resonance evaluation is needed (some progress was made with L. Leal, including direct capture contribution)


IPPE Sphere Leakage Spectrum
Sh_Cf_Fe70
Spectrum (1/MeV)
Eyeguide
e71
e80
jeff33
e80Fe_X29r34ojCr4
IPPE Cf-252 Sphere D=70 cm
Maximum Difference
-47.385 %
at X= .030984000
Ratios
Energy (MeV)

Chromium cross sections

- There is a problem with the ~5 keV resonances in $^{50,53}Cr$
- Raw measurements from ORNL/JRC and RPI agree in shape, but differ strongly after multiple scattering corrections
- ZPR-6/10 benchmark is highly sensitive to Cr cross sections near 5 keV
- **New measurement is needed to resolve the discrepancy in measured data?** (e.g. Lead-Slowing-Down measurement)

News from ICSBEP (from J. Bess)

- ICSBEP Handbook available Sep 2019
- IRPhEP Handbook available Dec 2019
- Key benchmarks of interest to nuclear data:
  - LCT099 – Ti cross section
  - LCT103 – U7Mo (~20% ^{235}U) plates
  - KRITZ-LWR-RESR-004 – Rod lattices 20 – 250 ºC
  - MSRE-MSR-RESR-001 – Molten salt & graphite
  - TREAT-FUND-RESR-002 – Graphite & hydrogen sensitivity in fuel
- See additional slide-pairs on the CSEWG 2019 web site for more information

Conclusions

- Code validation for ACE was successful (9 codes)

- LEU-COMP-THERM-078, 080, 096 benchmarks show sensitivity to oxygen data
- Lower elastic cross sections below 0.3 MeV in “e80” are only partly responsible for the negative bias in reactivity
- Higher absorption cross sections in “e80” (e.g. the alpha-emission) most probably affect assemblies with harder spectra
- Before re-tuning ENDF/B-VIII it is essential to sort out the oxygen cross sections in the MeV energy region

Conclusions (Cont.)

- Strong decrease of reactivity at higher temperatures as a function of enrichment with ENDF/B-VIII.0 data shown by O. Cabellos was alarming
  - Preliminary analysis of LCT026 benchmark (up to 231 deg.C) does not show any degraded performance of ENDF/B-VIII.0
  - More data testing is needed.
- Patched to ^{56}Fe were made,
  - new resonance evaluation is warranted
- Problems with ^{50,53}Cr resonance remain,
  - new measurement is needed to resolve contradicting measurements
- New release of ICSBEP and IRPhE handbooks