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Features of Fe evaluations emerging from data validation

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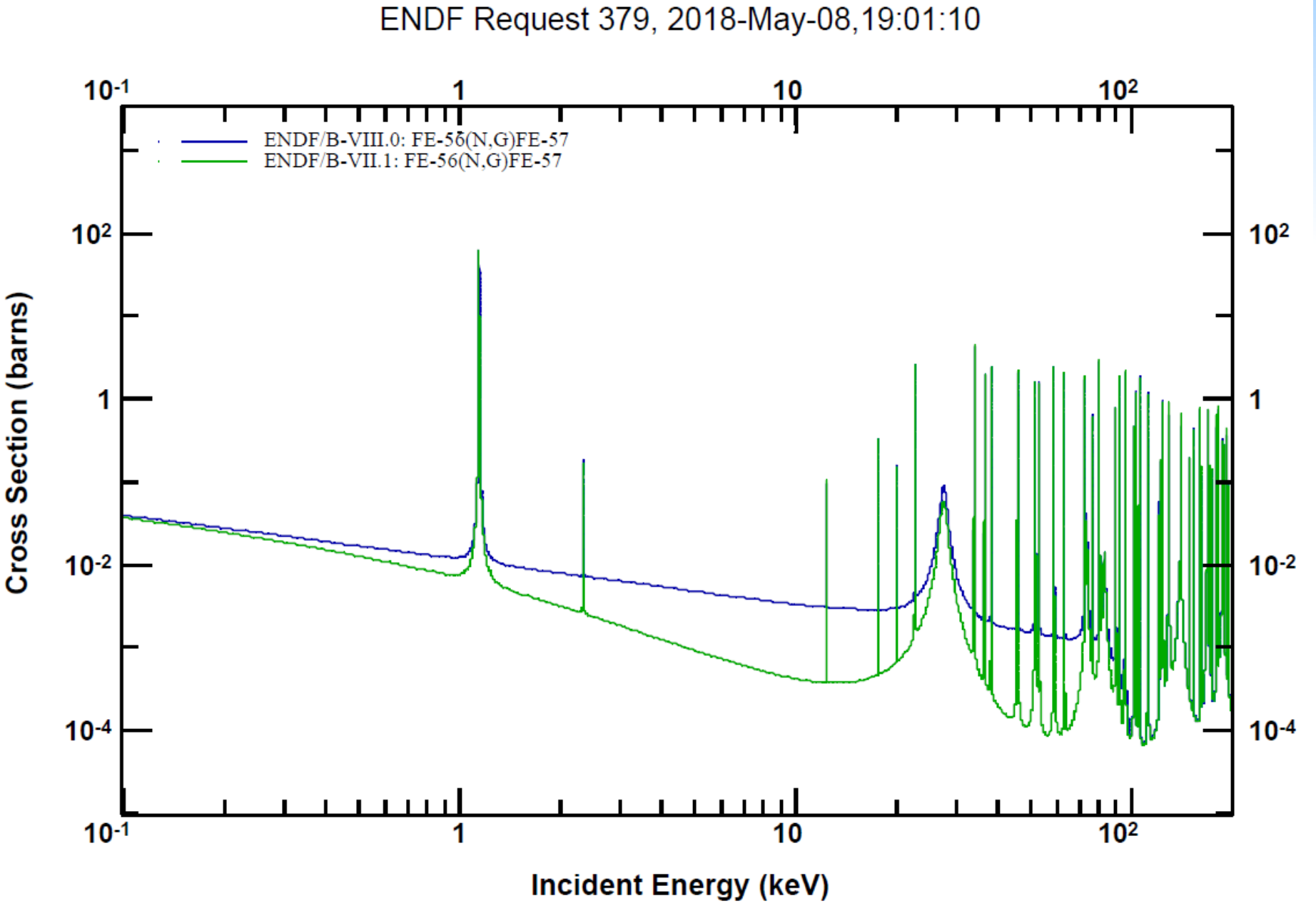
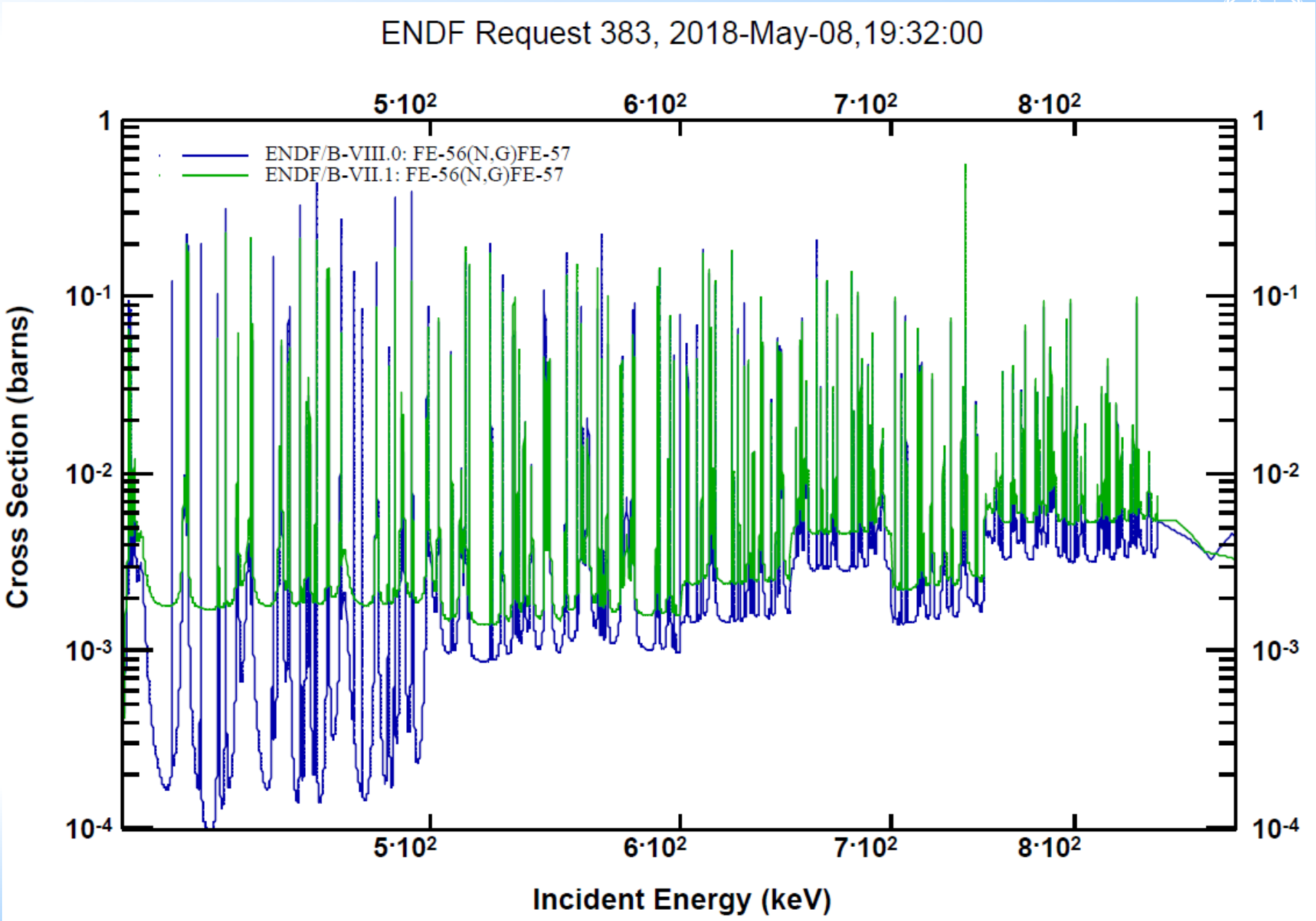
Context

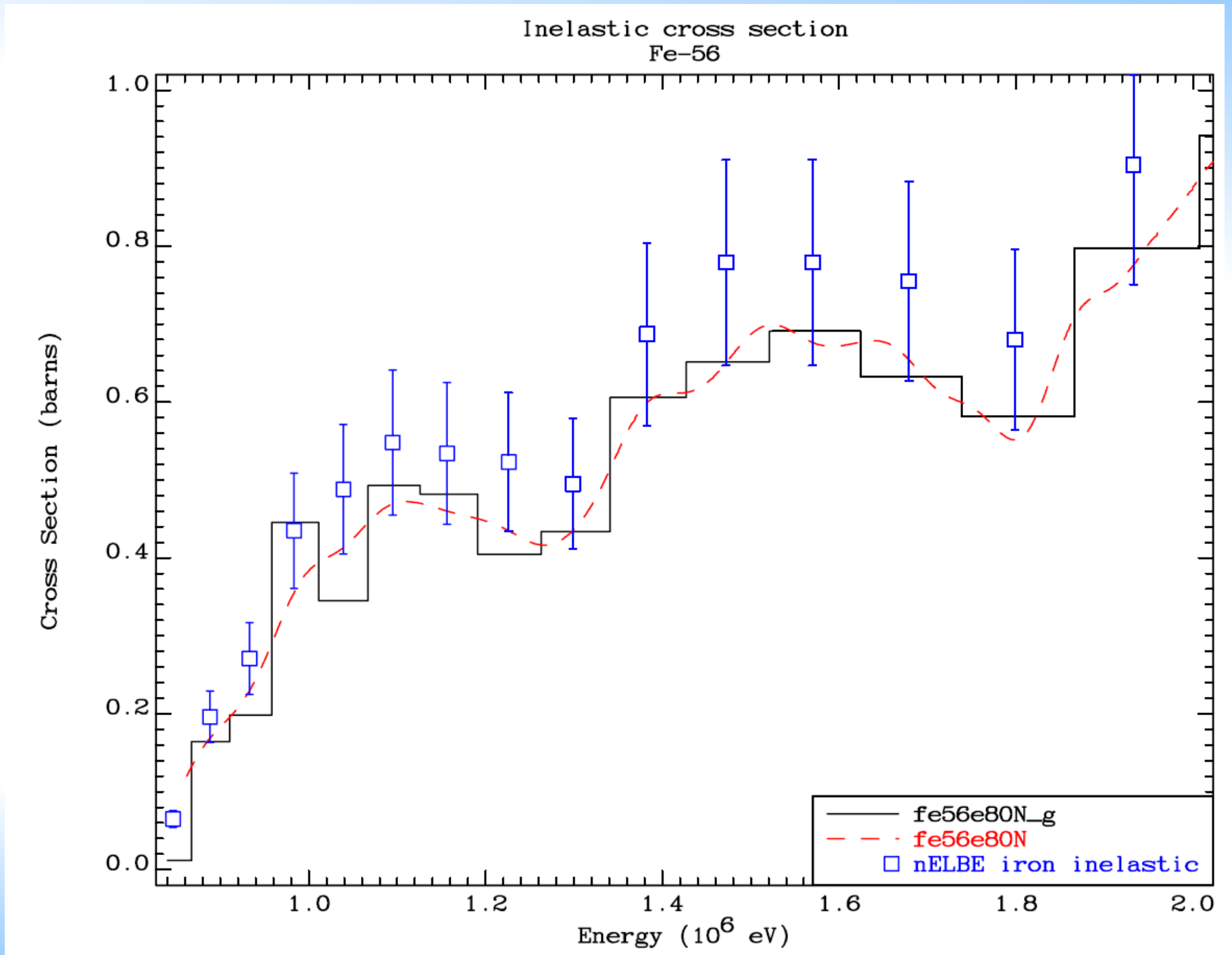
- Iron is an important structural material, affecting almost all benchmarks
- Several features/problems are similar to those encountered in actinides

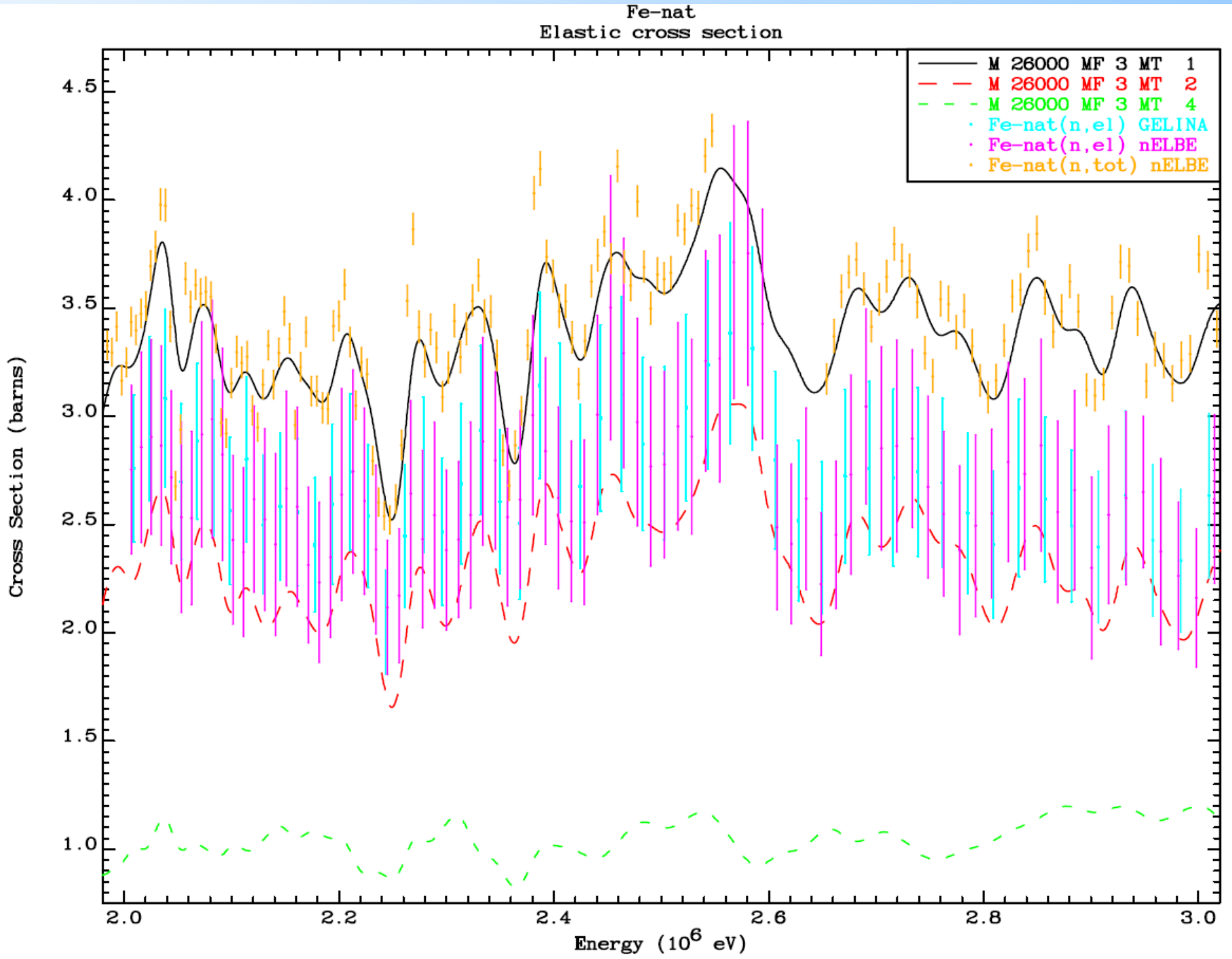
Scope

- ^{56}Fe resonance file in CIELO-1 is essentially by Froehner
  - Background to capture added at *E* 10-30 keV
    - Bound level at -24 keV ? Direct capture?
    - Minimum total x.s. consistent with Liou & Chrien, NSE 70, 150-154 (1979)
  - Background reduced at the upper end of RRR
    - RPI measurements
- Inelastic ^{56}Fe cross section scaled-down (post ENDF/B-VIII.0)
  - nELBE & IRMM new experiments
  - Evidence from ^{252}Cf leakage benchmarks
- Total ^{56}Fe cross section slightly reduced near 3 MeV
- Inelastic ^{57}Fe increased (low threshold)
  - Important contribution in some criticality benchmarks


ENDF Request 379, 2018-May-08,19:01:10
ENDF/B-VIII.0: FE-56(N,G)FE-57
ENDF/B-VII.1: FE-56(N,G)FE-57
Cross Section (barns)
Incident Energy (keV)
10-1
1
10
10²
10-2
10-4


ENDF Request 383, 2018-May-08,19:32:00
ENDF/B-VIII.0: FE-56(N,G)FE-57
ENDF/B-VII.1: FE-56(N,G)FE-57
Cross Section (barns)
Incident Energy (keV)
1
10-1
10-2
10-3
10-4
5·10²
6·10²
7·10²
8·10²

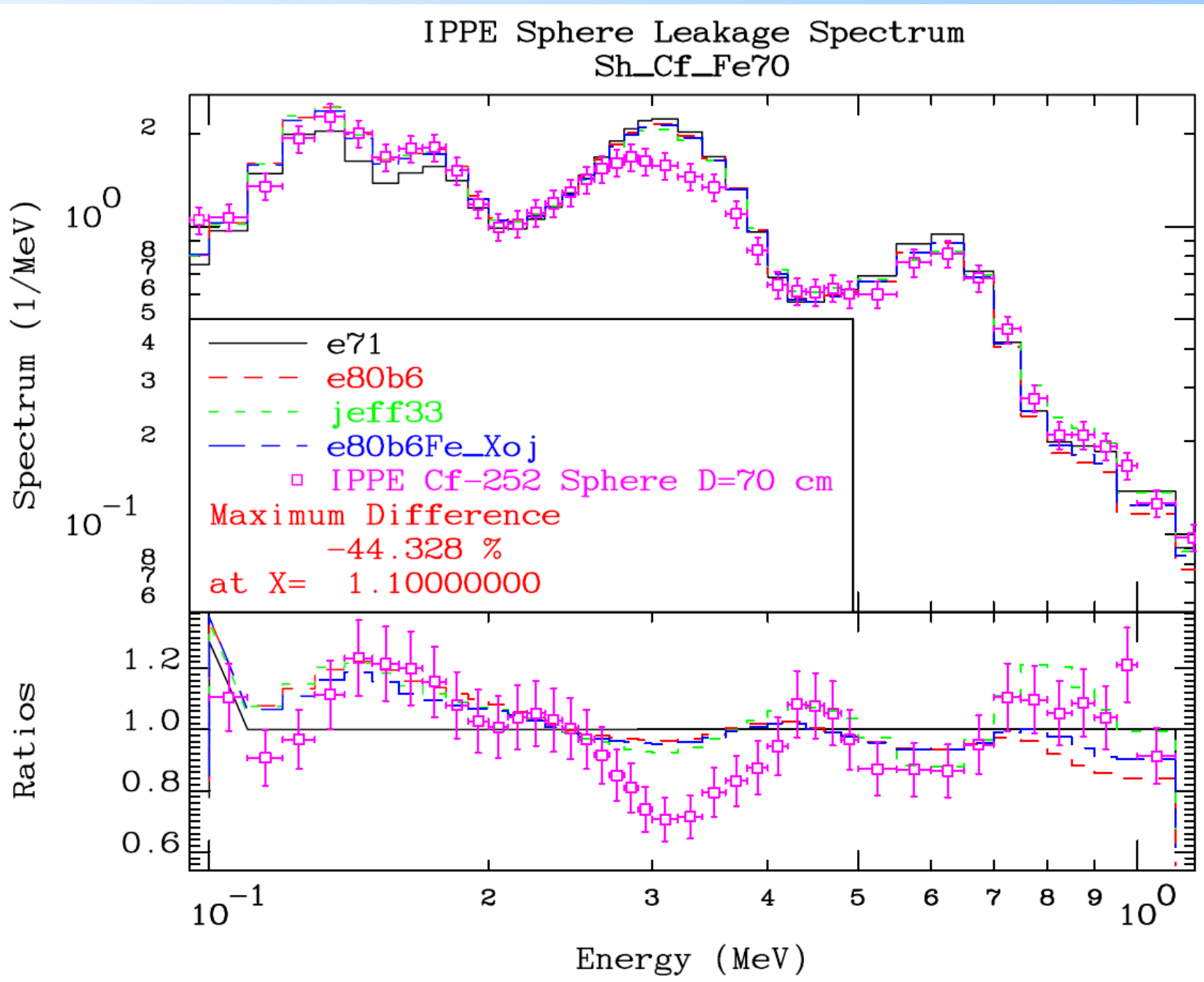

Inelastic cross section
Fe-56
Cross Section (barns)
Energy (10^6 eV)
1.0
0.8
0.6
0.4
0.2
0.0
1.0
1.2
1.4
1.6
1.8
2.0
fe56e80N_g
fe56e80N
nELBE iron inelastic

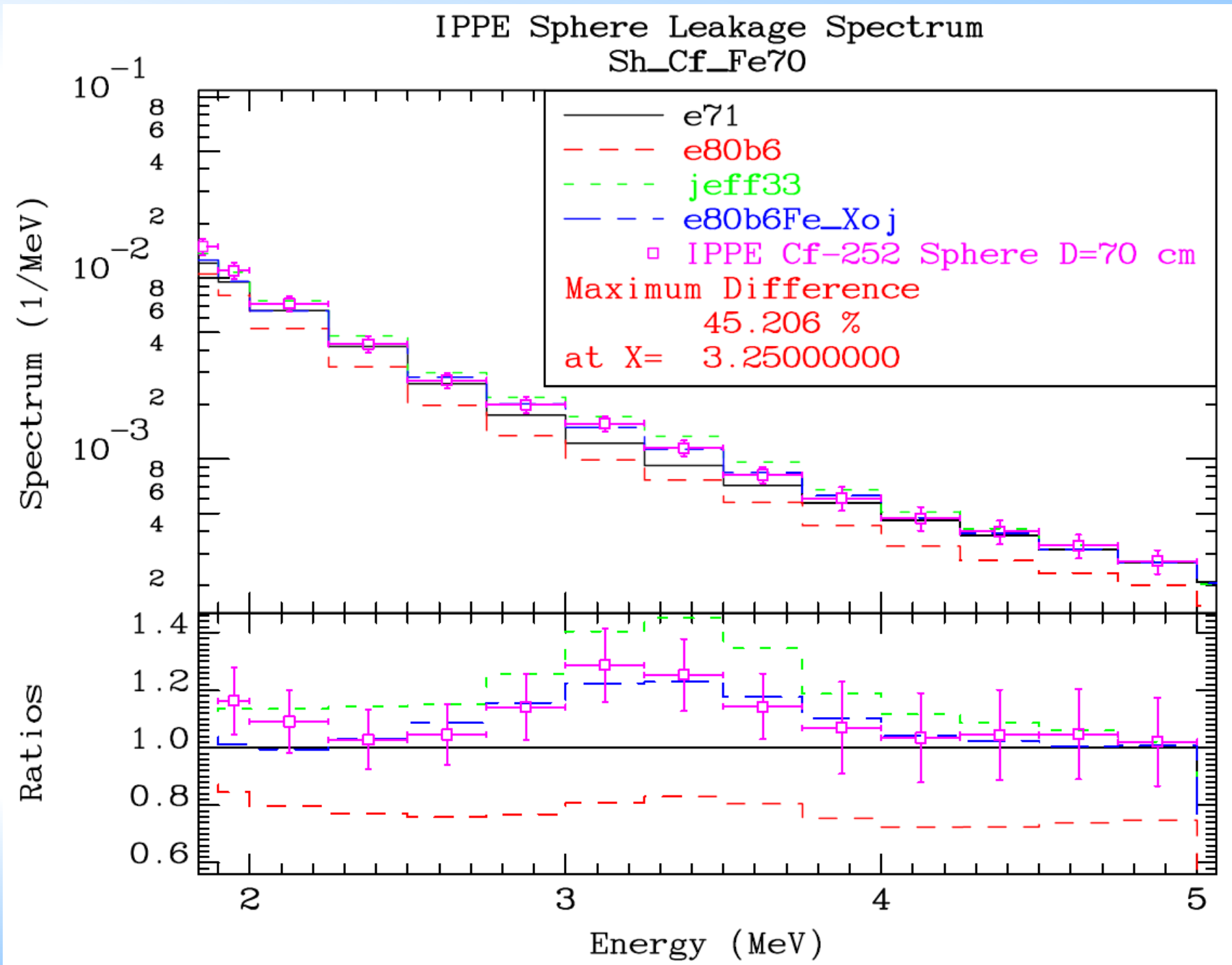

Fe-nat
Elastic cross section
M 26000 MF 3 MT 1
M 26000 MF 3 MT 2
M 26000 MF 3 MT 4
Fe-nat(n,el) GELINA
Fe-nat(n,el) nELBE
Fe-nat(n,tot) nELBE
Cross Section (barns)
Energy (10^6 eV)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
2.0
2.2
2.4
2.6
2.8
3.0

Integral performance

- Leakage spectra from spheres with ^{252}Cf(sf) source
  - All libraries overestimate spectrum near 300 keV
  - ENDF/B-VIII underestimated leakage spectrum above ~2 MeV; the improved file “Xoj” removes this deficiency by:
    - Reducing inelastic, increasing elastic (fixed total)
    - Slightly decreasing the total near 3 MeV

More details in INDC(NDS)-0757


IPPE Sphere Leakage Spectrum
Sh_Cf_Fe70
Spectrum (1/MeV)
Ratios
Energy (MeV)
e71
e80b6
jeff33
e80b6Fe_Xoj
IPPE Cf-252 Sphere D=70 cm
Maximum Difference
-44.328 %
at X= 1.10000000

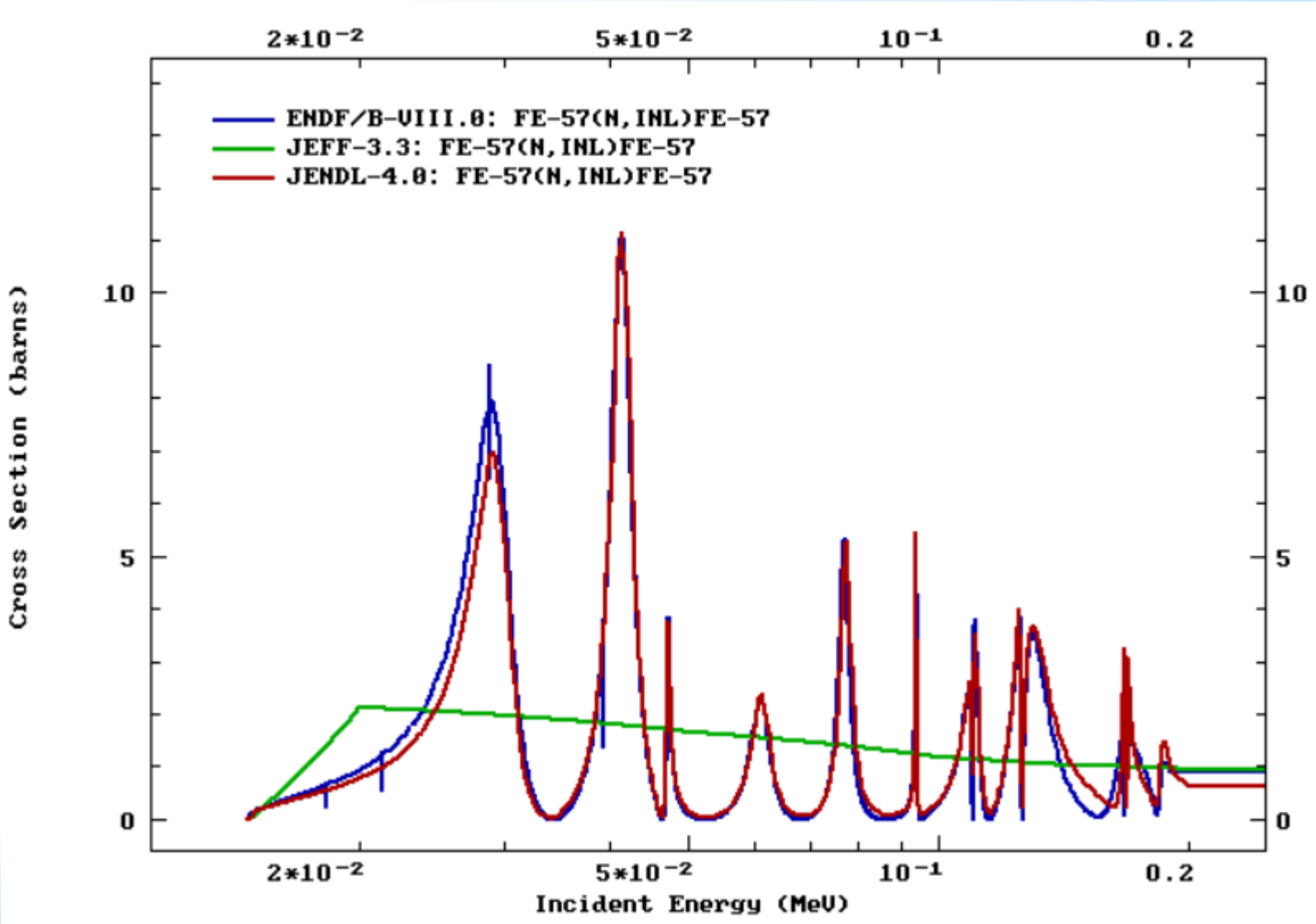

IPPE Sphere Leakage Spectrum
Sh_Cf_Fe70
e71
e80b6
jeff33
e80b6Fe_Xoj
IPPE Cf-252 Sphere D=70 cm
Maximum Difference
45.206 %
at X= 3.25000000
Spectrum (1/MeV)
Ratios
Energy (MeV)

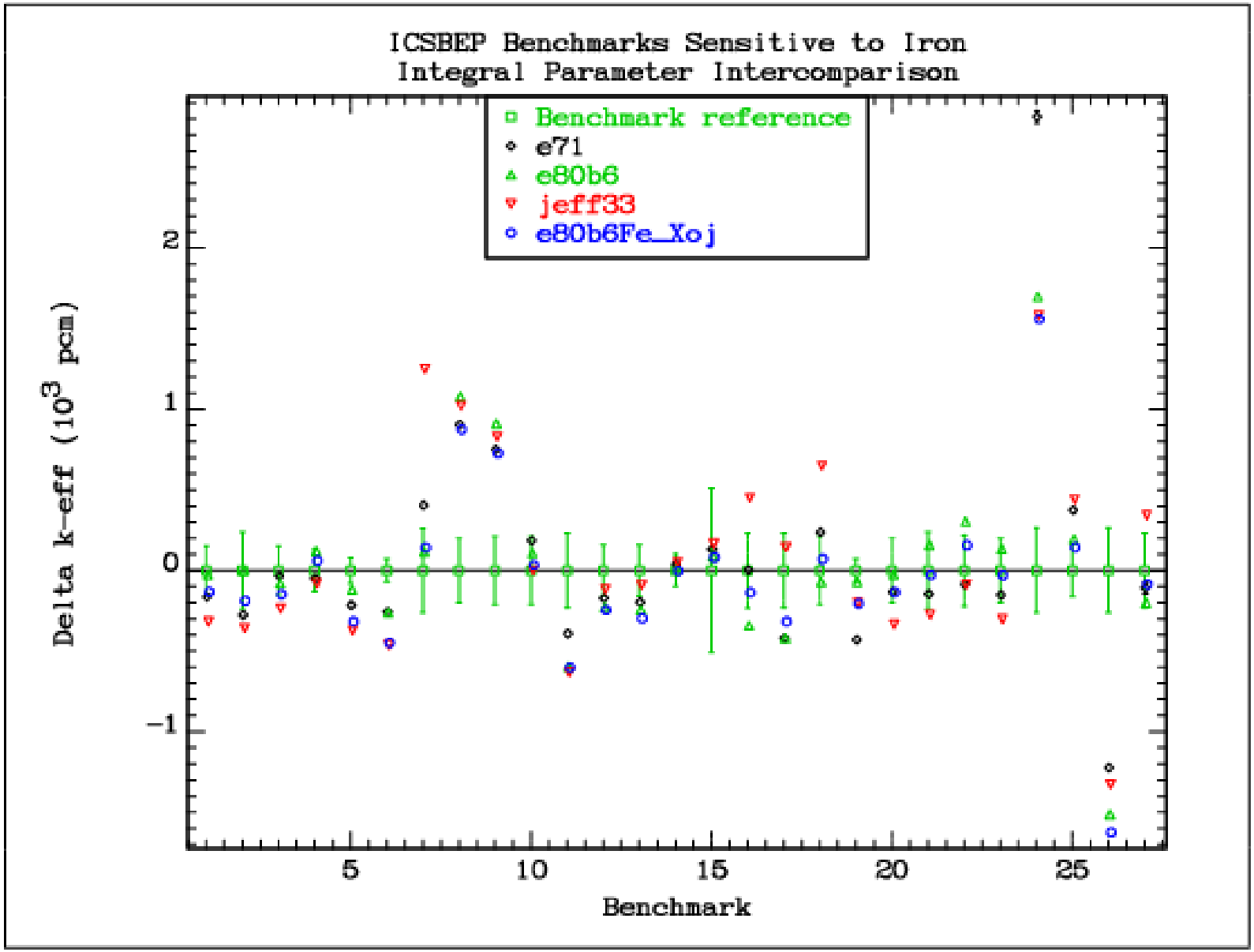
Integral performance (cont.)

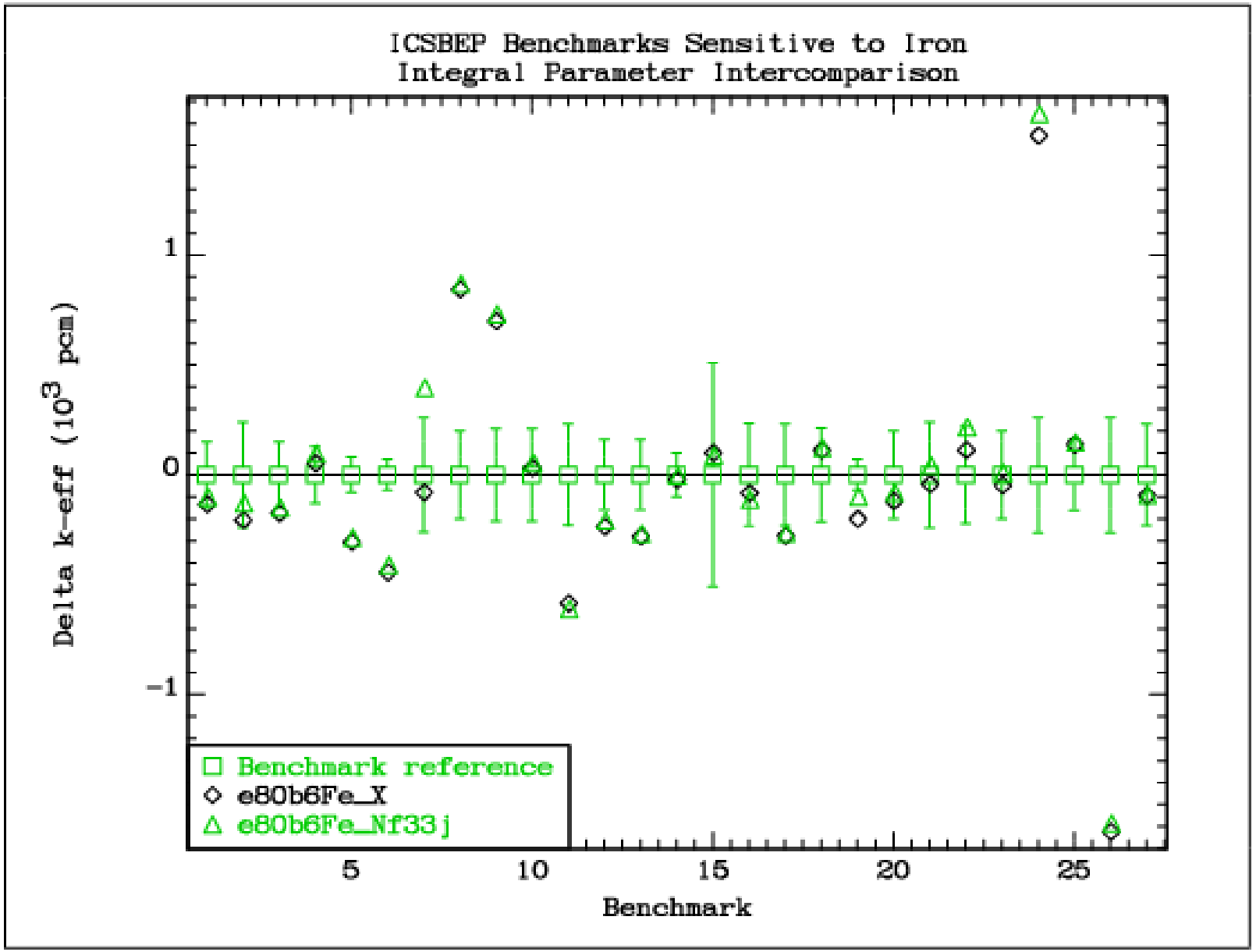
- Criticality benchmarks from ICSBEP
  - Performance with improved evaluations “Xoj” is maintained
  - Net effect of the increase of the inelastic cross section of ^{57}Fe is very large for ZPR-9/34 (label “NF33j”

More details in INDC(NDS)-0757

^{57}Fe(n,inl)


ENDF/B-VIII.0: FE-57(N,INL)FE-57
JEFF-3.3: FE-57(N,INL)FE-57
JENDL-4.0: FE-57(N,INL)FE-57
Cross Section (barns)
Incident Energy (MeV)
2*10-2
5*10-2
10-1
0.2
10
5
0


ICSBEP Benchmarks Sensitive to Iron
Integral Parameter Intercomparison
Benchmark reference
e71
e80b6
jeff33
e80b6Fe_Xoj
Delta k-eff (10^3 pcm)
2
1
0
−1
5
10
15
20
25
Benchmark


ICSBEP Benchmarks Sensitive to Iron
Integral Parameter Intercomparison
Delta k-eff (10^3 pcm)
1
0
-1
5
10
15
20
25
Benchmark
Benchmark reference
e80b6Fe_X
e80b6Fe_Nf33j

No.	ICSBEP Label	Short name	Common name
1	HEU-MET-FAST-013	hmf013	VNIITF-CTF-SS-13
2	HEU-MET-FAST-021	hmf021	VNIITF-CTF-SS-21
3	HEU-MET-FAST-024	hmf024	VNIITF-CTF-SS-24
4	HEU-MET-FAST-087	hmf087	VNIITF-CTF-Fe
5	HEU-MET-FAST-088	hmf088-001	FKBN-2/SS-PE-1
6	HEU-MET-FAST-088	hmf088-002	FKBN-2/SS-PE-2
7	HEU-MET-INTER-001	hmi001	ZPR-9/34
8	HEU-MET-THERM-013	hmt013-002	Planet_Fe-2
9	HEU-MET-THERM-015	hmt015	
10	IEU-MET-FAST-005	imf005	VNIIEF-CTF-5
11	IEU-MET-FAST-006	imf006	VNIIEF-CTF-6
12	LEU-COMP-THERM-042	lct042-001	lct042-001
13	LEU-COMP-THERM-042	lct042-002	lct042-002
14	LEU-COMP-THERM-043	lct043-002	IPEN/MB-01
15	LEU-MET-THERM-015	lmt015-001	RB-Vinca(01)
16	MIX-COMP-FAST-001	mcf001	ZPR-6/7
17	MIX-COMP-FAST-005	mcf005-s	ZPR-9/31
18	MIX-COMP-FAST-006	mcf006-s	ZPPR-2
19	PU-MET-FAST-015	pmf015	BR-1-3
20	PU-MET-FAST-025	pmf025	pmf025
21	PU-MET-FAST-026	pmf026	pmf026
22	PU-MET-FAST-028	pmf028	pmf028
23	PU-MET-FAST-032	pmf032	pmf032
24	PU-MET-INTER-002	pmi002	ZPR-6/10
25	PU-MET-INTER-003	pmi003-001s	ZPR-3/58(U)
26	PU-MET-INTER-004	pmi004-001s	ZPR-4/59(Pb)
27	IEU-COMP-INTER-005	ici005	ZPR-6/6A

Conclusions

- ^{56}Fe resonance data need re-evaluation
  - Be careful with energy calibration
  - Check bound levels, direct capture
  - Match newly-available experimental data
  - Do not miss observed resonances (e.g. Berthold data)
  - Check σ_{inl}/σ_{el} ratio (e.g. RPI data)
- ^{57}Fe inelastic has low threshold and resonance structure – match model calculations on average

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Thank you!