

Benchmarking and Validation of CIELO Evaluated Data Files

A.Trkov¹, R.Capote¹, G. Žerovnik^{2,3}

¹ IAEA, Vienna, Austria

² JSI, Ljubljana, Slovenia

³ JRC IRMM, Geel, Belgium



IAEA

International Atomic Energy Agency

Background

The IAEA is committed to:

- contribute to the international effort (the CIELO pilot project) of improving the evaluated nuclear data for the most important nuclides for the fission nuclear reactors, namely:
 ^{239}Pu , ^{238}U , ^{235}U , ^{56}Fe , ^{16}O , ^1H
- Improve the availability of validated nuclear data processing codes to the users in Member States.

Scope

^{238}U , ^{235}U , ^{56}Fe (^{16}O Hale, H_2O CAB)

- Evaluation basic principles
- General features of the tested evaluations
- Selection of benchmarks
- Benchmark results and compensating effects
- Data processing features

Evaluation basic principles

- Use the best physics in nuclear code modelling of reaction cross sections
- Respect the differential experimental data, applying corrections due to updated standards and weeding out outliers (with justification)
- Fine-tuning of less-accurately known parameters in the evaluations based on clean integral measurements

Benchmarking is an integral part of the evaluation process!

^{238}U – Fast energy range

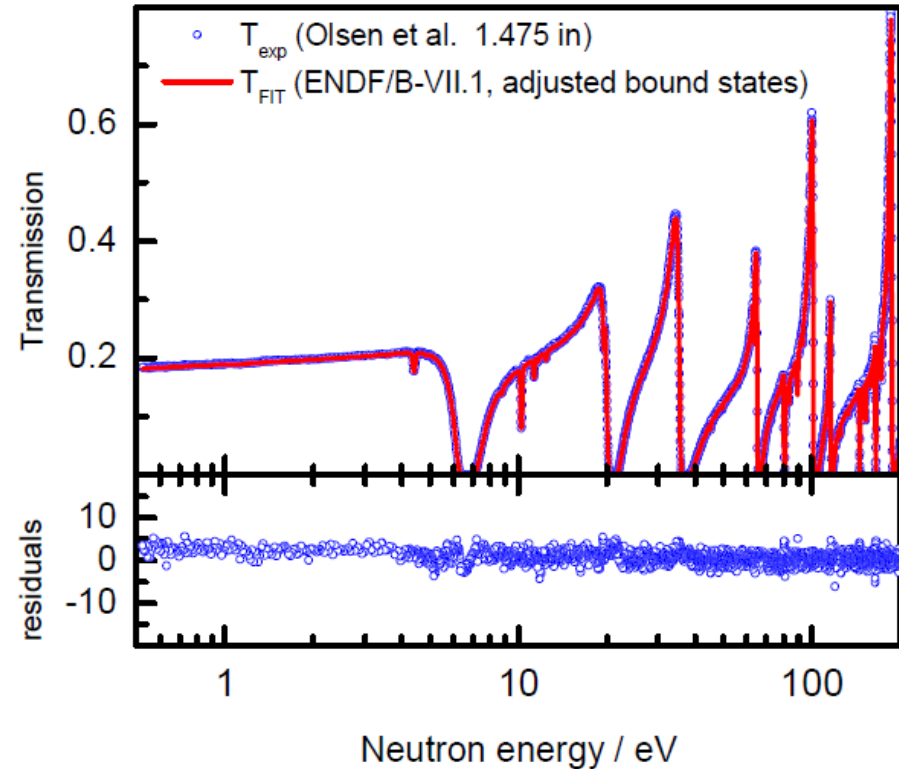
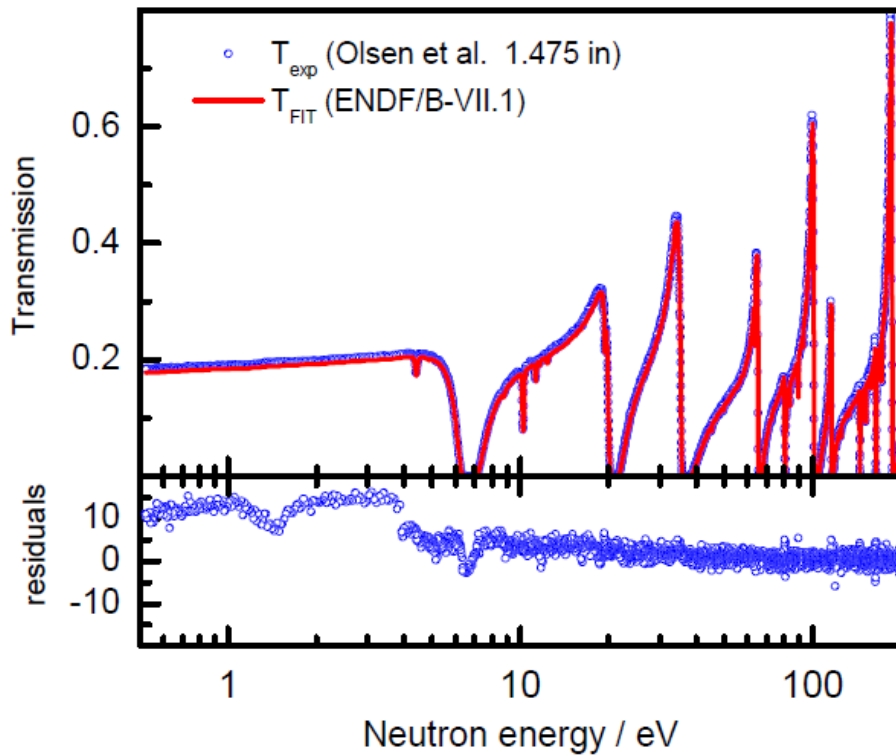
Empire calculation “u238ib44”

- DCCOMP (see presentation by R. Capote)
- Matching of “Standards” fission and capture within the model to get competing reaction channels right
- Replace fission and capture with ENDF/B-VII.1 (because it agrees with the “Standards”)

^{238}U Resonance range

- ENDF/B-VII.1 starter resonance file
- New work from IRMM:
 - Modified parameters of the bound states to fit Olsen data
 - Residual function greatly reduced (no need to renormalize Olsen data)
 - No impact on benchmarks sensitive to the thermal energy range
 - No change to thermal capture cross section
 - Slight change to the elastic cross section for consistency with measured coherent scattering length

^{238}U Resonance range (cont.)



^{238}U Resonance range (cont.)

- Work at IRMM (cont.)
 - New set of unresolved resonance parameters (URR) consistent with total from OMP, evaluated inelastic x.s. and “Standards” capture
 - Testing of RRR-URR boundary (10 keV or 20 keV)
 - Testing on benchmarks showed no differences in results – 20 keV boundary can be adopted
 - Work continues to incorporate new data and determine the covariance information

^{238}U Resonance range (cont.)

New data to be considered in the evaluation:

- new transmission (thin & thick sample) GELINA data
- new capture data from GELINA (12 m)

Resonance analysis

- simultaneous analysis including above + transmission data from Olsen and Harvey
- still waiting for the nTOF data and LANL data in a format suitable for a resonance shape analysis.
- ENDF/B-VII.1 starter but radiation width reduced from 23 meV to 22.5 meV instead of 23 meV)

^{238}U - PFNS

- Evaluation submitted by P. Talou for the IAEA CRP on PFNS

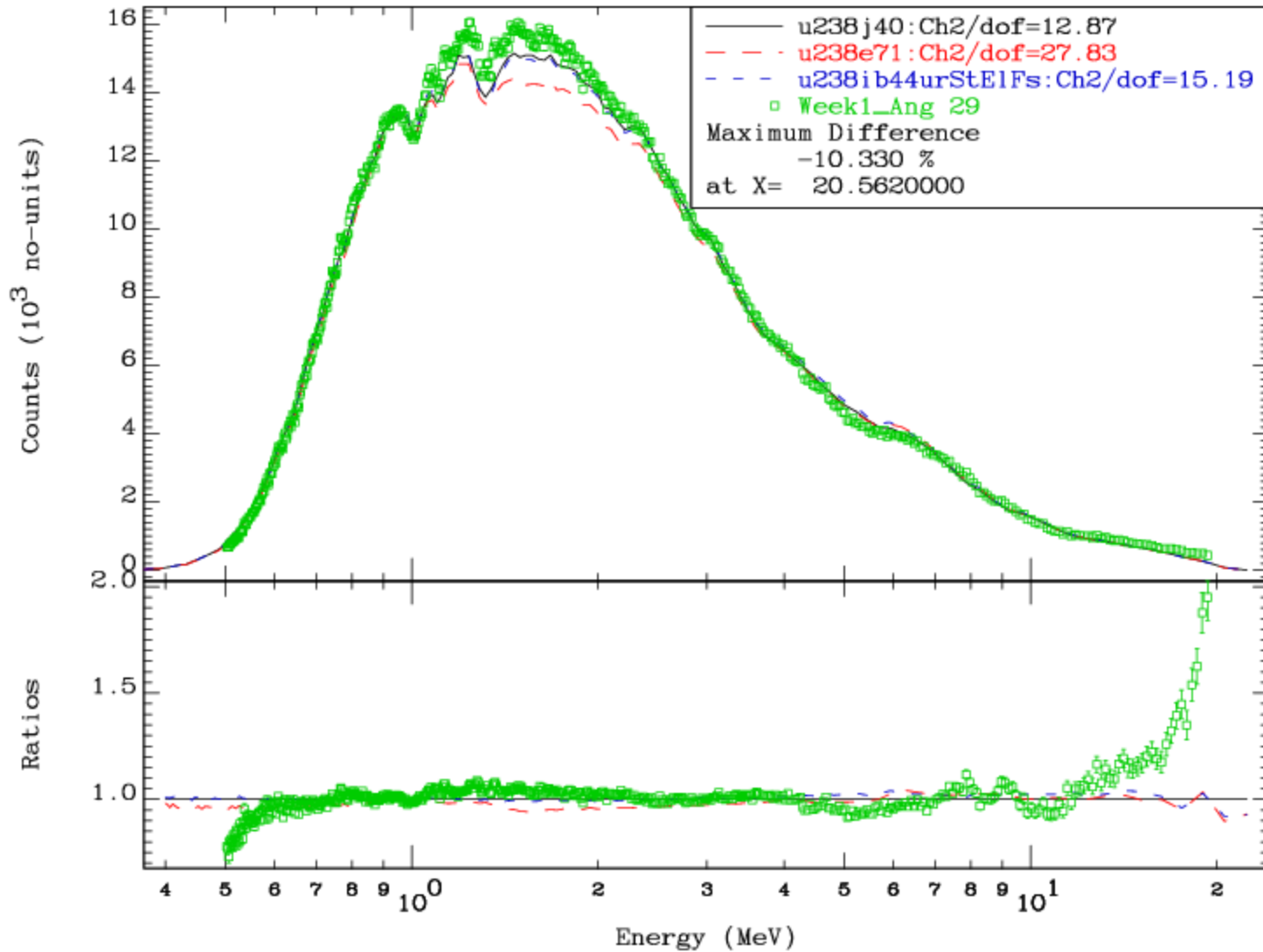
^{238}U - RPI and criticality benchmarks

- Capture and fission same as ENDF/B-VII.1
- Main changes to elastic and inelastic
- Criticality benchmarks:
 - The impact is expected to be small, mainly in assemblies reflected by ^{238}U
 - Inelastic and elastic evaluation was guided by the RPI benchmark

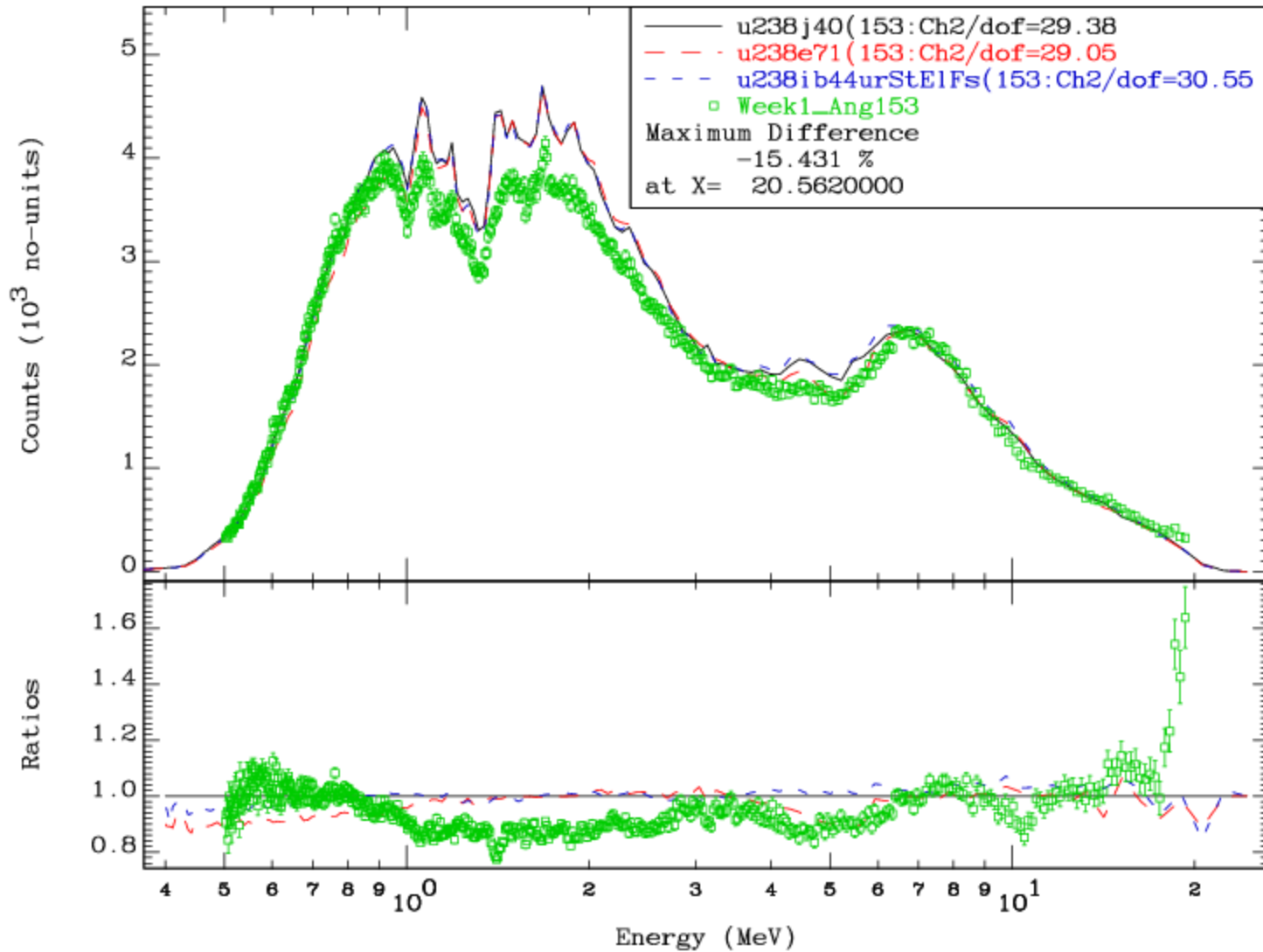
^{238}U - RPI benchmark

- The benchmark is highly selective to scattering data in the range 0.5-10 MeV
- Generally, the agreement with measurements is good
- Considerable improvement with the new evaluation
- Further information was released from RPI, some details are not yet fully understood

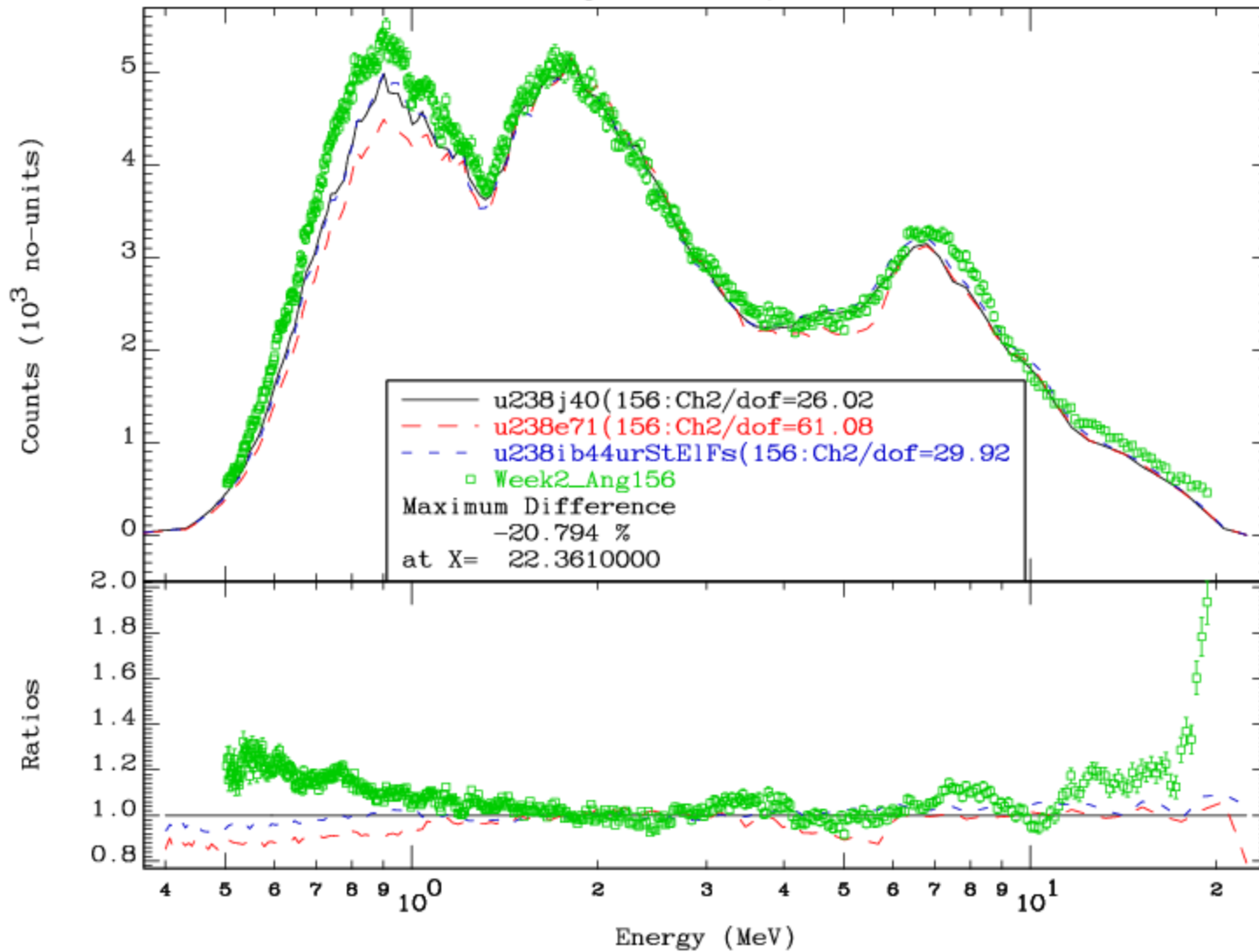
RPI-u-238 Benchmark
Spectrum raw yield



RPI-u-238 Benchmark
Spectrum raw yield



RPI-u-238 Benchmark
Spectrum raw yield



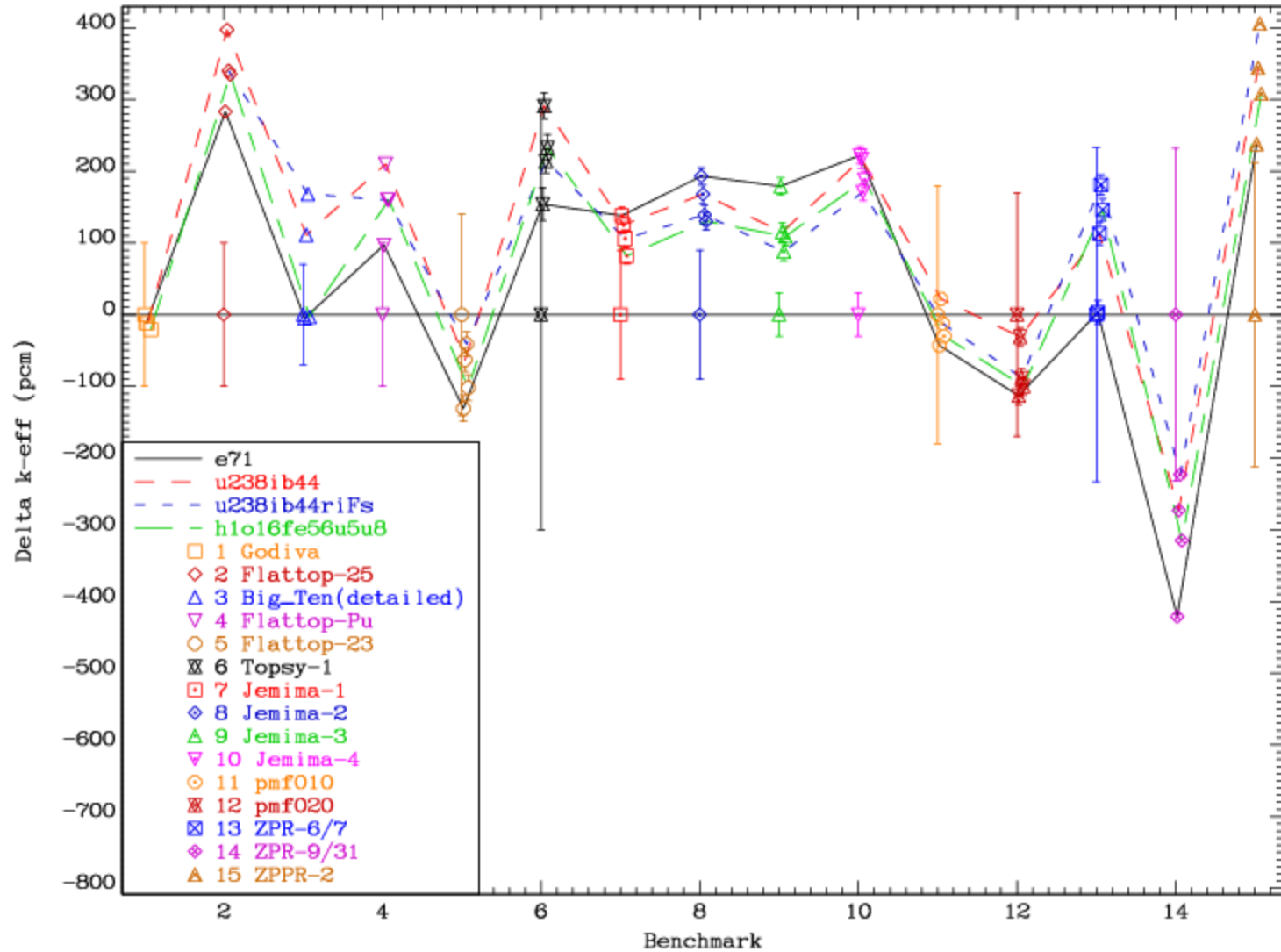
^{238}U - criticality benchmarks (ICSBEP)

- Improvement is observed for several fast benchmarks
- There are significant compensating effects, particularly with ^{235}U
- Big old outliers remain
- Thermal lattices are little affected by ^{238}U , but strongly by ^{235}U ; the bias of about 300 pcm could be compensated by ^{238}U (or ^{235}U ?)

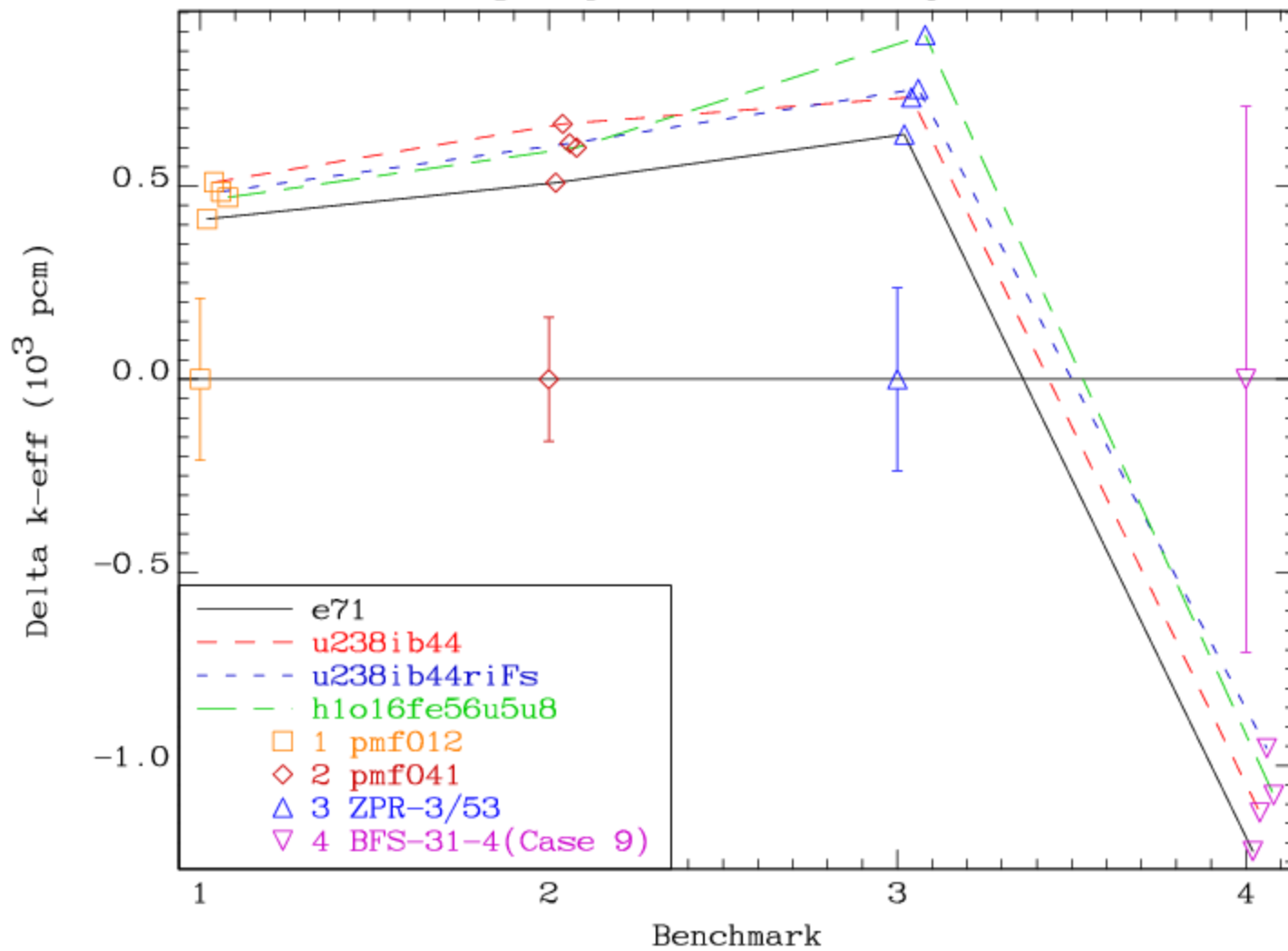
U-238 fast reactor benchmarks

ICSBEP name	Short name	Common name
HEU-MET-FAST-001	hmf001	Godiva
HEU-MET-FAST-028	hmf028	Flatop-25
IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
PU-MET-FAST-006	pmf006	Flatop-Pu
U233-MET-FAST-006	umf006	Flatop-23
HEU-MET-FAST-002	hmf002-1	Topsy-1
IEU-MET-FAST-001	imf001-1	Jemima-1
IEU-MET-FAST-001	imf001-2	Jemima-2
IEU-MET-FAST-001	imf001-3	Jemima-3
IEU-MET-FAST-001	imf001-4	Jemima-4
PU-MET-FAST-010	pmf010	pmf010
PU-MET-FAST-012	pmf012	pmf012
PU-MET-FAST-020	pmf020	pmf020
PU-MET-FAST-041	pmf041	pmf041
MIX-MET-INTER-004	mmi004	ZPR-3/53
MIX-COMP-FAST-001	mcf001	ZPR-6/7
MIX-COMP-FAST-005	mcf005-s	ZPR-9/31
MIX-COMP-FAST-006	mcf006-s	ZPPR-2
MIX-MISC-FAST-001	mif001-09	BFS-31-4

ICSBEP Benchmark Summary Results
Integral parameter intercomparison



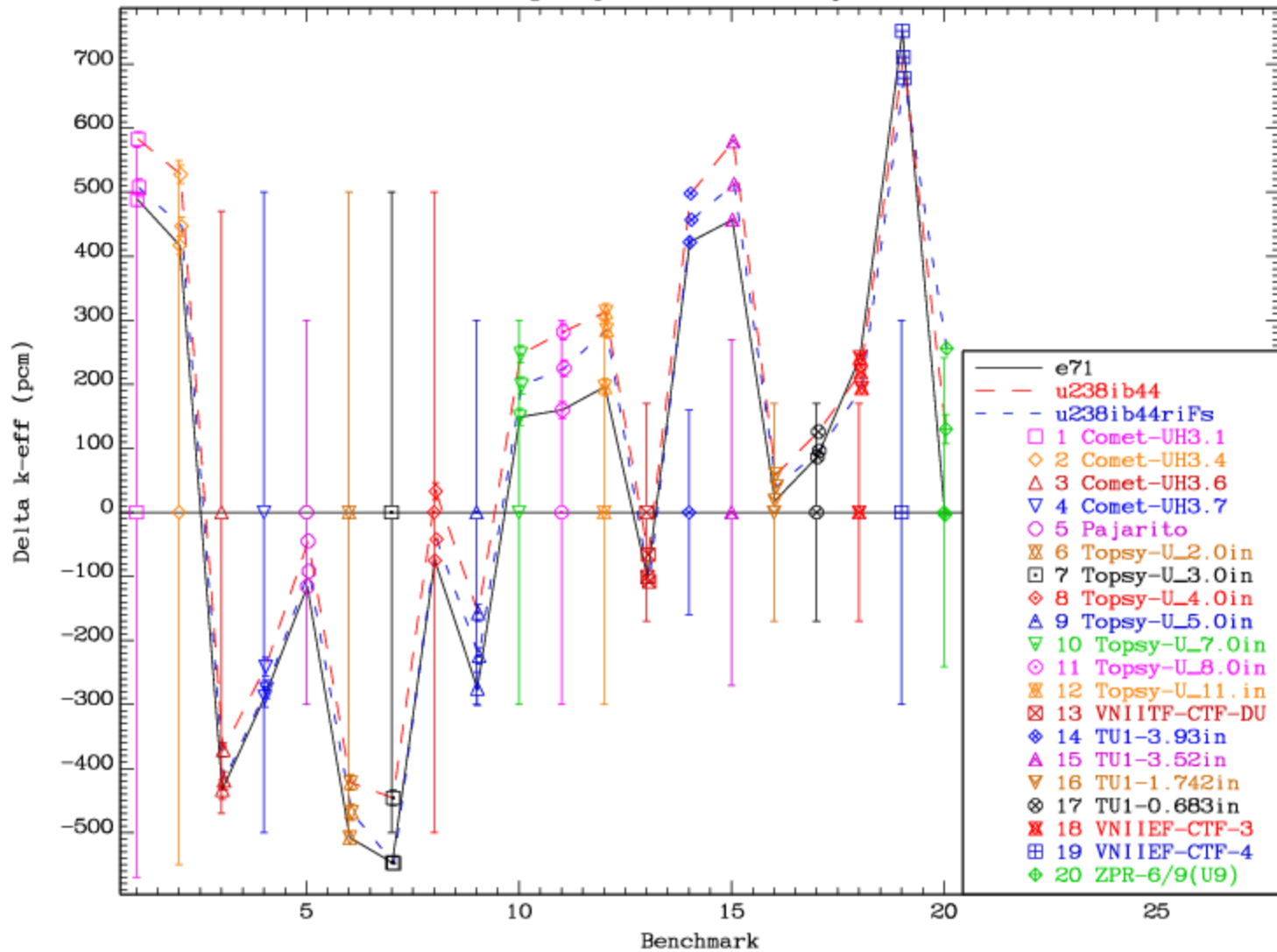
ICSBEP Benchmark Summary Results
Integral parameter intercomparison



Intermediate-enriched and ^{238}U reflected benchmarks

ICSBEP name	Short name	Common name
PU-MET-FAST-026	pmf026	pmf026
HEU-MET-FAST-061	hmf061	ZPPR-21F
PU-MET-FAST-033	pmf033	ZPPR-21A
HEU-MET-FAST-088	hmf088-1	hmf088-1
HEU-MET-FAST-088	hmf088-2	hmf088-2
PU-MET-FAST-025	pmf025	pmf025
HEU-MET-FAST-087	hmf087	VNIITF-CTF-Fe
HEU-COMP-INTER-003	hci003-1	COMET-UH3-1
HEU-COMP-INTER-003	hci003-4	COMET-UH3-4
HEU-COMP-INTER-003	hci003-6	COMET-UH3-6
HEU-COMP-INTER-003	hci003-7	COMET-UH3-7
HEU-MET-FAST-072	hmf072-1	ZEUS_Fe/Cu-1
HEU-MET-FAST-072	hmf072-3	ZEUS_Fe/Cu-3
HEU-MET-FAST-084	hmf084-14	Comet-W_1.0in
HEU-MET-FAST-084	hmf084-25	Comet-W_0.5in
PU-MET-FAST-032	pmf032	pmf032
HEU-MET-FAST-013	hmf013	VNIITF-CTF-SS-13
IEU-MET-FAST-005	imf005	VNIIEF-CTF-5
IEU-MET-FAST-005	imf005-s	VNIIEF-CTF-5s
HEU-MET-FAST-021	hmf021	VNIITF-CTF-SS-21
HEU-MET-FAST-085	hmf085-5	Comet-Th_2in
PU-MET-FAST-028	pmf028	pmf028
PU-MET-FAST-026	pmf026	pmf026

ICSBEP Benchmark Summary Results
Integral parameter intercomparison

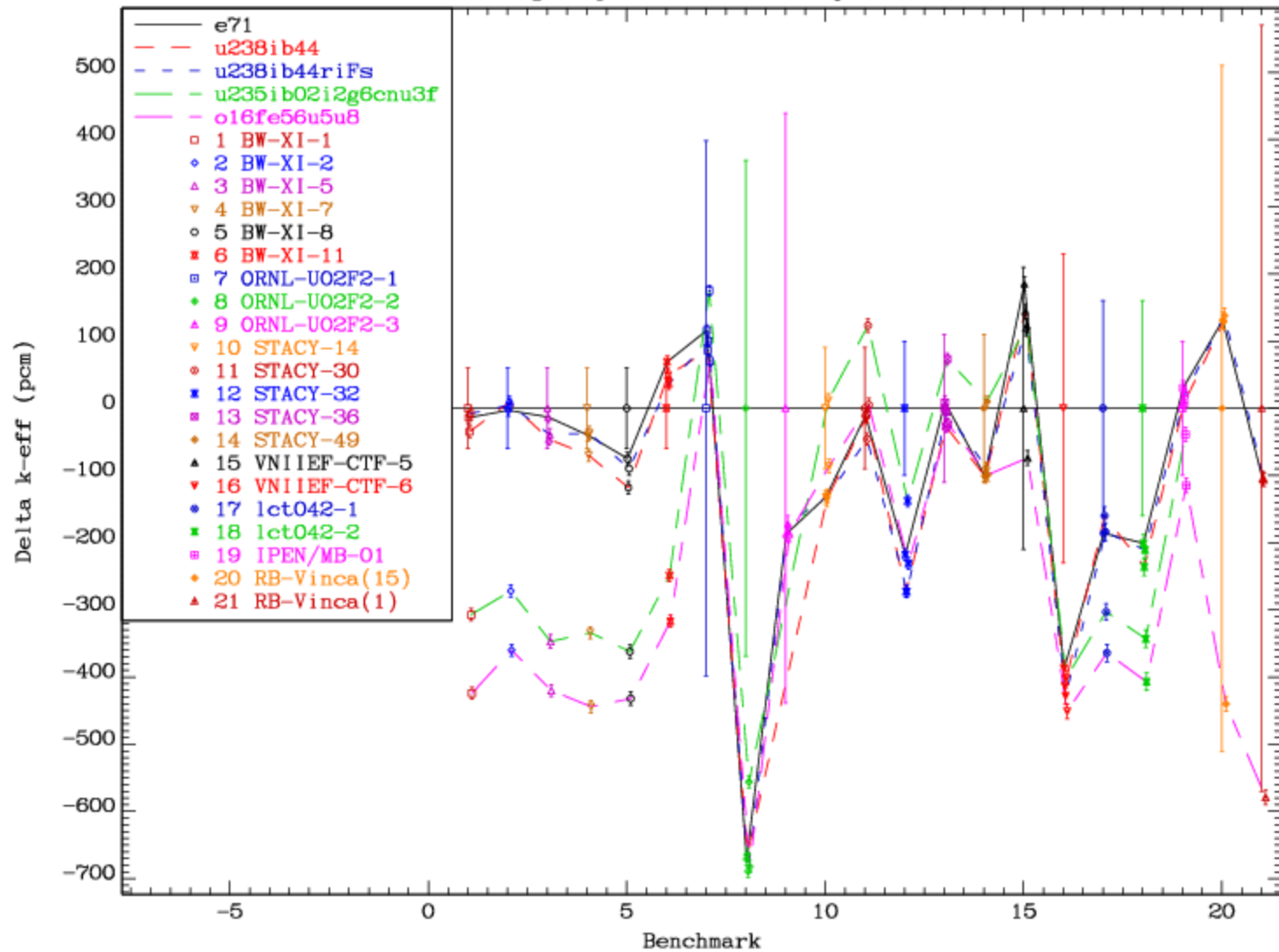


Thermal lattices and solutions

ICSBEP name	Short name	Common name
LEU-COMP-THERM-008	lct008-01	BW-XI-01
LEU-COMP-THERM-008	lct008-02	BW-XI-02
LEU-COMP-THERM-008	lct008-05	BW-XI-05
LEU-COMP-THERM-008	lct008-07	BW-XI-07
LEU-COMP-THERM-008	lct008-08	BW-XI-08
LEU-COMP-THERM-008	lct008-11	BW-XI-11
LEU-SOL-THERM-002	lst002-1	ORNL-UO2F2-1
LEU-SOL-THERM-002	lst002-2	ORNL-UO2F2-2
LEU-SOL-THERM-002	lst002-3	ORNL-UO2F2-3
LEU-SOL-THERM-007	lst007-14	STACY-14
LEU-SOL-THERM-007	lst007-30	STACY-30
LEU-SOL-THERM-007	lst007-32	STACY-32
LEU-SOL-THERM-007	lst007-36	STACY-36
LEU-SOL-THERM-007	lst007-49	STACY-49
IEU-MET-FAST-005	imf005	VNIIEF-CTF-5
IEU-MET-FAST-006	imf006	VNIIEF-CTF-6
LEU-COMP-THERM-042	lct042-1	lct042-1
LEU-COMP-THERM-042	lct042-2	lct042-2
LEU-COMP-THERM-043	lct043-2	IPEN/MB-01
LEU-MET-THERM-015	lmt015	RB-Vinca(15)
LEU-MET-THERM-001	lmt001	RB-Vinca(1)



ICSBEP Benchmark Summary Results
Integral parameter intercomparison



^{235}U – Fast energy range

- Empire calculation “u235ib02”
 - Model calculation similar to ^{238}U
 - Matching of “Standards” fission within the model to get competing reaction channels right
 - Replace fission and capture with ENDF/B-VII.1 (because fission agrees with the “Standards”)

^{235}U Resonance range

- Evaluation “ornl.v4” by L. Leal superseded by new evaluations:
 - “i1” matching approximately the thermal constants for Standards-2015 “mic.+mac.”, which are similar to the constants adopted in Standards-2006
 - “i2” matching the thermal constants for Standards-2015 “mic. Only”

^{235}U - PFNS

- GMA fit for Standards-2015 for incident thermal neutrons
- Evaluation submitted by P. Talou for the IAEA CRP on PFNS at higher energies

New evaluation has significantly lower average neutron energy for all incident neutron energies (see presentation by Chadwick)

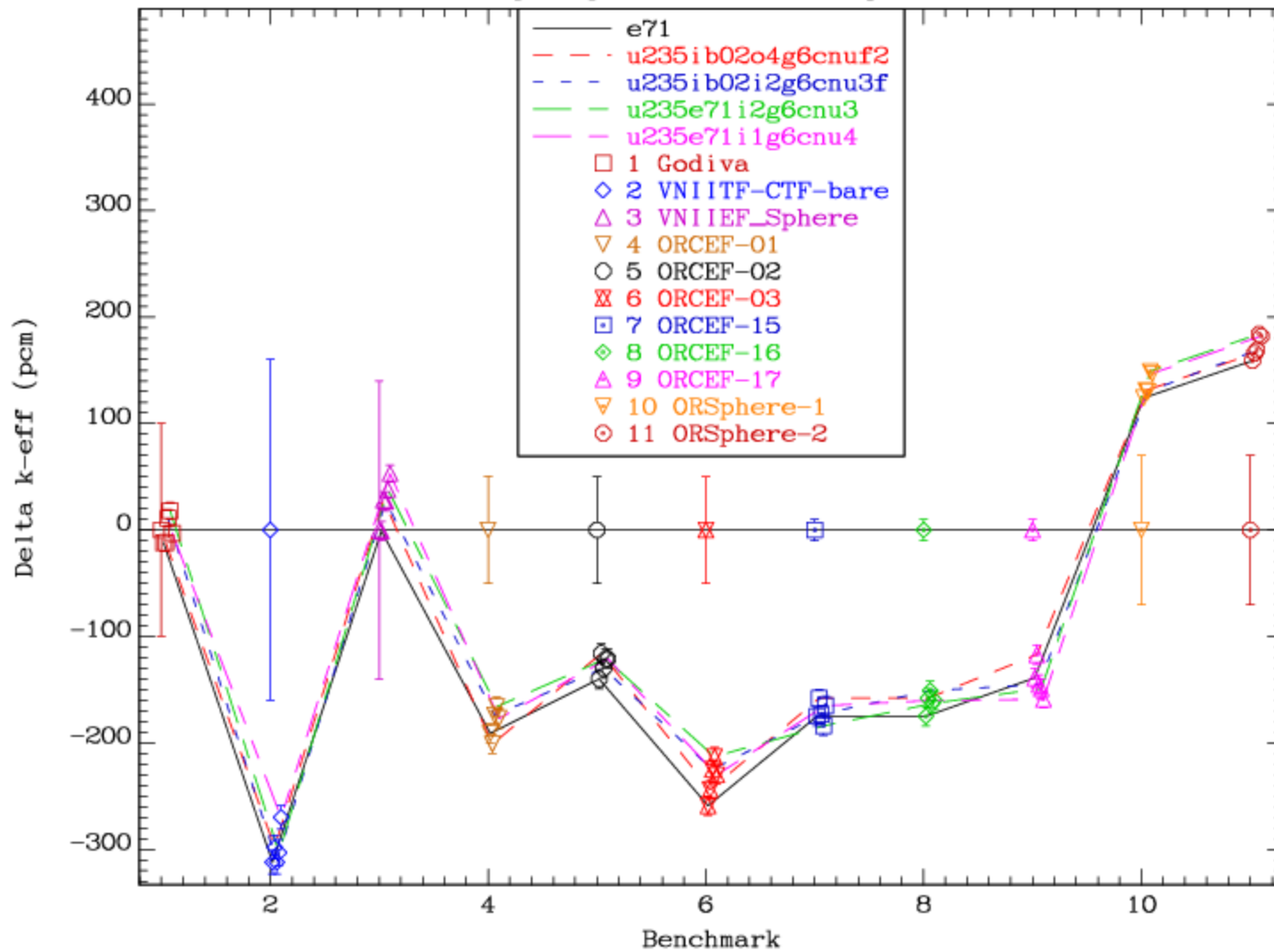
^{235}U - criticality benchmarks (ICSBEP)

- Decrease of inelastic cross section requires a 0.2% increase of $\bar{\nu}$ in 0.5-1 MeV range to restore performance for bare assemblies
- Lowering of E_{av} of PFNS has far-reaching consequences; reactivity of high-leakage HEU solutions increases greatly
- Performance is restored by changes to $\bar{\nu}$ (in accordance with “mic” Standards-2015”)
- ATLF-dependence improved by lowering $\bar{\nu}$ around the first resonance; same effect could (probably) be achieved by increasing α in the low-lying resonances

^{235}U bare assemblies

ICSBEP name	Short name	Common name
HEU-MET-FAST-001	hmf001	Godiva
HEU-MET-FAST-008	hmf008	VNIIEF-CTF-bare
HEU-MET-FAST-018	hmf018	VNIIEF_Sphere
HEU-MET-FAST-051	hmf051-01	ORCEF-01
HEU-MET-FAST-051	hmf051-02	ORCEF-02
HEU-MET-FAST-051	hmf051-03	ORCEF-03
HEU-MET-FAST-051	hmf051-15	ORCEF-15
HEU-MET-FAST-051	hmf051-16	ORCEF-16
HEU-MET-FAST-051	hmf051-17	ORCEF-17
HEU-MET-FAST-100	hmf100-1	ORSphere-1
HEU-MET-FAST-100	hmf100-2	ORSphere-2

ICSBEP Benchmark Summary Results
Integral parameter intercomparison

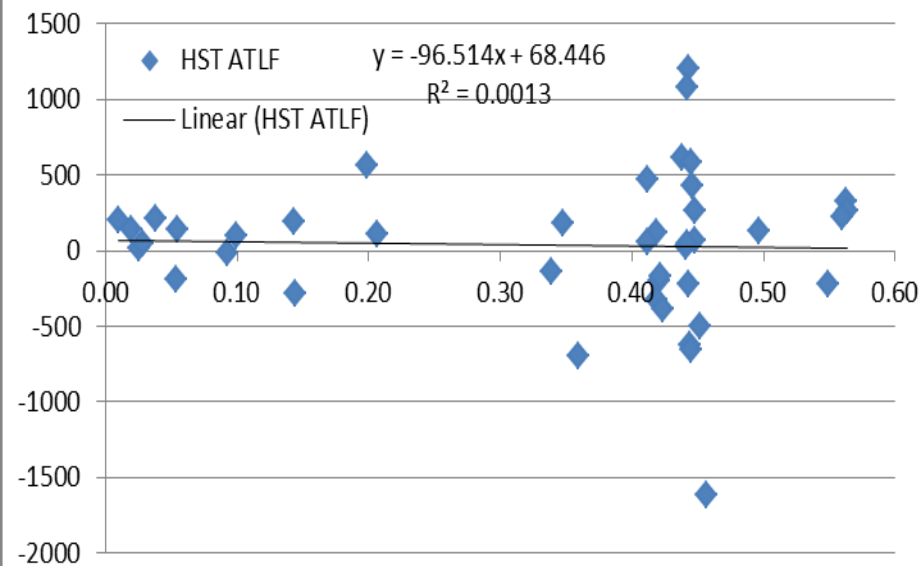


^{235}U - criticality benchmarks (Cont.)

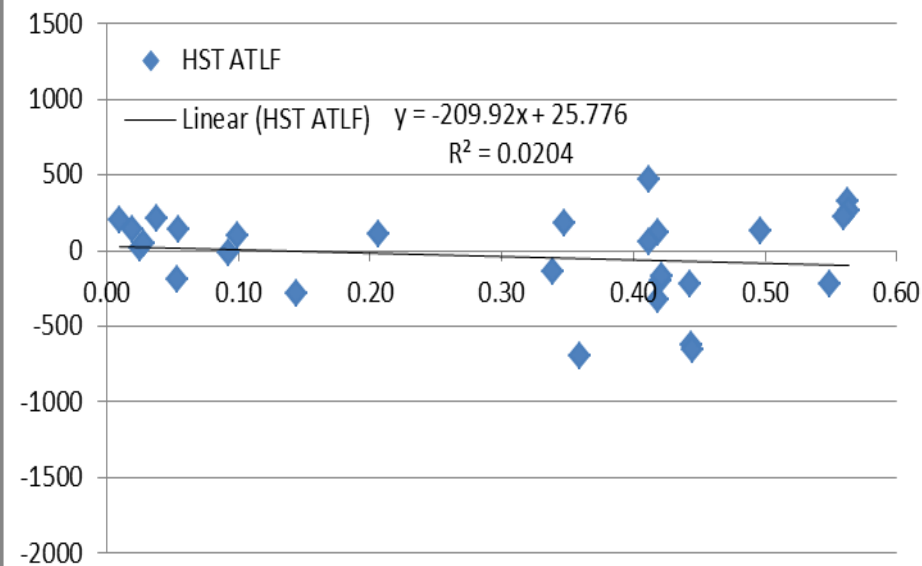
Fitting ATLF is tricky and subjective:

- LANL
 - fit C/E, unweighted
- IAEA
 - fit Δk ,
 - exclude hst043, hst050 (highly scattered)
 - Use benchmark uncertainties for weights

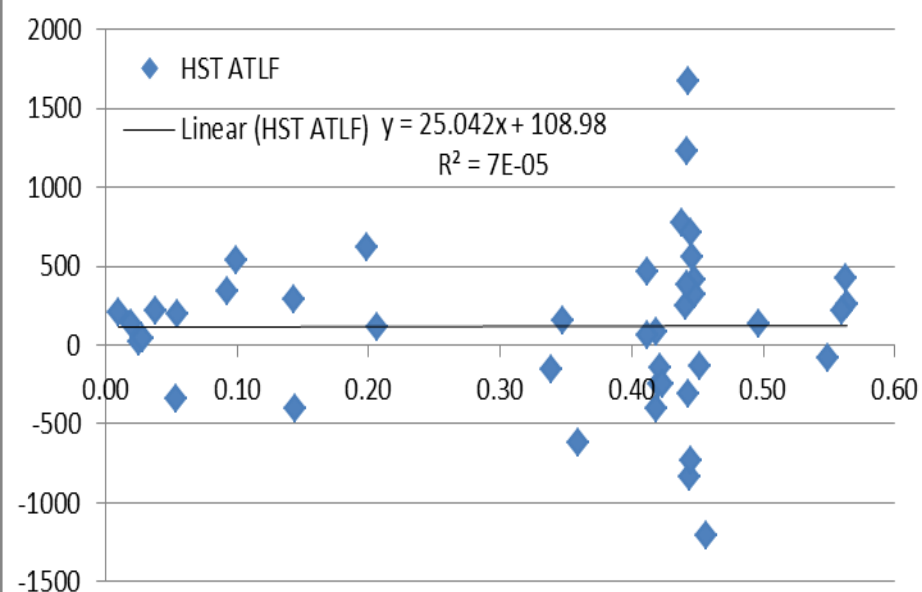
HST ATLF (Relative) 6-47



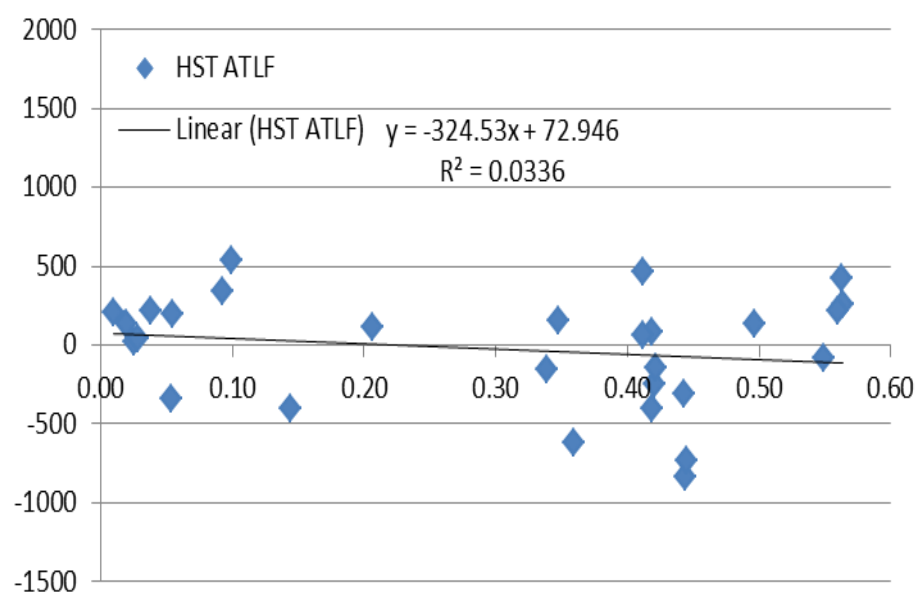
HST ATLF (Relative) 6-33



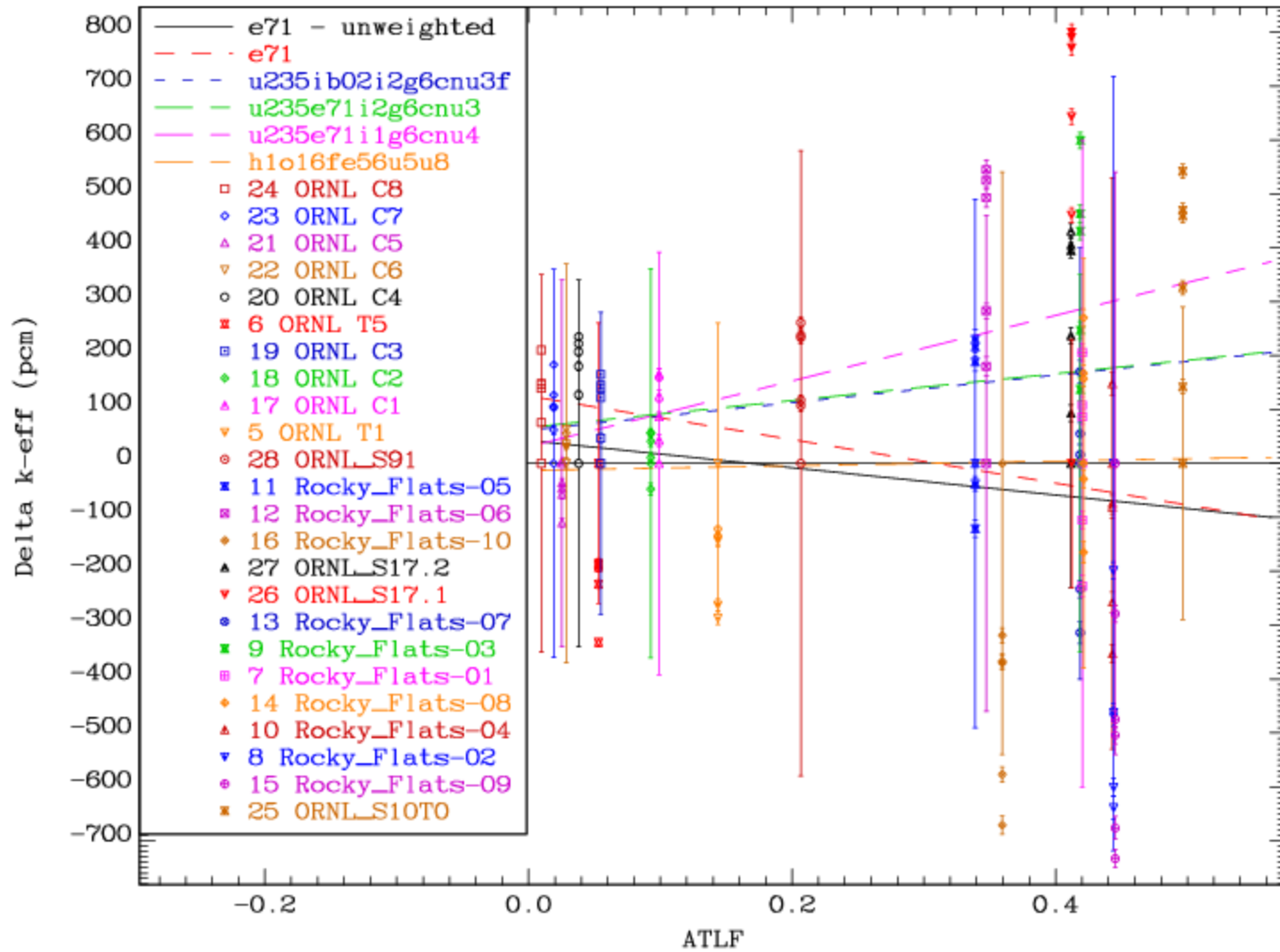
HST ATLF (delta_k) 6-47



HST ATLF (delta_k) 6-33



ICSBEP Benchmark Summary Results
Integral parameter intercomparison



^{235}U - criticality benchmarks (Cont.)

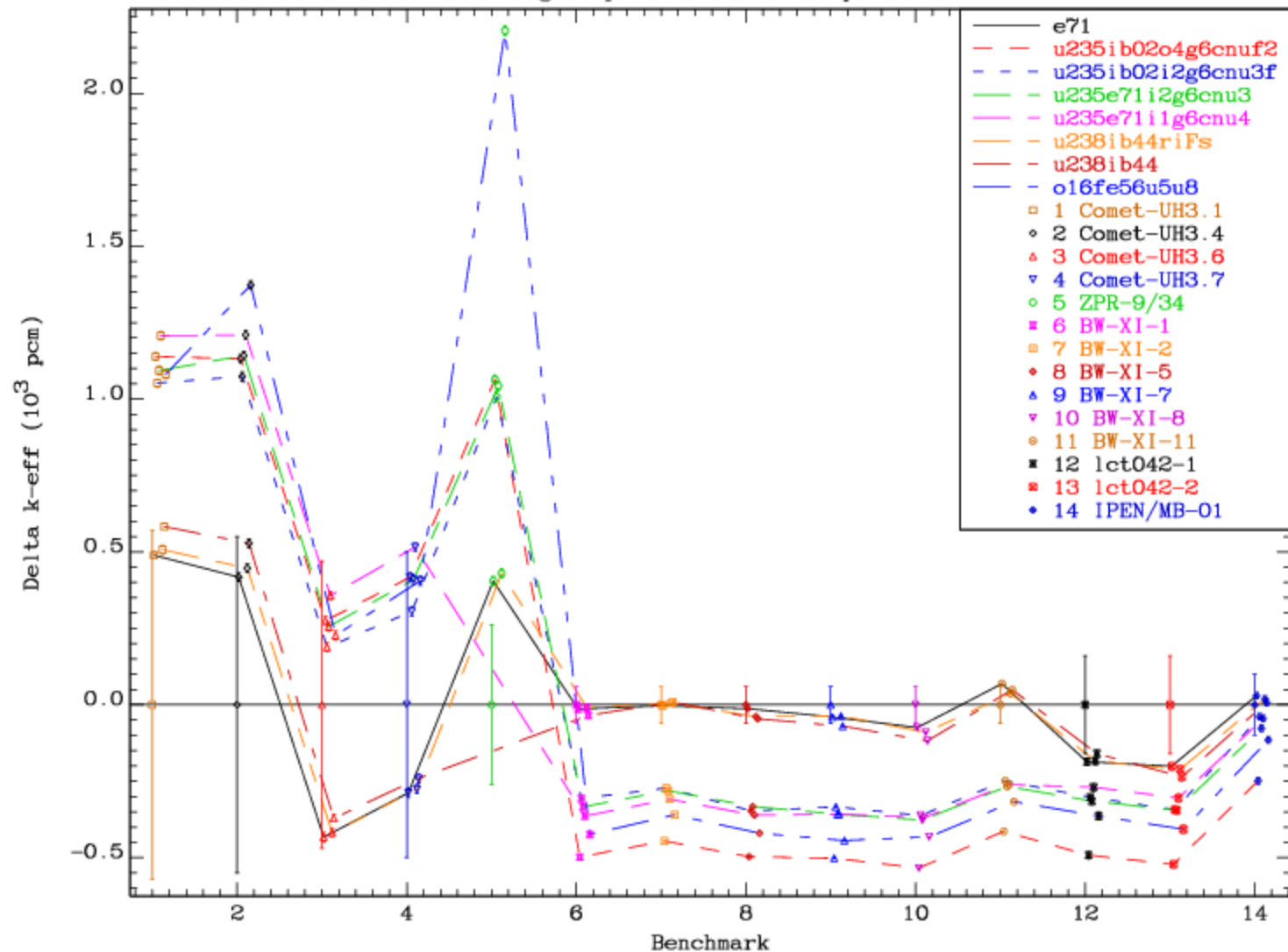
A few surprises?

- UH3 benchmarks show large positive reactivity swing (reason yet unknown)
- ZPR-9/34 is sensitive to capture in ^{235}U as well as capture in Fe
- Thermal lattices are underpredicted
- Compensating effect between materials are very important

Outliers

ICSBEP name	Short name	Common name
HEU-COMP-INTER-003	hci003-1	COMET-UH3-1
HEU-COMP-INTER-003	hci003-4	COMET-UH3-4
HEU-COMP-INTER-003	hci003-6	COMET-UH3-6
HEU-COMP-INTER-003	hci003-7	COMET-UH3-7
HEU-MET-INTER-001	hmi001	ZPR-9/34
LEU-COMP-THERM-008	lct008-01	BW-XI-1
LEU-COMP-THERM-008	lct008-02	BW-XI-2
LEU-COMP-THERM-008	lct008-05	BW-XI-5
LEU-COMP-THERM-008	lct008-07	BW-XI-7
LEU-COMP-THERM-008	lct008-08	BW-XI-8
LEU-COMP-THERM-008	lct008-11	BW-XI-11
LEU-COMP-THERM-042	lct042-1	lct042-1
LEU-COMP-THERM-042	lct042-2	lct042-2
LEU-COMP-THERM-043	lct043-2	IPEN/MB-01

ICSBEP Benchmark Summary Results
Integral parameter intercomparison



^{56}Fe – Evaluation features

- “ib04s”
 - Empire calculation Version 4 in the fast energy range
 - ORNL resonance parameters Version 4 up to 2 MeV
 - Smoothed angular from resonance parameters
- “c88”
 - Empire calculation in the fast energy range
 - Updated resonance parameters, reduced to 846 keV
 - JENDL-4.0 angular distributions in the resonance range
 - Cross sections and ang. distr. Up to 2 MeV from JEFF-3.2
- Another updated set of resonance data available, but not tested.

^{56}Fe - Criticality Benchmarks (ICSBEP)

- Benchmarks most sensitive to Fe capture and scattering, respectively
- UH3 benchmarks sensitive to capture and scattering

Benchmarks sensitive to ^{56}Fe capture

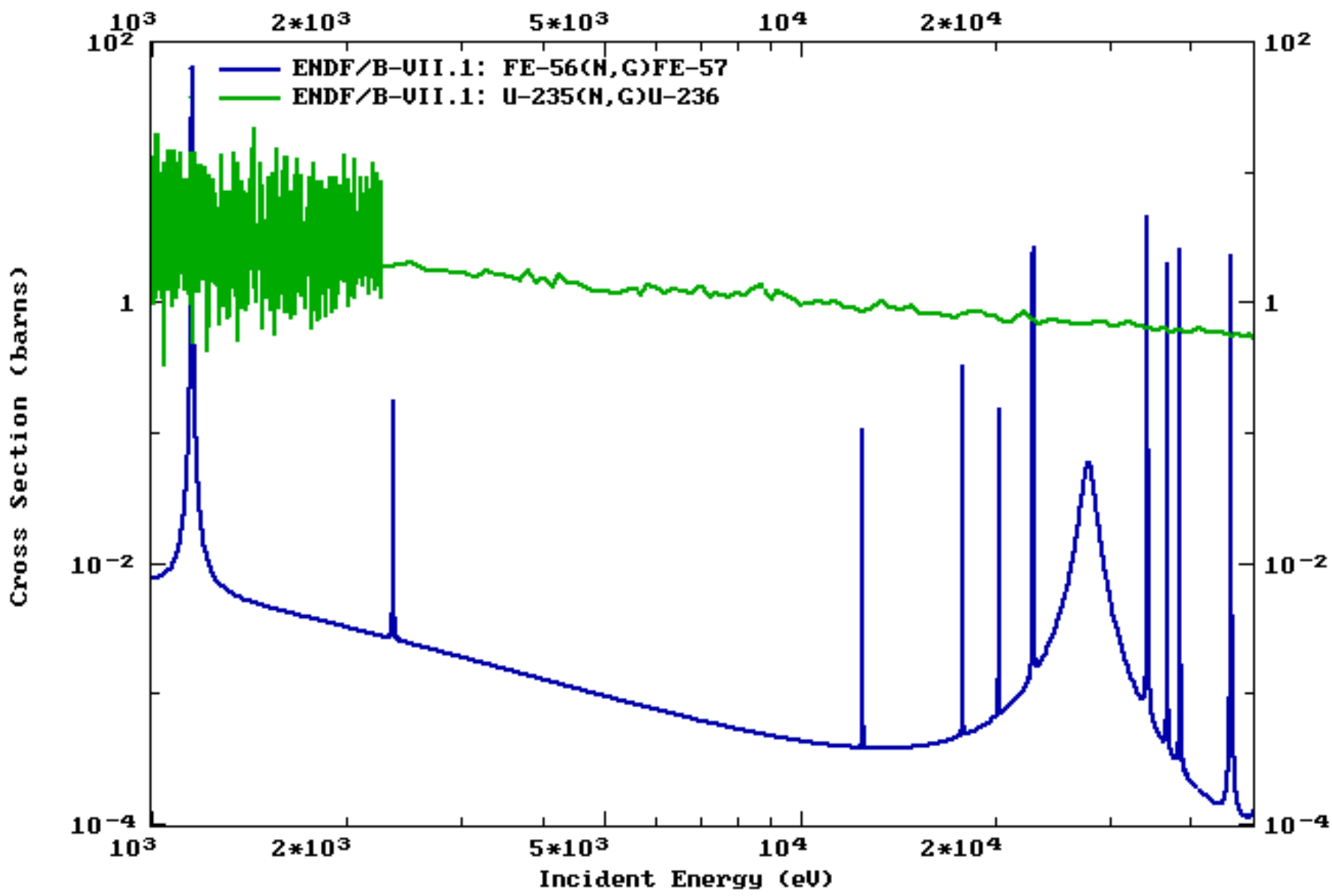
ICSBEP name	Short name	Common name
MIX-COMP-FAST-001	mcf001	ZPR-6/7
MIX-COMP-FAST-006	mcf006-s	ZPPR-2
MIX-COMP-FAST-005	mcf005	ZPR-9/31
MIX-COMP-FAST-005	mcf005-s	ZPR-9/31
IEU-COMP-INTER-005	ici005	ZPR-6/6A
HEU-MET-FAST-072	hmf072-1	ZEUS_Fe/Cu-1
HEU-MET-FAST-072	hmf072-3	ZEUS_Fe/Cu-3
IEU-MET-FAST-012	imf012	ZPR-3/41
MIX-MISC-FAST-002	mif002-1	BFS-49/1A
MIX-MISC-FAST-001	mif001-01	BFS-35-1
MIX-MISC-FAST-001	mif001-02	BFS-35-2
MIX-MISC-FAST-001	mif001-03	BFS-35-3
MIX-MISC-FAST-001	mif001-09	BFS-31-4
MIX-MISC-FAST-001	mif001-10	BFS-31-5
MIX-MISC-FAST-001	mif001-11	BFS-42
IEU-MET-FAST-010	imf010	ZPR-6/9 (U9)

Benchmarks sensitive to ^{56}Fe scattering

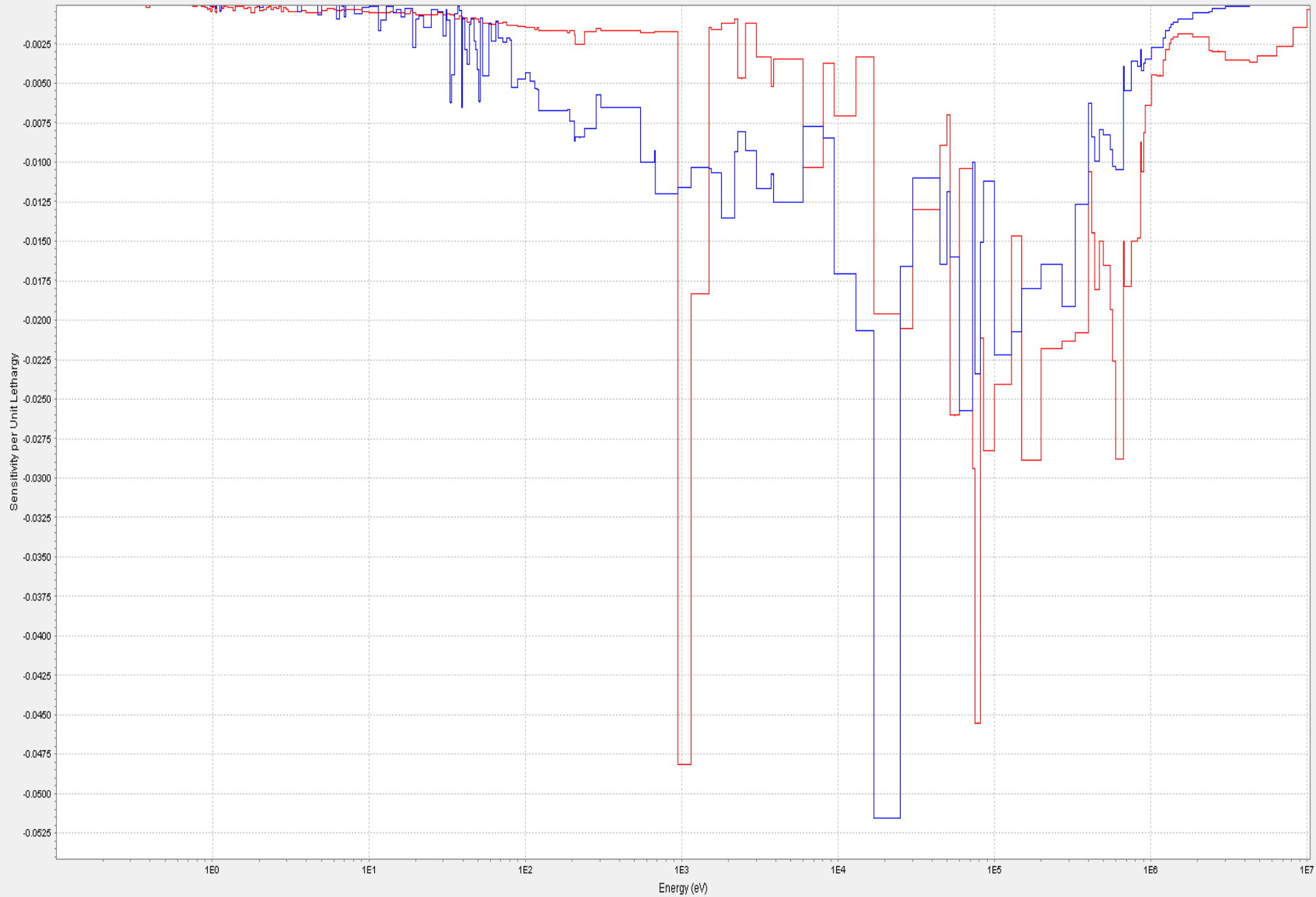
ICSBEP name	Short name	Common name
PU-MET-FAST-026	pmf026	pmf026
HEU-MET-FAST-061	hmf061	ZPPR-21F
PU-MET-FAST-033	pmf033	ZPPR-21A
HEU-MET-FAST-088	hmf088-1	hmf088-1
HEU-MET-FAST-088	hmf088-2	hmf088-2
PU-MET-FAST-025	pmf025	pmf025
HEU-MET-FAST-087	hmf087	VNIITF-CTF-Fe
HEU-COMP-INTER-003	hci003-1	COMET-UH3-1
HEU-COMP-INTER-003	hci003-4	COMET-UH3-4
HEU-COMP-INTER-003	hci003-6	COMET-UH3-6
HEU-COMP-INTER-003	hci003-7	COMET-UH3-7
HEU-MET-FAST-072	hmf072-1	ZEUS_Fe/Cu-1
HEU-MET-FAST-072	hmf072-3	ZEUS_Fe/Cu-3
HEU-MET-FAST-084	hmf084-14	Comet-W_1.0in
HEU-MET-FAST-084	hmf084-25	Comet-W_0.5in

Benchmarks sensitive to ^{56}Fe scattering

ICSBEP name	Short name	Common name
PU-MET-FAST-032	pmf032	pmf032
HEU-MET-FAST-013	hmf013	VNIITF-CTF-SS-13
IEU-MET-FAST-005	imf005	VNIIEF-CTF-5
IEU-MET-FAST-005	imf005-s	VNIIEF-CTF-5s
HEU-MET-FAST-021	hmf021	VNIITF-CTF-SS-21
HEU-MET-FAST-085	hmf085-5	Comet-Th_2in
PU-MET-FAST-028	pmf028	pmf028
PU-MET-FAST-026	pmf026	pmf026

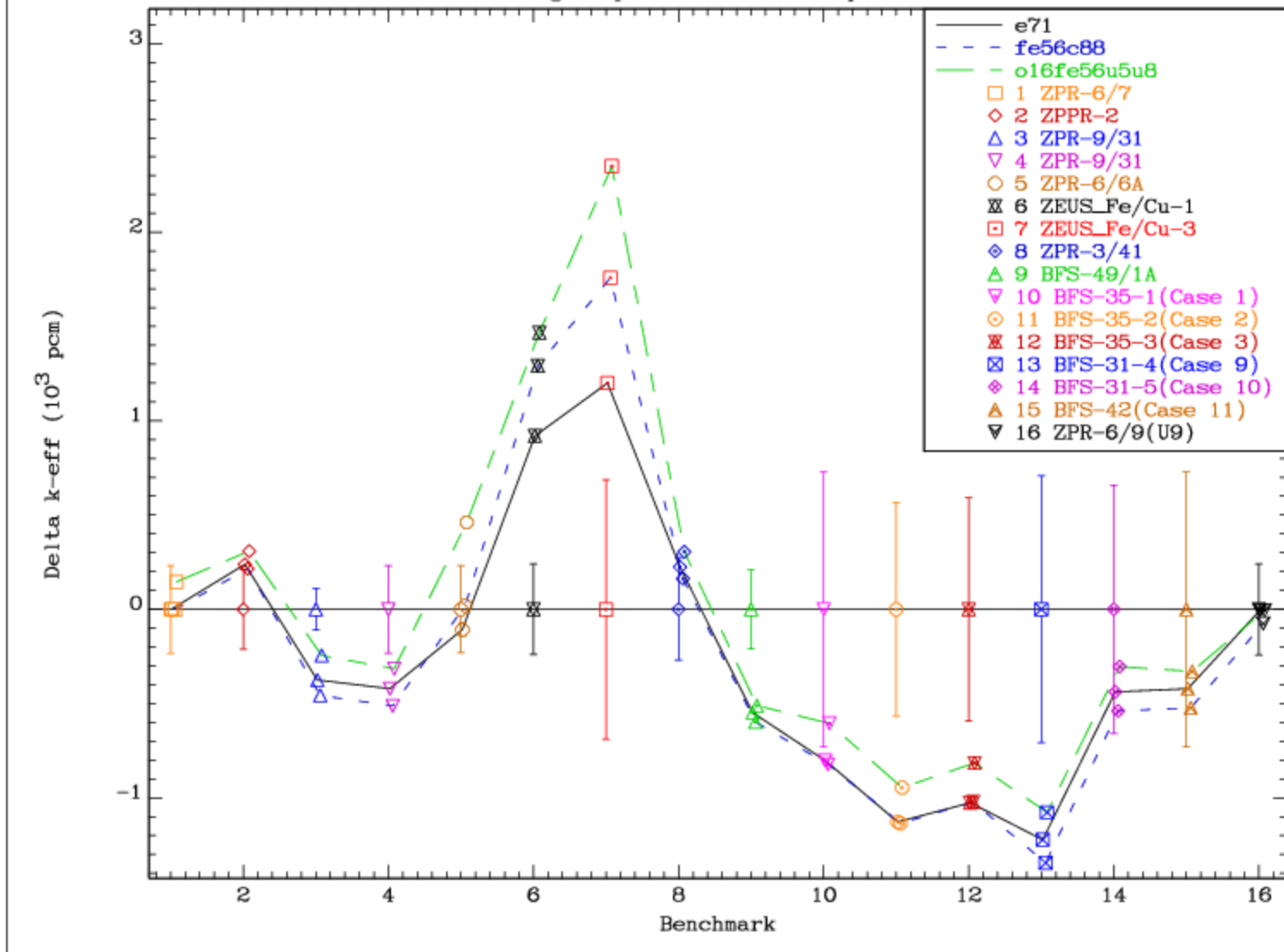


Sensitivity Plot

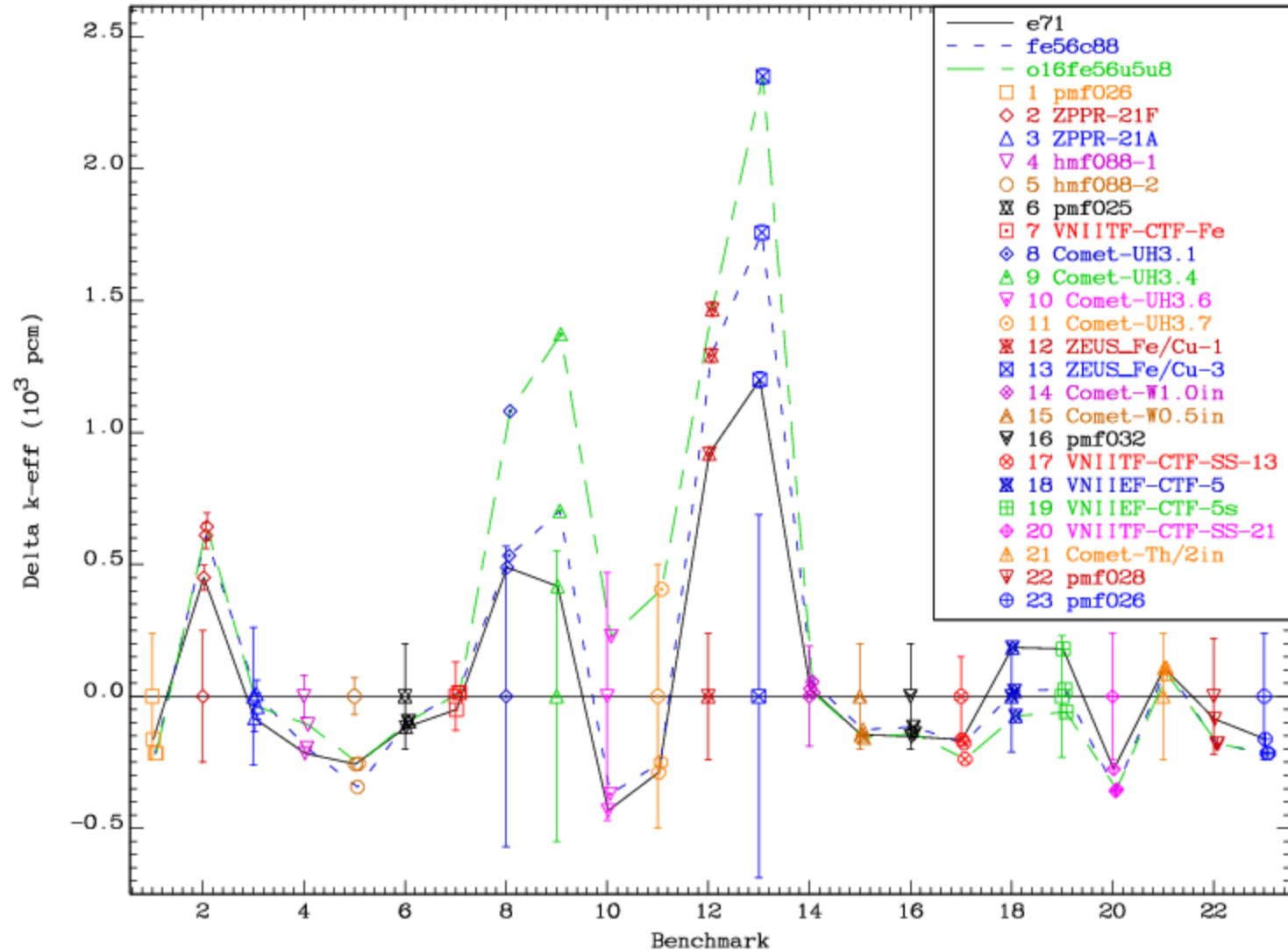


— HEU-MET-INTER-001-001 capture u-235 — HEU-MET-INTER-001-001 capture fe-0

ICSBEP Benchmark Summary Results
Integral parameter intercomparison



ICSBEP Benchmark Summary Results
Integral parameter intercomparison



^{56}Fe - Shielding benchmarks (SINBAD)

Evaluations taken into consideration:

- Basis file: ENDF/B-VII.1
- CIELO project intermediate files:
 - Ib04s, Ib88
- C/E comparison
- Calculations performed with MCNP v6.1
- Default libraries:
 - ENDF/B-VII.1 (transport), IRDFF v1.05 (dosimetry)

^{56}Fe - Shielding benchmarks (cont.)

SINBAD benchmarks sensitive to Fe:

- EURACOS Fe (abs.+rel. C/E comparison)
- ASPIS:
 - JANUS-1 (rel.)
 - NESDIP-2
 - NESDIP-3 (rel.)
- IPPE Fe spheres
- OKTAVIAN Fe
- ...

General Features of EURACOS Fe

- TRIGA thermal column n. source, converted to fast by fission plate
- Attenuation in Fe
- Reaction rate axial distributions (as a function of depth in Fe):
 - $^{32}\text{S}(n,p)$
 - $^{197}\text{Au}(n,\gamma)$ under Cd
 - $^{103}\text{Rh}(n,n')$ - *measurements normalized to the first value*
 - $^{115}\text{In}(n,n')$
- Experimental uncertainties:
 - Source (spectrum and spatial distribution)
 - Room return

EURACOS MCNP model (recent progress)

- Re-definition of the neutron source
- Improved variance reduction techniques
- Sensitivity study:
 - Source fission spectrum
 - Source positioning (in fission plate, before the fission plate, . . .)
 - Source (radial) distribution
 - Impurities in Fe
- Modelling of new activation detectors
- Neutron spectra calculations

Experimental setup

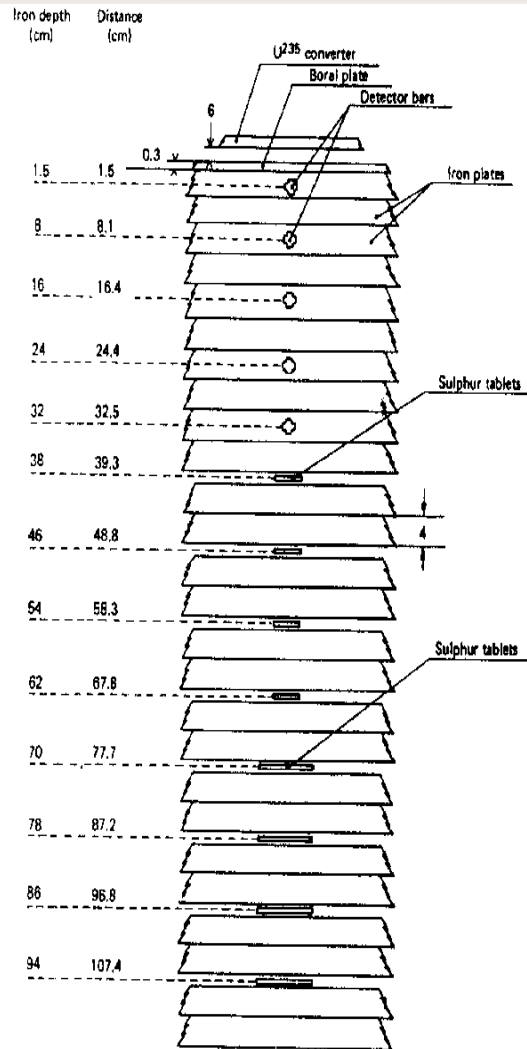


Fig. 4: SULPHUR DETECTOR POSITIONS IN THE IRON ASSEMBLY

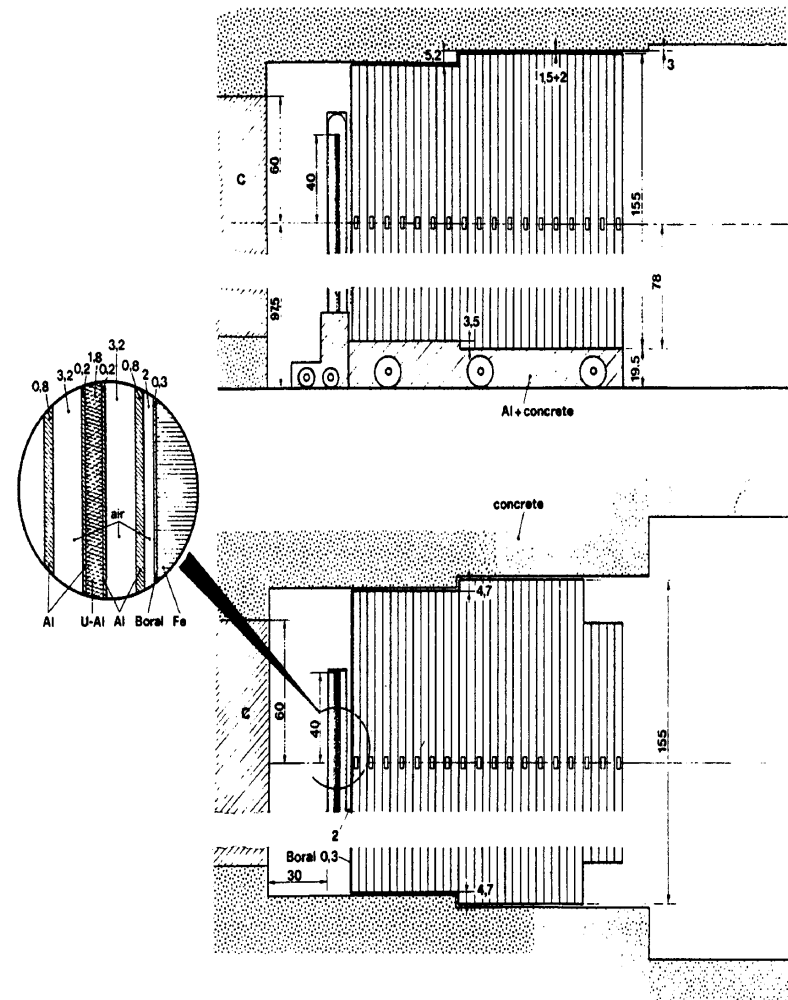
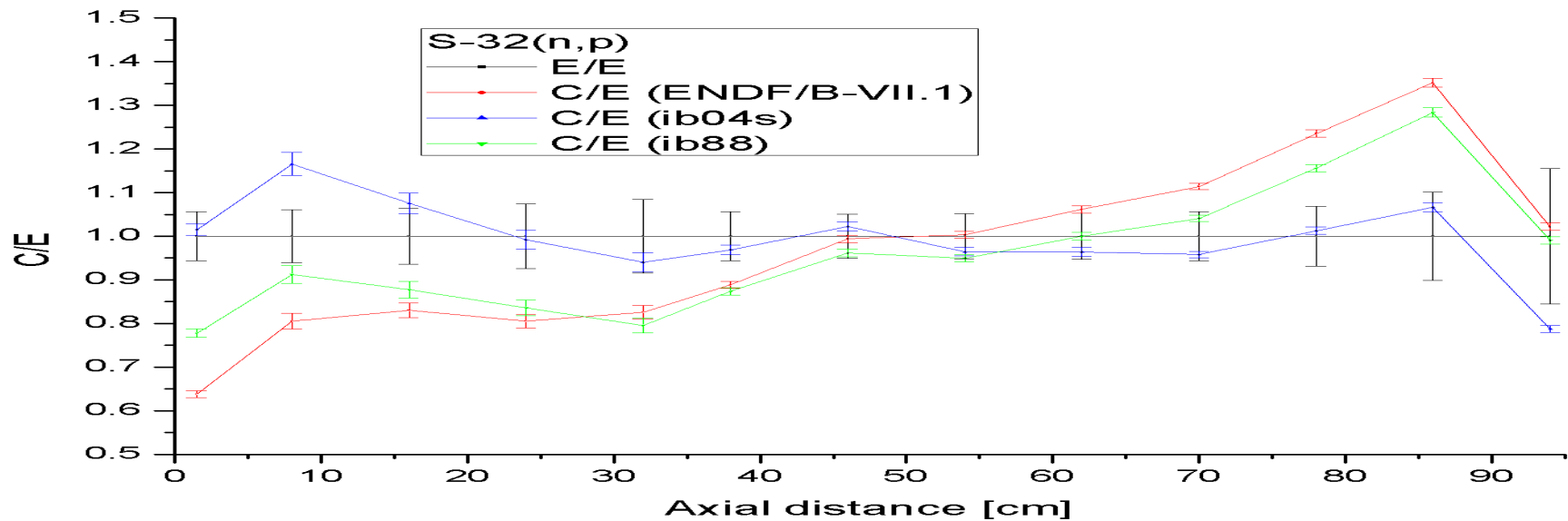
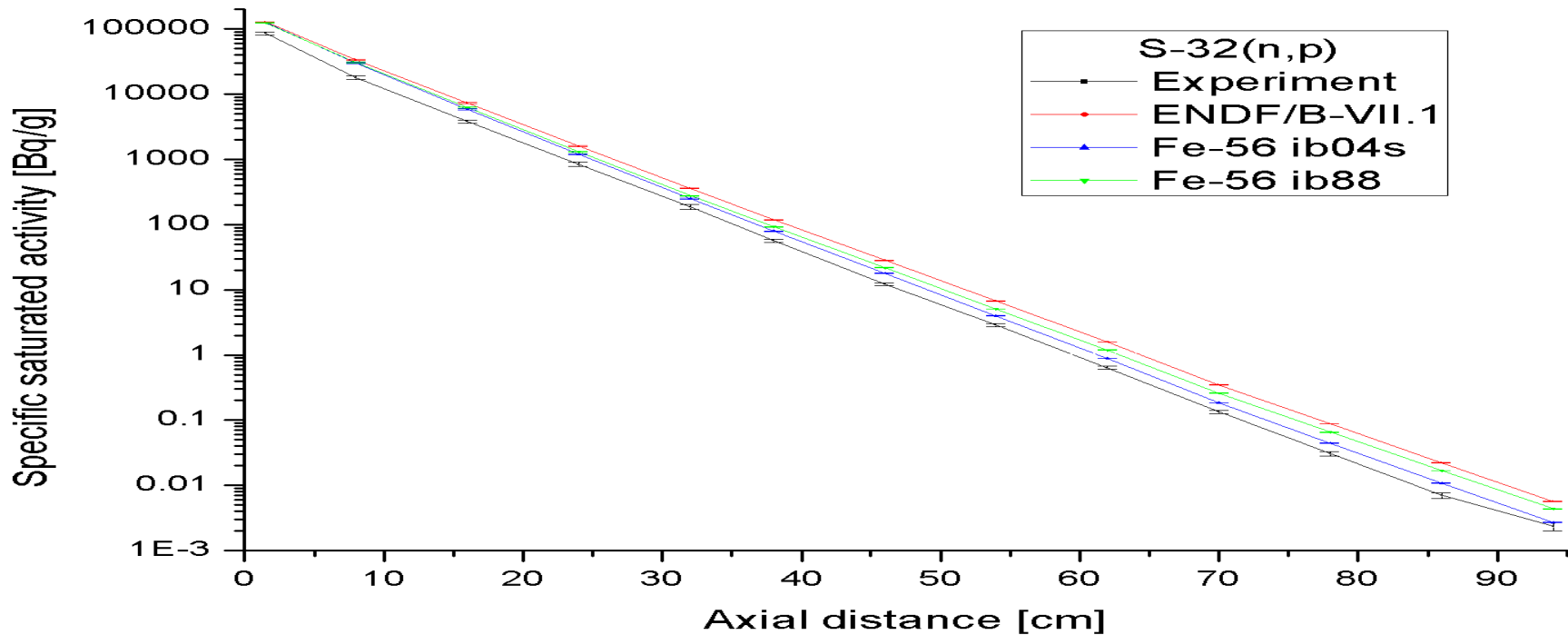
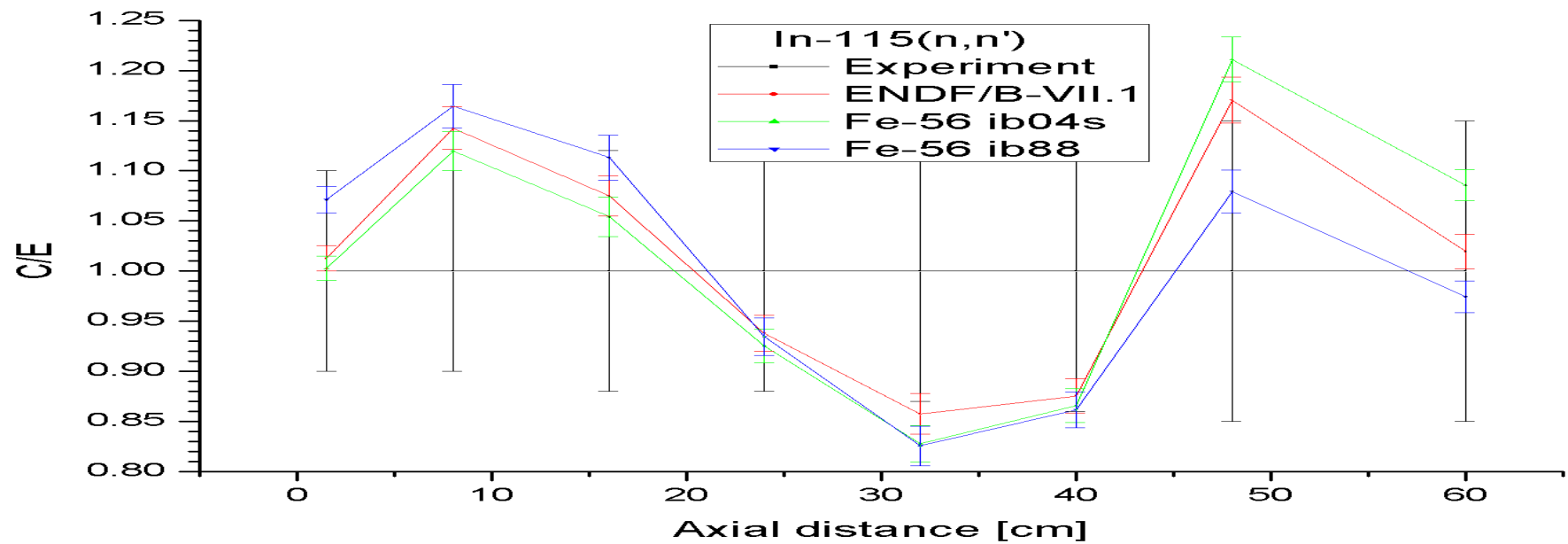
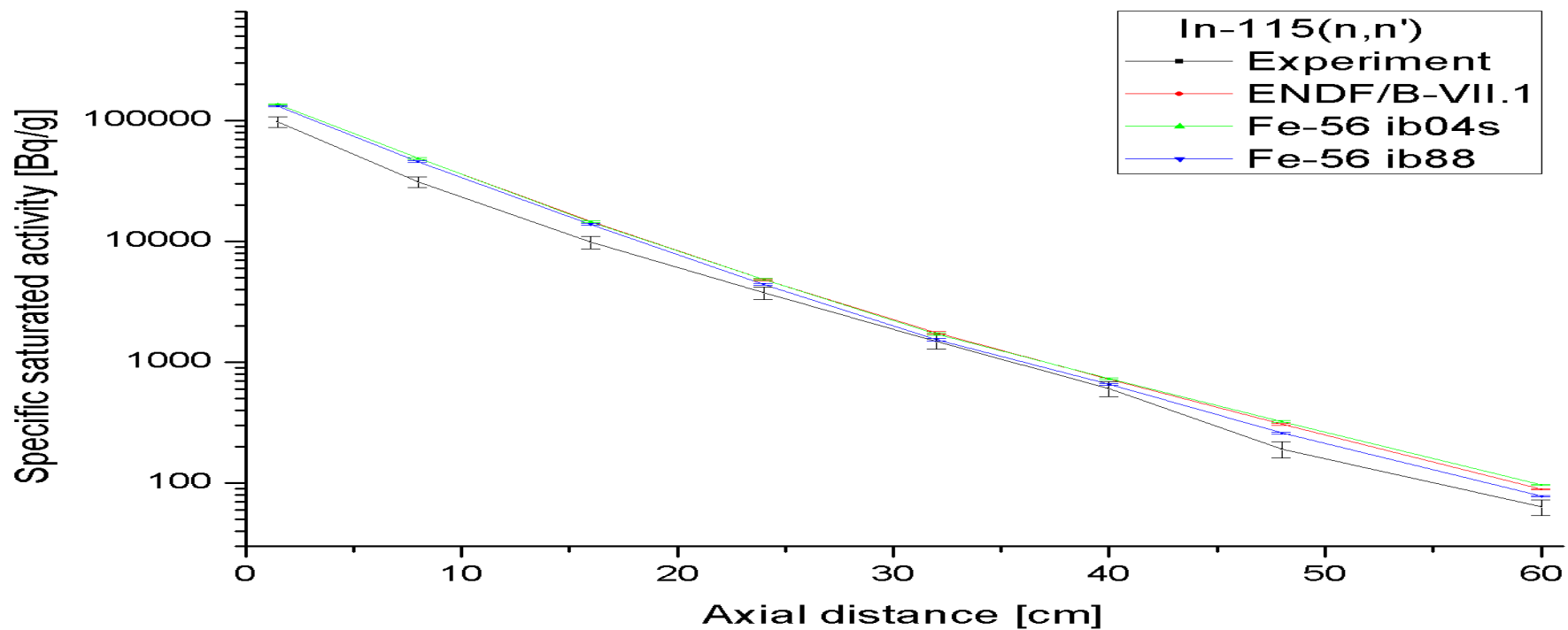
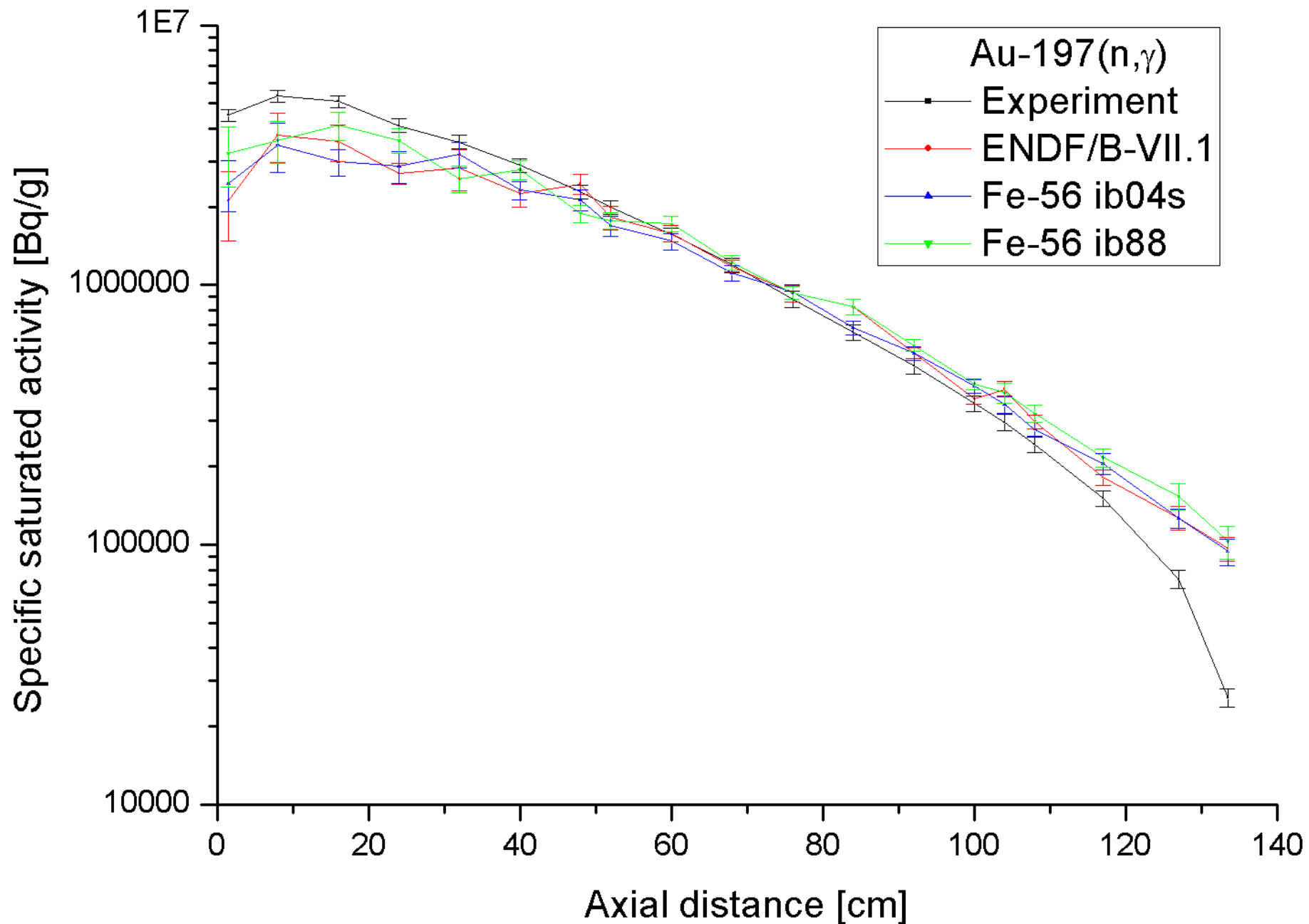


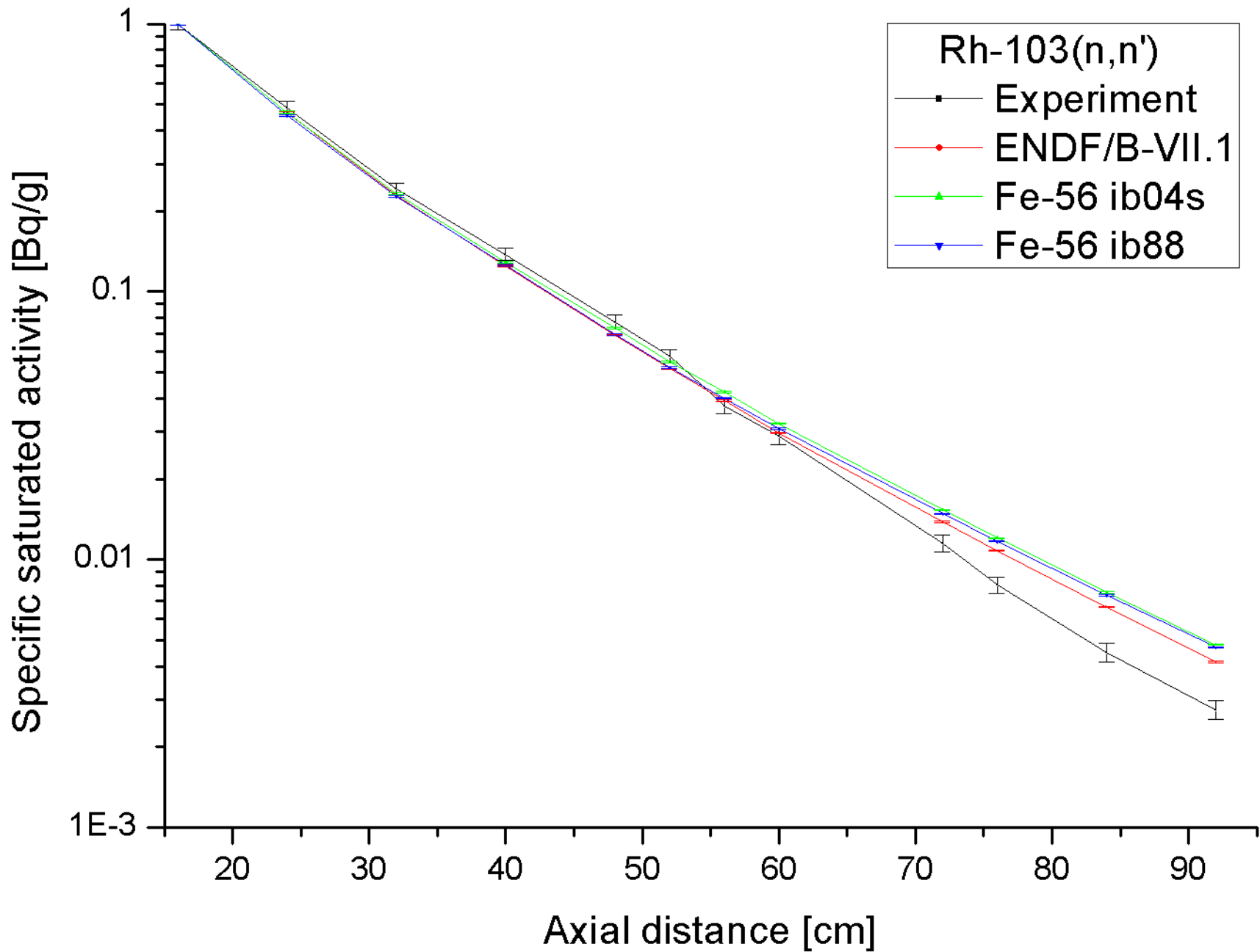
Fig. 2 Vertical and horizontal cross section of iron assembly including the Euracos II facility



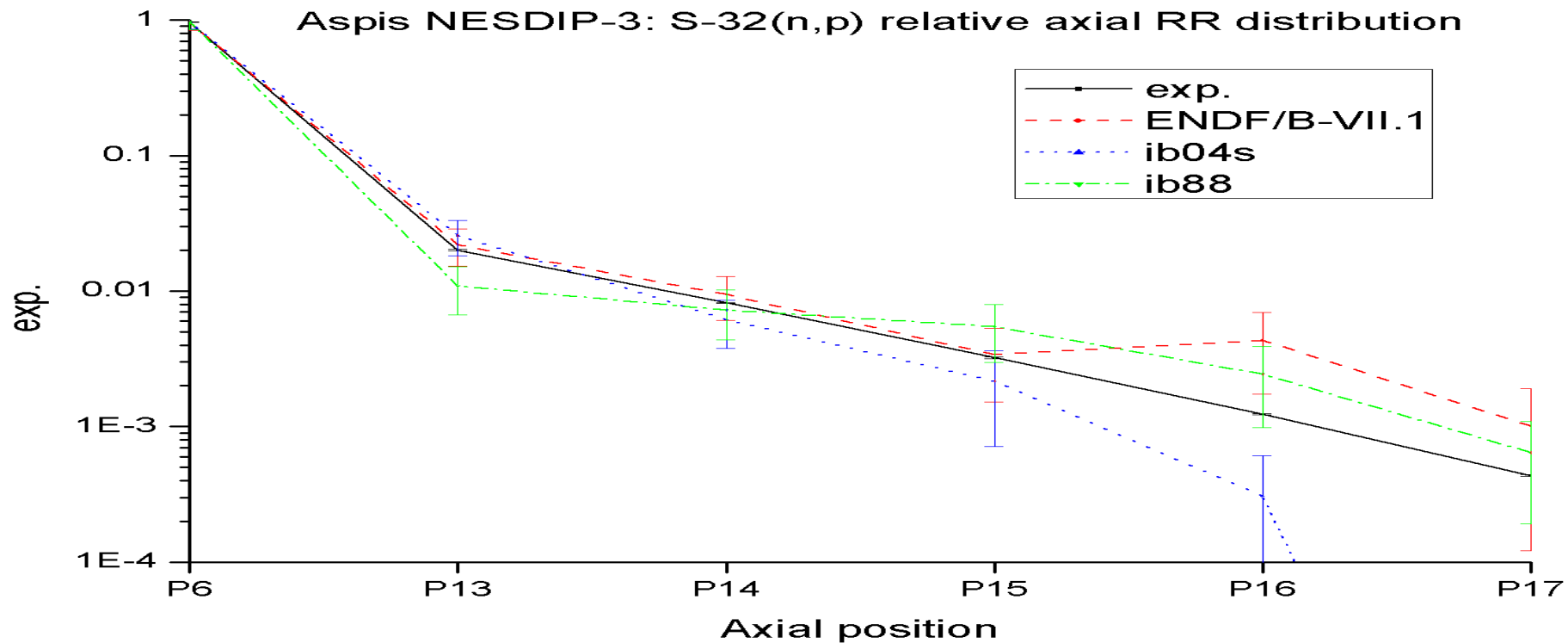




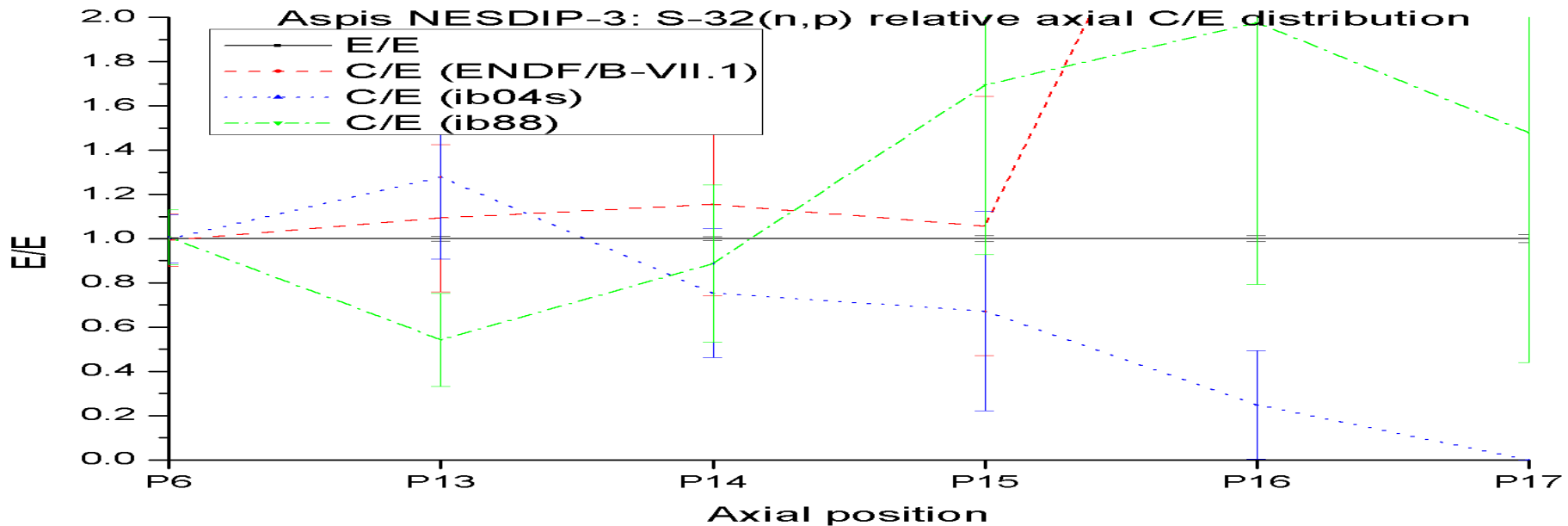




Aspis NESDIP-3: S-32(n,p) relative axial RR distribution



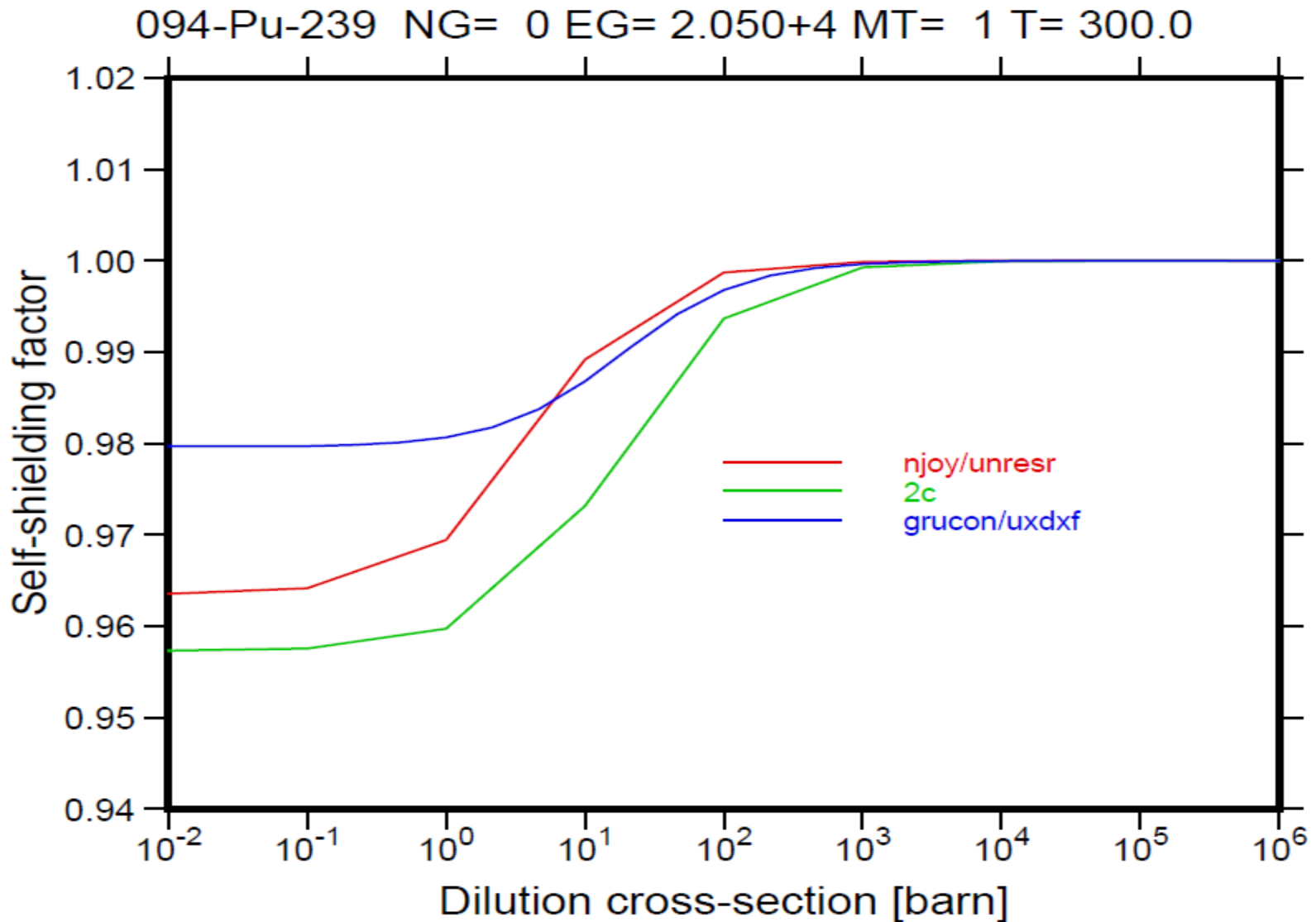
Aspis NESDIP-3: S-32(n,p) relative axial C/E distribution



Data processing

- Practically all benchmarking goes through NJOY processing – potential danger of “common mode failure”
- For example, differences in the self-shielded cross sections calculated with UNRESR and PURR from NJOY and GRUCON...
- There could be more...

Self-shielded cross sections



Summary for ^{238}U

- Evaluation in the fast range is stable; no great changes are expected
- URR evaluation is completed (IRMM)
- RRR evaluation with minor improvements is pending (IRMM)
- Evaluation will be finalised when the ^{235}U evaluation reaches maturity

Summary for ^{235}U

- New PFNS is a large perturbation to the evaluation, requiring extensive changes elsewhere
- Evaluation in the fast energy range can be refined (particularly inelastic)
- Two options for resonance evaluation are under investigation.
- Performance comparable to ENDF/B-VII.1 is achievable, but we want to do better
- There are outliers, which perform worse

Summary for ^{56}Fe

- Evaluation in the fast energy range can be improved (waiting for the release of RPI data), extended to 150 MeV and to the minor isotopes
- Extension of RRR to 2 MeV is challenging
- We are still gaining experience on the use of detailed angular distributions reconstructed from resonance parameters
- The goal of performance better than ENDF/B-VII.1 is not reached yet

Additional benchmarks results for Fe

General Features of ASPIS JANUS-1

- NESTOR graphite reflector n. source, converted by fission plate
- Attenuation in stainless and mild steel
- Reaction rate axial and lateral distributions:
 - $^{32}\text{S}(n,p)$
 - $^{55}\text{Mn}(n,\gamma)$ under Cd
 - $^{197}\text{Au}(n,\gamma)$ under Cd
 - $^{103}\text{Rh}(n,n')$
- For lateral distributions, no exp. unc. given!

Measurement positions

Figure 2
Schematic Side Elevation of the Experimental Shield of the JANUS Phase 1 in the ASPIS Trolley

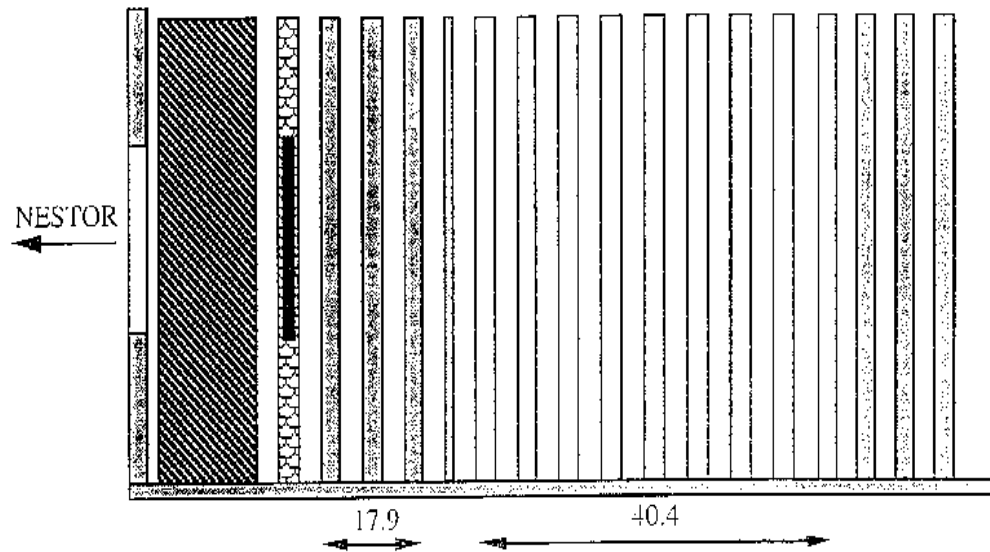
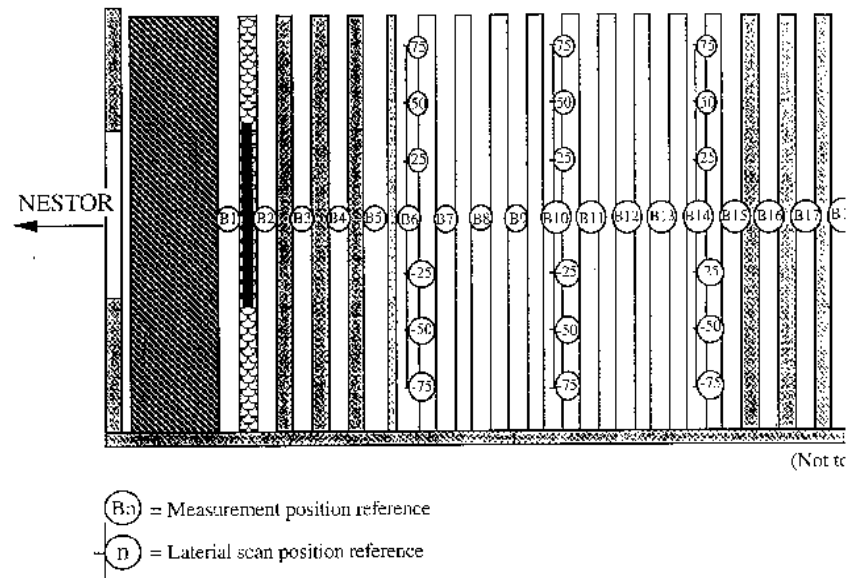
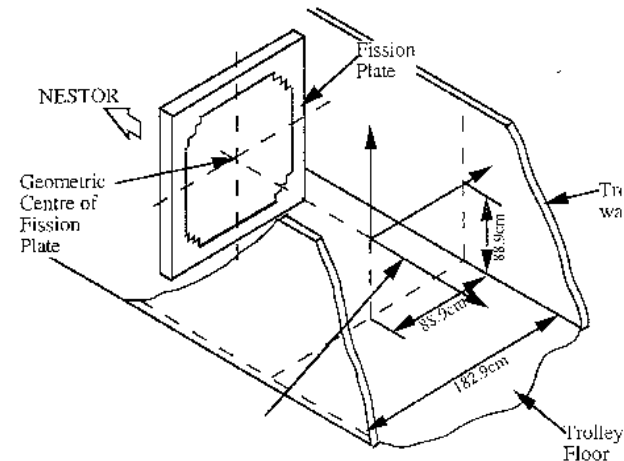








Figure 9
Measurement Locations for JANUS phase 1



Penetration measurements are located on the nuclear centre line as defined below



KEY

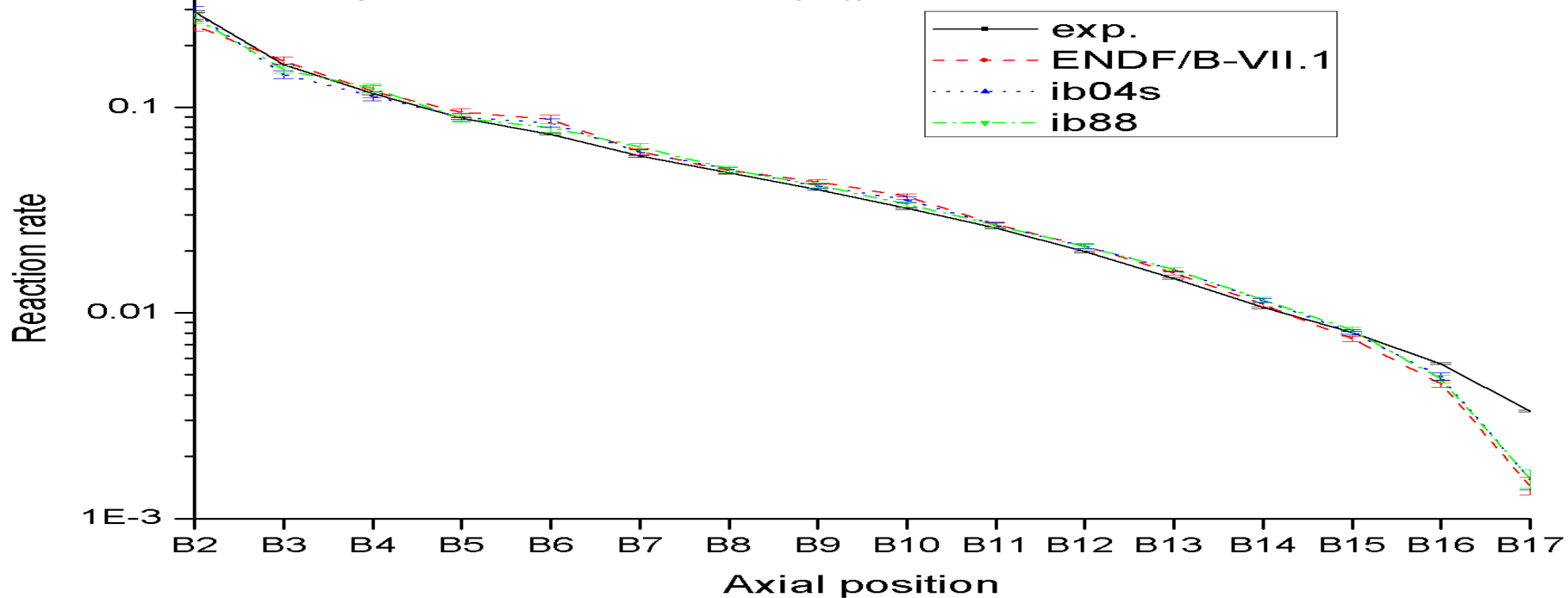
-  Fuel
-  Mild Steel
-  Stainless Steel
-  Fission Plate
-  Graphite
-  Aluminium

All components are 182.9cm wide by 191.0cm high

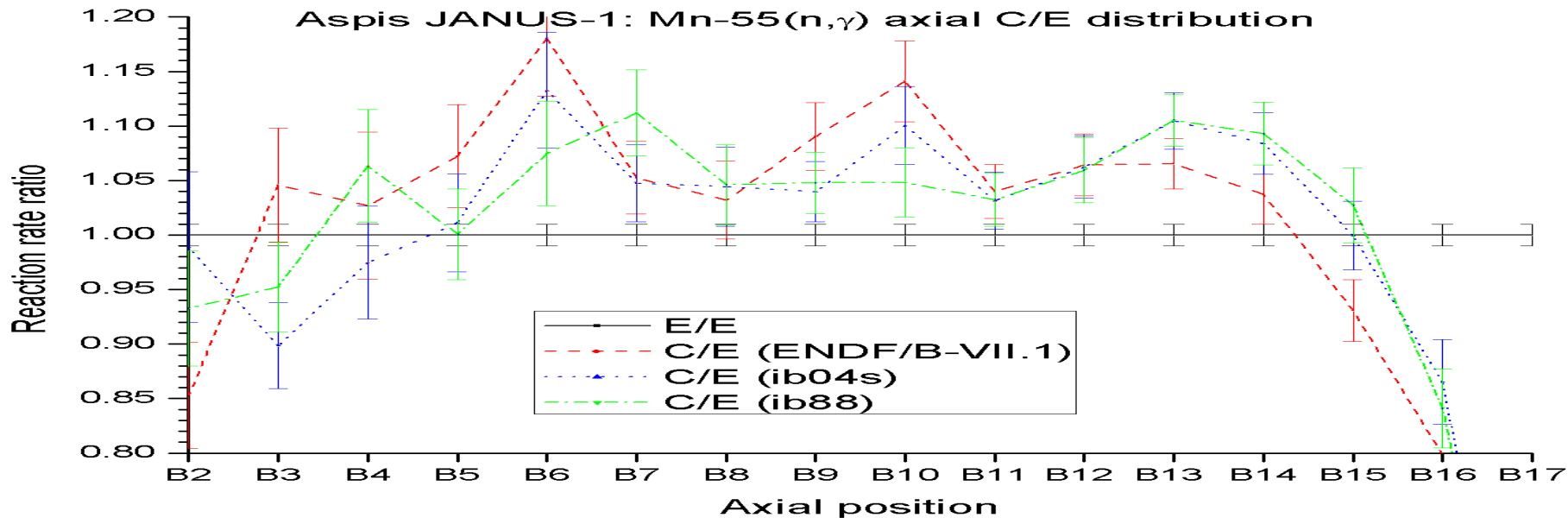
Dimensions Represent Nominal Material Thicknesses in cm

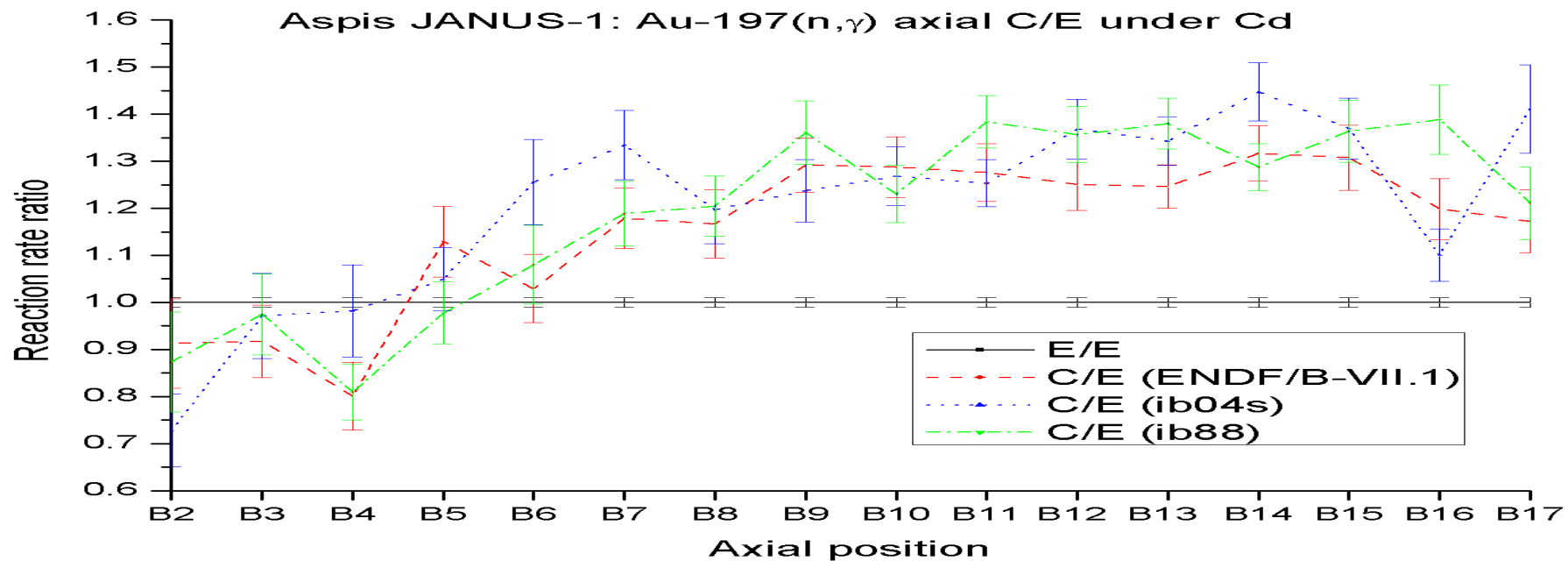
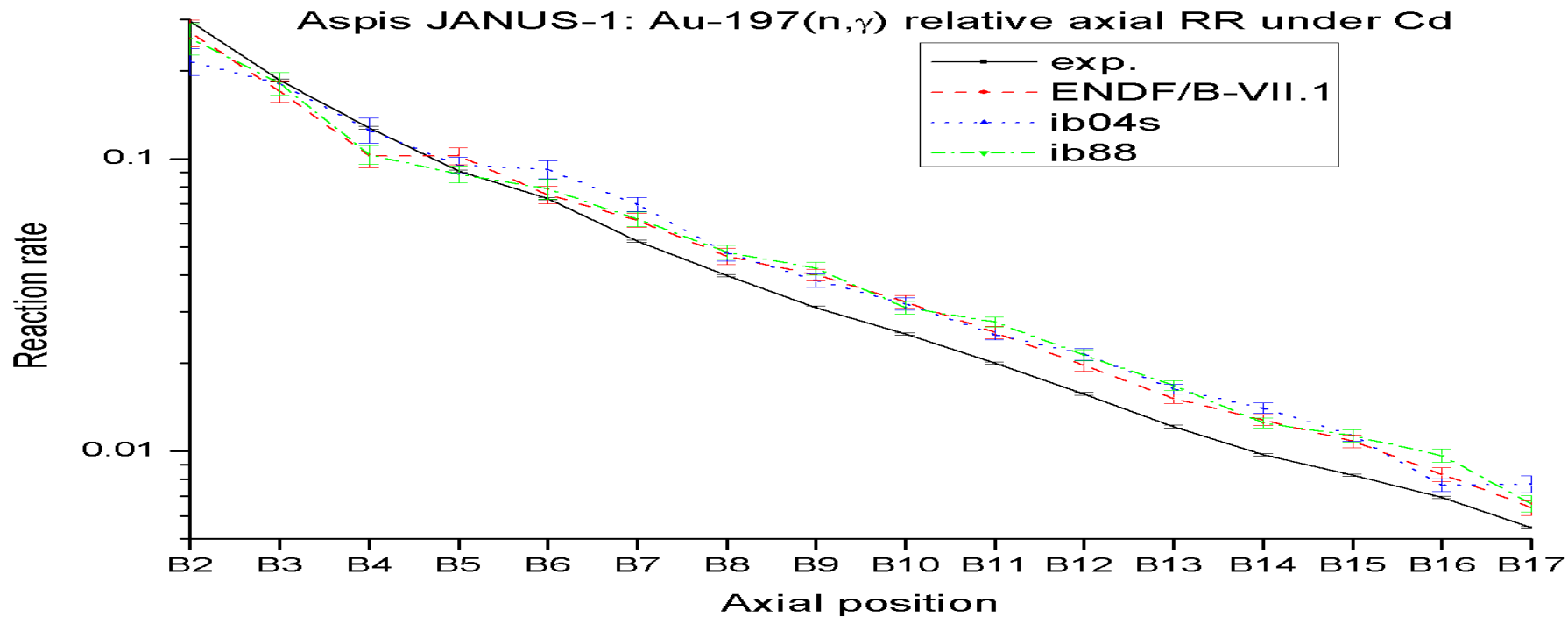
Not To Scale

Aspis JANUS-1: Mn-55(n, γ) relative axial RR distribution

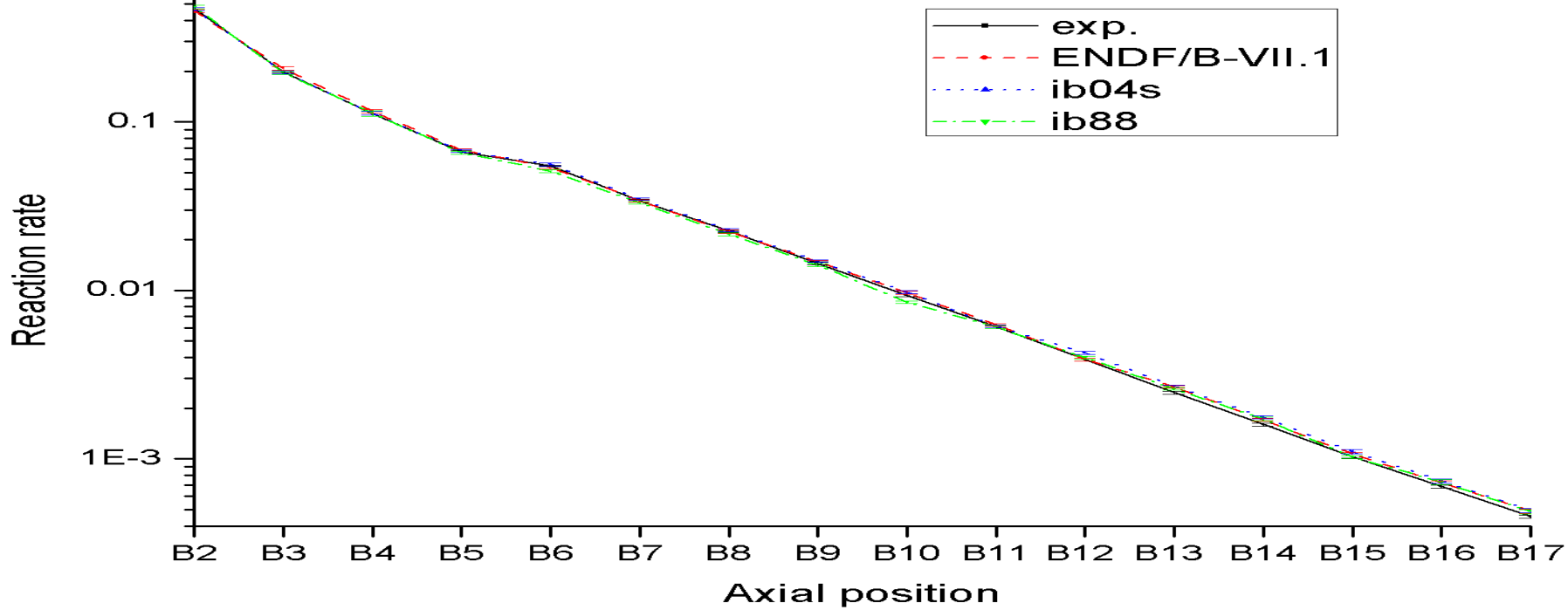


Aspis JANUS-1: Mn-55(n, γ) axial C/E distribution

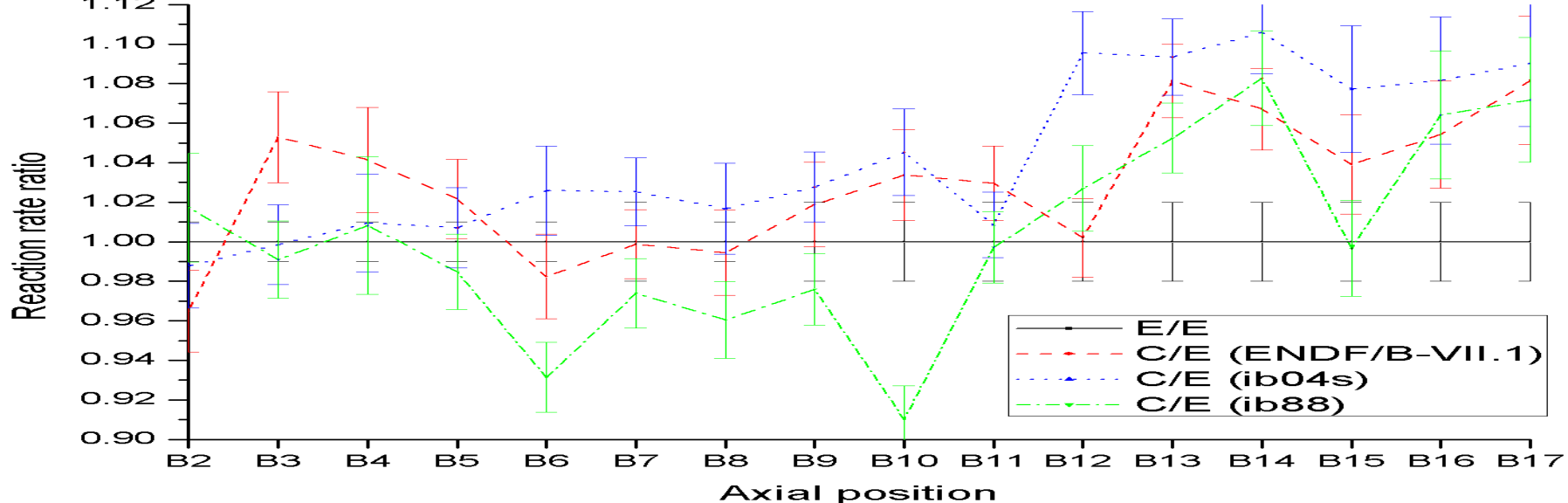




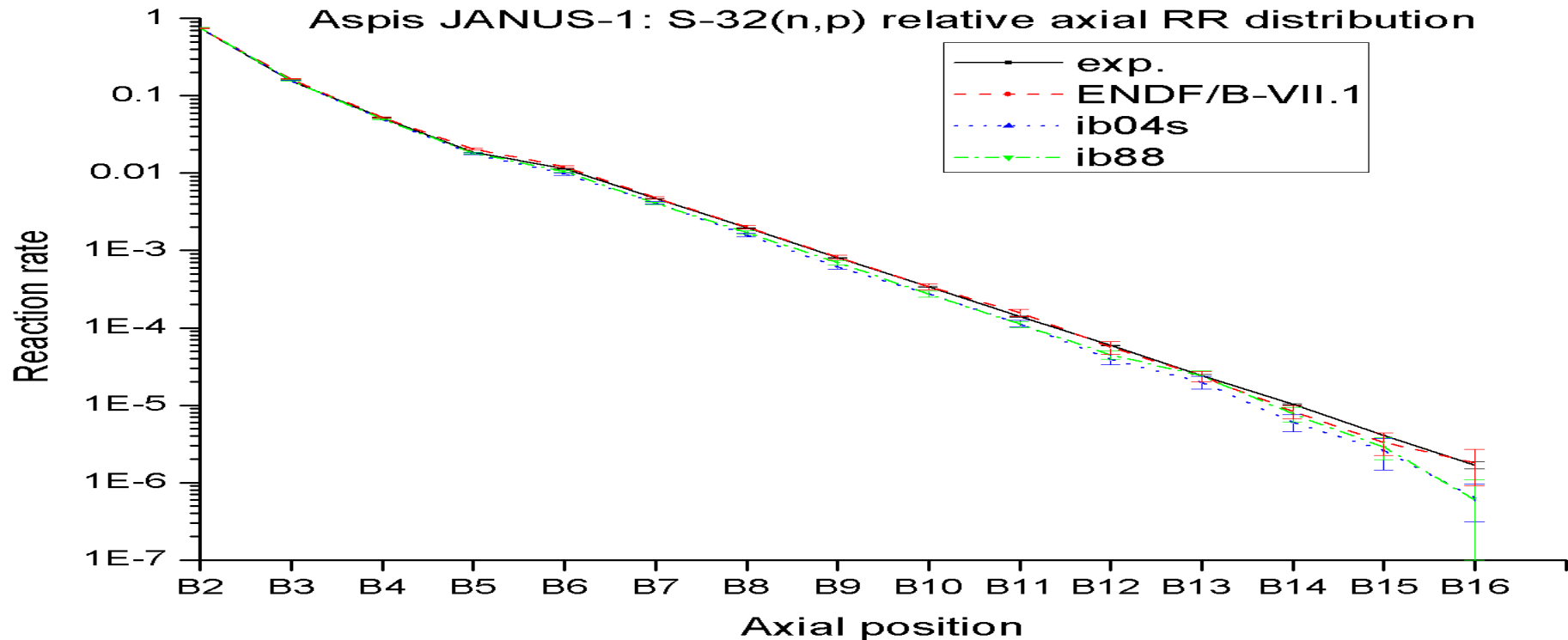
Aspis JANUS-1: Rh-103(n,n') relative axial RR distribution



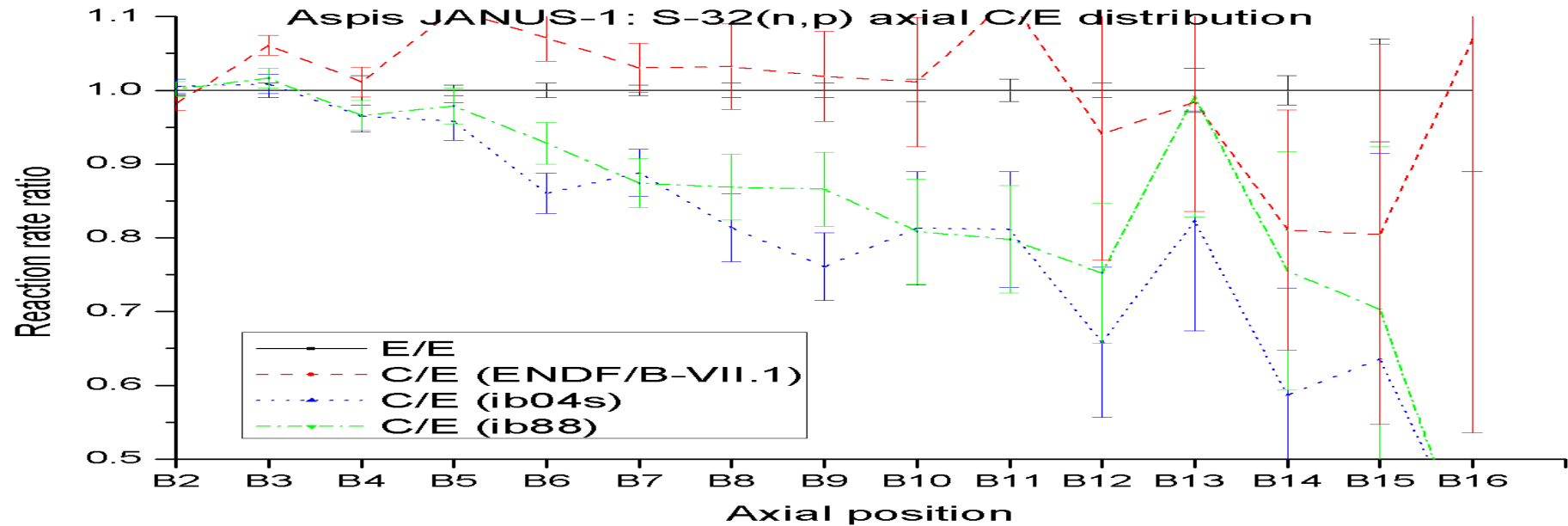
Aspis JANUS-1: Rh-103(n,n') axial C/E distribution



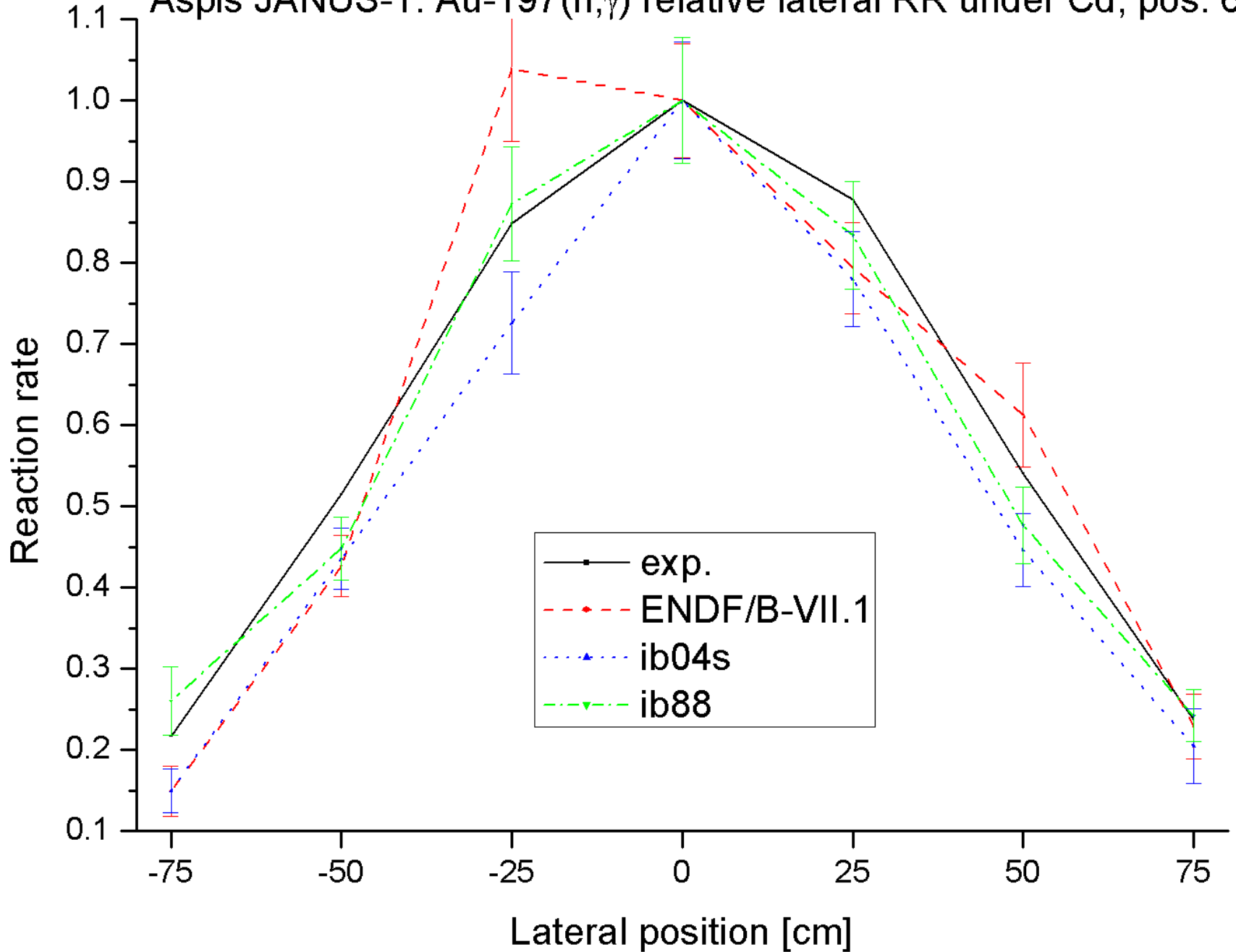
Aspis JANUS-1: S-32(n,p) relative axial RR distribution



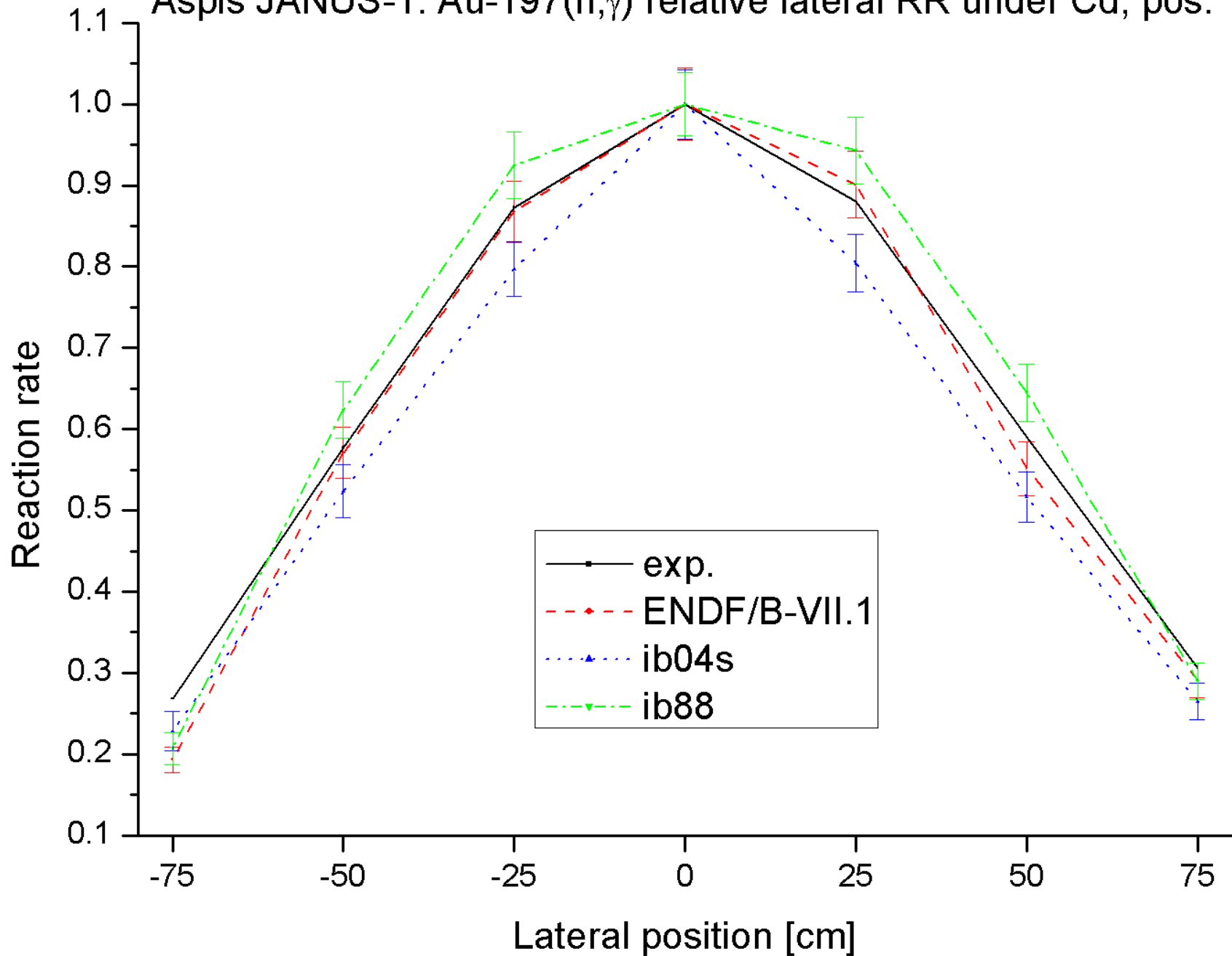
Aspis JANUS-1: S-32(n,p) axial C/E distribution



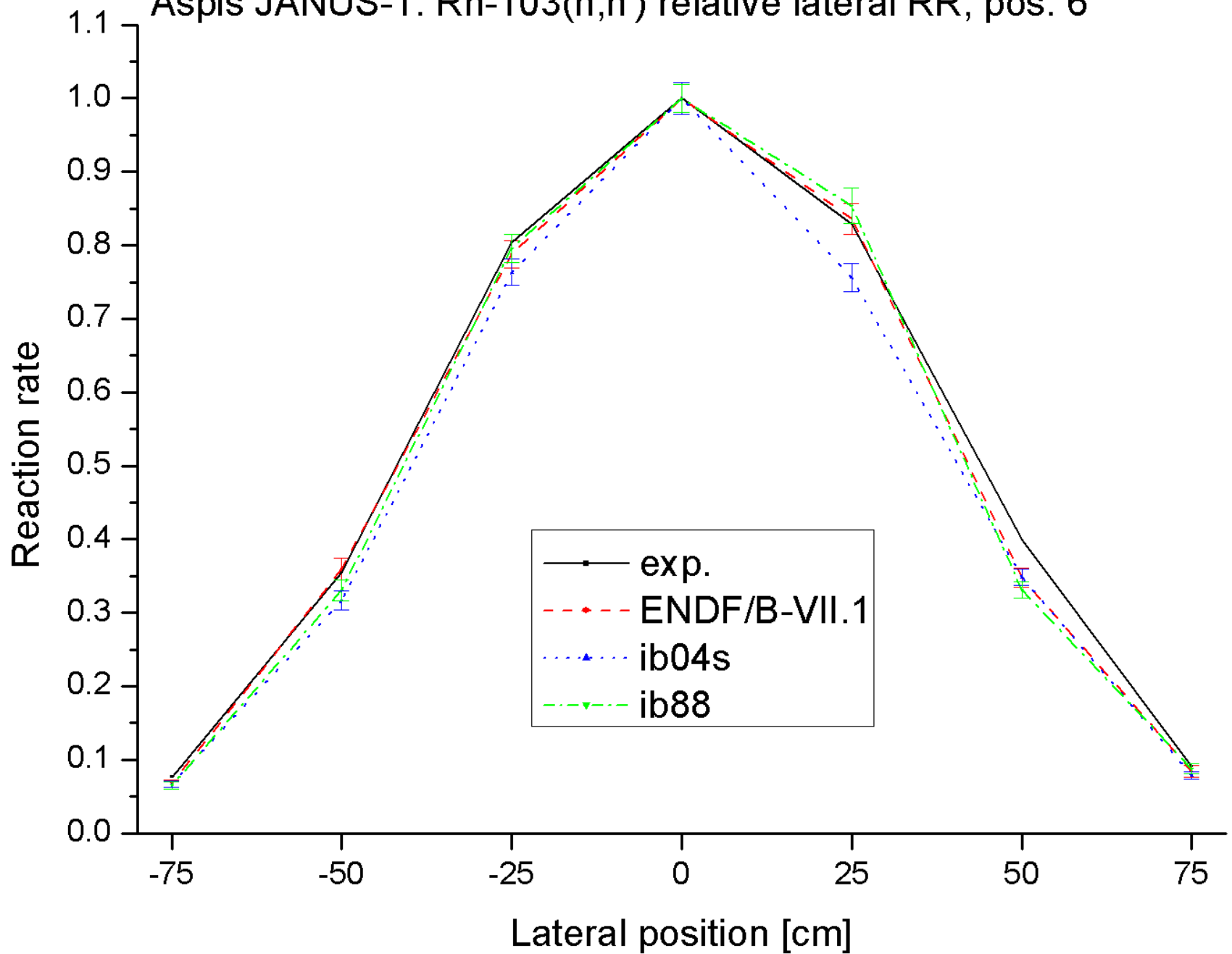
Aspis JANUS-1: Au-197(n, γ) relative lateral RR under Cd, pos. 6



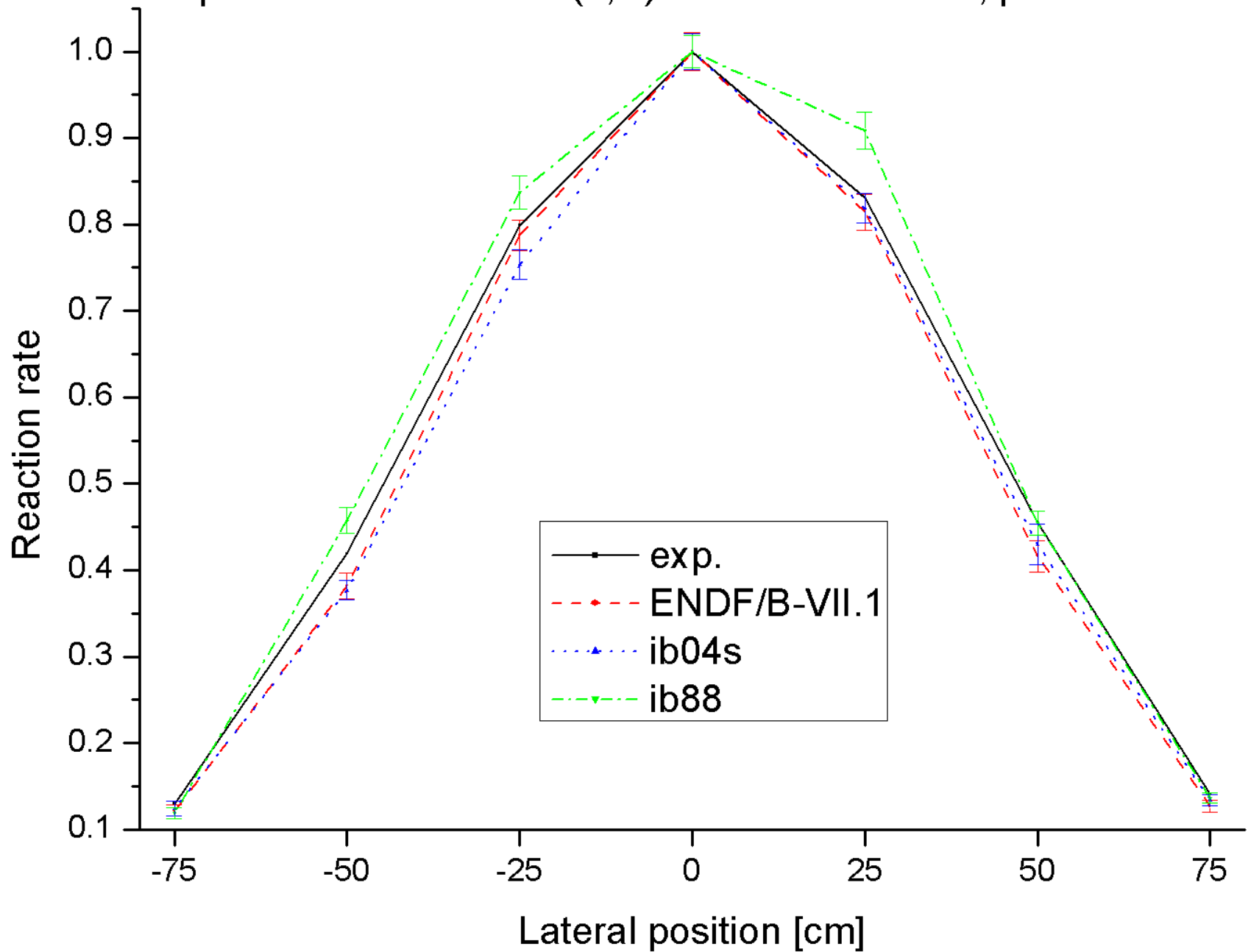
Aspis JANUS-1: Au-197(n, γ) relative lateral RR under Cd, pos. 14



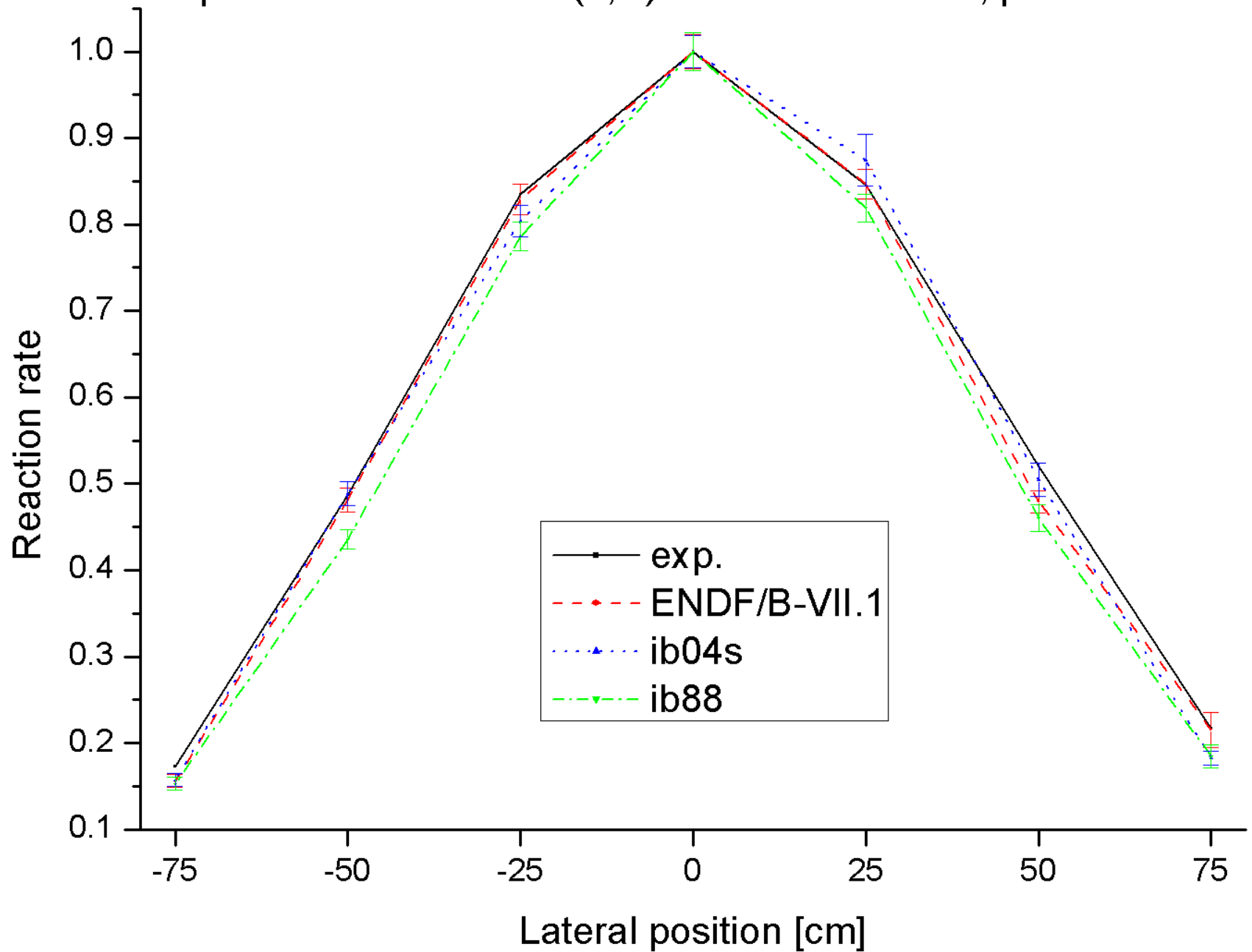
Aspis JANUS-1: Rh-103(n,n') relative lateral RR, pos. 6



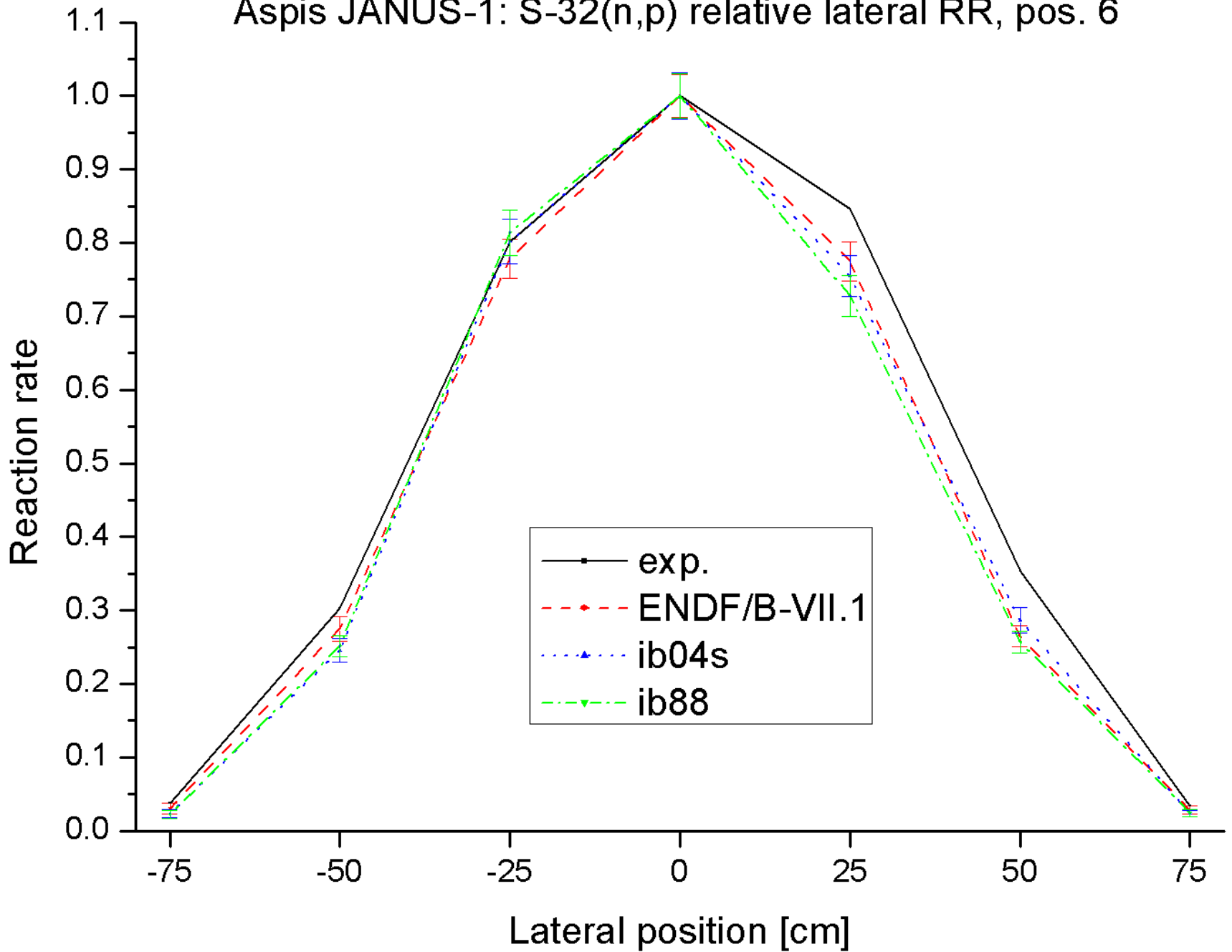
Aspis JANUS-1: Rh-103(n,n') relative lateral RR, pos. 10



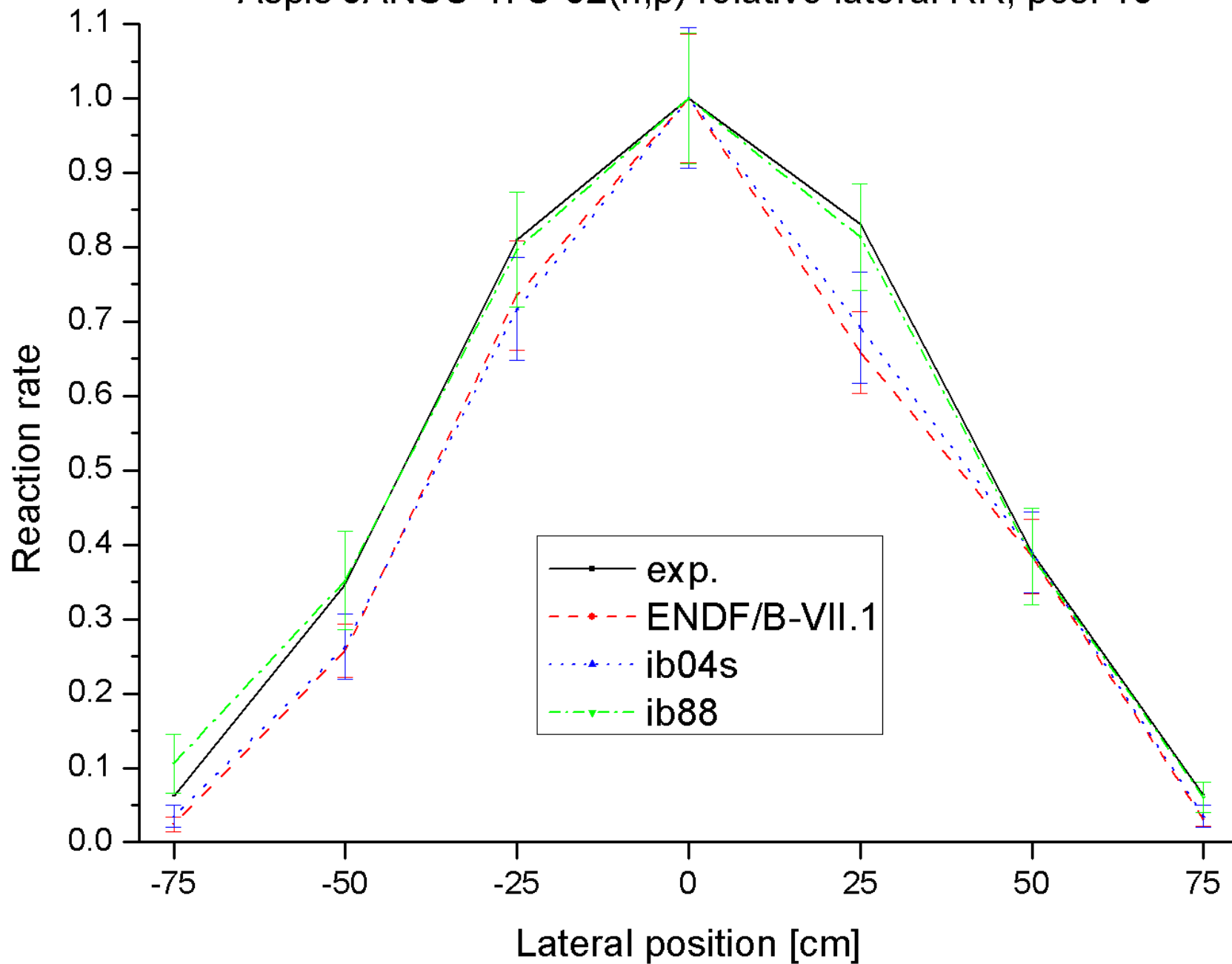
Aspis JANUS-1: Rh-103(n,n') relative lateral RR, pos. 14



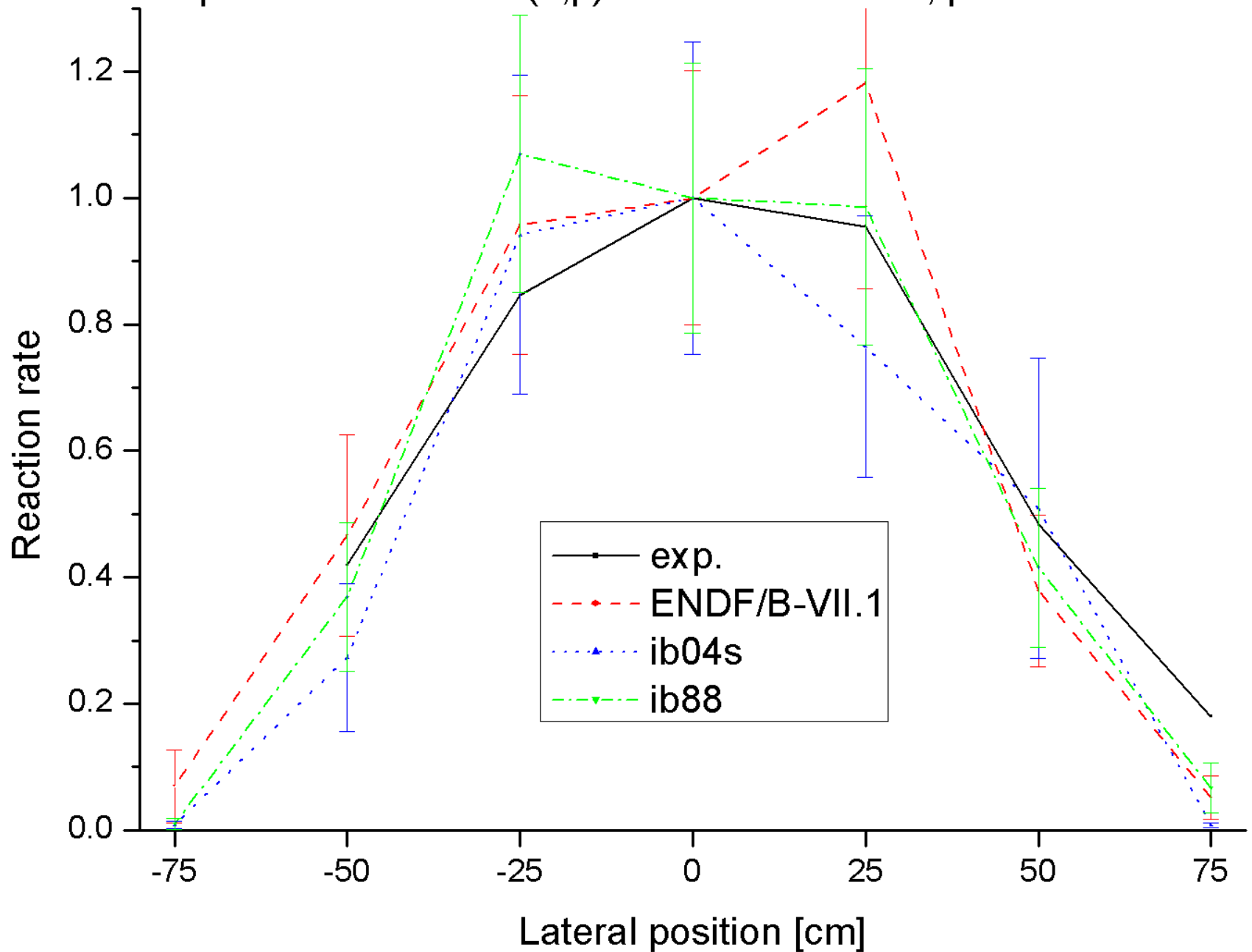
Aspis JANUS-1: S-32(n,p) relative lateral RR, pos. 6



Aspis JANUS-1: S-32(n,p) relative lateral RR, pos. 10



Aspis JANUS-1: S-32(n,p) relative lateral RR, pos. 14



General Features of ASPIS NESDIP-3

- NESTOR graphite reflector, neutron source converted by fission plate
- Attenuation in mild steel, SS, and water (simulating PWR shielding)
- Reaction rate axial distributions:
 - $^{32}\text{S}(n,p)$
 - $^{103}\text{Rh}(n,n')$

Measurement positions

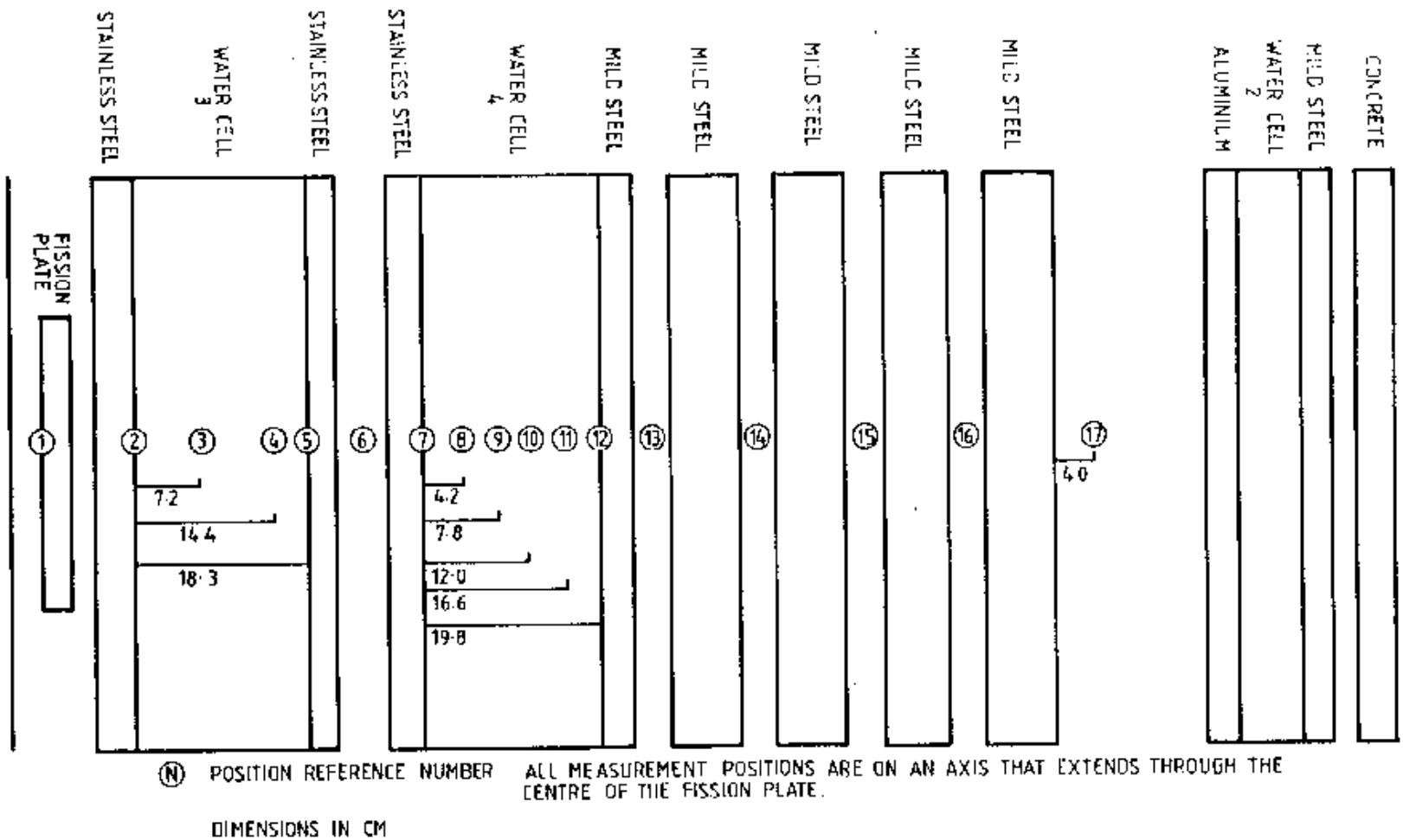
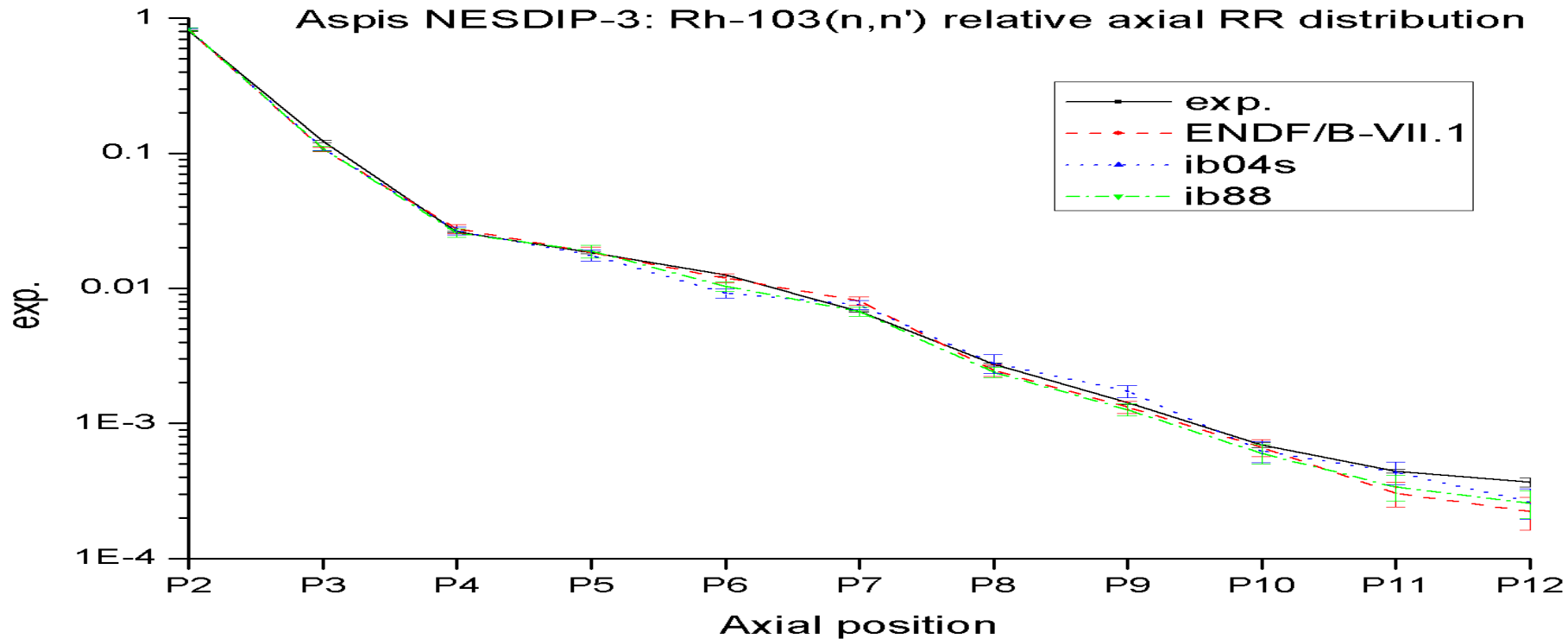


FIGURE 2
MEASUREMENT LOCATIONS IN THE 18/20 NESDIP ARRAY



Aspis NESDIP-3: Rh-103(n,n') relative axial RR distribution



Aspis NESDIP-3: Rh-103(n,n') relative axial C/E distribution

