

Status of the TALYS Evaluated Nuclear Data Library - TENDL

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NRG Petten, the Netherlands
WPEC Meeting, OECD/NEA Data Bank
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TENDL contributors

NRG:

- [Dimitri Rochman](#) and [Arjan Koning](#): Creators of the TENDL library, checking and processing
- [Steven van der Marck](#): Criticality and shielding validation

CCFE

- [Jean-Christophe Sublet](#): Processing and activation, decay heat and inventory validation

JUKO Research:

- [Jura Kopecky](#): Differential and integral validation of activation reactions

University of Uppsala:

- [Stephan Pomp](#), [Henrik Sjöstrand](#): Validation of TENDL through Total Monte Carlo uncertainty propagation for criticality, and (fast) reactor systems

CEA Bruyeres-le-Chatel:

- [Eric Bauge](#): development of covariance models, mass production plans

NEA Data Bank:

- [Emmeric Dupont](#), [Nicholas Soppera](#): Feedback on completeness and format issues through JANIS, EXFOR validation

IAEA:

- [Robin Forrest](#), [Viktor Zerkin](#): library hosting, feedback on completeness and format issues, EXFOR validation

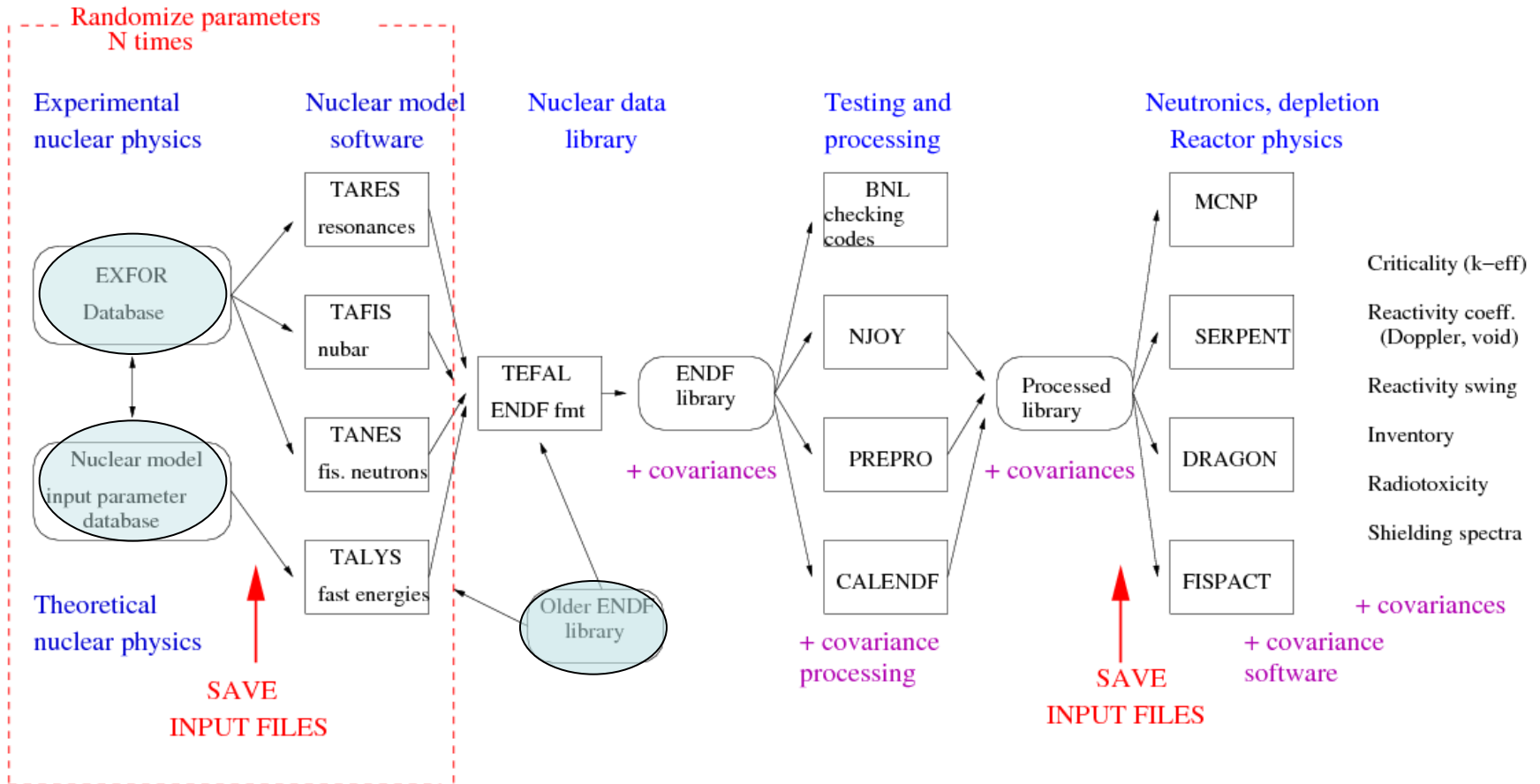
Contents

- The TENDL concept
- Differential validation
- Integral validation
- Conclusions

TENDL nuclear data library



Loop over nuclides : TENDL



A.J. Koning and D. Rochman, "Modern nuclear data evaluation with the TALYS code system", Nuclear Data Sheets 113, 2841 (2012).

TALYS Evaluated Nuclear Data Library: TENDL-2012

- Neutron, proton, deuteron, triton, Helium-3, alpha and gamma data libraries.
- 2430 targets (all isotopes with lifetime > 1 sec.)
- Complete reaction description in ENDF-6 format: MF1-MF40, up to 200 MeV
- MCNP-libraries (“ACE-files”), PENDF files and multi-group covariance data

Default: Global calculations by TALYS-1.48 and TARES (resonances)

which are overruled by

Adjusted TALYS calculations (340 input files) and Resonance Atlas-based TARES calculations

which are overruled by

TALYS-**normalization** to ~200 (experimental) evaluated reaction channels from other libraries (e.g. IRDFF, light nuclides, main channels of “big 3”)

“Best” TALYS input file for As-75

```

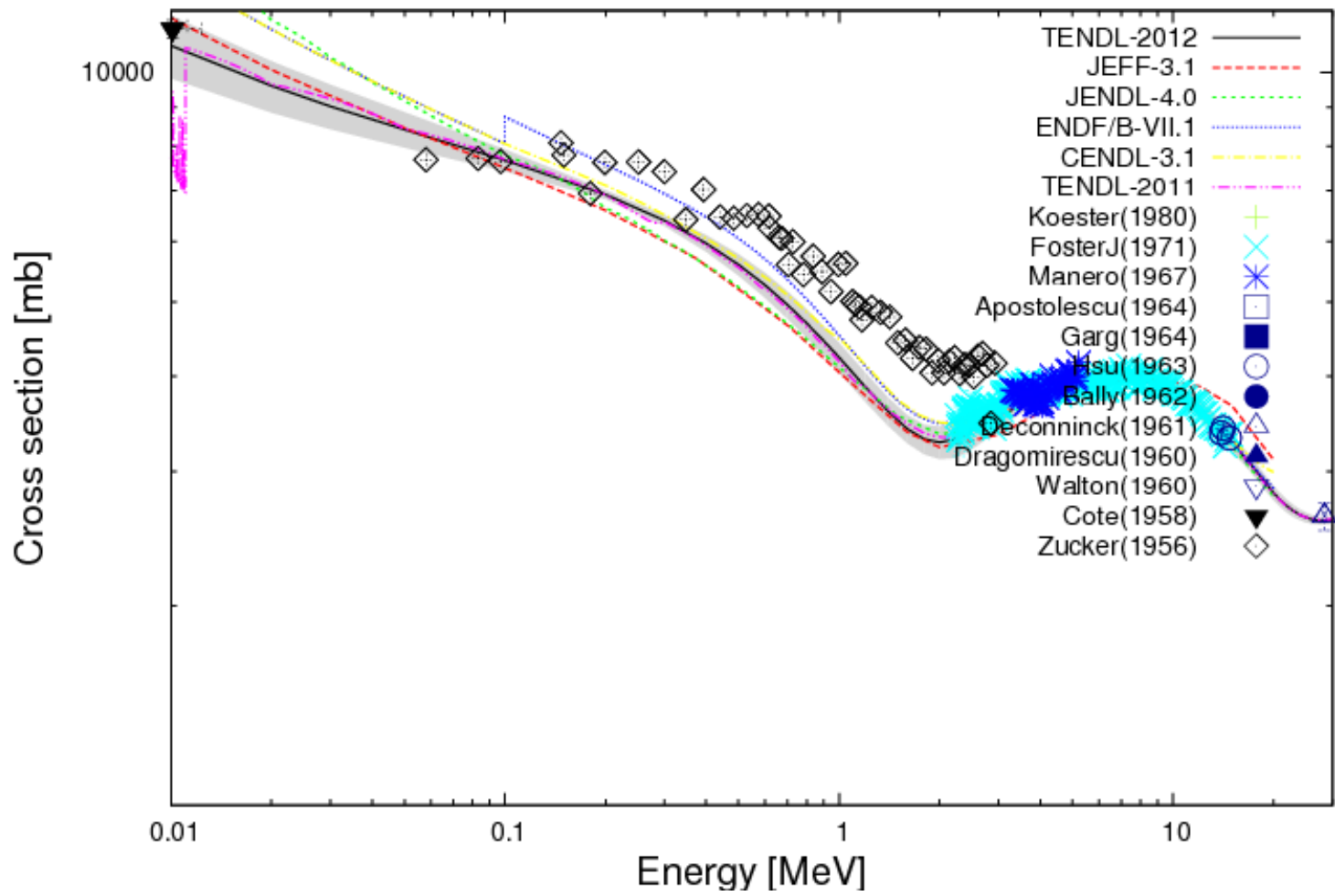
rvadjust n 1. 1. 6. 3.5 1.02
rvadjust n 1. 6. 20. 13. 0.99
gamgamadjust 33 76 1.80 0.10 ##
gnadjust 33 76 1.11 0.05 ##
gpadjust 33 76 1.11 0.05 ##
gnadjust 32 75 0.92
gpadjust 32 75 0.92
aadjust 33 76 0.95
aadjust 32 75 1.12
rvadjust p 0.89 0.02 ##
avadjust p 0.89 0.02 ##
rvadjust a 1.15
avadjust a 1.15

ldmodel 2
ldmodel 2 33 75
ldmodel 2 32 75
ldmodel 2 31 72
Rgamma 4.
branch 32 75 10 1 0 1.
branch 32 75 16 1 0 1.
branch 32 75 3 2 3 0.6 0 0.4
egradjust 33 76 0.8 E1
Cknock t 1.35
Cstrip t 1.35
Cknock a 0.65
Cstrip a 0.65
aadjust 31 72 1.20

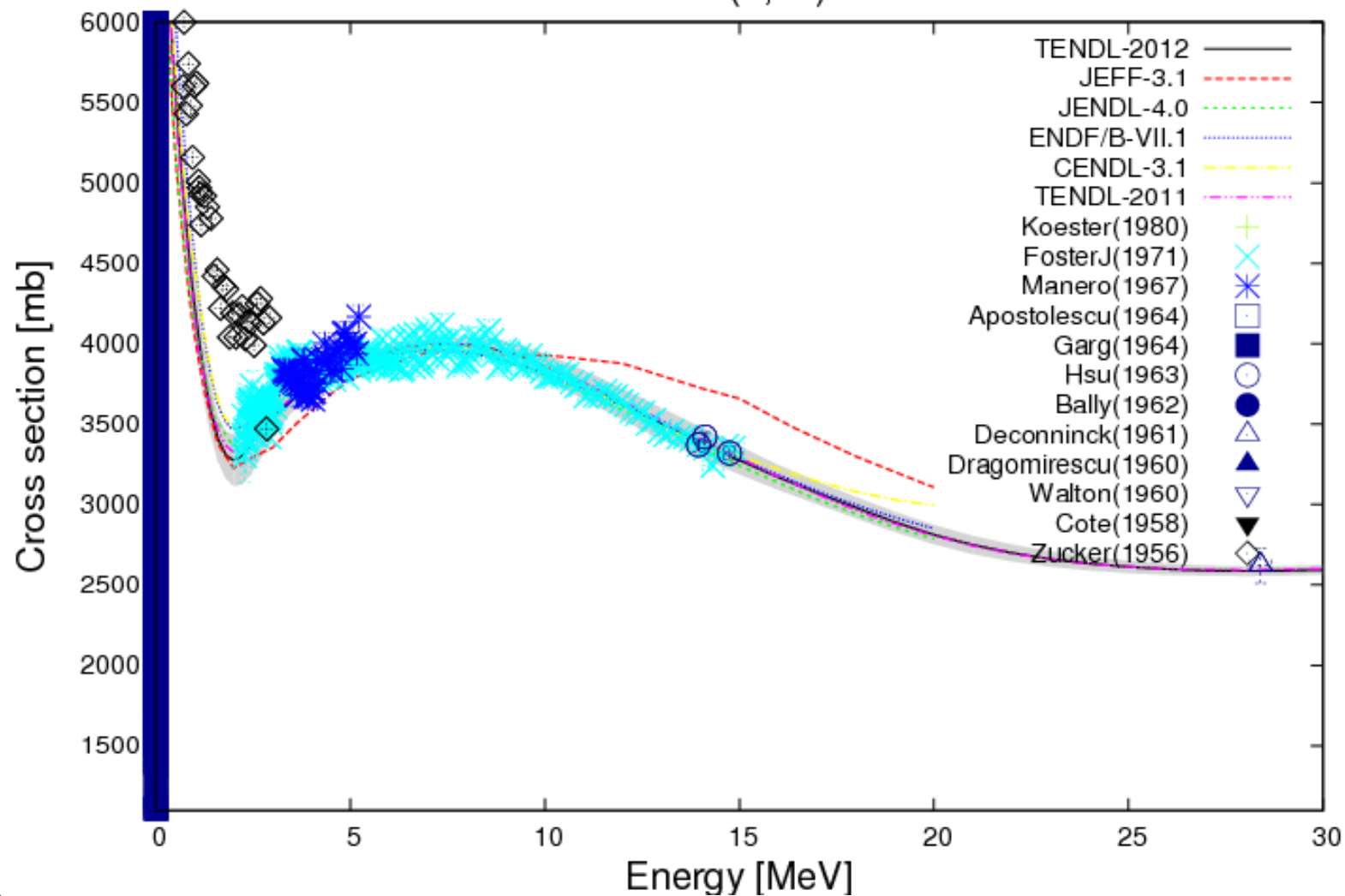
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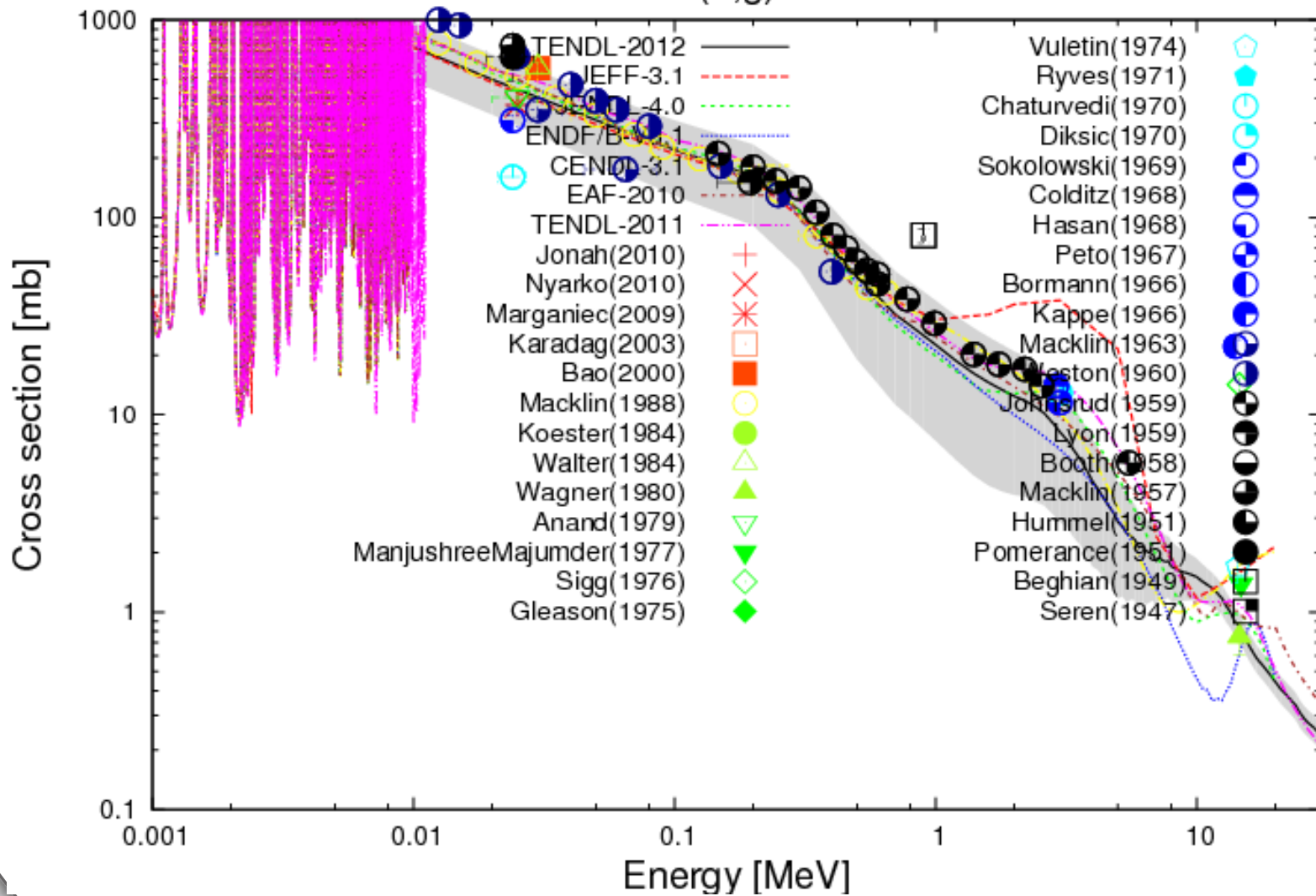
We have ~300 isotopic input files like this.

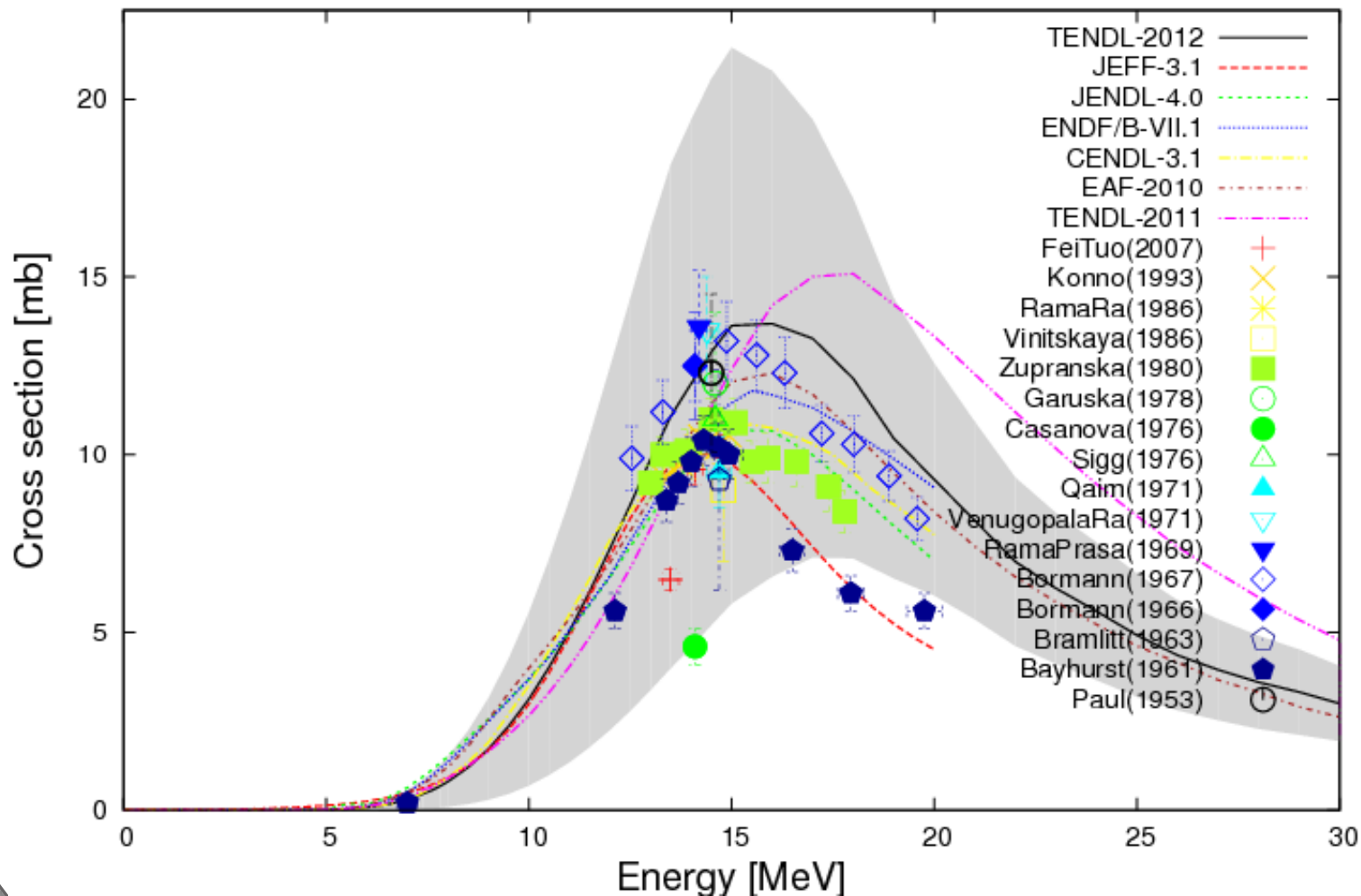
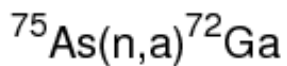
$^{75}\text{As}(n,\text{tot})$



$^{75}\text{As}(n,\text{tot})$

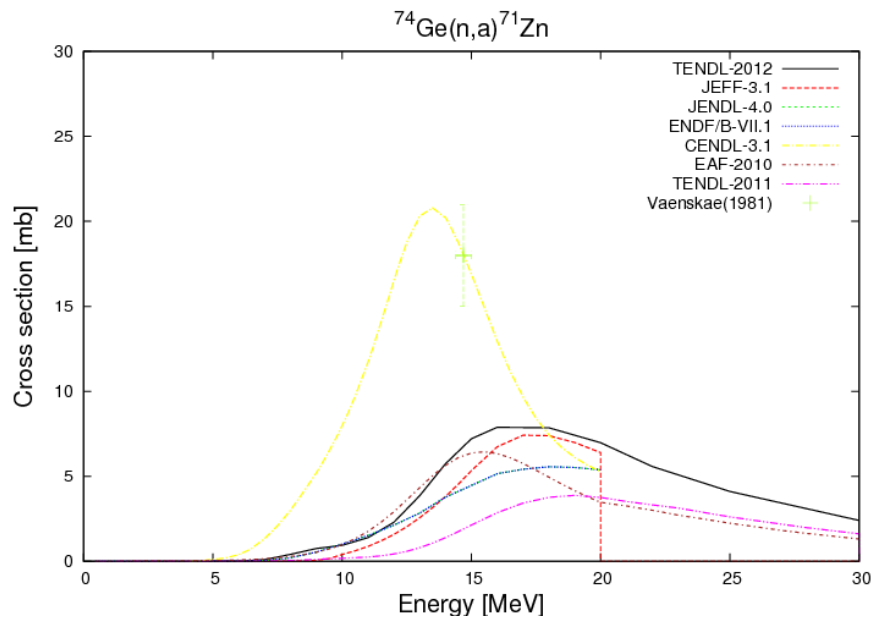


$^{75}\text{As}(n,g)^{76}\text{As}$


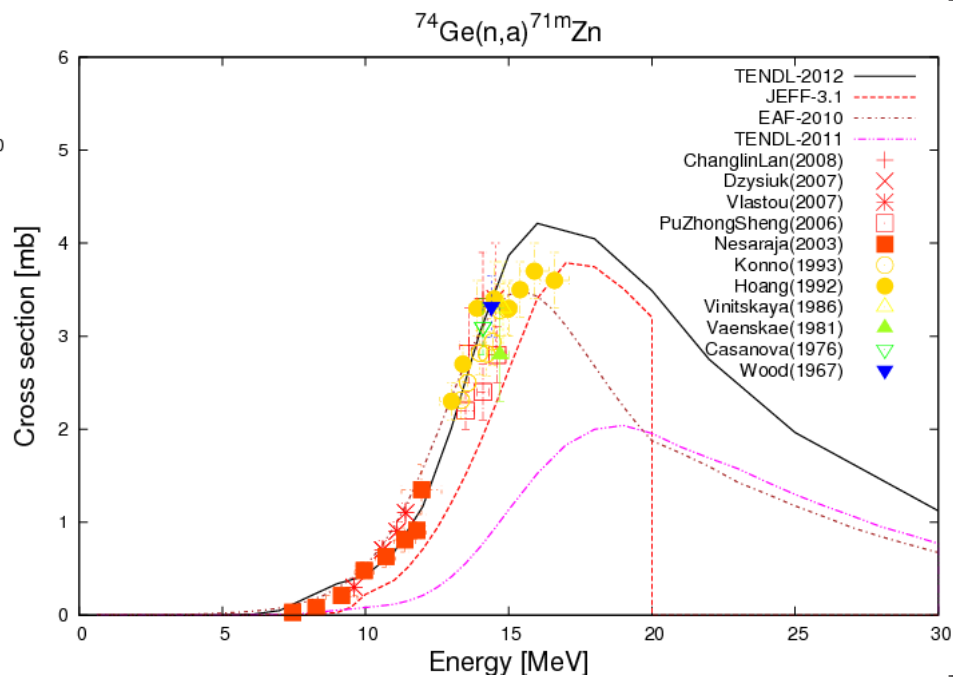


We have ~2500 pictures like this.

Isomeric information included



(By the way: what is the definition of a general purpose library?)



Global capture validation for Ga-Zr

Average over 41 nuclides

F-factor (C/E)	TENDL-2012	ENDF/B-VII.1	JEFF-3.1.1	JENDL-4.0	CENDL-3.1
Thermal	1.041	1.080	1.113	1.096	1.128
Res Int	1.181	1.174	1.159	1.164	1.194
MACS	1.197	1.245	1.291	1.212	1.309

Integral activation measurements (EASY-database). Example: As-75

F-factor	Spectrum	EAF-2010	TENDL-2012
As-75(n,p)m	FNS-5min	0.990	1.001
As-75(n,p)	FNS-5min	1.177	0.957
As-75(n,a)	D-Be2a	1.146	1.020

TENDL: Complete ENDF-6 data libraries

MF1: description and average fission quantities

MF2: resonance data

MF3: cross sections

MF4: angular distributions

MF5: energy spectra

MF6: double-differential spectra, particle yields and residual products

MF8-10: isomeric cross sections and ratios

MF12-15: gamma yields, spectra and angular distributions

MF31: covariances of average fission quantities

MF32: covariances of resonance parameters

MF33: covariances of cross sections

MF34: covariances of angular distributions

MF35: covariances of fission neutron spectra and particle spectra

MF40: covariances of isomeric data

Processing steps

• NJOY-99.385

- moder
- reconr
- broadr
- unresr
- heatr
- gaspr
 - purr
 - groupr
 - acer
 - ...

➤ PREPRO-2012

- linear
- recent
- sigma1
- sixpack
- activate
- merger
- dictin
- groupie

• CALENDF-2010

- calendf
- regroupt
- lecritp
-

PT file

ENDF file

Basic format and physics verification

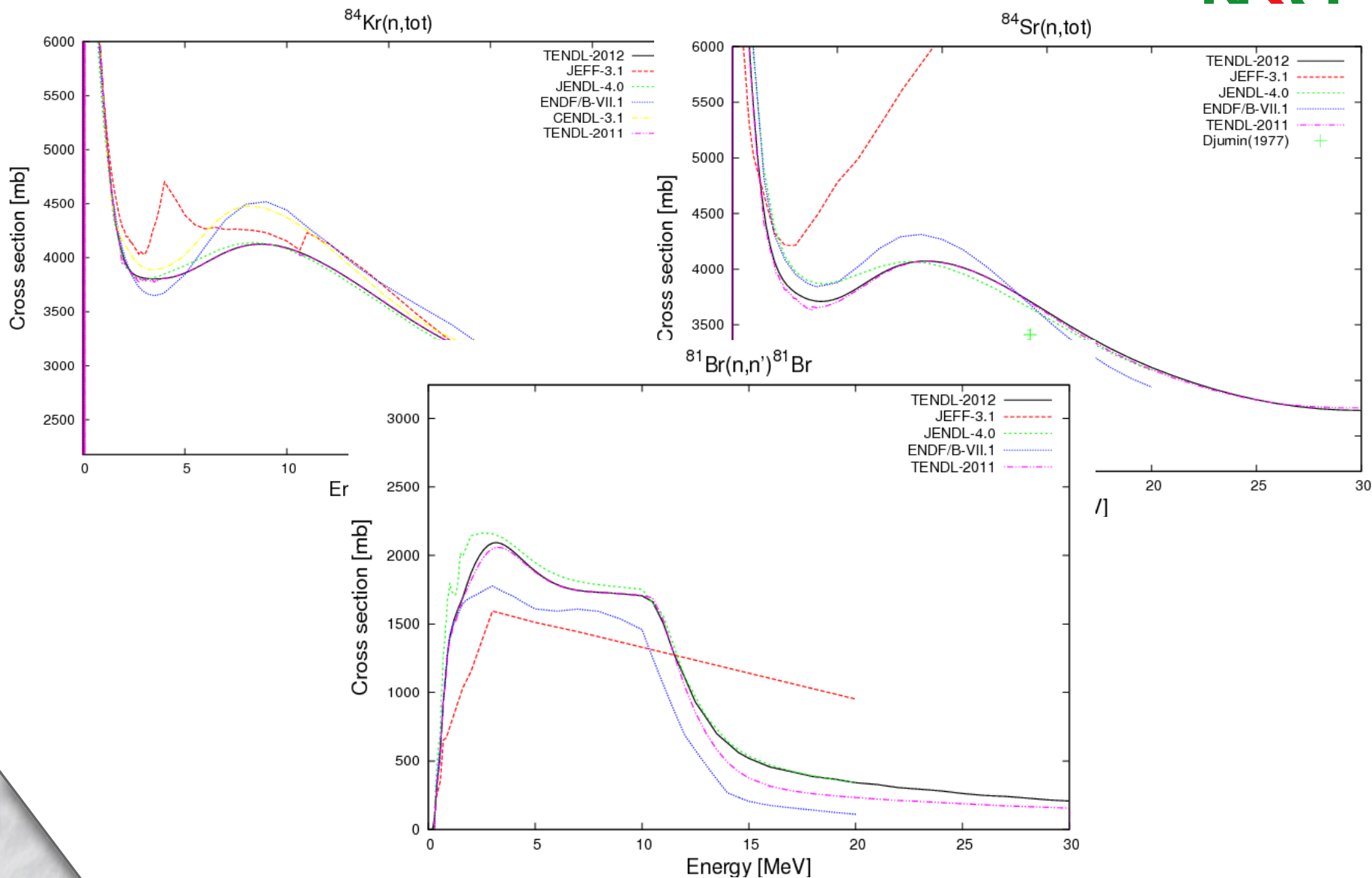
2430 (nuclides) x 7 (projectiles) data libraries are tested and processed with:

- CHECKR, FIZCON, PSYCHE and INTER
- FUDGE (is ENDF2GND2ENDF = ENDF ?)
- PREPRO-2010
- NJOY-99.364
- MCNPX-2.7

Scripts which search for all the possible warning and error messages by the above codes have been used. Now all problems for these 17010 data libraries are almost gone. Additional feedback on TENDL-2012:

- Some covariance identifiers (Eastwood, CCFE)
- Discontinuity in damage (Konobeyev, KIT, MacFarlane, LANL)
- TRIPOLI-specific issues (Jouanne, CEA Saclay)

It may be time to replace some old JEFF files!



TENDL4JEFF



New neutron data evaluations for all Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y and Zr isotopes have been made and (with exception of Y and Zr) are proposed for adoption in JEFF-3.2

Isotopes with lifetime > 1 year which are missing or for which all other libraries in the world are questionable:

- C-13, O-17,18, Ne-20,21,22, Mg-27, Si-31,32, P-31
- S-32,33,34,36, Cl-36, Ar-39,41, K-39,40,41, Ca-41,45
- Sc-46, V-49,50, Cr-51, Mn-53,54, Co-57, Ni-63, Cu-64
- Zn-64,66,67,68,70, Tc-98, Rh-104, Cd-109
-Tm, Yb, Os, Pt,.....etcetera

About a 100 nuclides in this category are proposed for JEFF-3.2

With 478 isotopic evaluations JEFF-3.2 will have the second largest general purpose file collection in the world!

TENDL-2012 integral testing (Steven van der Marck, ND-2013)



- ❖ Released 15 January 2013
- ❖ Contents
 - ✓ 2430 neutron ENDF + ACE files
 - ✓ 'Random' evaluations (Br, Zr, Nb, Mo, Cd, In, I, Xe, La, Nd Sm, Eu, Gd, Pb, Th, $^{234-239}\text{U}$, $^{238-242}\text{Pu}$, $^{241-243}\text{Am}$, $^{242,245}\text{Cm}$)
 - ✓ 2430 ENDF files for proton, deuteron, triton, ^3He , α , γ

- ❖ Compare with NDS, December 2012
 - ✓ ENDF/B-VII.1 December 2011
 - ✓ JENDL-4.0 April 2011
 - ✓ JEFF-3.1.1 January 2009

- ❖ Processed with NJOY-99.364
 - Exceptions ^{14}C , ^{144}Tb , $^{177\text{m}},^{178\text{n}},^{179\text{n}}\text{Hf}$, $^{192\text{m}}\text{Os}$, $^{198\text{m}}\text{Au}$, $^{206\text{m}}\text{Tl}$



Criticality safety: ~2000 cases

COMP

	therm	inter	fast	mixed
LEU	388			
IEU	5	4	1	
HEU	134	6		8
MIX	39		5	
PU		1		30
²³³ U	8			
Total	574	11	6	38

MET

	therm	inter	fast	mixed
LEU	23			
IEU			17	
HEU	49	5	139	5
MIX			31	
PU		1	98	6
²³³ U			10	
Total	72	6	295	11

Criticality safety: ~2000 cases

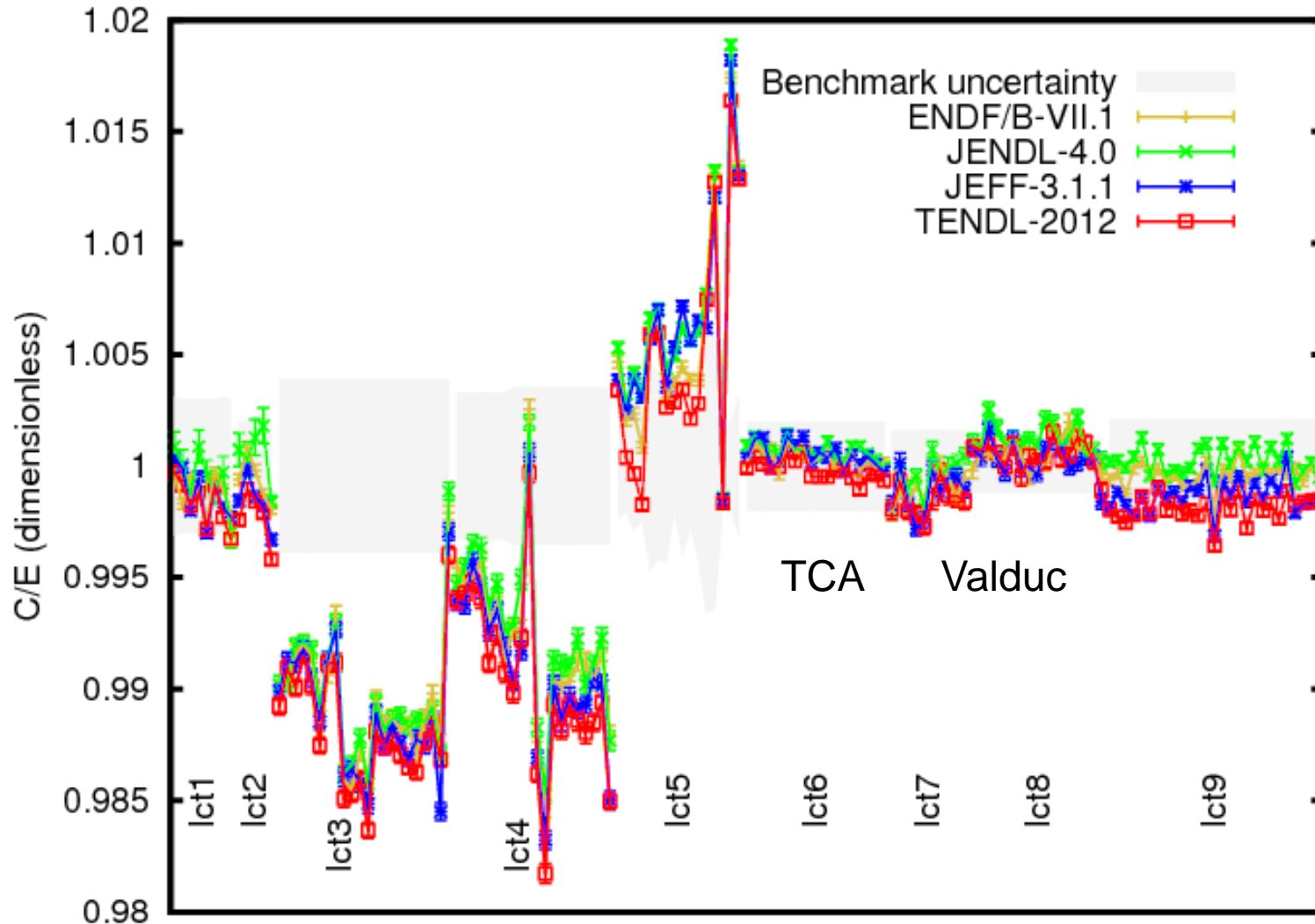
SOL

	therm	inter	fast	mixed
LEU	67			
IEU	13			
HEU	339			
MIX	53			
PU	368			
²³³ U	59			
Total	899			

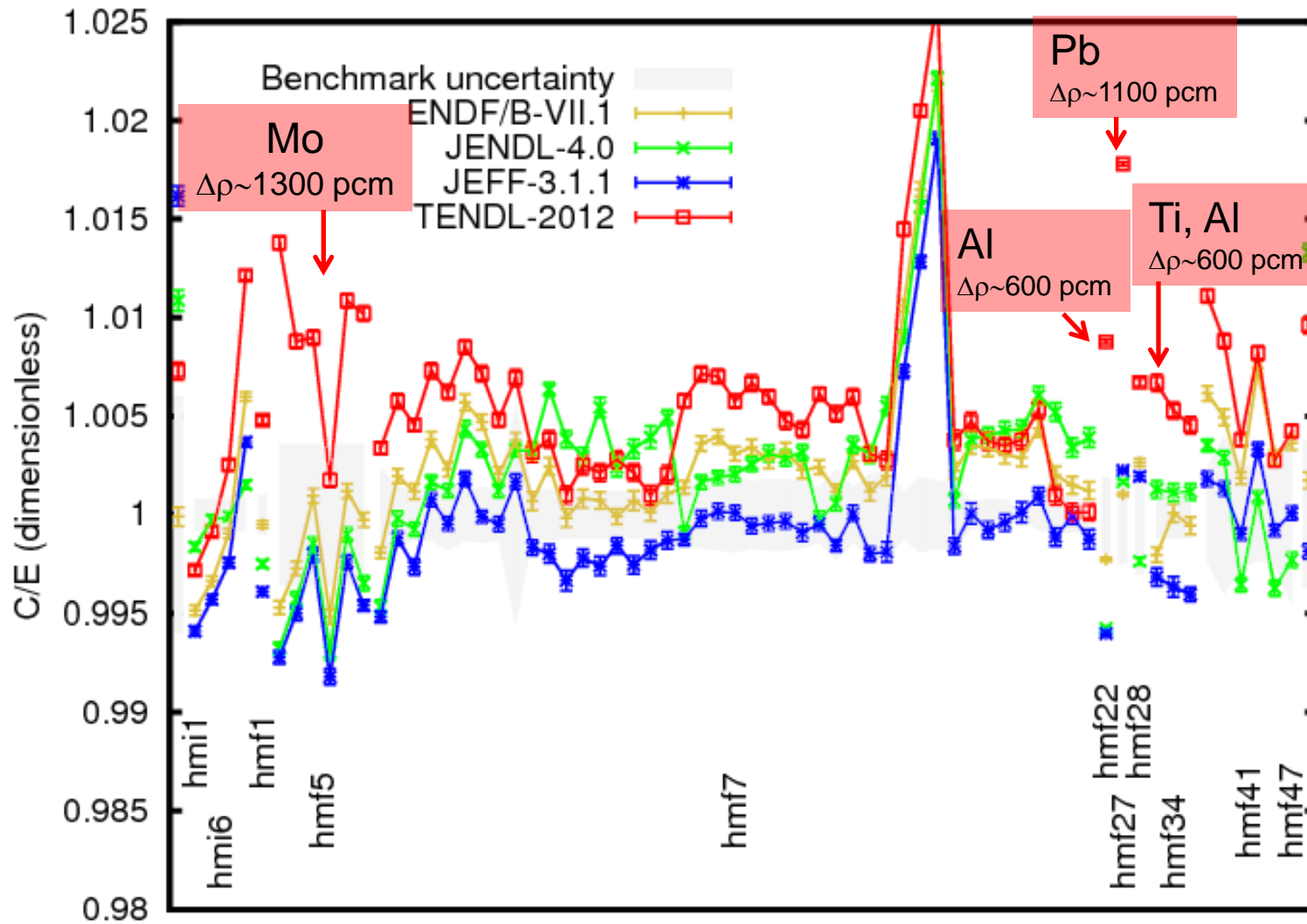
MISC

	therm	inter	fast	mixed
LEU				
IEU				
HEU				
MIX	46		10	
PU				
²³³ U				
Total	46		10	

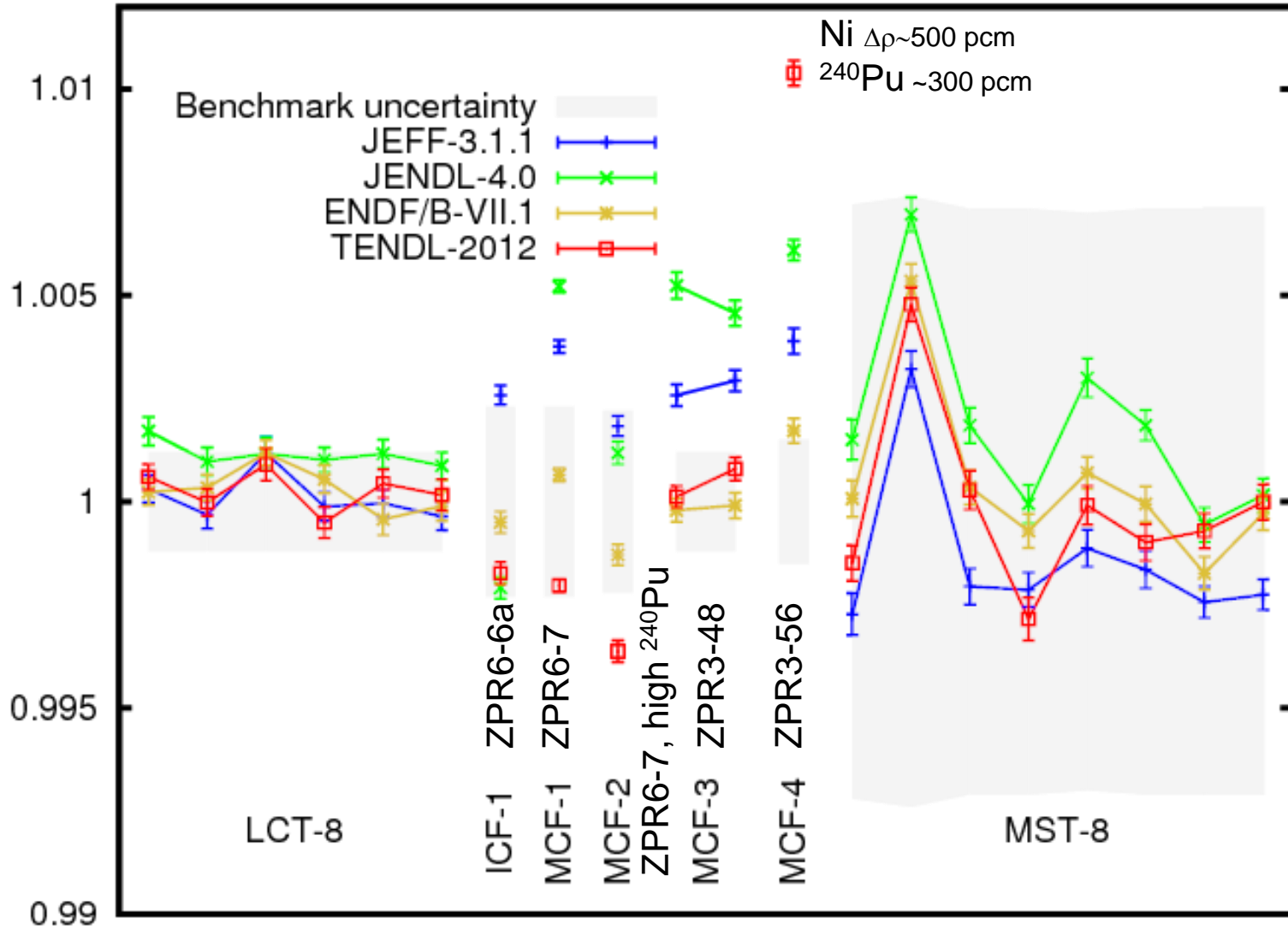
Criticality safety: leu-comp-therm



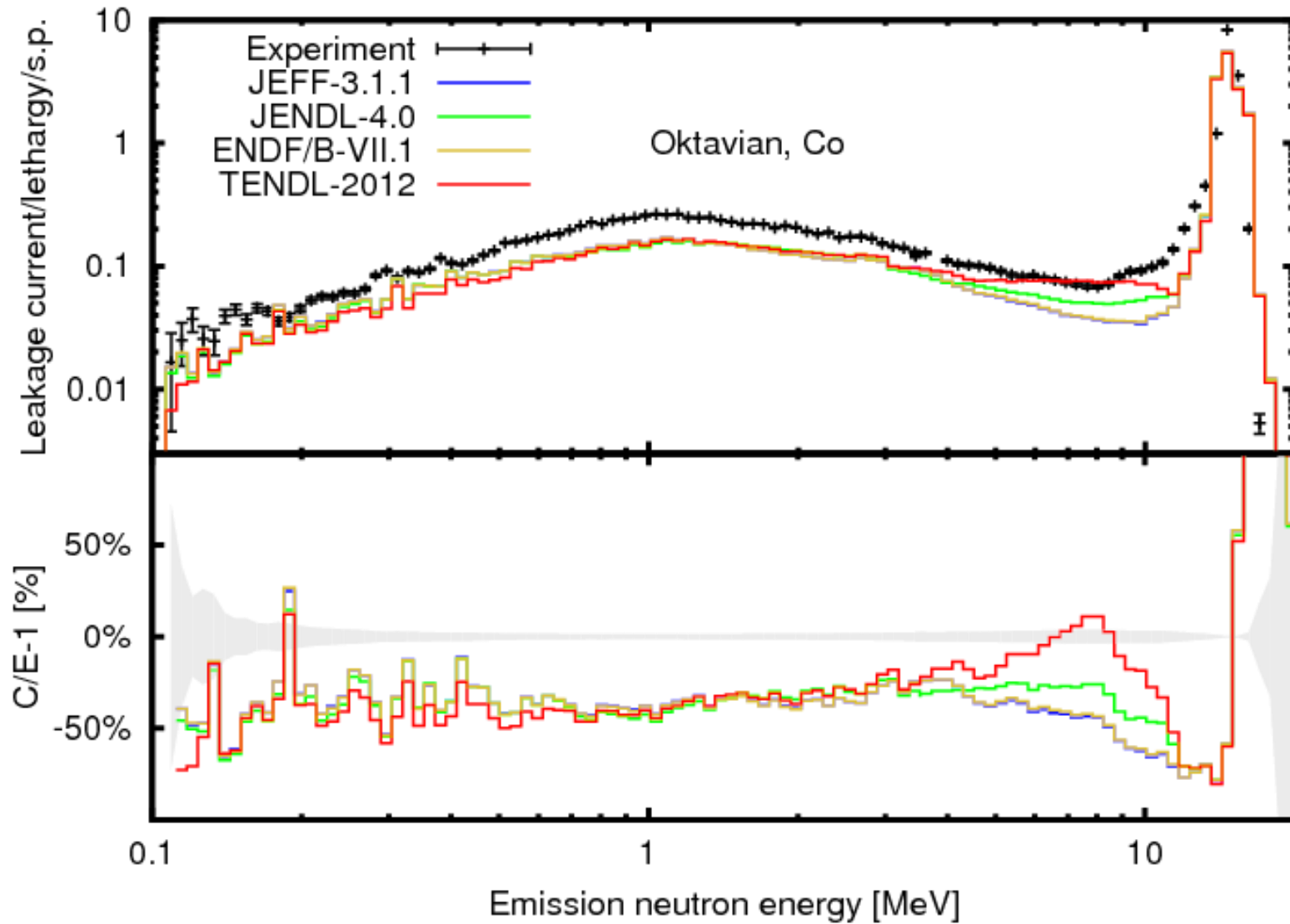
Criticality safety: heu-met-fast



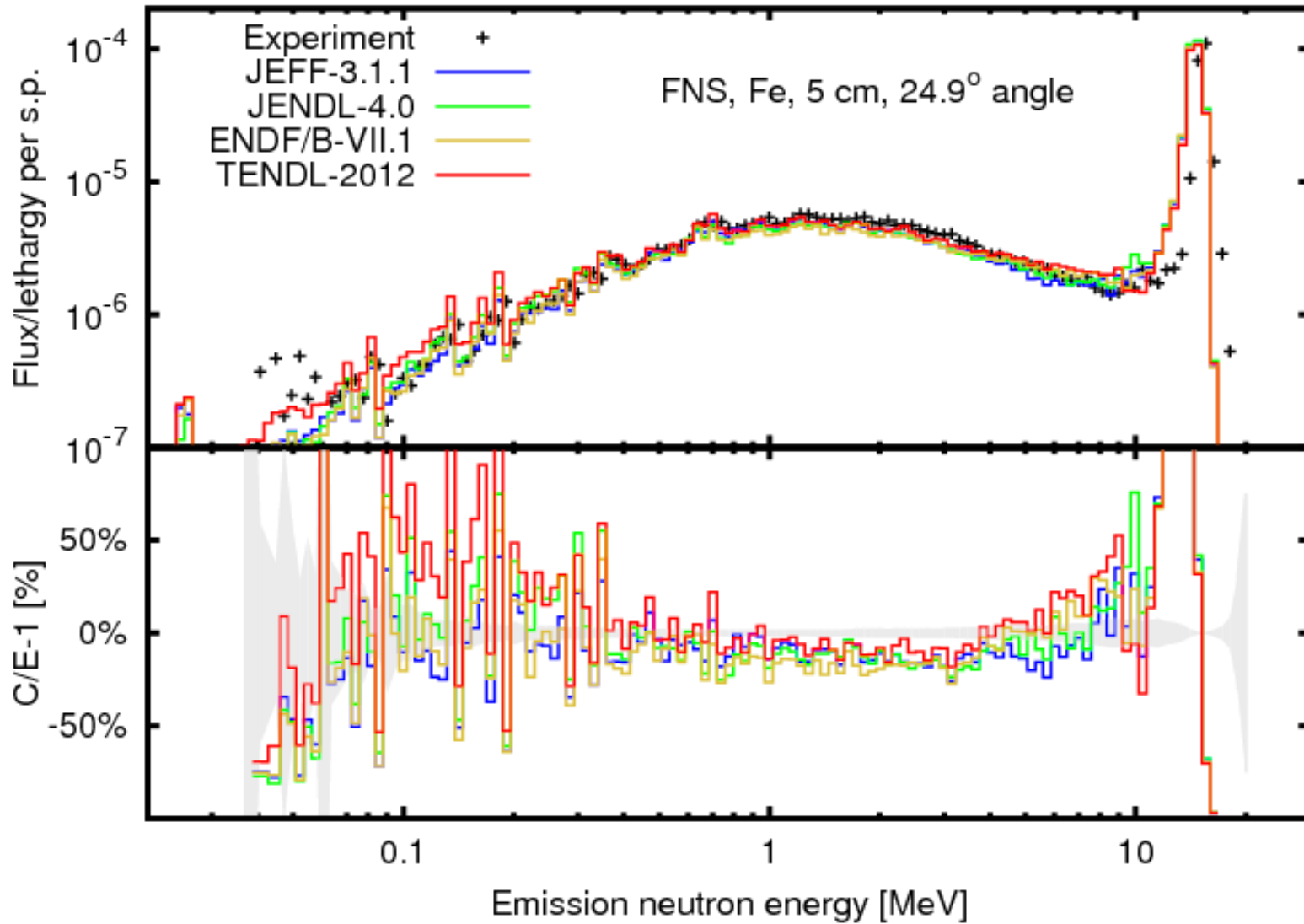
Criticality safety: Na



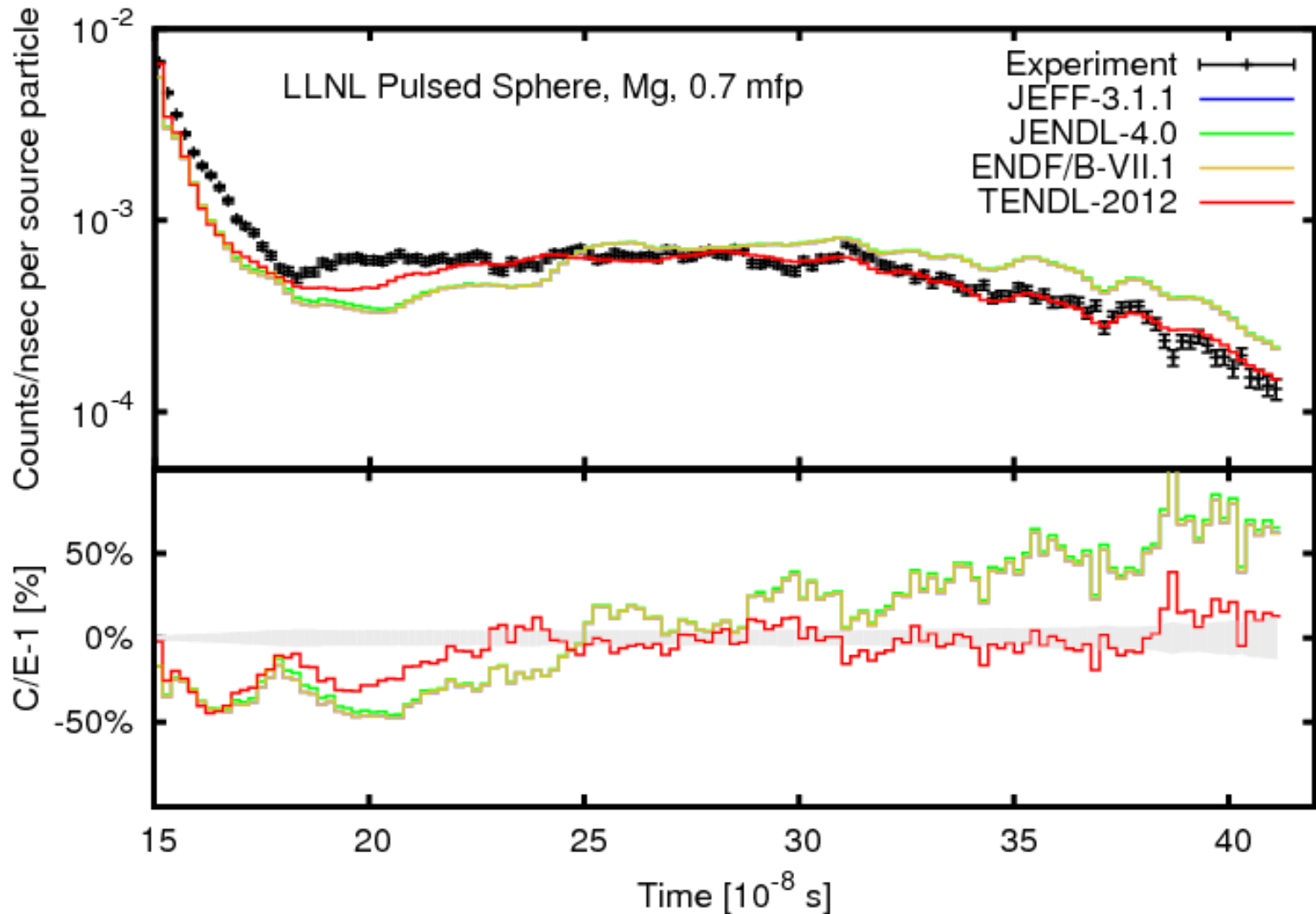
Shielding example: Oktavian, Co



Shielding example: FNS, 5cm, 24.9°



Shielding example: LLNL, Mg, 0.7 mfp



TENDL criticality and shielding testing summary

- ❖ Criticality safety
 - ✓ On average, good performance for LEU-COMP-THERM
 - ✓ Poorer results in fast range, especially due to reflectors
 - ✓ Outliers due to Ti, Ni, Mo, Pb, ...

- ❖ Shielding
 - ✓ Similar results compared to other libraries
 - ✓ Occasionally differences, such as for Co, Mg, Mn

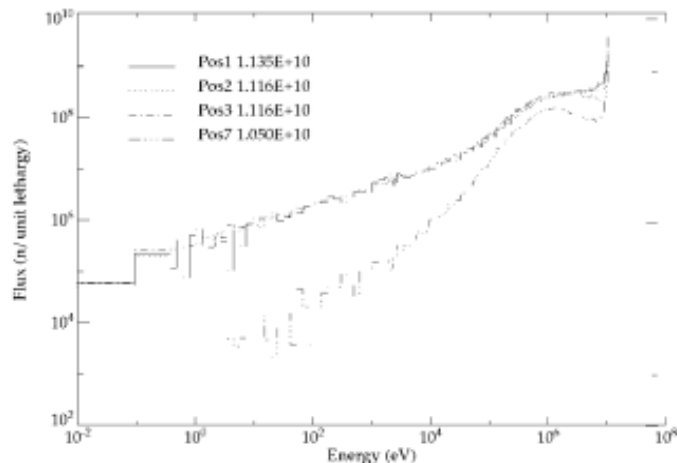
- ❖ Benchmark results are a good starting point for further improvements to TENDL

Decay heat validation of TENDL-2012

Jean-Christophe SUBLET, Mark R Gilbert, A Koning and D
Rochman

UK Atomic Energy Authority, Culham Science Centre, Abingdon OX14 3DB, United Kingdom
*Nuclear Research and Consultancy Group NRG, Westerduinweg 3, NL-1755 ZG Petten, The
Netherlands*

14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium bearing titanium target; Fusion Neutron Source

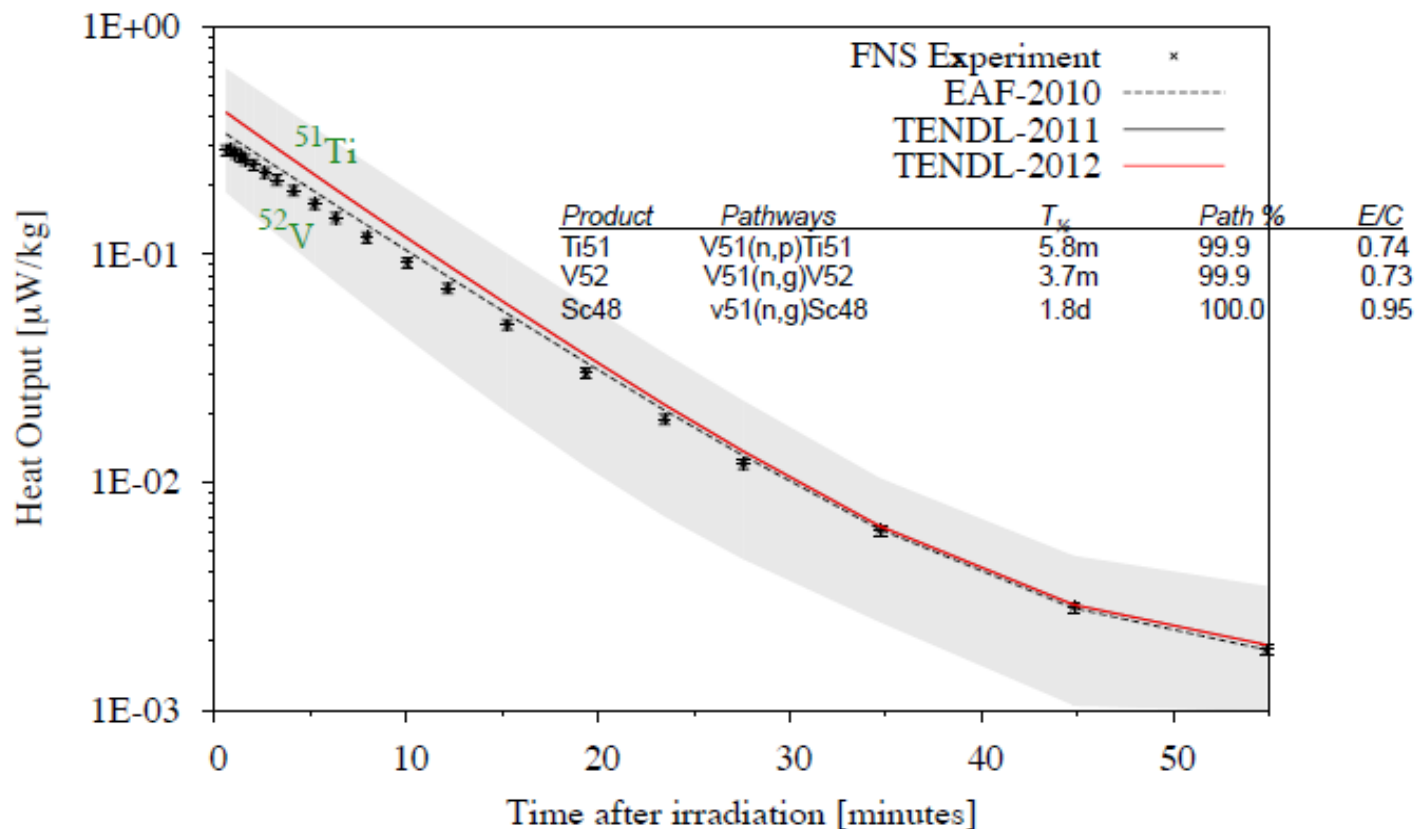


FNS Neutron spectra, neutron fluence monitored by $^{27}\text{Al}(n,\alpha)\text{Na}^{24}$

Two experimental campaigns: 1996 and 2000; 74 materials

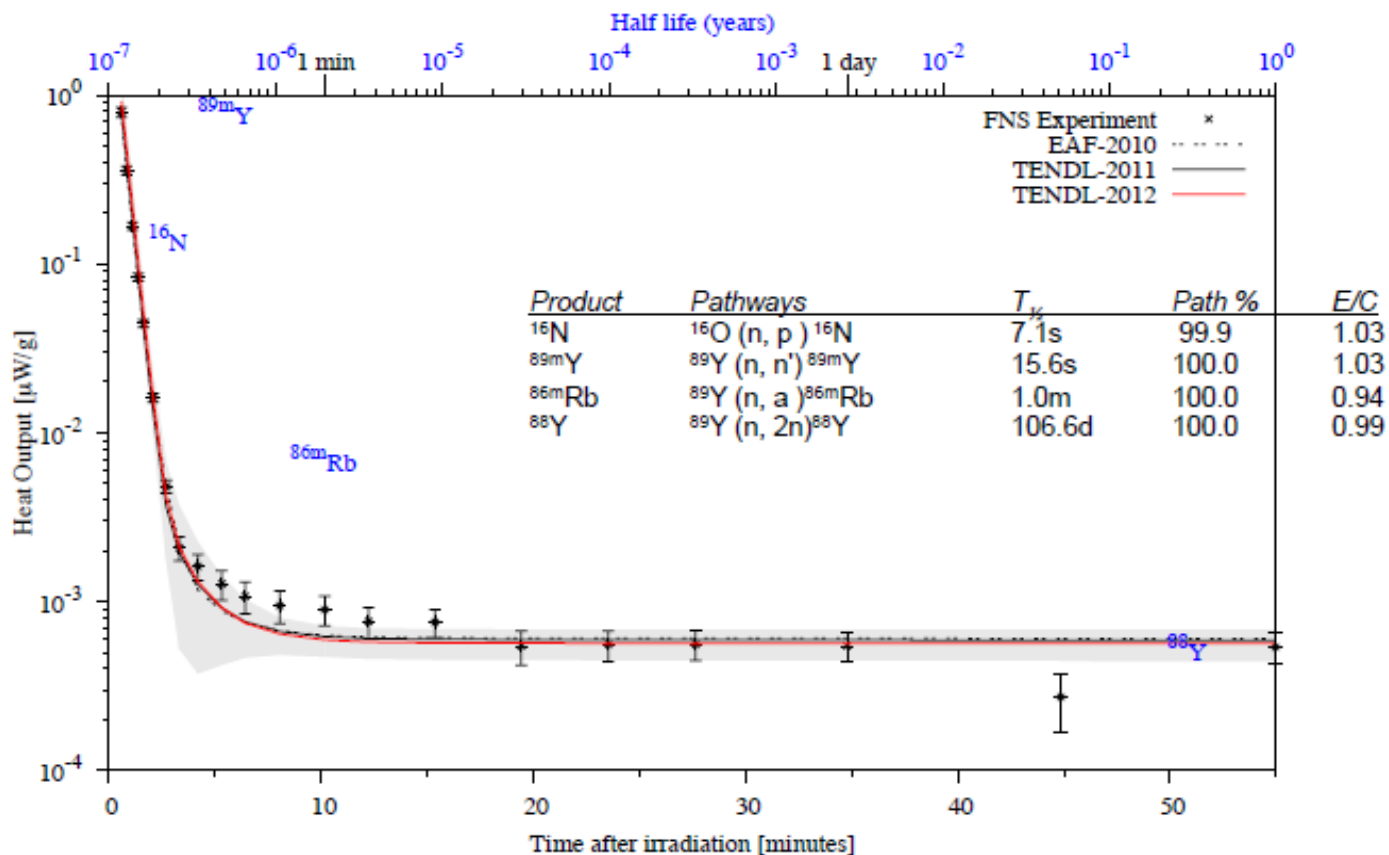
Z	Element	Form	Z	Element	Form
9	F	CF2	49	In	Metallic Foil
11	Na	Na2CO3	50	Sn	SnO2
12	Mg	MgO	51	Sb	Metallic Powder
13	Al	Metallic Foil	52	Te	TeO2
14	Si	Metallic Powder	53	I	IC6H4OH
15	P	P3N5	55	Cs	Cs2CO3
16	S	Powder	56	Ba	BaCO3
17	Cl	C2H2Cl2	57	La	La2O3
19	K	K2CO3	58	Ce	CeO2
20	Ca	CaO	59	Pr	Pr6O11
21	Sc	Sc2O3	60	Nd	Nd2O3
22	Ti	Metallic Foil	62	Sm	Sm2O3
23	V	Metallic Foil	63	Eu	Eu2O3
24	Cr	Metallic Powder	64	Gd	Gd2O3
25	Mn	Metallic Powder	65	Tb	Tb4O7
26	Fe	Metallic Foil	66	Dy	Dy2O3
27	Co	Metallic Foil	67	Ho	Ho2O3
28	Ni	Metallic Foil	68	Er	Er2O3
29	Cu	Metallic Foil	69	Tm	Tm2O3
30	Zn	Metallic Foil	70	Yb	Yb2O3
31	Ga	Ga2O3	71	Lu	Lu2O3
32	Ge	GeO2	72	Hf	Metallic Powder
33	As	As2O3	73	Ta	Metallic Foil
34	Se	Metallic Powder	74	W	Metallic Foil
35	Br	BrC6H4COOH	75	Re	Metallic Powder
37	Rb	Rb2CO3	76	Os	Metallic Powder
38	Sr	SrCO3	77	Ir	Metallic Powder
39	Y	Y2O3	78	Pt	Metallic Foil
40	Zr	Metallic Foil	79	Au	Metallic Foil
41	Nb	Metallic Foil	80	Hg	HgO
42	Mo	Metallic Foil	81	Tl	Tl2O
44	Ru	Metallic Powder	82	Pb	Metallic Foil
45	Rh	Metallic Powder	83	Bi	Metallic Powder
46	Pd	Metallic Foil	Alloy	SS-304	Metallic Foil
47	Ag	Metallic Foil	Alloy	SS-316	Metallic Foil
48	Cd	Metallic Foil	Alloy	NiCr	Metallic Foil
49	In	Metallic Foil	Alloy	Inc600	Metallic Foil

FNS-00 5 Min. Irradiation - V



Decay power: FNS JAERI Yttrium

FNS-00 5 Min. Irradiation - Y₂O₃



Conclusions: TENDL-2012

- TALYS Evaluated Nuclear Data Library (TENDL):
 - 2430 target nuclides (stable or lifetime > 1 sec)
 - Includes evaluated experimental data
 - For incident neutrons, protons, deuterons, photons, etc.
 - Up to 200 MeV and including all reaction information + covariance data
 - Available in ENDF-6, PENDF and ACE (MCNP) format
 - Already heavily used in MCNP(X), FISPACT etc.
- 2012: Zooming in: New neutron data evaluations for all Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y and Zr isotopes have been made and (with exception of Y and Zr) are proposed for adoption in JEFF-3.2
- A further ~100 (relatively unimportant) nuclides are included for JEFF-3.2
- Good validation for thermal criticality systems, decay heat and integral activation measurements. Work to be done for fast critical systems.

Outlook: TENDL-2013

- Zoom in on Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn (for among others F4E)
- Work on fast critical benchmarks
- Consistent Backward-Forward Monte Carlo evaluation for all nuclides
- Use CEA-2012 evaluations for U and Pu as starting point for Total Monte Carlo and the “Petten method” (Monte Carlo optimization)

Data evaluation will always requires particular attention per nuclide and reaction channel, i.e. can not be “totally” automated. But:

- Current world libraries: Evaluation = editing the data library
- TENDL: Evaluation = Input files + scripts driving TALYS, EXFOR + existing NDL's (the shoulders of giants). Library production, processing and validation is automated.

We will see which method will prevail.....