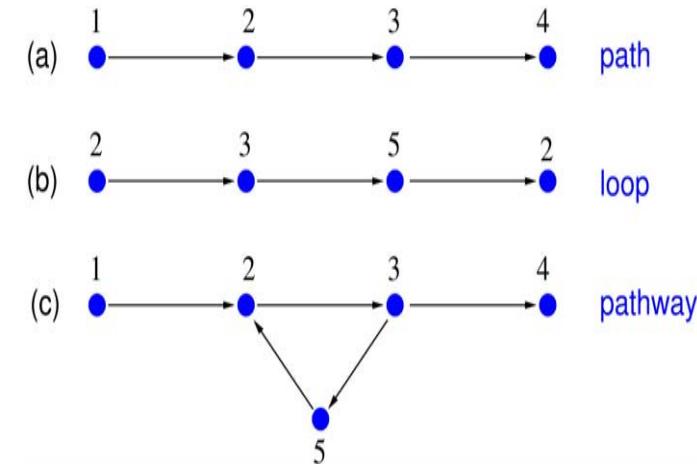


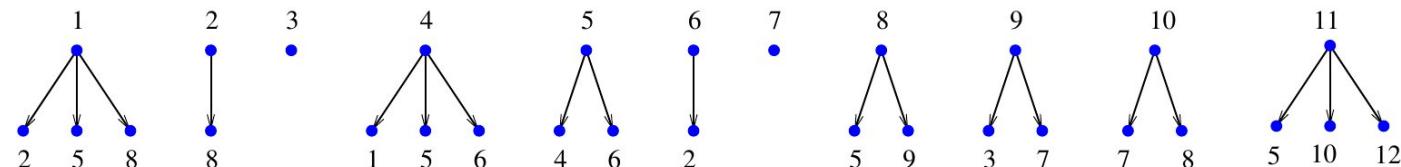


## Extended pathways search

- Pathway = path + loop(s)
- Finds reaction/decay chains
- Identifies important
  - Nuclides
  - Reactions
  - Decays
- Used for uncertainty and sensitivity calculations
- Simple previous approach could fail through combinatorial explosion

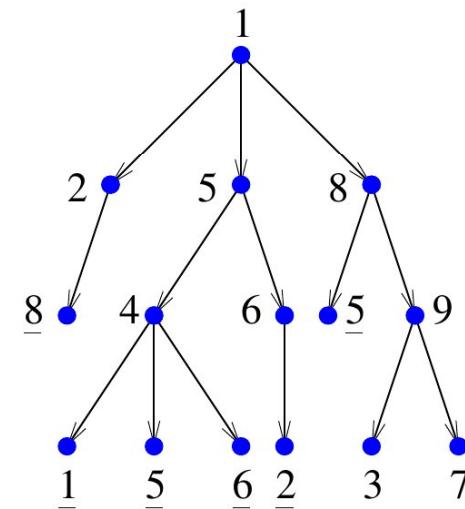


# Pathways – single visit tree



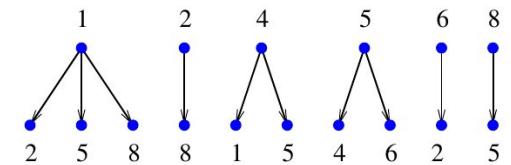
Adjacency lists

- tree search gives reduced p-d set
- pruning controlled using
  - path\_floor
  - loop\_floor
  - max\_depth
- TENDL library
  - 3873 nuclides, ~240000 reactions
  - ~160,000 p-d pairs (57/nuclide)
  - single visit breadth-first search BFS typically < 50 p-d (parent-daughter)

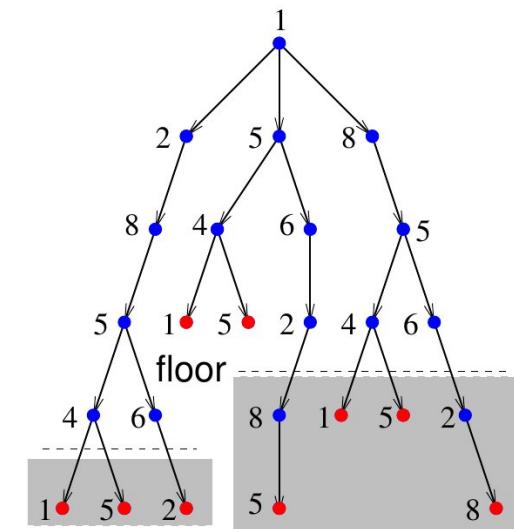


Single visit BFS tree for nuclide 1

- build full tree for reduced p-d set
  - leaf node if
    - repeat nuclide (loop)
    - path inventory below path floor
    - path depth greater than max depth
  - combine paths and loops
  - control keywords
    - UNCERTAINTY (path\_floor, loop\_floor, max\_depth)
    - SORTDOMINANT (topxx)
    - TOLERANCE (absolutetol\_path, relativetol\_path)
    - ZERO
    - LOOKAHEAD
    - PATHRESET



## nuclide 1 to 4 path edges



## full tree with pruning

paths: 154 1854 12854

loops: 1541 545



- Initiated by `ZERO` keyword
- Combined `topxx` from dominant lists
- May miss late cooling time dominant nuclides
- Some typical ‘fixes’ to increase the depth of the simulation for more demanding simulations:
  - Reduce `path_floor` (prune fewer pathways)
  - Increase `topxx` (more dominant nuclides)
  - Use `LOOKAHEAD` (finds dominant nuclides at late times)
  - Use `PATHRESET` (re-calculates pathways at requested time)



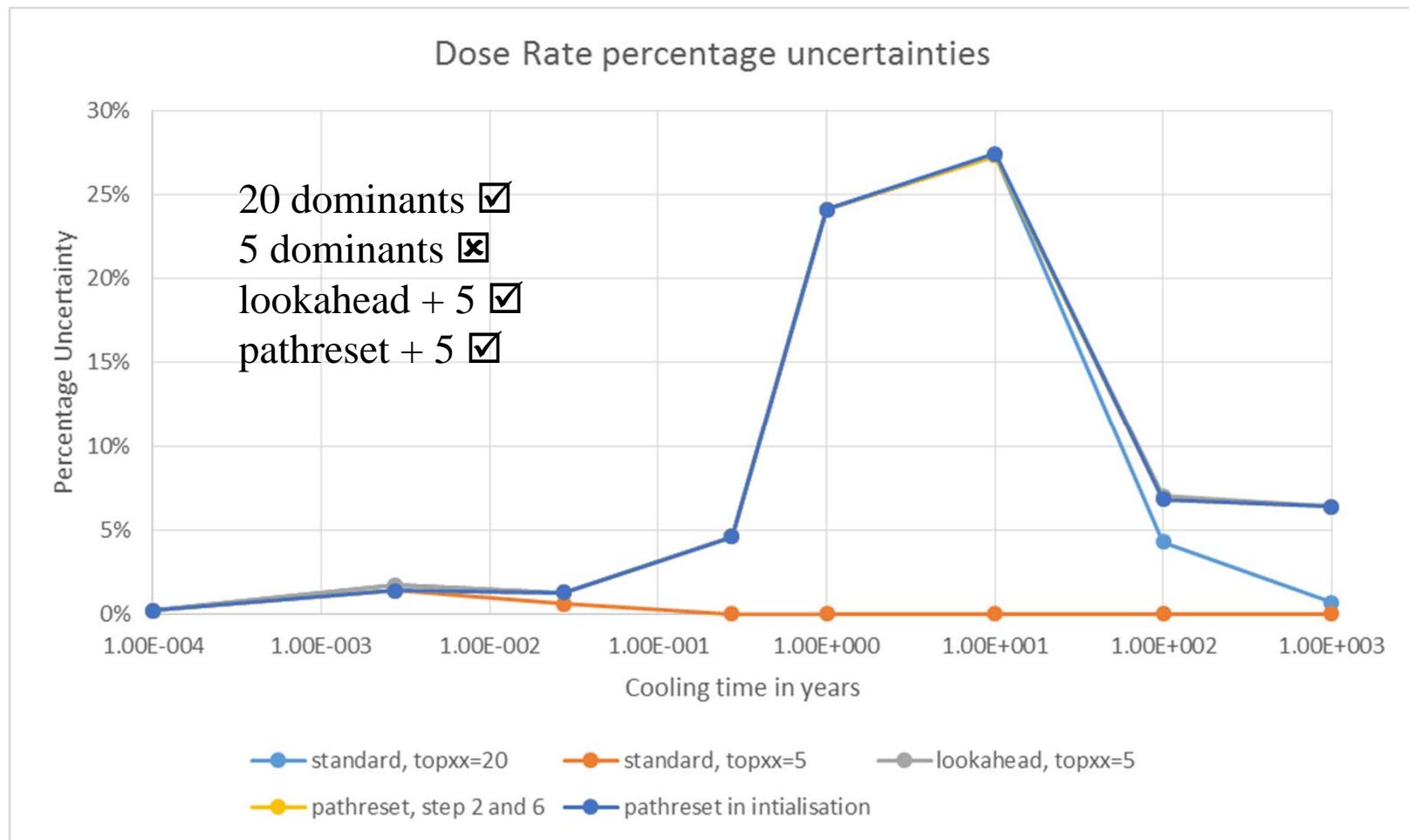
- LOOKAHEAD causes two-pass cooling:
- at ZERO, integrate cooling steps to get late time dominant nuclides
- merge additional dominants with dominant list at ZERO
- use merged list in pathways calculation



- Save dominant list at ZERO, *i.e.* the end of irradiation
- PATHRESET in cooling phase:
  - At PATHRESET keyword, check for new dominant nuclides
  - If no new dominant nuclides, do nothing
  - If found, redo pathways calculation with current dominant list
- PATHRESET in initialisation phase
  - Same as PATHRESET at all cooling steps

# Example: dose rate for SS316

- standard cases show late cooling time underestimates uncertainty; 25% at 1-10 years cooling





## Verification & Validation

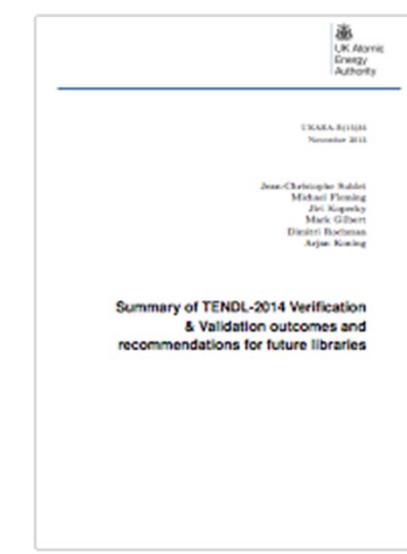
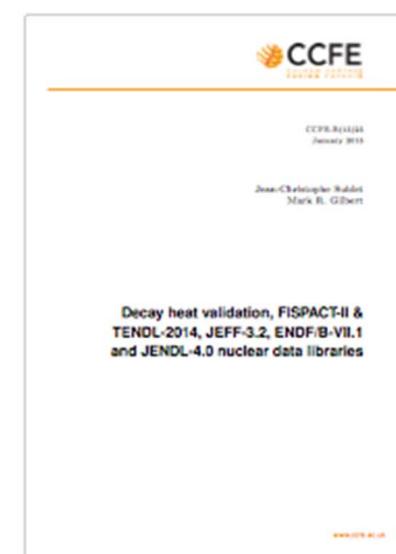
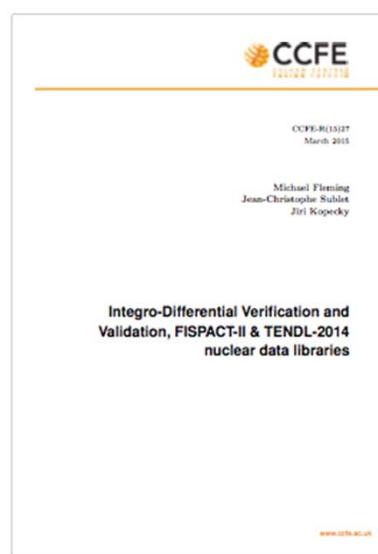
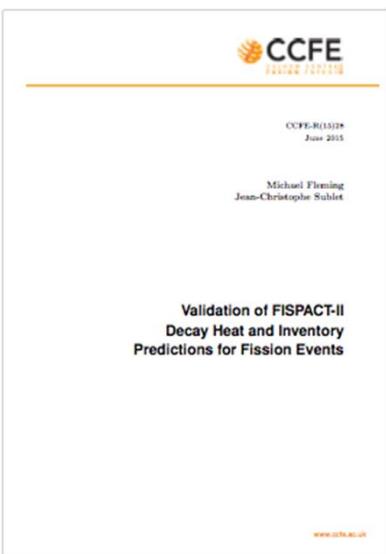
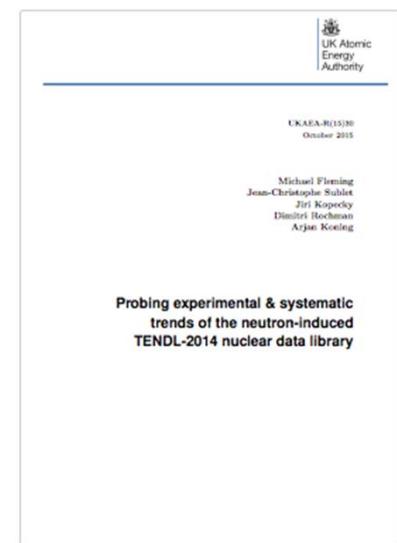
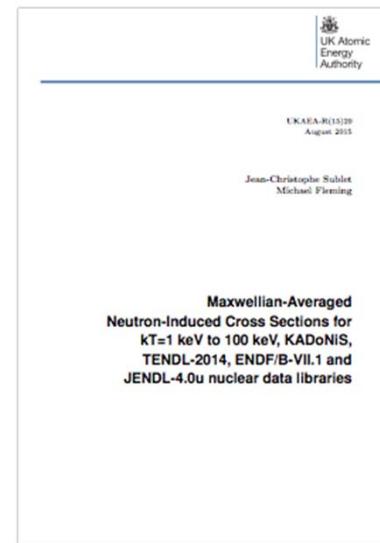
### Basic physics



- For a nuclear observables code like FISPACT-II, V&V takes several forms:
  - Comparison of nuclear data inputs against experimental data in a variety of forms
  - Consistency of nuclear data where no or limited experimental data is available
  - Completeness of the nuclear data to avoid error-by-omission (common and extremely problematic issue)
  - Checking code results against expected values and consistency of data handling between inputs
  - Validating code results against experimental data



- FISPACT-II and libraries are subject of various validation reports:
  - CCFE-R(15)25 Fusion decay heat
  - CCFE-R(15)27 Integral fusion
  - CCFE-R(15)28 Fission decay heat
  - UKAEA-R(15)29 Astro s-process
  - UKAEA-R(15)30 RI/therm/systematics
  - UKAEA-R(15)35 Summary report

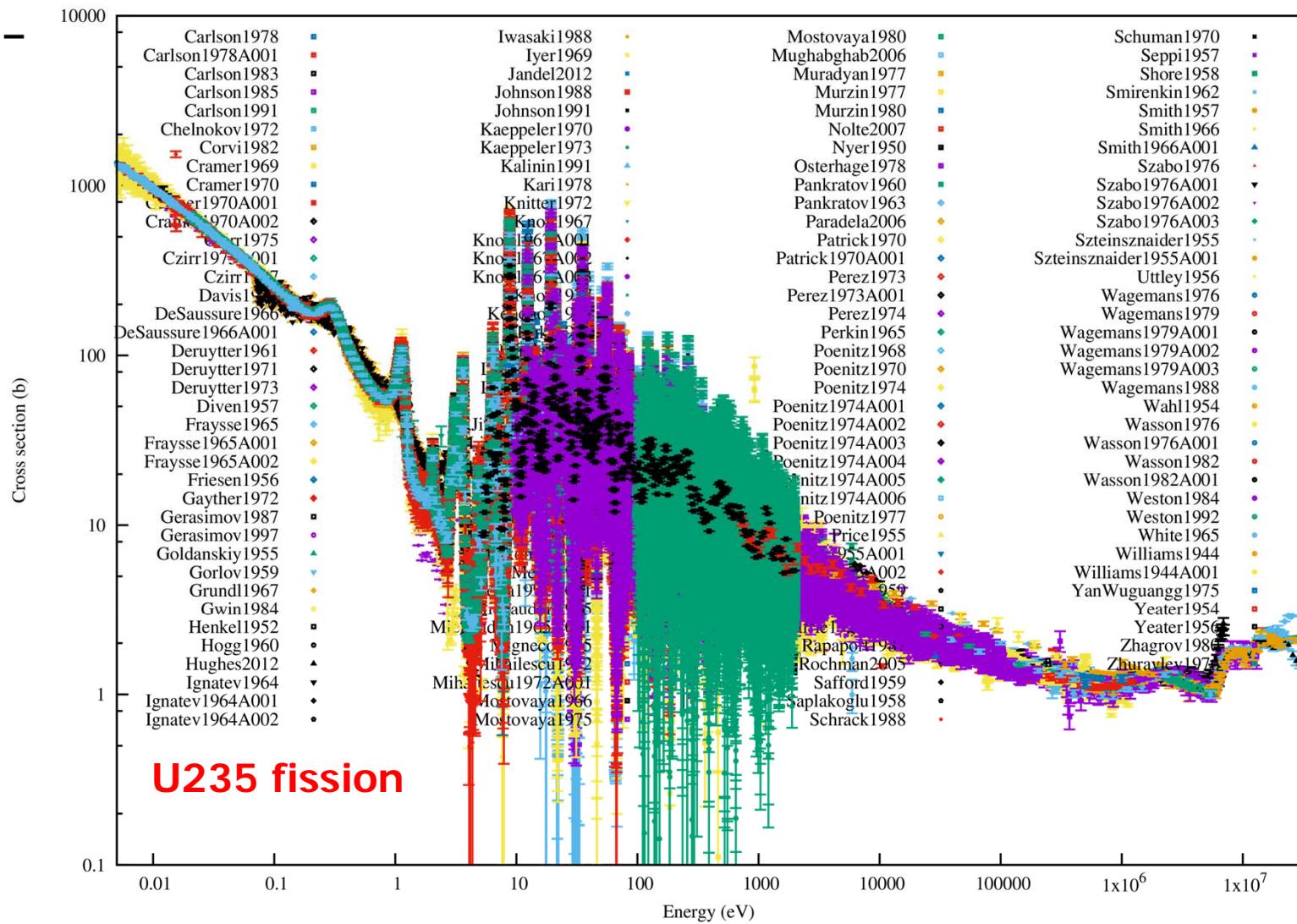




Typically these are divided into differential & integral:

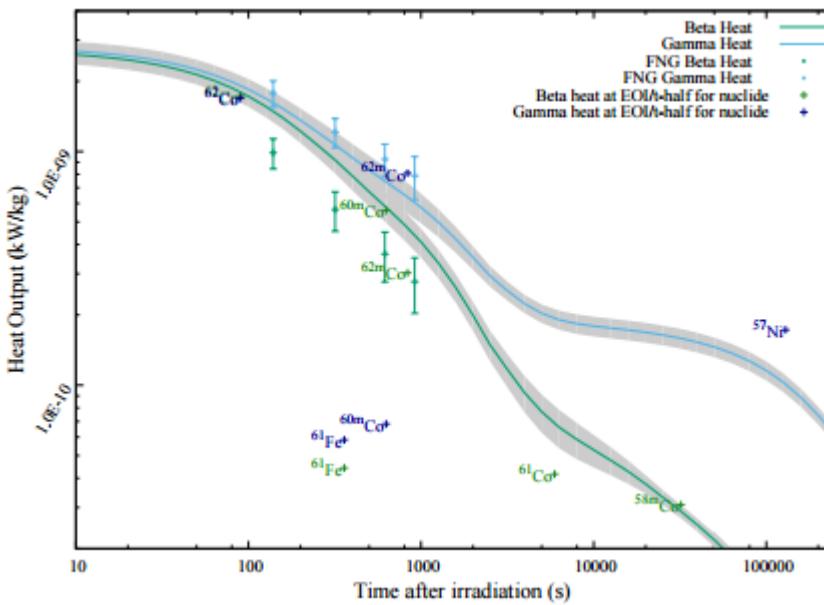
- Differential
  - C/E with the latest EXFOR database
  - C/C with other ENDF's files
  - SACS: Statistical Analysis of Cross Section
- Integral
  - Activation-transmutation; activity, gamma, decay heat
    - FISPACT-II validation suite (~500 reaction rates, thousands of integral E, time dependent, fast system)
  - MACS and RI: Maxwellian-averaged cross sections and astrophysical reaction rates, resonance integrals
  - Decay heat and inventories predictions for fission events

- Ideally we need differential (mono-energetic) measurements for cross-sections over all channels, energies

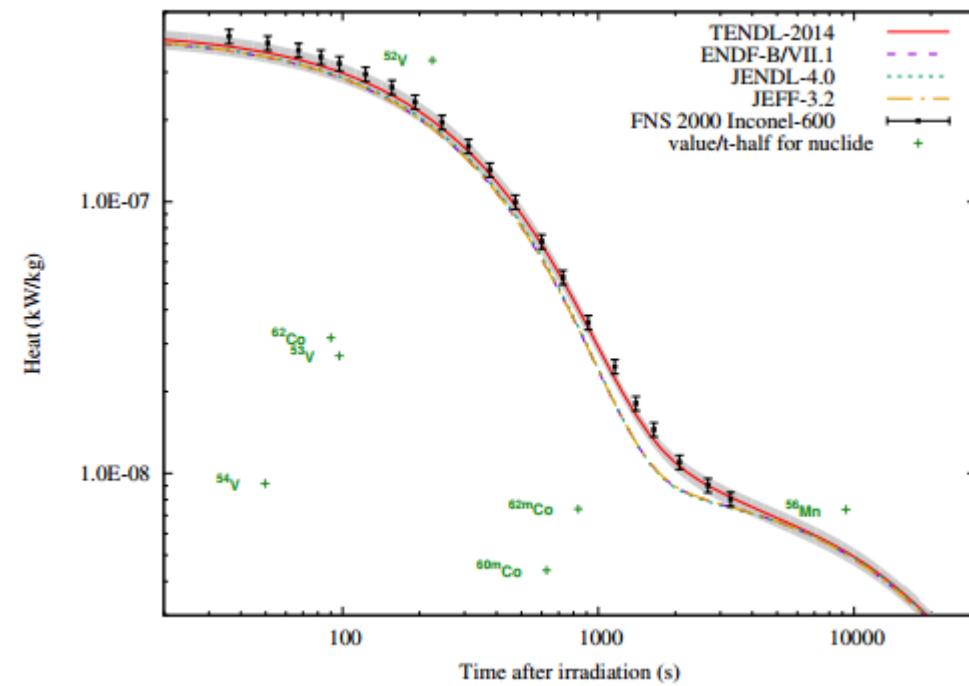


- But there are some 2800 nuclides with half-life above 1s and each with many reaction channels –
  - Very few are known well
  - Many have little or **zero** measurements
- Regardless of data, we often are required to generate simulation data for some application, 2 options:
  - Ignore the problem and the channels using some legacy file which doesn't contain the reactions
  - Use a technological library (TENDL) which contains the best available data
- FISPACT-II uniquely handles all TENDL data, but this requires more complex probing than simply checking against differential experiments

- Integral cross sections are inferred from post-irradiation measurements such as gamma-decays or calorimetric data

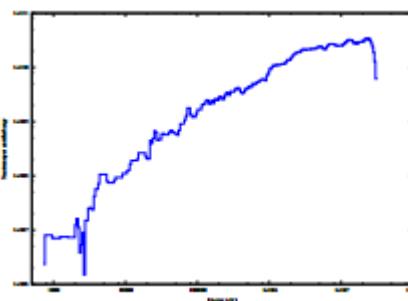
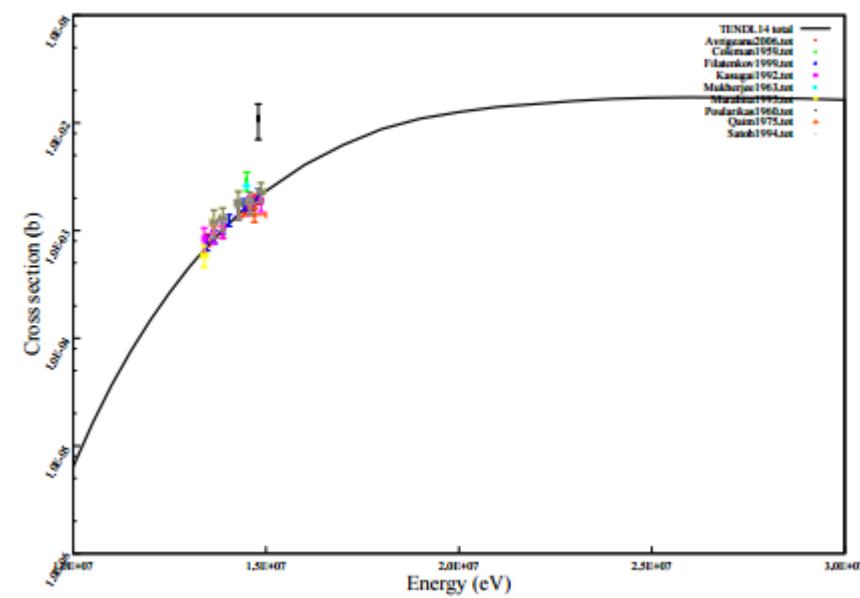
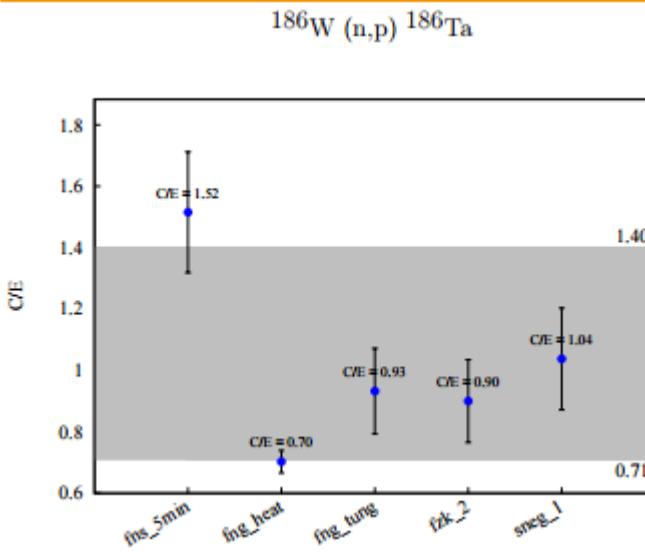


Spectroscopic heat from ENEA  
FNG campaign

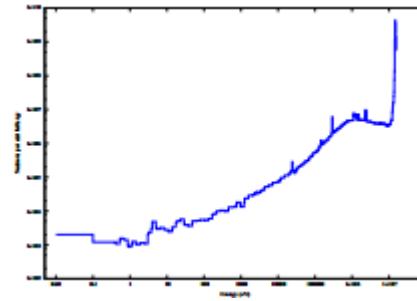


Total heat calorimetric  
measurements from JAEA  
FNS campaign

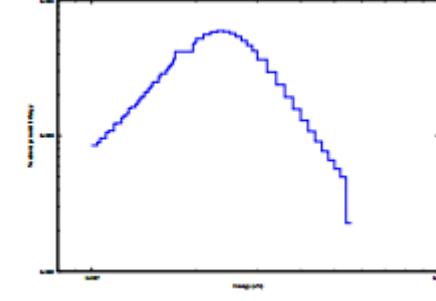
- The best approach is to use multiple experiments from different systems, covering int. and diff. experiments



Spectrum >100 MeV



Total heat FNS



D-Be gamma exp

- Often the measured nuclide can come from multiple reactions, or the heat may come from multiple radio-nuclides
  - Must de-convolve the experiment using simulation and pathways analyses (invalidating some experiments!)

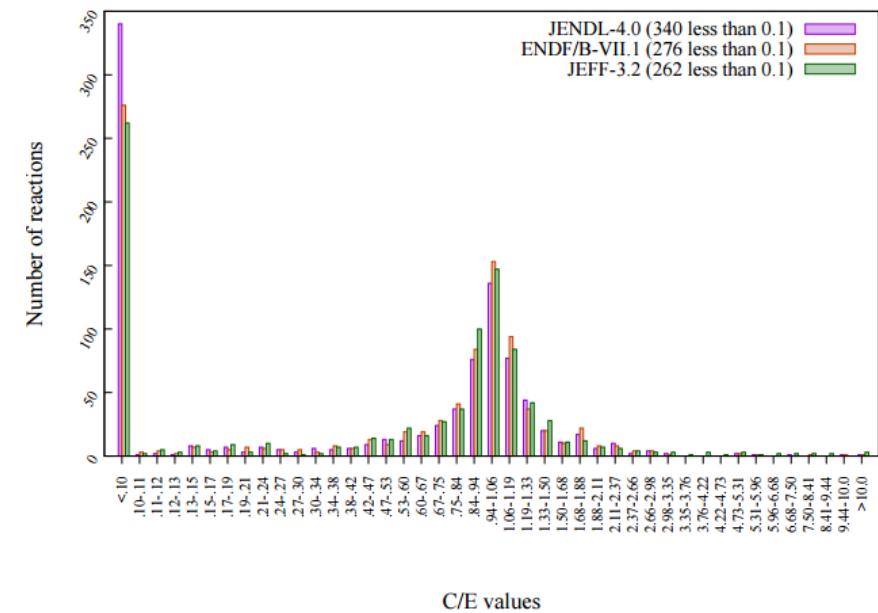
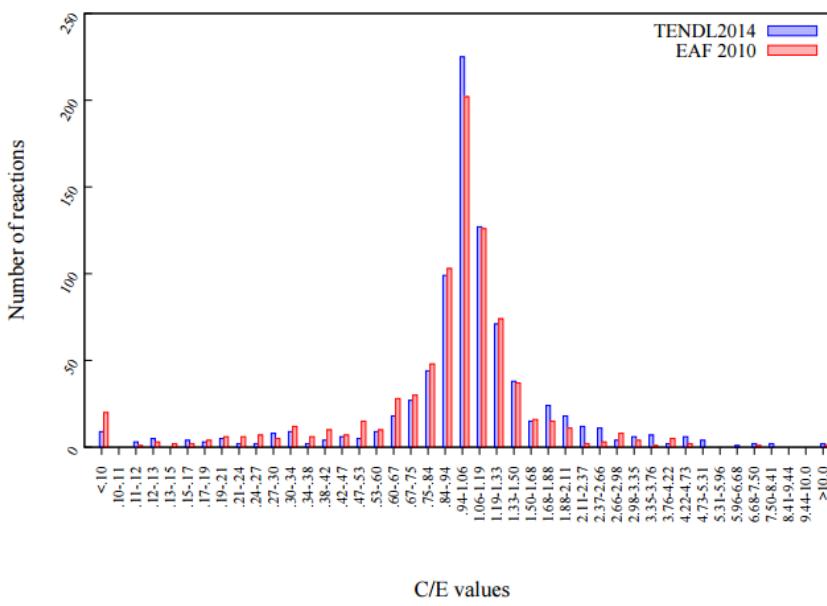
Product	Pathway(s)	%
Ta182	W182(n,p)Ta182	49.4
	W182(n,p)Ta182m(IT)Ta182	41.3
	W182(n,p)Ta182m(IT)Ta182m(IT)Ta182	3.7
	W183(n,d)Ta182	1.8
Sc47	Ti47(n,p)Sc47	41.2
	Ti48(n,np)Sc47	25.9
	Ti48(n,d)Sc47	18.1
	V50(n,a)Sc47	9.7
	V51(n,na)Sc47	5.4
In117	Sn117(n,p)In117	87.9
	Sn117(n,p)In117m(IT)In117	1.5
	Sn118(n,np)In117	6.9
	Sn118(n,d)In117	3.1
	Sn120(n,a)Cd117m(b-)In117	0.9

OK for total, not  
for isomeric

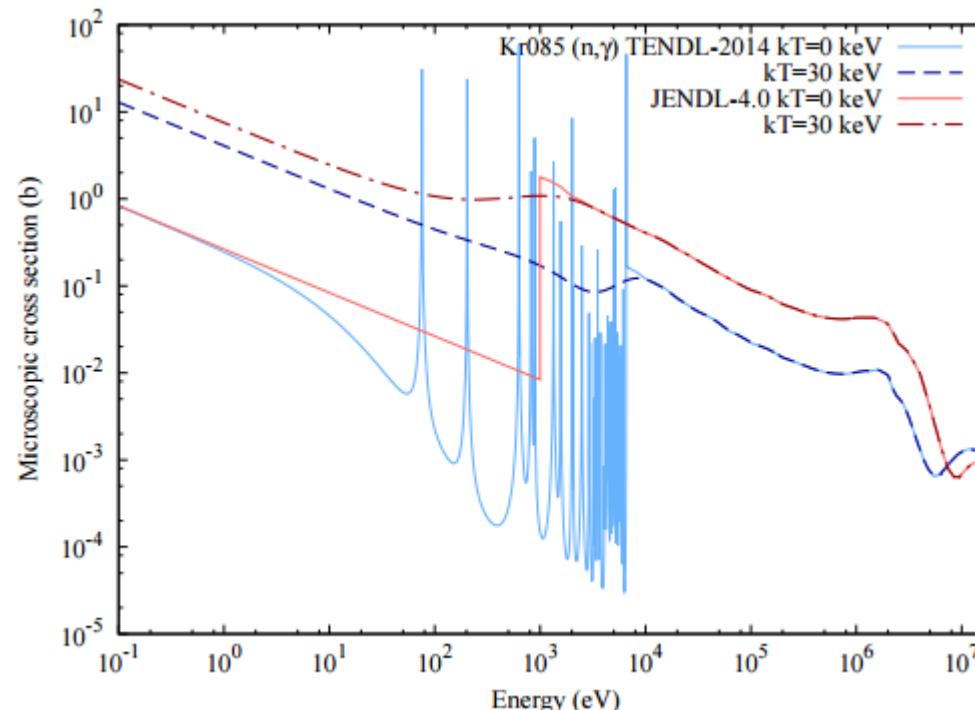
Too convoluted for  
experiment to isolate  
Sc47 as a product

Because minor paths  
have some data, we  
may use this for  
dominant pathway

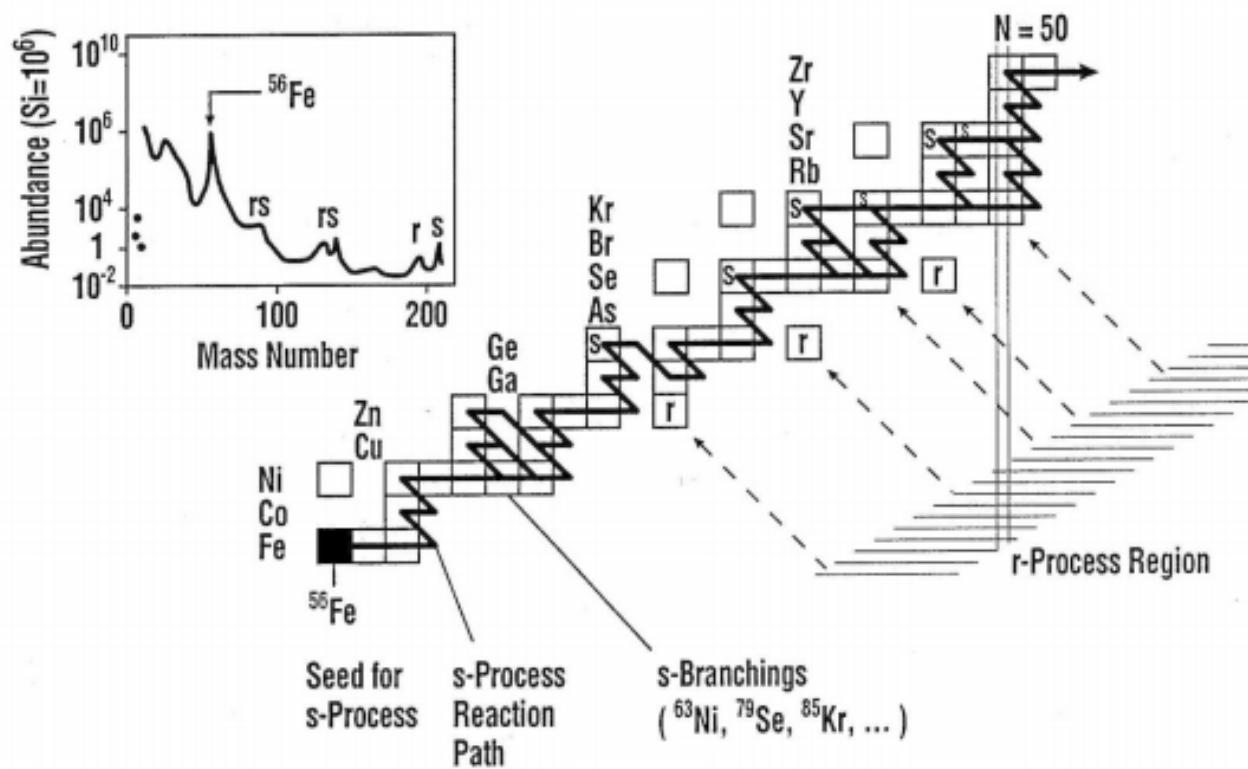
- Well-known libraries: ENDF/B-VII.1, JENDL-4.0u, JEFF-3.2 do not contain *at least 1/3 of reaction channels*
- TENDL-2014/15 outperform EAF, are complete and do not rely upon hand-modification – *allowing predictive capability*



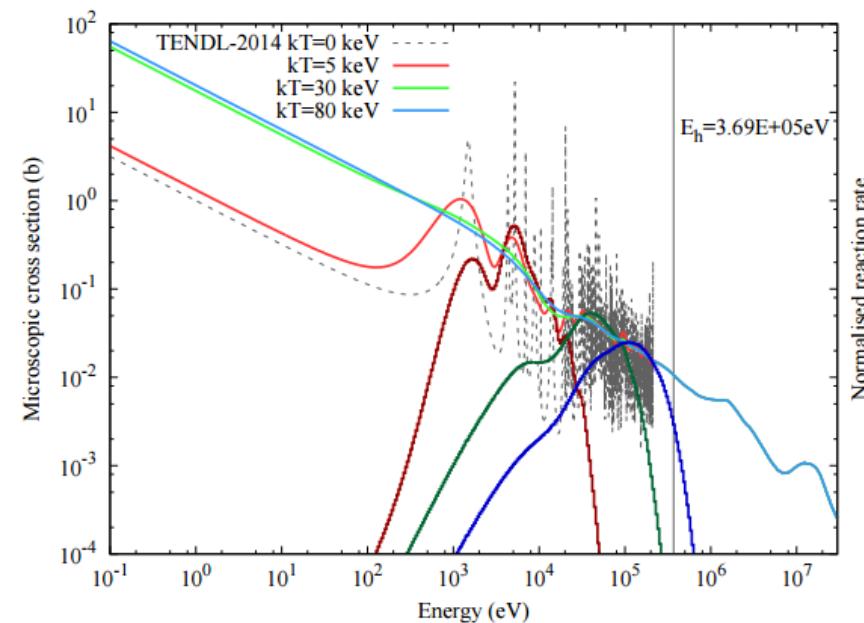
- Neutron capture and many other reactions are exothermic, allowing the reaction at any incident energy
- These reactions possess resonance structure which often determines reaction rate (aside from thermal spectra systems)
- Either the resonances have been measured, we statistically resolve them or (in non-TENDL) we get unphysical straight lines...



- Stellar nucleosynthesis offers an alternative (or complement) for resonance features
- Neutron capture is integral to element distribution in universe

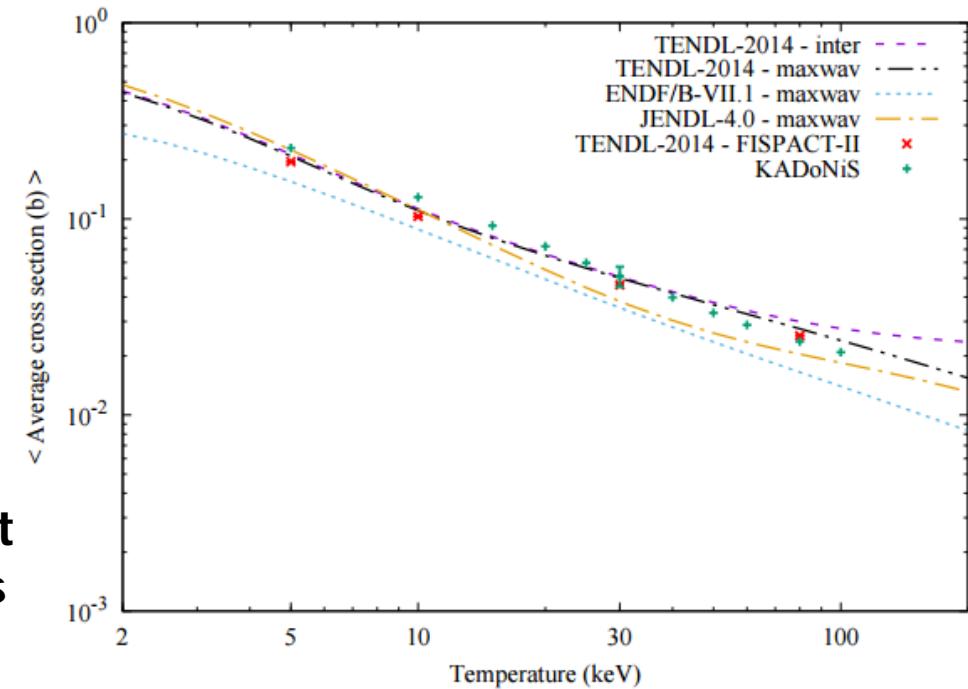


- The KADoNiS database includes some 357 nuclides over 11 Maxwellian-averaged temperatures for RR comparison

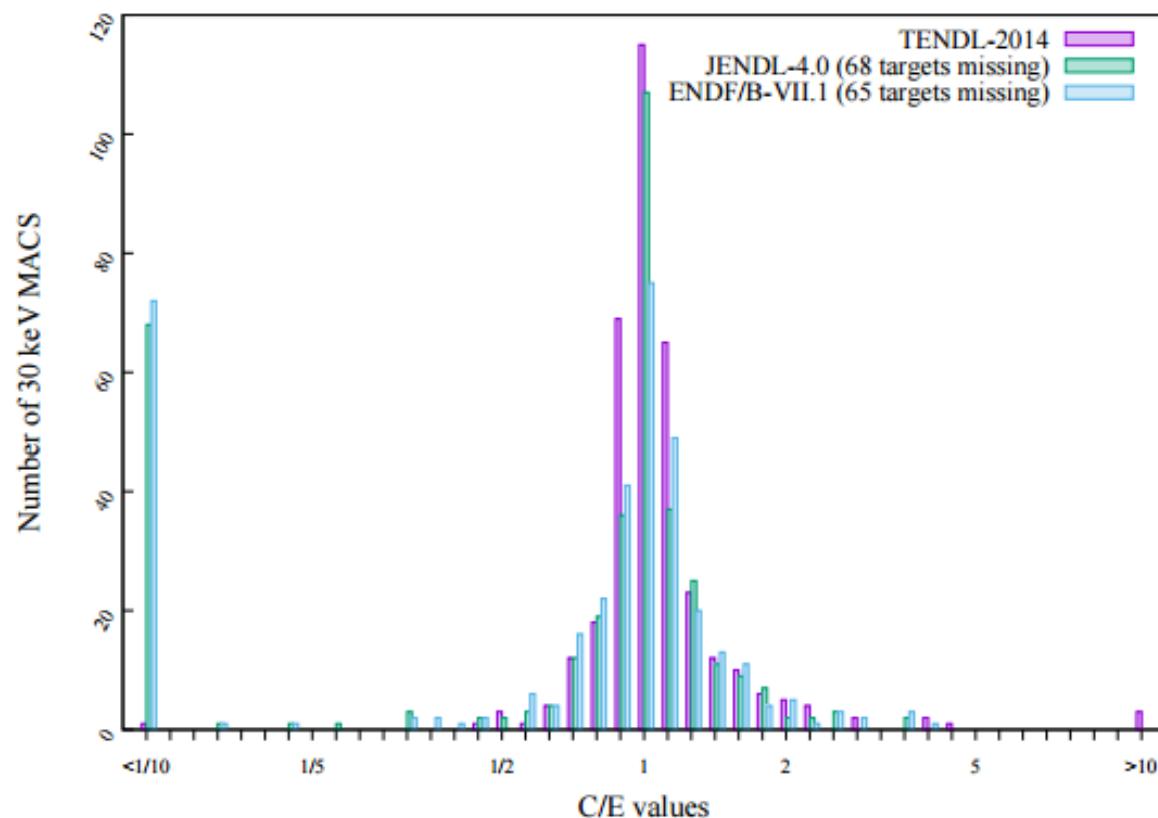


Temperature-dependent  
averaged cross-sections

### Broadened cross-sections



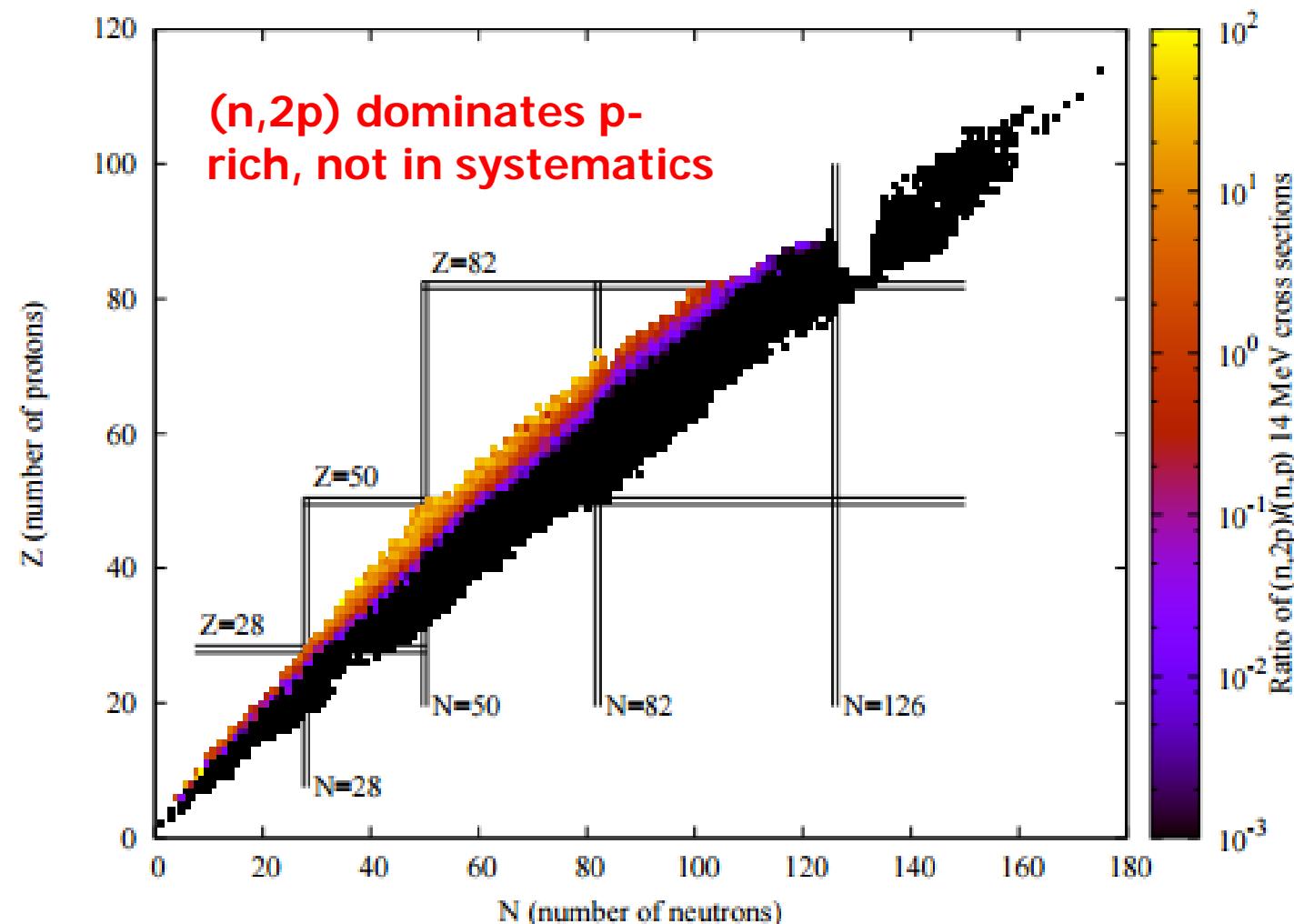
- About 20% of the channels are not in ENDF/B and JENDL, although TENDL of course includes all
- TENDL based on intelligent ‘stealing’ of best resonance parameter descriptions, so at least as good as legacy libraries



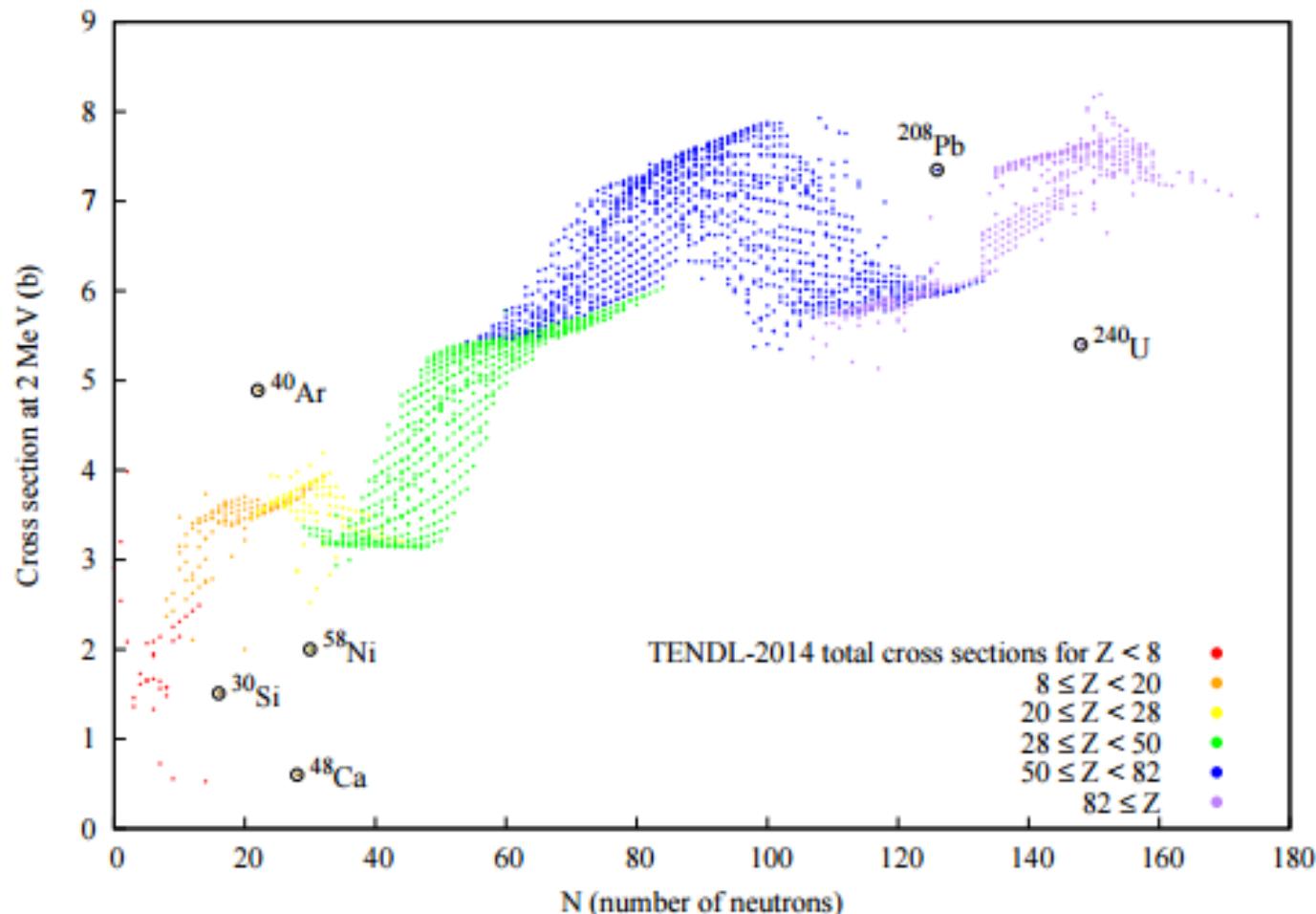


- For those without experiments, we can perform verification, consistency checks and look for outliers in global systematics
- A few options have been considered:
  - Use legacy systematics which were chi-square fitted to existing data (wary of extrapolation outside relevance)
  - Identify sensitive quantities and check trends
  - Probe any/all quantities and identify outliers

- For example, ( $n,p$ ) systematics for EAF were compared, here at 14 MeV



- Trends (here in total) help find programming glitches after various effects (shell, high-energy resolved resonances, etc) have been taken into account



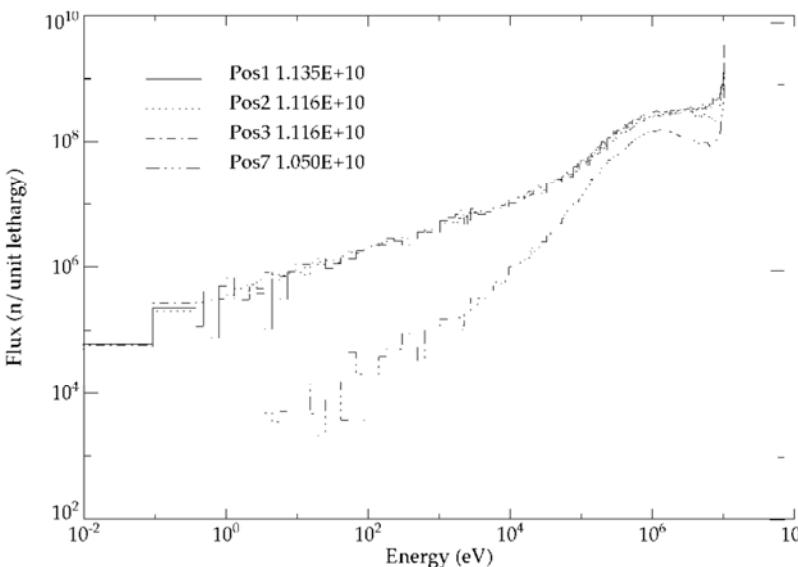
- For activation-based studies, complete nuclear data is required to prevent extreme simulation errors
- Where data exists, FISPACT-II and the nuclear data libraries have been tested
  - Legacy libraries fail in many scenarios, but TENDL offers complete simulation with predictive power
- UKAEA have performed extensive testing of TENDL against experiments covering a variety of systems/regimes and against systematics
- For application-specific studies, direct comparison of code outputs and observables is the best validation – see next



## Verification & Validation

## Applications

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

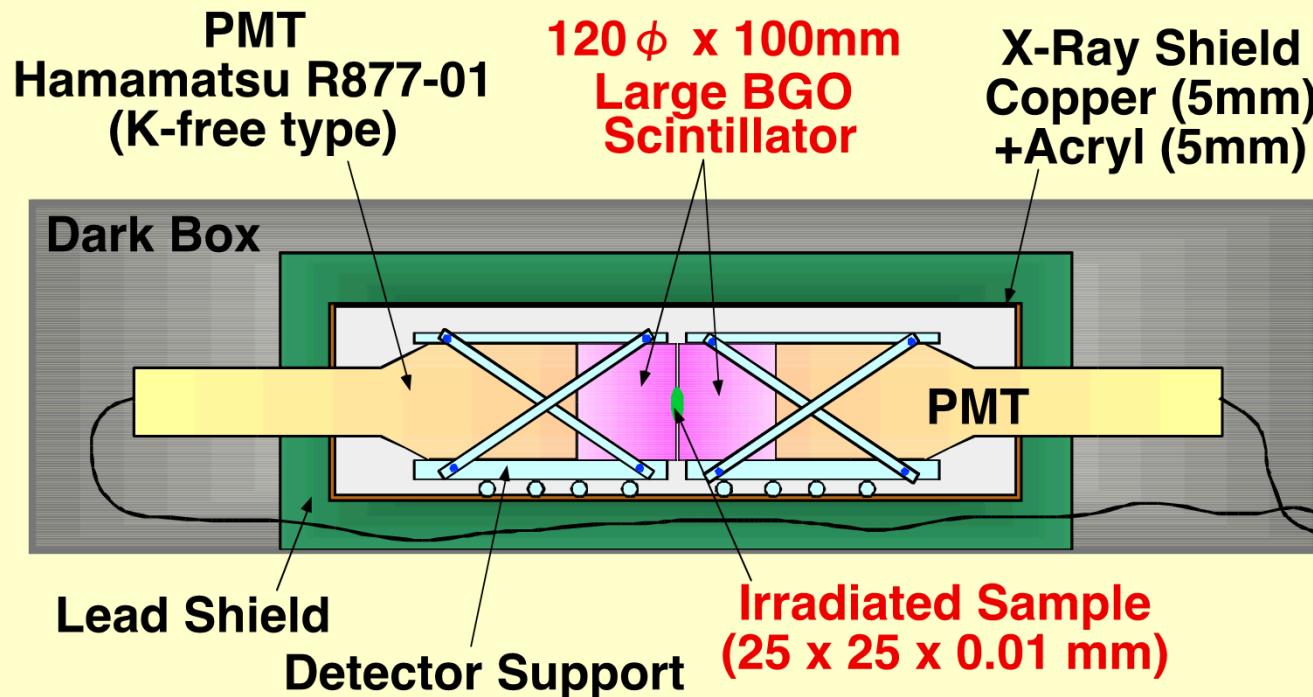


FNS Neutron spectra, neutron fluence monitored by  $^{27}\text{Al}(\text{n},\text{a})\text{Na}^{24}$

Two experimental campaigns:  
1996 and 2000; 74 materials

Z	Element	Form	Z	Element	Form
9	Fluorine	$\text{CF}_2$	46	Palladium	Metallic Foil
11	Sodium	$\text{Na}_2\text{CO}_3$	47	Silver	Metallic Foil
12	Magnesium	$\text{MgO}$	48	Cadmium	Metallic Foil
13	Aluminium	Metallic Foil	49	Indium	Metallic Foil
14	Silicon	Metallic Powder	50	Tin	$\text{SnO}_2$
15	Phosphorus	$\text{P}_3\text{N}_5$	51	Antimony	Metallic Powder
16	Sulphur	Powder	52	Tellurium	$\text{TeO}_2$
17	Chlorine	$\text{C}_2\text{H}_2\text{Cl}_2$	53	Iodine	$\text{IC}_6\text{H}_4\text{OH}$
19	Potassium	$\text{K}_2\text{CO}_3$	55	Caesium	$\text{Cs}_2\text{O}_3$
20	Calcium	$\text{CaO}$	56	Barium	$\text{BaCO}_3$
21	Scandium	$\text{Sc}_2\text{O}_3$	57	Lanthanum	$\text{La}_2\text{O}_3$
22	Titanium	Metallic Foil	58	Cerium	$\text{CeO}_2$
23	Vanadium	Metallic Foil	59	Praseodymium	$\text{Pr}_6\text{O}_{11}$
24	Chromium	Metallic Powder	60	Neodymium	$\text{Nd}_2\text{O}_3$
25	Manganese	Metallic Powder	62	Samarium	$\text{Sm}_2\text{O}_3$
26	Iron	Metallic Foil	63	Europium	$\text{Eu}_2\text{O}_3$
Alloy	SS304	Metallic Foil	64	Gadolinium	$\text{Gd}_2\text{O}_3$
Alloy	SS316	Metallic Foil	65	Terbium	$\text{Tb}_4\text{O}_7$
27	Cobalt	Metallic Foil	66	Dysprosium	$\text{Dy}_2\text{O}_3$
Alloy	Inconel-600	Metallic Foil	67	Holmium	$\text{Ho}_2\text{O}_3$
28	Nickel	Metallic Foil	68	Erbium	$\text{Er}_2\text{O}_3$
Alloy	Nickel-chrome	Metallic Foil	69	Thulium	$\text{Tm}_2\text{O}_3$
29	Copper	Metallic Foil	70	Ytterbium	$\text{Yb}_2\text{O}_3$
30	Zinc	Metallic Foil	71	Lutetium	$\text{Lu}_2\text{O}_3$
31	Gallium	$\text{Ga}_2\text{O}_3$	72	Hafnium	Metallic Powder
32	Germanium	$\text{GeO}_2$	73	Tantalum	Metallic Foil
33	Arsenic	$\text{As}_2\text{O}_3$	74	Tungsten	Metallic Foil
34	Selenium	Metallic Powder	75	Rhenium	Metallic Powder
35	Bromine	$\text{BrC}_6\text{H}_4\text{COOH}$	76	Osmium	Metallic Powder
37	Rubidium	$\text{Rb}_2\text{CO}_3$	77	Iridium	Metallic Powder
38	Strontium	$\text{SrCO}_3$	78	Platinum	Metallic Foil
39	Yttrium	$\text{Y}_2\text{O}_3$	79	Gold	Metallic Foil
40	Zirconium	Metallic Foil	80	Mercury	$\text{HgO}$
41	Niobium	Metallic Foil	81	Thallium	$\text{TI}_2\text{O}$
42	Molybdenum	Metallic Foil	82	Lead	Metallic Foil
44	Ruthenium	Metallic Powder	83	Bismuth	Metallic Powder
45	Rhodium	Metallic Powder			

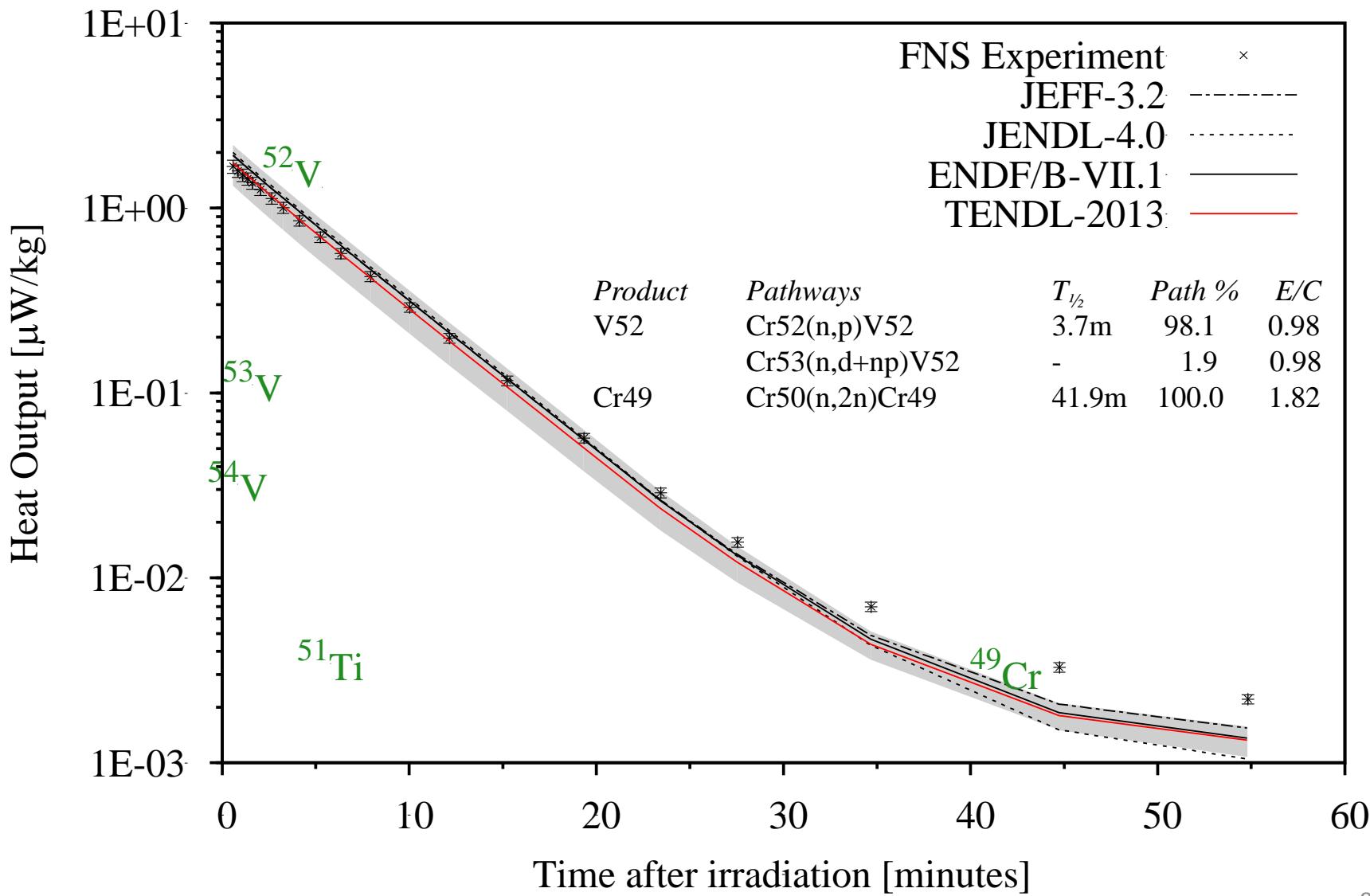
## WHOLE ENERGY ABSORPTION SPECTROMETER



**Detection Efficiency ~ 100 %**  
**for both beta- and gamma-rays**

random-walk uncertainty

FNS-00 5 Min. Irradiation - Cr



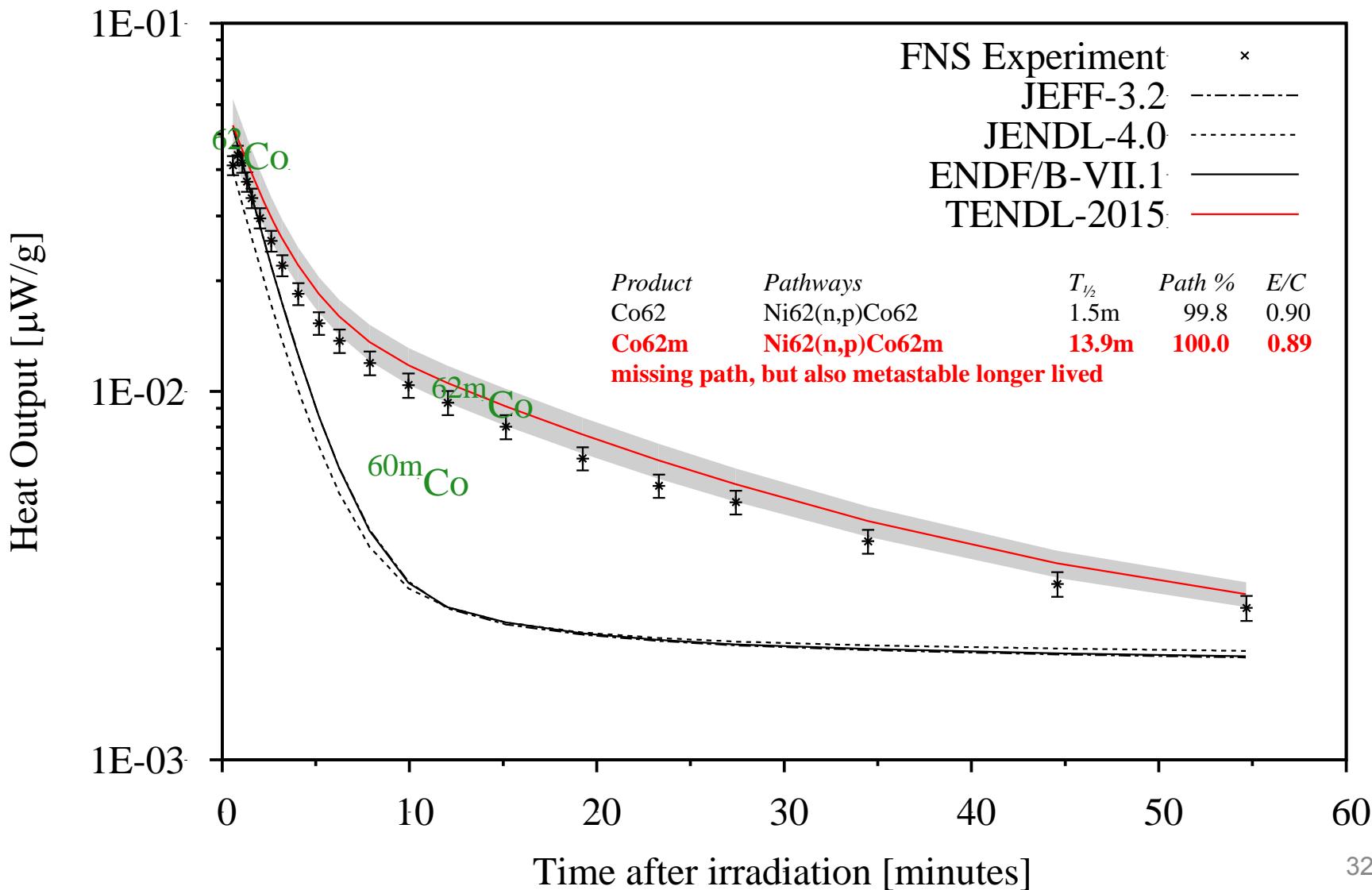


Times	FNS EXP. 5 mins	TENDL-2013	ENDF/ B-VII.1	JEFF-3.2	JENDL-4.0		
M in.	$\mu\text{W/g}$	$\mu\text{W/g}$	E/C	E/C	E/C		
0.58	1.68E + 00	+ / -8%	1.76E + 00	+ / -25% 0.96	0.87	0.87	0.84
0.85	1.58E + 00	+ / -8%	1.66E + 00	+ / -25% 0.95	0.87	0.87	0.84
1.10	1.51E + 00	+ / -8%	1.58E + 00	+ / -25% 0.96	0.87	0.87	0.84
1.37	1.44E + 00	+ / -8%	1.49E + 00	+ / -25% 0.96	0.88	0.88	0.85
1.62	1.37E + 00	+ / -7%	1.42E + 00	+ / -25% 0.96	0.87	0.87	0.85
2.05	1.26E + 00	+ / -7%	1.30E + 00	+ / -25% 0.97	0.88	0.88	0.85
2.65	1.13E + 00	+ / -7%	1.15E + 00	+ / -26% 0.98	0.88	0.89	0.86
3.27	1.00E + 00	+ / -7%	1.02E + 00	+ / -26% 0.98	0.89	0.89	0.86
4.13	8.53E - 01	+ / -7%	8.64E - 01	+ / -26% 0.99	0.89	0.89	0.86
5.25	6.95E - 01	+ / -6%	6.97E - 01	+ / -26% 1.00	0.90	0.90	0.87
6.35	5.67E - 01	+ / -6%	5.66E - 01	+ / -26% 1.00	0.90	0.91	0.88
7.93	4.26E - 01	+ / -6%	4.20E - 01	+ / -26% 1.02	0.92	0.92	0.89
10.03	2.90E - 01	+ / -6%	2.83E - 01	+ / -26% 1.03	0.93	0.93	0.90
12.15	1.98E - 01	+ / -6%	1.90E - 01	+ / -26% 1.04	0.94	0.94	0.91
15.23	1.16E - 01	+ / -6%	1.08E - 01	+ / -26% 1.08	0.97	0.98	0.95
19.33	5.70E - 02	+ / -6%	5.06E - 02	+ / -25% 1.13	1.02	1.02	1.00
23.43	2.88E - 02	+ / -6%	2.38E - 02	+ / -24% 1.21	1.10	1.09	1.09
27.55	1.56E - 02	+ / -6%	1.21E - 02	+ / -22% 1.29	1.18	1.16	1.19
34.68	6.98E - 03	+ / -6%	4.37E - 03	+ / -17% 1.60	1.50	1.43	1.62
44.75	3.28E - 03	+ / -6%	1.80E - 03	+ / -17% 1.82	1.76	1.58	2.18
54.82	2.21E - 03	+ / -6%	1.32E - 03	+ / -18% 1.67	1.62	1.44	2.10

Product	Pathways	$T_{1/2}$	Path %	E/C	$\Delta E\%$
V52	Cr52(n,p)V52	3.7m	98.1	0.98	7%
	Cr53(n,d+ np)V52		1.9	0.98	7%
Cr49	Cr50(n,2n)Cr49	41.9m	100.0	1.82	6%

## Random walk uncertainty

## FNS-00 5 Min. Irradiation - Ni



# Decay power: FNS JAERI Ni

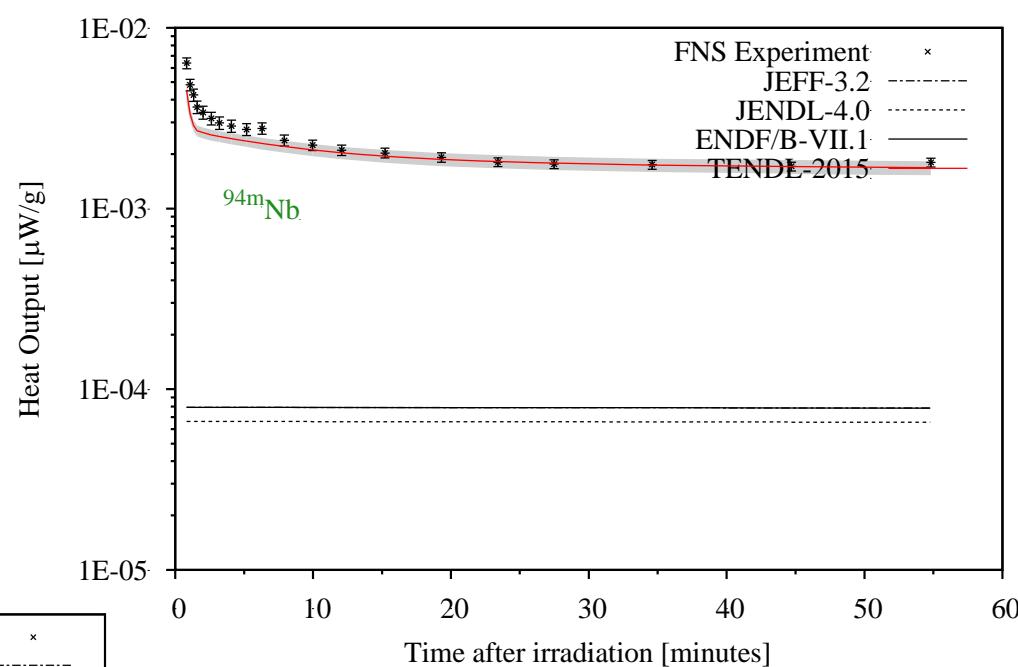
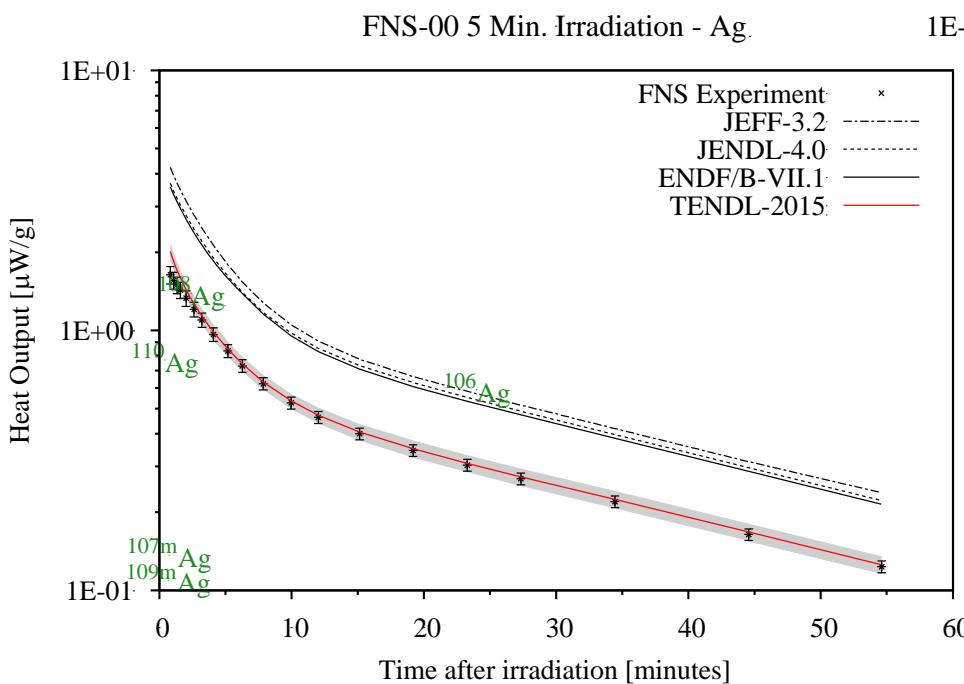
Times	FNS EXP. 5 mins	TENDL-2013	ENDF/ B-VII.1	JEFF-3.2	JENDL-4.0
M in.	μW/g	μW/g	E/C	E/C	E/C
0.58	4.11E-02 + / -6%	4.90E-02 + / -22% 0.84	0.79	0.79	1.04
0.83	4.38E-02 + / -6%	4.55E-02 + / -22% 0.96	0.94	0.94	1.23
1.08	4.18E-02 + / -6%	4.24E-02 + / -21% 0.99	1.00	1.00	1.30
1.33	3.71E-02 + / -6%	3.95E-02 + / -21% 0.94	0.99	0.99	1.29
1.58	3.35E-02 + / -6%	3.70E-02 + / -21% 0.90	0.99	0.99	1.29
2.02	2.95E-02 + / -6%	3.32E-02 + / -20% 0.89	1.05	1.05	1.35
2.62	2.56E-02 + / -6%	2.89E-02 + / -20% 0.89	1.17	1.17	1.49
3.22	2.20E-02 + / -7%	2.55E-02 + / -20% 0.86	1.27	1.27	1.60
4.07	1.84E-02 + / -7%	2.19E-02 + / -21% 0.84	1.46	1.46	1.82
5.17	1.53E-02 + / -7%	1.86E-02 + / -22% 0.83	1.79	1.79	2.16
6.27	1.37E-02 + / -7%	1.63E-02 + / -23% 0.84	2.22	2.22	2.60
7.88	1.19E-02 + / -7%	1.39E-02 + / -24% 0.86	2.85	2.84	3.15
9.95	1.04E-02 + / -8%	1.20E-02 + / -24% 0.87	3.44	3.42	3.57
12.05	9.32E-03 + / -8%	1.06E-02 + / -24% 0.88	3.59	3.62	3.59
15.15	8.02E-03 + / -7%	9.02E-03 + / -24% 0.89	3.40	3.44	3.40
19.25	6.58E-03 + / -7%	7.47E-03 + / -24% 0.88	2.99	3.01	2.97
23.32	5.54E-03 + / -7%	6.29E-03 + / -23% 0.88	2.62	2.64	2.59
27.42	5.00E-03 + / -7%	5.39E-03 + / -22% 0.93	2.43	2.45	2.39
34.48	3.92E-03 + / -8%	4.27E-03 + / -22% 0.92	1.96	1.97	1.92
44.58	3.00E-03 + / -8%	3.29E-03 + / -23% 0.91	1.54	1.55	1.50
54.68	2.58E-03 + / -8%	2.72E-03 + / -24% 0.95	1.35	1.36	1.31

Product	Pathways	T <sub>1/2</sub>	Path %	E/C Δ E%
Co62	Ni62(n,p)Co62	1.5m	99.8	0.90 6%
Co62m	Ni62(n,p)Co62m	13.9m	100.0	0.89 7%

# Decay power: FNS JAERI

When you do not account for isomer production channels....

The responses are missed entirely !!



Hunt for the isomers, the short lived...

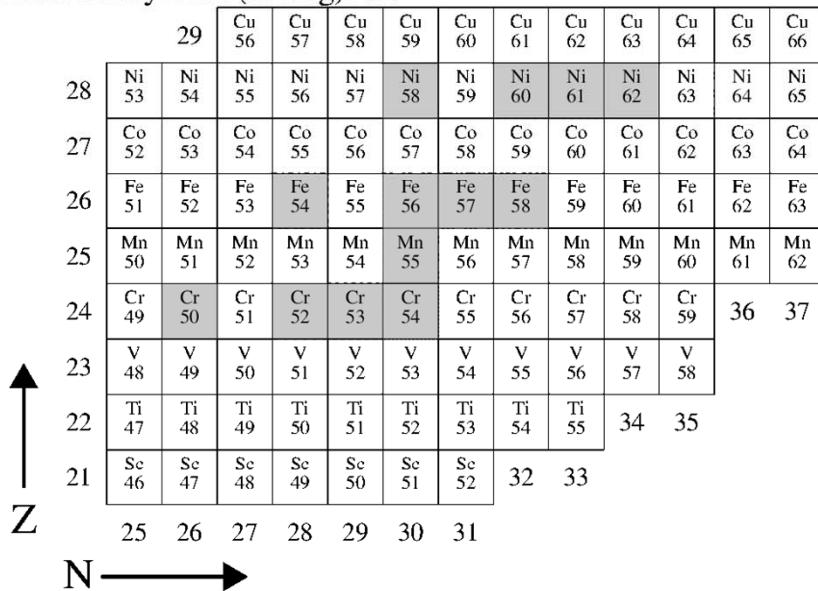
Most are lost in seconds, minutes...



# Decay power simulation with FISPACT-II

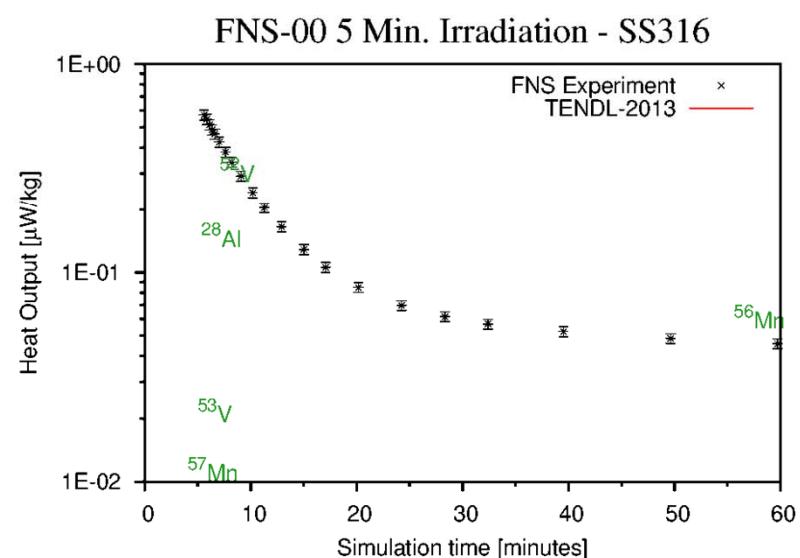
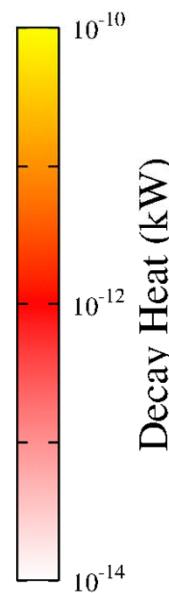
Time: 0.00 seconds

Total Decay Heat (kW/kg): 0.0



N →

Simulation of SS316 irradiated in JAEA FNS  
m - metastable state(s) > 50%



M.R. Gilbert & J.-Ch. Sublet CCFE-R(14)21 JAEA FNS Decay heat validation  
M. R. Gilbert et al., "Inventory Visualisation techniques" Nucl. Sci. Eng. (2014)



- Fission provides a convoluted system to simulate – including 1000+ radioactive fission products
- Fission can be handled as a independent or cumulative quantity, as post-prompt neutron or equilibrium (reactor)
  - FISPACT-II can process either depending on application, but handles ***full decay for all products***, eliminating benefit of cumulative
- Post-irradiation decay heat is a well-measured quantity for various fissile nuclides, including spectroscopic heat

- Example: liquid-He boil-off calorimetry for LANL OWR irradiation of various samples

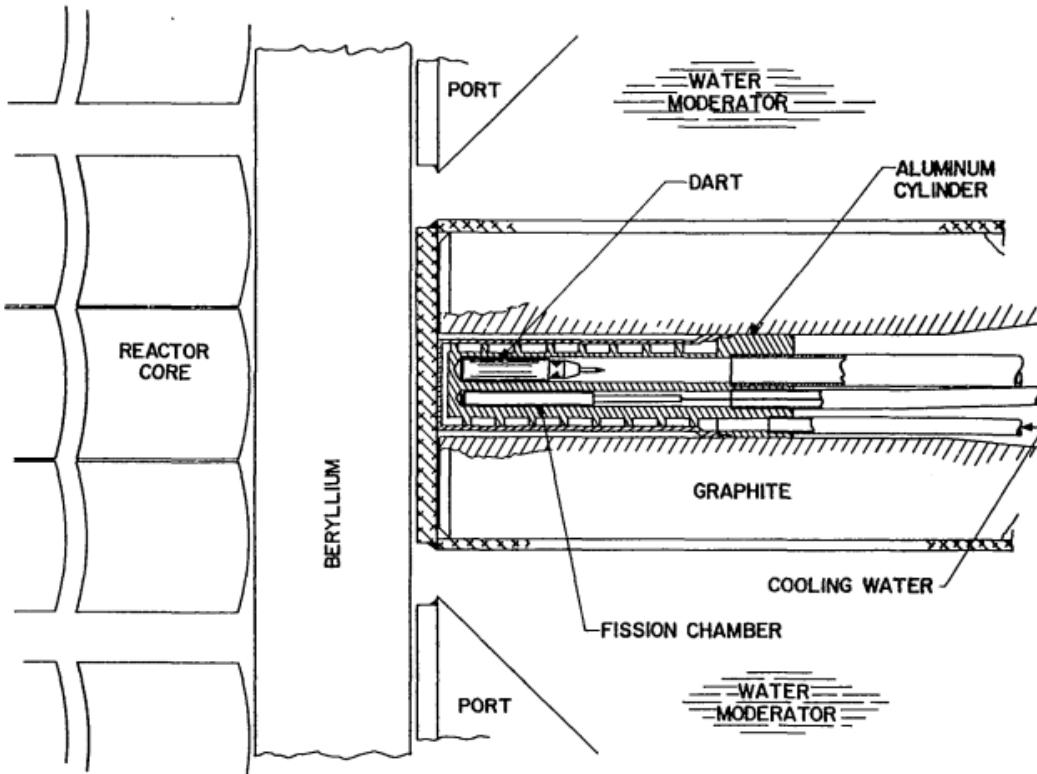


Fig. 2.

Facility used for sample irradiation. The facility is located in one of the 152-mm-diam ports of the 8-MW OWR. The port walls are made of aluminum. The fission chamber adjacent to the sample was used to control the reactor power during irradiation.

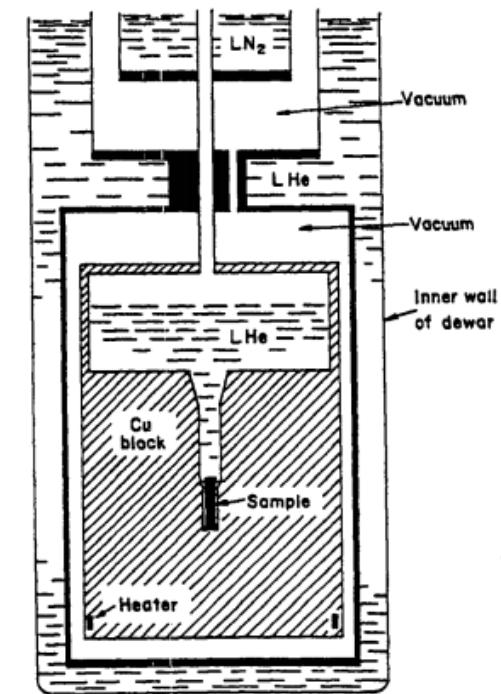


Fig. 3.

Active portion of the boil-off calorimeter. Radiation from the sample was absorbed in the copper block and was used to evaporate liquid helium from the reservoir in the top of the block. Heat leak into the copper block was prevented by the vacuum jacket and the outer helium bath.

- Simulation of 5.5 hours thermal irradiation using full independent yields, followed by cooling periods below. Note measurements from 10 s cooling up to ~1 day.

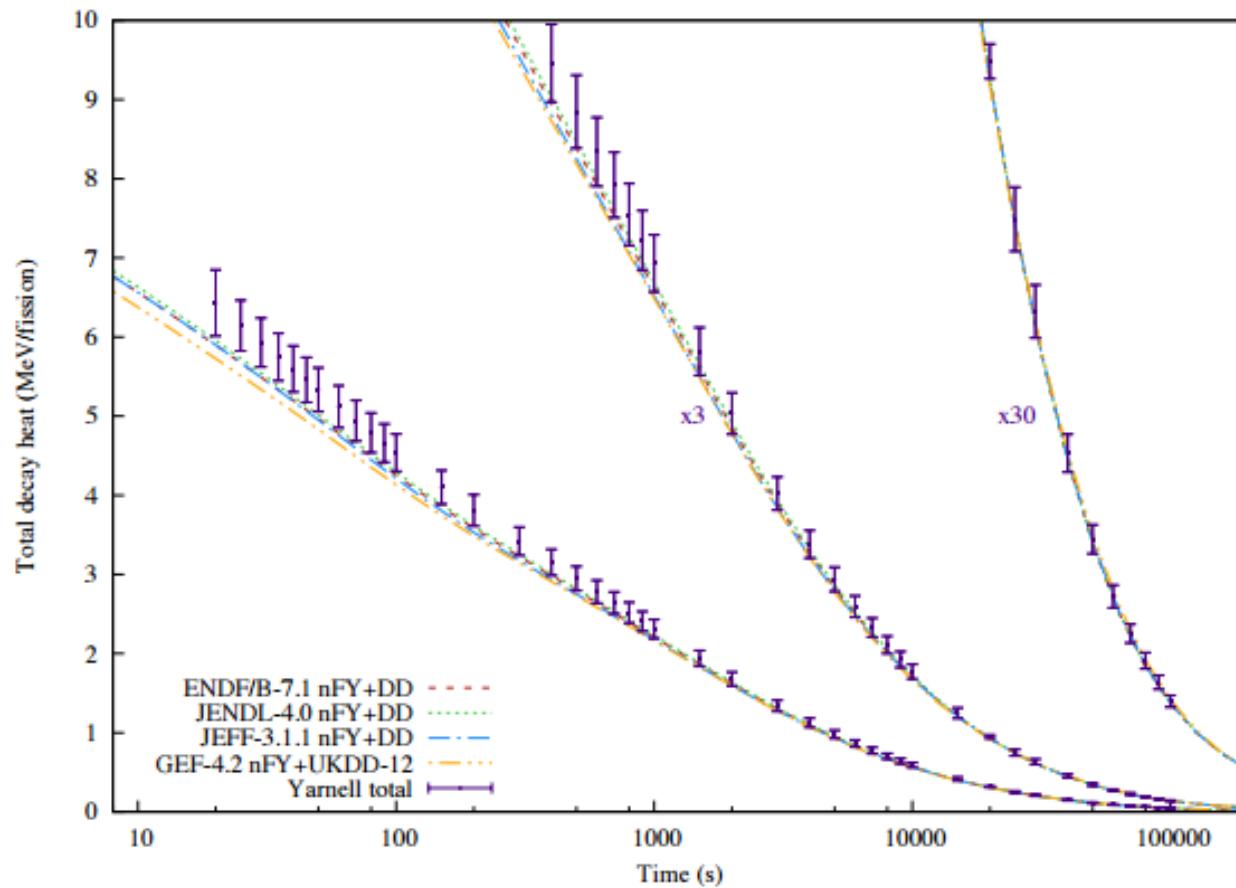
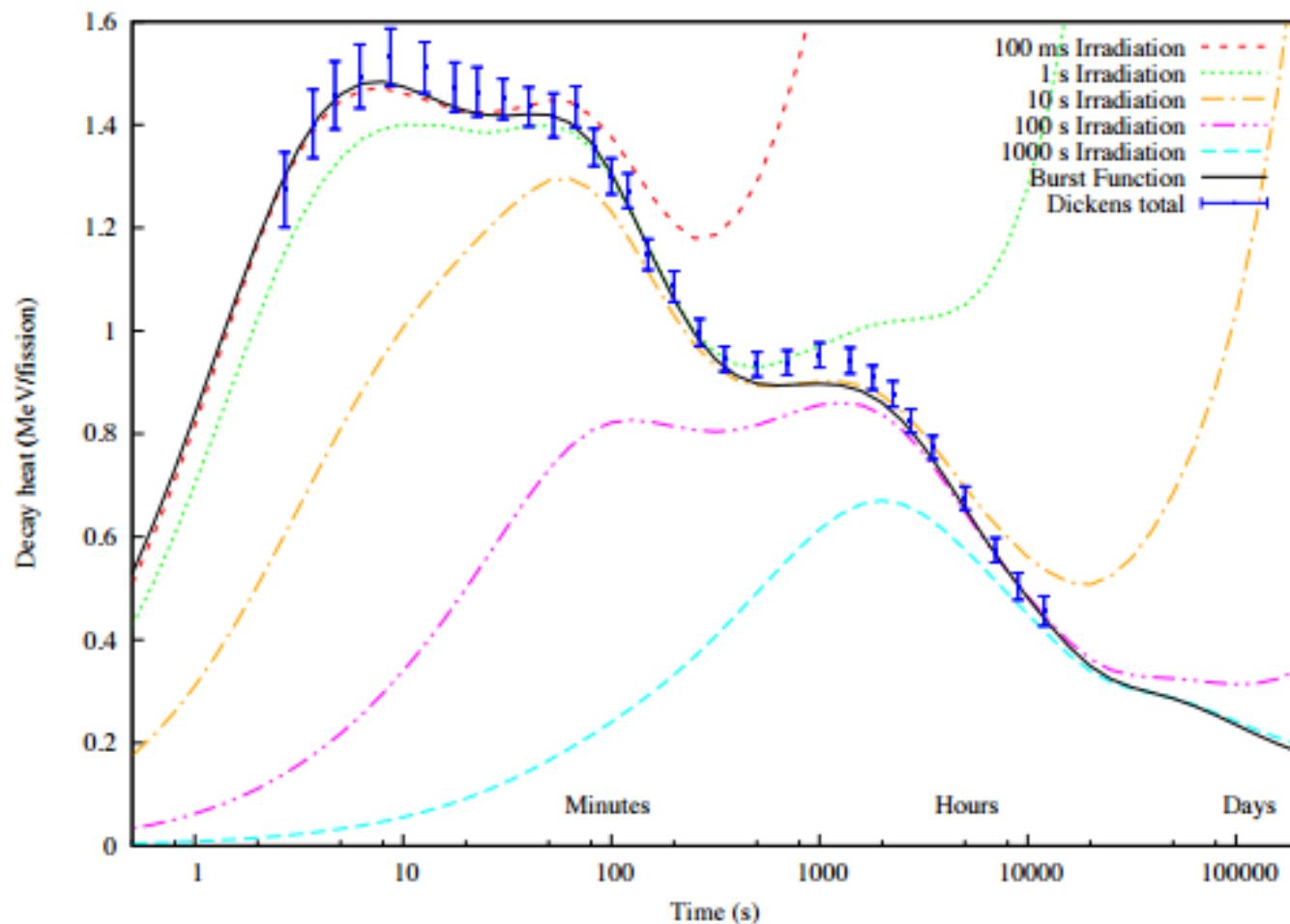
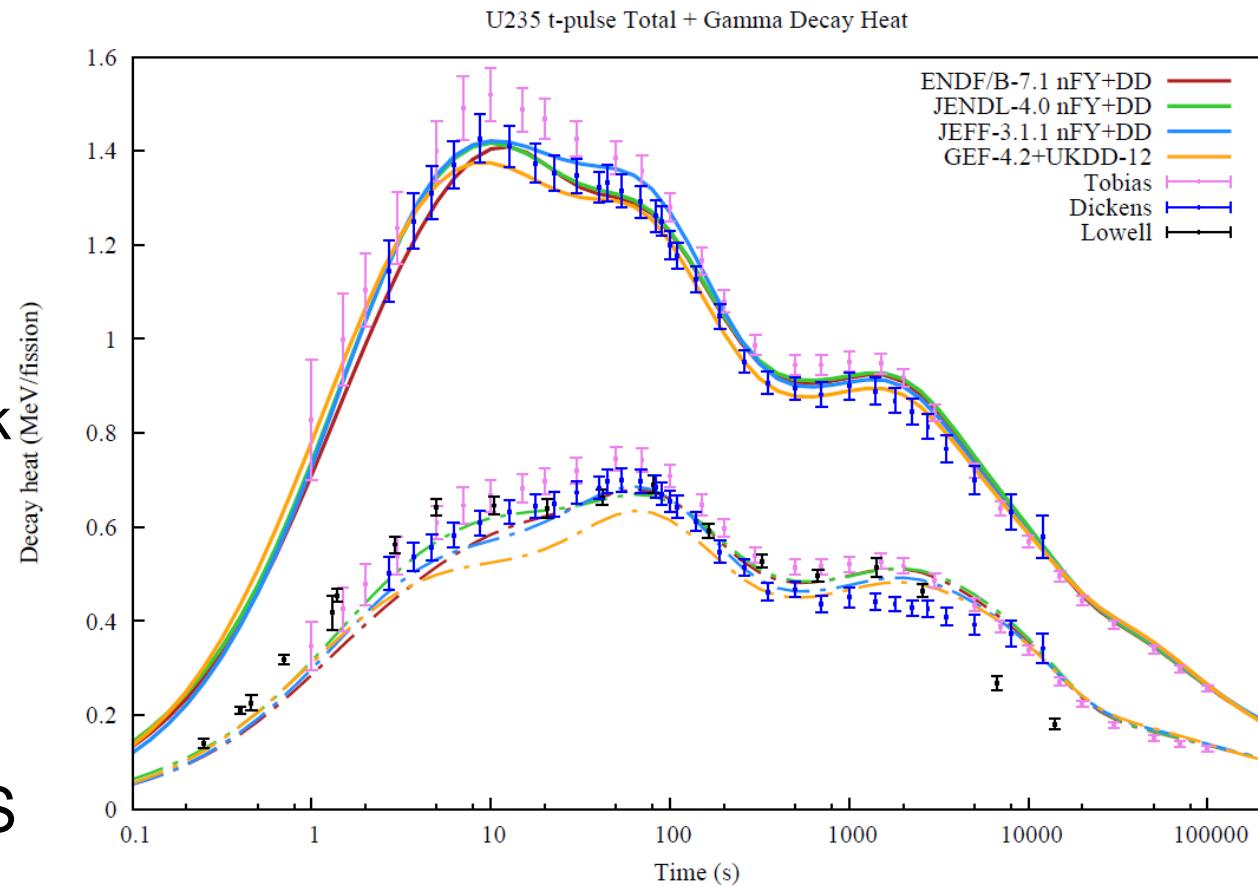


Figure 38: Total decay heat from thermal 2E4s irradiation of  $^{233}\text{U}$ .

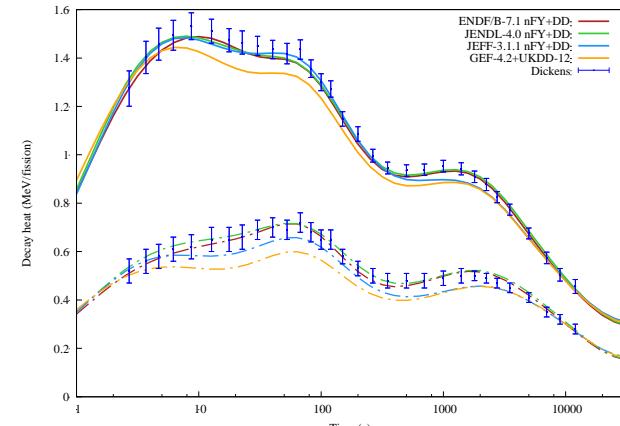
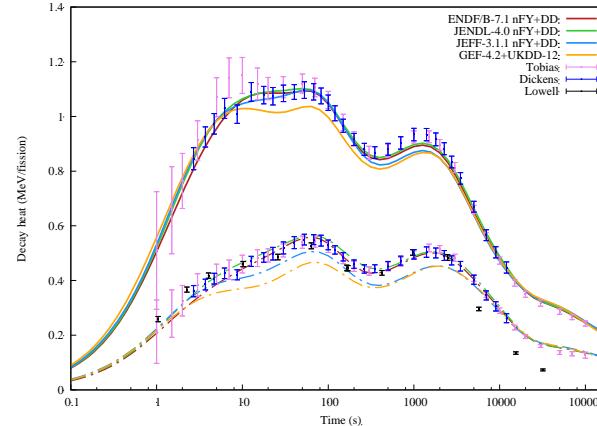
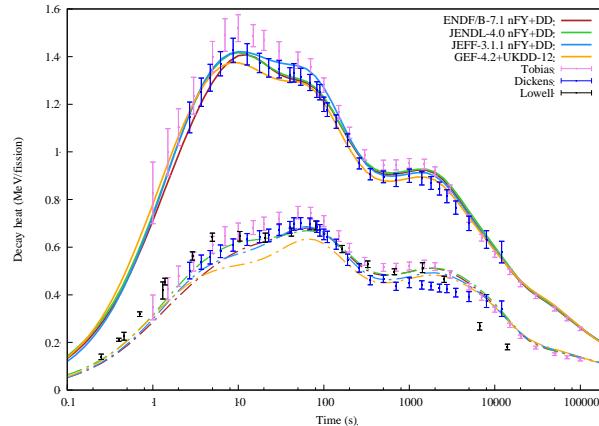
- A near-theoretical case is the fission ‘pulse’, which is idealised as a infinitesimal irradiation, built from re-normalised finite



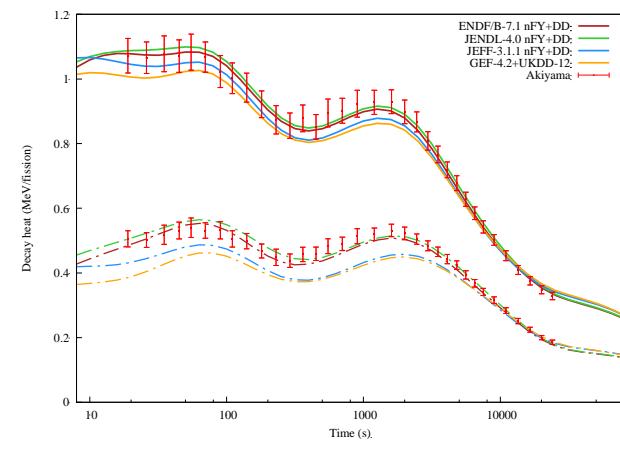
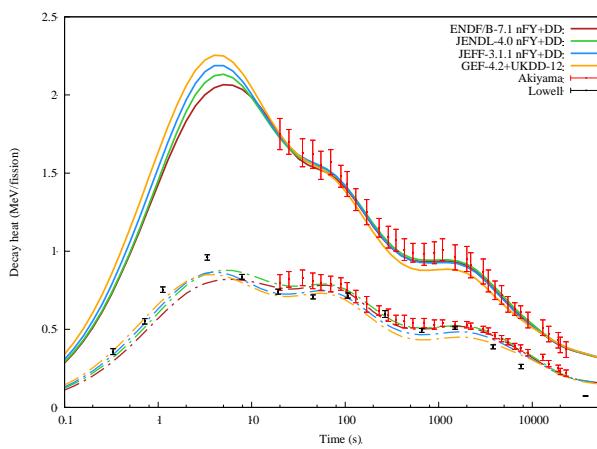
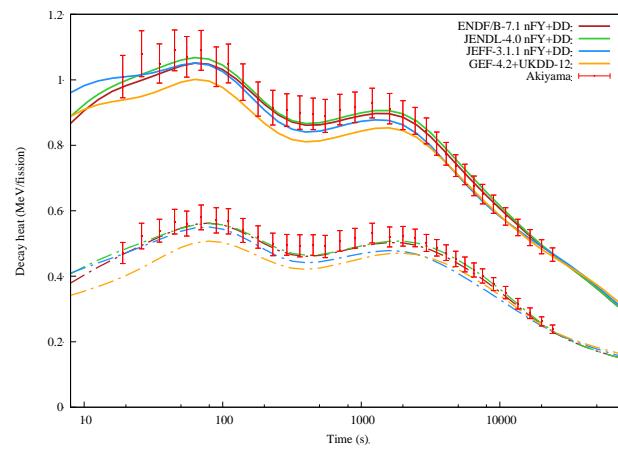
- Comparison between libraries for U235 total and gamma contributions to decay heat - note gamma deficiency
- ENDF/B, JENDL include TAGS to correct  $\gamma$  heat
- FISPACT-II can track all nuclides for in-depth study
- Contribution to DH needs for  $\nu$  + TAGS



# Standard pulse simulations

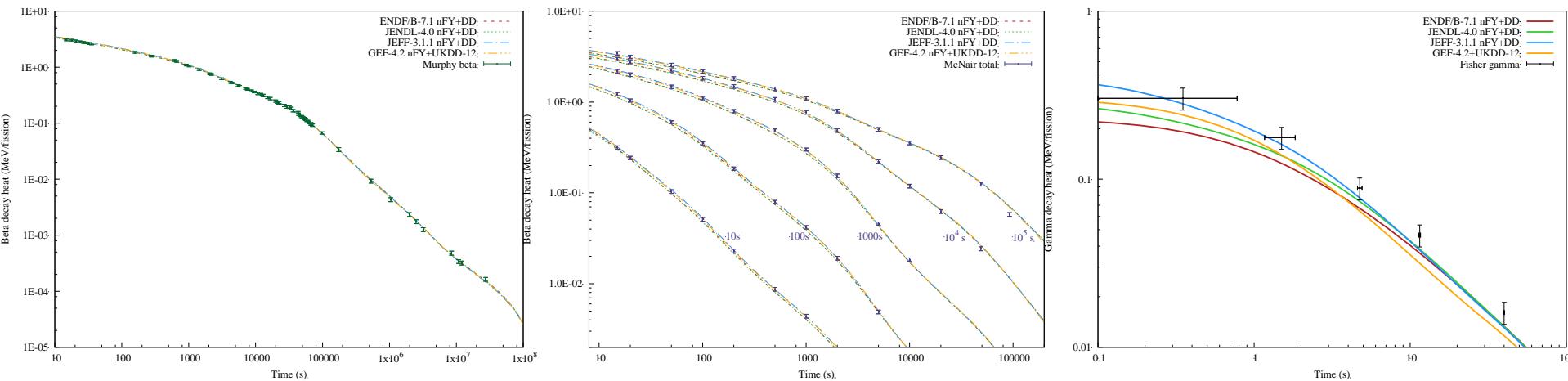


- Top (left to right): thermal U5, P9, P1 total and gamma heat
- Bottom (left to right): fast U3, U8, P9 total and gamma heat
- Note Pandemonium still in JEFF-3.1.1 for gamma (3.3?)

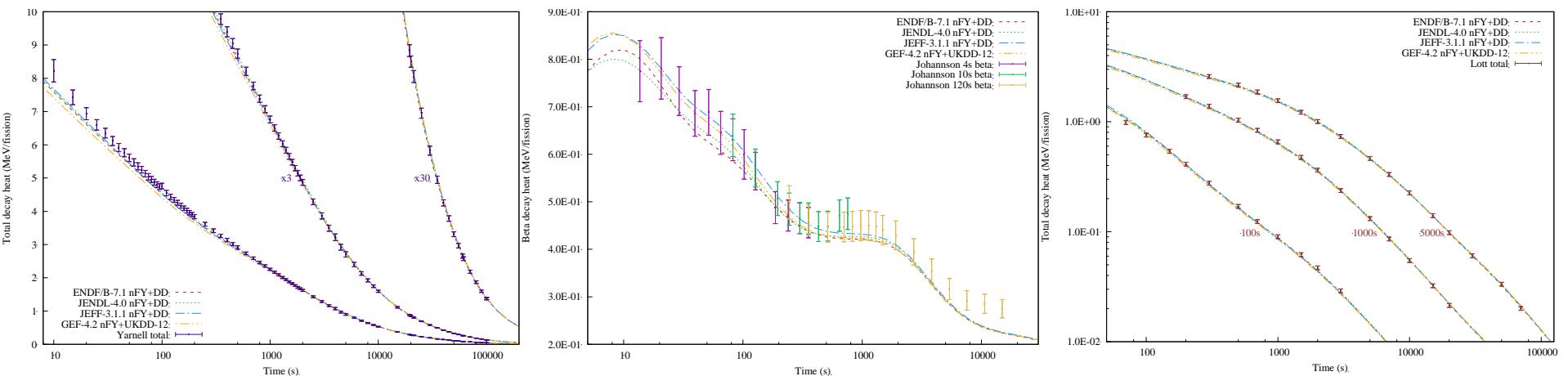




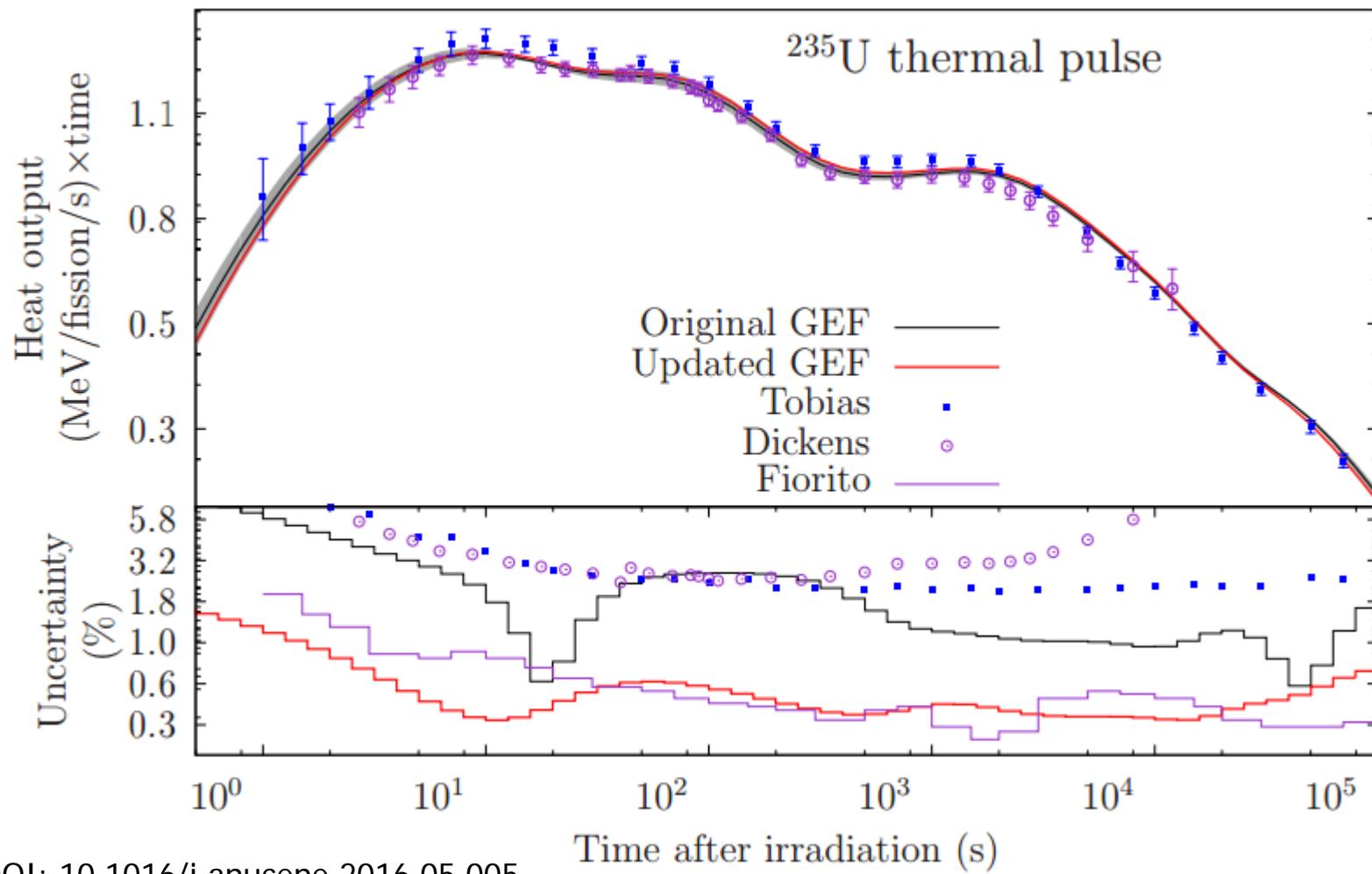
# Non-pulse simulations



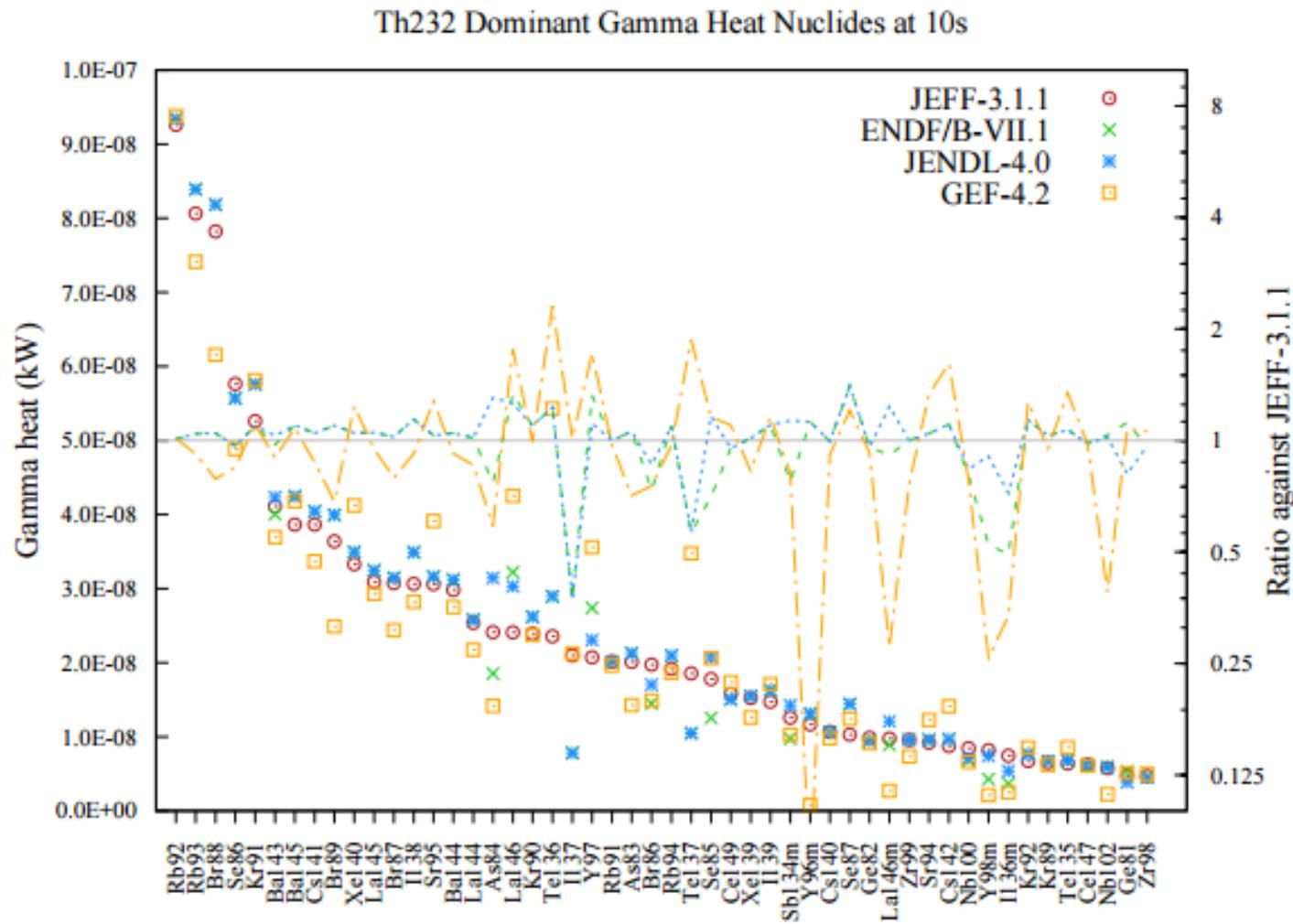
- Top (left to right): ZEBRA long P9, HERALD P9, GODIVA-II Th232
- Bottom (left to right): LANL U5 LHBoC, Studsvik U5 beta, CEA U5 calor
- As with pulse, these are a small subset of those in CCFE-R(15)28



- For these benchmarks, fission yields and decay data are being tested (and the code). TMC sample nFY for uncertainty



- By permuting the input data, we can also probe where differences in evaluations exist and contribute



- Collaboration with PSI, using modern CASMO-SIMULATE to compare inventory predictions for variety of assemblies:
  - BWR and PWR with mix of UO<sub>2</sub>, MOX, Gd
  - Includes Takahama, Atrium-10, TMI-1, Beznau

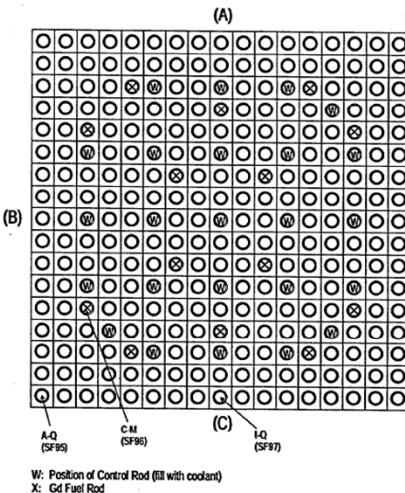
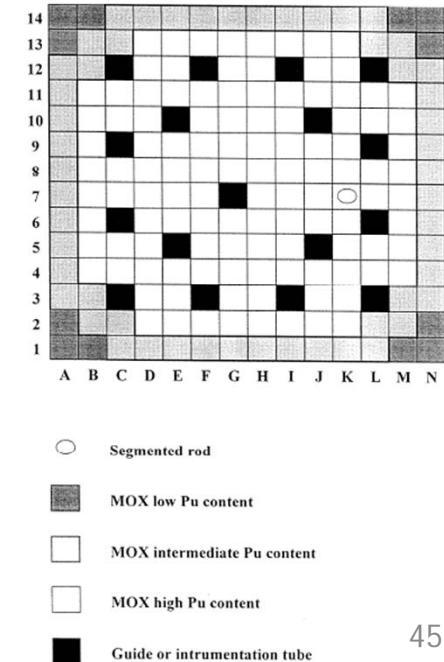


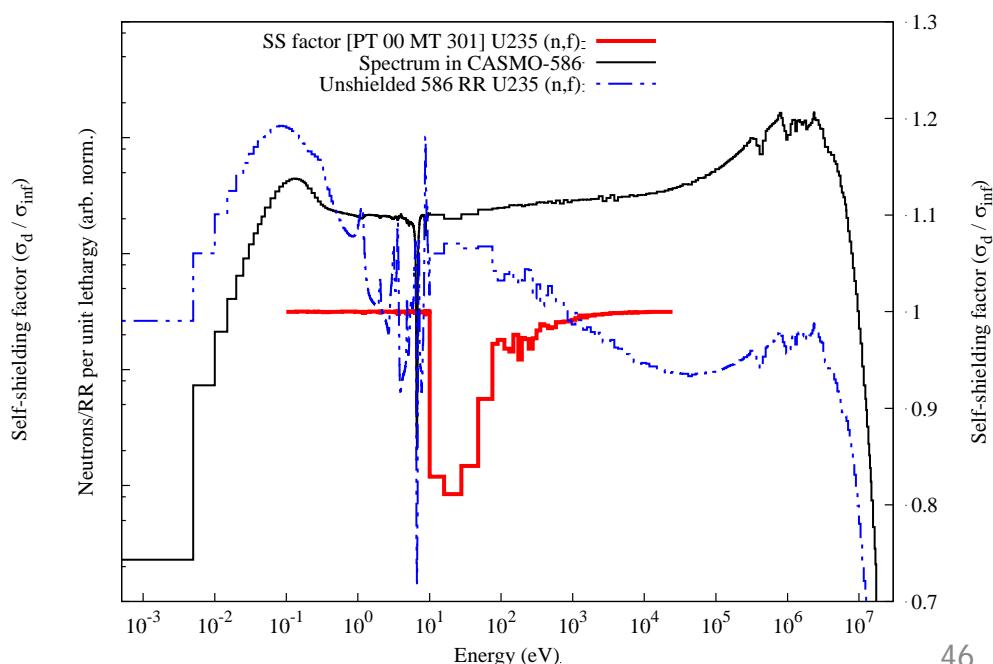
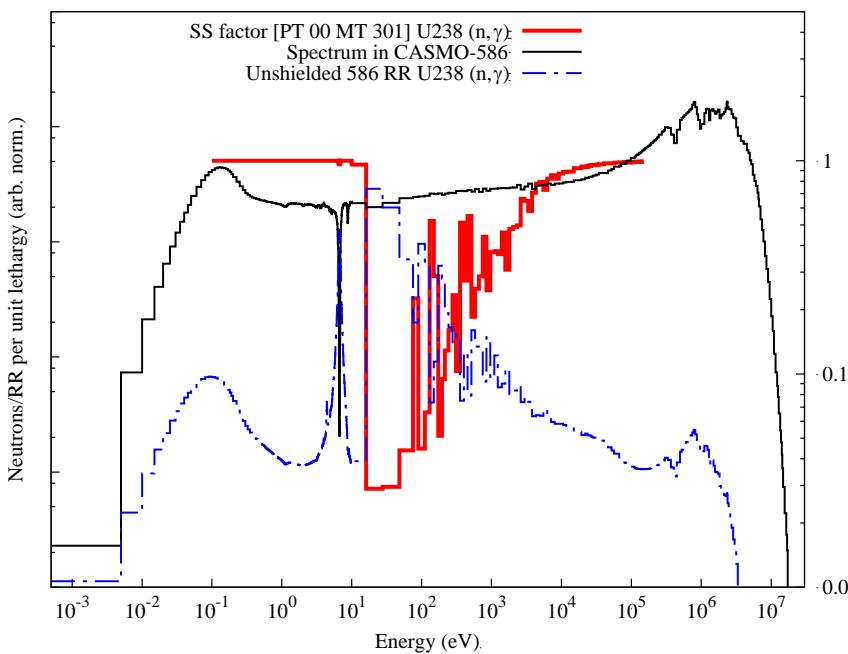
Figure 1 Positions of assay fuel rods in Takahama-3 assemblies NT3G23 and NT3G24

a	b	c	d	e	f	g	h	k	l
Pu1	Pu2	Pu3	Pu3	Pu3	Pu4	Pu3	Pu3	Pu2	Pu1
Pu2	Pu4	Pu4	Pu5	Pu4	Pu6	Pu6	Pu4	Pu4	Pu2
Pu3	Pu4	Pu6	Pu6	Pu6	Pu6	Pu6	Pu6	Pu4	Pu3
Pu3	Pu5	Pu6	Pu6	Pu6	Gd	Pu6	Pu6	Pu3	Pu3
Pu3	Pu4	Pu6	Pu6				Pu5	Pu4	Pu4
Pu4	Pu6	Pu6	Gd				Gd	Pu4	Pu3
Pu3	Pu6	Pu6	Pu6	Pu5	Gd	Pu5	Pu5	Pu3	
Pu3	Pu4	Pu6	Pu6	Pu5	Gd	Pu4	Pu4	Pu3	
Pu2	Pu4	Pu6	Pu4	Pu4	Pu5	Pu4	Pu4	Pu2	Pu1
Pu1	Pu2	Pu3	Pu3	Pu4	Pu3	Pu3	Pu2	Pu1	

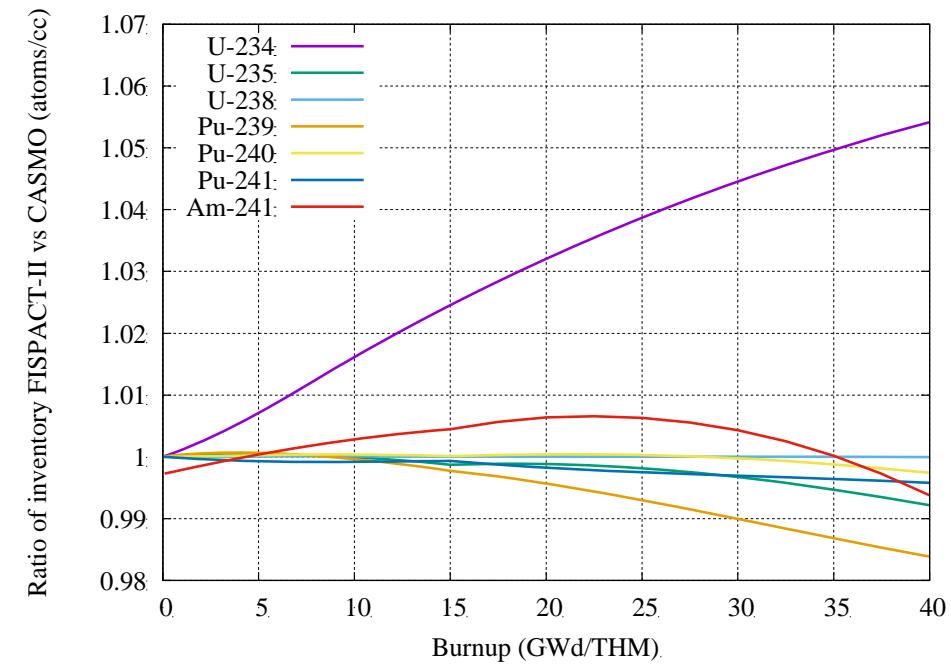
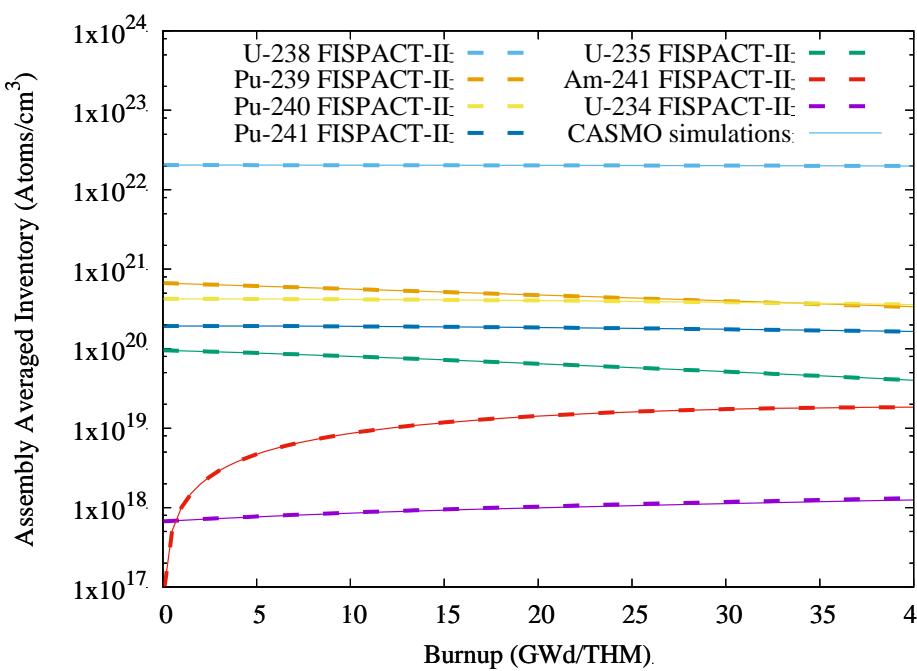
Figure 28: TMI-1 Fuel Assembly Layout



- Added 586 CASMO data for ENDF/B-VII.1, with CALENDF PTs for self-shielding. Applied to major actinides, but can in principle apply to any nuclide
- Left:** U8 capture RR and SSFs **Right:** U5 fission RR+SSFs  
Note: CASMO 586 treatment of <10 eV requires no SSFs! No so for >10 eV, where significant SS occurs and must be accounted for.

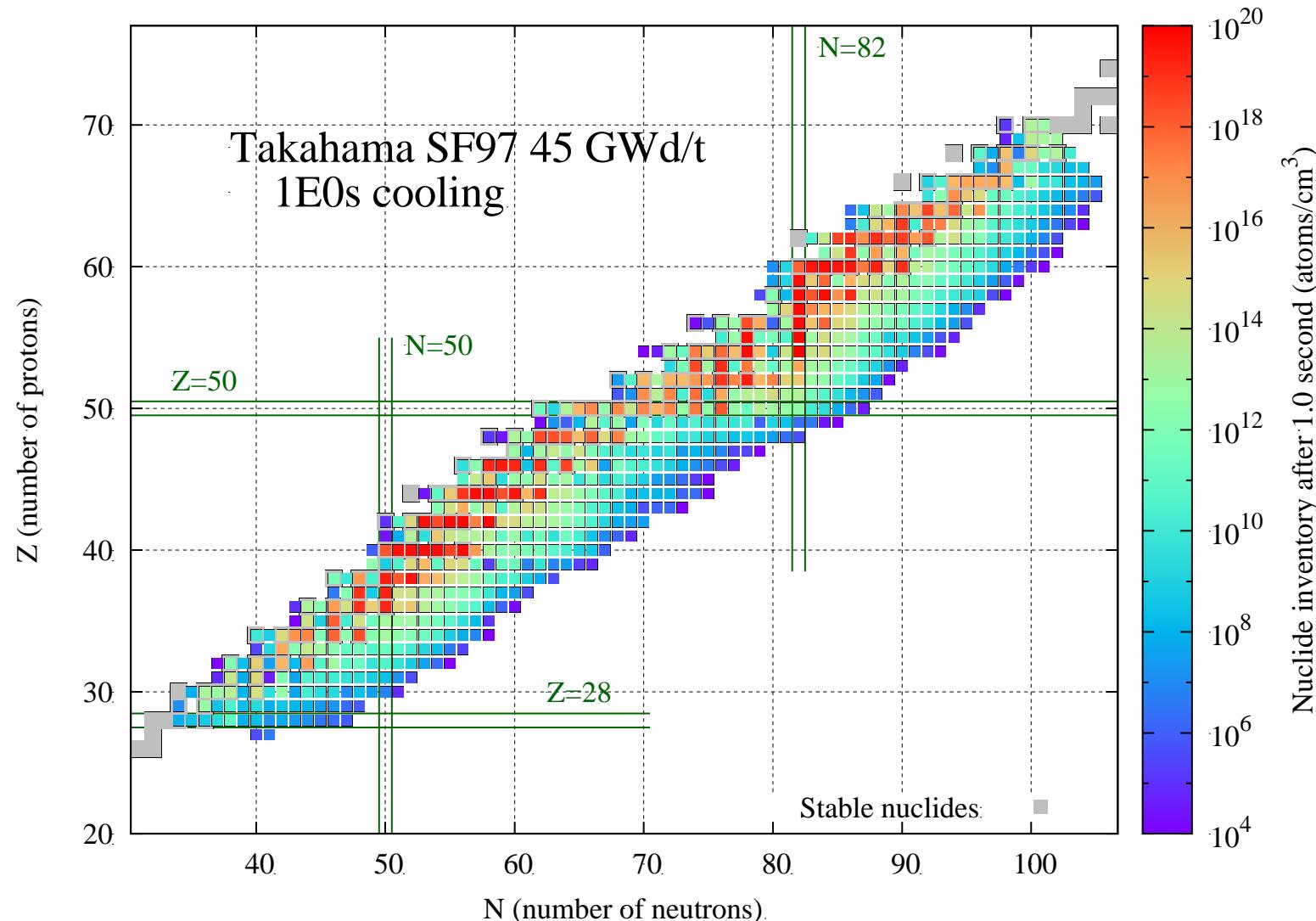


- In all examples, normalisation using POWER keyword of FISPACT-II (normalising flux based on full Kerma) to CASMO power density, converted to W/cc.
- Ratios are to CASMO simulation, following the spectra changes over 40 GWd/te, **below:** BWR MOX simulation



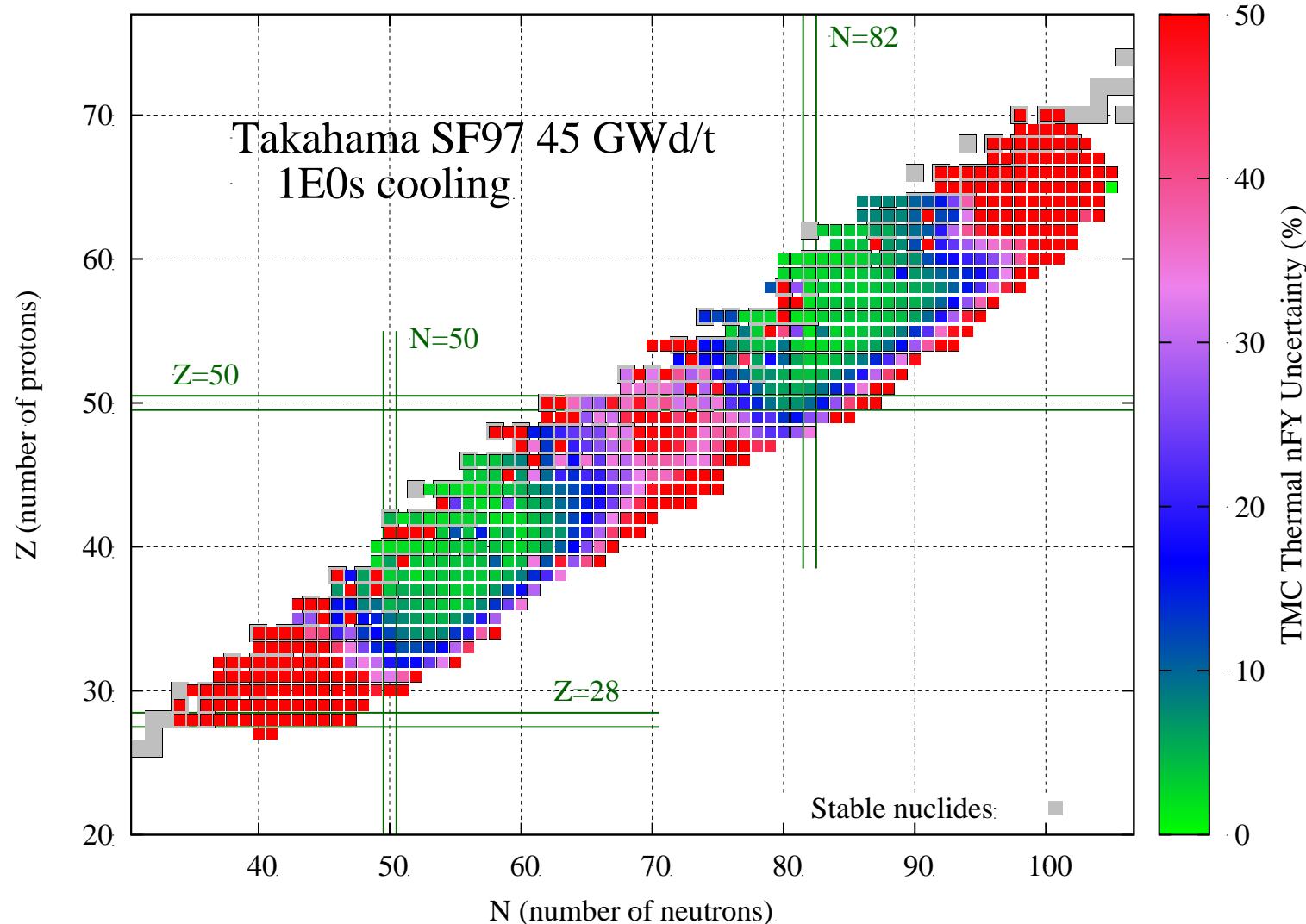
# Not your typical LWR simulation

- Unlike legacy codes, FISPACT-II uses all independent yields and decays to follow every nuclide

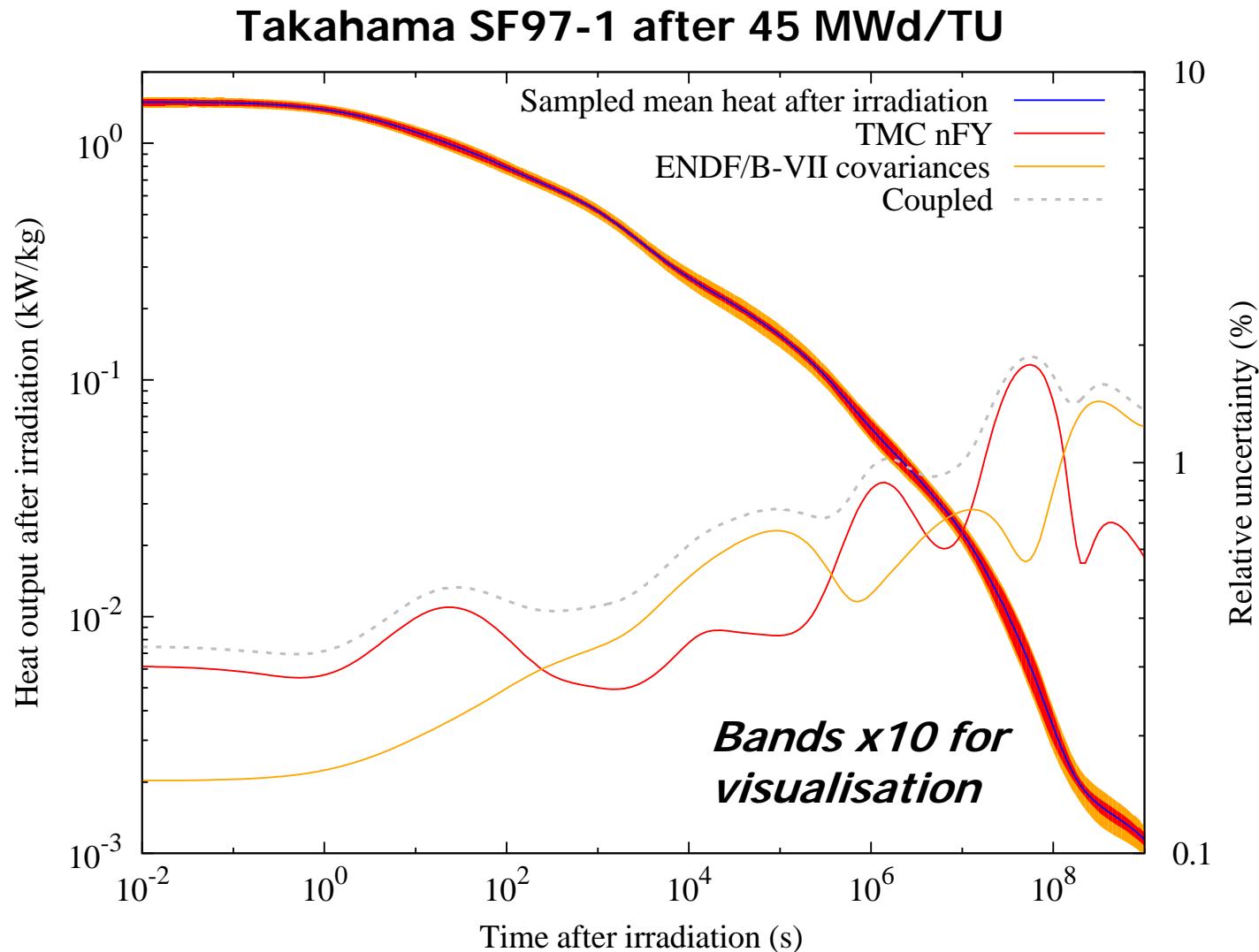


- Ability to handle technologically-generated TALYS, GEF(Y)

*In next chapter: Total Monte-Carlo Uncertainty methods*



- Coupling FISPACT-I covariance UQP for reaction rates with TMC we can provide coupled uncertainties:
  - From unc. of fissions and production of fissionable nuclides
  - From unc. in fission yields
  - And the coupled nFY + RR unc.



- Validation of FISPACT-II and its nuclear data libraries through multi-faceted effort covering a variety of code applications
- Each of the following completed (November 2015):
  - ✓ Detailed analysis of fusion total heat measurements done at JAEA/FNS
  - ✓ Validation of all existing integro-differential activation experiments
  - ✓ Simulation of complete set of material properties under irradiation
  - ✓ In-depth simulations of fission decay heat with break-down of nFY/decay/spectroscopic analysis
  - ✓ Massive validation against library of integral data from integral resonance, astrophysics and fission sources + statistical verification
- See CCFE-R(15)25,26,27,28 UKAEA-R(15)29,30,31,32,33,35

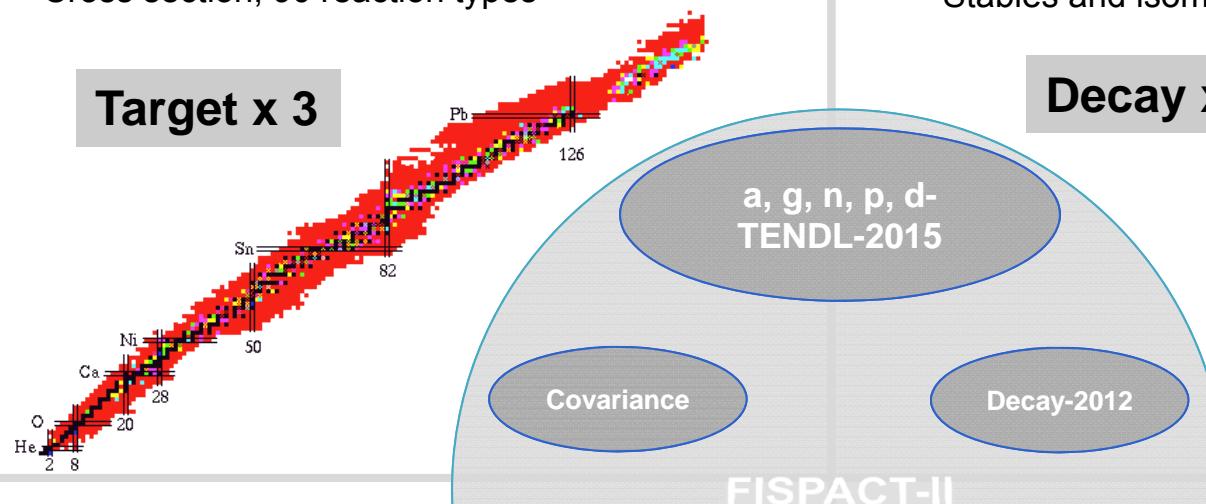
[http://www.ccfc.ac.uk/fispact\\_validation.aspx](http://www.ccfc.ac.uk/fispact_validation.aspx)

- **No comparable system has undergone equivalent V&V, weathered proof**

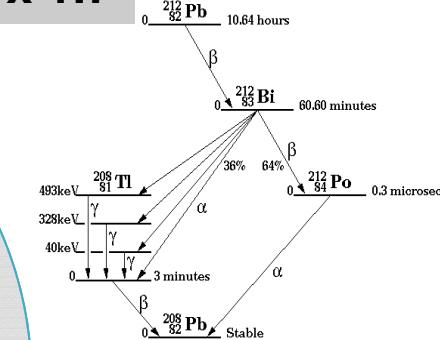
- 2809 targets ( $H^1$  to  $Fl^{281}$ )
- Cross section, 90 reaction types

- Decay data: 3873 nuclides; 24 types
- Stables and isomeric states; g, m, n, o,..

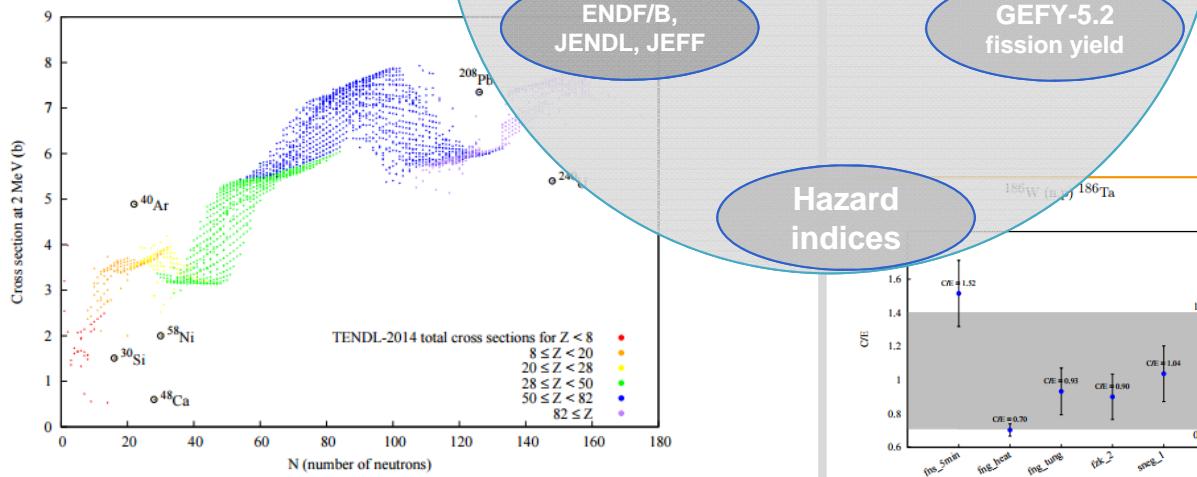
**Target x 3**



**Decay x 1.7**



**Validation: SACS**



V&V, C/E integral and differential with uncertainty

