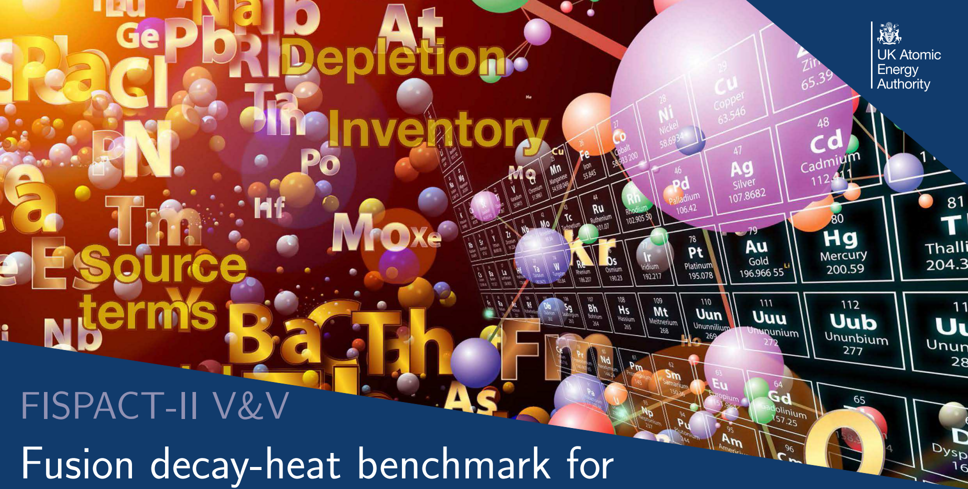

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FISPACT-II V&V

Fusion decay-heat benchmark for nuclear data validation

Advanced interrogation capabilities with FISPACT-II

Mark Gilbert, United Kingdom Atomic Energy Authority

FISPACT-II workshop

June 19-21, 2019, OECD/NEA, Paris

This work was funded by the RCUK Energy Programme
[Grant number EP/P012450/1]

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CULHAM CENTRE FOR FUSION ENERGY

Introduction

- Validation & Verification (V&V) is an important part of the development and release of FISPACT-II
- A suite of automated validation benchmarks have been created to test new releases of both the FISPACT-II code and the nuclear data libraries
  - against international experimental databases
- Results are compiled into open access pdf reports (see `fispact.ukaea.uk`)
  - thousands of pages in total providing a near-complete coverage of the physics landscape for neutron interactions

FISPACT-II validation

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- V&V exercises recently repeated for new FISPACT-II-4.0

UK Atomic Energy Authority

UKAEA-R(18)004
February 2018

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky

Integro-Differential Verification and Validation, FISPACT-II & TENDL-2017 nuclear data libraries

UK Atomic Energy Authority

UKAEA-R(18)003
February 2018

Michael Fleming
Jean-Christophe Sublet

Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events

UK Atomic Energy Authority

UKAEA-R(18)005
February 2018

Michael Fleming
Jean-Christophe Sublet
Arjan Koning
Dimitri Rochman

Maxwellian-Averaged Neutron-Induced Cross Sections for kT=1 keV to 100 keV, KADoNiS, TENDL-2017,-2014, ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0u, and EAF-2010 nuclear data libraries

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CCFE-R(18)002
September 2018

Mark R. Gilbert
Jean-Christophe Sublet

Fusion decay heat validation, FISPACT-II & TENDL-2017, EAF2010, ENDF/B-VIII.0, JEFF-3.3, and IRDFF-1.05 nuclear data libraries

www.ccfe.ac.uk

- focussing particularly on TENDL-2017
- but also benchmarking ENDF/B-VIII.0, JEFF-3.3 (and others)
- decay heat validation against (Japan-FNS) fusion experiments
- integral & differential xs validation against EXFOR
- fission decay heat and criticality benchmarks
- astrophysics testing (KADoNiS)

- In conjunction with J.-Ch. Sublet (IAEA) & M. Fleming (NEA)

available from http://fispact.ukaea.uk

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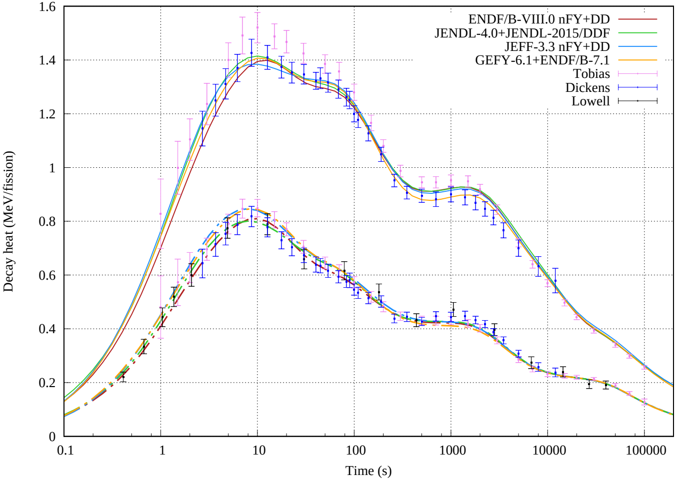
Other validation efforts (1)

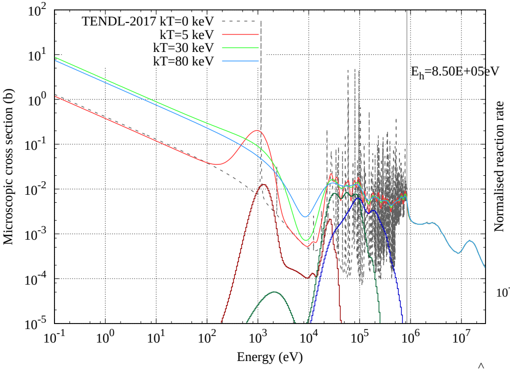
- Fission decay heat
- Comparison of simulated fission pulse decay heat to carefully interpreted experimental data
- e.g. ^{235}U thermal (0.0253 eV) pulse comparison



- total and β-generated decay heat
- simulated with latest ENDF/B, JEFF, and JENDL libraries
- Also included in exercise: ^{233}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{232}Th, and ^{237}Np

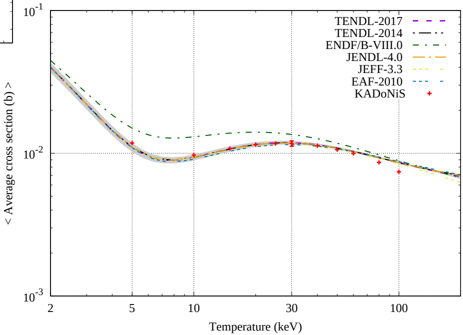
UKAEA-R(18)003

Other validation efforts (2)



- Maxwellian-averaged neutron xs comparison
- using KADoNiS astrophysics experimental database, which includes data for 357 nuclides at temperatures ranging from 5 keV (58 million K) to 100 keV (1.2 billion K)

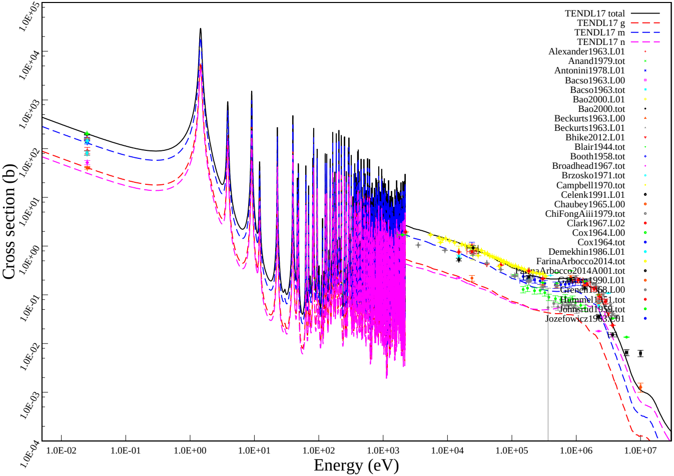
- e.g. ^{56}Fe results:
- TENDL-2017 xs & comparison to KADoNiS of average xs at various temperatures for different libraries



UKAEA-R(18)005

Other validations (3)

- Integro-differential V&V
- Comparison of cross section data against integral and differential data in the EXFOR database
- more than 400 reactions currently assessed this way (more could be added)



- e.g. ^{115}In(n,γ) differential data compared to TENDL-2017
- obvious complexity associated with three metastable states of ^{116}In and potential for mis-attribution

UKAEA-R(18)004

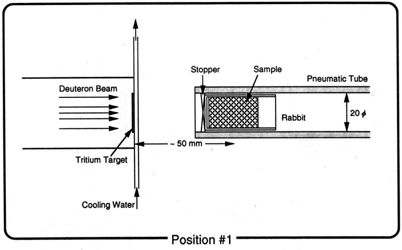
Fusion decay heat benchmark

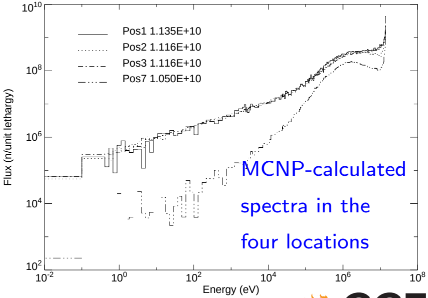
- Experiments performed at the Fusion Neutron Source (FNS) at JAEA in 1996-2000
- aimed at providing fusion-relevant decay-power data for important structural materials
- accurate experimental measurements with detailed records are ideal for simulation benchmarking

F. Maekawa M. Wada, Y. Ikeda *et al.*
Tech. Rep. JAERI-Data/Code 98-024, JAERI-Data/Code 98-021, & JAERI 99-055. http://www.jaea.go.jp/jaeri/
Maekawa *et al.*, Fus. Eng. Des. 47 (2000) 377-388 & J. Nucl. Sci. Tech. 39 (2002) 990-993

The experiment

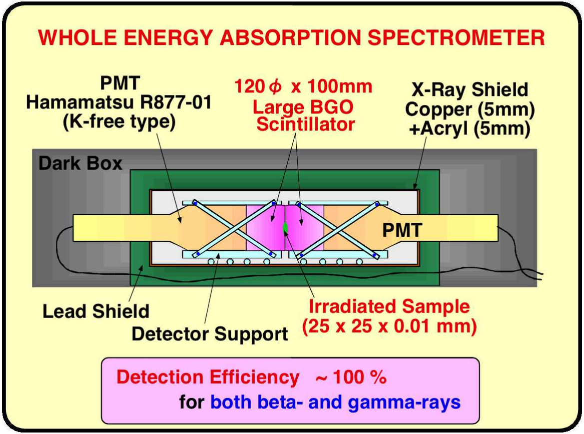
- 2 mA deuteron beam onto a tritium target producing a fusion neutron spectrum with fluxes of $\sim 10^{10}$ n cm^{-2} s^{-1} at the sample location
- samples irradiated for 5 minutes or 7 hours (4 different experimental set-ups)
- for the short irradiations, a rapid rabbit extraction system was used to make the samples available for immediate measurement





The experiment

- time-dependent decay heat of each sample was measured using a WEAS system
  - providing almost 100% detector efficiency
  - around 1 hour of recording for the 5-minute irradiations (starting from less than 1 minute after irradiation)
  - & up to a year of measurements from the 7-hour-irradiated samples



Z	Material	Form	Z	Material	Form
9	Fluorine	CF_2	46	Palladium	Metallic Foil
11	Sodium	Na_2CO_3	47	Silver	Metallic Foil
12	Magnesium	MgO	48	Cadmium	Metallic Foil
13	Aluminium	Metallic Foil	49	Indium	Metallic Foil
14	Silicon	Metallic Powder	50	Tin	SnO_2
15	Phosphorus	P_3N_5	51	Antimony	Metallic Powder
16	Sulphur	Powder	52	Tellurium	TeO_2
17	Chlorine	$C_2H_2Cl_2$	53	Iodine	IC_6H_4OH
19	Potassium	K_2CO_3	55	Caesium	Cs_2O_3
20	Calcium	CaO	56	Barium	$BaCO_3$
21	Scandium	Sc_2O_3	57	Lanthanum	La_2O_3
22	Titanium	Metallic Foil	58	Cerium	CeO_2
23	Vanadium	Metallic Foil	59	Praseodymium	Pr_6O_{11}
24	Chromium	Metallic Powder	60	Neodymium	Nd_2O_3
25	Manganese	Metallic Powder	62	Samarium	Sm_2O_3
26	Iron	Metallic Foil	63	Europium	Eu_2O_3
Alloy	SS304	Metallic Foil	64	Gadolinium	Gd_2O_3
Alloy	SS316	Metallic Foil	65	Terbium	Tb_4O_7
27	Cobalt	Metallic Foil	66	Dysprosium	Dy_2O_3
Alloy	Inconel-600	Metallic Foil	67	Holmium	Ho_2O_3
28	Nickel	Metallic Foil	68	Erbium	Er_2O_3
Alloy	Nickel-chrome	Metallic Foil	69	Thulium	Tm_2O_3
29	Copper	Metallic Foil	70	Ytterbium	Yb_2O_3
30	Zinc	Metallic Foil	71	Lutetium	Lu_2O_3
31	Gallium	Ga_2O_3	72	Hafnium	Metallic Powder
32	Germanium	GeO_2	73	Tantalum	Metallic Foil
33	Arsenic	As_2O_3	74	Tungsten	Metallic Foil
34	Selenium	Metallic Powder	75	Rhenium	Metallic Powder
35	Bromine	BrC_6H_4COOH	76	Osmium	Metallic Powder
37	Rubidium	Rb_2CO_3	77	Iridium	Metallic Powder
38	Strontium	$SrCO_3$	78	Platinum	Metallic Foil
39	Yttrium	Y_2O_3	79	Gold	Metallic Foil
40	Zirconium	Metallic Foil	80	Mercury	HgO
41	Niobium	Metallic Foil	81	Thallium	Tl_2O
42	Molybdenum	Metallic Foil	82	Lead	Metallic Foil
44	Ruthenium	Metallic Powder	83	Bismuth	Metallic Powder
45	Rhodium	Metallic Powder			

Simulations

- Detailed experimental information (irradiation times, measurement times, material compositions, etc.) have been translated into a set of FISPACT-II input files
  - these can be rapidly repeated for different nuclear data libraries
- Latest version of exercise compares results from TENDL-2017, ENDF/B-VIII.0, JEFF-3.3, and EAF2010 neutron cross section libraries
  - in some cases it is also possible to produce a meaningful comparison with the IRDFF-1.05 dosimetry file
- where available, the decay data file associated with each xs library is used (i.e. for JEFF and ENDF/B)
- otherwise the "dec_2012" decay database distributed with FISPACT-II is used – applies to TENDL-2017
  - 3875 nuclides
  - a combination of data from JEFF-3.1.1, JEF-2.2 to produce the EAF2010 decay file, UK evaluations in UKPADD6.1-6.9, and supplemented from ENDF/B-VII

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Typical results and presentation

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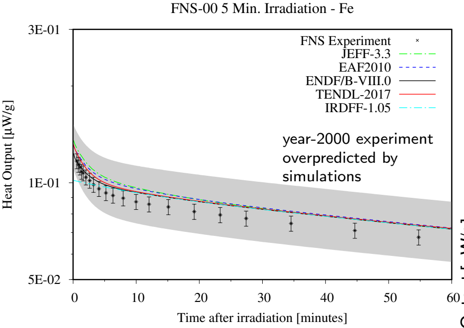
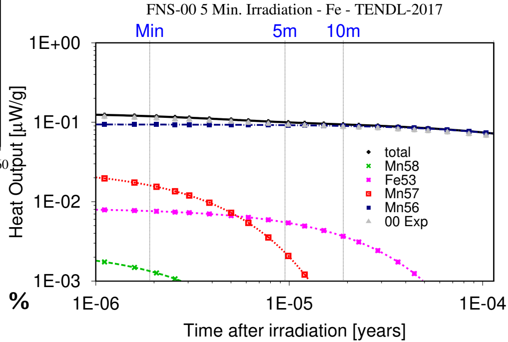
- 5 minute irradiation of pure iron



- decay heat curves from simulations with different libraries vs. experiment



- Pathway analysis for identified radionuclides

Product	$T_{1/2}$	Pathways	Path %
Mn58	1.09m	Fe58(n,p)Mn58	98.4
Mn57	1.42m	Fe57(n,p)Mn57	100.0
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Mn56	2.58h	Fe56(n,p)Mn56	99.5

- nuclide contribution breakdown for TENDL-2017 vs. experiment
- showing ^{56}Mn dominance

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Typical results and presentation

- tabulated comparison against each experimental measurement
- and tabulated characteristic E/C values for important radionuclides

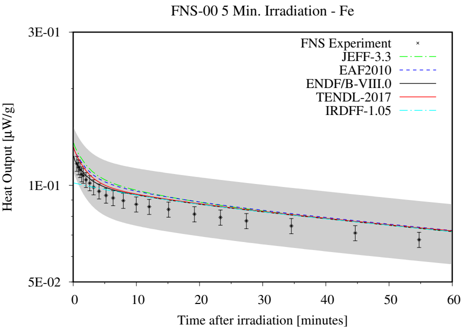
Times	FNS EXP. 5 mins		TENDL-2017			ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
Min.	μW/g		μW/g		E/C	E/C	E/C	E/C	E/C
0.58	$1.17E{-}01$	+/-5%	$1.24E{-}01$	+/-16%	0.94	1.00	0.91	0.94	1.15
0.83	$1.14E{-}01$	+/-5%	$1.22E{-}01$	+/-17%	0.94	0.99	0.90	0.93	1.13
1.08	$1.12E{-}01$	+/-5%	$1.19E{-}01$	+/-17%	0.94	0.99	0.90	0.93	1.11
1.35	$1.08E{-}01$	+/-5%	$1.17E{-}01$	+/-17%	0.93	0.97	0.89	0.92	1.08
1.60	$1.07E{-}01$	+/-5%	$1.15E{-}01$	+/-17%	0.93	0.98	0.90	0.92	1.07
2.03	$1.04E{-}01$	+/-5%	$1.12E{-}01$	+/-18%	0.93	0.97	0.89	0.92	1.04
2.63	$1.02E{-}01$	+/-5%	$1.08E{-}01$	+/-18%	0.94	0.97	0.90	0.92	1.02
3.23	$9.87E{-}02$	+/-5%	$1.05E{-}01$	+/-19%	0.94	0.96	0.90	0.92	1.00
4.10	$9.58E{-}02$	+/-5%	$1.02E{-}01$	+/-19%	0.93	0.95	0.90	0.91	0.98
5.20	$9.30E{-}02$	+/-5%	$9.98E{-}02$	+/-20%	0.93	0.94	0.90	0.91	0.96
6.32	$9.13E{-}02$	+/-5%	$9.79E{-}02$	+/-20%	0.93	0.94	0.90	0.91	0.95
7.93	$8.96E{-}02$	+/-5%	$9.58E{-}02$	+/-20%	0.93	0.94	0.90	0.91	0.95
9.98	$8.73E{-}02$	+/-5%	$9.39E{-}02$	+/-20%	0.93	0.94	0.90	0.91	0.94
12.03	$8.58E{-}02$	+/-5%	$9.24E{-}02$	+/-20%	0.93	0.93	0.91	0.91	0.93
15.10	$8.41E{-}02$	+/-5%	$9.05E{-}02$	+/-21%	0.93	0.93	0.91	0.92	0.93
19.20	$8.13E{-}02$	+/-5%	$8.82E{-}02$	+/-21%	0.92	0.93	0.91	0.91	0.93
23.32	$7.94E{-}02$	+/-5%	$8.61E{-}02$	+/-21%	0.92	0.93	0.92	0.91	0.93
27.42	$7.75E{-}02$	+/-5%	$8.42E{-}02$	+/-21%	0.92	0.92	0.92	0.91	0.92
34.53	$7.47E{-}02$	+/-5%	$8.11E{-}02$	+/-21%	0.92	0.92	0.92	0.92	0.92
44.65	$7.10E{-}02$	+/-5%	$7.73E{-}02$	+/-21%	0.92	0.92	0.92	0.91	0.92
54.75	$6.77E{-}02$	+/-5%	$7.37E{-}02$	+/-21%	0.92	0.92	0.92	0.91	0.92
mean % diff. from E					8	5	10	9	7

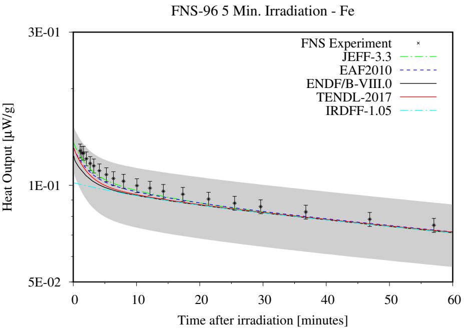
Product	$T_{1/2}$	E/C	%ΔE	$\%\Delta C^{nuc}$
Mn56	2.58h	0.94	5%	21%

Interpretation

UK Atomic Energy Authority

- interpretation of iron 5-minute experiments:
- year-2000 experimental batch is overpredicted by the simulations
- but identical simulations underpredict the 1996 batch.
    - suggests an experimental problem
- otherwise the libraries nicely capture the time-evolution profile





(IRDFF-1.05 contains the $^{56}Fe(n,p)^{56}Mn$ channel and can thus simulate the behaviour beyond 5-minutes of cooling)

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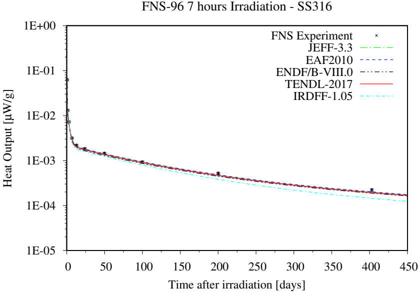
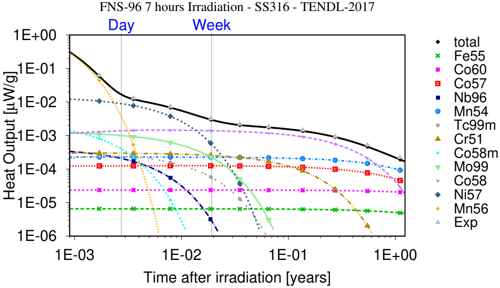
A complex case

- 7 hour irradiation of 316 stainless steel





- a good fit with the major libraries despite the relative complexity
  - the IRDFF dosimetry file misses ^{57}Co production from ^{58}Ni(n,np)
  - all library predictions are within a few % of the experiment at all decay times

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
mean % diff. from E	6	9	7	4	19

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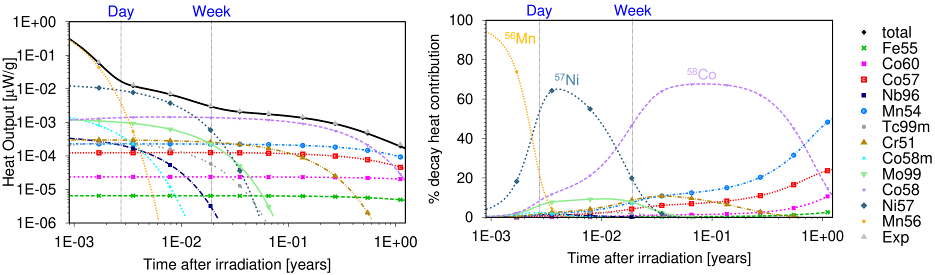
SS316 nuclide contributions

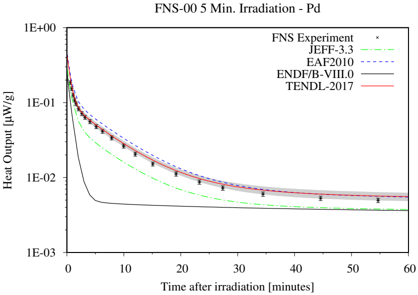
- the complexity can sometimes prevent understanding
- analyzing the % contributions to the decay heat as a function of time can identify the important nuclides

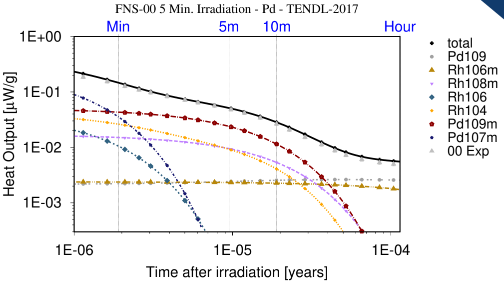


- despite numerous (minor) contributions, there are clear regions of single nuclide dominance
  - ^{56}Mn less than one day after irradiation
  - ^{57}Ni from 1 day to a few days
  - ^{58}Co from 1 week to almost a 10 months
  - after 1 year there is a split contribution from several nuclides

A case where TENDL-2017 is best

- 5 minute irradiation of pure palladium



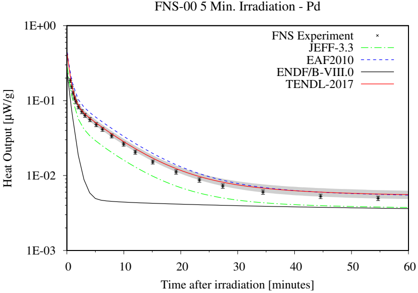


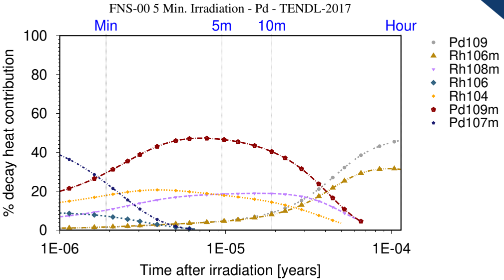
- a complex case with many contributing nuclides
  - particularly metastables: ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh
  - a mixture of (n,2n) and (n,p) reactions dominate
  - TENDL-2017 outperforms all others

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	8	64	32	24

A case where TENDL-2017 is best

- 5 minute irradiation of pure palladium

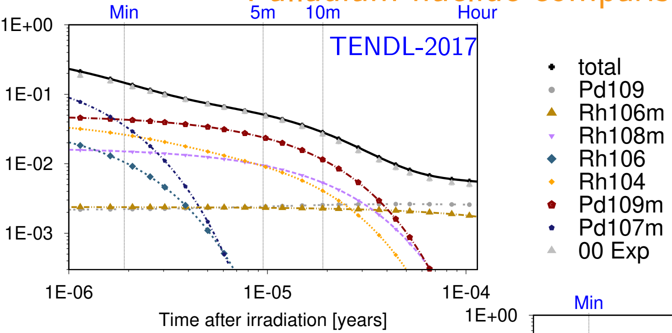




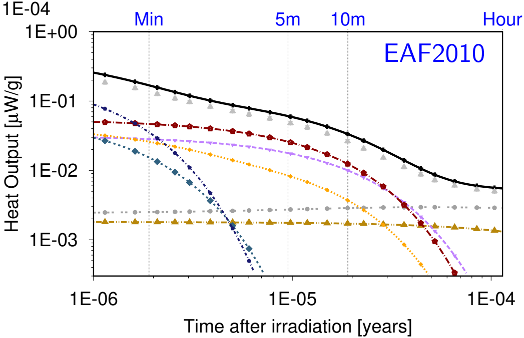
- a complex case with many contributing nuclides
  - particularly metastables: ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh
  - a mixture of (n,2n) and (n,p) reactions dominate
  - TENDL-2017 outperforms all others

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	8	64	32	24

Palladium nuclide comparisons



- EAF2010 overpredicts ^{108m}Rh production
- ENDF/B-VIII.0 & JEFF-3.3 (not shown) miss ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh



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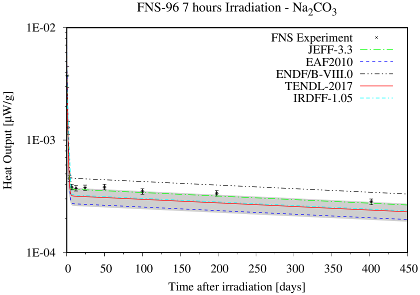
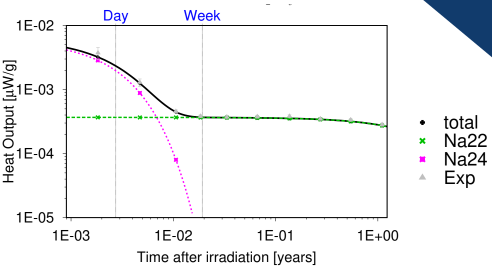
A case where JEFF-3.3 is best

- 7 hour irradiation of sodium

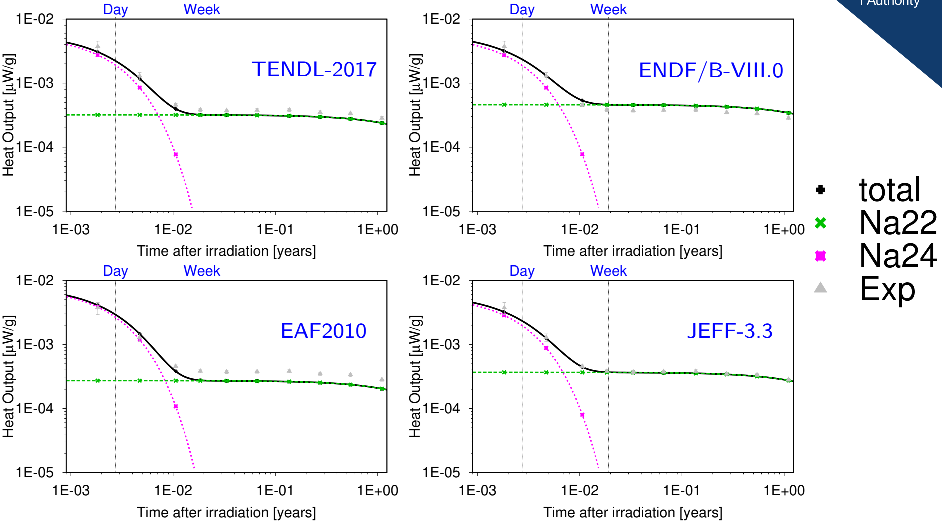




- only JEFF-3.3 matches closely the experimental measurements
  - other libraries either under or over predict the production of ^{22}Na
  - this could be a coincidence due to an experimental artefact – especially since the IRDFF dosimetry file underpredicts

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
mean % diff. from E	16	18	4	24	15

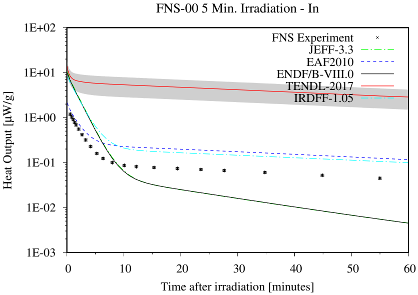
Sodium nuclide comparisons

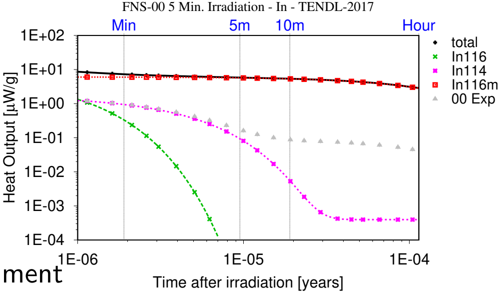


- ^{23}Na(n,γ)^{24}Na
- ^{23}Na(n,2n)^{22}Na

A case where all are wrong (1)

- 5 minute irradiation of pure Indium





- no library is close to the experiment
- the TENDL-2017 nuclide profiles suggest an overestimate of ^{116m}In production
  - ^{116m}In decay profile matches the experimental measurements beyond 5 minutes of cooling
  - incorrect distribution of ^{115}In(n,γ) to ^{116}In, ^{116m}In, ^{116n}In? ($T_{1/2}$=14.2s, 54.6m, and 2.2s, respectively)

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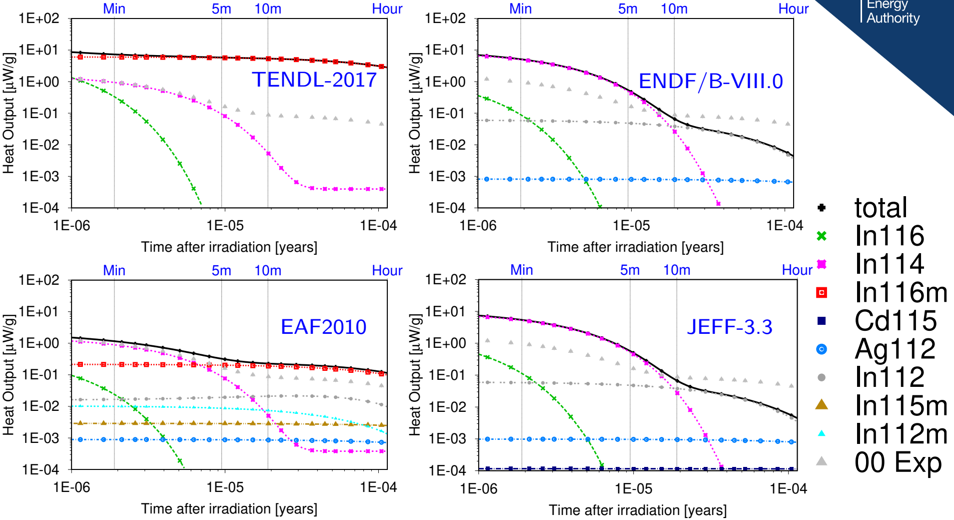
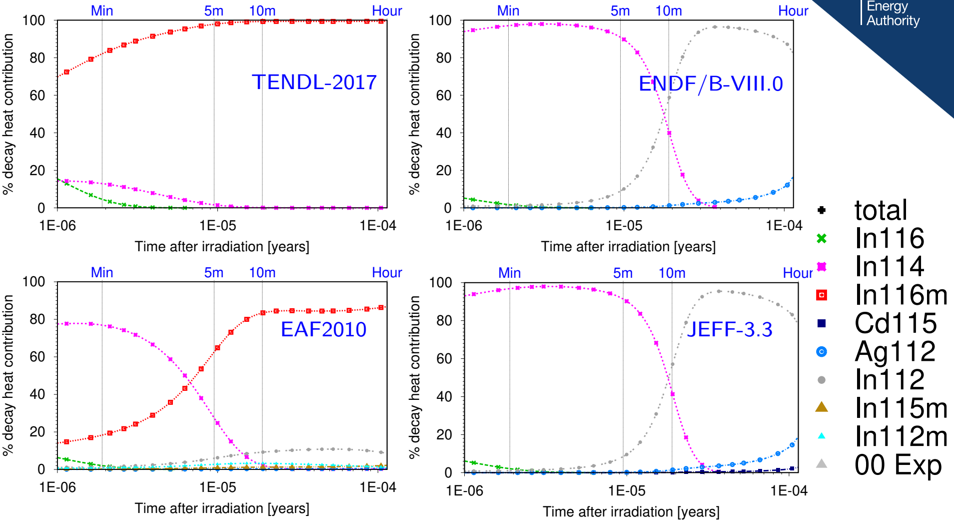
Indium nuclide comparisons



- JEFF-3.3, ENDF/B-VIII.0 miss ^{116m}In completely
- EAF2010 predicts many other contributing nuclides, but agrees with TENDL-2017 on ^{116m}In dominance

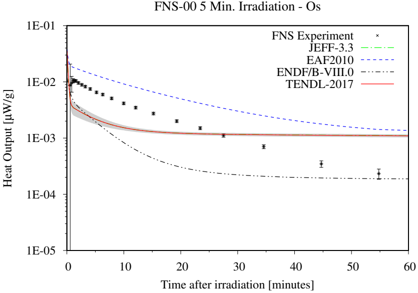
Indium nuclide comparisons

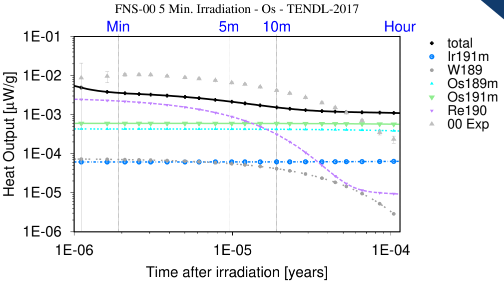


- JEFF-3.3, ENDF/B-VIII.0 miss ^{116m}In completely
- EAF2010 predicts many other contributing nuclides, but agrees with TENDL-2017 on ^{116m}In dominance

A case where all are wrong (2)

- 5 minute irradiation of pure Osmium

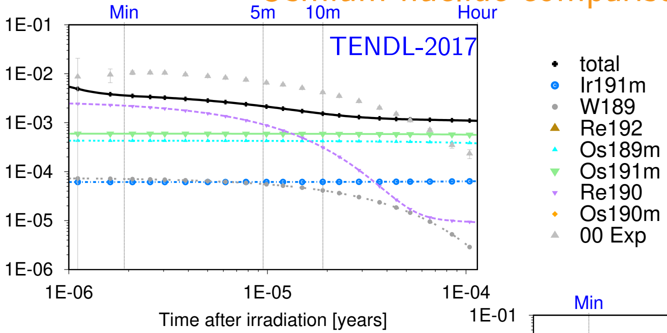


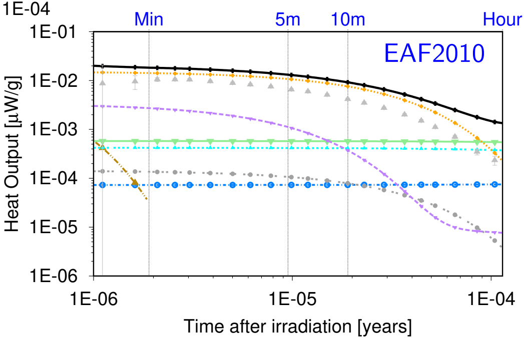


- no library predicts the correct decay-profile or heat magnitudes
  - JEFF-3.3 and TENDL-2017 are identical and under and overpredict at different times
  - EAF2010 always overpredicts, while ENDF/B-VIII.0 underpredicts

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	78	62	78	152

Osmium nuclide comparisons





- The EAF2010 profile is the best match and is attributed to $^{190}Os(n,n')^{190m}Os$
- this channel is missing from the group-wise processed version of TENDL-2017 (& JEFF-3.3 & ENDF/B-VIII.0)

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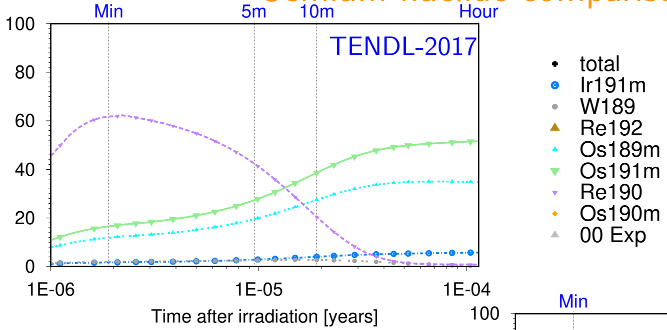
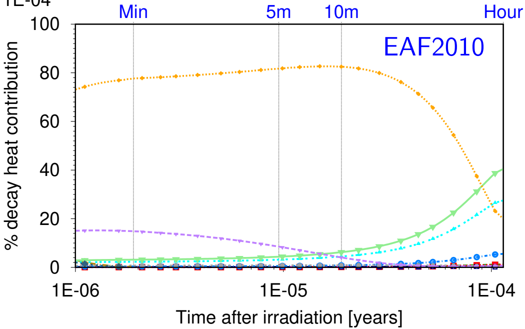
Osmium nuclide comparisons



- The EAF2010 profile is the best match and is attributed to ^{190}Os(n,n′)^{190m}Os
- this channel is missing from the group-wise processed version of TENDL-2017 (& JEFF-3.3 & ENDF/B-VIII.0)



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statistical summary

- Summary tables compare the average % deviation from experiment across all samples
- e.g. lighter elements/alloys from 5 minute experiments:

material	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
Fluorine	2	3	2	8
Sodium	22	41	23	26
Magnesium	7	6	7	5
Aluminium	7	8	14	8
Silicon	10	15	7	7
Phosphorus	5	12	6	11
Sulphur	27	72	41	76
Chlorine	12	45	46	32
Potassium	7	12	3	22
Calcium	12	13	17	14
Scandium	8	64	8	9
Titanium	5	7	2	3
Vanadium	15	14	13	11
Chromium	18	15	14	12
Manganese	12	16	25	13
Iron	8	5	10	9
SS304	3	2	3	3
SS316	6	5	6	2
Cobalt	10	4	6	10
Inconel-600	6	16	10	14
Nickel	10	40	7	7
Nickel-chrome	5	14	4	9
Copper	4	3	5	6

- green indicates a better than 10% agreement on average
- orange: better than 50%
- red: worse than 50%

statistical summary (2)

- heavier elements/alloys from 5 minute experiments:

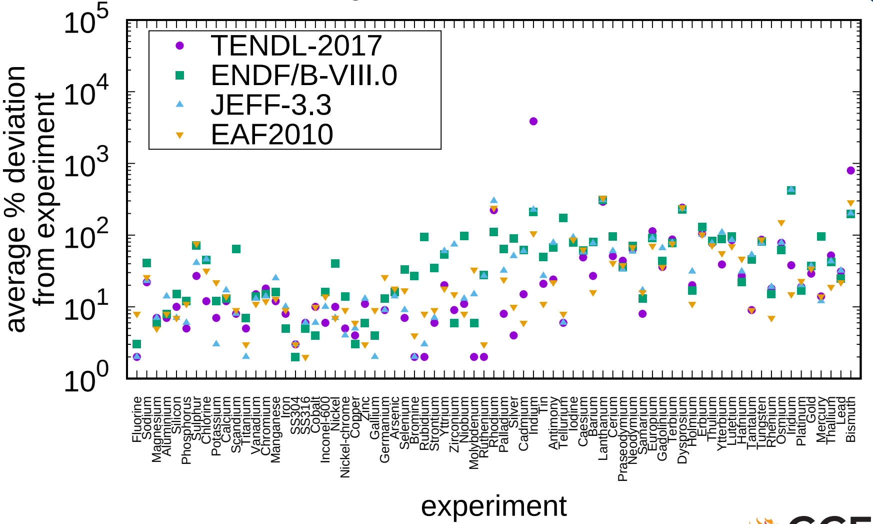
material	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
Caesium	49	61	58	63
Barium	27	80	77	16
Lanthanum	292	310	307	330
Cerium	51	95	60	41
Praseodymium	44	36	33	38
Neodymium	63	71	59	68
Samarium	8	13	17	16
Europium	113	91	91	71
Gadolinium	36	44	66	36
Terbium	87	78	78	76
Dysprosium	241	229	232	244
Holmium	20	17	31	11
Erbium	105	131	101	102
Thulium	77	83	77	72
Ytterbium	39	88	109	56
Lutetium	85	96	85	70
Hafnium	27	22	31	47
Tantalum	9	46	53	9
Tungsten	86	81	77	87
Rhenium	18	15	19	7
Osmium	78	62	78	152
Iridium	38	423	429	15
Platinum	19	17	20	23
Gold	29	37	37	34
Mercury	14	95	12	14
Thallium	52	42	43	19
Lead	31	25	32	22
Bismuth	795	199	200	287

- % deviation suggests a worse agreement at higher Z

statistical summary (3)

UK Atomic Energy Authority

- % deviation across all 5 minute experiments
- deviation increases at higher Z



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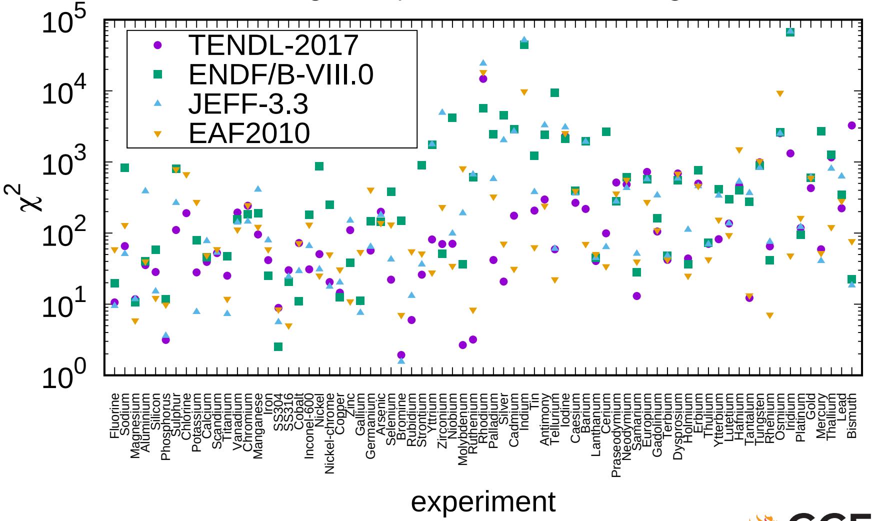
χ^2 test

- χ^2 variation for 5 minute experiments
- less clear trend $\Rightarrow$ higher experimental errors at high Z

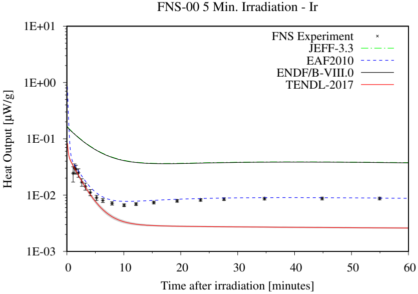


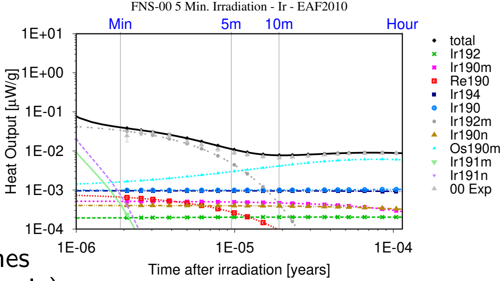
Summary

- The FNS experimental results from Japan offer a unique validation benchmark for inventory simulations in fusion-relevant conditions
    - they test the cross section data for a significant fraction of stable nuclides
- Automation of benchmarking against these experiments with FISPACT-II allows rapid testing of libraries
    - quickly provides a global impression of data quality
    - but each individual experiment and associated simulations can have unexpected subtleties
    - overall libraries perform well, particularly at low Z
    - no library succeeds for every case
    - new libraries still have something to learn from older ones ...

A case where the “legacy” is best

- 5 minute irradiation of pure Iridium



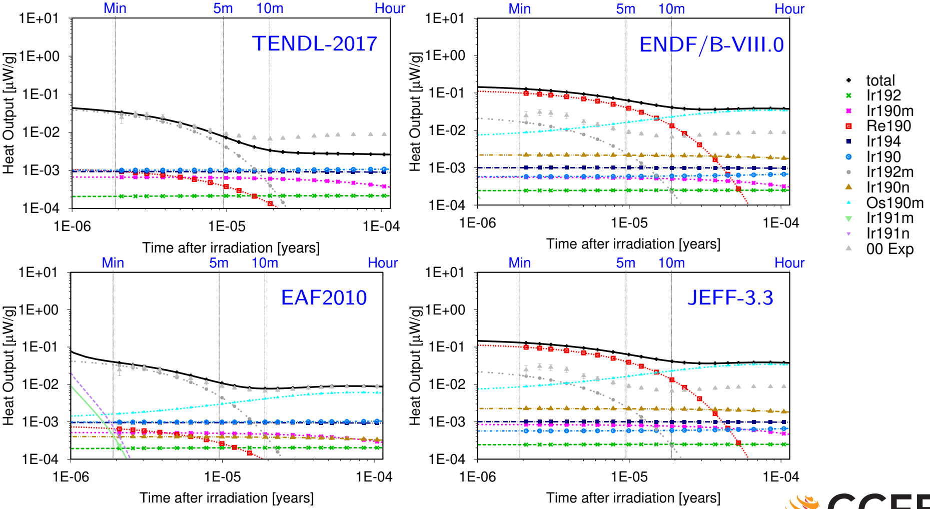


- Only EAF2010 correctly matches the experimental profile (and scale)
  - the observed decay heat originates from ^{192m}Ir in the first 5 minutes of cooling
  - at longer times ^{190m}Os dominates

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	38	423	429	15

Iridium nuclide comparisons

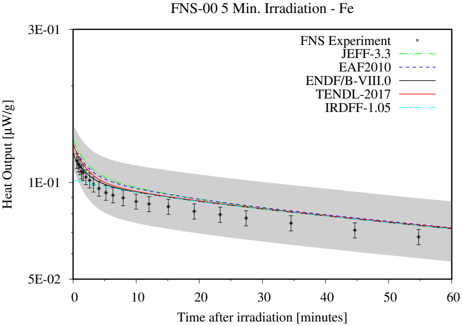
- TENDL-2017 underpredicts ^{191}Ir(n,2n)^{190n}Ir(β^+)^{190m}Os
- ENDF/B-VIII.0 and JEFF-3.3 overestimate this path and predict a different dominant nuclide (^{193}Ir(n,α)^{190}Re) at short cooling times



FISPACT-II inputs & outputs

.gra files

- e.g. irradiation of pure iron



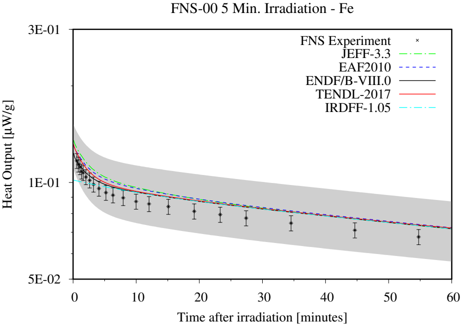
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from `.gra` files

```
GRAPH 1 2 1 3
UNCERTAINTY 2
```

- `UNCERTAINTY` keyword included to provide uncertainty estimates
- `GRAPH <<n>> <<show>> <<uncert>> <<list>>`
  - instructs FISPACT-II to output `<<n>>` blocks of summary data in an additional output file with a .gra stub
  - `<<show>>` equal to 2 makes the output suitable for `GNUPLOT` plotting (+ a *template* .plt file is written)

.gra files

- e.g. irradiation of pure iron



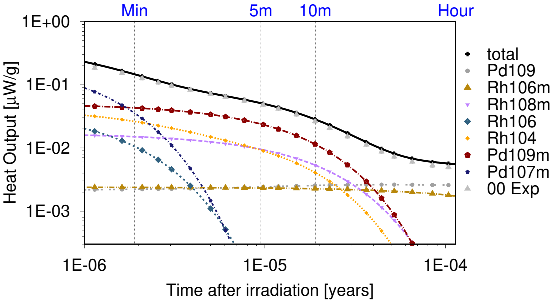
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from .gra files

```
GRAPH 1 2 1 3
UNCERTAINTY 2
```

- UNCERTAINTY keyword included to provide uncertainty estimates
- GRAPH <<n>> <<show>> <<uncert>> <<list>>
  - <<uncert>> equal to 1 includes the uncertainties in the .gra file (and plot)
  - <<list>>: list of <<n>> graphs required 1=activity;2=dose;3=decay-heat...

Nuclide graphs

- e.g. irradiation of palladium



- recently developed capability to extract nuclide contribution breakdown to radiological quantities
- curves extracted directly from `.grn` files

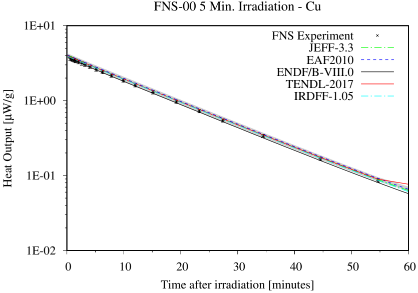
```
NUCGRAPH 1 1.0 1 2
```

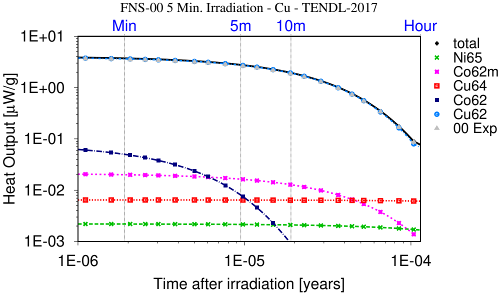
- `NUCGRAPH <<n>> <<floor>> <<uncert>> <<list>>`
- instructs FISPACT-II to output `<<n>>` blocks of data in .grn file 1=activity;2=decay-heat;3=dose...
- for each radiological quantity (block) as a function of time:
  - total with uncertainty (if `<<uncert>>` equals 1)
  - contribution to quantity from any nuclide that contributes `<<floor>>` % or more at any time

Additional Examples

A good agreement case

- 5 minute irradiation of pure copper



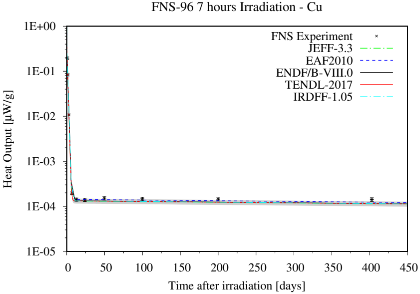


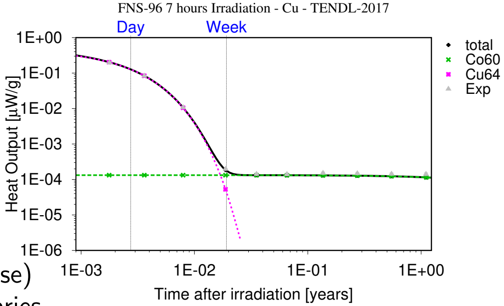
- a straightforward case entirely dominated by ^{62}Cu
  - ^{63}Cu(n,2n)^{62}Cu
  - all library predictions are within a few % of the experiment at all decay times

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
mean % diff. from E	4	3	5	6	3

Copper at longer times

- 7 hour irradiation of pure copper





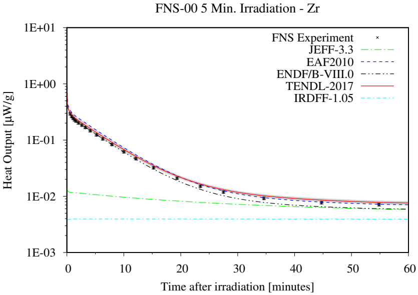
- two-nuclide contribution profile (different nuclides to 5 minute case) and good agreement with all libraries
  - ^{63}Cu(n,α)^{60}Co (including isomeric transition via ^{60m}Co)
  - ^{65}Cu(n,2n)^{64}Cu

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
mean % diff. from E	9	9	9	5	12

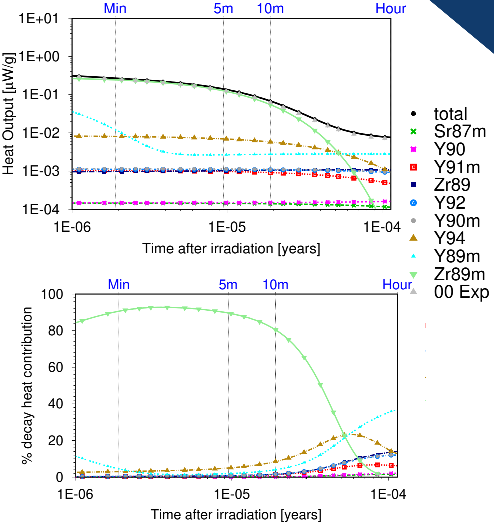
A problem for JEFF-3.3?

UK Atomic Energy Authority

- 5 minute irradiation of pure zirconium



TENDL-2017 results



- JEFF-3.3 underpredicts during the first 30 minutes of cooling
  - other libraries produce a good match to the experiment (IRDFF-1.05 only captures the low-level production of ^{89}Zr via ^{90}Zr(n,2n))

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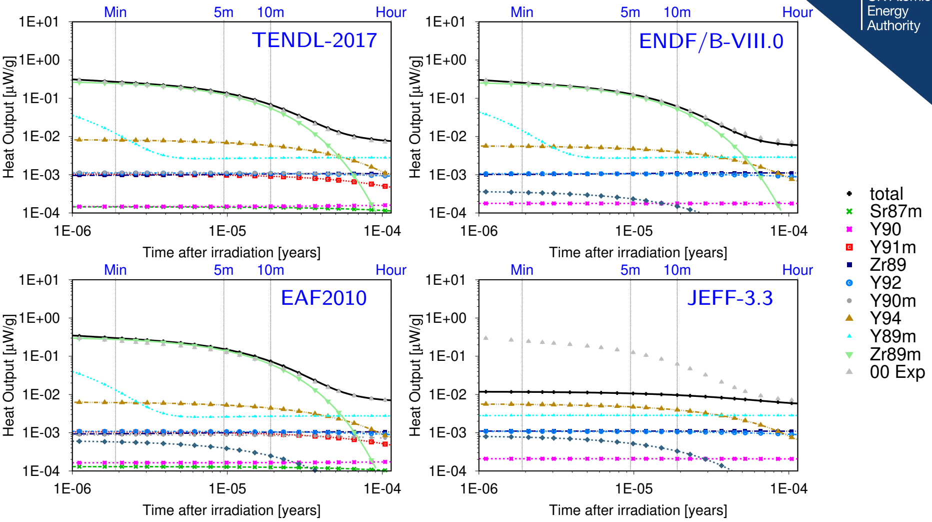
Zr nuclide contributions



- JEFF-3.3 does not include the ^{90}Zr(n,2n)^{89m}Zr channel
  - this is unexpected because it was included in JEFF-3.2

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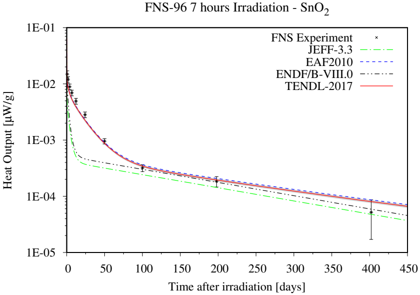
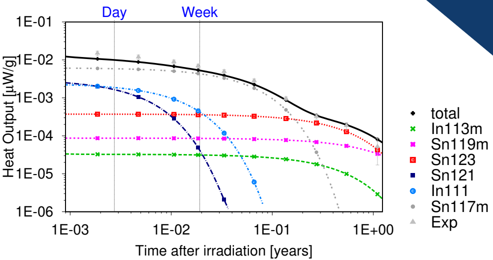
Multiple metastable importance

- 7 hour irradiation of pure tin



TENDL-2017 results

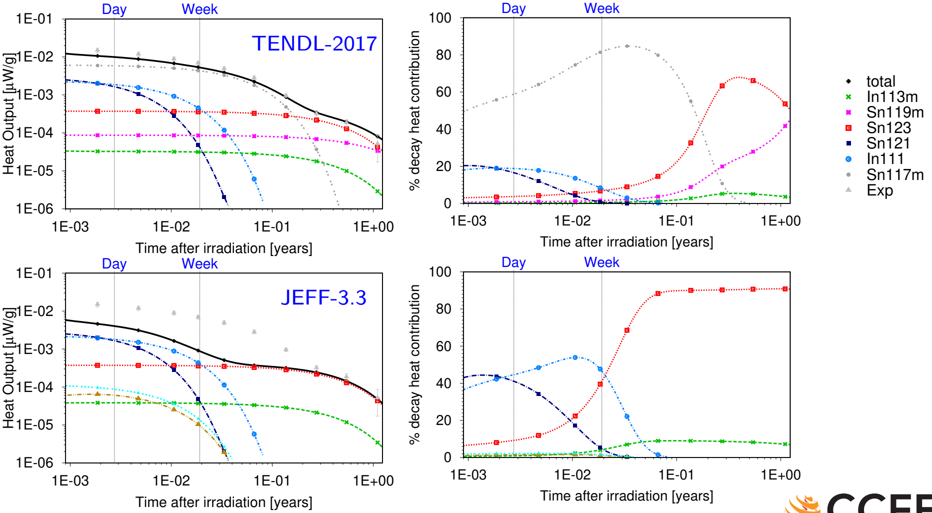


- TEND-2017 and EAF2010 produce a good match to the measured profile
  - although the absolute decay heat values are not very close to the experiment
- However, JEFF-3.3 and ENDF/B-VIII.0 clearly get the profile wrong

	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	22	50	60	23

Tin nuclide comparisons

- TENDL result shows importance of two metastable nuclides
  - ^{119m}Sn and ^{117m}Sn produced via (n,2n) reactions
- JEFF & ENDF/B include the (n,2n)s but only to ground-states



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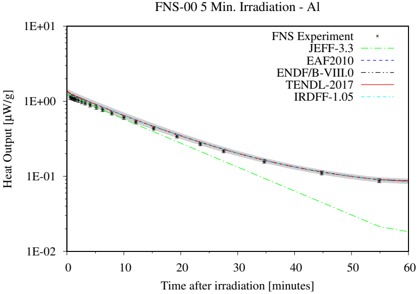
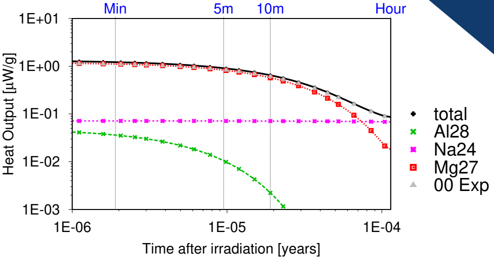
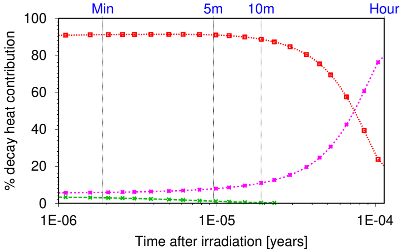
A problem for JEFF-3.3?

- 5 minute irradiation of pure aluminium



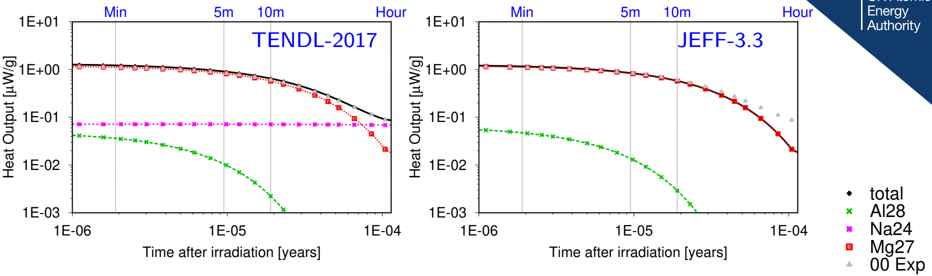
TENDL-2017 results





- beyond 20 minutes of cooling JEFF-3.3 underpredicts the experimentally measured decay heat
    - all other libraries produce a good match to the experiment

Aluminium nuclide contributions



- JEFF-3.3 does not predict any ^{24}Na via ^{27}Al(n,α)
  - analysis of the raw ENDF-6 JEFF-3.3 reveals that the MF 9 entries for this reaction are incorrect
    (MF 9 is necessary to split between ^{24}Na and ^{24m}Na)
  - causes incorrect processing to group-wise format
  - TENDL-2017 doesn't include the ^{24m}Na channel
    (the MF 3 entry is correct in both JEFF-3.3 and TENDL-2017)