

FISPACT-II V&V

Fusion decay-heat benchmark for nuclear data validation

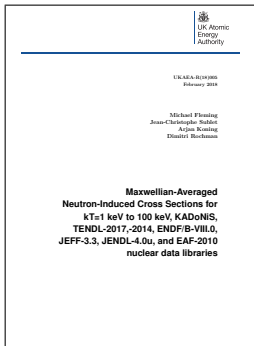
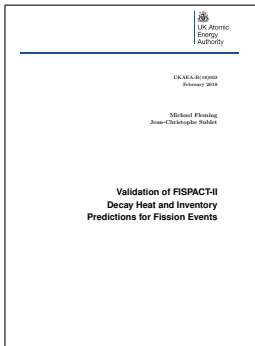
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FISPACT-II workshop

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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

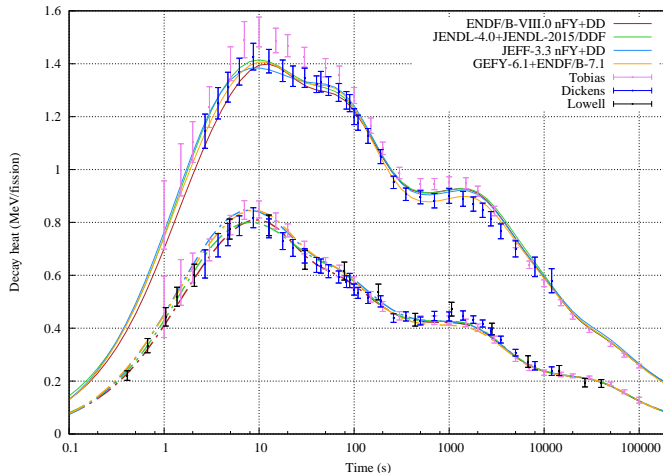
FISPACT-II validation



- V&V exercises with FISPACT-II focusing on TENDL
 - ▶ 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)

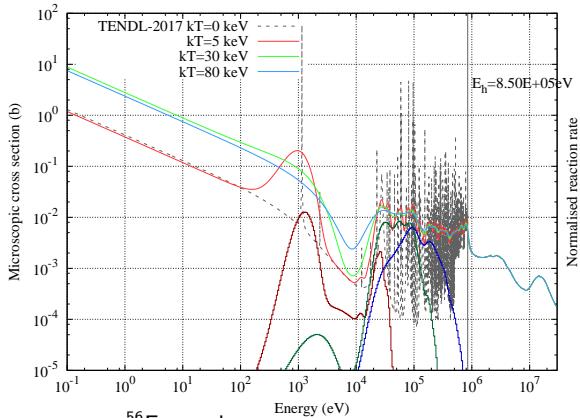
Other validation efforts (1)

- 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



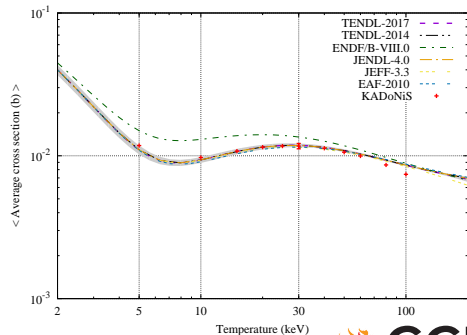
- total and β -generated decay heat
- simulated with latest ENDF/B, JEFF, and JENDL libraries
- Also included in exercise:
 ^{233}U , ^{238}U , ^{239}Pu , ^{241}Pu ,
 ^{232}Th , and ^{237}Np

Other validation efforts (2)



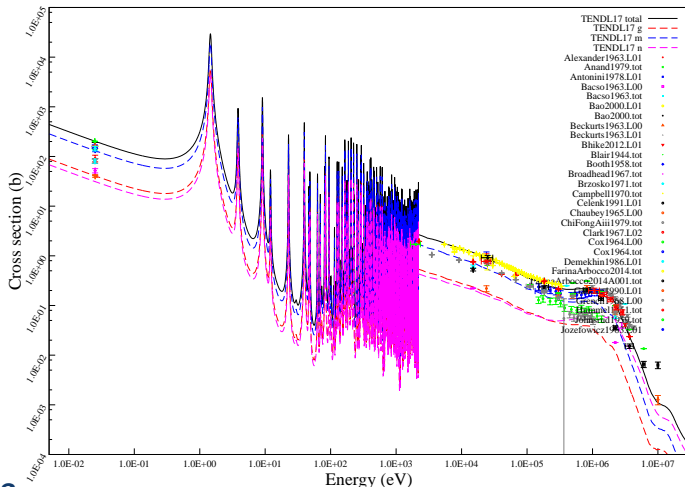
- e.g. ^{56}Fe results:
- TENDL-2017 xs & comparison to KADoNiS of average xs at various temperatures for different libraries

- 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)



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

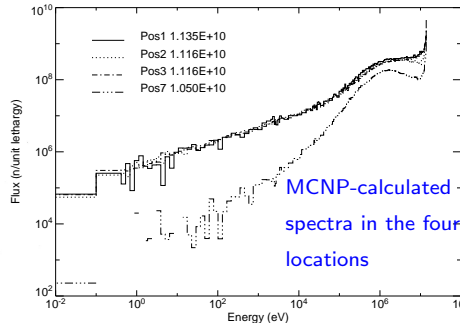
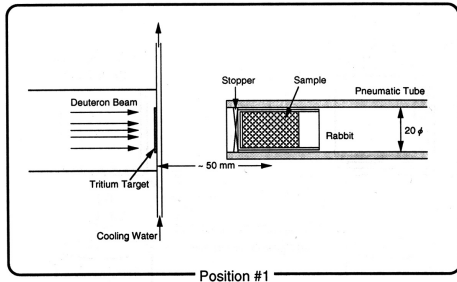
- Experiments performed at the Fusion Neutron Source (FNS) at JAEA in 1996-2000
- aimed at providing fusion-relevant decay-power data for important structural materials
- accurate experimental measurements with detailed records are ideal for simulation benchmarking

Experiment reports & papers: 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

Simulation paper: Gilbert, Sublet, *Nuclear Fusion* **59** (2019) 086045
Latest report: Gilbert, Vilkhivskaya, Sublet, UKAEA-CCFE-RE(20)04 (2020)
available from fispact.ukaea.uk/documentation-2/reports/

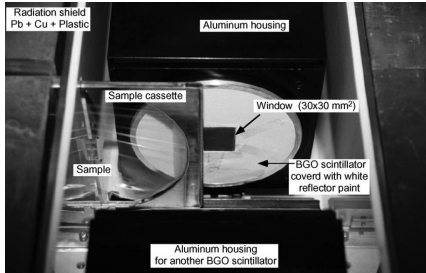
The experiment

- 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

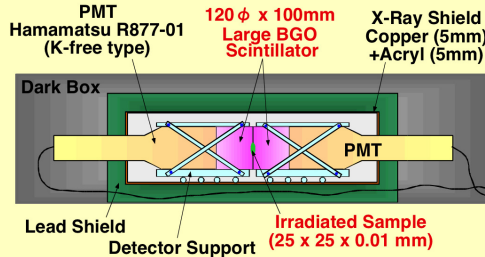


The experiment

- 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



WHOLE ENERGY ABSORPTION SPECTROMETER



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

Z	Material	Form	Z	Material	Form
9	Fluorine	CF ₂	46	Palladium	Metallic Foil
11	Sodium	Na ₂ CO 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 ₃ N ₅	51	Antimony	Metallic Powder
16	Sulphur	Powder	52	Tellurium	TeO ₂
17	Chlorine	C ₂ H ₂ Cl ₂	53	Iodine	IC ₆ H ₄ OH
19	Potassium	K ₂ CO ₃	55	Caesium	Cs ₂ O ₃
20	Calcium	CaO	56	Barium	BaCO ₃
21	Scandium	Sc ₂ O ₃	57	Lanthanum	La ₂ O ₃
22	Titanium	Metallic Foil	58	Cerium	CeO ₂
23	Vanadium	Metallic Foil	59	Praseodymium	Pr ₆ O ₁₁
24	Chromium	Metallic Powder	60	Neodymium	Nd ₂ O ₃
25	Manganese	Metallic Powder	62	Samarium	Sm ₂ O ₃
26	Iron	Metallic Foil	63	Europium	Eu ₂ O ₃
Alloy	SS304	Metallic Foil	64	Gadolinium	Gd ₂ O ₃
Alloy	SS316	Metallic Foil	65	Terbium	Tb ₄ O ₇
27	Cobalt	Metallic Foil	66	Dysprosium	Dy ₂ O ₃
Alloy	Inconel-600	Metallic Foil	67	Holmium	Ho ₂ O ₃
28	Nickel	Metallic Foil	68	Erbium	Er ₂ O ₃
Alloy	Nickel-chrome	Metallic Foil	69	Thulium	Tm ₂ O ₃
29	Copper	Metallic Foil	70	Ytterbium	Yb ₂ O ₃
30	Zinc	Metallic Foil	71	Lutetium	Lu ₂ O ₃
31	Gallium	Ga ₂ O ₃	72	Hafnium	Metallic Powder
32	Germanium	GeO ₂	73	Tantalum	Metallic Foil
33	Arsenic	As ₂ O ₃	74	Tungsten	Metallic Foil
34	Selenium	Metallic Powder	75	Rhenium	Metallic Powder
35	Bromine	BrC ₆ H ₄ COOH	76	Osmium	Metallic Powder
37	Rubidium	Rb ₂ CO ₃	77	Iridium	Metallic Powder
38	Strontium	SrCO ₃	78	Platinum	Metallic Foil
39	Yttrium	Y ₂ O ₃	79	Gold	Metallic Foil
40	Zirconium	Metallic Foil	80	Mercury	HgO
41	Niobium	Metallic Foil	81	Thallium	Tl ₂ O
42	Molybdenum	Metallic Foil	82	Lead	Metallic Foil
44	Ruthenium	Metallic Powder	83	Bismuth	Metallic Powder
45	Rhodium	Metallic Powder			

- mixture of metallic foils, powders, oxides, and alloys

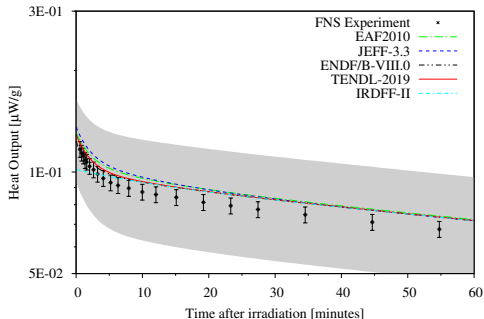
Simulations

- 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-2019, 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-II 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-2019
 - ▶ 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
 - ▶ a new decay_2020 file has recently been prototyped & also tested against the FNS benchmark

Typical results and presentation

5 minute irradiation of pure iron

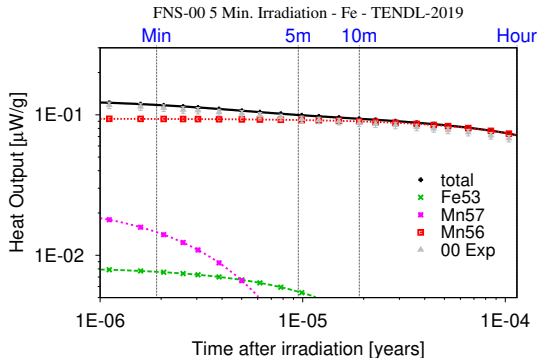
FNS-00 5 Min. Irradiation - Fe



decay heat curves from simulations with different libraries vs. experiment

- experimental artefact likely cause of slight disagreement – otherwise simulation captures the profile well

Product	$T_{1/2}$	Pathways	Path %
Mn57	1.42m	Fe57(n,p)Mn57	99.5
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Mn56	2.58h	Fe56(n,p)Mn56	99.7



- nuclide contribution breakdown for TENDL-2019 vs. experiment
- showing ^{56}Mn dominance

Typical results and presentation

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

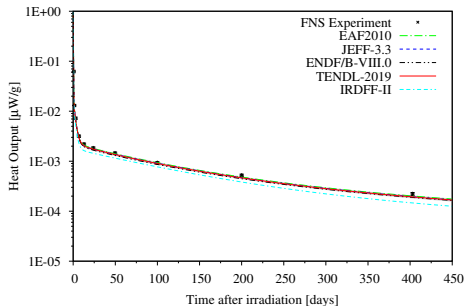
Times	FNS EXP. 5 mins		TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDF-II
Min.	$\mu\text{W/g}$		$\mu\text{W/g}$		E/C	E/C	E/C	E/C
0.58	$1.17E-01$	+/-5%	$1.22E-01$	+/-28%	0.96	1.00	0.94	0.91
0.83	$1.14E-01$	+/-5%	$1.19E-01$	+/-29%	0.96	1.00	0.94	0.91
1.08	$1.12E-01$	+/-5%	$1.17E-01$	+/-29%	0.96	0.99	0.93	0.91
1.35	$1.08E-01$	+/-5%	$1.15E-01$	+/-29%	0.94	0.98	0.92	0.90
1.60	$1.07E-01$	+/-5%	$1.13E-01$	+/-29%	0.95	0.98	0.93	0.90
2.03	$1.04E-01$	+/-5%	$1.10E-01$	+/-30%	0.95	0.97	0.92	0.90
2.63	$1.02E-01$	+/-5%	$1.07E-01$	+/-30%	0.95	0.97	0.92	0.90
3.23	$9.87E-02$	+/-5%	$1.04E-01$	+/-31%	0.94	0.96	0.92	0.90
4.10	$9.58E-02$	+/-5%	$1.02E-01$	+/-31%	0.94	0.95	0.91	0.90
5.20	$9.30E-02$	+/-5%	$9.93E-02$	+/-32%	0.94	0.94	0.91	0.90
6.32	$9.13E-02$	+/-5%	$9.75E-02$	+/-32%	0.94	0.94	0.91	0.90
7.93	$8.96E-02$	+/-5%	$9.56E-02$	+/-33%	0.94	0.94	0.91	0.90
9.98	$8.73E-02$	+/-5%	$9.37E-02$	+/-33%	0.93	0.93	0.91	0.90
12.03	$8.58E-02$	+/-5%	$9.22E-02$	+/-33%	0.93	0.93	0.91	0.91
15.10	$8.41E-02$	+/-5%	$9.02E-02$	+/-34%	0.93	0.93	0.92	0.91
19.20	$8.13E-02$	+/-5%	$8.79E-02$	+/-34%	0.93	0.93	0.91	0.91
23.32	$7.94E-02$	+/-5%	$8.58E-02$	+/-34%	0.93	0.93	0.91	0.92
27.42	$7.75E-02$	+/-5%	$8.39E-02$	+/-34%	0.92	0.92	0.91	0.92
34.53	$7.47E-02$	+/-5%	$8.09E-02$	+/-34%	0.92	0.92	0.92	0.92
44.65	$7.10E-02$	+/-5%	$7.71E-02$	+/-34%	0.92	0.92	0.91	0.92
54.75	$6.77E-02$	+/-5%	$7.36E-02$	+/-34%	0.92	0.92	0.91	0.92
mean % diff. from E					7	5	9	10
mean χ^2					1.59	1.20	2.75	3.62

Product	$T_{1/2}$	E/C	% ΔE	% ΔC^{nuc}
Mn56	2.58h	0.96	5%	35%

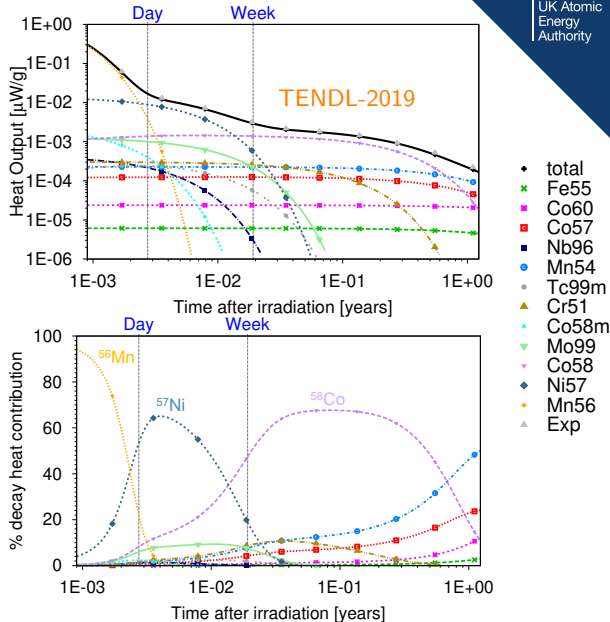
A complex case

7 hour irradiation of 316 stainless steel

FNS-96 7 hours Irradiation - SS316



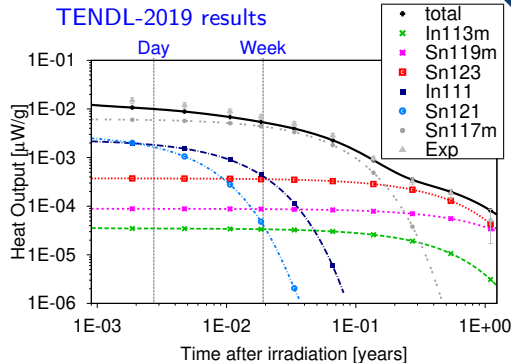
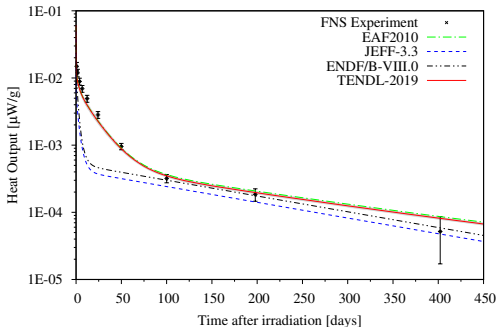
- a good fit with all major data libraries despite the relative complexity
 - predictions are within a few % of the experiment at all decay times
- numerous (minor) contributions but importance dominance of ^{56}Mn , ^{57}Ni , and ^{58}Co at different times



Multiple metastable importance

- 7 hour irradiation of pure tin

FNS-96 7 hours Irradiation - SnO_2

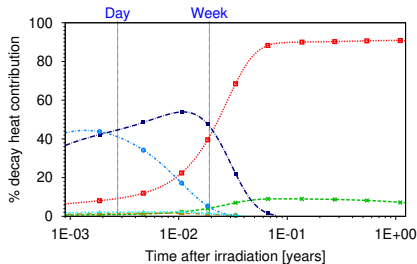
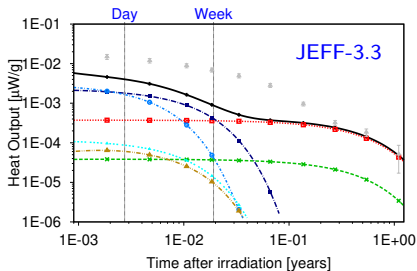
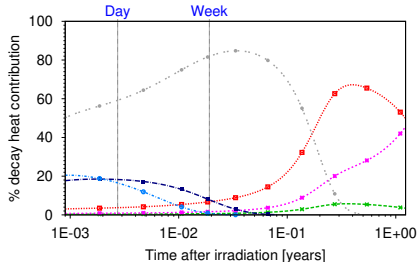
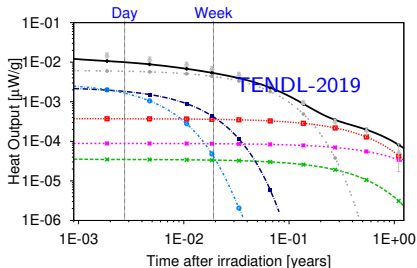
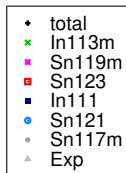


- TEND-2019 and EAF2010 produce a good match to the measured profile
 - but absolute decay heat values are not very close to the experiment
- JEFF-3.3 and ENDF/B-VIII.0 get the profile wrong

	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	22	51	23	61
mean χ^2	2.29	25.28	2.21	33.51

Tin nuclide comparisons

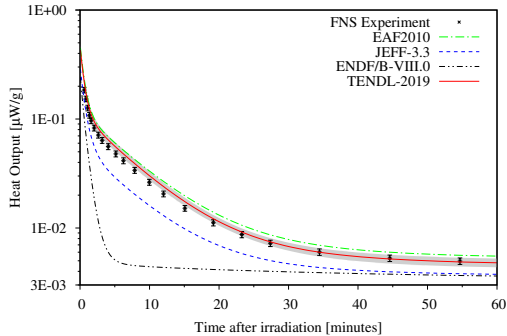
- TENDL result shows importance of two metastable nuclides
 - ▶ ^{119m}Sn and ^{117m}Sn produced via (n,2n) reactions
- JEFF & ENDF/B include the (n,2n)s but only to ground-states



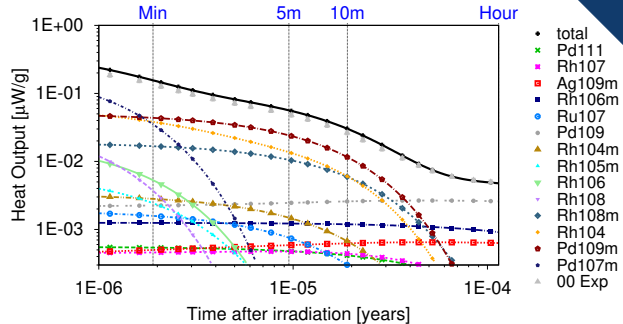
A case where TENDL is best

- 5 minute irradiation of pure palladium

FNS-00 5 Min. Irradiation - Pd



FNS-00 5 Min. Irradiation - Pd - TENDL-2019



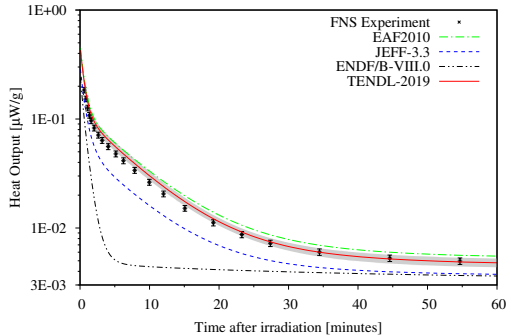
- a complex case with many contributing nuclides
 - particularly metastables: ^{108m}Rh , ^{109m}Pd , and ^{106m}Rh
 - a mixture of (n,2n) and (n,p) reactions dominate
 - TENDL-2017 outperforms all others

	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	12	66	23	32
mean χ^2	4.77	121.59	14.31	26.91

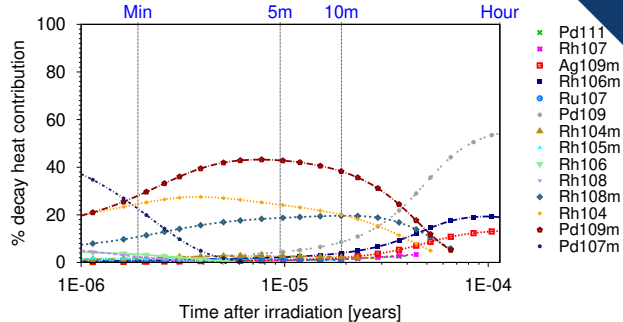
A case where TENDL is best

- 5 minute irradiation of pure **palladium**

FNS-00 5 Min. Irradiation - Pd



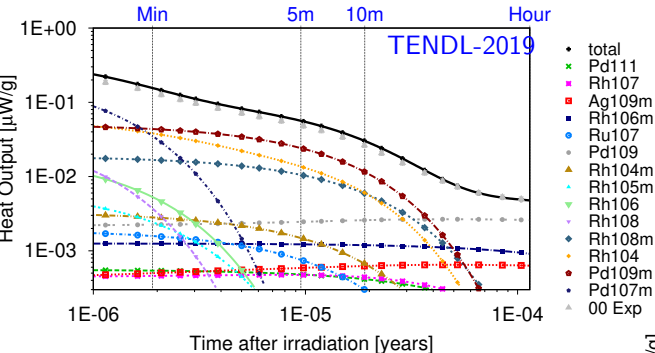
FNS-00 5 Min. Irradiation - Pd - TENDL-2019



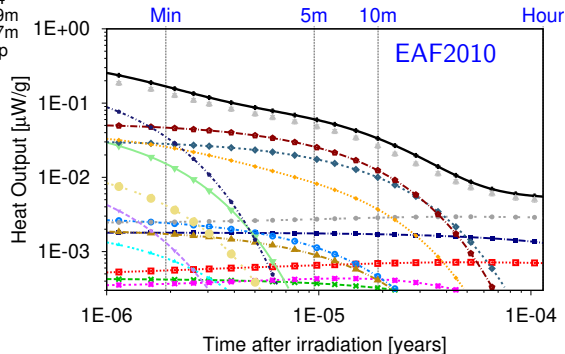
- a complex case with many contributing nuclides
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Palladium nuclide comparisons



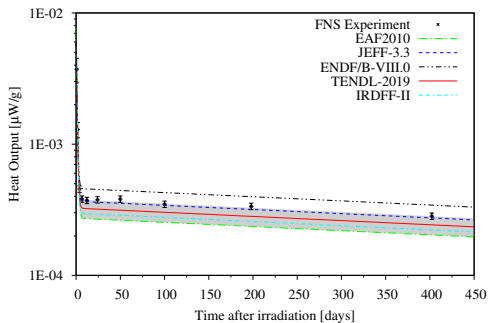
- EAF2010 overpredicts $^{108\text{m}}\text{Rh}$ production
- ENDF/B-VIII.0 & JEFF-3.3 (not shown) miss $^{108\text{m}}\text{Rh}$, $^{109\text{m}}\text{Pd}$, and $^{106\text{m}}\text{Rh}$



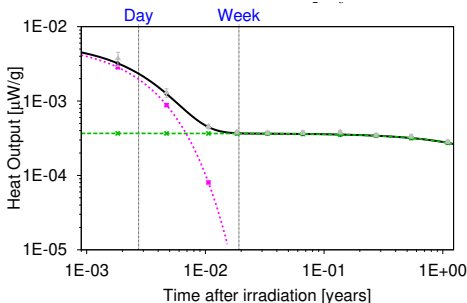
A case where JEFF-3.3 is best

7 hour irradiation of sodium

FNS-96 7 hours Irradiation - Na_2CO_3



JEFF-3.3 results

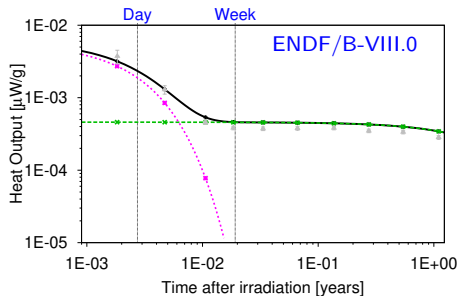
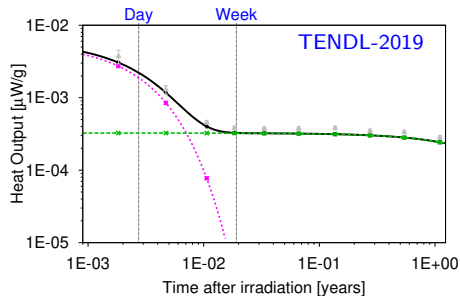


only JEFF-3.3 matches closely the experimental measurements

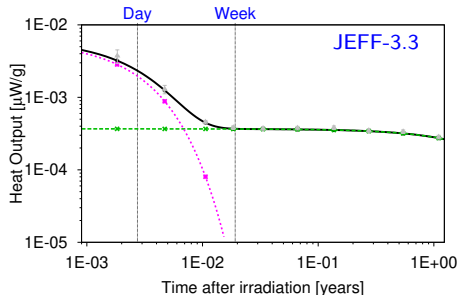
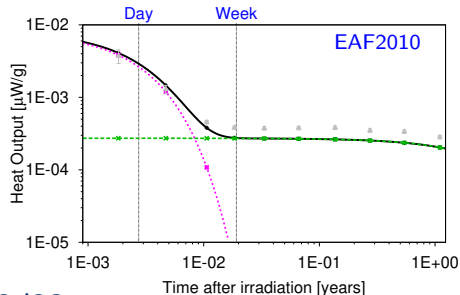
- ▶ other libraries either under or over predict the production of ^{22}Na
- ▶ this could be a coincidence due to an experimental artefact – especially since the IRDFF dosimetry file underpredicts

	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
mean % diff. from E	14	17	24	5	21
mean χ^2	5.58	10.23	19.27	0.47	12.27

Sodium nuclide comparisons



- total
- x Na22
- Na24
- ▲ Exp

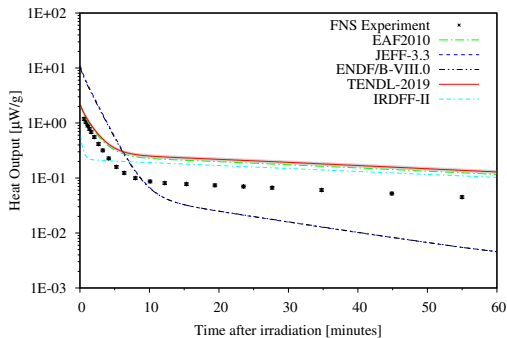


- $^{23}\text{Na}(n,\gamma)^{24}\text{Na}$
- $^{23}\text{Na}(n,2n)^{22}\text{Na}$

A case where all are wrong (1)

- 5 minute irradiation of pure Indium

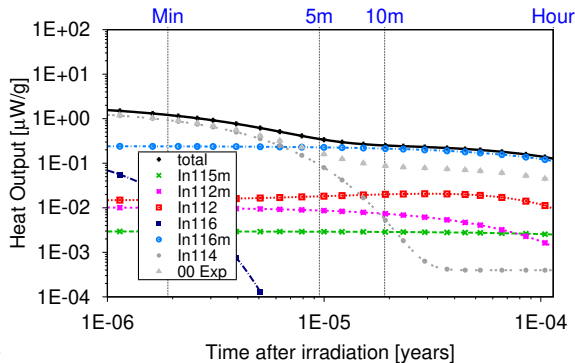
FNS-00 5 Min. Irradiation - In



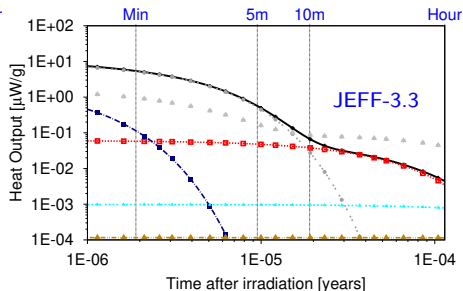
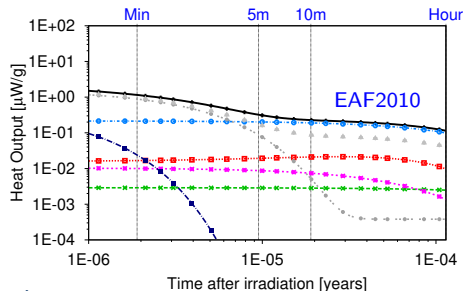
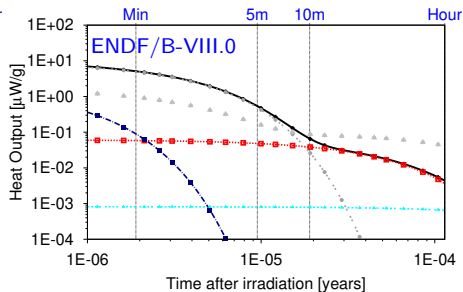
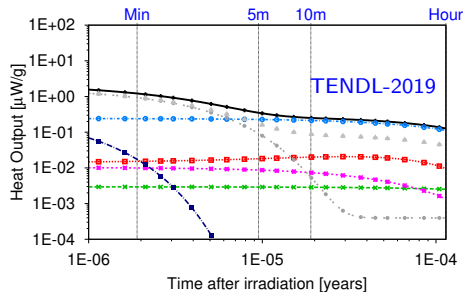
- no library is close to the experiment
- the TENDL-2019 nuclide profiles suggest an overestimate of $^{116\text{m}}\text{In}$ production

- $^{116\text{m}}\text{In}$ decay profile matches the experimental measurements beyond 5 minutes of cooling
- incorrect distribution of $^{115}\text{In}(n,\gamma)$ to ^{116}In , $^{116\text{m}}\text{In}$, $^{116\text{n}}\text{In}$?
($T_{1/2}=14.2\text{s}$, 54.6m , and 2.2s , respectively)

TENDL-2019 results

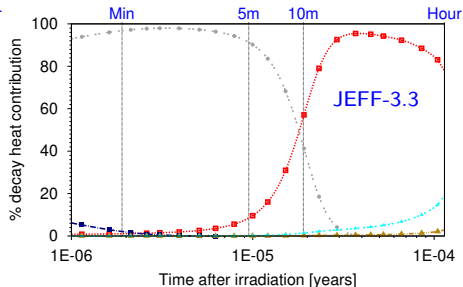
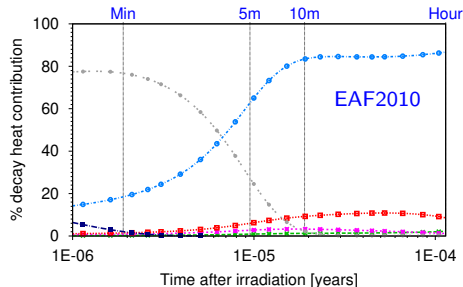
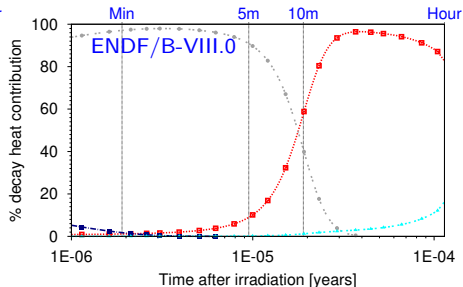
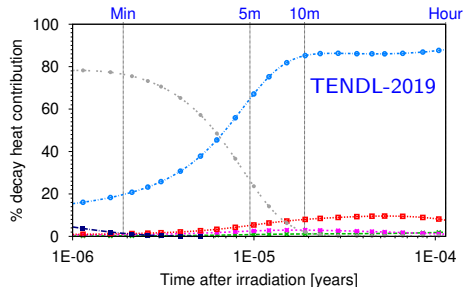


Indium nuclide comparisons



- total
 - × In115m
 - In112m
 - In112
 - In116
 - In116m
 - In114
 - ▲ 00 Exp
 - ▲ Ag112
- JEFF-3.3, ENDF/B-VIII.0 miss $^{116\text{m}}\text{In}$ completely
 - EAF2010 & predict more contributing nuclides, but agree on $^{116\text{m}}\text{In}$ dominance

Indium nuclide comparisons

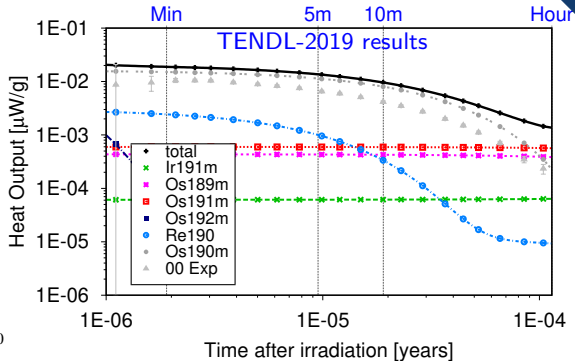
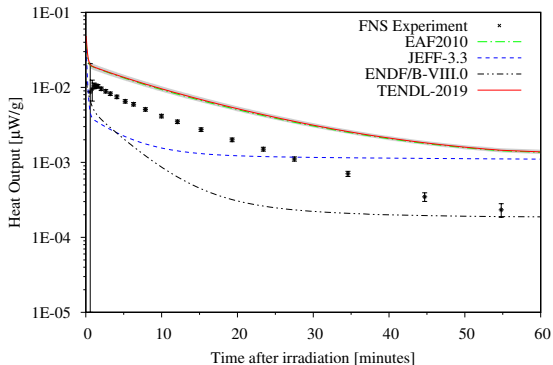


- total
 - × In115m
 - In112m
 - In112
 - In116
 - In116m
 - In114
 - ▲ 00 Exp
 - ▲ Ag112
- JEFF-3.3, ENDF/B-VIII.0 miss ^{116m}In completely
 - EAF2010 & predict more contributing nuclides, but agree on ^{116m}In dominance

A case where all are wrong (2)

5 minute irradiation of pure Osmium

FNS-00 5 Min. Irradiation - Os



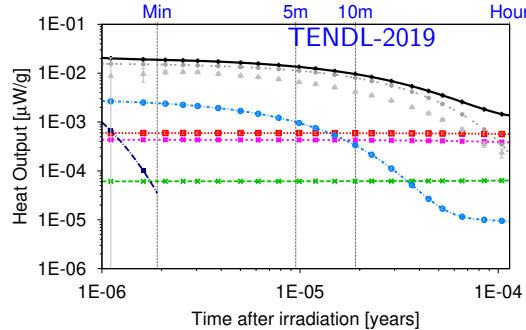
no library predicts the correct decay-profile or heat magnitudes

- ▶ EAF2010 and TENDL-2019 are identical and overpredict
- ▶ JEFF-3.3 over and under predicts at different times, while ENDF/B-VIII.0 underpredicts

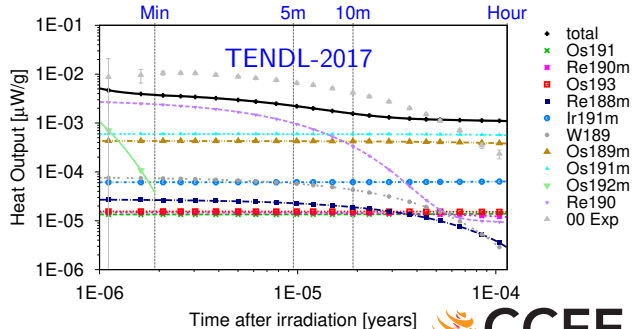
	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	160	63	155	80
mean χ^2	501.94	127.59	467.62	118.99

Osmium nuclide comparisons

- The EAF2010 profile was identified as the best match and is attributed to $^{190}\text{Os}(n,n')^{190m}\text{Os}$

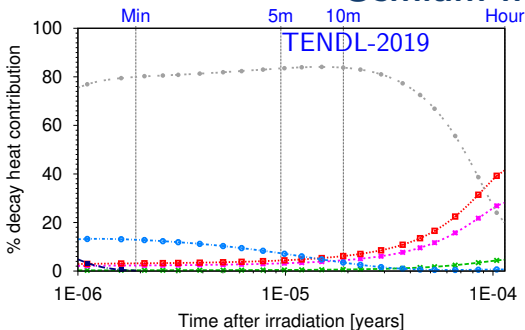


- this channel was missing from the group-wise processed version of TENDL-2017 (& JEFF-3.3 & ENDF/B-VIII.0)
- but now included in TENDL-2019

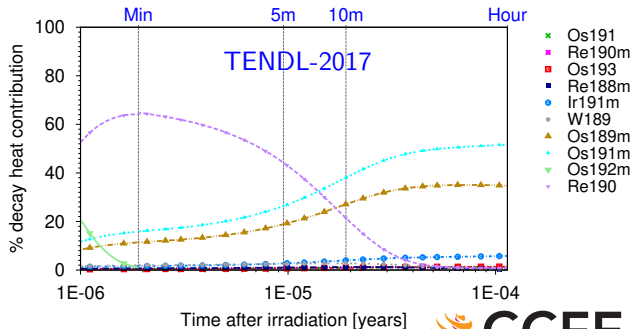


Osmium nuclide comparisons

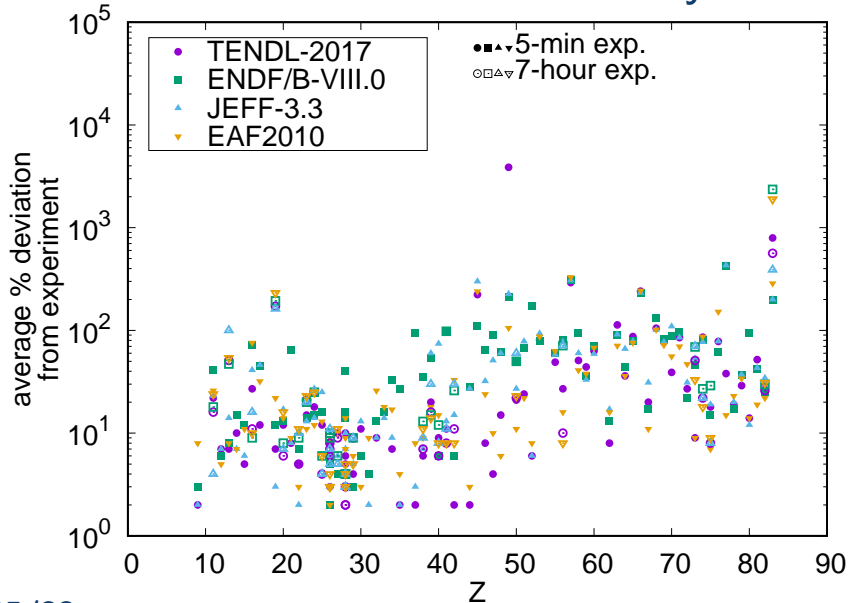
- The EAF2010 profile was identified as the best match and is attributed to $^{190}\text{Os}(n,n')^{190m}\text{Os}$



- this channel was missing from the group-wise processed version of TENDL-2017 (& JEFF-3.3 & ENDF/B-VIII.0)
- but now included in TENDL-2019

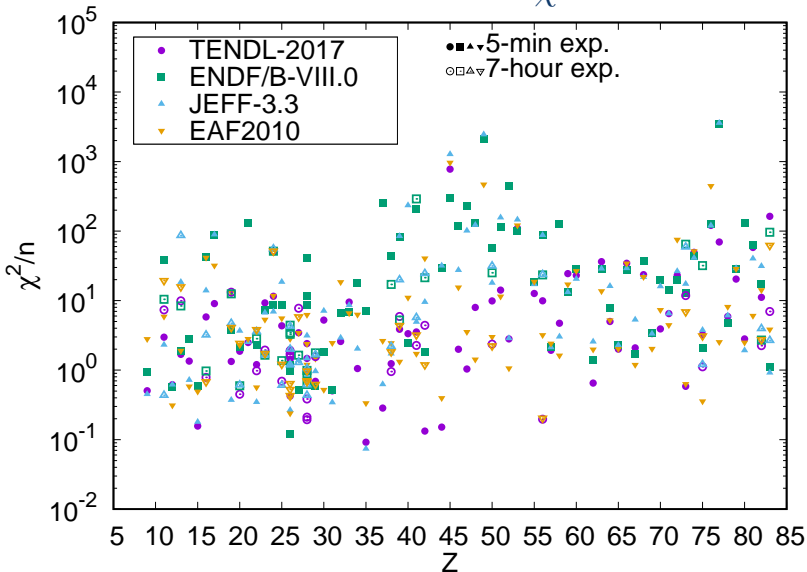


Statistical analysis



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

χ^2 test

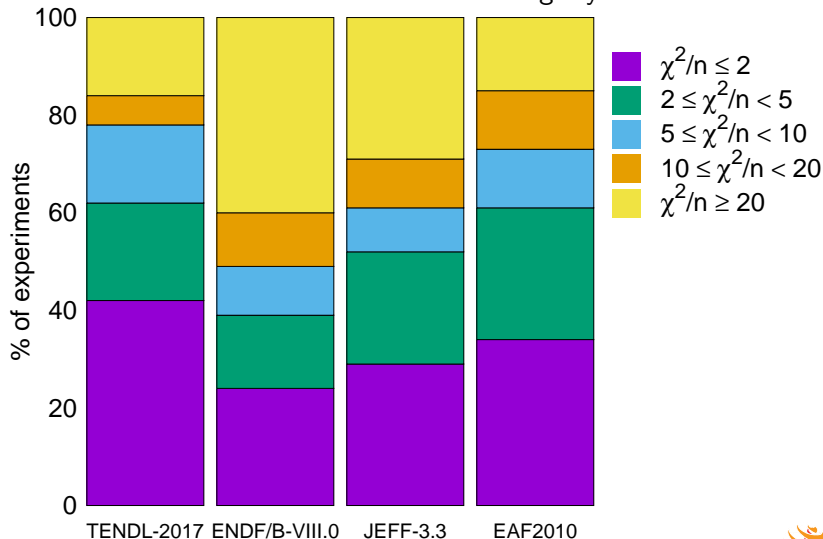


- χ^2/n variation for all experiments
- less clear trend
⇒ higher experimental errors at high Z

$$\chi^2 = \left(\frac{D_{sim} - D_{exp}}{\Delta D_{exp}} \right)^2$$

n values per experiment

- TENDL performs better than other modern libraries & slightly better than EAF2010



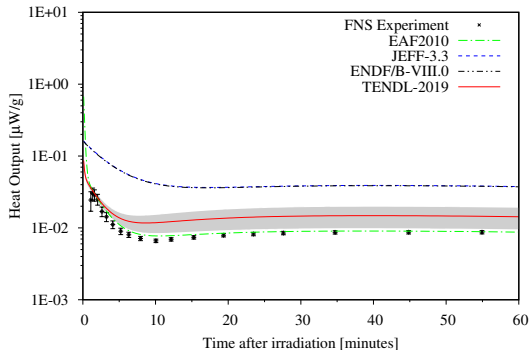
Summary

- 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

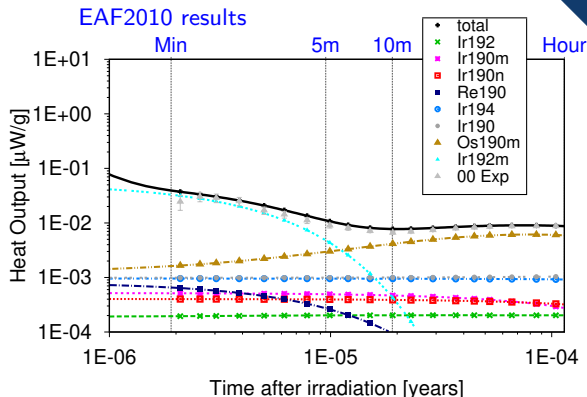
5 minute irradiation of pure Iridium

FNS-00 5 Min. Irradiation - Ir



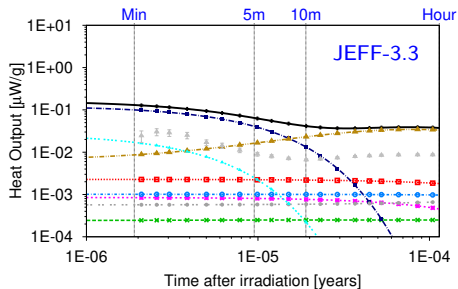
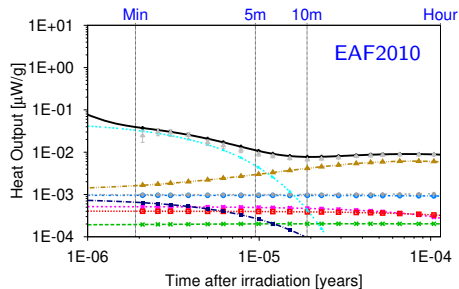
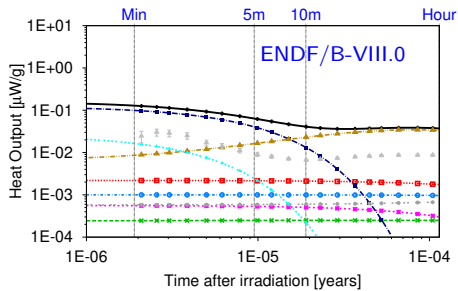
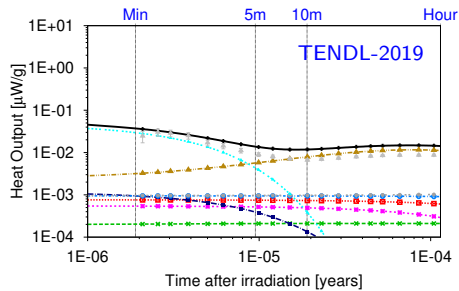
Only EAF2010 correctly matches the experimental profile (and scale)

- the observed decay heat originates from ^{192m}Ir in the first 5 minutes of cooling
- at longer times ^{190m}Os dominates



	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	52	419	13	425
mean χ^2	94.41	3453.56	2.29	3550.01

Iridium nuclide comparisons

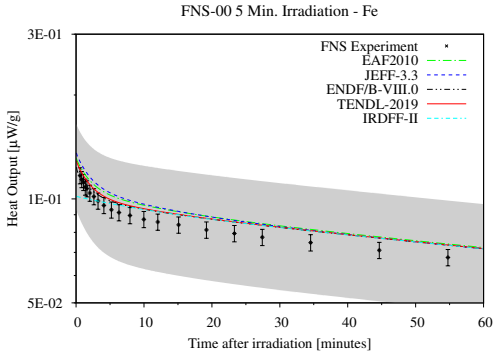


- TENDL-2017 underpredicts $^{191}\text{Ir}(n,2n)^{190\text{n}}\text{Ir}(\beta^+)^{190\text{m}}\text{Os}$
- ENDF/B-VIII.0 and JEFF-3.3 overestimate this path & predict a different dominant nuclide ($^{193}\text{Ir}(n,\alpha)^{190}\text{Re}$) at short times

FISPACT-II inputs & outputs

.gra files

- e.g. irradiation of pure **iron**



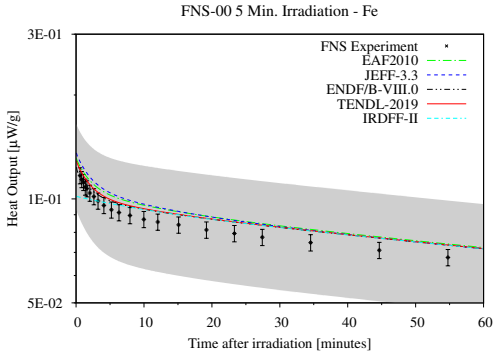
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from **.gra** files

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 GNUPLLOT plotting (+ a *template* .plt file is written)

.gra files

- e.g. irradiation of pure **iron**



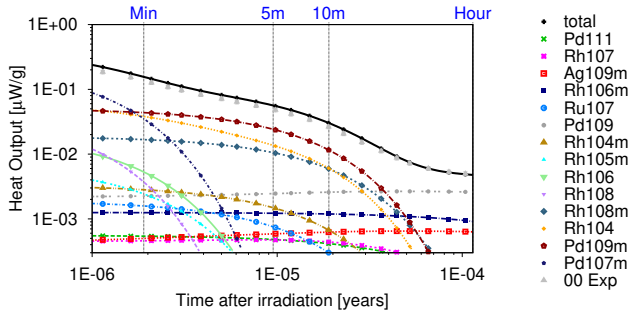
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from **.gra** files

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**



- 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