FISPACT-II V&V

Fusion decay-heat benchmark for nuclear data validation

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FISPACT-II workshop

November 23 - December 3, 2020

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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

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FISPACT-II validation

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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

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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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UKAEA-CCFE-RE(20)04
April 2020

Mark R. Gilbert
Olga Vilkhivskaya
Jean-Christophe Sublet

Fusion decay heat validation, FISPACT-II & TENDL-2019, ENDF/B-VIII.0, JEFF-3.3, EAF2010, and IRDFF-II nuclear data libraries

www.ccfe.ac.uk

- 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)

available from http://fispact.ukaea.uk

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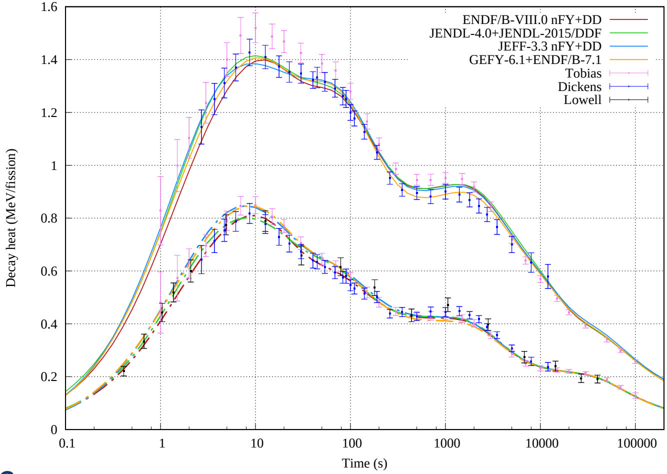
Other validation efforts (1)

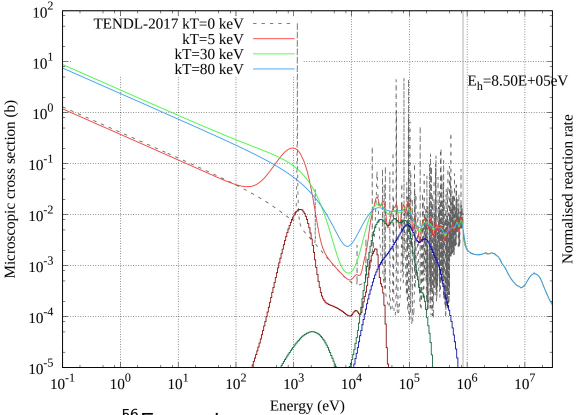
- Fission decay heat
- Comparison of simulated fission pulse decay heat to carefully interpreted experimental data
- e.g. ^{235}U thermal (0.0253 eV) pulse comparison



- 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

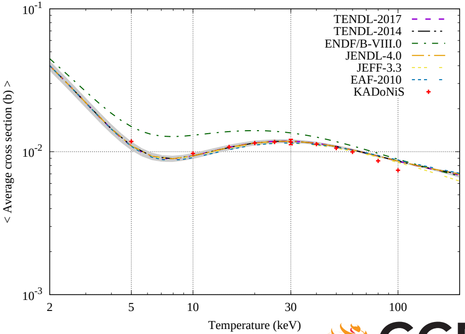
UKAEA-R(18)003

Other validation efforts (2)



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

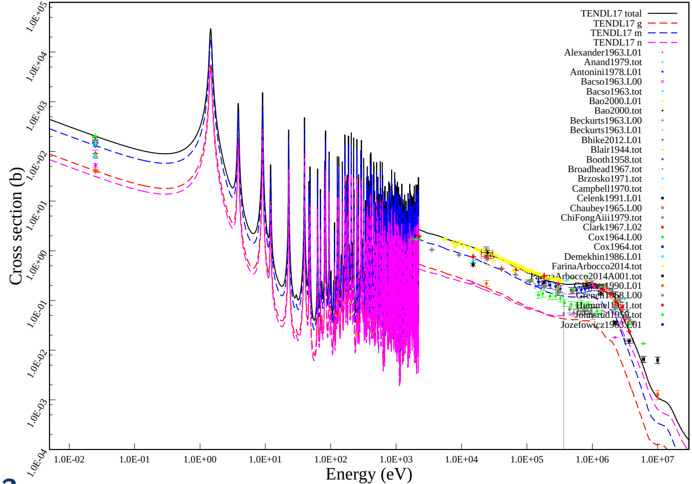
- Maxwellian-averaged neutron xs comparison
- using KADoNiS astrophysics experimental database, which includes data for 357 nuclides at temperatures ranging from 5 keV (58 million K) to 100 keV (1.2 billion K)



UKAEA-R(18)005

Other validations (3)

- <u>Integro-differential V&V</u>
- 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

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Fusion decay heat benchmark

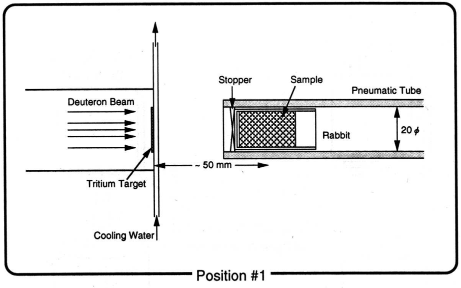
- Experiments performed at the Fusion Neutron Source (FNS) at JAEA in 1996-2000
- aimed at providing fusion-relevant decay-power data for important structural materials
- accurate experimental measurements with detailed records are ideal for simulation benchmarking

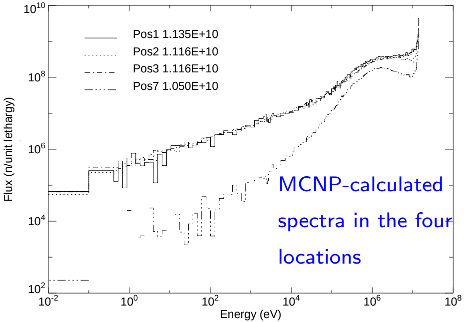
Experiment reports & papers: F. Maekawa M. Wada, Y. Ikeda *et al.* Tech. Rep. JAERI-Data/Code 98-024, JAERI-Data/Code 98-021, & JAERI 99-055. http://www.jaea.go.jp/jaeri/
Maekawa *et al.*, Fus. Eng. Des. 47 (2000) 377-388 &
J. Nucl. Sci. Tech. 39 (2002) 990-993

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

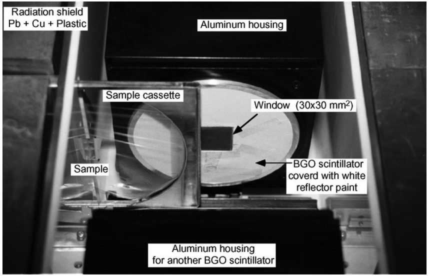
- 2 mA deuteron beam onto a tritium target producing a fusion neutron spectrum with fluxes of $\sim 10^{10}$ n cm^{-2} s^{-1} at the sample location
- samples irradiated for 5 minutes or 7 hours (4 different experimental set-ups)
- for the short irradiations, a rapid rabbit extraction system was used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

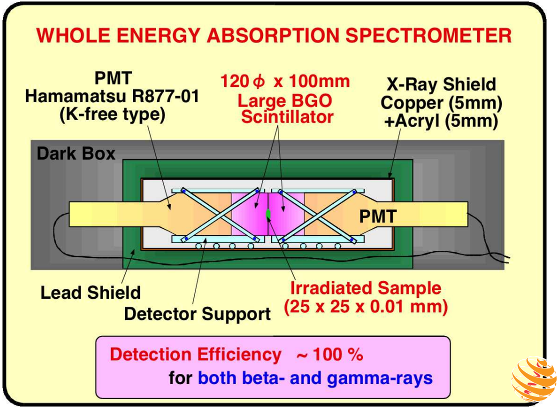




The experiment

- 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





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			

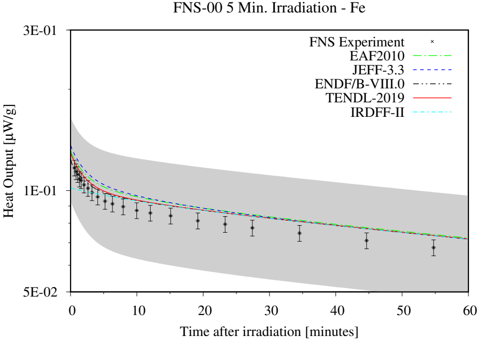
- mixture of metallic foils, powders, oxides, and alloys

Simulations

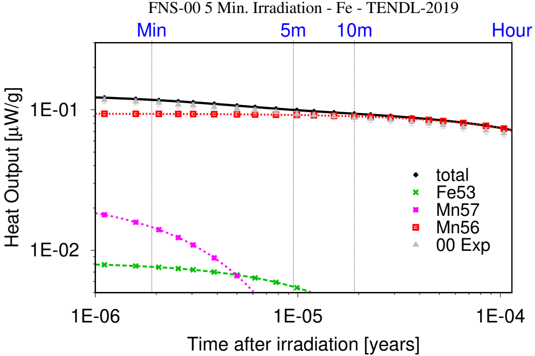
- Detailed experimental information (irradiation times, measurement times, material compositions, etc.) have been translated into a set of FISPACT-II input files
  - these can be rapidly repeated for different nuclear data libraries
- Latest version of exercise compares results from TENDL-2019, ENDF/B-VIII.0, 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



- 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	IRDFF-II
Min.	μW/g		μW/g		E/C	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	1.15
0.83	$1.14E-01$	+/-5%	$1.19E-01$	+/-29%	0.96	1.00	0.94	0.91	1.13
1.08	$1.12E-01$	+/-5%	$1.17E-01$	+/-29%	0.96	0.99	0.93	0.91	1.11
1.35	$1.08E-01$	+/-5%	$1.15E-01$	+/-29%	0.94	0.98	0.92	0.90	1.08
1.60	$1.07E-01$	+/-5%	$1.13E-01$	+/-29%	0.95	0.98	0.93	0.90	1.07
2.03	$1.04E-01$	+/-5%	$1.10E-01$	+/-30%	0.95	0.97	0.92	0.90	1.04
2.63	$1.02E-01$	+/-5%	$1.07E-01$	+/-30%	0.95	0.97	0.92	0.90	1.03
3.23	$9.87E-02$	+/-5%	$1.04E-01$	+/-31%	0.94	0.96	0.92	0.90	1.00
4.10	$9.58E-02$	+/-5%	$1.02E-01$	+/-31%	0.94	0.95	0.91	0.90	0.98
5.20	$9.30E-02$	+/-5%	$9.93E-02$	+/-32%	0.94	0.94	0.91	0.90	0.96
6.32	$9.13E-02$	+/-5%	$9.75E-02$	+/-32%	0.94	0.94	0.91	0.90	0.95
7.93	$8.96E-02$	+/-5%	$9.56E-02$	+/-33%	0.94	0.94	0.91	0.90	0.95
9.98	$8.73E-02$	+/-5%	$9.37E-02$	+/-33%	0.93	0.93	0.91	0.90	0.94
12.03	$8.58E-02$	+/-5%	$9.22E-02$	+/-33%	0.93	0.93	0.91	0.91	0.93
15.10	$8.41E-02$	+/-5%	$9.02E-02$	+/-34%	0.93	0.93	0.92	0.91	0.94
19.20	$8.13E-02$	+/-5%	$8.79E-02$	+/-34%	0.93	0.93	0.91	0.91	0.93
23.32	$7.94E-02$	+/-5%	$8.58E-02$	+/-34%	0.93	0.93	0.91	0.92	0.93
27.42	$7.75E-02$	+/-5%	$8.39E-02$	+/-34%	0.92	0.92	0.91	0.92	0.92
34.53	$7.47E-02$	+/-5%	$8.09E-02$	+/-34%	0.92	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	0.92
54.75	$6.77E-02$	+/-5%	$7.36E-02$	+/-34%	0.92	0.92	0.91	0.92	0.92
mean % diff. from E					7	5	9	10	7
mean χ^2					1.59	1.20	2.75	3.62	1.89

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

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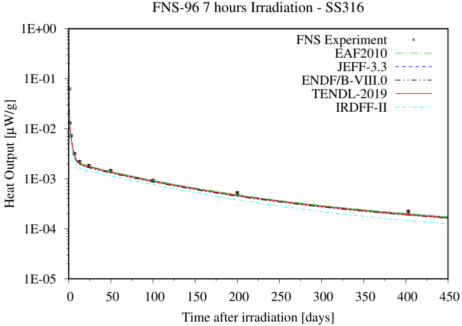
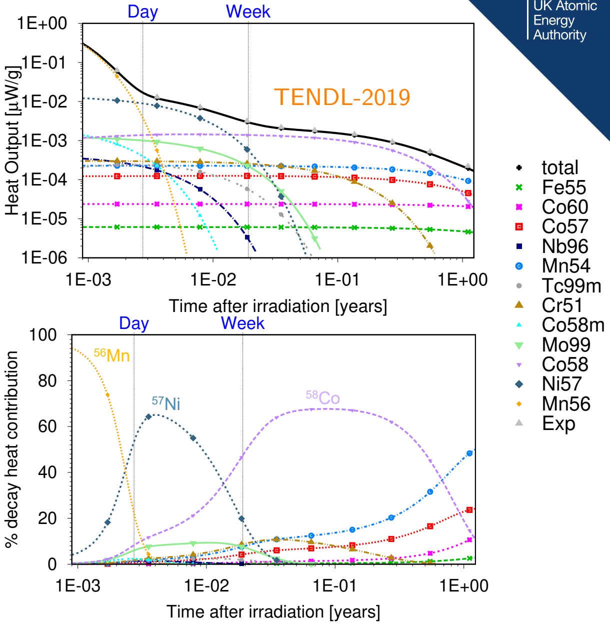
A complex case

- 7 hour irradiation of 316 stainless steel

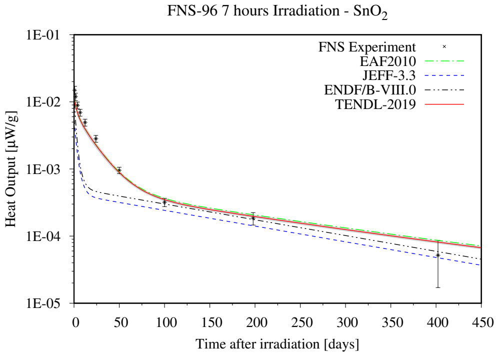


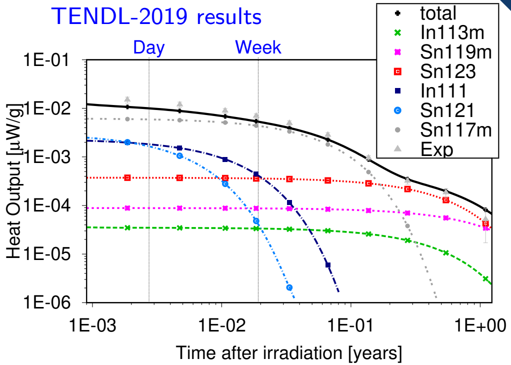


- a good fit with all major data libraries despite the relative complexity
  - predictions are within a few % of the experiment at all decay times
- numerous (minor) contributions but importance dominance of ^{56}Mn, ^{57}Ni, and ^{58}Co at different times

Multiple metastable importance

- 7 hour irradiation of pure tin





- 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

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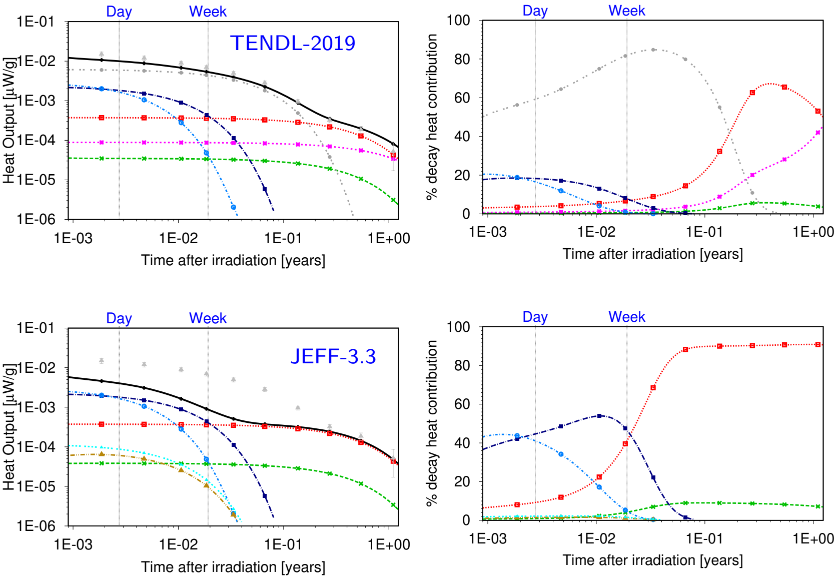
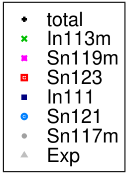
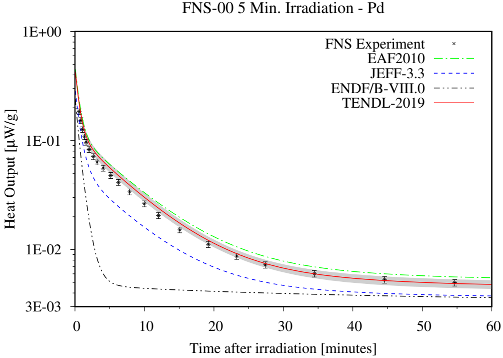


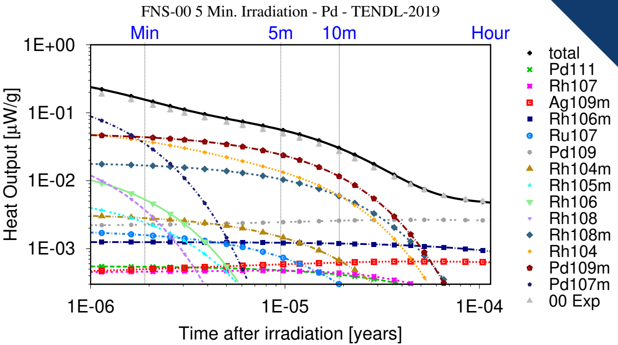
- TENDL result shows importance of two metastable nuclides
  - ^{119m}Sn and ^{117m}Sn produced via (n,2n) reactions
- JEFF & ENDF/B include the (n,2n)s but only to ground-states



A case where TENDL is best

- 5 minute irradiation of pure palladium



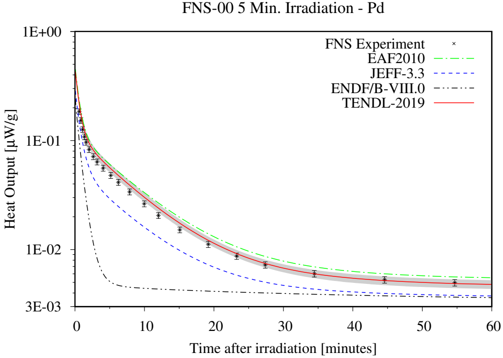


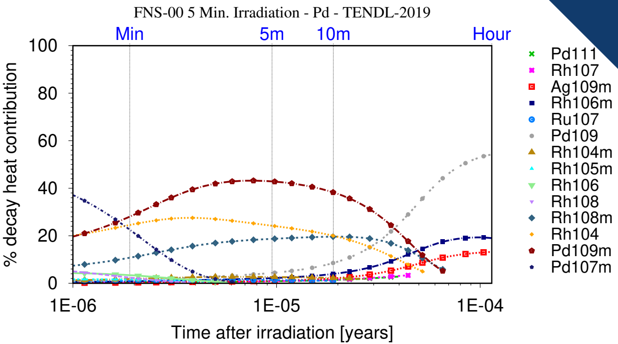
- a complex case with many contributing nuclides
  - particularly metastables: ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh
  - a mixture of (n,2n) and (n,p) reactions dominate
  - TENDL-2017 outperforms all others

	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





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mean % diff. from E	12	66	23	32
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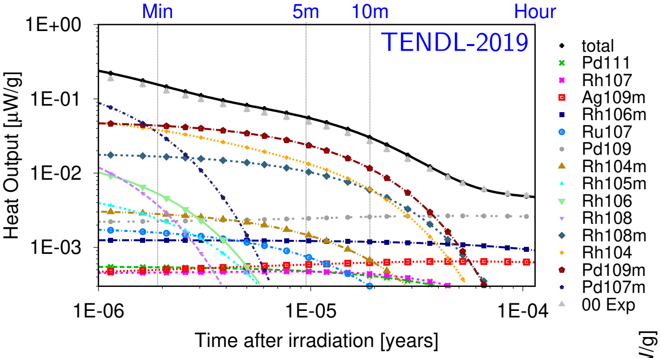
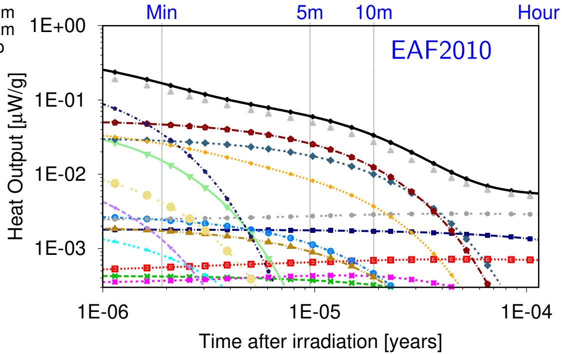
Palladium nuclide comparisons

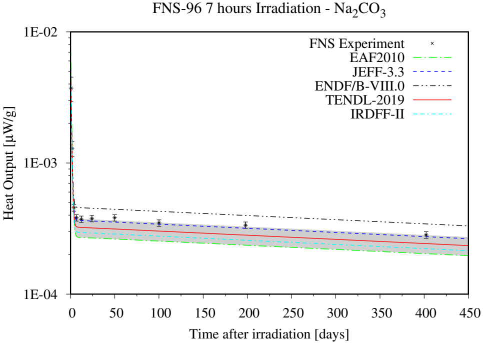


- EAF2010 overpredicts ^{108m}Rh production
- ENDF/B-VIII.0 & JEFF-3.3 (not shown) miss ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh

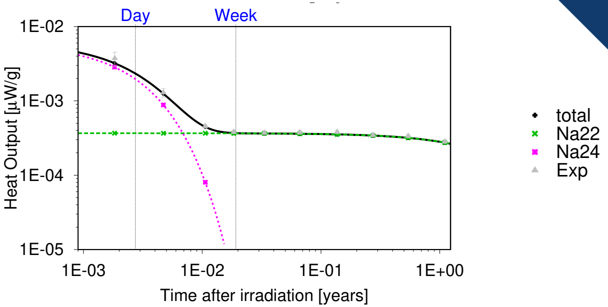


A case where JEFF-3.3 is best

- 7 hour irradiation of sodium



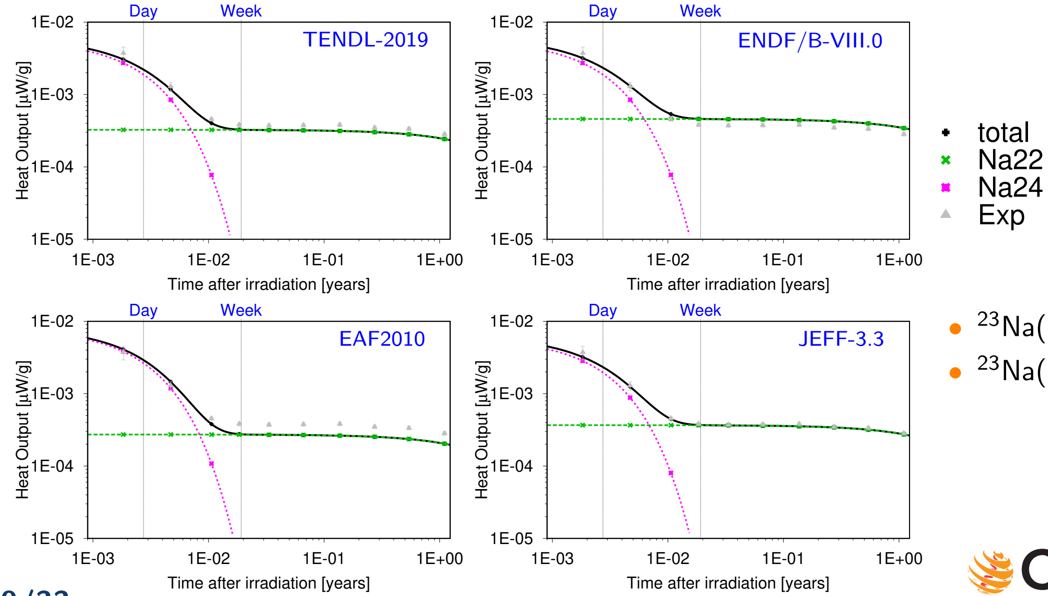
JEFF-3.3 results



- 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

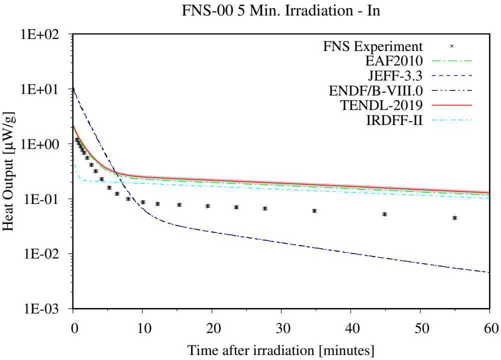
Sodium nuclide comparisons

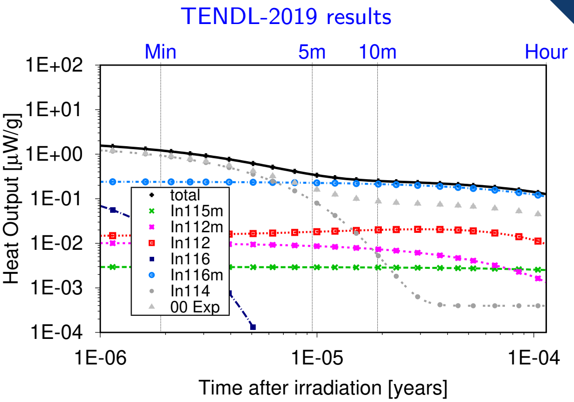


- $^{23}Na(n,\gamma)^{24}Na$
- $^{23}Na(n,2n)^{22}Na$

A case where all are wrong (1)

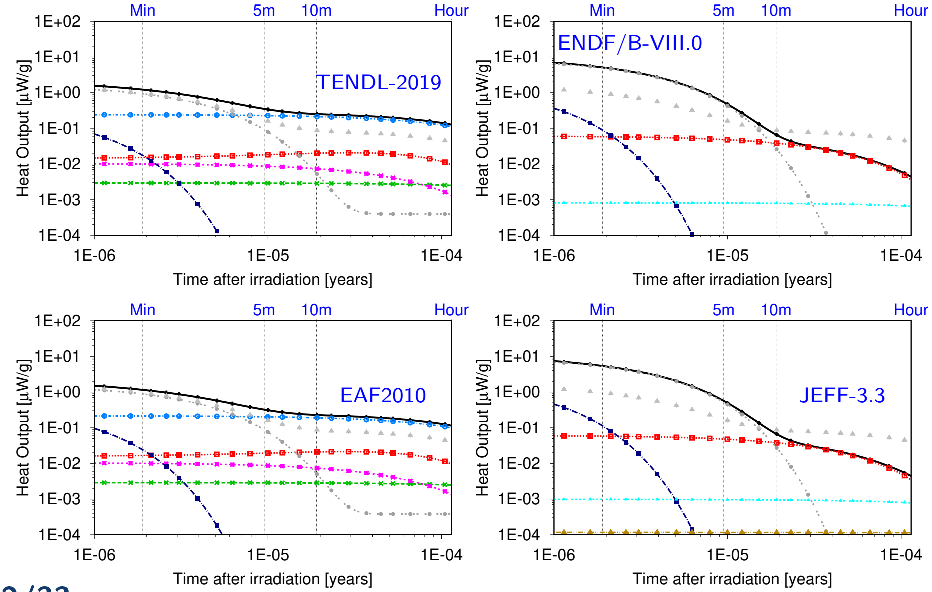
- 5 minute irradiation of pure Indium





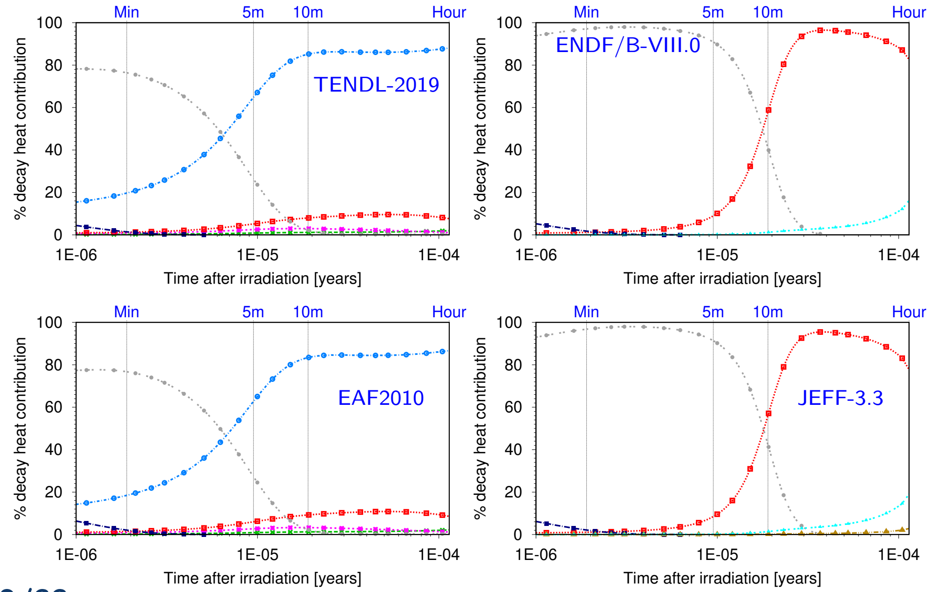
- no library is close to the experiment
- the TENDL-2019 nuclide profiles suggest an overestimate of ^{116m}In production
  - ^{116m}In decay profile matches the experimental measurements beyond 5 minutes of cooling
  - incorrect distribution of ^{115}In(n,γ) to ^{116}In, ^{116m}In, ^{116n}In? ($T_{1/2}$=14.2s, 54.6m, and 2.2s, respectively)

Indium nuclide comparisons



- JEFF-3.3, ENDF/B-VIII.0 miss ^{116m}In completely
- EAF2010 & predict more contributing nuclides, but agree on ^{116m}In dominance

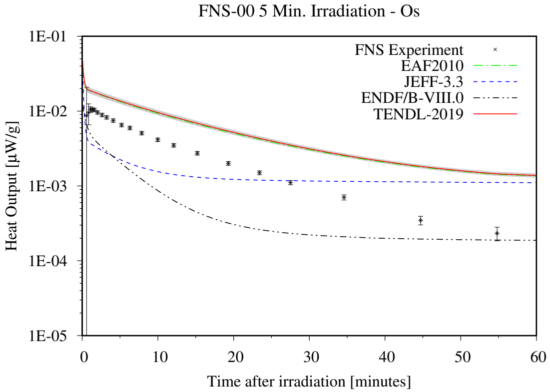
Indium nuclide comparisons

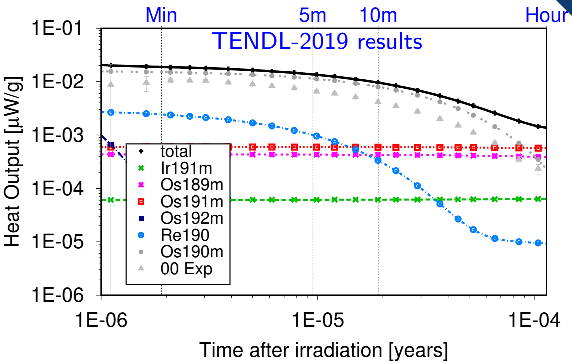


- JEFF-3.3, ENDF/B-VIII.0 miss ^{116m}In completely
- EAF2010 & predict more contributing nuclides, but agree on ^{116m}In dominance

A case where all are wrong (2)

- 5 minute irradiation of pure Osmium

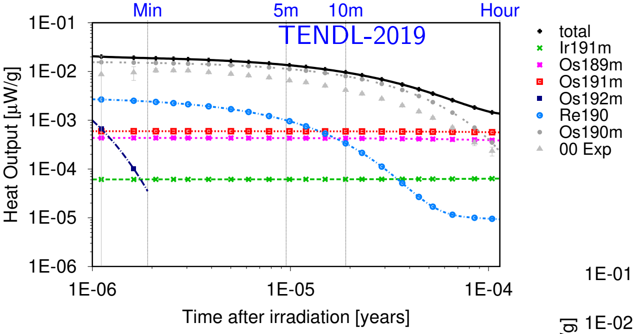




- no library predicts the correct decay-profile or heat magnitudes
  - EAF2010 and TENDL-2019 are identical and overpredict
  - JEFF-3.3 over and under predicts at different times, while ENDF/B-VIII.0 underpredicts

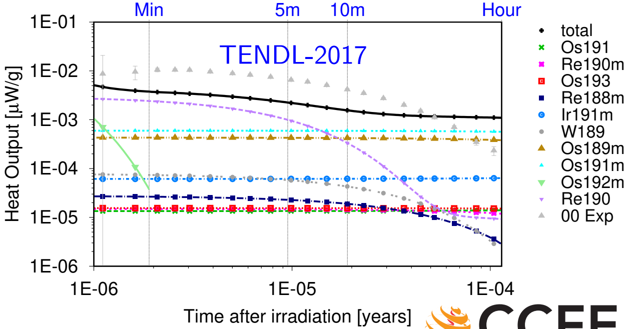
	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3
mean % diff. from E	160	63	155	80
mean χ^2	501.94	127.59	467.62	118.99

Osmium nuclide comparisons

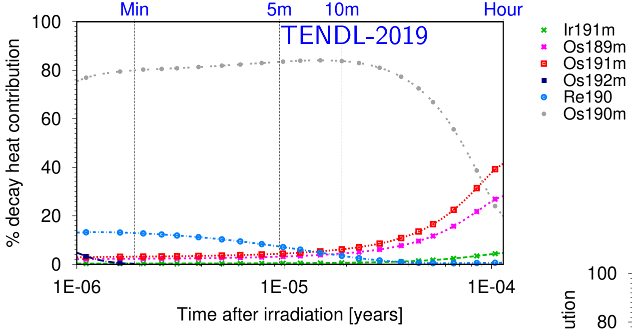


- The EAF2010 profile was identified as the best match and is attributed to $^{190}Os(n,n')^{190m}Os$

- 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 $^{190}\mathrm{Os}(n,n')^{190m}\mathrm{Os}$

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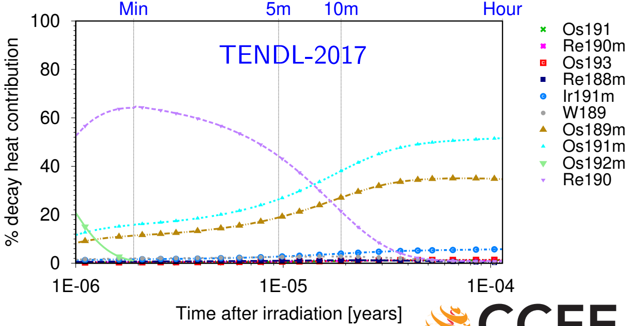

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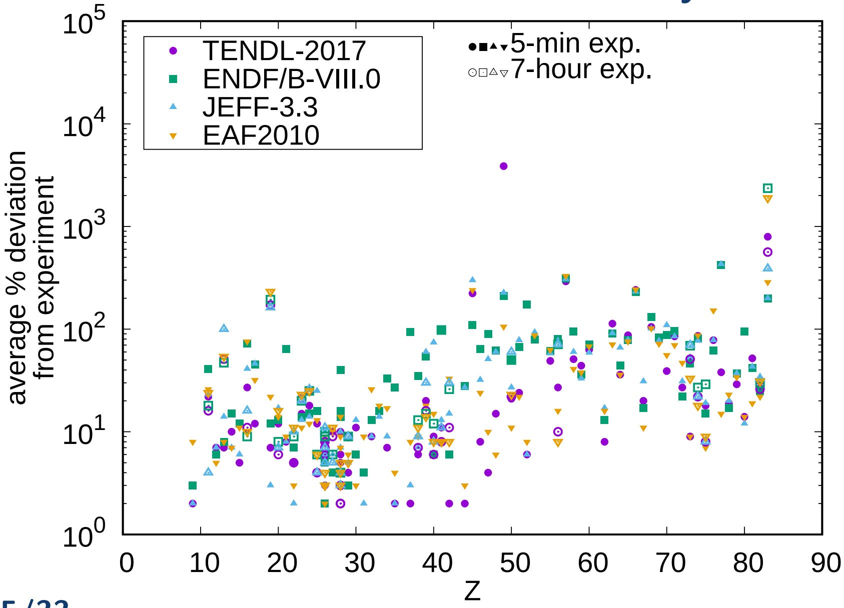
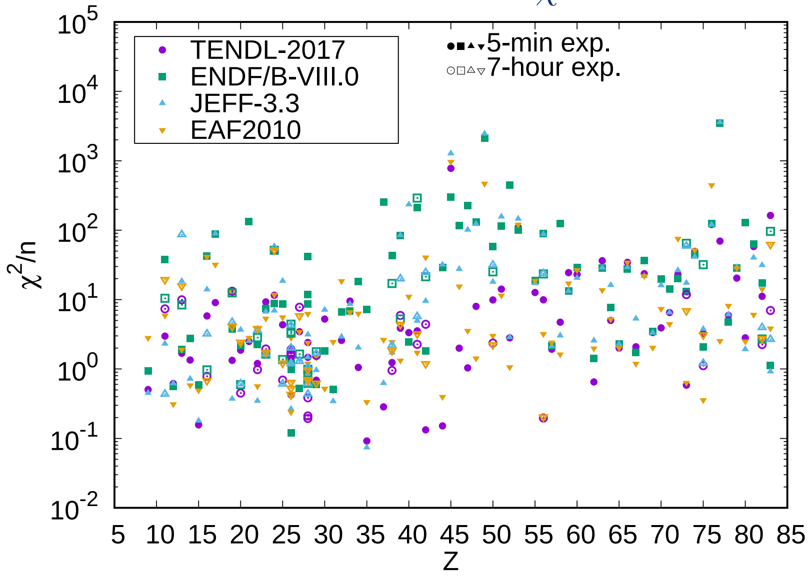
Statistical analysis



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

χ^2 test



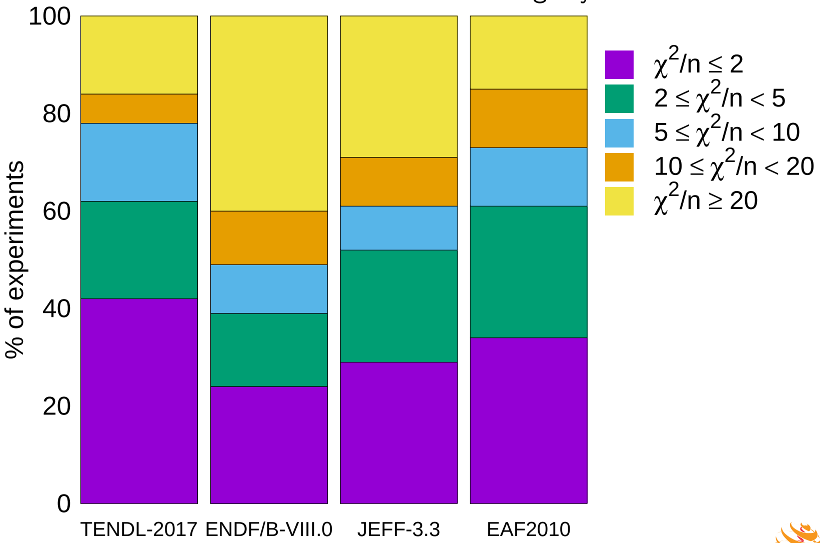
- χ^2/n variation for all experiments
- less clear trend
  $\Rightarrow$ higher experimental errors at high Z

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

n values per experiment

χ^2 test

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



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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 ...

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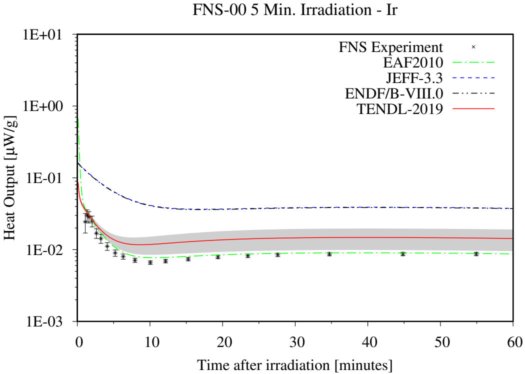
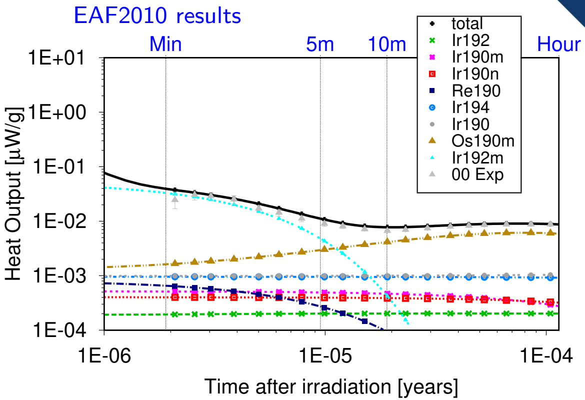
A case where the "legacy" is best

- 5 minute irradiation of pure Iridium

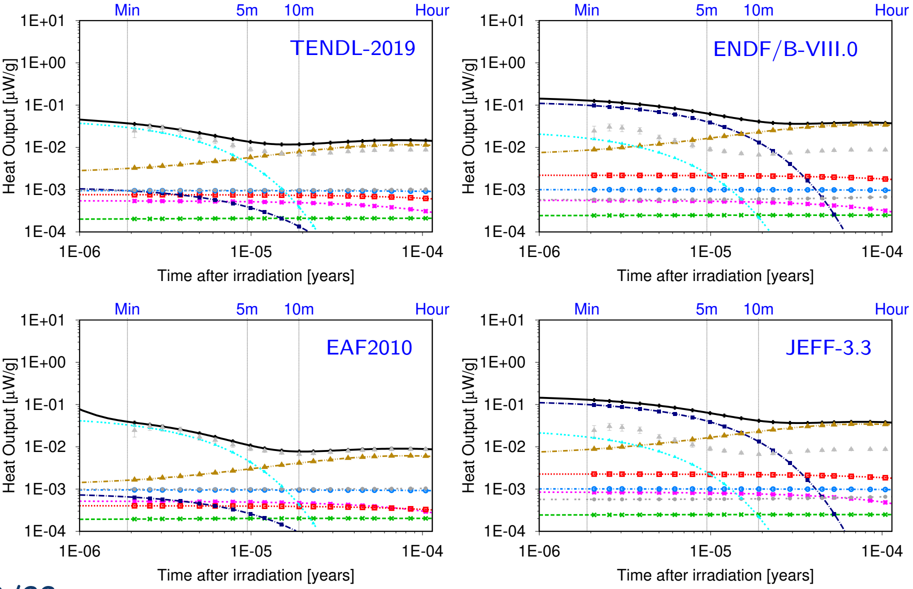




- Only EAF2010 correctly matches the experimental profile (and scale)
  - the observed decay heat originates from ^{192m}Ir in the first 5 minutes of cooling
  - at longer times ^{190m}Os dominates

	TENDL-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



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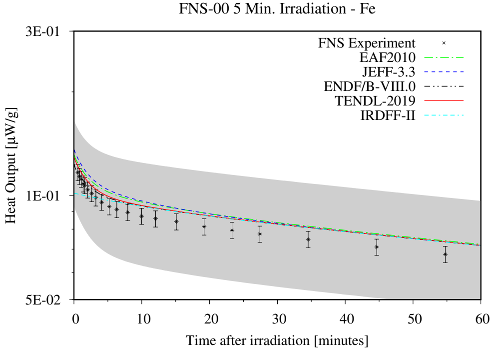
- TENDL-2017 underpredicted ^{191}Ir(n,2n)^{190n}Ir (β^+) ^{190m}Os (corrected now for TENDL-2019)
- ENDF/B-VIII.0 and JEFF-3.3 overestimate this path & predict a different dominant nuclide (^{193}Ir(n,α)^{190}Re) at short times

FISPACT-II inputs & outputs

.gra files

- e.g. irradiation of pure iron



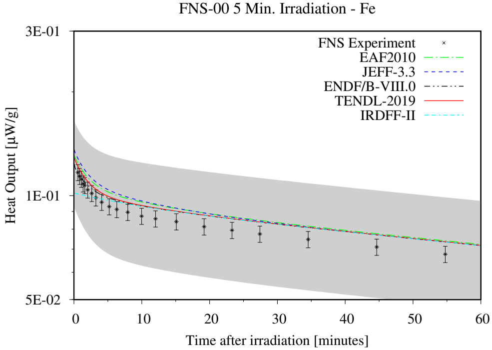
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from `.gra` files

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

.gra files

- e.g. irradiation of pure iron



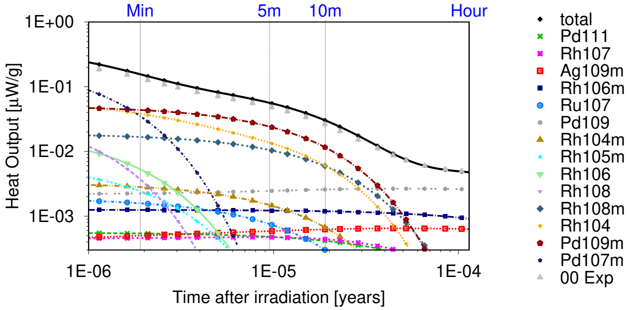
- separate FISPACT-II simulation for each different nuclear data library (and for each different material)
- curves extracted directly from `.gra` files

```
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



- 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