



Decay-heat validation of simulations with fusion neutrons

(+ nuclear heating importance)

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IAEA Technical meeting on nuclear heating theory and data, 19-22 April 2022

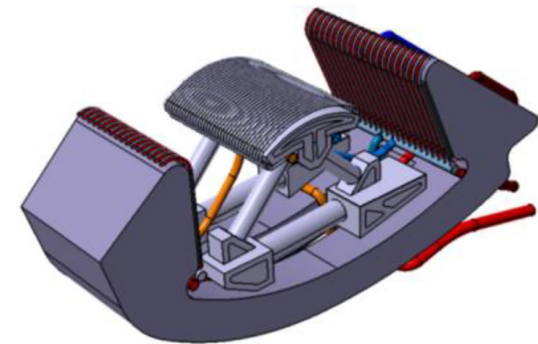
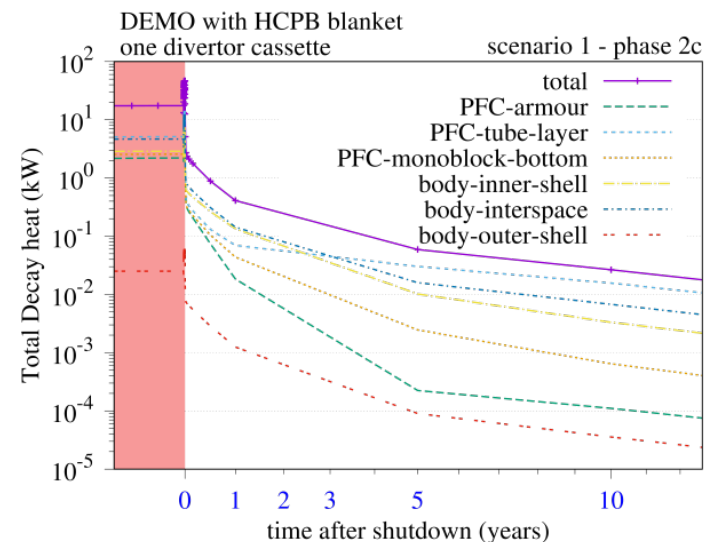
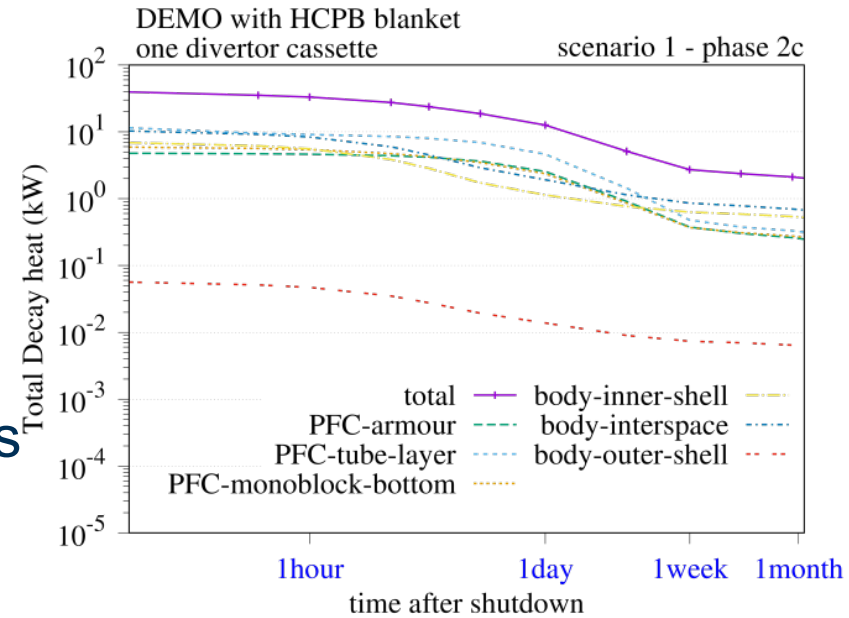
Contents

- Why decay heat predictions are important for fusion engineering
- FNS Decay heat benchmark to test codes and libraries
- Nuclear heating evaluations; contribution of photons

Decay heat

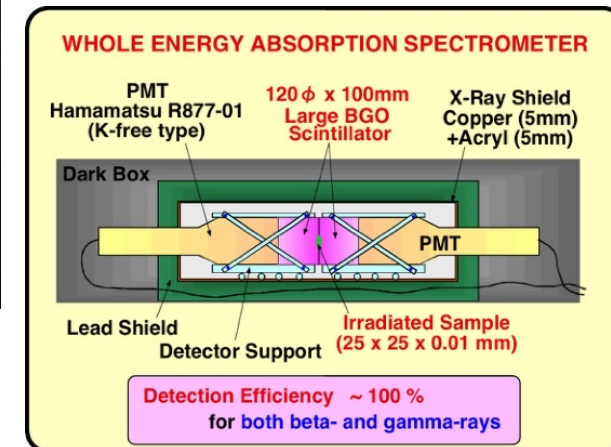
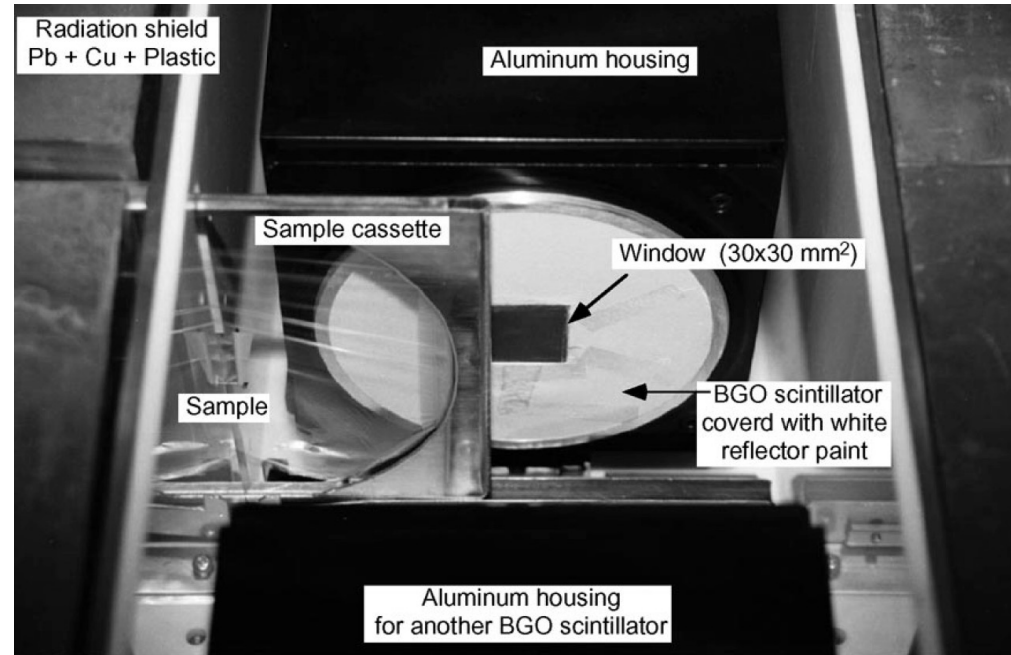
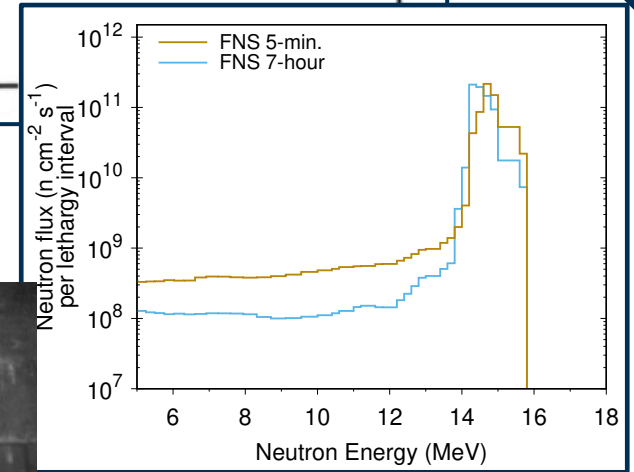
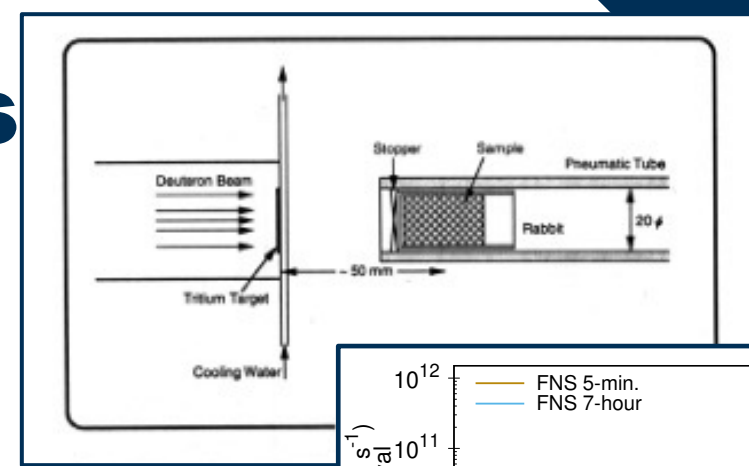
Motivation for high accuracy in decay heat predictions

- Fusion is moving towards engineering delivery of prototype and near-commercial reactors
- Cooling requirements, both during and after operation, are critical engineering parameters
- Large uncertainty is not acceptable when designing cooling plants and will jeopardize net energy gain
- A single divertor cassette on DEMO may have cooling requirements of 10s of kW at shutdown
 - One of 54 in this design
 - Mixture of steels, W, copper-alloys



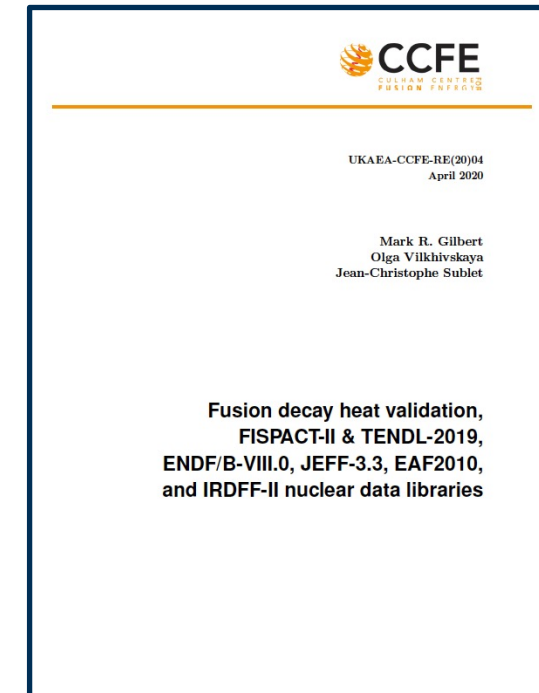
FNS decay-heat experiments

- JAEA experiments in 1996-2000 aimed at providing fusion-relevant decay-power data for important materials
- 2 mA deuteron beam onto a tritium target producing 14 MeV-peaked neutron fluxes of $\sim 10^{10}$ n/cm²/s
- Decay heat measured after 5-minute or 7-hour irradiations using Whole Energy Absorption Spectrometer (WEAS)



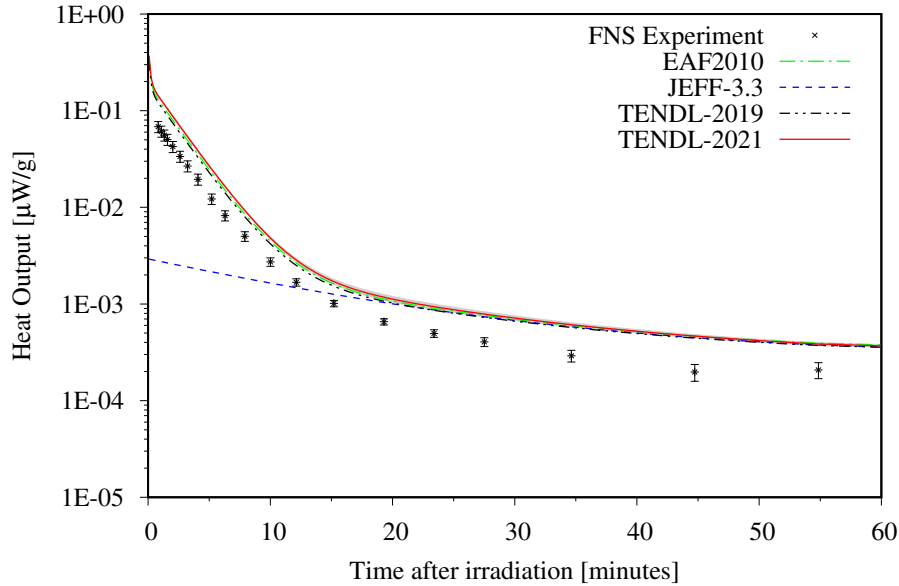
Z	Material	Form	Z	Material	Form
9	Fluorine	CF ₂	46	Palladium	Metallic Foil
11	Sodium	Na ₂ CO ₃	47	Silver	Metallic Foil
12	Magnesium	MgO	48	Cadmium	Metallic Foil
13	Aluminium	Metallic Foil	49	Indium	Metallic Foil
14	Silicon	Metallic Powder	50	Tin	SnO ₂
15	Phosphorus	P ₃ N ₅	51	Antimony	Metallic Powder
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			

- Measurements for 73 different materials
- Crafted into a simulation benchmark to test decay-heat predictions with inventory codes (FISPACT-II) and different nuclear data libraries
- Latest version:
- Mostly tests cross sections (not decay data)
- Data and benchmark guidance available on CoNDERC website <https://nds.iaea.org/conderc/>

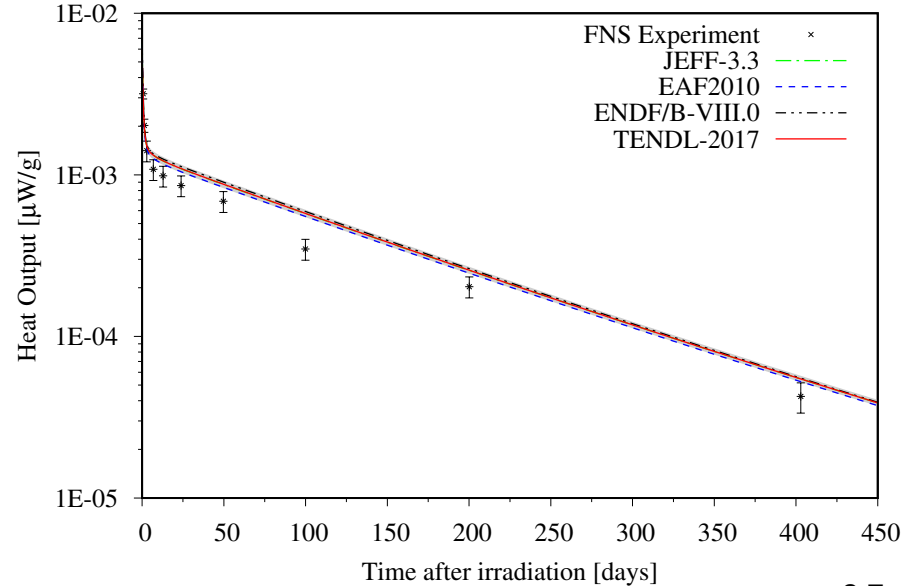


Typical benchmark output: W

FNS-00 5 Min. Irradiation - W

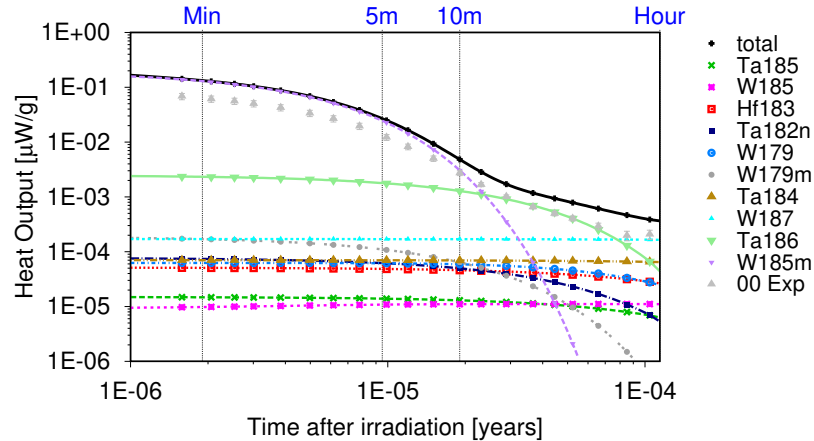


FNS-96 7 hours Irradiation - W

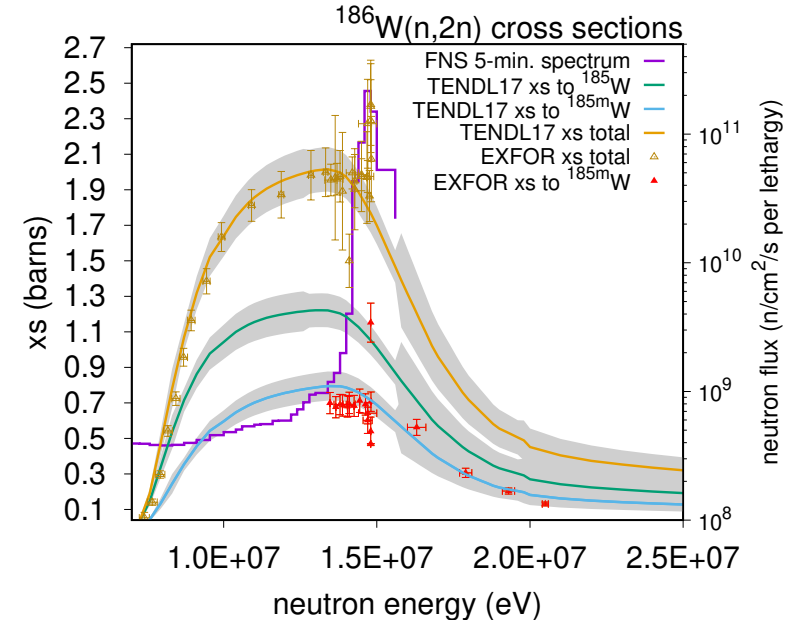
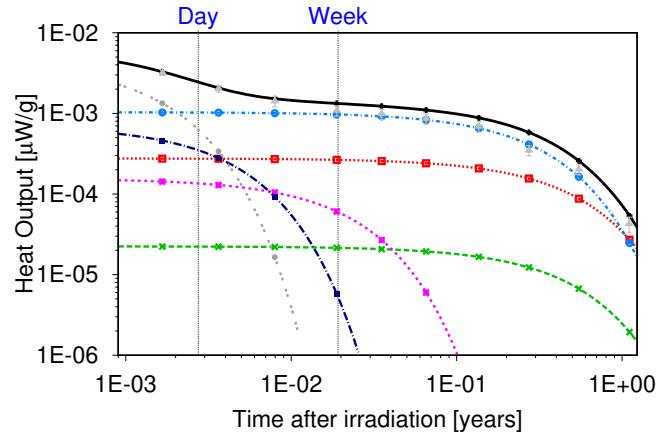


- Simulations overpredict relative to experiments after both 5-min and 7-hour irradiation
- Potential unresolved issue with $^{186}\text{W}(n,2n)$

FNS-00 5 Min. Irradiation - W - TENDL-2021

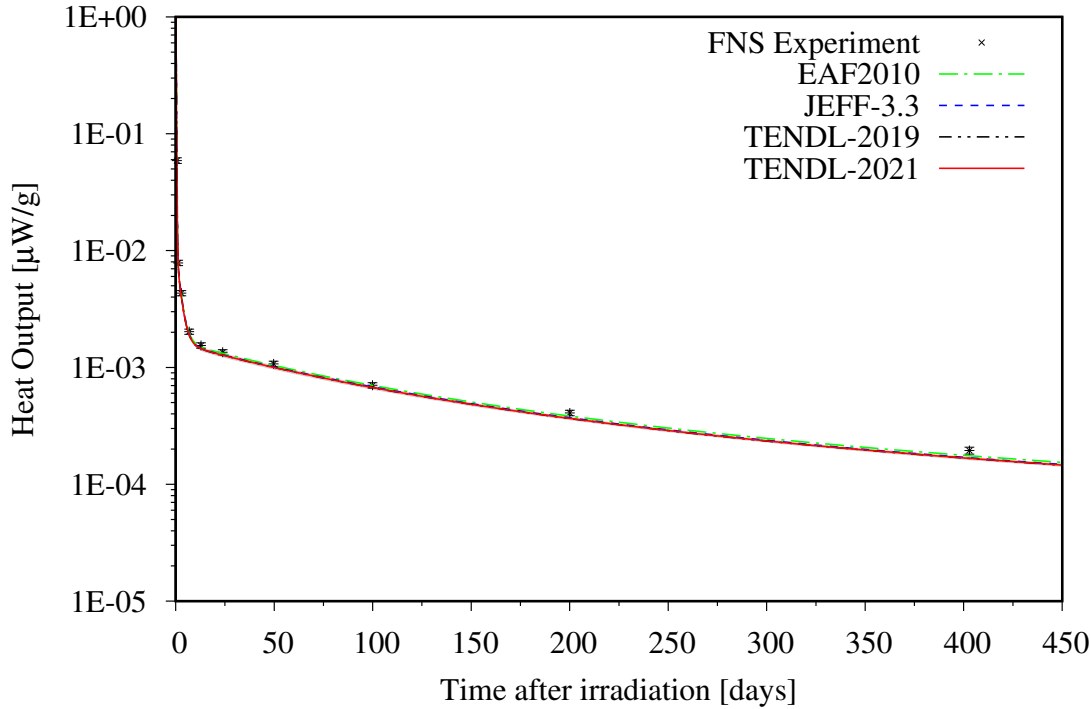


FNS-96 7 hours Irradiation - W - TENDL-2021

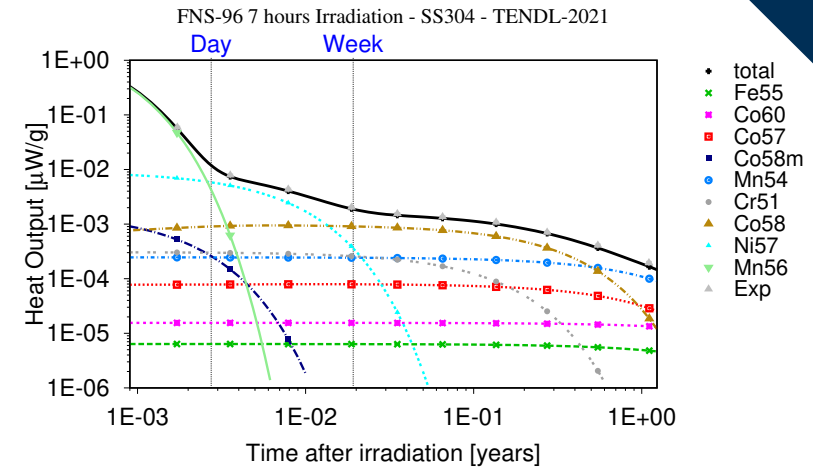


Good performance: SS304

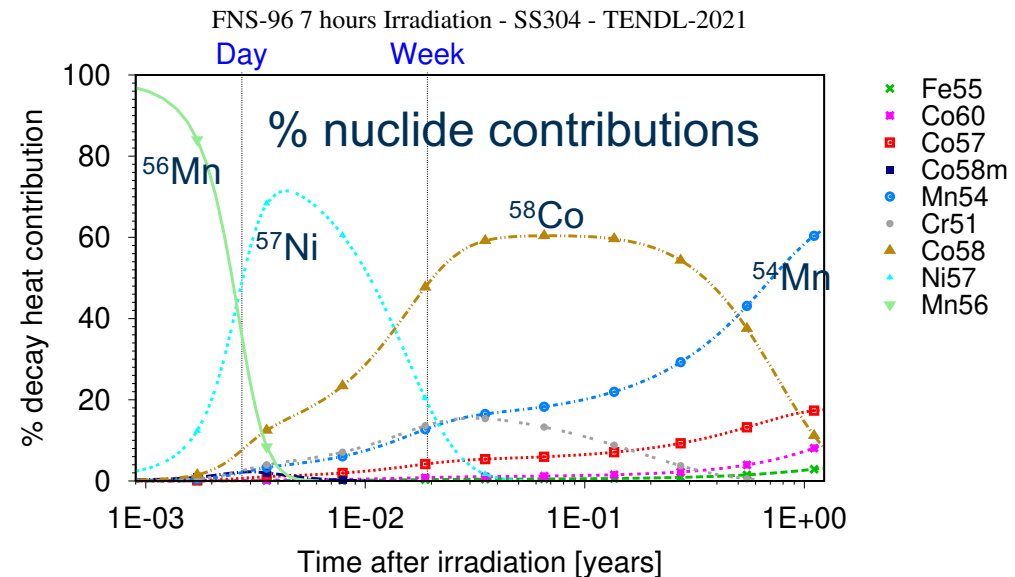
FNS-96 7 hours Irradiation - SS304



Product	$T_{1/2}$	Pathways	Path %
Mn56	2.58h	Fe56(n,p)Mn56	99.8
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Co58	70.87d	Ni58(n,p)Co58	80.0
		Ni58(n,p)Co58m(IT)Co58	20.0
Mn54	312.16d	Fe54(n,p)Mn54	53.1
		Mn55(n,2n)Mn54	46.8

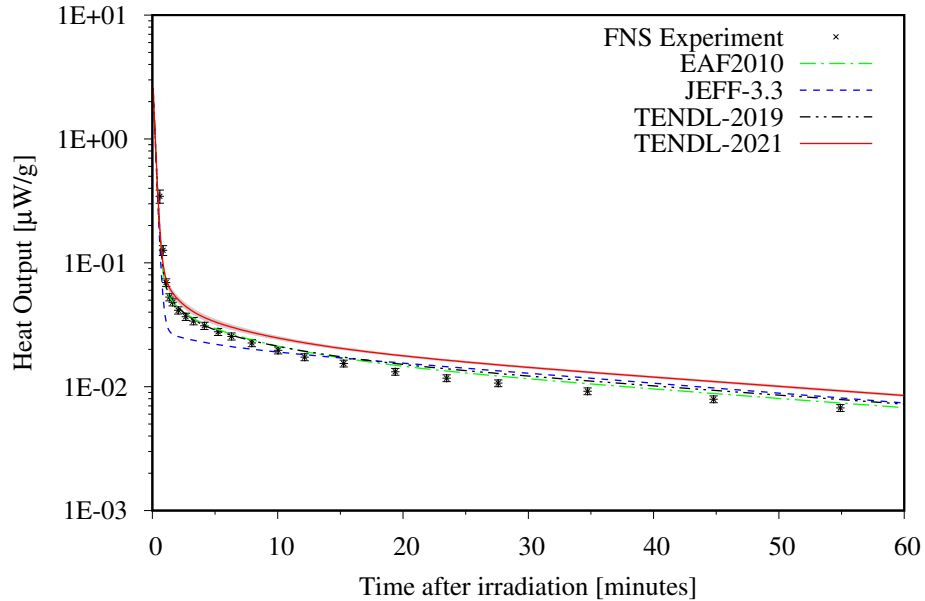


- Benchmark provides excellent validation of decay heat predictions for many materials, even complex alloys
- Sometimes requiring close match of several reaction channels over several orders of decay times

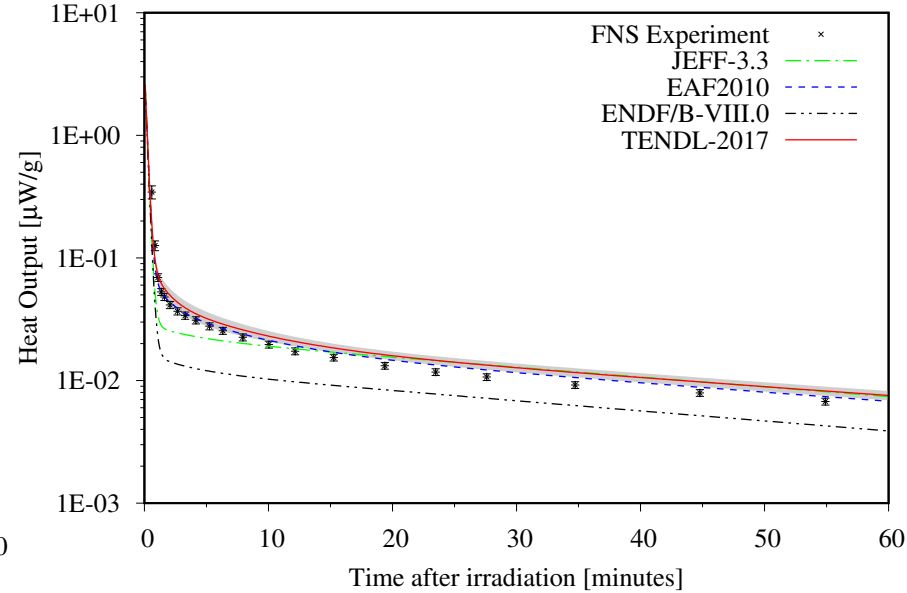


Metastable importance: tin

FNS-00 5 Min. Irradiation - SnO₂



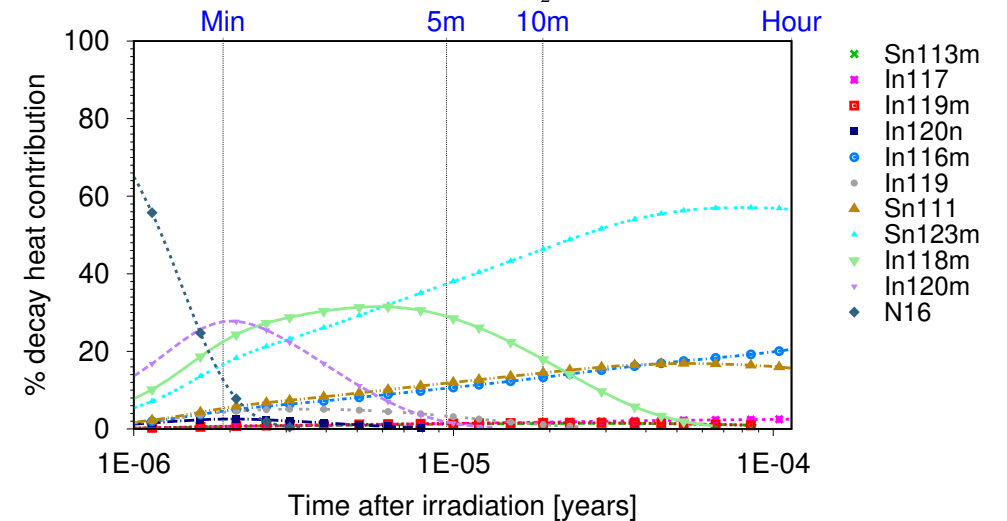
FNS-00 5 Min. Irradiation - SnO₂



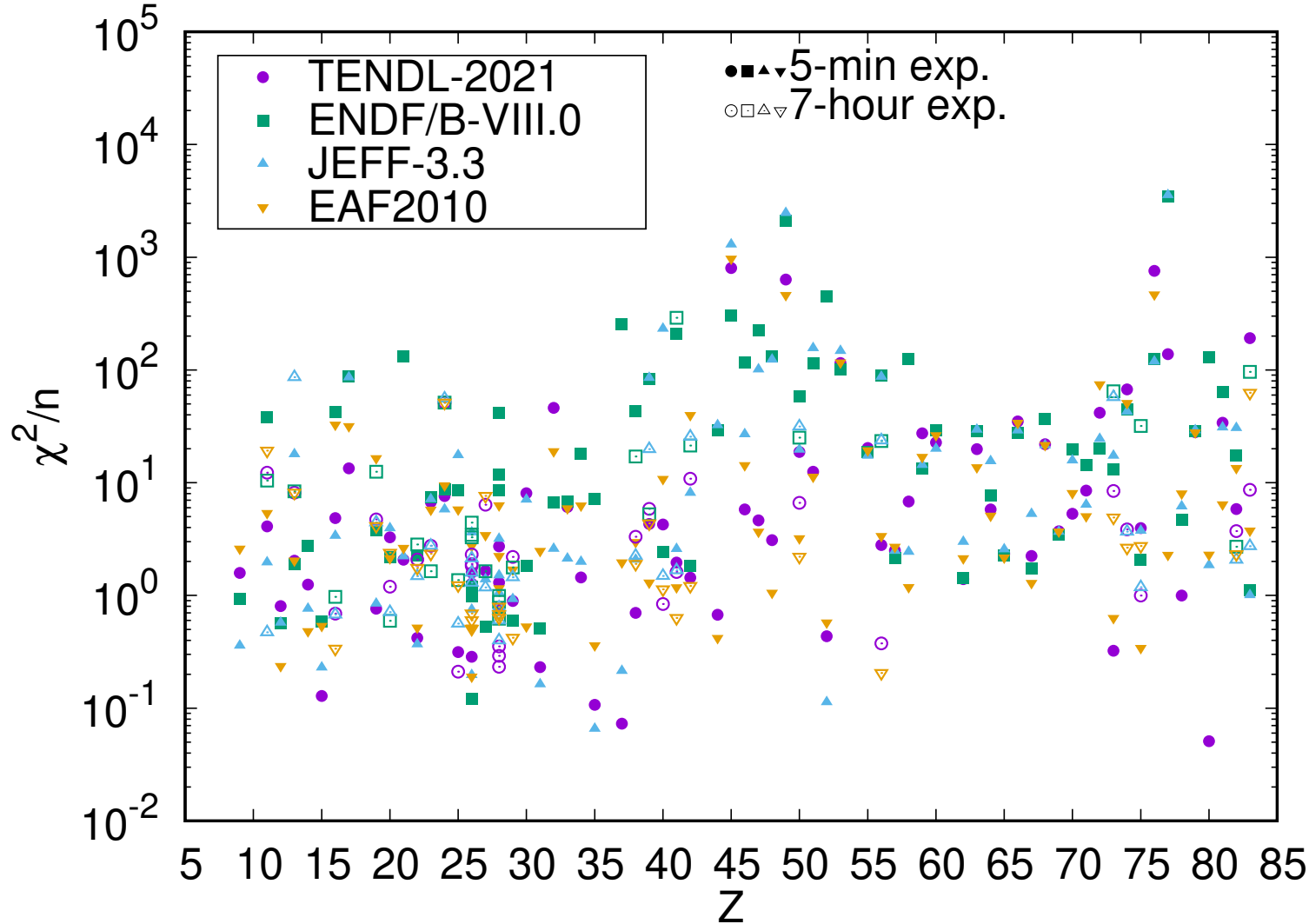
Measurements were taken soon after exposure, allowing validation of the production of short-lived metastables in some materials, and even ¹⁶N ($T_{1/2}=7\text{s}$)

Product	$T_{1/2}$	Pathways	Path %
In120m	46.21s	Sn120(n,p)In120m	100.0
In118m	4.45m	Sn118(n,p)In118m	88.6
		Sn118(n,p)In118n(IT)In118m	10.4
Sn123m	40.06m	Sn124(n,2n)Sn123m	99.9

FNS-00 5 Min. Irradiation - SnO₂ - TENDL-2021



Overall performance of libraries

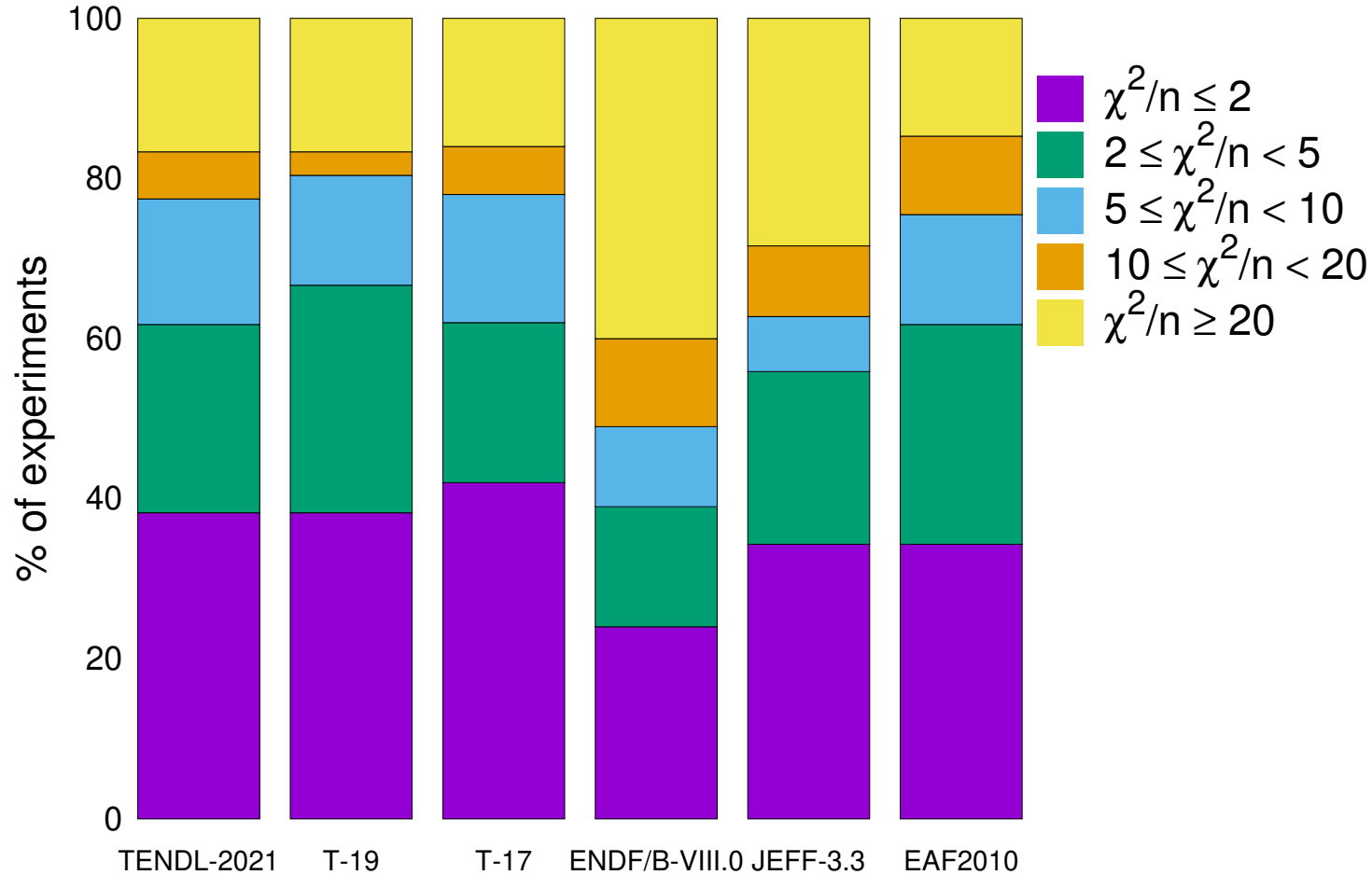


- Deviations from experiment increase with Z
- χ^2 values are reasonably consistent across the materials (high Z materials typically had larger errors in the experiments)

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

n – number of measurements in experiment

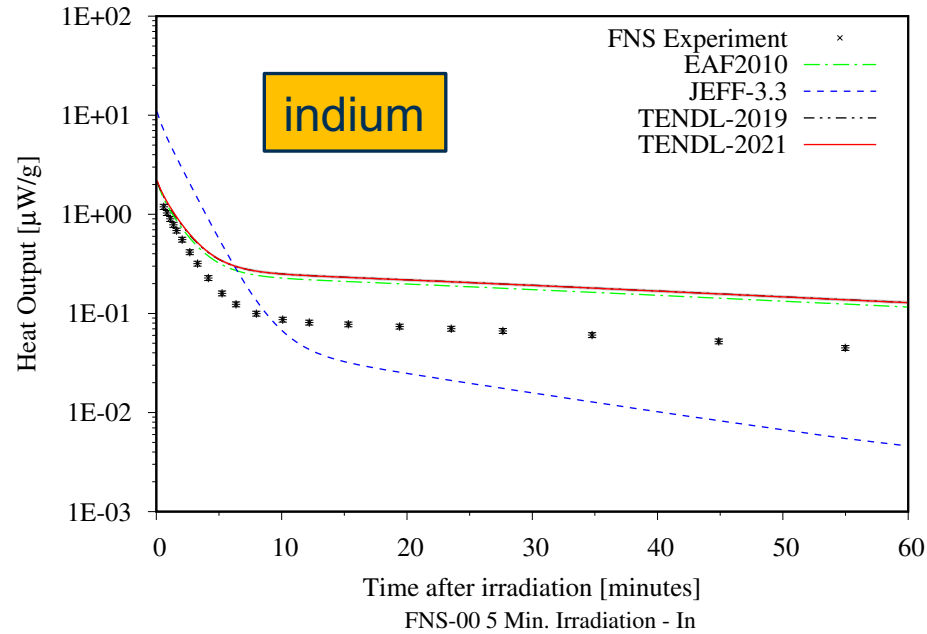
Library comparison



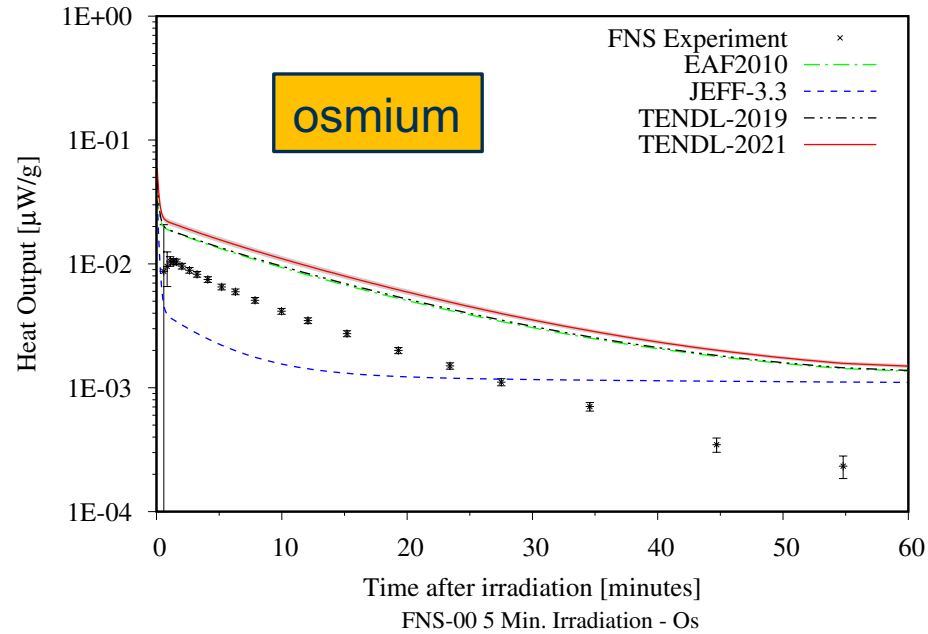
- Measuring performance based on χ^2 shows TENDL libraries do about as well as fusion-tailored EAF2010
- No improvements recently; is this the limit of agreement for this benchmark?....

Still room for improvement?

FNS-00 5 Min. Irradiation - In

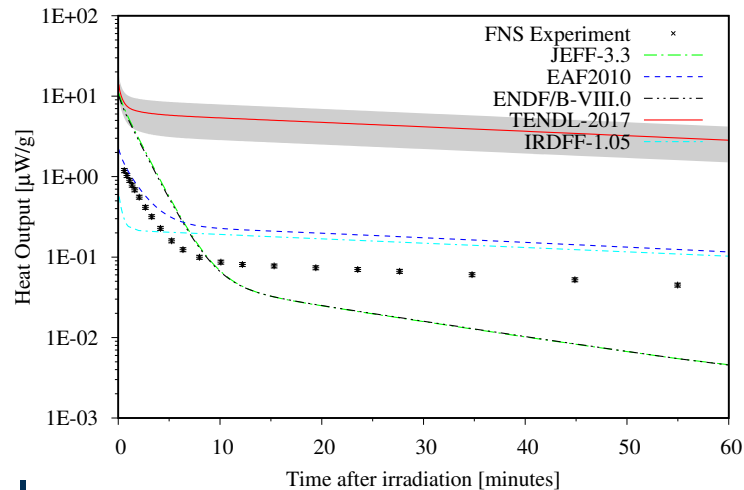


FNS-00 5 Min. Irradiation - Os

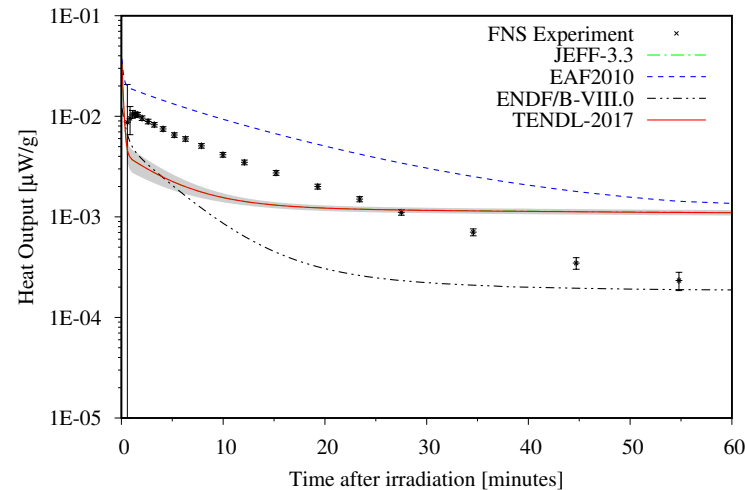


- Fundamental disagreement in decay profiles still exist for these two materials with all libraries

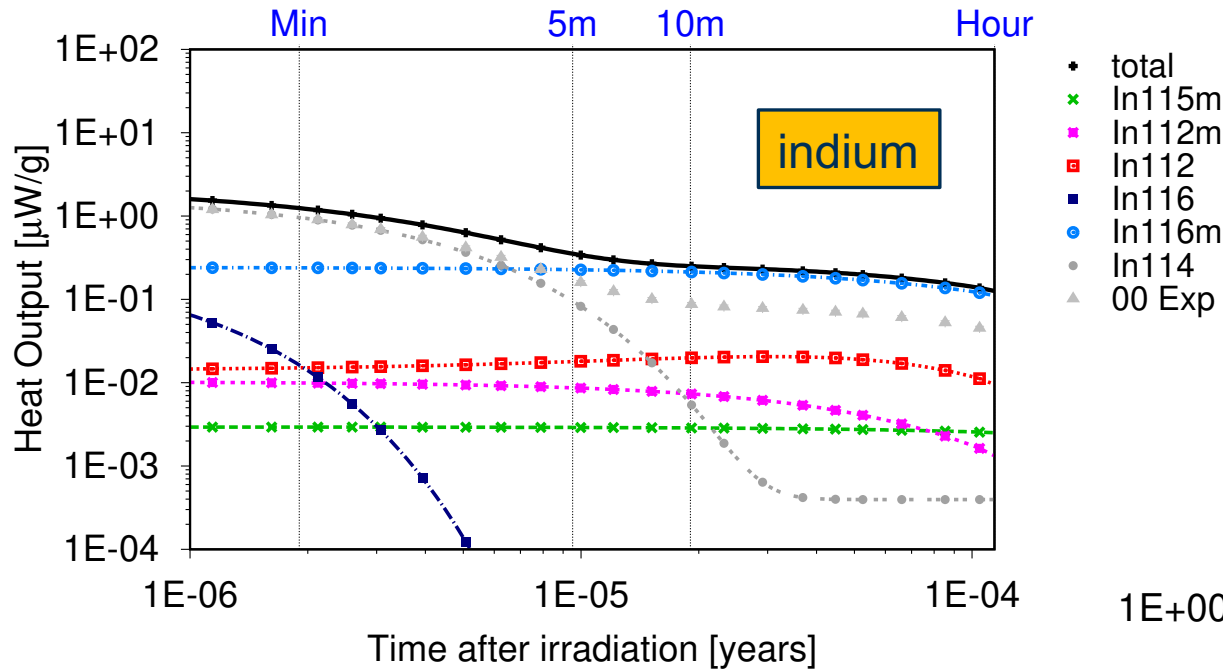
FNS-00 5 Min. Irradiation - In



FNS-00 5 Min. Irradiation - Os



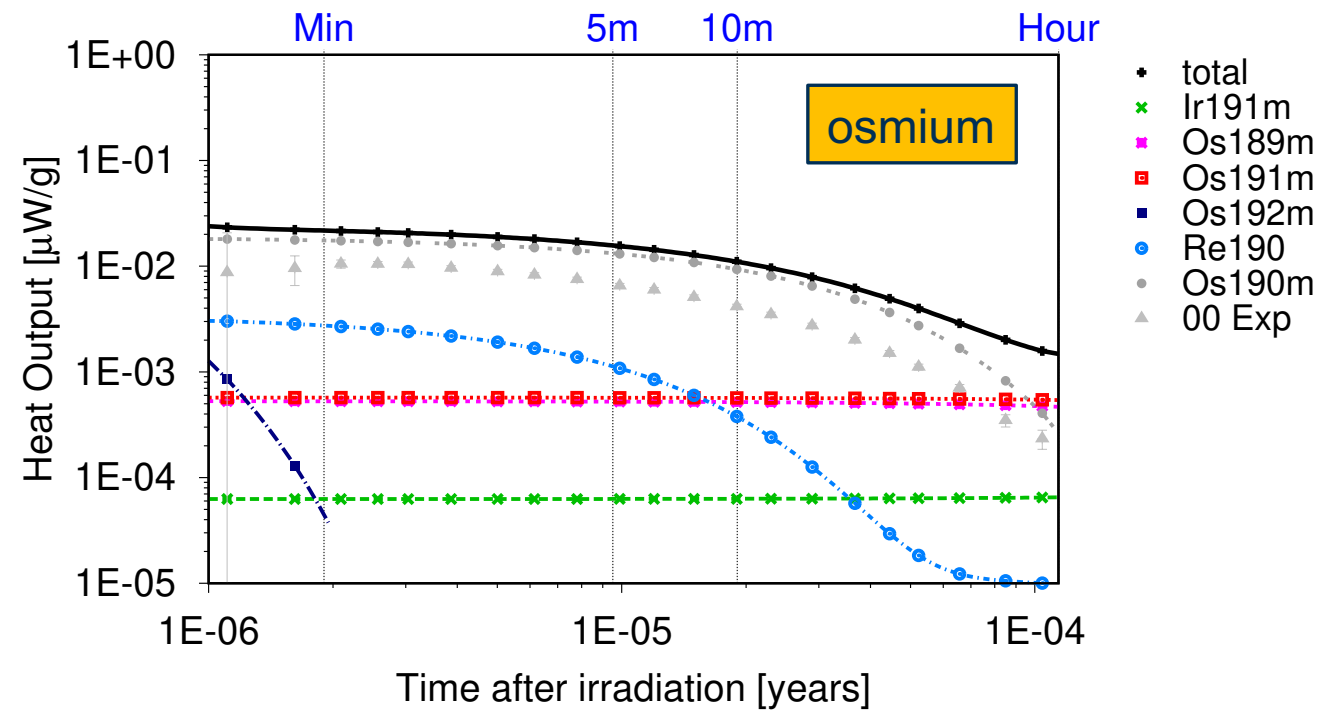
FNS-00 5 Min. Irradiation - In - TENDL-2021



- Too much $^{115}\text{In}(n,\gamma)^{116\text{m}}\text{In}$?
- Experimental limitation (improperly characterized thermal fluxes)?

- Too much $^{190}\text{Os}(n,n')^{190\text{m}}\text{Os}$?
- Incorrect production pathway?

FNS-00 5 Min. Irradiation - Os - TENDL-2021

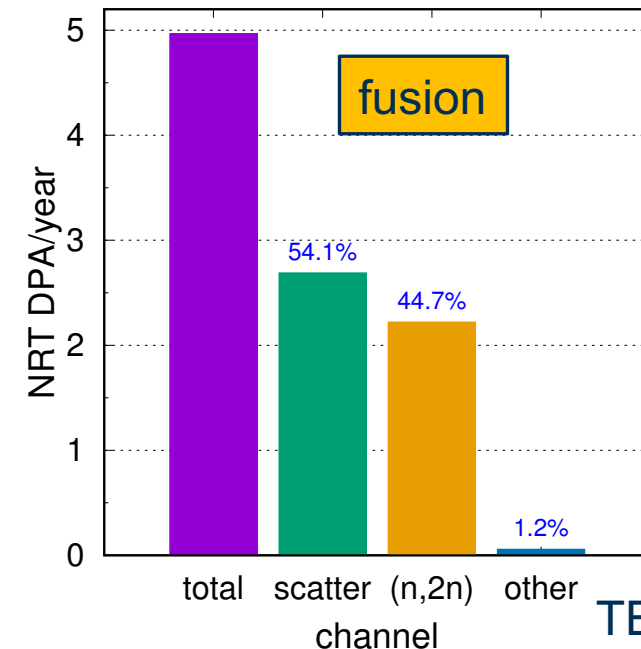
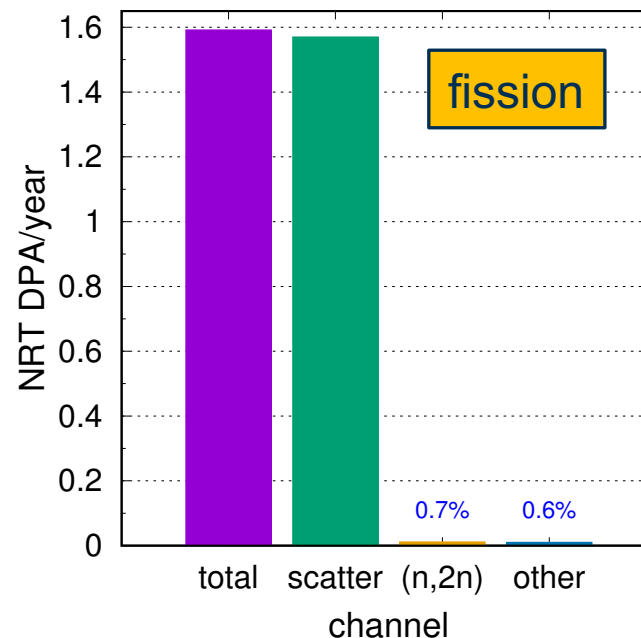


Nuclear heating

Importance of nuclear heating predictions for fusion material testing

- Qualifying performance of materials being considered for future fusion reactors relies on a combination of ion irradiation and campaigns in fission test reactors
- It is important to understand the damage evolution and the origin of that damage
- Comparison between techniques and relevance of fission experiments for fusion needs accurate prediction of nuclear damage dose
- E.g., dpa in W
- Damage created by (n,2n) reactions predicted to be important in fusion, but almost absent in fission

Gilbert, Sublet, J. Nucl. Mater. **504** (2018) 101



Nuclear heating fusion vs fission

DEMO	W/g	Fusion total (mt 301)	Fusion photon (442)	Fusion nonelastic (303)	Fusion Elastic (302)
W		2.731	2.650 (97%)	2.727	4.279e-3
Fe		1.683	1.191 (71%)	1.646	3.666e-2
Be		3.645	2.885e-3 (0%)	2.078	1.567

HFR	W/g	Fission total	Fission photon	Fission nonelastic	Fission Elastic
W		10.479	10.358 (99%)	10.476	3.794e-3
Fe		1.997	1.626 (81%)	1.954	4.277e-2
Be		2.146	8.369e-7 (0%)	4.451e-1	1.701

- Damage-dose prediction based on dpa does not (?) include energy from photons, which in materials like W is most of the energy deposited in materials (local deposition assumption in NJOY-HEATR)
- Could explain anecdotal evidence of self-annealed materials under neutron exposure (compared to ion irradiation) – photons may provide enough energy to anneal damage – ongoing work
- Accurate nuclear heating predictions would then become critical for predicting material performance

Summary

- Decay heat predictions are important for design engineering of fusion power plants (~ few 100s of W cooling required per kW of decay heat)
- Benchmarking of decay heat predictions against experiments under fusion conditions demonstrate good performance across a range of materials
 - Improvements have slowed recently – possible limit of benchmark, but some materials still show clear discrepancies
- Further experiments, particularly on primary fusion materials, including new alloys (steels), are needed
- Nuclear heating calculations could be critical to understand the observed damage in neutron-irradiated materials and thus to predict performance evolution