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FISPACT-II

Nuclear data validation efforts

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Consultancy Meeting:
International Radiation Characterization Benchmark Experiment Project (IRCBEP)

August 6-8, 2018, IAEA, Vienna

Research Councils UK Energy For a Low Carbon Future
This work was funded by the RCUK Energy Programme
[Grant number EP/P012450/1]

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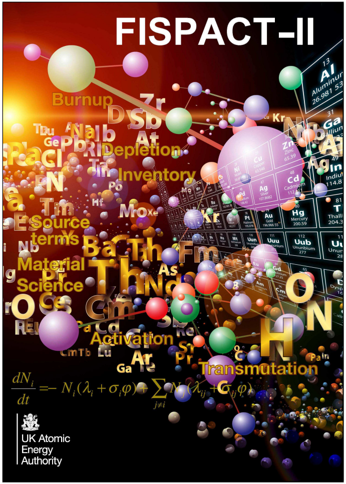
Inventory simulation platform



- multiphysics platform for predicting the inventory changes in materials under both neutron and charged-particle interactions
  - calculates activation, transmutation, burn-up, dpa, PKAs, gas production, etc.
- can read data from the most up-to-date international nuclear libraries, including
  - TENDL-2017, ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, . . .

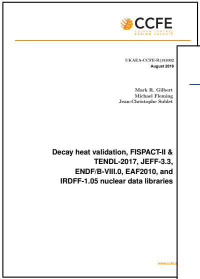
Sublet, Eastwood, Morgan, Gilbert, Fleming, and Arter
"**FISPACT-II: An Advanced Simulation System for Activation, Transmutation and Material Modelling**"
Nucl. Data Sheets **139** (2017) 77137

http://fispact.ukaea.uk

Introduction

- Validation & Verification (V&V) is an important part of the development and release of the FISPACT-II platform
- 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

TENDL & FISPACT-II validation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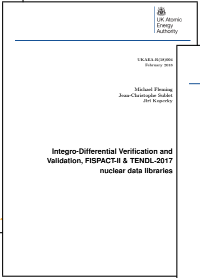
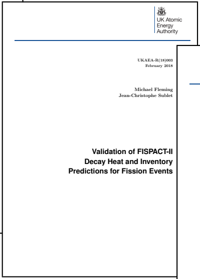
CULHAM CENTRE FUSION ENERGY
UKAEA-CCFE-R(18)002
August 2018
Mark R. Gilbert
Michael Fleming
Jean-Christophe Sublet
Decay heat validation, FISPACT-II & TENDL-2017, JEFF-3.3, ENDF/B-VIII.0, EAF2010, and IRDFF-1.05 nuclear data libraries


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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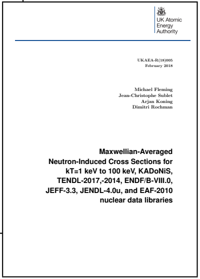
UKAEA-R(18)003
February 2018
Michael Fleming
Jean-Christophe Sublet
Validation of FISPACT-II Decay Heat and Inventory Predictions for Fission Events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UKAEA-R(18)005
February 2018
Michael Fleming
Jean-Christophe Sublet
Arjan Koning
Dimitri Rochman
Maxwellian-Averaged 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

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

- 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)

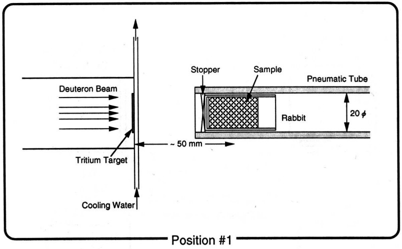
Fusion decay heat benchmark

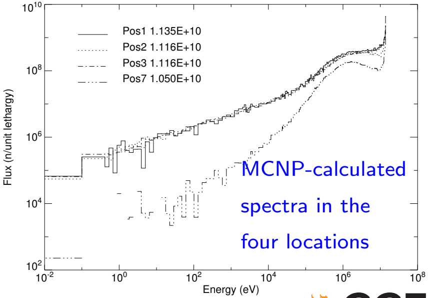
- Experiments performed at the Fusion Neutron Source (FNS) at JAEA in 1996-2000
- aimed at providing fusion-relevant decay-power data for important structural materials
- accurate experimental measurements with detailed records are ideal for simulation benchmarking

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/

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





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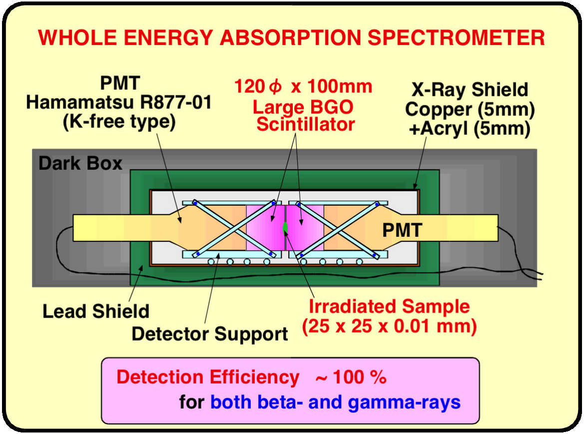
The experiment

- 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



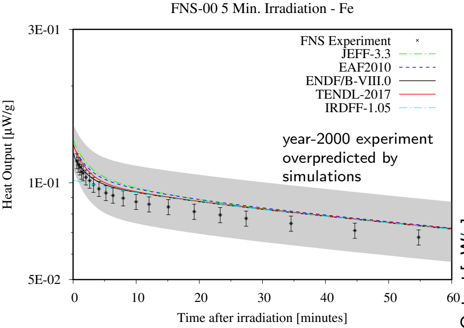
Z	Material	Form	Z	Material	Form
9	Fluorine	CF_2	46	Palladium	Metallic Foil
11	Sodium	Na_2CO_3	47	Silver	Metallic Foil
12	Magnesium	MgO	48	Cadmium	Metallic Foil
13	Aluminium	Metallic Foil	49	Indium	Metallic Foil
14	Silicon	Metallic Powder	50	Tin	SnO_2
15	Phosphorus	P_3N_5	51	Antimony	Metallic Powder
16	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

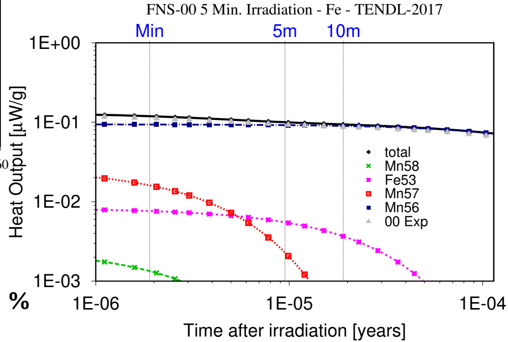
- Detailed experimental information (irradiation times, measurement times, material compositions, etc.) have been translated into a set of FISPACT-II input files
  - these can be rapidly repeated for different nuclear data libraries
- Latest version of exercise compares results from TENDL-2017, ENDF/B-VIII.0, 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 new "dec_2012" decay database distributed with FISPACT-II is used
  - 3873 nuclides
  - a combination of data from JEFF-3.1.1, JEF-2.2 to produce the EAF2010 decay file, UK evaluations in UKPADD6.10, and supplemented from ENDF/B-VII.1

Typical results and presentation

- 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

Typical results and presentation

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

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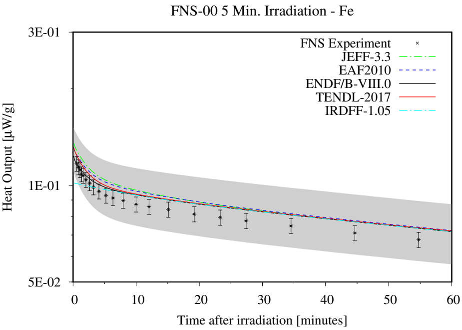
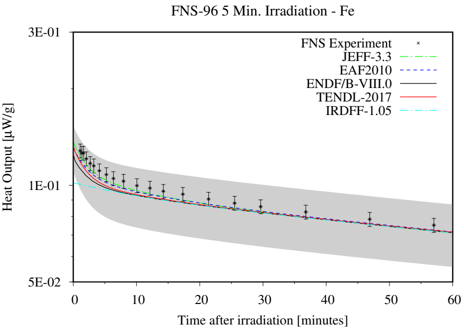
Times	FNS EXP. 5 mins		TENDL-2017			ENDF/B-VIII.0	JEFF-3.3	EAF2010	IRDFF-1.05
Min.	μW/g		μW/g		E/C	E/C	E/C	E/C	E/C
0.58	1.17E−01	+/-5%	1.24E−01	+/-16%	0.94	1.00	0.91	0.94	1.15
0.83	1.14E−01	+/-5%	1.22E−01	+/-17%	0.94	0.99	0.90	0.93	1.13
1.08	1.12E−01	+/-5%	1.19E−01	+/-17%	0.94	0.99	0.90	0.93	1.11
1.35	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 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

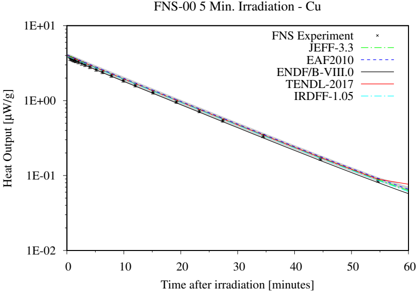


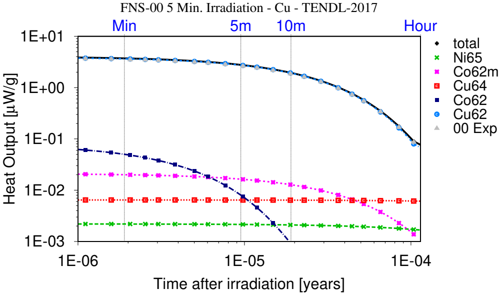


(IRDFF-1.05 contains the ^{56}Fe(n,p)^{56}Mn channel and can thus simulate the behaviour beyond 5-minutes of cooling)

A good agreement case

- 5 minute irradiation of pure copper



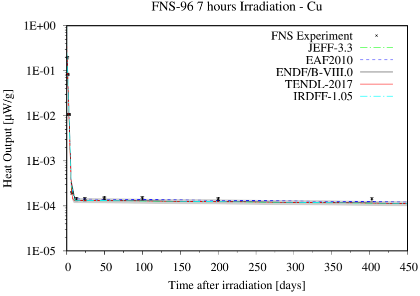


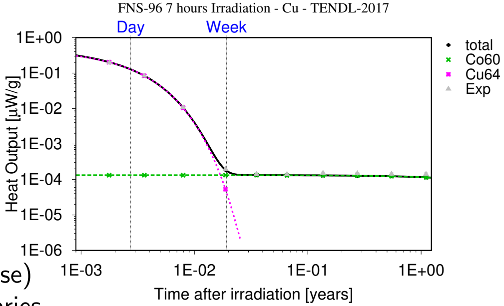
- a straightforward case entirely dominated by ^{62}Cu
  - ^{63}Cu(n,2n)^{62}Cu
  - all library predictions are within a few % of the experiment at all decay times

	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



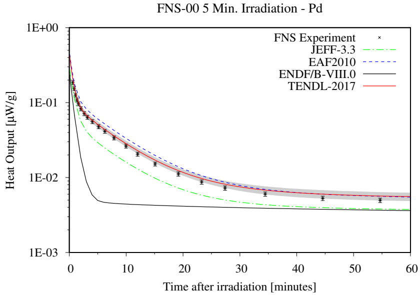


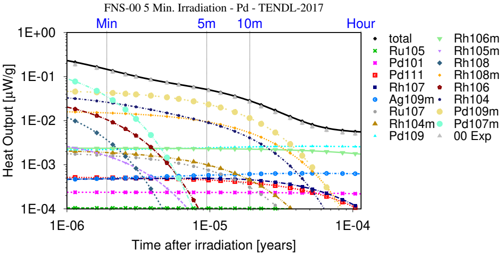
- two nuclide contribution profile (different nuclides to 5 minute case) and good agreement with all libraries
  - ^{63}Cu(n,α)^{60}Co (including isomeric transition via ^{60m}Co)
  - ^{65}Cu(n,2n)^{64}Cu

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

A case where TENDL-2017 is best

- 5 minute irradiation of pure palladium



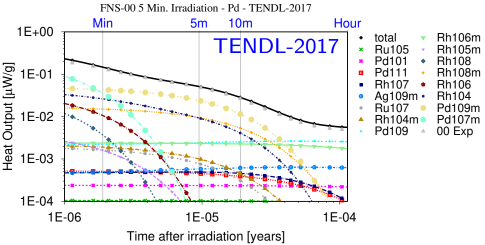


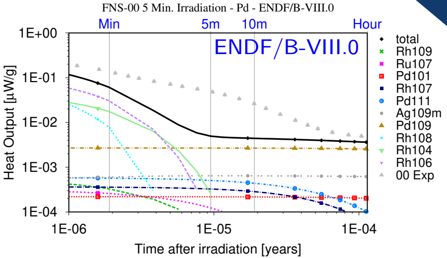
- a complex case with many contributing nuclides
  - particularly metastables: ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh
  - a mixture of (n,2n) and (n,p) reactions dominate
  - TENDL-2017 outperforms all others

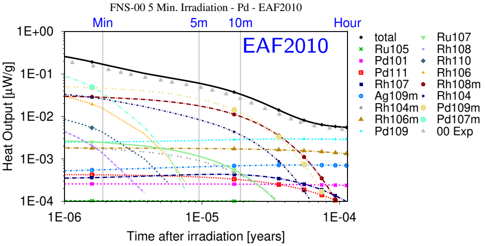
	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	8	64	32	24

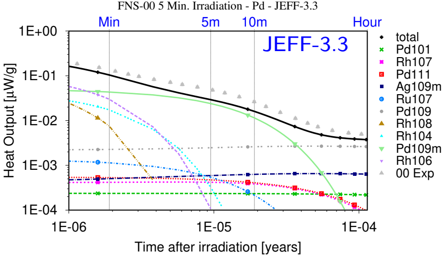
Palladium nuclide comparisons

- EAF2010 overpredicts ^{108m}Rh production
- ENDF/B-VIII.0 misses ^{108m}Rh, ^{109m}Pd, and ^{106m}Rh
- JEFF-3.3 misses ^{108m}Rh and ^{106m}Rh









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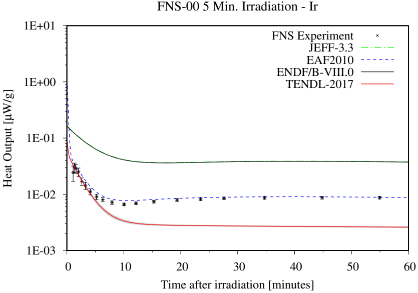
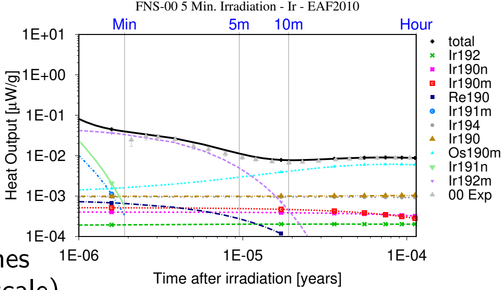
A case where the "legacy" is best

- 5 minute irradiation of pure Iridium



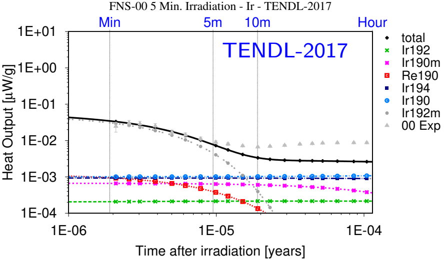


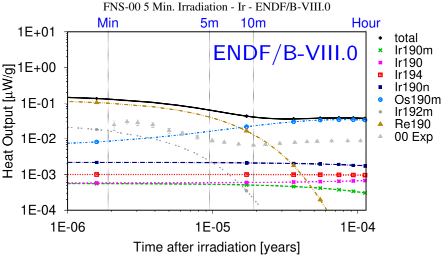
- Only EAF2010 correctly matches the experimental profile (and scale)
  - the observed decay heat originates from ^{192m}Ir in the first 5 minutes of cooling
  - at longer times ^{190m}Os dominates

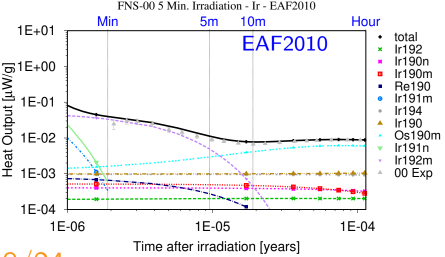
	TENDL-2017	ENDF/B-VIII.0	JEFF-3.3	EAF2010
mean % diff. from E	38	423	429	15

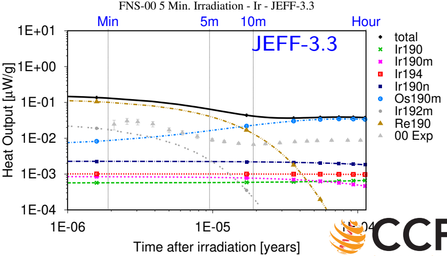
Iridium nuclide comparisons

- 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



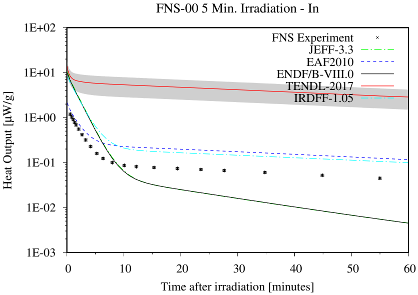


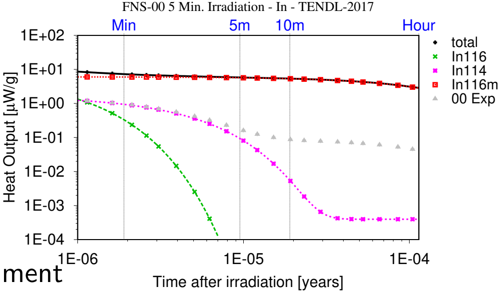




A case where all are wrong

- 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
  - 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)
  - but this could also be due to a poor characterisation of the neutron spectrum in the thermal range

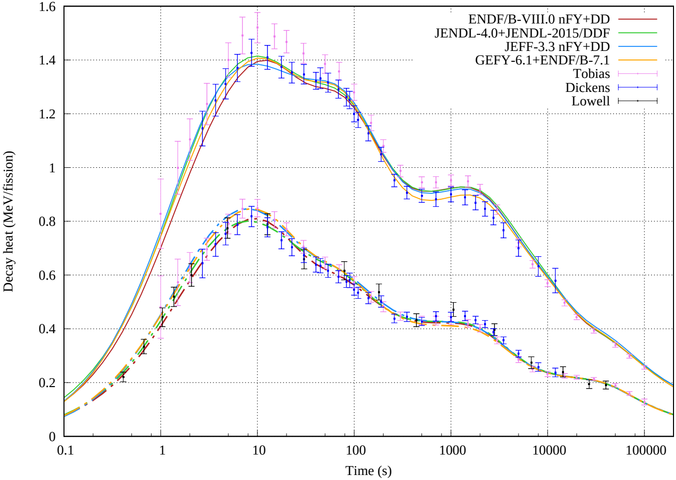
decay heat statistical summary

- Summary tables compare the 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

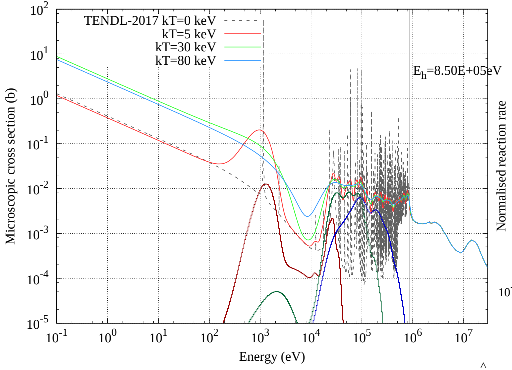
Other validation efforts (1)

- 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



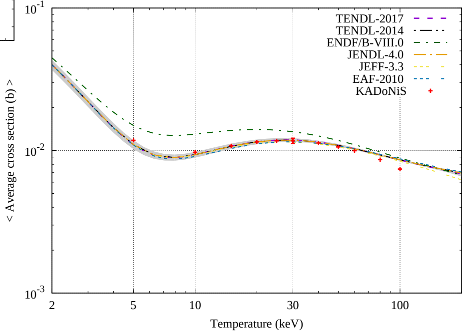
- total and β-generated decay heat
- simulated with latest ENDF/B, JEFF, and JENDL libraries
- Also included in exercise: ^{233}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{232}Th, and ^{237}Np

Other validation efforts (2)



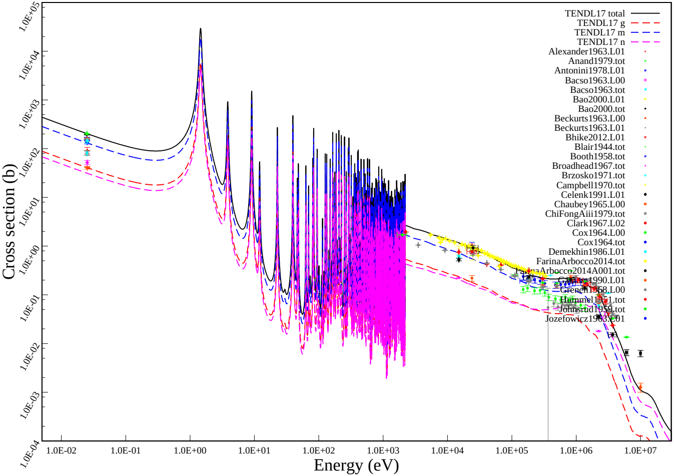
- e.g. ^{56}Fe results:
- TENDL-2017 xs & comparison to KADoNiS of average xs at various temperatures for different libraries

- 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}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

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Summary

- The suite of validation exercises (largely automated) performed for FISPACT-II and the extensive nuclear data libraries it is able to access represent an unprecedented test of an inventory simulation platform
  - exploring a large amount of the physics landscape for neutron interactions
- developed over a number of years at UKAEA
  - in a relatively mature state with well constructed programs, scripts, and input file sets

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