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Disclaimer

Neither the authors nor the United Kingdom Atomic Energy Authority accept responsibility for consequences arising from any errors either in the present documentation or the FISPACT-II code, or for reliance upon the information contained in the data or its completeness or accuracy.

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Executive Summary

The calculation of activation inventories is a key input to virtually all aspects of the operation, safety and environmental assessment of nuclear plants. For the licensing of such devices, regulatory authorities will require proof that the calculations for structural materials and fuel inventories, and calculations to which these quantities are the inputs, are either correct or conservative. An important aspect of activation-transmutation is decay heat power.

In power plants decay power arises after shutdown from the energy released in the decay of the products of neutron interaction by α, γ and β emissions. Computation of the decay power is performed by sophisticated computer codes, which solve the large number of coupled differential equations governing the generation and decay chains for the many nuclides involved. They rely on a large volume of nuclear data that includes both neutron activation-transmutation cross sections and radioactive decay data.

Validation of decay power computational predictions by means of direct comparison with integral data and measurement of sample structural materials under high energy relevant neutron spectra generate confidence in the values calculated. It also permits an assessment of the adequacy of the methods and of the nuclear data, and indicates any inaccuracy or omission that may have led to erroneous results.

No experimental data on decay power existed for most fission reactor materials other than reactor fuel, or for materials under high energy irradiation conditions typical of fusion, until a series of experiments were performed using the Fusion Neutron Source FNS facility at the Japan Atomic Energy Agency JAEA. Many elements and some alloy micro-samples were irradiated in a simulated D-T neutron field for times up to 7 hours and the resulting decay power generated was measured for cooling times of up to a year or more. Using the highly sensitive Whole Energy Absorption Spectrometer (WEAS) method, both β and γ emission decay energies were measured at selected cooling times as early as a few tens of seconds after the irradiation ended. This report details the comparison of these experimental measurements to simulations performed by the inventory code FISPACT-II using different nuclear data libraries: TENDL-2019, EAF2010, ENDF/B-VIII.0, and JEFF-3.3. Additionally, and only where appropriate because its reaction/nuclide coverage is limited (deliberately), results obtained using the IRDFF-II dosimetry library have also been compared. This is, to our knowledge, the most detailed comparison of this type that has been undertaken.

Overall the results of this particular validation exercise indicate that the calculational methods and nuclear databases, with some notable exceptions and variability, generally allow predictions, with quantifiable margins, of the decay power of the tested materials against cooling time. This exercise tested the specific production pathways, as well as the decay data in some cases, associated with the nuclides that dominate the decay heat.

Contents

1 Introduction

Safety and Environmental (S&E) impact issues have acquired increasing importance for the development of power plants. As part of future programmes and especially in connection with engineering feasibility studies, S&E and research and development (R&D) analyses require a sound and reliable database for the neutron-induced primary and secondary responses. The words primary and secondary define two very different types of response: the former relates to neutronic and gamma-ray time independent responses when the plant is in operation, while the latter refers to time dependent responses which are important after shutdown. In power plants, decay heat will arise after shutdown from the energy released in the decay of the products of particle interactions.

The calculation of activation inventories is an important input to virtually all aspects of S&E analysis. For licensing, the regulatory authorities will require proof of either the correctness or conservatism of the calculations of activation-transmutation and of calculations which use activation-transmutation as input. The radioactive inventory and residual decay power generation depend on the specific design of the plant and its components, its geometrical configuration and material choices, as well as the given irradiation conditions: power, operational scenario, and neutron source distribution. It is essential to include in the plant development properly performed activation inventory calculations that are consistent with the overall plant design. An important aspect of activation is residual decay power. The residual decay power, in the event of a postulated accident in which cooling is lost, might induce structural damage in certain plant components. Temperature transients may promote gas-generating chemical reactions and, in plants of high power density, may promote the mobilisation of activation, transmutation or fission products.

There is thus a strong motivation to limit accidental temperature transients and to ensure that the design and material-choices provide for removal of decay heat, preferably by passive means. Safety studies assess the efficiency of the design in this regard using computer models which require, as a starting point, an accurate assessment of the decay heat levels in the plant. Computation of the decay power is performed by sophisticated computer codes which solve the large number of coupled differential equations which govern the generation and decay chains for the many nuclides involved. They rely on a large volume of nuclear data, both neutron activation-transmutation cross sections and radioactive decay data.

Validation of decay power predictions from such codes by means of direct comparison with integral data measurements of sample structural materials under neutron spectra allow confidence to be given to the decay power values calculated. It also permits an assessment of the adequacy of the methods and nuclear data, and indicates any inaccuracy or omission that may have led to erroneous code predictions. Safety authorities world-wide tend to request experimental validation results that can be used to assess the adequacy of the safety features. It is clear that certain safety margins can be derived from such a validation exercise, if relevant to plant operation, materials and design, and applied as bounding conditions in S&E analyses.

Little experimental data exists for structural material samples irradiated under relevant neutron spectra and even when data does exist the measured quantities are either specific activity and/or γ spectroscopy. In particular, no experimental data on decay power has previously existed for fission plant structural materials and for materials under high energy irradiation conditions (i.e. fusion). It was to fill this gap that a series of experiments were performed using the Fusion Neutron Source (FNS) facility at the Japan Atomic Energy Agency JAEA [1, 2, 3] . Material samples were irradiated in a simulated D-T neutron field and the resulting decay power was measured for cooling times of up to thirteen months. Using the highly sensitive Whole Energy Absorption Spectrometer (WEAS) method, both β and γ emission decay energies were measured at selected cooling times and, quite impressively, as soon as a few tens of seconds after the end of irradiation.

In this report we have utilised the experimental database from JAEA to perform an extensive benchmark validation exercise of the FISPACT-II [4] inventory code and the latest versions of several international nuclear reaction data libraries, including TENDL-2019[5]. This benchmark exercise has been developed over a number of years and now forms a key part of European efforts to validate TENDL and JEFF libraries. This present version, focussing on TENDL-2019, builds on earlier reports [6, 7, 8] and the benchmark, together with the extensive analysis tooled developed with it (and used in this report), have recently been highlighted by a publication in Nuclear Fusion [9]

2 Experimental set-up

2.1 FNS assembly

14 MeV neutrons are generated by a 2 mA deuteron beam impinging on a stationary tritium-bearing titanium target. The total neutron flux at the sample location, for this experiment, is in the range of 1.0×10^{10} [n cm^{-2} s^{-1}], the same order of magnitude as in the first wall of the Joint European Torus (JET) fusion experiment when operating with D-T plasma. However, the irradiation time at the FNS were of 5 minutes and 7 hours in comparison with the few seconds flat burn achieved during the DTE1 JET fusion campaign. The DTE1 campaign culminated in a single 16MW fusion shot. As a point of reference, the total flux in a power plant is typically expected to be in the region of 10^{13} or 10^{15} [n cm^{-2} s^{-1}], three to five orders of magnitude higher than in JET or FNS, and also for much longer irradiation times.

Thin samples, 25x25 mm^2 in area, and typically 10 μm thick, have been used, either as metallic foil or powder sandwiched between tape. Use of a thin sample minimises the self-absorption of β rays emitted in the sample itself and allows their measurement. A total of 74 different materials have been used across the different phases of the

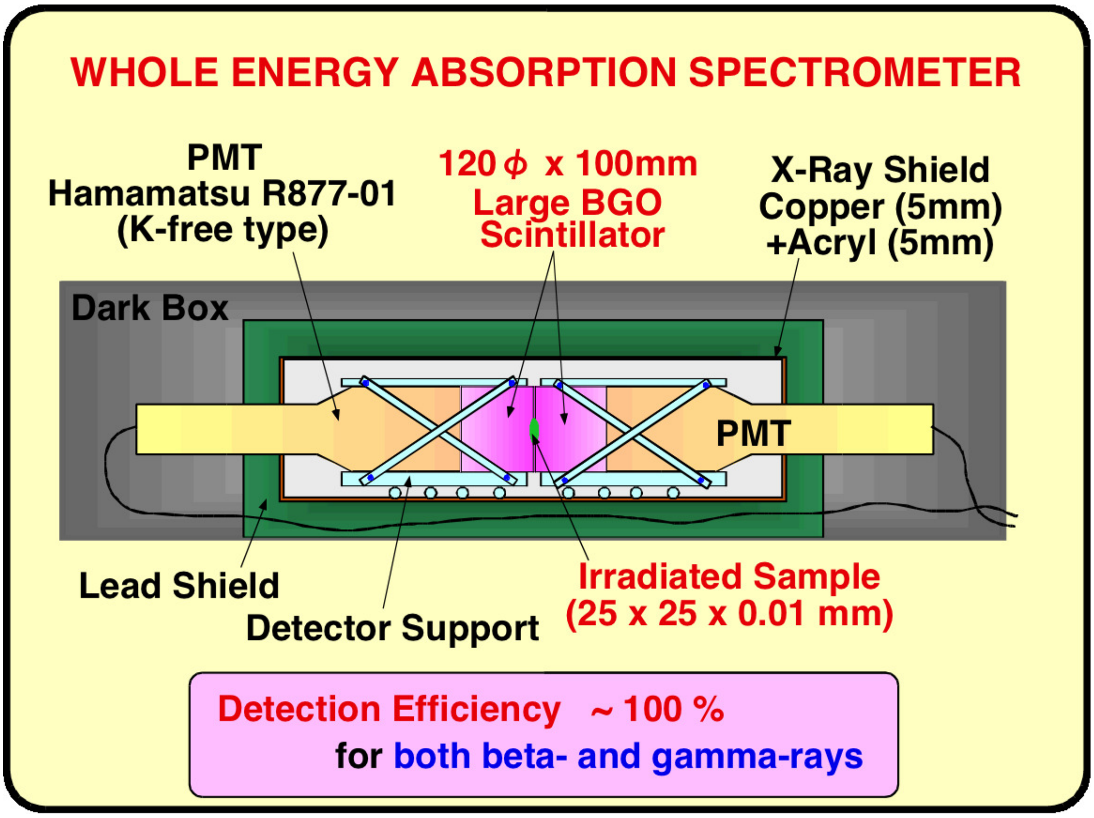


Figure 1: Whole Energy Absorption Spectrometer WEAS set-up

experiment.

The decay energy in each irradiated sample was measured in the Whole Energy Absorption Spectrometer (WEAS), which comprises two large bismuth-germanate BGO scintillators in a geometric arrangement provides almost 100 % detection efficiency for both β and γ-rays (see Figure 1). Correction factors need to be applied for γ-ray efficiency and for β and electron energy loss in the sample itself (less than 15% generally), and for other effects such as the decay heat due to the plastic tape used for the powder samples. The overall experimental uncertainty totals between 6 to 10% in most cases, although it rises to higher levels at particular cooling time for certain samples. The WEAS provides high sensitivity, down to powers less than 1 pW, which is valuable for measurement of some nuclides with long half-lives. It also has a wide dynamic range: measurements of up to a few mW have been achieved in the experiments.

2.2 Irradiation conditions

Three types of irradiation have been performed in order to extract the maximum information possible from such experiments. First, a 5 minute irradiation rapidly followed by a time dependent series of decay power measurements from tens of seconds up to one hour of cooling was used. Such prompt measurements are made possible by the use of a small sample rapidly transported from the irradiation zone to the measurement areas by means of pneumatic tubes. This particular type of measurement allows very short half-life nuclides to be detected and measured. Second, a 7 hour irradiation was performed for some of the samples, followed by a more relaxed time-dependent series of decay power measurements spanning from half a day up to a year of cooling. And third, in order to broaden the scope of the study and enlarge the materials database, the number of studied materials was increased from 32 to 74, covering many more elements of interest, but with published results only on the 5 minute irradiation experiments.

In the 5 minute irradiation experiments, three different positions were used: positions 1, 2, 3; while only one sample position, 7, was used for the 7 hour irradiations. The experimental set-ups in for each position are depicted in Figure 2. Different neutron spectra, in the 175 Vitamin-J group structure, were calculated using the Monte Carlo code MCNP [3] with a geometrical configuration corresponding to the different assembly positions and are plotted in Figure 3. Slight spectral differences exist between position 1, 2 and 3; however, the neutron flux profiles indicate a marked 14 MeV fusion peak and very few neutrons at energies lower than one MeV. The flux profile corresponding to position 7 is sufficiently shifted from the others to be treated separately. It is clear from Figure 3 and the fact the calculated standard deviation is large (typically greater than 20% [3]) for the energy groups below 100 eV, that few reaction rates can be well characterised at these energies. This means that if the energies below 100 eV are important in the production pathways of a measured radionuclide, no clear conclusion should be drawn from the comparison. Note that a nominal 0.5 to 1% standard deviation convergence criteria for reaction rates in all the neutron energy bins was not achieved in the Monte Carlo simulation, although the standard deviation of the total fluxes was below a few percent. This highlights the fact that in Monte Carlo simulations the total-flux standard deviation is not a good indicator of the quality of the neutron flux spectra, particularly in their low energy tails.

Originally in 1996, 32 relevant materials were irradiated at JAEA/FNS, for 5 minutes and 7 hours, and decay heat values measured over a wide range of cooling times: from a few tens of seconds up to 400 days and compared to predictions with previous activation databases [10, 11]. These results are referred to as FNS-96 in this report. Additionally, in 1998-99, 74 samples - one for each of naturally occurring elements, but excluding very light element and noble gases - were prepared for a new measurement campaign in the same assembly. The experimental results are referred to in this report as FNS-00, having been released officially in 2000.

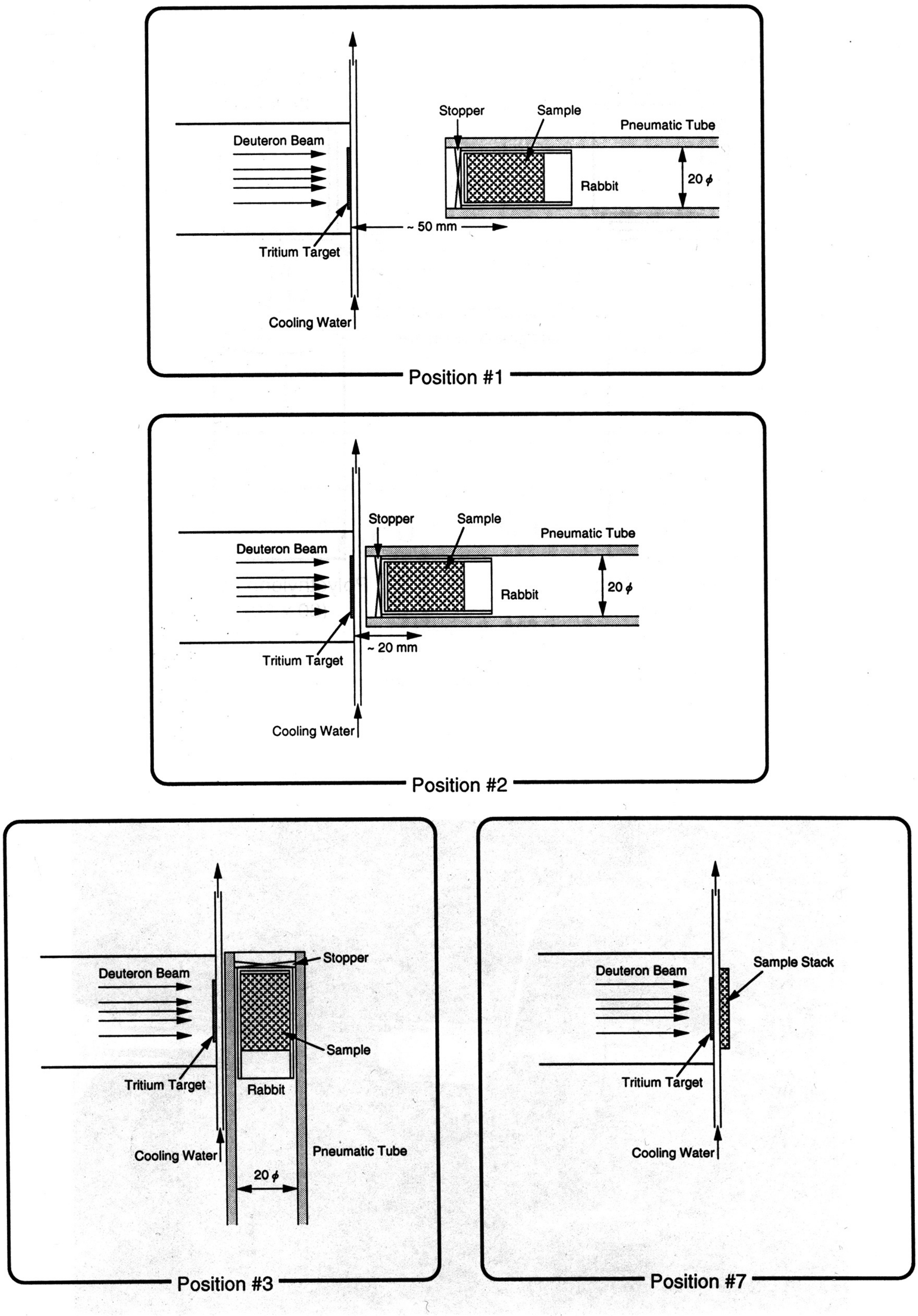


Figure 2: JAEA FNS four set up assemblies

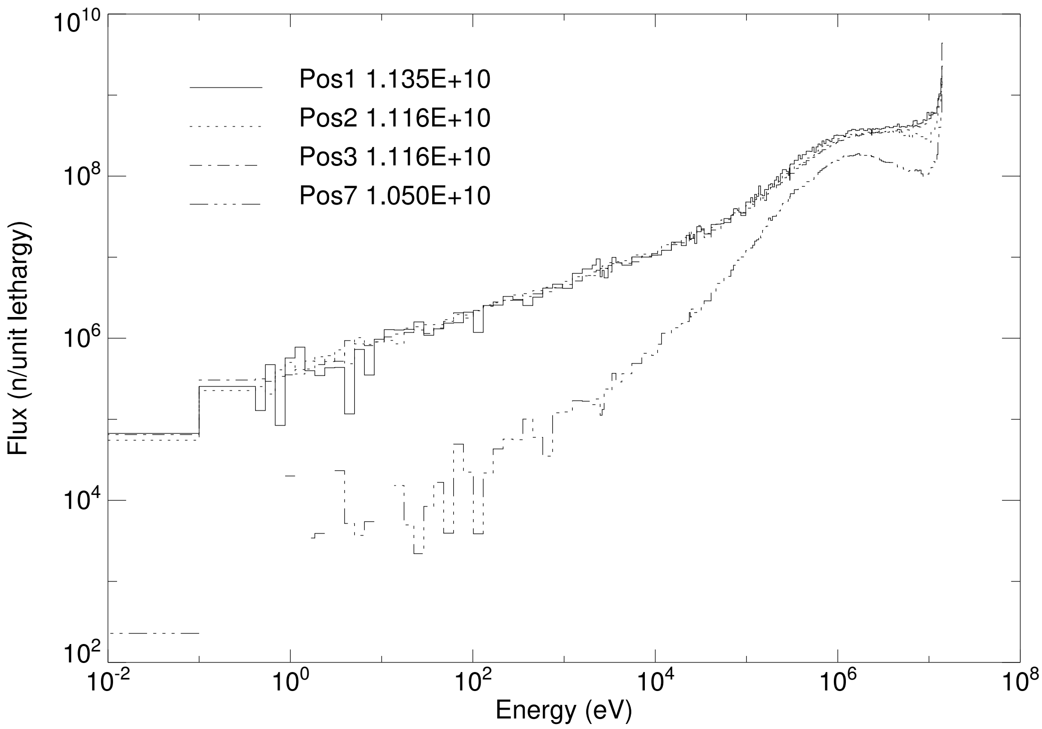


Figure 3: FNS Neutron spectra, neutron fluence monitored by $^{27}Al(n,\alpha)^{24}Na$

2.3 Material data

For each of the material samples, the percentage elemental weight has been supplied by JAEA. These tend to correspond to the theoretical weight distribution calculated from the compound or material fractions of the major isotopes. No impurity levels have been given and thus no isotopes other than the major ones have been used in the input data of the calculation scheme. The lack of real chemical analysis of the irradiated samples, although not thought to be important at the preparatory stage of this validation exercise, will be shown to be a drawback for certain materials that seem to have contained a specified (by the manufacturer), but un-quantified, amount of impurities. If those levels of impurities are not known then the code predictions cannot be accurate, and so the comparison will be inconclusive at times when impurities are proven to be important. Table 1 gives a complete list of the irradiated samples and their experimental form.

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			

Table 1: Irradiated sample materials. A superscript * next to the material name indicates the 5 minute irradiation experiments were also compared to simulations with the the IRDFF-II nuclear data library (in addition to the other libraries discussed in this report), while the § indicates IRDFF-II comparison to the 7-hour experiments.

3 Calculated predictions

The FISPACT-II [4, 12] inventory simulation platform has been used to perform this validation exercise. Several different, major cross section databases have been accessed using the FISPACT-II code [12]: TENDL-2019[5], EAF2010[13], JEFF-3.3[14], ENDF/B-VIII.0[15], and IRDFF-II[16]. In addition to cross sections the other basic quantities required by an inventory code are information on the decay properties (such as half-life or decay scheme) of all the nuclides considered. These data are available in a handful of evaluated decay data libraries. FISPACT-II is able to read the data directly in ENDF-6 [17] format, requiring no pre-processing to be done. The now well verified and validated eaf_dec_2010 library based primarily on the JEFF-3.1.1 and JEF-2.2 radioactive decay data libraries, with additional data from the latest UK evaluations, UKPADD6.10, contained data for 2233 nuclides. However, to handle the extension in incident particle type, energy range, and number of targets, many more nuclides must be included. A 3873-nuclide decay library dec_2012 was assembled from eaf_dec_2010 complemented with all of JEFF-3.1.1 and a handful of ENDF/B-VII.1 decay files. This new decay library was used by default in the simulations. However, ENDF/B-VIII.0 and EAF2010 have their own dedicated libraries, and so these were used in those cases, while JEFF-3.3 requires a decay library in non-ENDF-6 format, and thus simulations for that library were performed with eaf_dec_2010.

The modern (EAF2010 excluded) groupwise libraries used in the calculation scheme all correspond to either a 1102 or 709 group structure [12] collapsed using a 1/E micro flux weighting function. These calculations required the collapse of the nuclear data libraries for each flux at positions 1, 2, 3 and 7 (see figure 2).

FISPACT-II also includes the capability to identify the dominant radionuclides to a particular radiological quantity (including decay heat), and can subsequently perform an analysis of their major production pathways and associated uncertainties (in the case of TENDL, based on Bayesian Monte Carlo BMC covariance date) – all of which has been used in the detailed comparative analysis shown in the present work.

4 Comparison of the results

For each material sample and irradiation condition (which combines the flux spectrum, irradiation time [5 minutes or 7 hours], and experimental cooling times) calculations have been performed with FISPACT-II and compared to the corresponding experimental data. Tabular and graphical comparisons of the results are presented. On the primary graphs FNS experimental measurements are plotted (as points) and include the uncertainties as vertical lines, while the grey shaded area corresponds to the calculation uncertainty derived from TENDL-2019. Simulated data results with each data library are plotted as lines. The 5 minute irradiation results are presented first followed by those for the 7 hour irradiations, where available. Graphs corresponding to the 5-minute irradiations of the year 2000 campaign are given first, followed by the results of the year 1996 experiments, where they exist experimentally.

Care needs to be taken when interpreting the graphs, particularly in view of the log-linear scales. Such plots allow a direct visual interpretation of the performance of each library in simulating a particular experiment. A departure from equivalence in the decay profile between experiment and calculation would indicate a mismatch in terms of half-life in one or more of the important/dominant nuclides produced (or in some cases, not produced) during the experiment/simulation – this is generally rare as decay data is mature. Meanwhile, a properly shaped profile at the wrong heat level is normally a signal that the cross sections for the associated production pathways are incorrect.

A table (for the 2000 5-minute or 1996 7-hour experiments only) follows the graphs and gives more information, showing the experimental and simulated (for TENDL-2019 only) decay heats and uncertainties at each experimental measurement time. The tables also include E/C (experimental/calculation) values for each library considered and evaluates the mean % difference of each simulation from the experiment (i.e. the average over all experimental data points of $|E - C| * 100/E$ – see section 5). For this latest report, we also estimate the mean χ^2 of the simulation deviation. By taking into account the experimental error via $\chi^2 = ((C - E)/\Delta E)^2$ we can address the imbalance caused by poor simulation matches to experiments with high uncertainty (which would otherwise have a high mean % deviation). The mean (χ^2/n values, where n is the number of data points in the experiment, are given for each library in the table.

These tables and graphs are followed by a more detailed analysis for the TENDL-2019 results (again, just for the 2000 5-minute or 1996 7-hour experiments, as appropriate). First, characteristic E/C values are defined for each dominant radionuclide (as identified by FISPACT-II) by taking the global E/C value associated with the decay-time at which the nuclide first contributes more than 75% of the total decay heat. If a nuclide never attains such a level of dominance during the TENDL-2019 simulation, then no E/C values are given as this would be inappropriate (the integrated decay heat experiment & simulation cannot say anything meaningful about the contribution from that nuclide). For each nuclide and E/C value, the table also includes the % experimental error (%ΔE) and FISPACT-II uncertainty % for the nuclide (%ΔC^{nuc}) at the selected decay-time.

Secondly, the contributions from dominant radionuclides are plotted in graphical form, which is a recently developed automatic output from FISPACT-II [18]. Such plot shows the time-evolution in the total decay heat result along with separate evolving curves for each FISPACT-II-identified dominant nuclide (all are included regardless of whether they were included in the E/C analysis table). In this main section of the report for each experiment only the nuclide contribution plot for TENDL-2019 simulations are included. At the end of the section (after the pathways and comments) additional plots are shown for other libraries and the absolute contributions plots are complimented by % contribution plots – this is a new feature for the current report making it easier to observe which radionuclides give important contributions to the total decay heat in each simulation as a function of time. These plot-pairs for each library simulation (absolute decay-heat and % contributions) provide a detailed visual representation of the importance of different nuclides and can be used to assess the relative contribution of different nuclides, which, combined with the E/C (see above) and pathway (see below) analyses, allows for a judgement to be made on whether the experimental result is able to validate the calculational approach for production pathways and decay data. An additional plot final plot is also given – replicating the standard out from previous validation exercises [7] – showing the important nuclides labelled at the position of their heat level at shutdown from the TENDL-2019 simulations on the ordinate and half-life on the abscissa.

A pathway analysis is also tabulated for all the dominant nuclides (regardless of whether they were included in the E/C analysis table). This uses the standard code-word options (UNCERT and LOOKAHEAD were required, see the description in [12]) for pathway analyses and no special attempt was made to perform individually-designed calculations for each experiment. The table includes, for each dominant radionuclide, the half-life and all important production routes, with % production values. This table is presented separately to the E/C analysis above because it includes all dominant nuclides for completeness, but the data can be used in conjunction with that former table to interpret the specific reactions that were responsible for the important contributions to the simulated decay heat. Note that the pathway analysis presented (including the % contributions of each path to the production of a particular nuclide) are based on simulation outputs with TENDL-2019– this is an important observation since there are cases where other libraries predict completely different dominant nuclides (and/or production paths), which is not capture in these tables.

Careful consideration needs to be given when analysing experimental data such as that produced from FNS. The fact is that the measured quantities may, or may not, be directly related to the pathways of production of a particular radionuclide, which is why the 75% criteria was introduced in the E/C analysis above. However, even in this case, there is only a strong possibility, not a certainty, that the major radionuclides measured are the ones predicted by the code, and further that their amount has been properly calculated before their respective decay power is derived. Although improbable, it could be the case, for example, that a 20% under prediction in terms of atomic amount of a nuclide is balanced by a 20% over prediction through the decay data scheme. This would lead to a perfect E/C value, even though the simulation is different to the experiment. Such possibilities of error compensation, though unlikely, could exist, which makes unequivocal interpretation of the results problematic. However, such difficult-to-detect scenarios are made less probable when the experimental results are compared to results from different activation codes, cross section libraries and decay data [3], as here – especially if combined with analysis of C/E values for the cross sections themselves.

The remainder of this report presents, as described above, the analysis for each of the 74 materials samples that have been irradiated. For convenience, the complete set of comments for each experiment are include first, but these are also given again at the end of each material & batch section. At the end of the report, a further discussion is given, along with summary tables showing the quality of predictions for each library.

Comments on each experiment

Fluorine 5-minute

(Page 52) The agreement between experiment and simulation is excellent for both fluorine samples at all cooling times. TENDL-2019, JEFF-3.3, and ENDF/B-VIII.0 are in agreement at all cooling times, while EAF2010 and IRDFF-II show disagreement at decay-times beyond ∼5 minutes – those two libraries appear to slightly underpredict F18 production via (n,2n) reactions on F19 in F18 production via the (n,2n) reaction on F19. For the 2000 experiment, the F18 production of the TENDL-2019 et al. gives a good match, while for the 1996 experiment, it is EAF and IRDFF whose F18 prediction is closed to the measurements. The variation between the two experimental data sets clearly demonstrates that experiments do not always lead to the same measurements, even when carried out in the same assembly set-up, and here the discrepancy makes it difficult to identify the best prediction. However, there is a 10% uncertainty in F18 production with TENDL-2019 (see the E/C table), which easily encompass this experimental fluctuation (as shown by the grey error bands). Note, O19 production via (n,p) on F19 is not important for dosimetry, so IRDFF-II only captures the decay-heat profile when F18 dominates.

Sodium 5-minute

(Page 57) Clearly the two experimental batches are discrepant for sodium and do not exhibit the same decay-heat plateau beyond 10-minutes, which the simulations say is primarily due to Na24. Many factors could have influenced the experimental set-up including the presence of impurities in the sample. All libraries show good agreement to the 2000 result (IRDFF-II does not include the (n,p) reaction to produce Ne23, which dominates at short-timescales with the other libraries). The TENDL-2019 Na23 capture cross section seems to represent the 2000 experiment well, although the uncertainties are relatively high in both cases.

Sodium 7-hour

(Page 62) For the longer experiment on sodium, most of the library simulations seems to either under or overpredict the measurement, with only JEFF-3.3 matching closely the result at all decay times. The heat arising from Na22 seems to be underpredicted by around 40% by EAF2010, and 20% by TENDL-2019 and 30% by IRDFF-II (a change to the (n,2n) channel on Na23 compared to IRDFF-1.05), while ENDF/B-VIII.0 overpredicts by around 15%. The wide variation between the simulated results makes it difficult to draw any concrete conclusions (JEFF-3.3 could be a good match by chance).

Magnesium 5-minute

(Page 66) There is good agreement at all cooling times (with the caveat that IRDFF-II does not include the reaction data for the production of the short-lived Na25 or Ne23 nuclides from Mg). Na24 production-rates via (n,p) reactions on Mg24 are well predicted by all libraries for magnesium.

Aluminium 5-minute

(Page 70) For aluminium an excellent agreement can be seen, for both batches, for the production route of the Mg27 radionuclide with all libraries, although TENDL-2019 is a slightly worse match than with the previous TENDL-2017 (the mean deviation in the latter case was 7% compared to 13% here), seemingly due to a slight increase in Mg27 production. TENDL-2019 variance reflects well the experimental uncertainty. JEFF-3.3 misses the production of the long-lived Na24 nuclide via (n,α) reactions and so begins to deviate from the experiment from around 10 minutes. The IRDFF-II result is noticeably somewhat worse than the previous IRDFF-1.05 results, possibly because of the addition of the (n,X) channel between Al27 and Na24.

Aluminium 7-hour

(Page 75) Apart from JEFF-3.3 – which predicts no Na24 whatsoever despite its obvious dominance in the other cases – all libraries show good agreement up to around 7 days of cooling. Beyond this the simulations deviate significantly from the experiment, which could be due to unknown impurities in the sample, such as Mn and Fe, whose presence at the thousands of ppm level could easily account for the missing decay heat observed in the simulations. On the other hand, all the simulations could be severely underestimating the production of H3 via (n,t) reactions on Al2 and, besides this, there is some variation in the prediction, with TENDL and IRDFF prediction of H3 lower than the other three.

Silicon 5-minute

(Page 79) In the pure silicon simulations of the 2000 5-minute experiment (an earlier 1996 experiment is omitted here due to an unacceptable level of undocumented impurities in the silicon oxide sample used in that case) both Al29 and Mg27 contribute significantly to the decay heat beyond around 15 minutes of cooling, and so it is not possible to reliably attribute E/C values to either of these radionuclides. At shorter cooling times Al28 dominates (see the nuclide contribution chart). All libraries agree well with the experiment, although IRDFF-II deviates at longer times because it doesn't contain data on the necessary reactions to produce Al29 or Mg27.

Phosphorus 5-minute

(Page 83) IRDFF-II is only concerned with the longer-lived Si31 nuclide and so doesn't include data for the reactions that produce the shorter-lived nuclides in phosphorus but captures well the experimental decay heat level associated with that former nuclide (as do the general-purpose libraries). Al28 dominates the decay heat in the simulations with the other libraries at times less than 30-40 minutes and there is good agreement between the simulated results and the experimental decay heat measured for this nitrate sample – although the experimental uncertainty is a suspiciously uniform 16%.

Sulphur 5-minute

(Page 87) The two sets of experimental measurements following 5-minute exposures do not agree, despite the fact that they should have been performed on identical sulphur samples. There is good agreement between TENDL-2019, JEFF-3.3 and the most recent 2000 experiment, while EAF2010 seems to match well with the earlier 1996 experiment. It is difficult to interpret anything more from these results because of such discrepant experimental measurements, although the library simulations all seem to reproduce the time-evolution profile of the experiments well, suggesting that the predicted radionuclide distribution – P34 dominance at first followed by a combination of Si31 and P32 – is a good fit to the experimental reality. Interestingly, ENDF/B-VIII.0 appears to predict a significantly smaller amount of Si31 compared to JEFF, TENDL and EAF because it lacks the (n,2p) production route from S32.

Sulphur 7-hour

(Page 92) This is an unambiguous, text-book case of a single important radionuclide (P32) producing all of the measured decay heat. All of the libraries (including IRDFF-II) correctly capture the behaviour both qualitatively and quantitatively, although only TENDL-2019 contains covariance data for the crucial (n,p) channel on S32. A better reproduction of the cross section structure has been achieved in 2-5 MeV region in TENDL-2019, potentially contributing to a slight improvement compared to TENDL-2017.

Chlorine 5-minute

(Page 96) All of the libraries show reasonable agreement with the short-term (<5 minute) experimental behaviour in Chlorine, which is predominantly from S37. However, JEFF-3.3 and ENDF/B-VIII.0 fail to produce the either Cl34 or Cl34m nuclide (via (n,2n) reactions on Cl35), which predominant in simulations with TENDL-2019 and EAF2010 beyond around 15 minutes of cooling, and so only those latter libraries show some agreement with the experiment beyond this point. However, even in those cases, there is discrepancy (overprediction), which may be a sign of an incorrectly allocated branching ratios or decay-heat contributions for the short-lived metastable and even shorter-lived ground-state that it decays to (which creates the secular equilibrium shown in the plots). Note that the E/C table is omitted here because the simulations predict non-negligible contributions from several radionuclides at all measurement times (see the nuclide contribution graph).

Potassium 5-minute

(Page 100) The extremely rapid measurement – made barely 34 seconds after the irradiation – of the decay heat from the potassium sample with more than 30 wt.% oxygen allows for a glimpse of the contribution of the short-lived N16 isotope. After this has decayed, first K38 and then Cl38 are the predominant contributors to decay heat (the latter is also joined by Ar41 at around 30% at 1 hour of cooling). All included libraries seem to show a some overprediction of production for K38, in particular. TENDL-2019 is the best match (and seems to show less overprediction of Cl38 and Ar41) followed by JEFF-3.3.

Potassium 7-hour

(Page 105) Here the experimental uncertainties are rather high, making a detailed analysis and comparison difficult. The decay-heat profiles appear generally well-shaped with all libraries. Although a better agreement between the experiment and TENDL-2019 results (compared to TENDL-2017) are observed for the experimental measurements at 0.65 and 1.71 days, which could be a sign of an improvement in the evaluation of the (n,γ) channel on K41, producing the K42 radionuclide that dominates the first few cooling times. Notice that K40 is nearly stable on the experimental timescale here.

Calcium 5-minute

(Page 109) For the latest, 2000 experiment there is a good agreement for simulations with all included libraries, even at short cooling times, although TENDL-2019 and

JEFF-3.3. seem to underpredict K44 slightly (from (n,p) reaction on Ca44) compared to EAF and ENDF/B. For the earlier, 1996 experiment the measurements are systematically higher, resulting in an apparent underprediction in the simulations. One possible explanation for this is that the CaO powder used in the experiment was very fine and was used in very small amounts, sandwiched between plastic tape. The contribution from that tape had to be extracted from the raw measured data, but because it may have been a very significant contribution to the decay heat, the signal-to-noise ratio would have been high and so there may be an unavoidable random variation in the results – a situation that may have also occurred in the SrCO3, Y2O3, and SnO2 samples discussed later. The profile associated with the predominant K44 radionuclide seems to be well-represented by the simulations in all considered cases (despite the aforementioned difference for JEFF and TENDL).

Calcium 7-hour

(Page 114) All libraries considered produce a good agreement to the measurements and the data points are all within TENDL-2019's uncertainty band. This is an impressive result given the somewhat complex, multi-nuclide picture, with dominant ($> 50\%$) contributions from K42 and Ca47 at different cooling times, combined with more minor, 10-20% contributions from Sc47, Ar37 and K43.

Scandium 5-minute

(Page 118) Here the scandium simulations yield good agreement for the production of Sc44, apart from ENDF/B-VIII.0, which overpredicts by a factor of 2. TENDL-2019 shows a particularly excellent agreement for Sc44 production via (n,2n), where the simulated decay-heat beyond 1 minute of cooling is always within the experimental uncertainty (JEFF-3.3 is equally good, suggesting identical underlying data). In principle, this experiment should be used to reduce the cross section uncertainty for Sc45(n,2n), see figure A1 in the appendix. There is more disagreement at cooling times below 1 minute where N16 (from the oxygen in the sample) is important and where there appears to be an underprediction of its production.

Titanium 5-minute

(Page 122) The 5-minute graphs exhibit some unexplained differences between the two experimental batches - reflected in the overprediction by most libraries for the year 2000 experiment, but under prediction of the 1996 case. The routes of production of the identified important isotopes are relatively complex, although the simulations with the four general purpose libraries are in agreement and seem to capture the main profile of the decay heat; it is dominated by first Sc50 (< 5 minutes of cooling) and then Sc48 ($\sim$50% with Sc49+Ti45 (both $\sim$20%) afterwards. IRDFF-II includes the relevant Ti48(n,p)Sc48 channel for this case, but underpredicts due to the absence of the production channels for Sc50 and Sc49.

Titanium 7-hour

(Page 127) An excellent agreement exists at all cooling times for all libraries (even IRDFF-II, although it is not as good as IRDFF-1.05), even with the relatively complex production routes of Sc46, which dominates at decay times beyond around 14 days and is produced from reaction routes that include (n,p), (n,np) and (n,d) channels.

Vanadium 5-minute

(Page 131) The two sets of experimental measurements here are clearly discrepant with one another – particularly at cooling times beyond 30 minutes, where the identical simulation with all general purpose libraries appear to underpredict the 1996 results but produce very good agreement in the 2000 experiment. IRDFF-II only contains the (n,α) reaction to produce the longer-lived Sc48 radionuclide and even here appears to overestimate the production by a factor of 2 compared to the others. The Ti51 (from (n,p) on V51) profile with JEFF, TENDL, EAF, and ENDF/B nicely captures the experimental profile for all but the last two measurements (where Sc48 becomes important).

Vanadium 7-hour

(Page 136) An excellent agreement is seen with TENDL, JEFF, ENDF/B, and EAF libraries at all but the last 50-day cooling step, where the experimental uncertainty is quoted as 58%. IRDFF-II reproduces the simulated profile (dominated in the simulations by Sc48 from (n,α) reactions on V51), but with a twofold overprediction that was not the case with IRDFF-1.05. In the final cooling step, V49 (from (n,2n)) is predicted to contribute around 90% of the decay-heat with all of the general purpose libraries, but the large discrepancy compared to the experiment makes it difficult to draw any definitive conclusions – is it an underpredicted channel in the simulations, or an unaccounted for impurity in the experiment?

Chromium 5-minute

(Page 140) There is a good simulation.vs.experiment agreement up to around 30 minutes of cooling with all of the included libraries, which is precisely the timescale over which V52 dominates. V52 is primarily produced via (n,p) reactions on Cr52 (see the pathways table), but this reaction is missing from IRDFF (V52 is too short lived to be of interest for a dosimetry file) and so that library is not included here. At longer times there is deviation from the experiment, which could come from Al and Fe impurities. These may have been present in the sample at levels of up to 2000 and 6000 ppm, respectively (such levels of impurities have been measured in similar samples). Else there is an underprediction in the Cr50(n,2n)Cr49 channel, but further experiments would be needed to confirm this.

Chromium 7-hour

(Page 145) Some short-lived isotopes seem to be missing in all the simulations, almost certainly produced from impurities within the sample (as discussed for the 5 minute experiments earlier where only production of the very short-lived V52 nuclide was seen to follow the decay cooling in the experiment), but the overall agreement, completely dominated by Cr52(n,2n)Cr51, remains excellent. Note that IRDFF-1.05 included this important channel, but IRDFF-II misses it (due to shift to natural Cr data files?) and is omitted from the plots.

Manganese 5-minute

(Page 149) For Manganese, there is a good agreement at short cooling times for both batches with all general purpose libraries (IRDFF-II misses the Cr55 and V52 production). A slightly improved overall agreement with the experiment is noted for TENDL-2019 results compared to those with TENDL-2017, seemingly due a reduction in the cross section of the (n,α) channel that produces V52 (this is the dominant nuclide below 30 minutes).

Manganese 7-hour

(Page 154) All of the simulations are in good agreement with the experimental measurements (generally within the experimental uncertainty) for this simple case dominated by the Mn55(n,2n)Mn54 reaction path (also part of IRDFF-II).

Iron 5-minute

(Page 158) The two sets of calculated decay-heat curves, one for the experiment in 2000 and one for 1996, are in exact agreement (with some differences in the distribution of measured cooling times), as would be expected. However, the experimental decay results in the two batches disagree; one is just below the simulation curves (which are virtually identical with all libraries) and one above. This is suspicious and there is even more cause for concern with the reported data because the quoted uncertainty appears to be a simple, fixed standard deviation value, rather than an actual experimental error. IRDFF-II does not include the necessary reaction paths for the two short-lived radionuclides, Fe53 and Mn57, which the general purpose libraries predict (correctly) to be important in the first few minutes of cooling – for example, the dominant Mn56 contributes less than 80% of the decay-heat during the first minute of cooling (but is 100% after round 20 minutes and which IRDFF captures).

Iron 7-hour

(Page 163) As with the 5-minute experiments, there is generally good agreement for iron between the simulation and experiment, with the decay profiles associated with the dominant Mn56 and Mn54 nuclides (both produced via (n,p) reactions) appearing to well-capture the experimental profile. The simulated curves are generally within the experimental uncertainty.

SS304 5-minute

(Page 167) Remarkable agreement between experiment and simulation (with TENDL-2019, JEFF-3.3, EAF2010 and ENDF/B-VIII.0) for cooling times of up to 1 hour (IRDFF-II is discrepant below 20 minutes because it doesn't include the Cr52(n,p)V52 channel). All libraries capture the profile associated with the important Mn56 nuclide, which dominates beyond 10 minutes.

SS304 7-hour

(Page 172) A very clean and well defined agreement despite the complexity of the system, with many nuclides providing non-negligible contributions, and four-overlapping plateau regions where different predominant nuclides (see the % contribution plots). IRDFF-II only misses the channels for Co57 (from Ni58), which provides a 20% contribution towards the ends of the measurement time, but otherwise captures the important nuclides and production routes identified by TENDL-2019.

SS316 5-minute

(Page 176) Identically to SS304: Remarkable agreement between experiment and simulation (with TENDL-2019, JEFF-3.3, EAF2010 and ENDF/B-VIII.0) for cooling times of up to 1 hour (IRDFF-II is discrepant below 20 minutes because it doesn't include the Cr52(n,p)V52 channel). All libraries capture the profile associated with the important Mn56 nuclide, which dominates beyond 10 minutes.

SS316 7-hour

(Page 181) Virtually identical to the SS304 results and comparison: A very clean and well defined agreement despite the complexity of the system, with many nuclides providing non-negligible contributions, and four-overlapping plateau regions where different predominant nuclides (see the % contribution plots). IRDFF-II only misses the channels for Co57 (from Ni58), which provides a 20% contribution towards the ends of the measurement time, but otherwise captures the important nuclides and production routes identified by TENDL-2019.

Cobalt 5-minute

(Page 185) The two batches of measured experimental data sets are different when there is no reason for them to be (the simulated predictions are identical for the two batches – apart from some minor variations in the [measured] cooling times), and, furthermore, these unexplained differences lie outside of the quoted experimental uncertainty. Despite the obvious issues with the experimental results (it is not even clear that this is impurity related), simulations with the general purpose libraries nicely capture the decay profile measured in the experiments. Both TENDL-2019 and EAF2010 predict some minor contributions from Co60m at cooling times below 5 minutes, which JEFF-3.3 and ENDF/B-VIII.0 miss, but the contribution is too small for its inclusion (or not) to have any significant impact on the quality of predictions (especially given the experimental abnormalities). IRDFF-II is worse than IRDFF-1.05; seemingly overpredicting the production of the completely dominant Mn56 (via (n,α) on Co59) by a factor of two (2).

Cobalt 7-hour

(Page 190) Good agreement with all libraries for this relatively simple case, which is dominated by Co58 decay heat (produced via Co59(n,2n)Co58) at all cooling times greater than 1 day (see the % contribution plots). All simulation curves fall almost within the experimental uncertainties when this nuclide is dominant. At shorter cooling times, associated with the experimental measurements at 0.63 and 1.31 days, JEFF and ENDF/B seem to do better than either TENDL-2019 or EAF2010 (or IRDFF-II). For these first two cooling times, TENDL and EAF results seem to overpredict the experiment by around 20%, which almost exactly corresponds to the % contribution from Co58m predicted in the simulations with these two libraries. JEFF-3.3 and ENDF/B-VIII.0 on the other hand, only predict the production of Mn56 (via (n,α) on Co59), and at a level that EAF2010 and TENDL-2019 agree with – it appears that the Co58m contribution is unnecessary (and thus overpredicted) and doesn't reflect reality. The IRDFF-II issue at these first two cooling times appears, once again (as in the 5 minute experiment), more related to the overprediction of Mn56 compared to IRDFF-1.05.

Inconel-600 5-minute

(Page 194) Two main radionuclides are predicted (by the general purpose libraries) to dominate: V52 (mainly from Cr52(n,p)) during the first 20 minutes of cooling and then Mn56 (via Fe56(n,p)) for the remainder, up to 1-hour of cooling. The combined profile of these two nuclides seems to well capture the experimental profile, although the simulations all give a slight, systematic underprediction. As with the Cr experiment, IRDFF-II misses the production of V52, but does capture the production of Mn56. TENDL-2019 performs better than all other libraries, with the experimental points mostly within the simulation uncertainty. It is difficult to attribute the underestimation to anything specific in this complex material – certainly it is unlikely to be an issue with Cr52(n,p)V52 because that produced an overprediction in the Cr 5-minute experiments.

Inconel-600 7-hour

(Page 199) There is a very good agreement between the TENDL, JEFF, EAF, and ENDF/B libraries and experiment for this Inconel-600 alloy, with these libraries within a few % of the measurements at all decay times. IRDFF-II captures well the profile when first Ni57 and then Co58 dominate the decay heat, but misses the production of Co57 and Co60, which become important (along with Co58) in for the final 2 experimental measurements (or beyond around 100 days of cooling).

Nickel 5-minute

(Page 203) Here the two 5-minutes data-sets of experimental measurements differ (without explanation), but the predictions stay within 15% of the measurements at all cooling times for simulations with TENDL-2019 or EAF2010, and within 20% for JEFF-3.3. ENDF/B-VIII.0 performs badly as it lacks the metastable isomer production pathways, particularly Co60m and Co62m (both from (n,p) reactions on Ni isotopes according to the TENDL-2019 simulations). IRDFF-II also misses the production of these metastables, as well as the production of the short-lived Co62 (via (n,p) on Ni62)) and only has the simple decay-profile associated with the longer-lived Ni57.

Nickel 7-hour

(Page 208) Excellent agreement between experiment and simulation for the 4 general purpose libraries considered. Predictions show (correctly) that the decay-heat is dominated by Ni57 during the first few days of cooling and then by Co58. As with the Inconel 7-hour experiment, Co57 and Co60 join Co58 to contribute significantly in the final two cooling steps (IRDFF-II misses these two nuclides, but, as before, captures the profile associated with Co58 and Ni57).

Nickel-chrome 5-minute

(Page 212) The first 15 minutes of cooling time are dominated by the Cr-isotope produced V-52; a trend that was also seen in the Cr experiments. This early, chromium-dominated behaviour is well-captured by all the general purpose libraries. However, at later cooling time, ENDF/B-VIII.0 suffers (as it did in predictions for Ni) because it omits, in particular, the metastable Co62m isotope produced via (n,p) reactions on Ni62. As already noted (for Cr and Ni), IRDFF-II lacks the reaction channel to produce either the short-lived V52 from Cr or the Co isotopes from Ni – only the longer-lived Ni57 is produced, which TENDL-2019, JEFF-3.3 and EAF2010 predict contributes 50% at 1-hour of cooling – those three libraries all perform almost identically and well-match the experiment.

Nickel-chrome 7-hour

(Page 217) The Cr makes up around 20 weight % of the samples and the main radionuclides produced from Cr only have impact at shorter times (see the discussion of the 5-minute experiment), and so, unsurprisingly, the observations for this longer experiment are identical to those of pure Ni. Excellent agreement exits for simulations with TENDL, JEFF, EAF, and ENDF/B, while IRDFF-II misses the Co57 and Co60 that are important at 1-year of cooling.

Copper 5-minute

(Page 221) A good agreement between experiment and simulation (with all libraries) for both sample-runs for this straightforward case of (n,2n)-generated Cu62 decay-heat dominance at all cooling times. However, the experimental uncertainties seem rather uniform at 5 or 6%, which seems questionable given that the two experiments themselves differ by more than this amount.

Copper 7-hour

(Page 226) A simple, two-nuclide contribution profile – Cu64 during the first week and Co60 afterward – captures well the experimental result, with the simulated decay-heat values often within the experimental uncertainty for all libraries.

Zinc 5-minute

(Page 230) Both ENDF/B-VIII.0 and EAF2010 show remarkable agreement with the experiment, especially at cooling time beyond around 20 minutes where Zn63 (via (n,2n) reactions on Zn64) is particularly dominant. However, all libraries considered show very good agreement, with the short-term contribution from Cu66 ($\sim$30%) also well captured.

Gallium 5-minute

(Page 234) All included libraries produce a very good simulation agreement to the experimental measurements, mostly within the experimental uncertainty, demonstrating that the (n,2n) reactions involved in producing the two equally dominant Ga70 and Ga68 nuclides are well evaluated in the libraries.

Germanium 5-minute

(Page 238) A good agreement for most libraries, although there appears to be an underprediction of the short-lived N16 nuclide from O16, which dominates the very first cooling step. EAF2010 predictions seem to be too high in general, despite showing a near-identical nuclide contribution profile to the others. TENDL-2019 nicely follows the profile, particularly beyond 20 minutes of cooling where Ge75 (from (n,2n) reactions on Ge76) dominates.

Arsenic 5-minute

(Page 242) There is good agreement with all libraries, although there is an apparent and systematic overprediction once the short-lived N16 from oxygen has faded away (after about 1 minute of cooling). Since the quoted experimental uncertainties are relatively small – smaller than the overprediction by the libraries – it could indicate a need for slight revision of the (n,p) channel cross section that produces the Ge75 nuclide from As75 – this nuclides contributes 40-50% of the predicted decay-heat with all libraries. However, it is difficult to be definitive about this need as there are also several minor contributing nuclides: Ga72, As74, and As76.

Selenium 5-minute

(Page 246) A good agreement between simulation and experiment for TENDL-2019, JEFF-3.3 and EAF2010. TENDL-2019 is almost within the experimental uncertainties, JEFF-3.3 is slightly more outside, and EAF2010 produces the correct decay profile, but generally overpredicts by 15-30% (of the experiment). At short cooling times (less than around 1 minute) there are a complex set of important radionuclides and associated reaction pathways, but the majority of the decay cooling is dominated by Se81 (via (n,2n) reactions on Se82). ENDF/B-VIII.0 completely omits the various metastable nuclides that are predicted by the other libraries to be important during the first few minutes of cooling – particularly the Se79m whose decay profile is required to properly match the experimental shape between 1 and 10 minutes of cooling. Furthermore, ENDF/B-VIII/0 omits Se81m production and instead appears to combine its contribution via (n,2n) on Se82 into the Se81 production leading to an overprediction of that ground state nuclide and a complete misrepresentation of the profile.

Bromine 5-minute

(Page 251) Similarly, to the case with selenium, for bromine, ENDF/B-VIII.0 combines the contributions from Br81(n,2n) to both Br80 and Br80m into simply the production of Br80, which has a much shorter half-life than its metastable and thus a completely different decay profile. This leads to a significant overprediction of Br80 with that library and, even though it contributes only around 10% of the decay heat before 10 minutes of cooling (only becoming dominant at around 1-hour of cooling), this leads to a dramatic and obvious overprediction of the decay heat by the ENDF/B-VIII.0 library calculations. The predictions get worse for that library at later cooling after the previously dominant Br78 (also from (n,2n) reactions) falls away leaving Br80 to dominate. The other libraries considered produce excellent agreement to the experiment (particularly TENDL-2019 and JEFF-3.3) – well within the experimental uncertainties. This result demonstrates again the need to populate all reaction channel cross sections to create a truly general purpose library.

Rubidium 5-minute

(Page 255) TENDL-2019 properly matches this experiment, JEFF-3.3 and EAF2010 also perform well, but ENDF/B-VIII.0 does not capture the various channels to metastable nuclides – particularly the dominant Rb86m (at times less than 1.5 minutes) and Rb84 (dominant throughout the remainder of the experimental timescale) from (n,2n) reactions. This leads to a massive underprediction of the experiment by ENDF/B-VIII.0 in a situation where the pathways to the metastable nuclides are clearly validated by the C/E values obtained with the other libraries.

Strontium 5-minute

(Page 259) An interesting case where a metastable isomer (Sr87m) becomes dominant at the end of the measurement while a ground state nuclide (Rb88) contributes the most decay heat during the first 20-30 minutes (after the short-lived contribution of

N16 produced from oxygen has disappeared). TENDL-2019, JEFF-3.3 and EAF2010 also show excellent agreement to both experimental batches (even though there are some unexplained differences between the experiments). ENDF/B-VIII.0 underpredicts significantly at all times due to the missing contribution from Sr87m. Note that the N16 contribution appears underpredicted with all libraries, but this is more likely an experimental artefact than a problem with the well-characterised (n,p) channel on O16.

Strontium 7-hour

(Page 264) A good agreement with all libraries, except for the first cooling step with ENDF/B-VIII.0 where there is an underprediction due to the missing Sr87m metastable. A relatively complex picture, with three different overlapping nuclide contributions (Sr87m, Sr83, and then Sr85 as a function of time according to TENDL, JEFF, and EAF), so the level of agreement is very pleasing.

Yttrium 5-minute

(Page 268) Some large experimental uncertainties in the 2000 batch experiment for yttrium and the two batches (1996 vs. 2000) disagree significantly. Only TENDL-2019 and EAF2010 capture the dominance of Y89m at cooling times below around 3 minutes of cooling (JEFF and ENDF/B miss this nuclide). None of the libraries give very good agreement at intermediate cooling times ($\sim$3-10 minutes of cooling), but all give better agreement at longer times where the single ground-state nuclide Y88 (from (n,2n) on Y89) is completely dominant. Rb86m seems to be the underpredicted nuclide that would properly match the experiment profile at the intermediate times, and so its production via (n,α) on Y89 should be reviewed.

Yttrium 7-hour

(Page 273) All of the code predictions seem to underestimate the experimental measurement consistently and evenly to differing degrees up to 400 days of cooling, with EAF2010 the closest and JEFF-3.3 the worst. The response is predicted to be entirely due to the production of Y88 via Y89(n,2n), so this seems to suggest a need to re-evaluate the cross section for this reaction or the decay data associated with Y88 (if not backed up by differential measurements).

Zirconium 5-minute

(Page 277) As this element is part of fission fuel cladding and is this very important, unusually, ENDF/B-VIII.0 includes the necessary production of the metastable Zr89m nuclide, which dominates the decay-heat below 10 minutes of cooling. This nuclide is also produced (via (n,2n) reactions on Zr90) in simulations with TENDL-2019 and EAF2010, but JEFF-3.3 omits it (also unexpected because it was included in JEFF-3.2 – see [7]). In fact, ENDF/B-VIII.0 gives the best agreement to the early phase of the decay profile in the two 5-minute experiments and has the best (lowest) average deviation from the 2000 experiment. However, TENDL-2019 gives the best visual agreement to the experimental decay profile, with a fairly uniform 5-10% over-prediction, while ENDF/B-VIII.0 seems to underestimate the decay heat at longer cooling times (after Zr89m falls away) despite also predicting the Y89m metastable (TENDL-2019 and EAF2010 also have this), which dominates after around 20 minutes of cooling. IRDFF-II is included here, but it is only suitable to observe the small, constant (on the experimental timescale) contribution from Zr89 (from (n,2n) on Zr90).

Zirconium 7-hour

(Page 282) A complex simulation picture, with four different radionuclides contributing at least 20% of the decay-heat at some point during the simulations with all libraries considered, but excellent agreement exists between experiment and simulation (almost within experimental uncertainty in the case of TENDL-2019). Only in the last cooling step there is significant deviation, with all of the libraries underpredicting the experimental result. It is difficult to assess the cause of this – the Zn95 radionuclide and the Nb95 produced from it (via decay) follow the experimental profile at cooling times below 1-year, so their production seems properly simulated – perhaps an unknown impurity in the experimental sample? Alternatively, the decay properties of one or other of these nuclides may need adjustment.

Niobium 5-minute

(Page 287) ENDF/B-VIII.0 does very badly here, completely missing the production of metastables Nb94m, Nb92m, Y90m, and Y89m, which all provide contributions of at least 20% to the decay-heat at some time in the simulations with the other libraries. That library only contains the reaction channel to produce Y90 and thus dramatically underpredicts the measurements. All other libraries considered give a good agreement to both experimental batches and clearly well represent this relatively complex picture dominated by four competing metastable nuclides. JEFF-3.3, in particular, has improved relative to earlier versions of that library (see the JEFF-3.2 results in [7]). In IRDFF-II, Nb93(n,2n)Nb92m is the only reaction pathway that is relevant for this experiment, contributing more than 60% after around 30 minutes of cooling, and so this library performs better than ENDF/B-VIII.0 for this case.

Niobium 7-hour

(Page 292) A superb agreement is seen here for predictions with TENDL-2019, JEFF-3.3, EAF2010, and IRDFF-II, due to the correct production of Nb92m via (n,2n) reactions. As in the 5-minute experiments, ENDF/B-VIII.0 is severely discrepant because it misses the production of that metastable, instead producing a completely different, and obviously erroneous, profile of contributing nuclides.

Molybdenum 5-minute

(Page 296) There is slight, unexplained difference between the two otherwise identical experimental batches for molybdenum. However, TENDL-2019, JEFF-3.3, and ENDF/B-VIII.0 give good agreement to the experiments. TENDL-2019, in particular, produces a remarkably close match to the 2000 experiment, well within the experimental uncertainty, while ENDF/B-VIII.0 does the same when compared to the 1996 experiment. Unusually, EAF2010 seems to consistently overpredict, which suggests that an error in the Mo92(n,2n)Mo91 cross section has been corrected in the nuclear data field since the generation of that legacy-style library. There is a minor contribution (max. 20%) from Mo91m during the first 5-minutes of cooling in the TENDL-2019 (and EAF2010) simulations, which could explain why that library, in particular, produces a good, uniform match at all cooling times – JEFF-3.3. and ENDF/B-VIII.0 miss that metastable isomer and show a varying agreement profile, which is worse at shorter cooling times.

Molybdenum 7-hour

(Page 301) The complex decay heat picture predicted by TENDL-2019 (and EAF2010) – with many contributing nuclides, particularly beyond 10 days of cooling – reproduces the experimentally measured profile for 200 days of cooling. ENDF/B-VIII.0 and JEFF-3.3 begin to underestimate the decay heat from around 10 days of cooling, primarily because of the absence of two metastable radionuclides: Nb92m via Mo92(n,p) and Nb91m via Mo92(n,np), which provide important contributions in the simulations with EAF2010 and TENDL-2019 (Nb92m is actually dominant at the 24-minute measurement time).

Ruthenium 5-minute

(Page 305) A superb fit to the experiment can be seen in the predictions with both TENDL-2019 and EAF2010, even at short cooling times of less than around 10 minutes where the Tc102m metastable is seen to dominate (although not sufficiently for its reaction channel [(n,p) reactions on Ru102] to be fully-validated by the experiment) – Ru95 from (n,2n) reactions on Ru96 dominates at all later cooling times. The combined and overlapping profile from these two nuclides perfectly captures the experimental profile and the two libraries are within the experimental uncertainties at almost all cooling times. ENDF/B-VIII.0 and JEFF-3.3 both miss the production of the metastable and thus produce the wrong decay profile, while ENDF/B-VIII.0 also overpredicts the contribution from Ru95.

Rhodium 5-minute

(Page 309) The fit to the experimental measurement is poor with all libraries for this important element. The two predominant radionuclides are: Rh104, whose production route involves a branched capture channel (on Rh103), which cannot be well characterised in the FNS neutron spectrum; and, at least in simulations with TENDL-2019, EAF2010 JEFF-3.3, Rh103m, whose production is via a super-inelastic reaction. Despite the overprediction, the combination of these two nuclides, which are completely dominant (no other nuclide contributes more than 10% with TENDL, EAF, or JEFF), produces a profile that is a good match to the experimental profile. The predominance of non-threshold reactions in the simulations make it difficult to make any definitive conclusions or recommendations regarding the quality of the agreement (or lack of). ENDF/B-VIII.0 misses the production of Rh103m completely and produces a decay-profile that is not a good match to the experiment, despite having a seemingly lower average deviation from the measurements. IRDFF-II includes the channel to Rh103m and shows the same overprediction as TENDL-2019 (and others).

Palladium 5-minute

(Page 313) A nice agreement between experiment and simulations with TENDL-2019 – fairly remarkable given the complexity of the case (a large number of contributing nuclides with multiple production pathways). Shorter cooling times are dominated by metastable isomers, particularly Pd109m and Pd107m produced via (n,2n) reactions and Rh108m from (n,p). ENDF/B-VIII.0 misses all of these nuclides, while JEFF-3.3 does slightly better by including the channel to Pd109m but misses the others. Additionally, TENDL-2019 and EAF-2010 predict that Rh106m is important at longer cooling times underneath the predominant Pd109 (all libraries predict this), but JEFF and ENDF/B miss this (via (n,p) on Pd106). There have been some minor changes in TENDL-2019 compared to TENDL-2017; agreement to the experiment beyond 20 minutes of cooling has improved, while deviation has increased at very short cooling times (possibly due to a new overprediction of Rh104). EAF2010 includes the production of all the necessary metastables, but overpredicts the production of Rh108m, leading to a significant (25%) overprediction at cooling times less than around 20 minutes. This proves once again the strength of the TALYS modelling processes to produce a truly general purpose library with proper inclusion of all reaction channels.

Silver 5-minute

(Page 318) TENDL-2019 and EAF2010 both overpredict slightly at cooling times less than 5 minutes, while at longer cooling times EAF2010 underpredicts quite significantly. Overall, TENDL-2019 does very well in capturing the experimental profile, which is dominated by the decay of nuclides from two different (n,2n) production channels – to produce Ag108 and Ag106, which are both important during the initial cooling phase, while Ag106 is completely dominant beyond 10 minutes of cooling. JEFF-3.3 overpredicts the production of Ag108 and so performs badly during the first 10 minutes, while ENDF/B-VIII.0 overpredicts both (n,2n) channels and hence the decay-heat dramatically (by a factor of 2 at all cooling times).

Cadmium 5-minute

(Page 322) EAF2010 performs very well here, almost within the experimental uncertainty, while TENDL-2019 seems to overpredict by between 10 and 20% at all cooling times. Examining the simulations in detail, one notes that TENDL-2019 predicts significantly more decay heat from Cd105, which contributes around 10-20% of the decay-heat at all cooling times. Indeed, the total cross section for the (n,2n) reaction on Cd106 producing this nuclide is roughly twice as high with TENDL-2019 compared to EAF2010 – suggesting that the TENDL evaluation should be reassessed in this case. There may also be a need to adjust the production channels for Cd111m, which dominates the decay heat at all cooling times – it is produced primarily via (n,2n) reactions on Cd112 and TENDL-2017 and EAF2010 are nearly in agreement for that total cross section. However, an inelastic scattering channel on Cd111 also provides a non-negligible contribution and has a somewhat higher total cross section with TENDL-2019. At the same time, TENDL-2019 clearly outperforms both ENDF/B-VIII.0 and JEFF-3.3, which massively underpredict the experiment because they do not include either of the Cd111m production routes – they only capture the contribution from Cd105.

Indium 5-minute

(Page 327) TENDL-2019 and EAF2010 produce an overprediction for this element, particularly at cooling times greater than 5 minutes, when In116m becomes dominant. However, the overall decay-profile is a reasonably good match to the experimental profile (unlike the IRDFF-II result, which only represents the In116m and In116 contributions, and misses the In114 production). TENDL-2019 does much better than TENDL-2017 (see [6]) for this element, reflecting the adjustment in the In115(n,γ) channel to the different isomeric states, but there is evidence from this experiment for further adjustment. The In114 profile is the correct match for the measurements during the first 5-minutes of cooling, but there is still potentially some issue with the branching ratio to In116m (and In116n and In116), because its contribution and dominance at later cooling times is too high. An alternative explanation to the overprediction of In116m could be poor characterisation of the thermal profile in the FNS neutron spectrum, but this is not observed in experiments on other materials (in general). JEFF-3.3 and ENDF/B-VIII.0 fail to predict In116m at all, and also get the In114 contribution wrong, so those libraries have even greater issues for this case. The overprediction of In114 with those two libraries is due to incorrect summing of the In115(n,2n) contributions into one channel for In114 production, instead of including the correct (dominant) branching to In114m – a very longer-lived metastable. A rare case where IRDFF-II has multiple relevant reactions channels on the same element, but the profile and decay-heat level are not a good match to the experiment.

Tin 5-minute

(Page 332) The two experimental result sets differ, although the simulation with TENDL, JEFF, and EAF produce a much better agreement with the most recent, year-2000 one. TENDL-2019 and EAF2010 seem to match the decay profile the best. JEFF-3.3 has the wrong shape at cooling times of less than 10 minutes, apparently because of missing (n,p) channels to metastable In118m and In120m. An improvement of the agreement for the TENDL-2019 (compared to TENDL-2017) with the experiment is observed for cooling times between 1 and 10 minutes when In118m is important – the overprediction of that nuclide with TENDL-2017 has been corrected. ENDF/B-VIII.0 misses not only the short-term metastables, but also the longer-lived Sn123m (from (n,2n) on Sn124) whose contribution is predicted to be dominant with TENDL-2019 after around 10 minutes. This latter point actually disagrees with JEFF-3.3, where Sn111 is shown to be just as important; demonstrating that there is general uncertainty in certain aspects of this complex picture for a material with so many naturally occurring isotopes, although TENDL and EAF perform best, suggesting that the picture they predict is more likely to be correct.

Tin 7-hour

(Page 337) Only TENDL-2019 and EAF2010 properly capture (to within around 20%) the experimentally measured decay profile for this longer tin experiment. JEFF-3.3 and ENDF/B-VIII.0 both miss the production of the Sn117m metastable that is important out to 50 days of cooling. This case also shows the limit of the experimental measurement technique, with the large uncertainty after 13 months of cooling reflecting the fact that the heat output is approaching the pico-watt limit of sensitivity.

Antimony 5-minute

(Page 341) TENDL-2019 results are very similar to EAF2010, but both over-predict by around 20-30% at all cooling times, suggesting that there may need to be some re-evaluation of the (n,2n) channel on Sb121, which is responsible for the production of the Sb120 nuclide that is predicted to dominate at all cooling times measured. Still, these two libraries are performing better than either ENDF/B-VIII.0 or JEFF-3.3, which seem to get this reaction channel very wrong.

Tellurium 5-minute

(Page 345) An excellent simulation versus experiment comparison for TENDL-2019, JEFF-3.3 and EAF2010, even for the prediction of N16 from oxygen at very short cooling time. ENDF/B-VIII.0 seems to massively overpredict the production of the dominant Te129, which is almost certainly due to the incorrect summing of contributions from Te130(n,2n)Te129 and Te130(n,2n)Te129m into a single channel producing Te129. Te129m has a much longer half-life than its ground-state daughter (33.6 days versus 1.16 hours) and so does not contribute measurably to the decay-heat when properly accounted for.

Iodine 5-minute

(Page 349) A systematic overprediction with all of the general purpose libraries. At cooling times less than 1 minute N16 from oxygen dominates the decay heat, but this seems overpredicted by a factor of 2 in the simulations. Beyond 1-minute of cooling the (n,γ) reaction on I127 to produce the dominant I128 seems to have been overpredicted with all general libraries suggesting that the thermal part of that cross section may not be correct (or there is a problem in the characterisation of the neutron spectrum). IRDFF-II only contains the (n,2n) channel to produce the long-lived I126 from I127 and so shows a massive underprediction but is included here to illustrate the underlying decay-heat that will become dominant at longer cooling times.

Caesium 5-minute

(Page 353) A surprising, but not necessarily un-physical upward trend in the experimental heat measurements during the first 1.5 minutes of cooling is observed, which may be caused by a larger than expected subtraction of the tape contribution, or unidentified isomeric states (although there is nothing obvious missing). The simulations do not capture this part of the profile, showing, instead a simple two-nuclide profile from first N16 ad then Cs132 for all remaining decay times. The simulations and experiment all seem to agree on the longer term (10-60 minutes) dominance of the Cs132 nuclide from (n,2n) reactions, although the simulations seem to overpredict its contribution slightly.

Barium 5-minute

(Page 357) The 1996 sample may have contained some unidentified impurities, possibly Fluorine, which may explain the significant underestimation in the code predictions with EAF and TENDL that are not repeated in the comparison to the 2000 experiment. TENDL-2019 and EAF2010 nicely capture the profile of decay, which is a simple two nuclide picture. At short cooling times (less than around 20 minutes) and for most of the measurement points, Ba137m dominates, and an improved agreement with the experiment is observed for this experiment with TENDL-2019 in comparison to the TENDL-2017 results (by around 10%). ENDF/B-VIII.0 and JEFF-3.3 both fail to predict Ba137m production via (n,2n) reactions on Ba138 (and probably mis-attribute the Ba137m production to the stable Ba137 instead). At longer cooling times Cs138 predominates, and all library predictions converge to this contribution. However, TENDL and EAF seem to overpredict the total decay-heat for the final four measurements, but it is difficult to attribute this to a particular failing in the simulations as those two libraries predict many minor contributions from various metastable nuclides – many of which JEFF and ENDF/B miss and yet those to libraries are a better match to the experiment for those last four measurements.

Barium 7-hour

(Page 362) As was the case with the shorter, 5-minute experiments, ENDF/B-VIII.0 and JEFF-3.3 produce a mis-shaped decay profile, while TENDL-2019 and EAF2010 follow the experimental profile relatively well – even allowing for the large experimental uncertainty in the later cooling steps. The TENDL simulation shows that Ba135m and Ba133m are the important metastables governing the decay heat for the first few days of cooling (Bas135m from (n,2n) reactions dominates), which JEFF-3.3. and ENDF/B-VIII.0 omit. From around 2 weeks of cooling (the final two measurement times in this relatively short experiment), decay heat from Cs136 and Ba131 dominate. It is difficult to be sure which library produces the best prediction for these two nuclides because the experimental uncertainties are so large, but the decay profiles of all four seem to match the experiment in these final two data points.

Lanthanum 5-minute

(Page 367) The rather large and honest experimental uncertainties do not permit an in-depth investigation for this lanthanum experiment, although the overall trend seems to be well represented by the simulations with all of the general purpose libraries. IRDFF-II is included here, but it is only able to capture the contribution from the longer-lived (relative to these experimental timescales) La140 via neutron capture on La139.

Cerium 5-minute

(Page 371) A good agreement to the experiment exists up to 30 minutes cooling in simulations with TENDL-2019, EAF2010, and JEFF-3.3. At later cooling times the large experimental uncertainties might explain the significant disagreement observed, especially since the simulations suggest a set of fairly constant decay-heat contributions from longer-lived (relative to the experiment timescales) nuclides (i.e. there is no reason for the significant fall in decay heat between 35 and 45 minutes, so this could be an experimental artefact). ENDF/B-VIII.0 produces a misshapen decay profile because it fails to predict the Ce139m nuclide (via (n,2n) reactions) that dominates the profile in the first 10-15 minutes of cooling.

Praseodymium 5-minute

(Page 375) For Praseodymium, a systematic 30-50% (relative to the experiment) over-prediction exists in simulations with all libraries, indicating that the (n,2n) channel that produces the dominant Pr140 radionuclide may need to be corrected (the decay profile seems well-shaped so the decay data is reasonable). Interestingly, IRDFF-II, which includes the necessary (n,2n) reaction on Pr141 but omits the production channels for Pr142, seems to better capture the profile in the final cooling step. Even though the experimental uncertainties are too high at this time (and there could be issues with the spectrum characterisation at low energies) to make a definitive conclusion, it could be that the capture channels on Pr141 have over-estimated cross sections.

Neodymium 5-minute

(Page 379) There is a rather uniform and significant 50% over-prediction with TENDL-2019 (and with the other libraries considered) from around 5 minutes of cooling onwards. This appears to be a clear case where the cross sections – particularly the Nd150(n,2n) channel for the production of the Nd149 nuclides that dominates all measurements times beyond 10 minutes – may need some adjustment. At the same time, the production of Nd141m, which dominates at sub 5-minute cooling times, is also slightly overpredicted despite the simulations following the experimental decay profile well. Since this latter nuclide is produced via a branched (n,2n) channel on Nd142 that also creates the Nd141 radionuclide, which provides around 20% of the decay heat during Nd149 dominance, that channel may also need correcting.

Samarium 5-minute

(Page 383) A good agreement exists between all the general purpose libraries and the experiment, with TENDL-2019 marginally better than the others. All libraries show the same profile of contributing nuclides, although JEFF-3.3 and ENDF/B-VIII.0 don't predict as many contributions from metastable nuclides as the other two, particularly Sm143m, which provides relatively significant contributions to the decay-heat during the first 5 minutes, and this could explain why ENDF/B and JEFF underpredict the experiment during this time.

Europium 5-minute

(Page 387) As was observed with caesium, there is an upward trend in the decay-heat measurements at short cooling times (less than 5 minutes), which is not reproduced in the simulations with any library – either the tape contribution is overestimated or there are some missing isomeric states in the simulations. Certainly ENDF/B-VIII.0 and JEFF-3.3 have this problem as they fail to predict any of the three isomeric states that TENDL-2019 and EAF2010 find to be important (see the nuclide contribution charts), and, instead, only find the low level of decay heat attributed to the Pm150 nuclide. EAF2010 seems to be somewhat better than TENDL-2019 beyond 5 minutes of cooling and certainly those two libraries show a different distribution of the Eu152n, Eu152n, and Eu150m nuclides as a function of time – EAF2010 finds Eu152m much more predominant than TENDL-2019, which instead shows both isomeric states of Eu152 to be equally important. This demonstrates a different branching ratio within the (n,2n) cross section on Eu153, but there is too much disagreement compared to the experiment in both cases to draw any firm conclusions. Further investigation is warranted. Review of the EXFOR cross-section data shown in Figure A2 and recent findings by the authors in [19] add some further evidence for the need to re-evaluate and adjust the branching ratio (to reduce Eu152n and Eu152m production) for the ^{153}Eu(n,2n) reaction channel for future TENDL library releases.

Gadolinium 5-minute

(Page 391) Another case with a short timescale (less than 5-minute) increase in the decay heat in the experiments. Beyond this the predictions with three of the libraries (TENDL, EAF, and ENDF/B) appear to follow the measurement profile but with a slight overprediction of one of the contributing nuclides – almost certainly the long-lived Gd159 (from (n,2n) reactions on Gd160) whose flat contribution (on this timescale) becomes more and more dominant as cooling times increase (almost 90% at 1 hour). JEFF-3.3 completely omits the reaction for this nuclide and produces a clearly very discrepant decay profile.

Terbium 5-minute

(Page 395) None of the included libraries perform particularly well (IRDFF-II is omitted because it contains no terbium reactions), although the overall profile of each, nearly identical, curve seems to match the experimental profile (but not the heat level). The contribution from the short-lived Tb158m, which only TENDL and EAF predict, is completely swamped by N16 from oxygen (and so it is difficult to assess the prediction quality), and the plateau beyond around three minutes of cooling, which comes from Gd159 and Tb160 decay heat, seems to be a severe underprediction of the experiment. However, the associated measurements should be viewed with caution due to the large, uneven uncertainties.

Dysprosium 5-minute

(Page 399) All libraries massively overpredict the experimental decay heat at cooling times beyond around 1 minute (at shorter times the contribution from N16 seems to be underpredicted). The culprit is the constant, swamping contribution from Dy165 (its half-life is beyond the timescale of the experiment), whose decay profile does not match the experimental profile, which falls away throughout the measurement. In fact, the measurement profile would be better matched by the other decaying contributions from Tb162 and Tb163 (from (n,p) reactions), suggesting that the Dy165 should not be there at all and giving cause to question the neutron capture cross sections that produce it in the simulations (EAF, TENDL, and JEFF also predict significant Dy165m production via the same channel, and this too seems an overprediction).

Holmium 5-minute

(Page 403) TENDL-2019 and EAF2010 give a better match to the experimental profile than either JEFF-3.3 or ENDF/B-VIII.0, although ENDF/B, by chance, manages to have a slightly lower average deviation than TENDL-2019 with a clearly incorrect decay profile. EAF2010 is very good overall (ignoring the usual underprediction of N16 contributions at short timescales). For this lanthanide, the experiment gives a nice example of the importance of the correct branching ratios in an (n,2n) reaction that produces a ground-state and metastable with similar (but not identical) half-lives. The subtle ratio between the slightly longer-lived Ho164m and the ground-state it decays to is crucial in correctly predicting the profile. The fact that TENDL-2019 overpredicts slightly more than EAF2010 suggests that the (n,2n) channel on Ho165 and its branching ratio should be checked. Importantly, the time-evolution is a good match and it is worth remembering that a correction in the decay data has improved matters compared to earlier libraries [20].

Erbium 5-minute

(Page 407) At first glance the obvious disagreement in the shape profile of the measured decay-heat and the simulations is suggestive of a problem with the underlying half-life data for some nuclide, which would be a rare and interesting example if confirmed. However, closer inspection of the nuclide contributions from the simulations suggest, instead, that there could be an over-estimation of Er165 production via (n,2n) reactions, which dominates the simulated decay-heat beyond 10 minutes of cooling – precisely the region where the simulations are clearly discrepant from the experimental measurements. If this channel was adjusted downwards, then the simulations would be a much better match to the experiment.

Thulium 5-minute

(Page 412) A rare example in the lanthanides where IRDFF-II is able to simulate the experiment reasonably. As usual, no library is able to capture the measured response from N16 decay-heat at very short timescales (could there be some missing contributions from isomeric states?), but they all agree on the dominant, constant contribution from Tm168 at all cooling times beyond around 1.5 minutes (nearly 100% at all times where N16 does not contribute). The overall agreement, as measured by the mean % difference, does not look good, but this can be attributed to experimental problems, which see very high uncertainties below 10 minutes of cooling, some random fluctuations, and then a significant drop in decay-heat (again with high uncertainties) beyond 40 minutes of cooling – the simulations particularly disagree with this and there is no obvious reason to expect it.

Ytterbium 5-minute

(Page 416) The best agreement here is seen with TENDL-2019 simulations, followed by EAF2010 – both give nice agreement to the experimental profile, even allowing for the large experimental uncertainties beyond 20 minutes of cooling (the low χ^2 deviations demonstrate this). ENDF/B-VIII.0 and JEFF-3.3 overpredict, but for different reasons; ENDF/B-VIII.0 over-produces the short-lived Tm174 nuclide (via (n,p) reactions) and so is wrong in the 1-10 minute cooling phase. Meanwhile, results of Tm174 production with JEFF-3.3 look reasonable, whereas over-production of the Yb167 nuclide (via (n,2n) on Yb168) is apparent, causing an overprediction beyond 10 minutes of cooling.

Lutetium 5-minute

(Page 421) There is some structure in the experimental results that are not captured by the simulations, particularly below 5 minutes of cooling – the high quoted uncertainties suggest that there may have been problems in the experiment (such as an incorrect level of tape subtraction). ENDF/B-VIII.0 does not include the reaction channels to produce the Lu176m metastable that the other libraries predict to provide almost the entirety of the decay heat from Lutetium itself. This is clearly discrepant as the profile with the other libraries is a reasonable match to the experiment, although they mostly overpredict. There could be a justifiable need to correct one of the identified channels for Lu176m production. Notice that the absence of Lu176m production with ENDF/B, causes the identification of many minor nuclides (that are thus included in the pathway analysis), which otherwise are not important for the simulations with other libraries.

Hafnium 5-minute

(Page 425) The predicted contribution from Hf179m in the first ~2 minutes of cooling is a good fit to the experiment in simulations with EAF2010 and JEFF-3.3 – ENDF/B-VIII.0 fails to capture the production of this nuclide from a combination of Hf180(n,2n) and Hf178(n,γ), while TENDL-2019 seems to underpredict compared to the better result seen with TENDL-2017. At longer cooling times none of the simulated profiles is a good match for the shape of the decay evolution. One possibility, in examining the nuclide contribution charts of TENDL and EAF, is that a greater production of Lu180 could provide a closer match to the experiment between 2 and around 15 minutes of cooling, while a reduction in Hf180m would solve the overprediction at later cooling times and leave the Lu178 to dominate, whose profile seems to better fit the decay profile in the experiment for the last few cooling steps. A careful reassessment of the Hf180(n,p), Hf180(n,n′) reaction channels for the production of Lu180 and Hf180m, respectively, is advised.

Tantalum 5-minute

(Page 430) There are some noticeable and unexplained differences between the decay heat levels of the two 5-minute experiments for tantalum. The fact that the code predictions with TENDL-2019 (and EAF2010) agree very well with the more recent 2000 experiment suggests that the experimental techniques may have been improved between 1996 and 2000 leading to the latter being more representative of reality. TENDL-2019 and EAF2010 are both within the (rather large) experimental uncertainty for the 2000 experiment, while ENDF/B-VIII.0 and JEFF-3.3 both overpredict the result by more than 40% on average. This is again a situation where these two libraries sum the contributions of (n,2n) channels. In this case ENDF/B-VIII.0 and JEFF-3.3 assume that all of the (n,2n) reactions on Ta182 produce the unstable, short-lived ground-state Ta180, while in fact around half should have produced the stable Ta180m “metastable”, which does not contribute to decay heat. This is a glaring error because the stability of Ta180m is such an unusual and well-known anomaly that it should have been easy to get this correct.

Tantalum 7-hour

(Page 435) The decay profile seems properly shaped by first the heat from Ta180 at cooling times less than 3 days, and then contributions from Hf181 and predominantly Ta182 at later times. However, the Ta180 production seems to overestimate the experiment, while a 50% or more underprediction is evident at later cooling times. Potentially, both the (n,2n) and neutron capture channels on Ta181 should be reassessed. IRDFF-II only includes the ground-state branch of the neutron capture reaction (whose evaluation is closer to TENDL in the MeV region) to Ta182, and so underpredicts to a greater extent than the other libraries.

Tungsten 5-minute

(Page 439) A better than expected level of agreement is observed for this particularly troublesome, in nuclear data terms, element even at short cooling time for ENDF/B-VIII.0, TENDL-2019, and EAF2010. The decay profile predicted with those libraries nicely follows the experimental shape, although the systematic over-prediction on both experimental batches (more in the 2000 case) suggests that there needs to be some re-evaluation and in-depth analysis of the major production routes involved, in particular the (n,2n) channel to produce W185m, which dominates (generally more than 90%) all cooling times less than 10 minutes with those libraries. JEFF-3.3 clearly misrepresents the decay-shape by missing the production of W185m. Analysis of the available differential data for the entire W186(n,2n) channel in EXFOR reveals that the currently evaluated cross section for W185m in TENDL-2019 (and ENDF/B-VIII.0, EAF2010) is higher than the majority of data around 14 MeV, with EXFOR data falling largely outside of the TENDL-2019 uncertainty band (the data at 14 MeV could be biased by the one anomalously high data point at 15 MeV). If the experimental measurements are to be believed then they would indicate that the W186(n,2n)W185m production channel needs to be re-evaluated slightly ($\sim$0.85 factor), particularly at 14 MeV.
All general purpose libraries are in reasonable agreement with one another for the longer-term profile, predicting first Ta186 and then W187 dominance, but again, over-prediction is evident. IRDFF-II is only able to capture the contribution of the longer lived W187 radionuclide, whose production via neutron capture on W186 has important dosimetry applications.

Tungsten 7-hour

(Page 444) There seems to be a systematic 20-30% overestimation with all libraries in the production of W185, which is significant at all cooling times, but particularly dominant beyond 1 day of cooling. Production of this nuclide is via the same (n,2n) channel that caused overprediction of W185m in the 5-minute experiment, adding further evidence of the need to re-evaluate that channel. However, simulations with all libraries are in good agreement with the experiment during the first few days of cooling, where Ta184 (via (n,p) reactions on W184) is dominant. Note that it could, in fact, be W181, rather than W185, that is overpredicted here, since that nuclide contributes around 20% to the decay heat for much of the profile (and increases near the end), but again it would be an (n,2n) channel (this time on W182) that needs adjustment (TENDL-2019 appears to overestimate the EXFOR experimental cross section data for this channel).

Rhenium 5-minute

(Page 448) EAF2010 shows very good agreement to the 2000 batch of the 5 minute experiments on rhenium, nearly within the experimental uncertainties. The experimental result from the 1996 batch is significantly different, which is unexplained, but EAF2010 is still the best performer. The other three libraries considered are all in reasonable agreement with one-another, but overpredict the production of Re186, in particular, relative to EAF2010 and thus show a greater overprediction of both experimental batches compared to that legacy library. A re-evaluation of the predominant (n,2n) channel on Re187 may be required. There may also be a slight overprediction of the capture channel on the same target with all libraries, leading to an over-production of Re188, which contributes at least 20% of the decay-heat at all times and in all simulations (even EAF2010 is not in exact agreement with the 2000 experimental batch and so Re188 is an obvious culprit).

Rhenium 7-hour

(Page 453) A much better agreement, compared to the 5-minutes analysis, with TENDL-2019, JEFF-3.3 (which can be barely distinguished from the TENDL results), and EAF2010 for measured cooling times starting from 0.69 days. Note in this case the unusual occurrence of metastable isomer having a half-life greater than the ground (Re184m vs. Re184). The decay heat from this Re184m metastable becomes a significant factor in the final two experimental cooling times and ENDF/B-VIII.0's failure to produce it in simulations explains why that library is so discrepant beyond 100 days of cooling. Re186 dominates at cooling times less than 1 week, and all four libraries do a reasonable job of capturing the experiment in this region (EAF2010 is best here, while TENDL-2019 and JEFF-3.3 are better in the Re184 region). Overall, the relevant (n,2n) channels probably need further work to improve the agreement.

Osmium 5-minute

(Page 457) While JEFF-3.3 provides a significantly better comparison to the experimental decay heat magnitude in comparison to EAF2010, in reality it completely mis-represents the shape profile of the time evolution. EAF2010 is much better in this respect and it predicts that Os190m is the main contributor to the decay heat during all but the final experimental cooling time measured. Clearly, the production of this radionuclide via (n,n′) reactions on Os190 is massively overpredicted by the EAF2010 library, but it nonetheless gives the proper shape to the evolution. This channel has been embedded in TENDL-2019 (and that library closely follows EAF), however it still needs further analysis and scale-correction to be able to properly match the experiment. ENDF/B-VIII.0 has even greater trouble predicting this experiment, as it does not even generate the contributions from the Os191m and Os189m metastables that JEFF and TENDL find as the underlying base of decay heat. On the other hand, the high discrepancy between the experiment and simulations in the final few cooling times, where those metastables become important, show that the production channels of these are also in need of re-analysis.

Iridium 5-minute

(Page 462) EAF2010 and now TENDL-2019 are the only libraries that matches the experiment in this case, demonstrating that the observed decay-heat comes from Ir192m at short cooling times (less than 5 minutes) and then from Os190m at longer times; growth of the latter as Ir190n decays explains why the decay-heat increases in the experiments and simulations between 5 and 15 minutes of cooling. All other nuclides are shown to only provide minor contributions to the decay heat. TENDL-2019 has been dramatically improved in comparison to TENDL-2017, which didn't capture the Os190m production correctly, but EAF2010 is still much better. Adjustment of the (n,2n) channel on Ir191 is probably warranted in TENDL to reduce Ir90n production (perhaps a branching issue?).
Meanwhile JEFF-3.3 and ENDF/B-VIII.0 both predict the importance of Os190m, although they overpredict its production via (n,2n) reactions on Ir191 (primarily via the Ir190n metastable). More dramatically, they predict the dominance of a completely different nuclide, Re190, at short decay times of less than 5 minutes.

Platinum 5-minute

(Page 466) Since the only nuclide predicted to contribute significantly to the decay-heat by all libraries is Pt197m at all cooling times, the discrepancy between the simulations and experiment must be attributed to incorrect production rates of that nuclide. With TENDL-2019 (and the other libraries) there appears to be around a 20% overprediction in the decay-heat from Pt197m, although the experimental uncertainty and TENDL-2019 error bands do at least overlap. A case for correction of the (n,2n) reaction channel on Pt198 (maybe the branching ratio of that channel is wrong).

Gold 5-minute

(Page 470) No library prediction is particularly good, but at least TENDL-2019 and EAF2010 produce the correct two-step decay profile, with dominance in the first 1 minute of cooling by a short-lived nuclide, followed by nearly equal contributions from Au196 and Au196n at all remaining cooling times. Interestingly, while the two libraries agree on the contributing nuclides for the second stage, they predict different nuclides for the first 1 minute: TENDL-2019 predicts that Au196m should be dominant, while EAF2010 predicts in is Au197m. These nuclides have nearly identical half-lives and so the profile of each seems to capture the measurement profile well – it is difficult to judge which is correct, although TENDL-2019 also shows a minor Au197m contribution; further analysis is warranted.
Overall, both TENDL-2019 and EAF2010 overpredict by about 30% the experimental values. Meanwhile JEFF-3.3, ENDF/B-VIII.0, and IRDFF-II only capture Au196 production (i.e. the usual absence of metastable production channels) and thus underpredict (coincidently by about 30%) at all cooling times. all underpredict by a similar percentage.
Incorrect branching ratios for (n,2n) to Au196, Au196m, and Au196n in TENDL-2019 could still be the source of overprediction with that library.

Mercury 5-minute

(Page 474) A textbook case exemplifying the problem (for ENDF/B-VIII.0) when missing the production of isomeric states. TENDL-2019, JEFF-3.3, and EAF2010 all agree regarding the complete dominance of the Hg199m nuclide (at all but the first cooling step where the usual N16 signal is seen), produced by a combination of (n,2n) reactions on Hg200 and (n,n′) reactions on Hg199, but ENDF/B-VIII.0 does not include either of these channels and so massively underpredicts relative to the experiment. The other libraries are not perfect and there could be justification for modifying some of the production cross sections for this uniquely predominant metastable. IRDFF-II includes only the (n,n′) reaction channel on Hg199 for this simulation which explains underprediction of the experiment with that library.

Thallium 5-minute

(Page 478) Reasonable shape agreement for TENDL-2019 and JEFF-3.3, but only EAF2010 can be considered to produce a good overall agreement to the experiment. For TENDL-2019, in particular, the large discrepancies for cooling times between 1 and 30 minutes suggest that the production routes for the Hg205 and Tl206 nuclides that contribute and dominate almost equally in this time range may need re-evaluation. ENDF/B-VIII.0 clearly mis-represents the profile at cooling times below 30 minutes because, surprisingly, it does not contain the (n,p) channel to produce Hg205 from Tl205.

Lead 5-minute

(Page 482) The experimental data sets are somewhat different from one-another, resulting in a very different comparison to the simulations. The 1996 experiment seems to be better captured by the simulations (particularly from TENDL-2019) at cooling times beyond 10 minutes. The more recent, 2000 experiment is overpredicted by the simulations (with all libraries) at these cooling times. This is an interesting deviation from the previous comparison [7] with earlier version of the libraries, where, instead, the 2000 experiment was better captured by the simulations. For TENDL, this appears to originate from a 30% increase in the total cross section associated with the (n,n′) reaction on Pb204 between TENDL-2014 and TENDL-2017, that remained in TENDL-2019, which leads to an increase in Pb204m production and its contribution to the decay heat (at long cooling times, when this nuclide dominates, the total decay heat has increased by this same ∼30% factor). However, in both batches the short term heat predictions, dominated by decay heat of Tl208 from (n,p) reactions on Pb208 in the simulations, seem to be low compared with the measured ones (as was the case in [7]). After 30 minutes of cooling EAF2010 and IRDFF-II yield the closest match to the experiment – Pb204(n,′)Pb204m is an important dosimetry reaction and is included in the official IRDFF-II release.

Lead 7-hour

(Page 487) At shorter cooling times (below around 15 days) there is good agreement between the simulations and experiment (this is particularly clear in the nuclide contribution plots). However, at longer times (beyond around 20 days) – associated with the final two experimental data points – the simulations diverge (consistently with each other) from the experiment. This could be due to an unreported impurity in the sample, although an underestimation of Hg203 production from (n,α) reactions on Pb206 is not completely eliminated as a potential issue. In general, the experimental data is scarce and discrepant, and the experimental uncertainties are very large for these last points so more definitive analysis is not possible.

Bismuth 5-minute

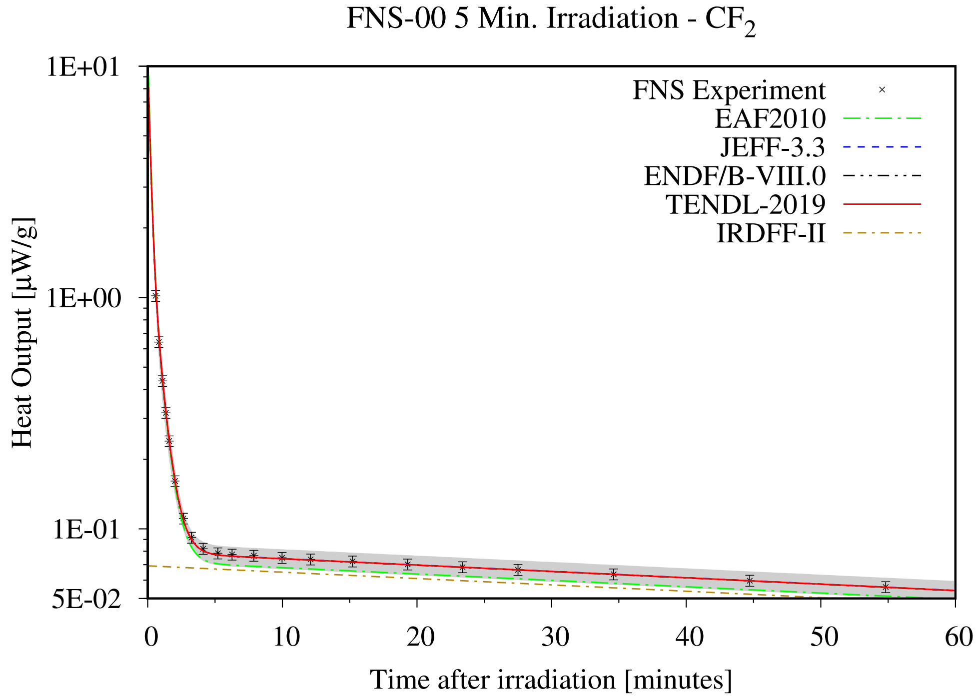
(Page 491) Some large differences and uncertainties can be seen between the two experimental data-sets. This is particularly true at cooling times beyond around 20 minutes. At shorter decay times (where the experimental uncertainties are lower), simulations with JEFF-3.3, EAF2010, and ENDF/B-VIII.0 are in reasonably good agreement with the experimental profile and measurements, while TENDL-2019 sits apart. While the former three predict near-complete dominance of Tl206 during the first 20-30-minutes of cooling, TENDL-2019 instead predicts a combined contribution from Tl206 and its first-level metastable – all via (n,α) reactions on Bi209. The overprediction by TENDL-2019 suggests that the branching ratio for this channel with that library is

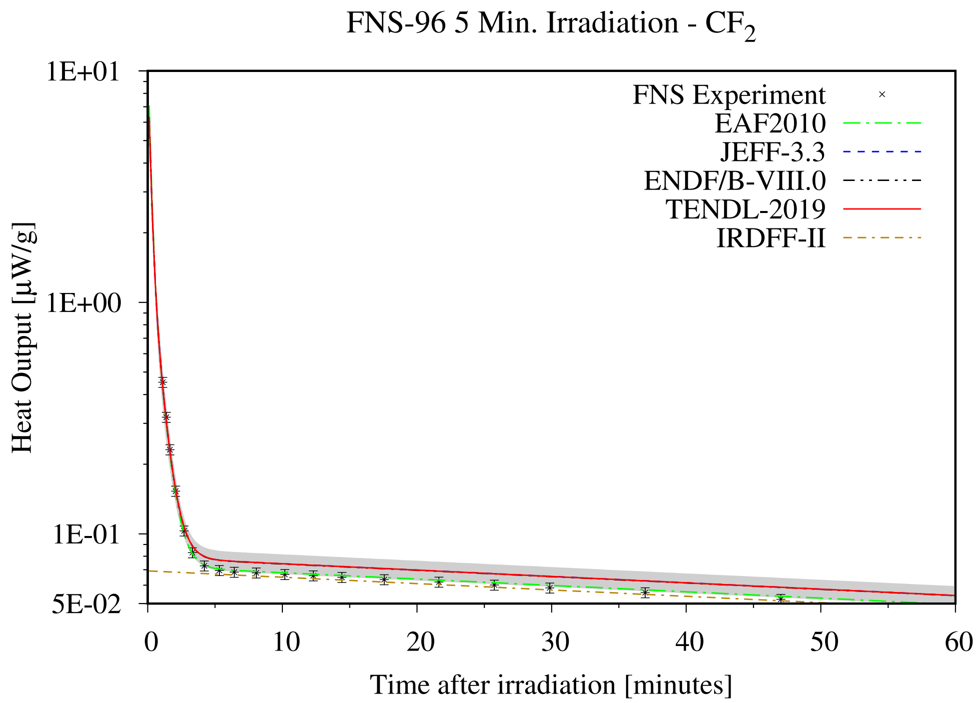
wrong (EAF2010 also predicts Tl206m, but at a much lower level).
Nothing can be gleaned from the later cooling steps, particular with respect to the production of Pb209 – there is too much uncertainty.

Bismuth 7-hour

(Page 496) A poor C/E agreement on this important element, but the experimental uncertainties are very large. As with the 5 minute experiments on bismuth, the simulations overpredict (to a varying degree depending on the library), although it is difficult to draw any conclusions about library deficiencies with such large experimental uncertainties.

Fluorine

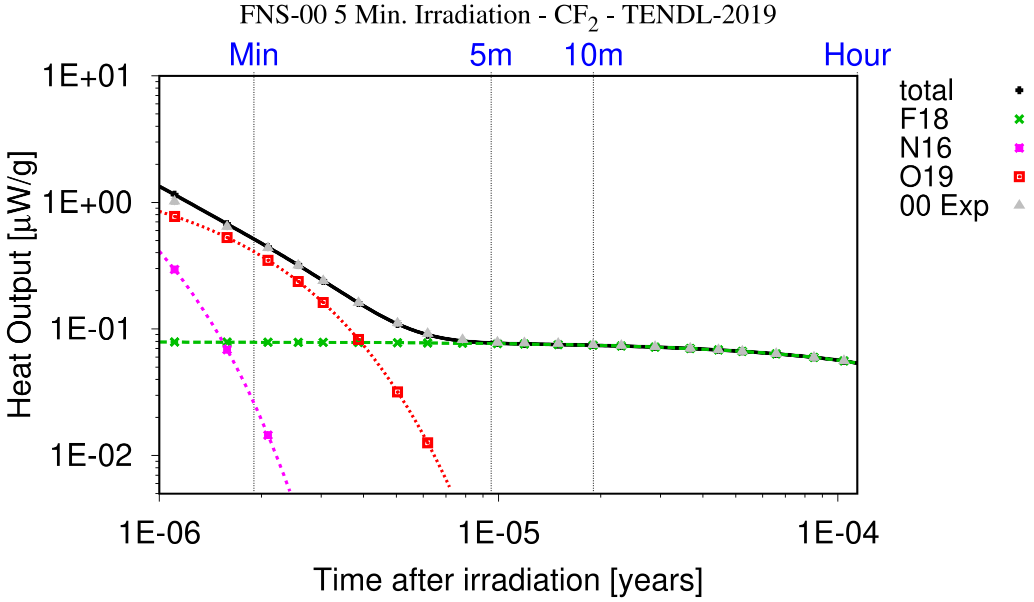

FNS-00 5 Min. Irradiation - CF2
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+01
1E+00
1E-01
5E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - CF2
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+01
1E+00
1E-01
5E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]

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	1.02E+00 +/-5%	1.15E+00 +/-18%	0.88	0.88	0.85	0.88	14.75
0.83	6.42E−01 +/-5%	6.76E−01 +/-20%	0.95	0.95	0.94	0.95	9.33
1.10	4.36E−01 +/-5%	4.43E−01 +/-20%	0.98	0.98	0.99	0.98	6.34
1.35	3.17E−01 +/-5%	3.19E−01 +/-19%	0.99	0.99	1.01	0.99	4.63
1.60	2.40E−01 +/-5%	2.40E−01 +/-17%	1.00	1.00	1.02	1.00	3.50
2.03	1.61E−01 +/-5%	1.61E−01 +/-14%	1.00	1.00	1.04	1.00	2.36
2.65	1.11E−01 +/-5%	1.10E−01 +/-10%	1.01	1.01	1.08	1.01	1.63
3.25	9.17E−02 +/-5%	9.01E−02 +/-9%	1.02	1.02	1.10	1.02	1.35
4.12	8.21E−02 +/-5%	8.04E−02 +/-9%	1.02	1.02	1.11	1.02	1.22
5.22	7.84E−02 +/-5%	7.72E−02 +/-10%	1.02	1.02	1.11	1.02	1.17
6.27	7.74E−02 +/-5%	7.62E−02 +/-10%	1.02	1.02	1.11	1.02	1.16
7.88	7.66E−02 +/-5%	7.53E−02 +/-10%	1.02	1.02	1.11	1.02	1.16
9.98	7.50E−02 +/-5%	7.43E−02 +/-10%	1.01	1.01	1.10	1.01	1.15
12.10	7.38E−02 +/-5%	7.33E−02 +/-10%	1.01	1.01	1.10	1.01	1.15
15.22	7.23E−02 +/-5%	7.19E−02 +/-10%	1.01	1.01	1.10	1.01	1.15
19.32	7.02E−02 +/-5%	7.00E−02 +/-10%	1.00	1.00	1.10	1.00	1.15
23.38	6.83E−02 +/-5%	6.83E−02 +/-10%	1.00	1.00	1.09	1.00	1.14
27.50	6.65E−02 +/-5%	6.65E−02 +/-10%	1.00	1.00	1.09	1.00	1.14
34.62	6.36E−02 +/-5%	6.36E−02 +/-10%	1.00	1.00	1.09	1.00	1.14
44.72	5.97E−02 +/-5%	5.97E−02 +/-10%	1.00	1.00	1.09	1.00	1.14
54.82	5.60E−02 +/-5%	5.60E−02 +/-10%	1.00	1.00	1.09	1.00	1.14
mean % diff. from E			2	2	8	2	34
mean χ^2			0.36	0.37	2.60	0.36	71.38

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
O19	26.91s	0.95	5%	25%
F18	1.83h	1.02	5%	10%

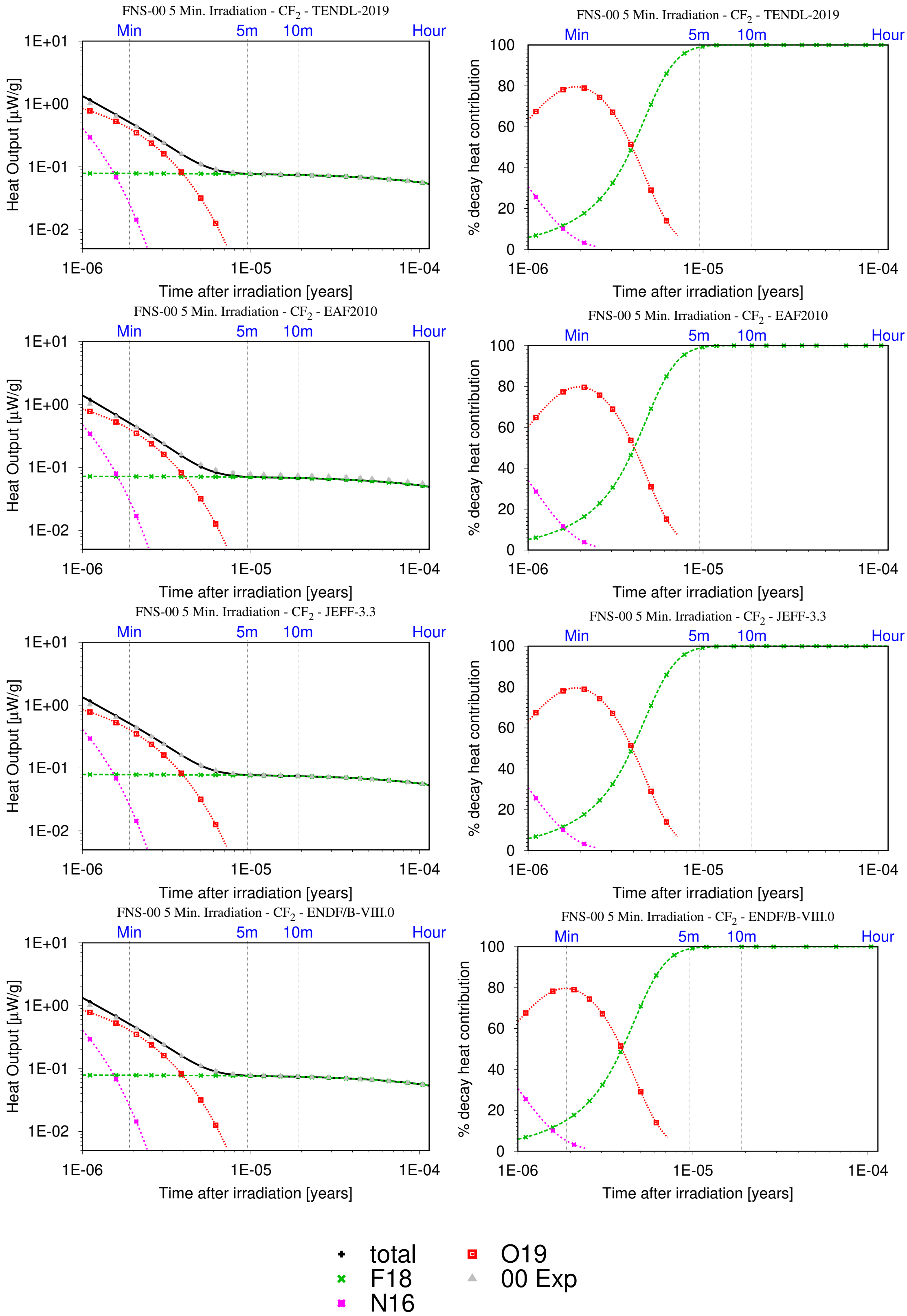


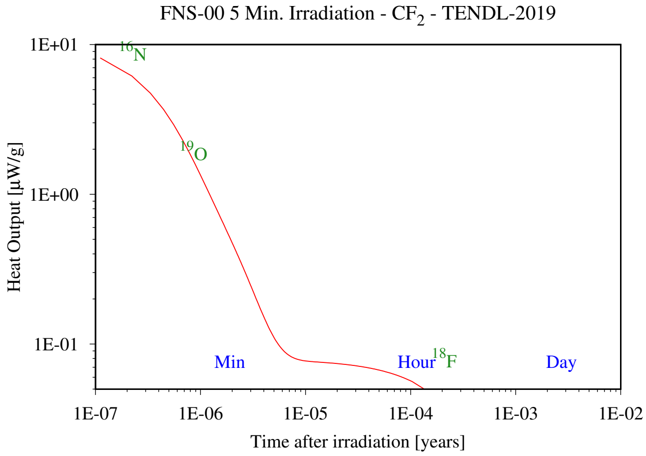
Fluorine, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	F19(n,α)N16	100.0
O19	26.91s	F19(n,p)O19	100.0
F18	1.83h	F19(n,2n)F18	100.0

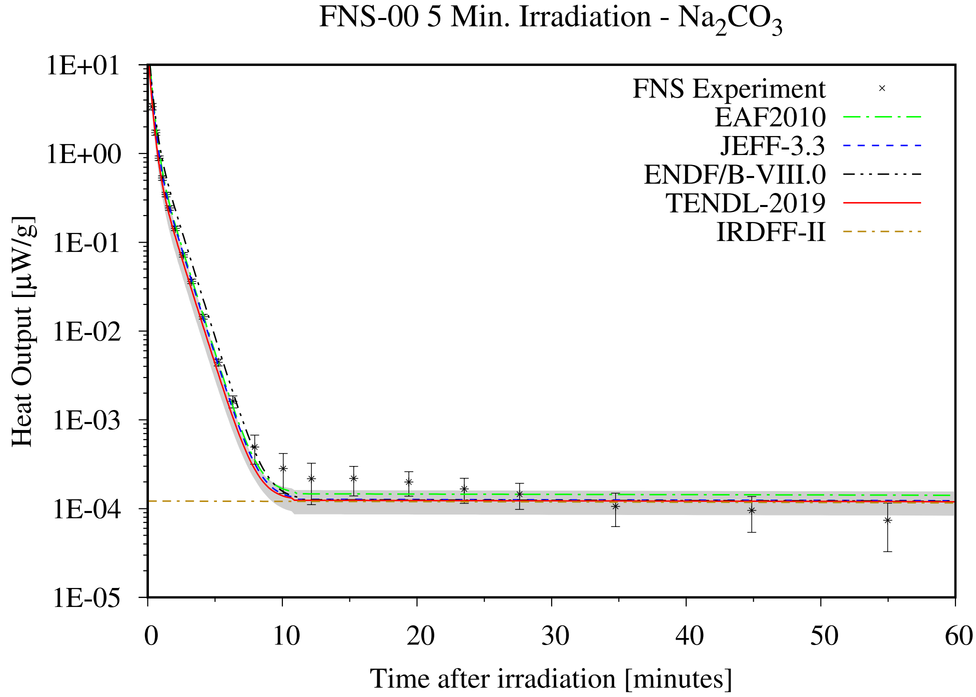
Comments on Fluorine 5-minute experiments:

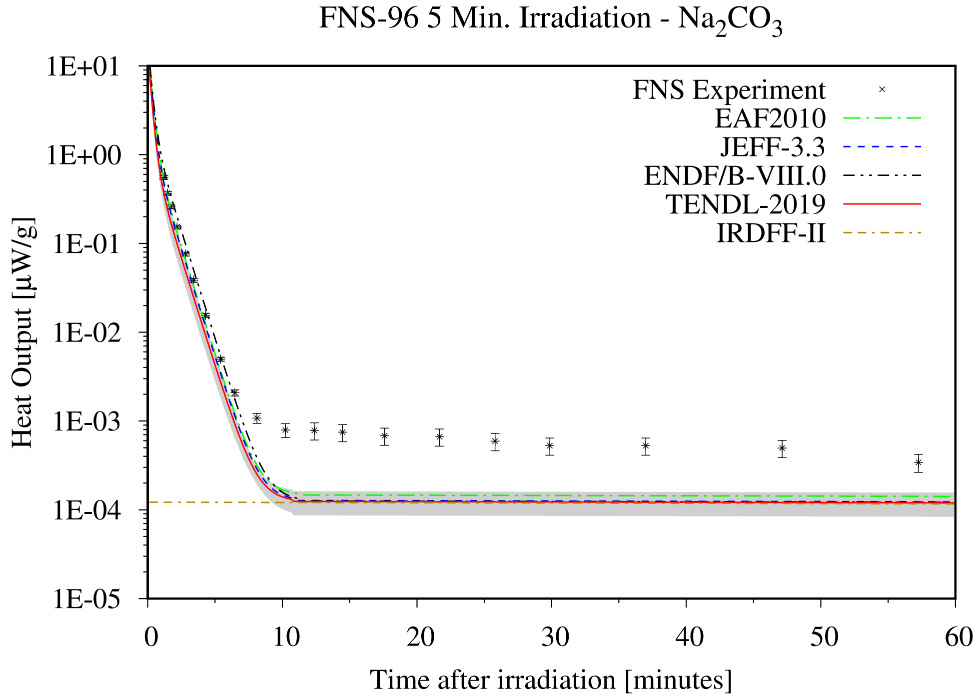
The agreement between experiment and simulation is excellent for both fluorine samples at all cooling times. TENDL-2019, JEFF-3.3, and ENDF/B-VIII.0 are in agreement at all cooling times, while EAF2010 and IRDFF-II show disagreement at decay-times beyond ∼5 minutes – those two libraries appear to slightly underpredict F18 production via (n,2n) reactions on F19 in F18 production via the (n,2n) reaction on F19. For the 2000 experiment, the F18 production of the TENDL-2019 et al. gives a good match, while for the 1996 experiment, it is EAF and IRDFF whose F18 prediction is closed to the measurements. The variation between the two experimental data sets clearly demonstrates that experiments do not always lead to the same measurements, even when carried out in the same assembly set-up, and here the discrepancy makes it difficult to identify the best prediction. However, there is a 10% uncertainty in F18 production with TENDL-2019 (see the E/C table), which easily encompass this experimental fluctuation (as shown by the grey error bands). Note, O19 production via (n,p) on F19 is not important for dosimetry, so IRDFF-II only captures the decay-heat profile when F18 dominates.


FNS-00 5 Min. Irradiation - CF2 - TENDL-2019
FNS-00 5 Min. Irradiation - CF2 - EAF2010
FNS-00 5 Min. Irradiation - CF2 - JEFF-3.3
FNS-00 5 Min. Irradiation - CF2 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
F18
N16
O19
00 Exp


FNS-00 5 Min. Irradiation - CF2 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
16N
19O
18F
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

Sodium

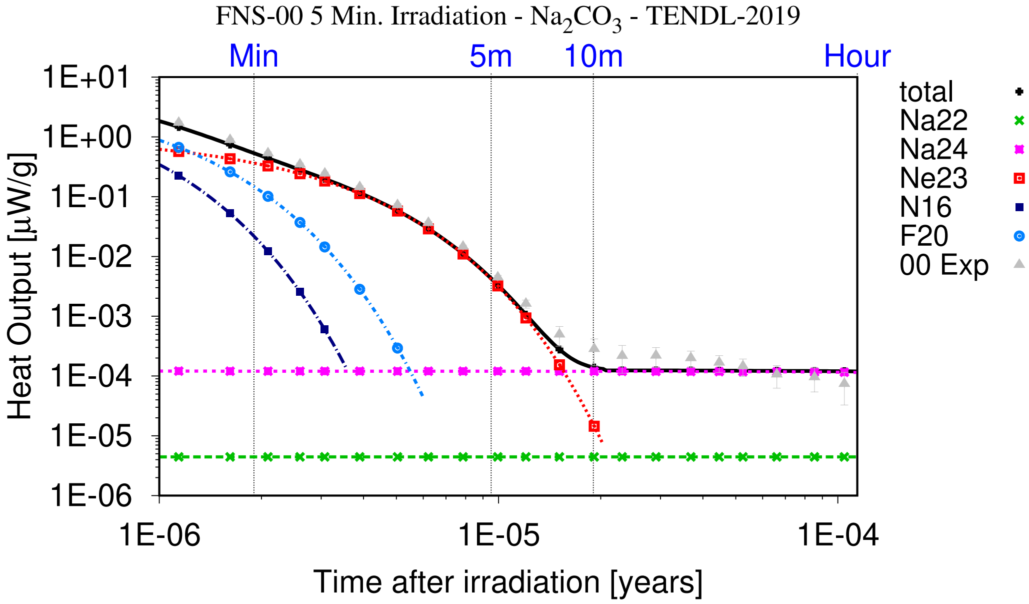

FNS-00 5 Min. Irradiation - Na2CO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Na2CO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]

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
0.33	3.38E+00 +/-8%	3.66E+00 +/-24%	0.92	0.62	0.63	0.72	> 1000
0.60	1.72E+00 +/-7%	1.46E+00 +/-25%	1.17	0.71	0.79	0.89	> 1000
0.85	8.86E−01 +/-6%	7.44E−01 +/-26%	1.19	0.66	0.81	0.90	> 1000
1.10	5.30E−01 +/-6%	4.40E−01 +/-28%	1.21	0.63	0.84	0.92	> 1000
1.37	3.45E−01 +/-6%	2.82E−01 +/-31%	1.22	0.62	0.87	0.95	> 1000
1.62	2.44E−01 +/-6%	1.98E−01 +/-33%	1.23	0.61	0.89	0.96	> 1000
2.05	1.44E−01 +/-6%	1.16E−01 +/-34%	1.24	0.61	0.91	0.98	> 1000
2.65	7.22E−02 +/-6%	5.81E−02 +/-35%	1.24	0.61	0.92	0.98	594.71
3.27	3.63E−02 +/-6%	2.91E−02 +/-35%	1.25	0.61	0.93	0.99	299.26
4.13	1.45E−02 +/-6%	1.11E−02 +/-35%	1.31	0.65	0.97	1.04	119.73
5.23	4.44E−03 +/-9%	3.33E−03 +/-34%	1.33	0.66	0.99	1.06	36.62
6.33	1.61E−03 +/-15%	1.06E−03 +/-31%	1.52	0.79	1.14	1.23	13.33
7.95	4.94E−04 +/-36%	2.77E−04 +/-24%	1.78	1.12	1.39	1.53	4.09
10.07	2.83E−04 +/-48%	1.39E−04 +/-27%	2.04	1.83	1.71	1.92	2.34
12.17	2.18E−04 +/-49%	1.24E−04 +/-30%	1.75	1.73	1.48	1.71	1.80
15.30	2.19E−04 +/-37%	1.24E−04 +/-30%	1.77	1.75	1.50	1.72	1.82
19.40	1.99E−04 +/-31%	1.23E−04 +/-30%	1.62	1.59	1.37	1.57	1.66
23.52	1.67E−04 +/-31%	1.23E−04 +/-30%	1.36	1.34	1.15	1.32	1.40
27.62	1.46E−04 +/-33%	1.23E−04 +/-30%	1.19	1.17	1.00	1.16	1.22
34.75	1.06E−04 +/-41%	1.22E−04 +/-30%	0.87	0.86	0.73	0.85	0.89
44.87	9.55E−05 +/-43%	1.21E−04 +/-30%	0.79	0.78	0.67	0.77	0.81
54.97	7.39E−05 +/-56%	1.20E−04 +/-30%	0.61	0.61	0.52	0.60	0.63
mean % diff. from E			27	45	25	21	72
mean χ^2			5.24	44.67	5.39	1.97	132.14

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Ne23	37.21s	1.22	6%	35%
Na24	14.96h	2.04	48%	31%

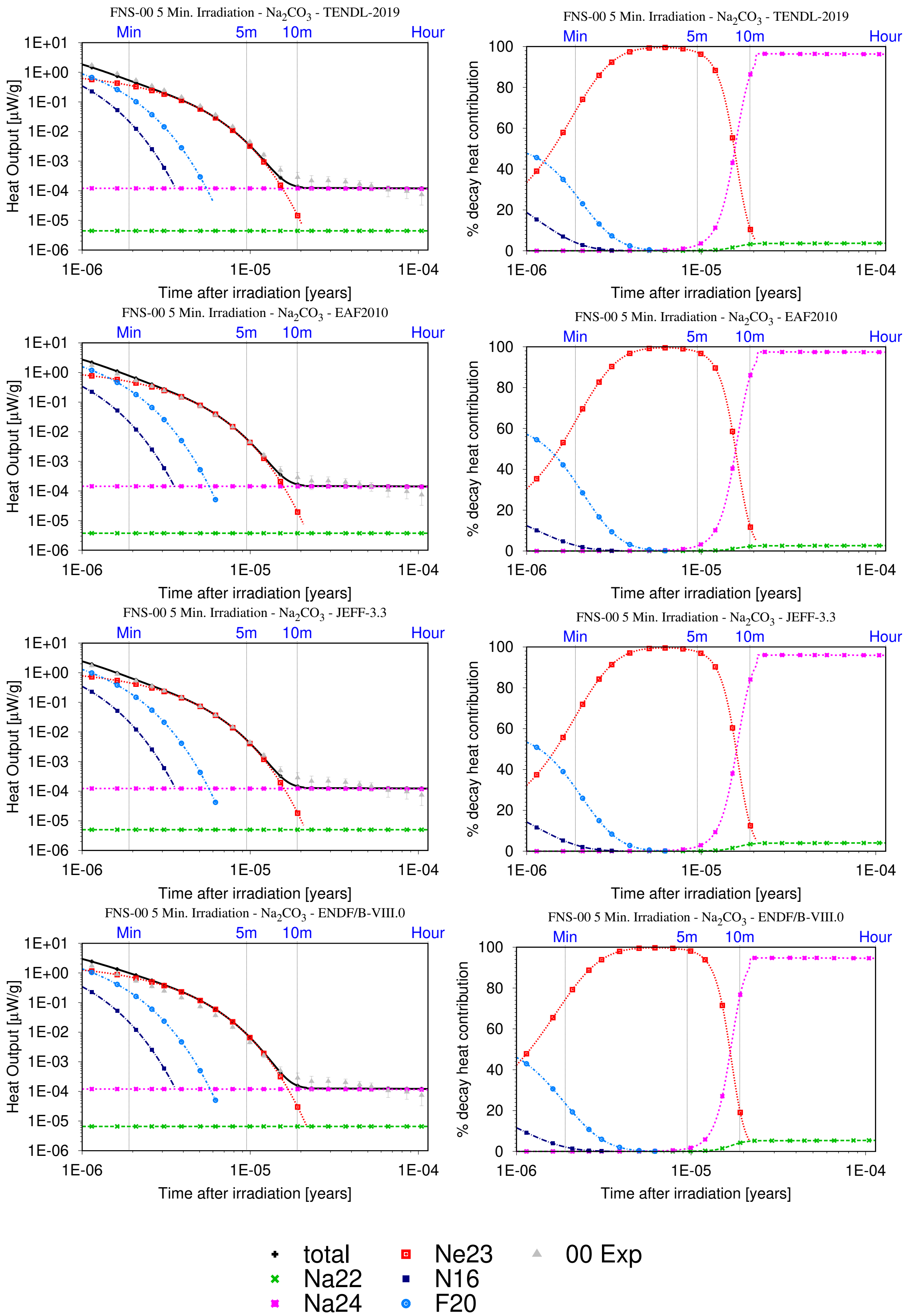


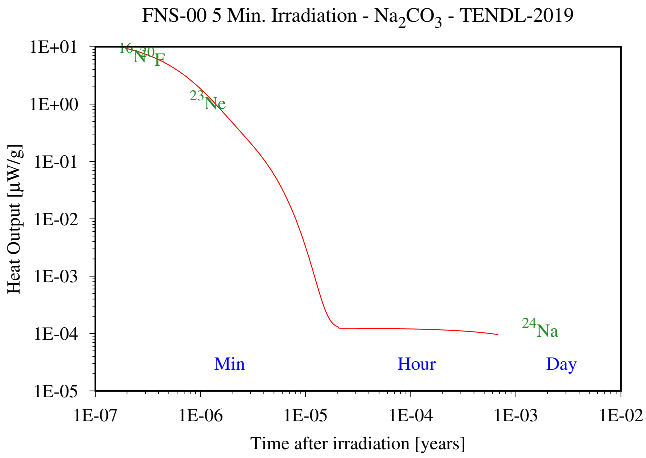
Sodium, TENDL-2019 5-minute pathway analysis

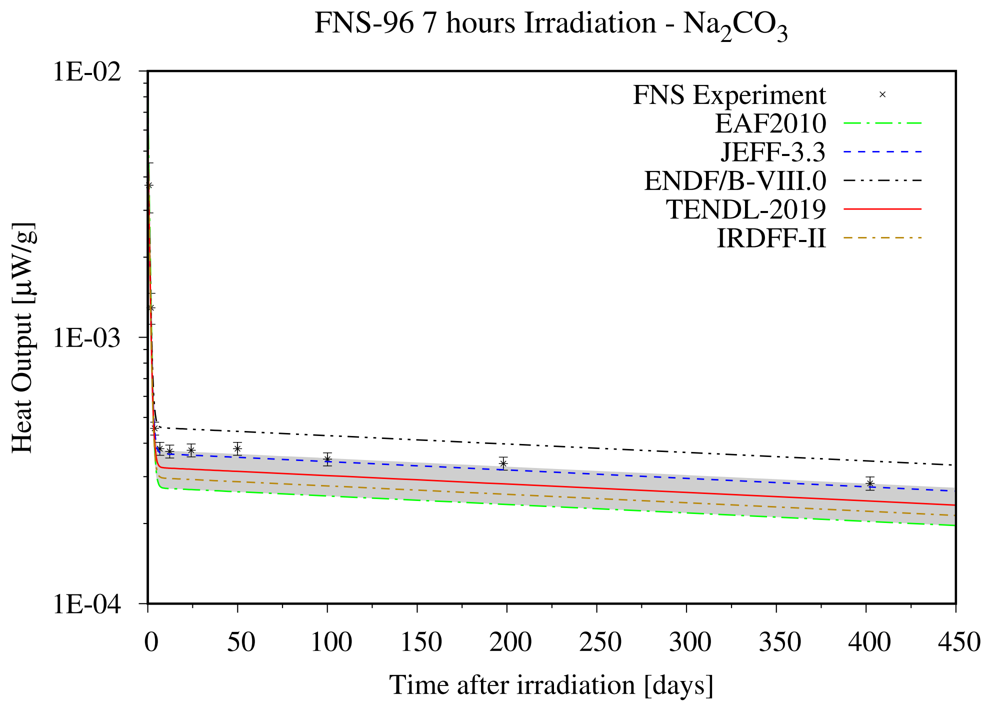
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
F20	11.03s	Na23(n,α)F20	100.0
Ne23	37.21s	Na23(n,p)Ne23	100.0
Na24	14.96h	Na23(n,γ)Na24	100.0
Na22	2.60y	Na23(n,2n)Na22	100.0

Comments on Sodium 5-minute experiments:

Clearly the two experimental batches are discrepant for sodium and do not exhibit the same decay-heat plateau beyond 10-minutes, which the simulations say is primarily due to Na24. Many factors could have influenced the experimental set-up including the presence of impurities in the sample. All libraries show good agreement to the 2000 result (IRDFF-II does not include the (n,p) reaction to produce Ne23, which dominates at short-timescales with the other libraries). The TENDL-2019 Na23 capture cross section seems to represent the 2000 experiment well, although the uncertainties are relatively high in both cases.


FNS-00 5 Min. Irradiation - Na_2CO_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Na_2CO_3 - EAF2010
FNS-00 5 Min. Irradiation - Na_2CO_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Na_2CO_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Na22
Na24
Ne23
N16
F20
00 Exp

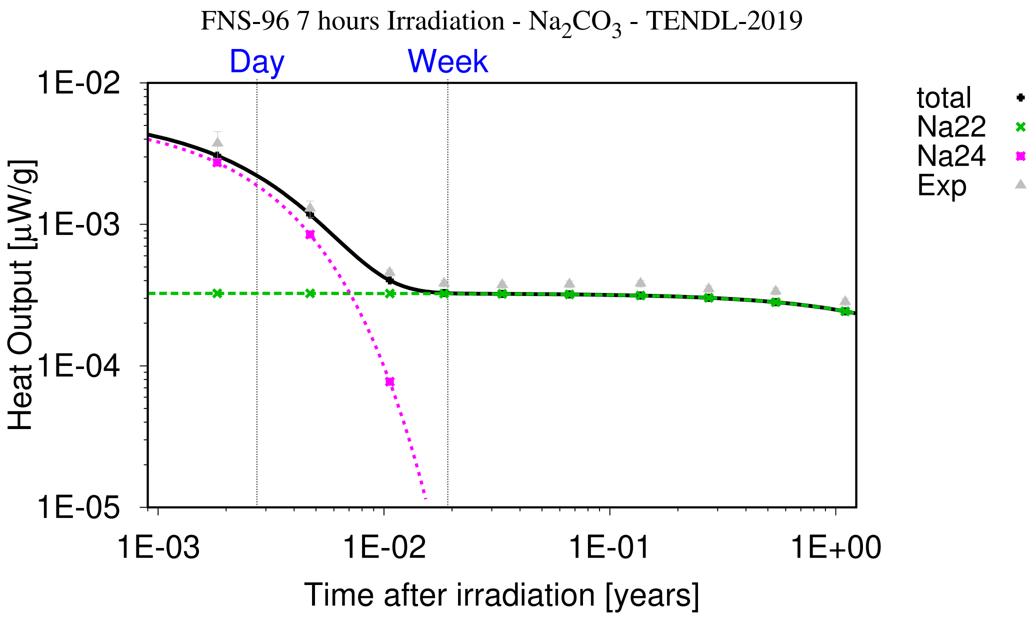

FNS-00 5 Min. Irradiation - Na2CO3 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
20F
23Ne
24Na
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.67	$3.73E{-}03$ +/-21%	$3.06E{-}03$ +/-42%	1.22	1.17	0.91	1.16	1.26
1.72	$1.29E{-}03$ +/-13%	$1.17E{-}03$ +/-35%	1.10	0.99	0.88	1.03	1.15
3.87	$4.55E{-}04$ +/-6%	$4.02E{-}04$ +/-16%	1.13	0.85	1.20	1.02	1.22
6.74	$3.82E{-}04$ +/-6%	$3.27E{-}04$ +/-16%	1.17	0.83	1.38	1.04	1.28
12.19	$3.73E{-}04$ +/-6%	$3.23E{-}04$ +/-16%	1.16	0.82	1.38	1.02	1.26
24.20	$3.77E{-}04$ +/-6%	$3.20E{-}04$ +/-16%	1.18	0.83	1.41	1.04	1.29
49.95	$3.82E{-}04$ +/-6%	$3.14E{-}04$ +/-16%	1.22	0.86	1.45	1.08	1.33
100.08	$3.49E{-}04$ +/-6%	$3.03E{-}04$ +/-16%	1.15	0.82	1.37	1.02	1.26
197.95	$3.36E{-}04$ +/-6%	$2.82E{-}04$ +/-16%	1.19	0.84	1.42	1.06	1.30
402.16	$2.83E{-}04$ +/-6%	$2.43E{-}04$ +/-16%	1.17	0.82	1.39	1.03	1.27
mean % diff. from E			14	17	24	5	21
mean χ^2			5.58	10.23	19.27	0.47	12.27

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Na24	14.96h	1.22	21%	47%
Na22	2.60y	1.13	6%	16%

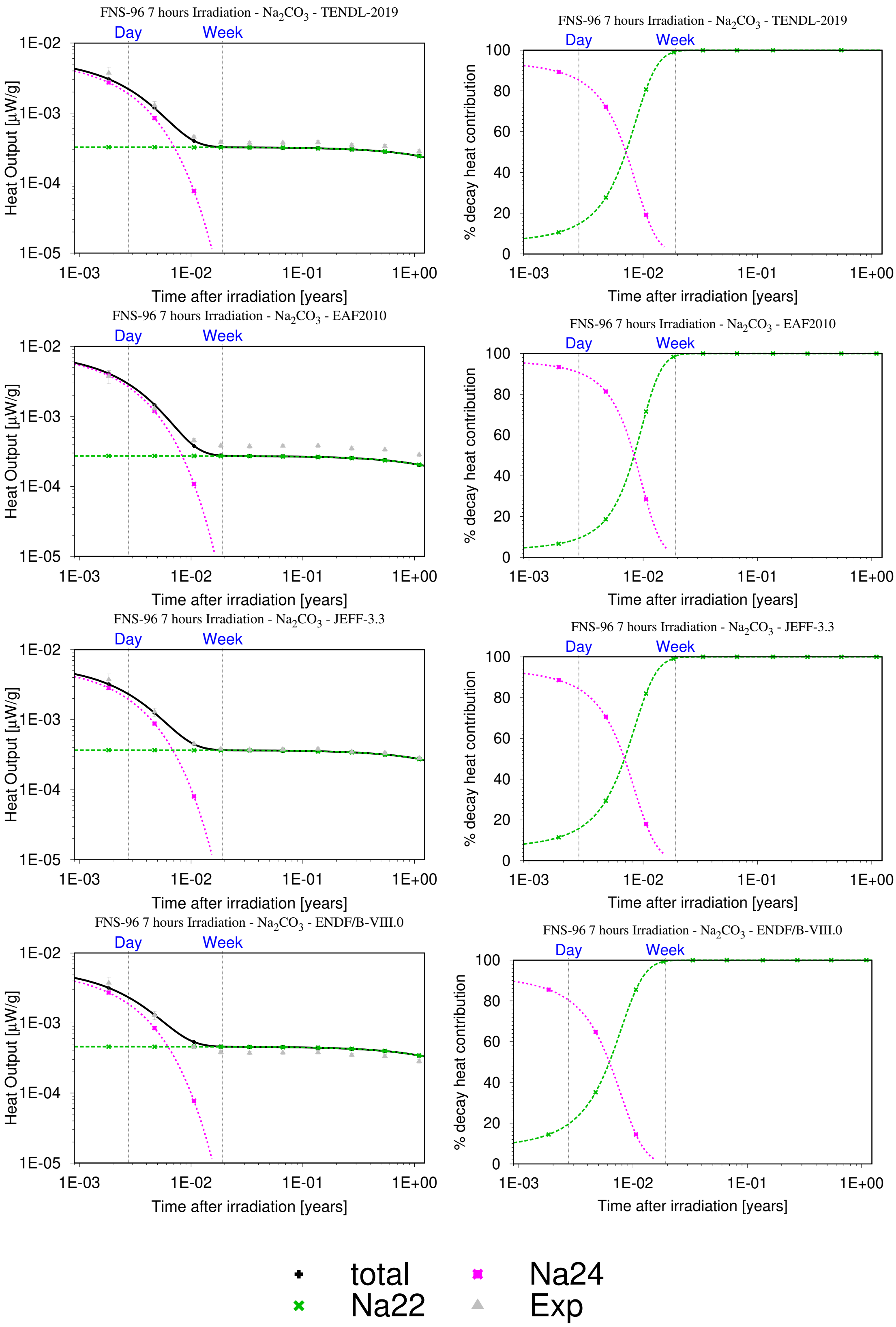


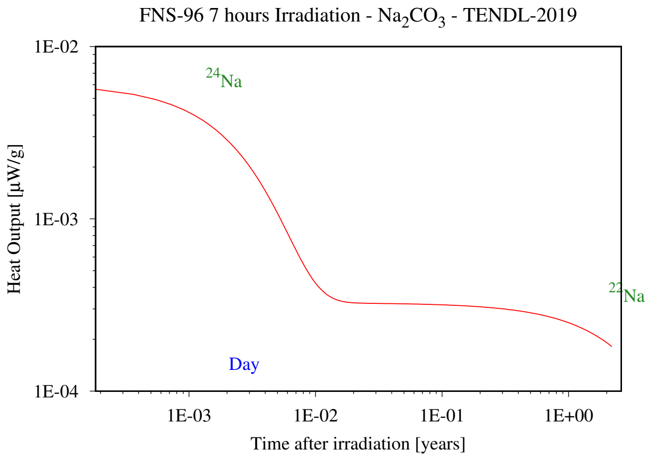
Sodium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Na24	14.96h	Na23(n,γ)Na24	100.0
Na22	2.60y	Na23(n,2n)Na22	100.0

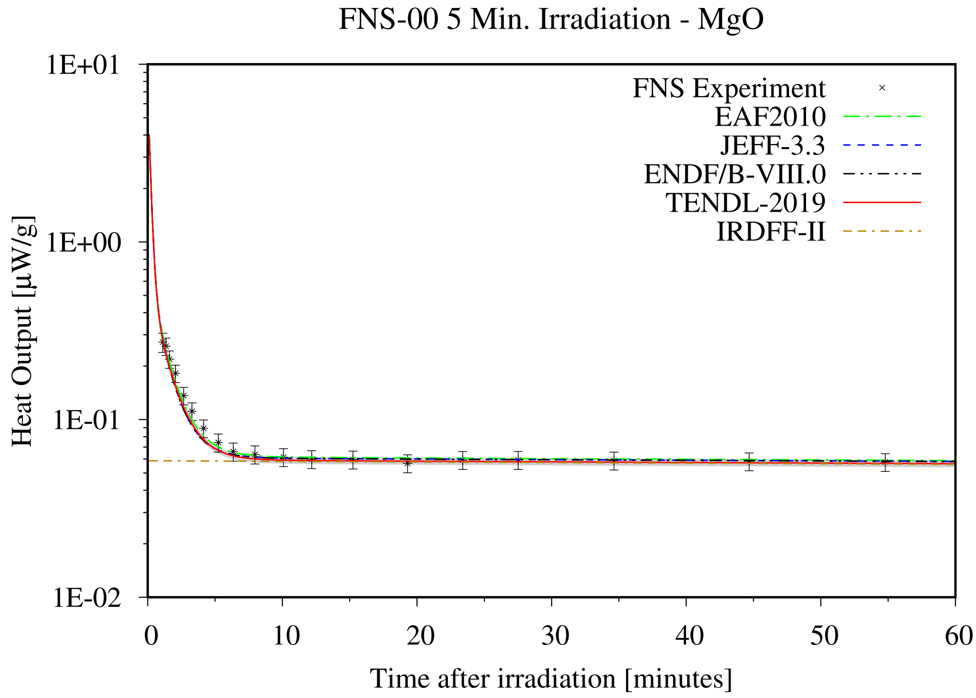
Comments on Sodium 7-hour experiments:

For the longer experiment on sodium, most of the library simulations seems to either under or overpredict the measurement, with only JEFF-3.3 matching closely the result at all decay times. The heat arising from Na22 seems to be underpredicted by around 40% by EAF2010, and 20% by TENDL-2019 and 30% by IRDFF-II (a change to the (n,2n) channel on Na23 compared to IRDFF-1.05), while ENDF/B-VIII.0 overpredicts by around 15%. The wide variation between the simulated results makes it difficult to draw any concrete conclusions (JEFF-3.3 could be a good match by chance).


FNS-96 7 hours Irradiation - Na_2CO_3 - TENDL-2019
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - Na_2CO_3 - EAF2010
FNS-96 7 hours Irradiation - Na_2CO_3 - JEFF-3.3
FNS-96 7 hours Irradiation - Na_2CO_3 - ENDF/B-VIII.0
total
Na24
Na22
Exp


FNS-96 7 hours Irradiation - Na2CO3 - TENDL-2019
1E-02
1E-03
1E-04
Heat Output [µW/g]
24Na
22Na
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

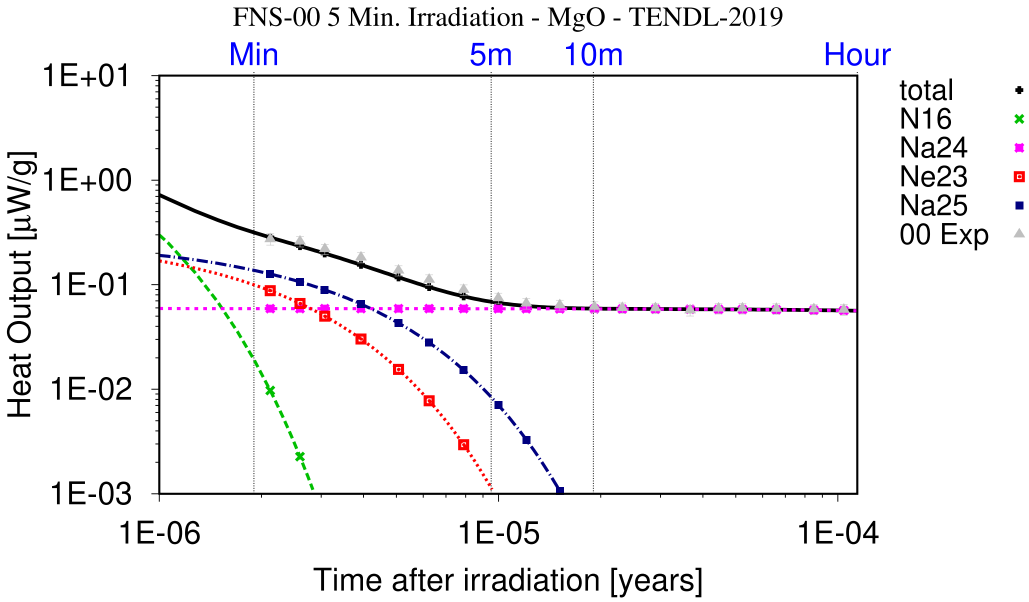
Magnesium



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
1.12	2.73E−01 +/-12%	2.83E−01 +/-8%	0.96	0.96	0.91	0.96	4.65
1.37	2.59E−01 +/-11%	2.34E−01 +/-8%	1.10	1.11	1.04	1.11	4.41
1.62	2.19E−01 +/-11%	1.99E−01 +/-8%	1.10	1.11	1.04	1.11	3.73
2.07	1.82E−01 +/-11%	1.55E−01 +/-7%	1.18	1.21	1.11	1.20	3.11
2.67	1.36E−01 +/-11%	1.18E−01 +/-6%	1.16	1.19	1.10	1.19	2.33
3.28	1.11E−01 +/-11%	9.49E−02 +/-5%	1.17	1.21	1.11	1.20	1.90
4.15	8.93E−02 +/-12%	7.74E−02 +/-4%	1.15	1.17	1.10	1.17	1.53
5.25	7.43E−02 +/-12%	6.71E−02 +/-4%	1.11	1.11	1.06	1.10	1.27
6.35	6.61E−02 +/-12%	6.26E−02 +/-4%	1.06	1.04	1.01	1.04	1.13
7.97	6.37E−02 +/-12%	6.01E−02 +/-4%	1.06	1.04	1.01	1.04	1.09
10.08	6.15E−02 +/-12%	5.91E−02 +/-4%	1.04	1.02	1.00	1.01	1.06
12.18	5.99E−02 +/-12%	5.88E−02 +/-4%	1.02	0.99	0.98	0.99	1.03
15.25	5.96E−02 +/-12%	5.86E−02 +/-4%	1.02	0.99	0.98	0.99	1.03
19.30	5.67E−02 +/-12%	5.84E−02 +/-5%	0.97	0.95	0.93	0.94	0.98
23.40	5.92E−02 +/-12%	5.82E−02 +/-5%	1.02	0.99	0.98	0.99	1.03
27.52	5.92E−02 +/-12%	5.80E−02 +/-5%	1.02	0.99	0.98	0.99	1.03
34.63	5.88E−02 +/-12%	5.76E−02 +/-5%	1.02	0.99	0.98	0.99	1.03
44.68	5.82E−02 +/-12%	5.72E−02 +/-5%	1.02	0.99	0.98	0.99	1.03
54.78	5.77E−02 +/-12%	5.67E−02 +/-5%	1.02	0.99	0.98	0.99	1.03
mean % diff. from E			6	6	5	6	27
mean χ^2			0.49	0.59	0.24	0.57	11.87

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ$\mathbf{C}^{nuc}$**
Na24	14.96h	1.15	12%	5%

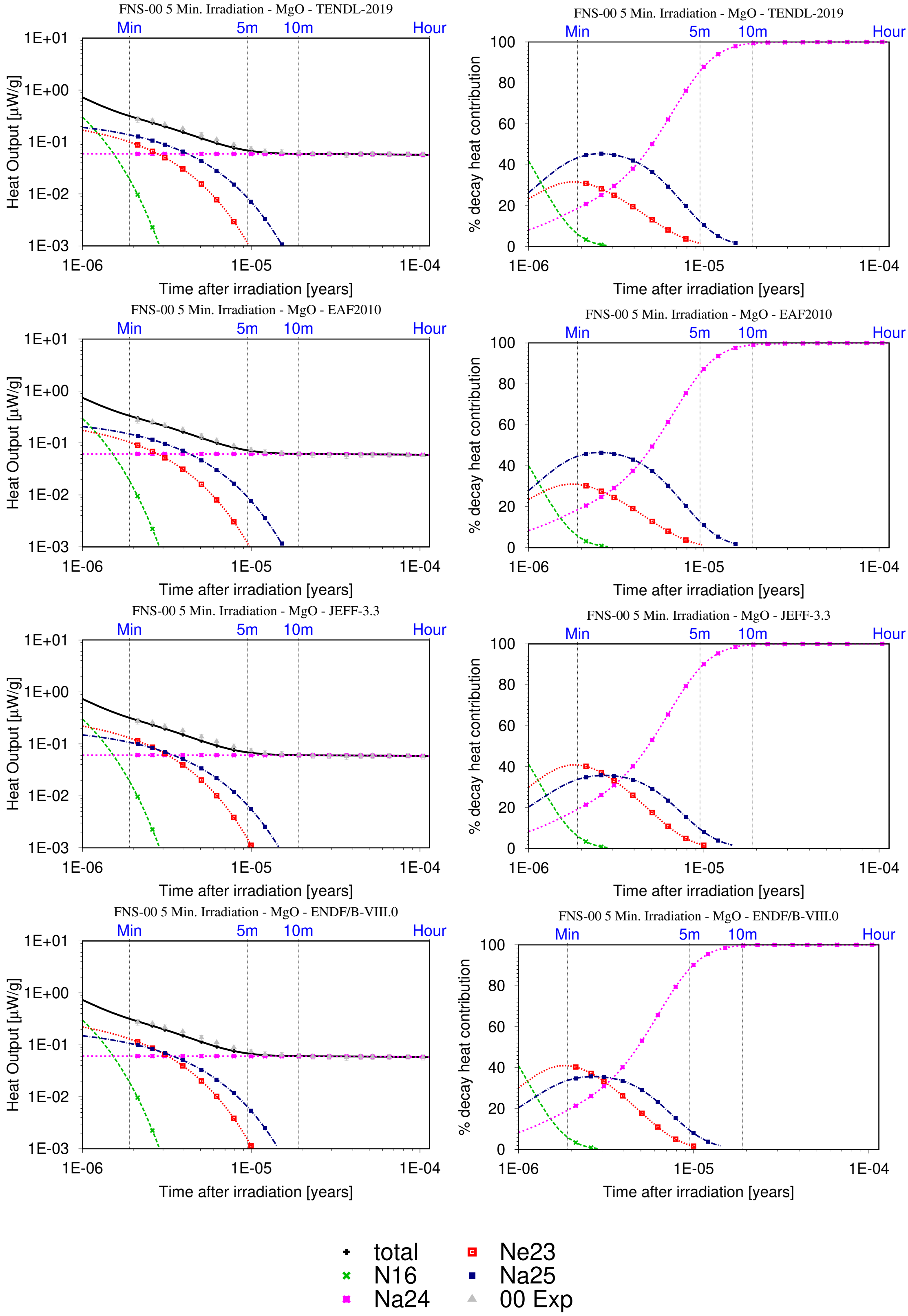


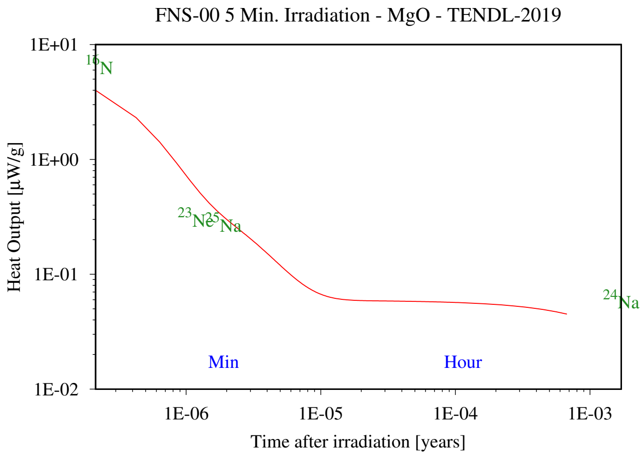
Magnesium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ne23	37.21s	Mg26(n,α)Ne23	100.0
Na25	59.60s	Mg25(n,p)Na25	96.5
		Mg26(n,d)Na25	3.4
Na24	14.96h	Mg24(n,p)Na24	99.1

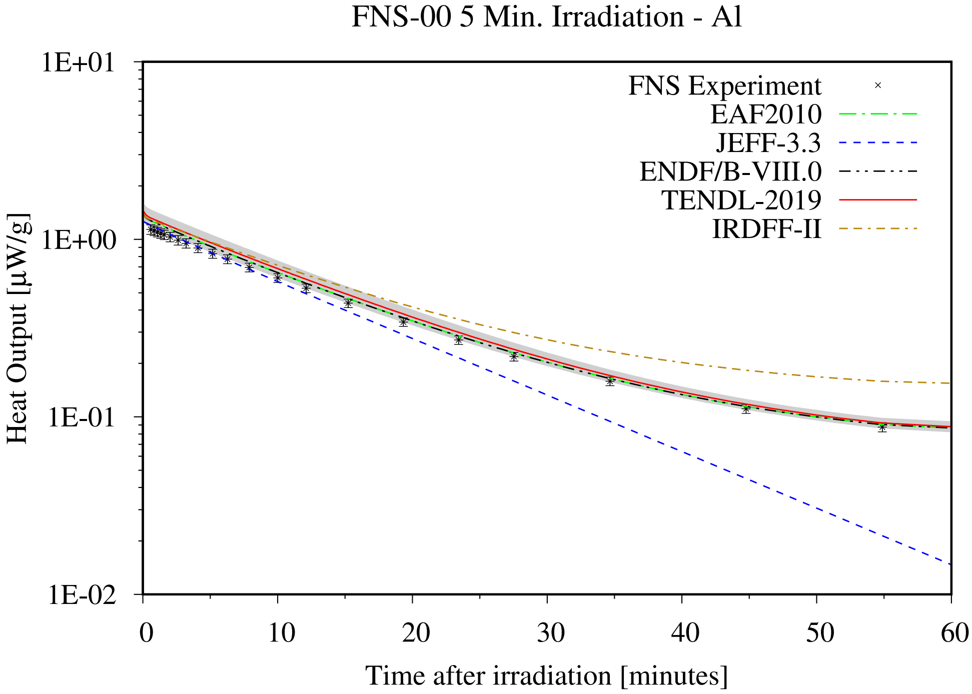
Comments on Magnesium 5-minute experiments:

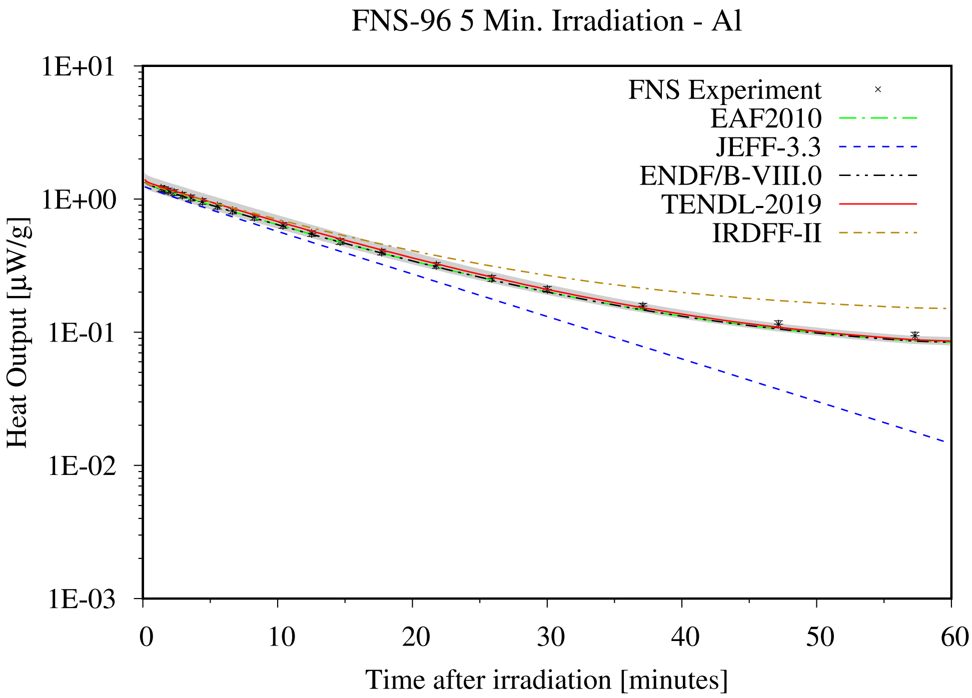
There is good agreement at all cooling times (with the caveat that IRDFF-II does not include the reaction data for the production of the short-lived Na25 or Ne23 nuclides from Mg). Na24 production-rates via (n,p) reactions on Mg24 are well predicted by all libraries for magnesium.


FNS-00 5 Min. Irradiation - MgO - TENDL-2019
FNS-00 5 Min. Irradiation - MgO - EAF2010
FNS-00 5 Min. Irradiation - MgO - JEFF-3.3
FNS-00 5 Min. Irradiation - MgO - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
N16
Na24
Ne23
Na25
00 Exp


FNS-00 5 Min. Irradiation - MgO - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
16N
23Ne
25Na
24Na
Min
Hour
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

Aluminium

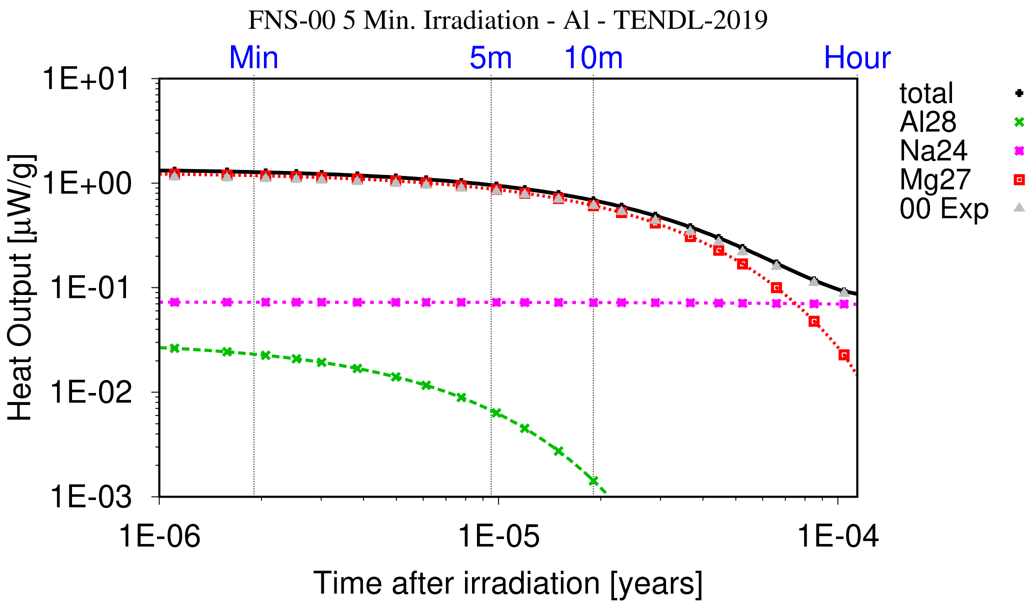

FNS-00 5 Min. Irradiation - Al
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+01
1E+00
1E-01
1E-02
0
10
20
30
40
50
60
Heat Output [µW/g]
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Al
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Heat Output [µW/g]
Time after irradiation [minutes]

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	1.14E+00 +/-6%	1.32E+00 +/-12%	0.86	0.89	0.89	0.95	0.88
0.83	1.12E+00 +/-6%	1.29E+00 +/-12%	0.86	0.90	0.89	0.95	0.88
1.08	1.10E+00 +/-6%	1.27E+00 +/-12%	0.87	0.90	0.90	0.95	0.88
1.33	1.08E+00 +/-6%	1.25E+00 +/-12%	0.87	0.90	0.90	0.96	0.88
1.58	1.06E+00 +/-6%	1.22E+00 +/-12%	0.87	0.90	0.90	0.96	0.88
2.02	1.03E+00 +/-6%	1.19E+00 +/-12%	0.87	0.91	0.90	0.97	0.88
2.62	9.88$E-$01 +/-6%	1.14E+00 +/-12%	0.87	0.91	0.91	0.97	0.88
3.22	9.49$E-$01 +/-6%	1.09E+00 +/-12%	0.87	0.91	0.91	0.98	0.88
4.08	8.93$E-$01 +/-6%	1.02E+00 +/-12%	0.87	0.91	0.91	0.99	0.87
5.18	8.31$E-$01 +/-6%	9.48$E-$01 +/-12%	0.88	0.92	0.92	1.00	0.87
6.28	7.73$E-$01 +/-6%	8.79$E-$01 +/-11%	0.88	0.93	0.92	1.01	0.86
7.90	6.95$E-$01 +/-6%	7.87$E-$01 +/-11%	0.88	0.93	0.93	1.03	0.86
10.02	6.06$E-$01 +/-6%	6.84$E-$01 +/-11%	0.89	0.93	0.93	1.05	0.85
12.12	5.30$E-$01 +/-6%	5.96$E-$01 +/-11%	0.89	0.94	0.94	1.07	0.84
15.23	4.37$E-$01 +/-6%	4.88$E-$01 +/-11%	0.89	0.94	0.94	1.11	0.82
19.33	3.42$E-$01 +/-6%	3.80$E-$01 +/-10%	0.90	0.95	0.95	1.18	0.79
23.43	2.71$E-$01 +/-6%	3.00$E-$01 +/-10%	0.90	0.95	0.95	1.26	0.76
27.53	2.18$E-$01 +/-6%	2.40$E-$01 +/-9%	0.91	0.95	0.95	1.37	0.73
34.67	1.59$E-$01 +/-6%	1.71$E-$01 +/-8%	0.93	0.96	0.96	1.68	0.68
44.77	1.11$E-$01 +/-6%	1.18$E-$01 +/-7%	0.94	0.97	0.97	2.46	0.61
54.87	8.76$E-$02 +/-6%	9.24$E-$02 +/-7%	0.95	0.97	0.97	4.08	0.55
mean % diff. from E			13	8	8	14	25
mean χ^2			4.85	1.99	2.04	17.87	27.99

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Mg27	9.46m	0.86	6%	13%
Na24	14.96h	0.95	6%	8%

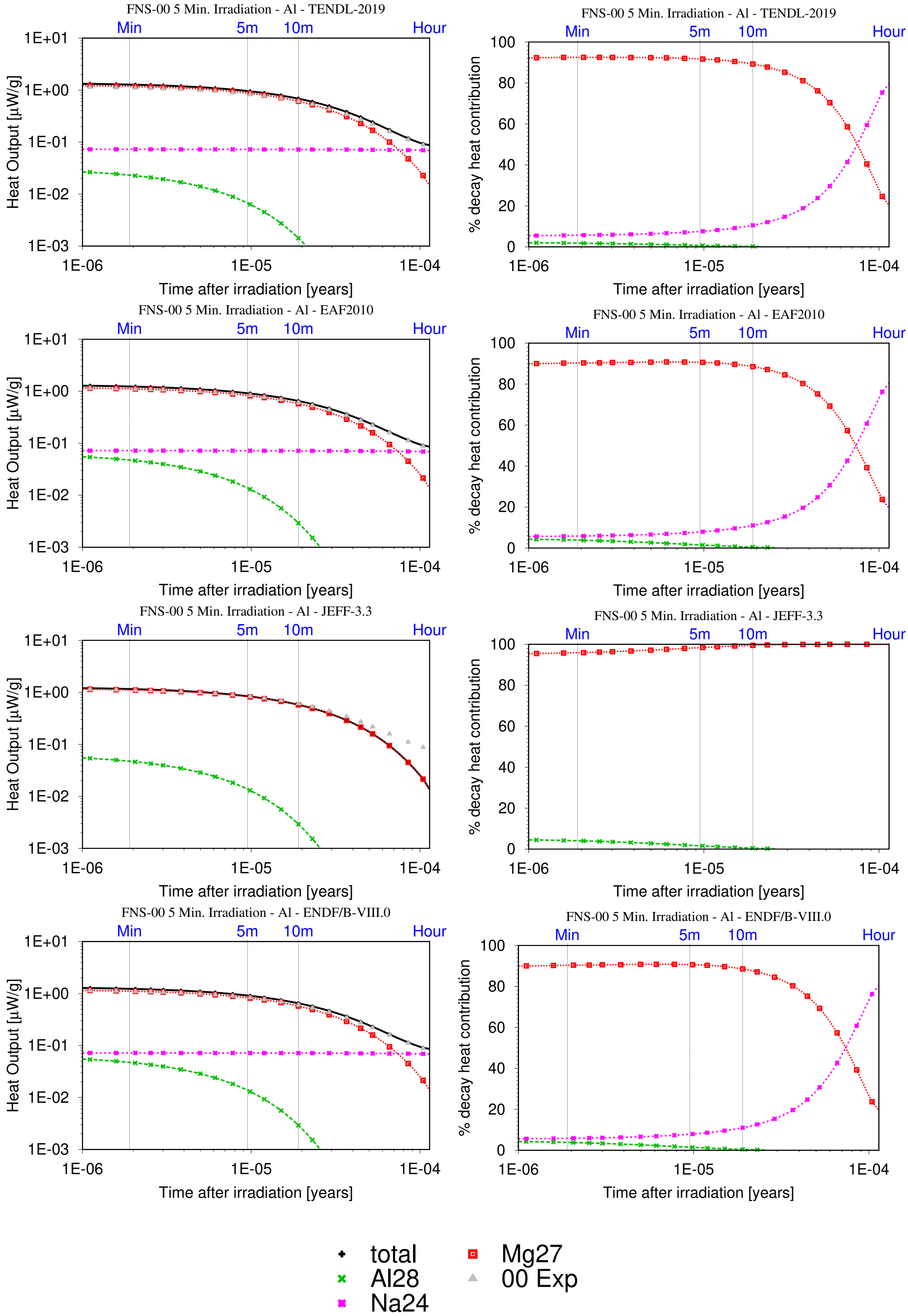


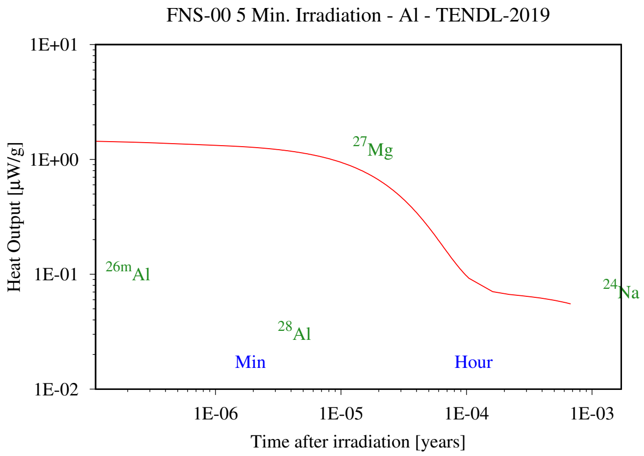
Aluminium, TENDL-2019 5-minute pathway analysis

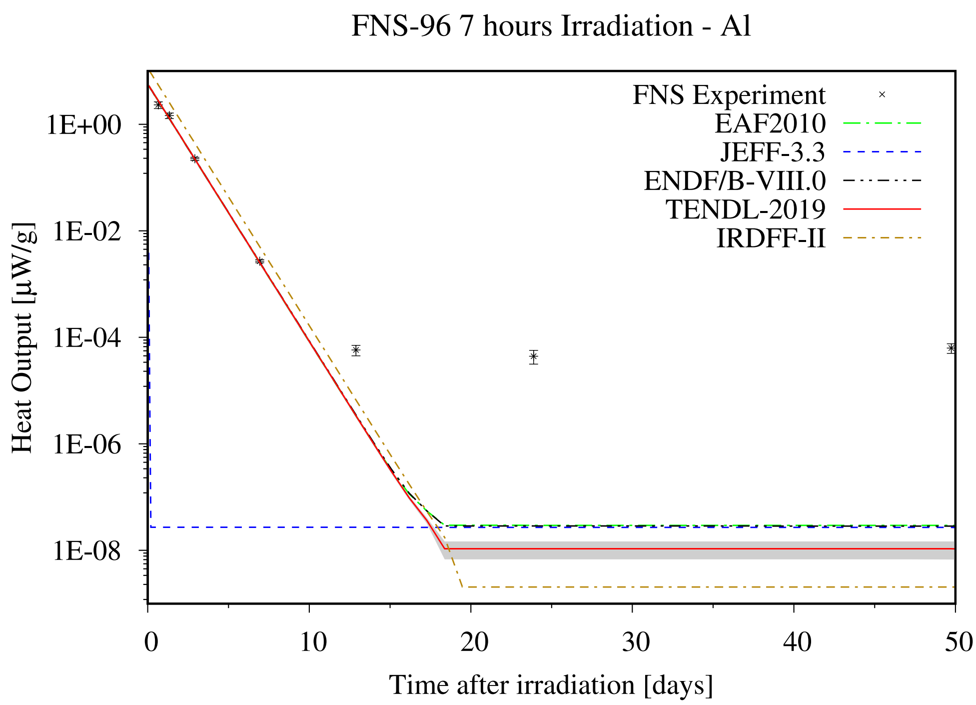
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Al28	2.24m	Al27(n,γ)Al28	100.0
Mg27	9.46m	Al27(n,p)Mg27	100.0
Na24	14.96h	Al27(n,α)Na24	100.0

Comments on Aluminium 5-minute experiments:

For aluminium an excellent agreement can be seen, for both batches, for the production route of the Mg27 radionuclide with all libraries, although TENDL-2019 is a slightly worse match than with the previous TENDL-2017 (the mean deviation in the latter case was 7% compared to 13% here), seemingly due to a slight increase in Mg27 production. TENDL-2019 variance reflects well the experimental uncertainty. JEFF-3.3 misses the production of the long-lived Na24 nuclide via (n,α) reactions and so begins to deviate from the experiment from around 10 minutes. The IRDFF-II result is noticeably somewhat worse than the previous IRDFF-1.05 results, possibly because of the addition of the (n,X) channel between Al27 and Na24.


FNS-00 5 Min. Irradiation - Al - TENDL-2019
FNS-00 5 Min. Irradiation - Al - EAF2010
FNS-00 5 Min. Irradiation - Al - JEFF-3.3
FNS-00 5 Min. Irradiation - Al - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Al28
Na24
Mg27
00 Exp

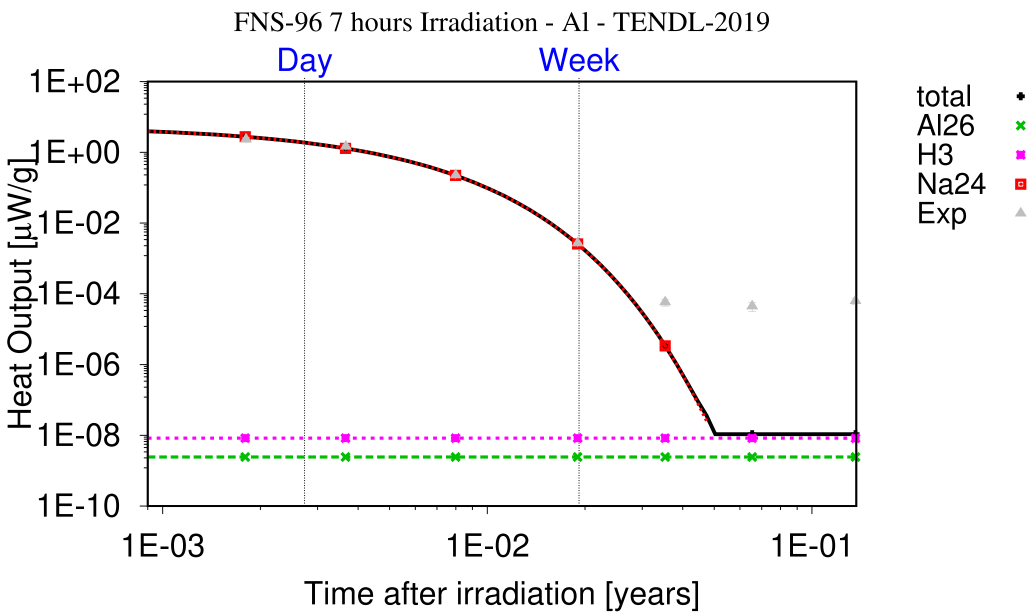

FNS-00 5 Min. Irradiation - Al - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
Time after irradiation [years]
1E-06
1E-05
1E-04
1E-03
27Mg
26mAl
28Al
24Na
Min
Hour



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.66	2.31E+00 +/-14%	2.76E+00 +/-9%	0.84	0.84	0.84	> 1000	0.42
1.34	1.46E+00 +/-12%	1.29E+00 +/-9%	1.12	1.13	1.13	> 1000	0.57
2.92	2.25E−01 +/-7%	2.23E−01 +/-9%	1.01	1.01	1.01	> 1000	0.51
6.93	2.68E−03 +/-7%	2.56E−03 +/-9%	1.05	1.03	1.05	> 1000	0.53
12.89	5.78E−05 +/-22%	3.40E−06 +/-9%	17.01	16.41	17.04	> 1000	8.62
23.89	4.40E−05 +/-29%	1.08E−08 +/-37%	> 1000	> 1000	> 1000	> 1000	> 1000
49.74	6.28E−05 +/-20%	1.07E−08 +/-37%	> 1000	> 1000	> 1000	> 1000	> 1000
mean % diff. from E			47	47	47	100	98
mean χ^2			8.15	8.09	8.16	86.36	78.72

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Na24	14.96h	0.84	14%	9%
H3	12.33y	4094.88	29%	47%

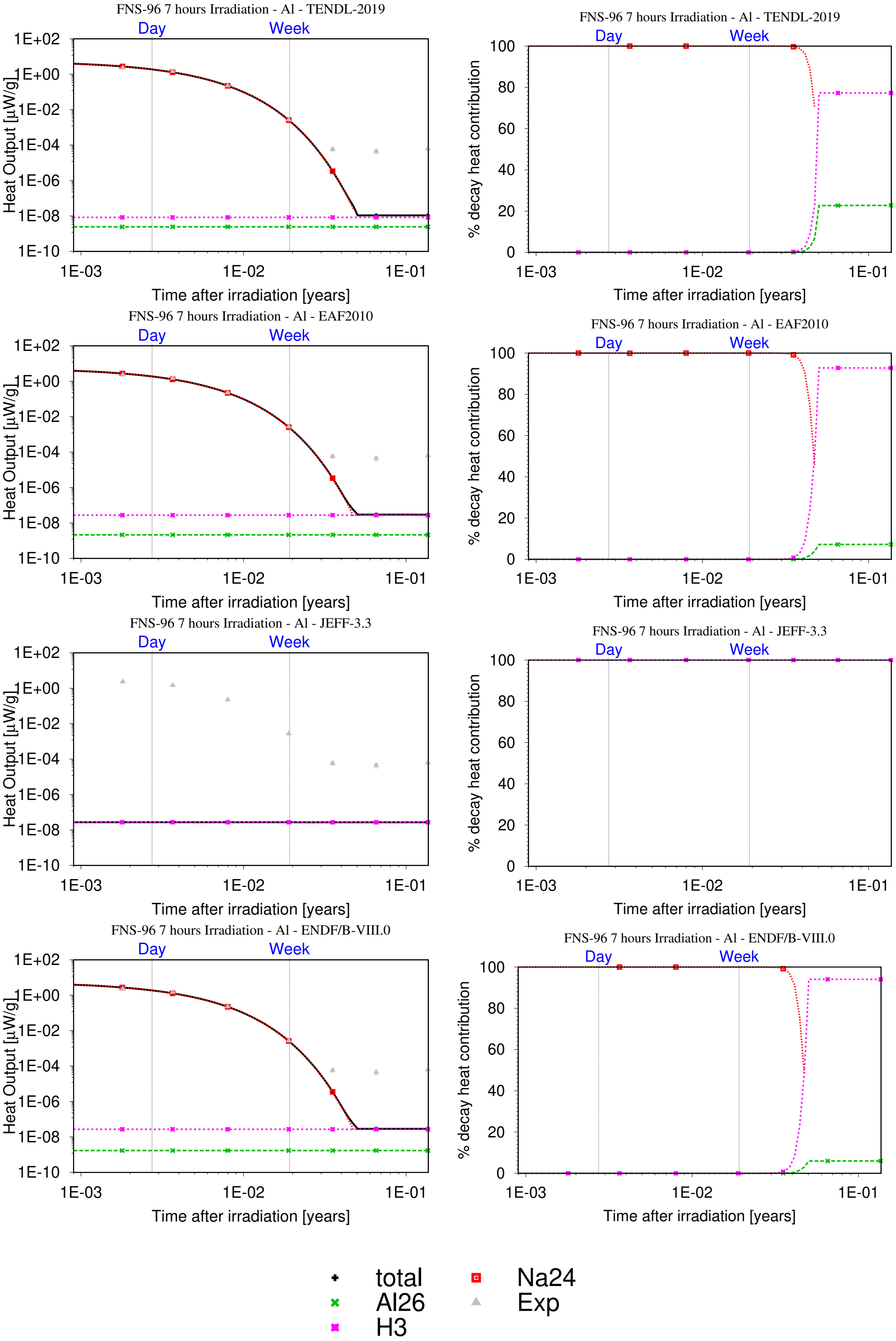


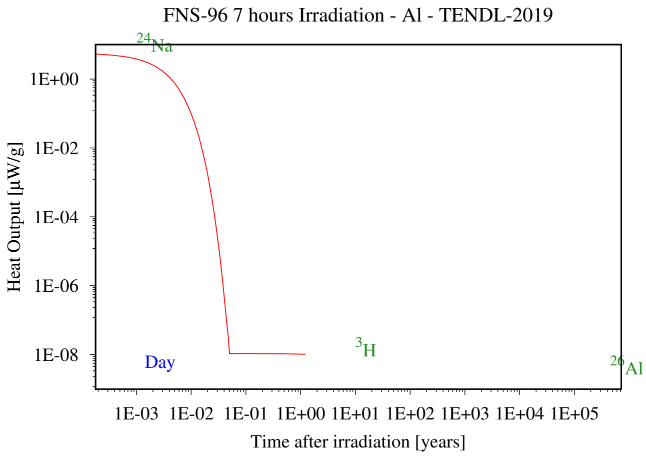
Aluminium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Na24	14.96h	Al27(n,α)Na24	100.0
H3	12.33y	Al27(n,t)H3	100.0
Al26	7.2 10^5y	Al27(n,2n)Al26	100.0

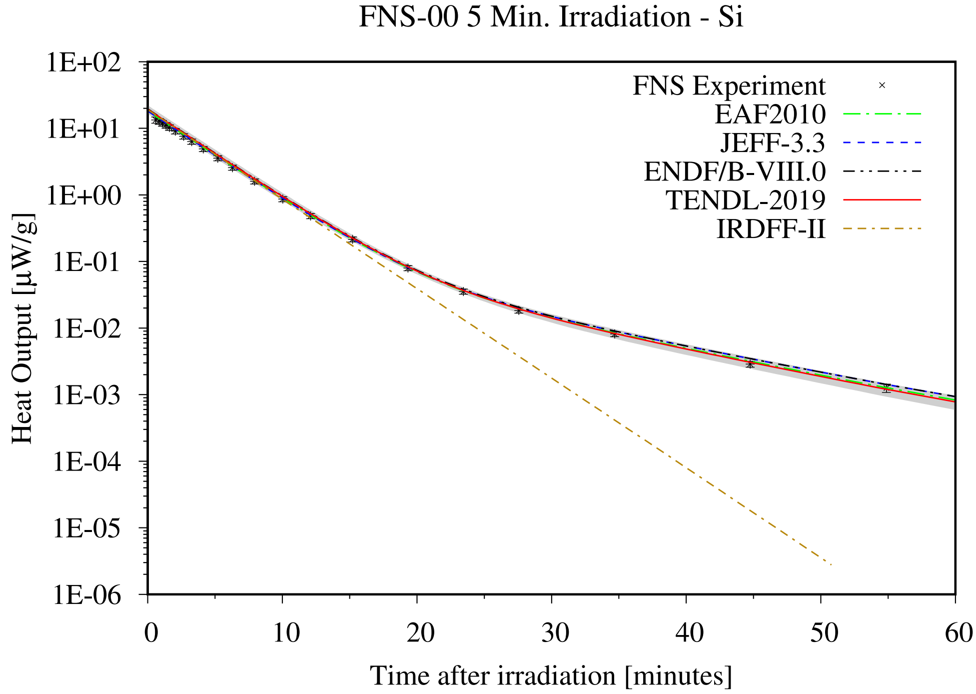
Comments on Aluminium 7-hour experiments:

Apart from JEFF-3.3 – which predicts no Na24 whatsoever despite its obvious dominance in the other cases – all libraries show good agreement up to around 7 days of cooling. Beyond this the simulations deviate significantly from the experiment, which could be due to unknown impurities in the sample, such as Mn and Fe, whose presence at the thousands of ppm level could easily account for the missing decay heat observed in the simulations. On the other hand, all the simulations could be severely underestimating the production of H3 via (n,t) reactions on Al2 and, besides this, there is some variation in the prediction, with TENDL and IRDFF prediction of H3 lower than the other three.


FNS-96 7 hours Irradiation - Al - TENDL-2019
FNS-96 7 hours Irradiation - Al - EAF2010
FNS-96 7 hours Irradiation - Al - JEFF-3.3
FNS-96 7 hours Irradiation - Al - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-03
1E-02
1E-01
1E+02
1E+00
1E-02
1E-04
1E-06
1E-08
1E-10
0
20
40
60
80
100
total
Al26
H3
Na24
Exp


FNS-96 7 hours Irradiation - Al - TENDL-2019
^{24}Na
^{3}H
^{26}Al
Day
Heat Output [µW/g]
1E+00
1E-02
1E-04
1E-06
1E-08
1E-03 1E-02 1E-01 1E+00 1E+01 1E+02 1E+03 1E+04 1E+05
Time after irradiation [years]

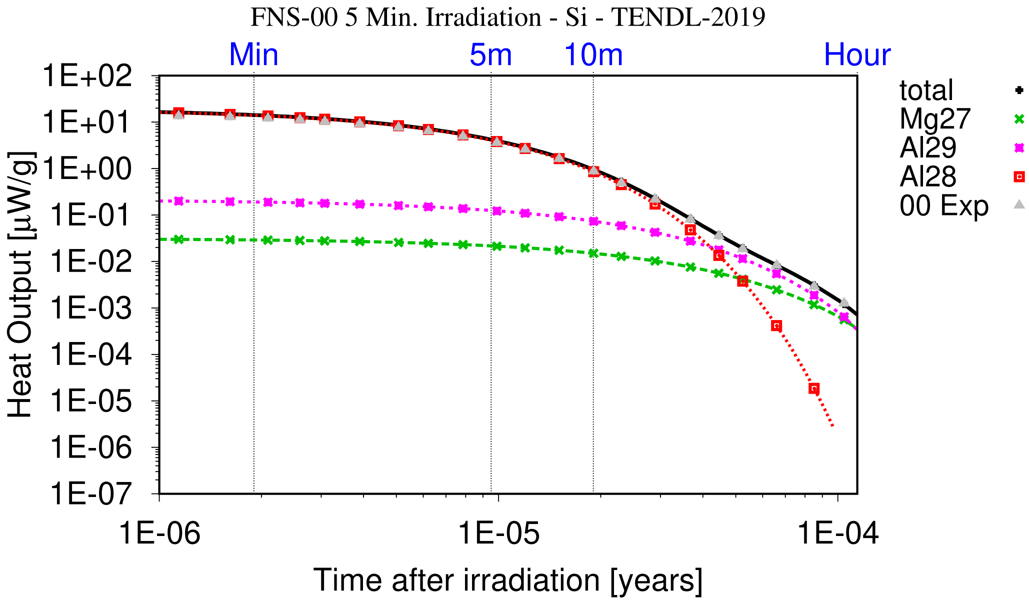
Silicon



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
0.60	1.33E+01 +/-10%	1.61E+01 +/-15%	0.83	0.82	0.88	0.88	0.84
0.85	1.28E+01 +/-10%	1.49E+01 +/-15%	0.86	0.85	0.91	0.91	0.87
1.10	1.19E+01 +/-10%	1.38E+01 +/-15%	0.87	0.85	0.91	0.92	0.88
1.37	1.11E+01 +/-10%	1.27E+01 +/-15%	0.88	0.86	0.92	0.93	0.89
1.62	1.03E+01 +/-10%	1.18E+01 +/-15%	0.87	0.86	0.92	0.93	0.89
2.05	9.08E+00 +/-10%	1.03E+01 +/-15%	0.88	0.87	0.93	0.93	0.90
2.67	7.59E+00 +/-9%	8.54E+00 +/-14%	0.89	0.88	0.94	0.94	0.91
3.27	6.34E+00 +/-9%	7.11E+00 +/-14%	0.89	0.88	0.94	0.94	0.91
4.13	4.91E+00 +/-9%	5.47E+00 +/-14%	0.90	0.89	0.95	0.95	0.92
5.20	3.57E+00 +/-9%	3.96E+00 +/-14%	0.90	0.89	0.95	0.95	0.93
6.30	2.57E+00 +/-9%	2.84E+00 +/-14%	0.90	0.89	0.95	0.96	0.94
7.93	1.60E+00 +/-9%	1.75E+00 +/-14%	0.92	0.90	0.97	0.97	0.97
10.03	8.67E−01 +/-9%	9.44E−01 +/-13%	0.92	0.91	0.97	0.97	1.01
12.10	4.83E−01 +/-9%	5.23E−01 +/-13%	0.92	0.91	0.97	0.97	1.07
15.22	2.15E−01 +/-9%	2.25E−01 +/-12%	0.96	0.94	1.00	0.99	1.25
19.33	7.97E−02 +/-9%	8.33E−02 +/-11%	0.96	0.93	0.98	0.97	1.65
23.45	3.53E−02 +/-9%	3.69E−02 +/-11%	0.96	0.92	0.97	0.94	2.61
27.57	1.84E−02 +/-9%	1.95E−02 +/-13%	0.94	0.89	0.94	0.90	4.85
34.68	8.16E−03 +/-9%	8.32E−03 +/-16%	0.98	0.90	0.96	0.90	19.52
44.75	2.88E−03 +/-10%	3.08E−03 +/-20%	0.94	0.82	0.90	0.83	163.08
54.87	1.26E−03 +/-14%	1.21E−03 +/-23%	1.04	0.88	0.98	0.88	0.00
mean % diff. from E			10	13	6	7	30
mean χ^2			1.33	2.06	0.48	0.76	18.11

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Al28	2.24m	0.83	10%	15%

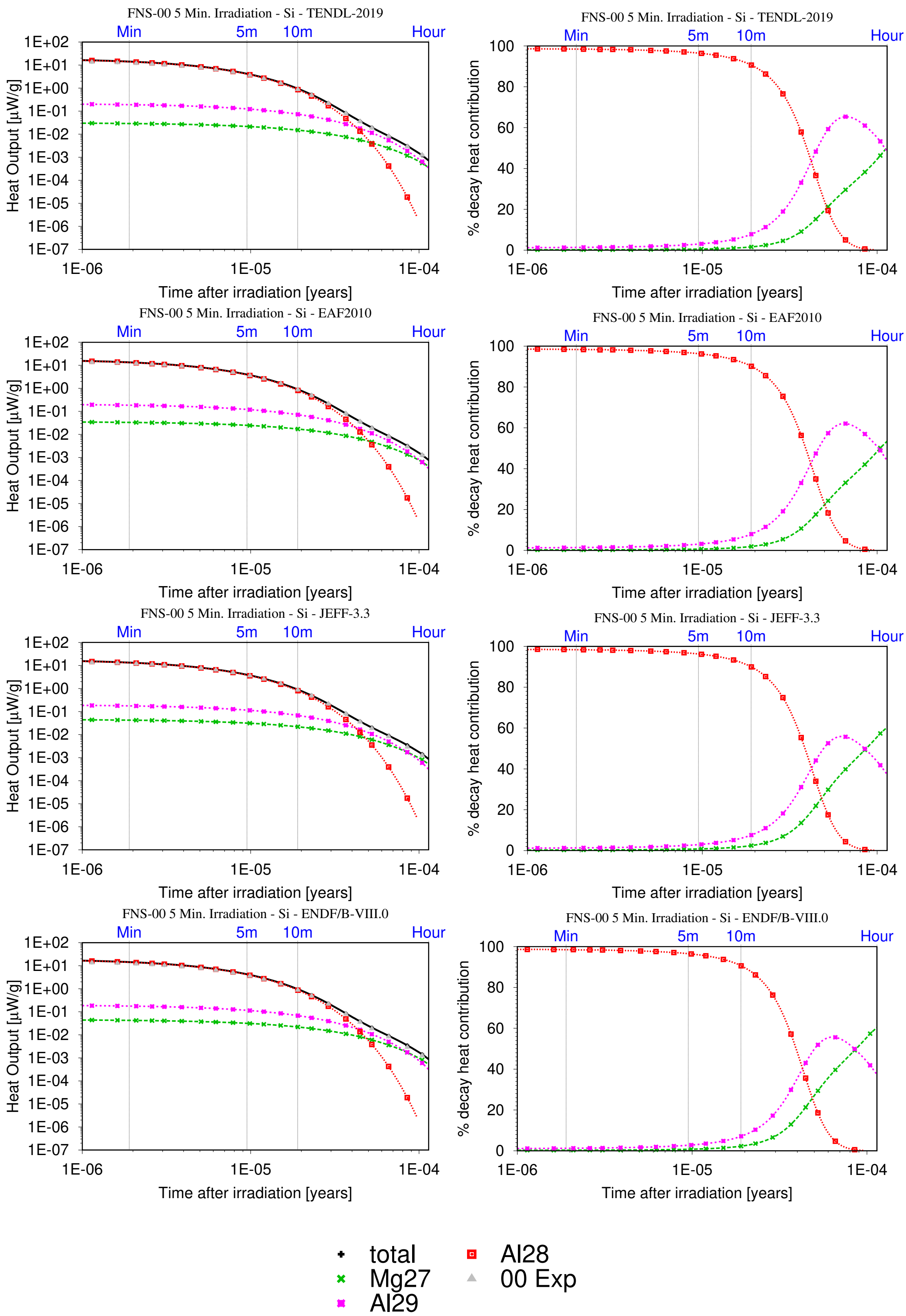


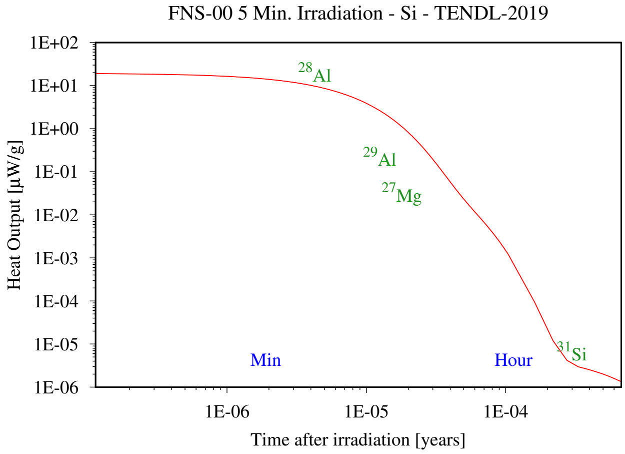
Silicon, TENDL-2019 5-minute pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Al28	2.24m	Si28(n,p)Al28	99.7
Al29	6.56m	Si29(n,p)Al29	99.1
Mg27	9.46m	Si30(n,α)Mg27	100.0

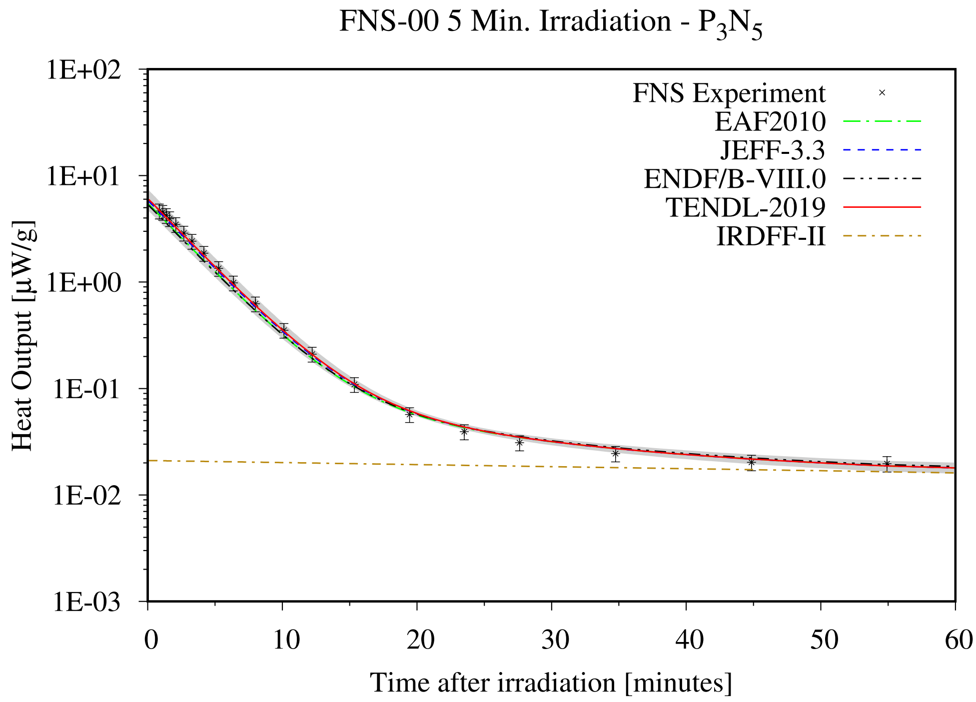
Comments on Silicon 5-minute experiments:

In the pure silicon simulations of the 2000 5-minute experiment (an earlier 1996 experiment is omitted here due to an unacceptable level of undocumented impurities in the silicon oxide sample used in that case) both Al29 and Mg27 contribute significantly to the decay heat beyond around 15 minutes of cooling, and so it is not possible to reliably attribute E/C values to either of these radionuclides. At shorter cooling times Al28 dominates (see the nuclide contribution chart). All libraries agree well with the experiment, although IRDFF-II deviates at longer times because it doesn't contain data on the necessary reactions to produce Al29 or Mg27.


FNS-00 5 Min. Irradiation - Si - TENDL-2019
FNS-00 5 Min. Irradiation - Si - EAF2010
FNS-00 5 Min. Irradiation - Si - JEFF-3.3
FNS-00 5 Min. Irradiation - Si - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Mg27
Al29
Al28
00 Exp


FNS-00 5 Min. Irradiation - Si - TENDL-2019
Heat Output [µW/g]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
28Al
29Al
27Mg
31Si
Min
Hour
1E-06
1E-05
1E-04
Time after irradiation [years]

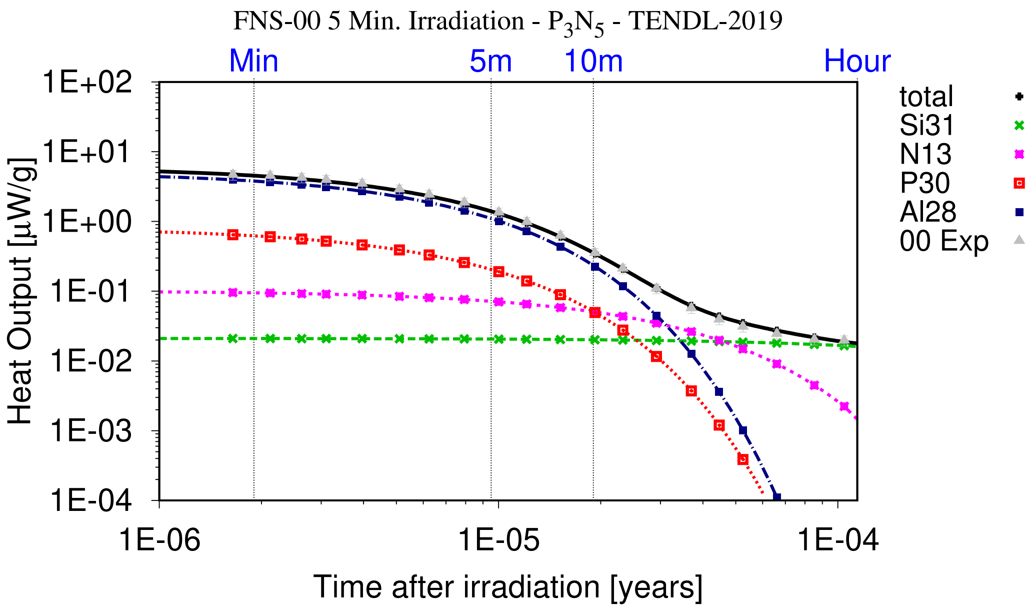
Phosphorus



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
0.87	$4.65E{+}00$ +/-16%	$4.72E{+}00$ +/-22%	0.99	1.12	1.10	1.02	221.80
1.12	$4.52E{+}00$ +/-16%	$4.38E{+}00$ +/-22%	1.03	1.17	1.15	1.07	215.65
1.38	$4.22E{+}00$ +/-16%	$4.04E{+}00$ +/-22%	1.04	1.19	1.16	1.09	201.86
1.63	$3.94E{+}00$ +/-16%	$3.75E{+}00$ +/-22%	1.05	1.19	1.17	1.09	188.59
2.08	$3.47E{+}00$ +/-16%	$3.28E{+}00$ +/-22%	1.06	1.20	1.18	1.10	166.43
2.68	$2.88E{+}00$ +/-16%	$2.75E{+}00$ +/-21%	1.05	1.19	1.17	1.09	138.61
3.28	$2.42E{+}00$ +/-16%	$2.31E{+}00$ +/-21%	1.05	1.19	1.17	1.09	116.52
4.17	$1.87E{+}00$ +/-16%	$1.78E{+}00$ +/-21%	1.05	1.18	1.17	1.09	90.27
5.27	$1.34E{+}00$ +/-16%	$1.30E{+}00$ +/-21%	1.04	1.17	1.15	1.07	65.34
6.37	$9.82E{-}01$ +/-16%	$9.48E{-}01$ +/-20%	1.04	1.16	1.15	1.07	47.97
8.00	$6.25E{-}01$ +/-16%	$6.03E{-}01$ +/-19%	1.04	1.15	1.15	1.07	30.73
10.12	$3.53E{-}01$ +/-16%	$3.46E{-}01$ +/-17%	1.02	1.12	1.12	1.05	17.51
12.22	$2.10E{-}01$ +/-16%	$2.09E{-}01$ +/-15%	1.01	1.09	1.10	1.03	10.55
15.35	$1.09E{-}01$ +/-16%	$1.11E{-}01$ +/-11%	0.98	1.04	1.05	1.00	5.54
19.45	$5.70E{-}02$ +/-16%	$6.19E{-}02$ +/-7%	0.92	0.94	0.95	0.93	2.95
23.52	$3.93E{-}02$ +/-16%	$4.36E{-}02$ +/-6%	0.90	0.90	0.91	0.90	2.07
27.62	$3.10E{-}02$ +/-16%	$3.49E{-}02$ +/-7%	0.89	0.88	0.89	0.89	1.66
34.75	$2.45E{-}02$ +/-16%	$2.73E{-}02$ +/-9%	0.90	0.88	0.90	0.90	1.35
44.85	$2.02E{-}02$ +/-17%	$2.18E{-}02$ +/-10%	0.93	0.91	0.93	0.93	1.17
54.92	$1.97E{-}02$ +/-17%	$1.88E{-}02$ +/-11%	1.05	1.02	1.05	1.05	1.19
mean % diff. from E			5	12	11	7	78
mean χ^2			0.15	0.66	0.54	0.23	28.22

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Al28	2.24m	0.99	16%	26%
Si31	2.62h	0.93	17%	13%

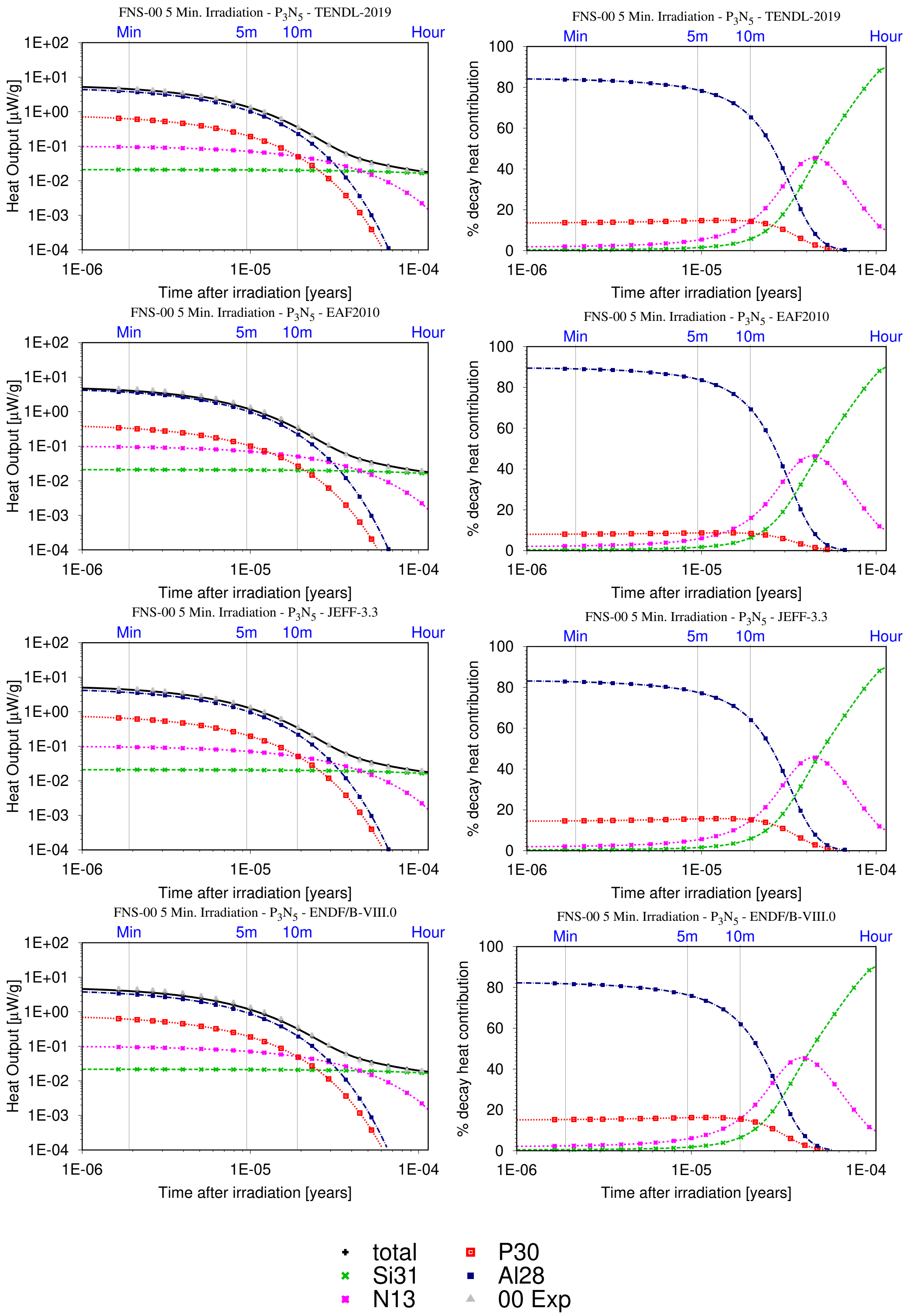


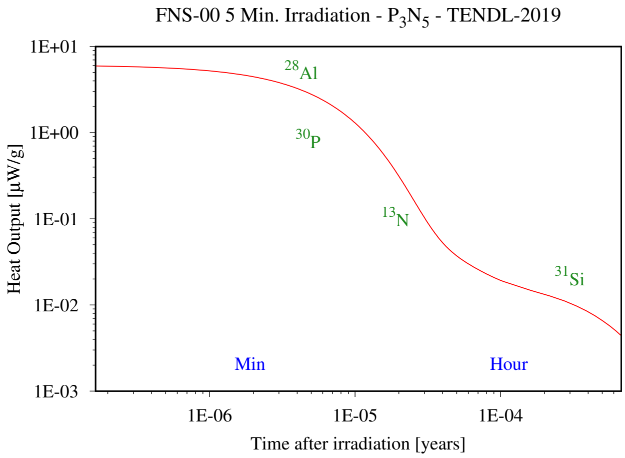
Phosphorus, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Al28	2.24m	P31(n,α)Al28	100.0
P30	2.50m	P31(n,2n)P30	100.0
N13	9.97m	N14(n,2n)N13	100.0
Si31	2.62h	P31(n,p)Si31	100.0

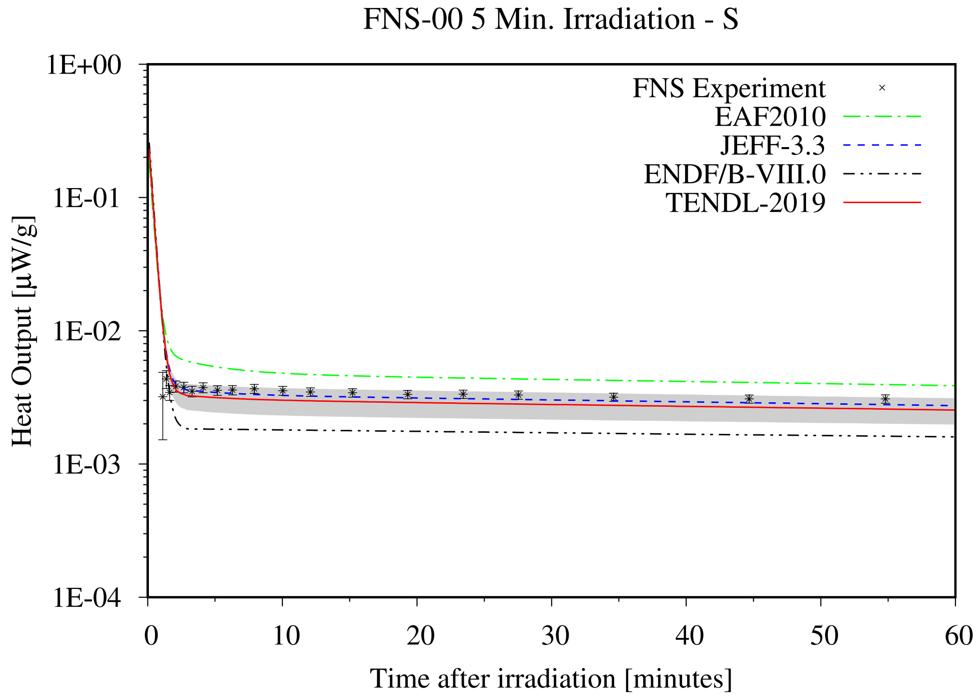
Comments on Phosphorus 5-minute experiments:

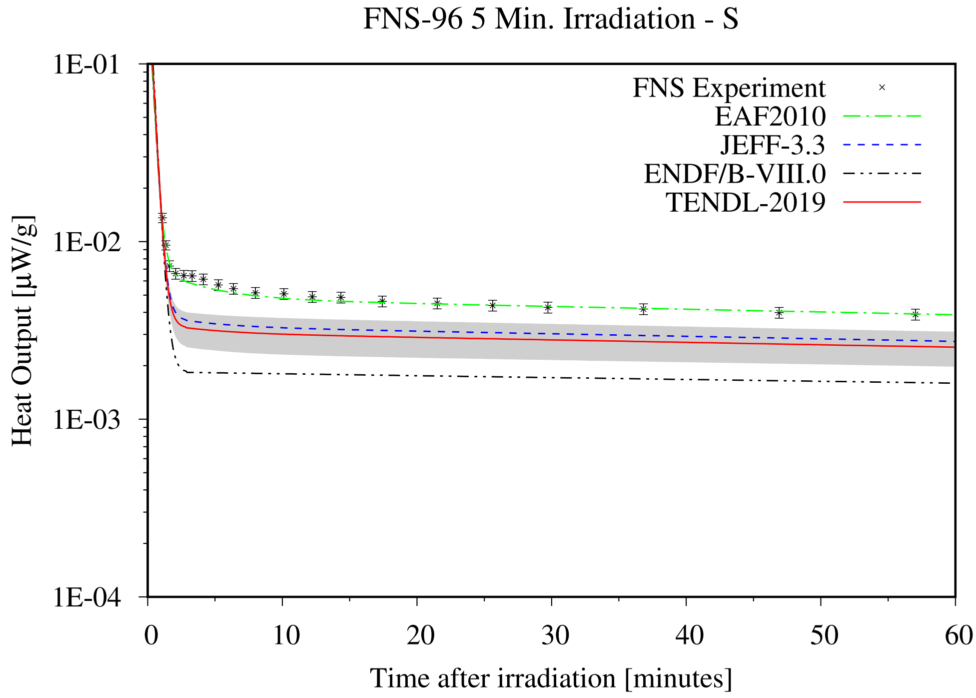
IRDFF-II is only concerned with the longer-lived Si31 nuclide and so doesn't include data for the reactions that produce the shorter-lived nuclides in phosphorus but captures well the experimental decay heat level associated with that former nuclide (as do the general-purpose libraries). Al28 dominates the decay heat in the simulations with the other libraries at times less than 30-40 minutes and there is good agreement between the simulated results and the experimental decay heat measured for this nitrate sample – although the experimental uncertainty is a suspiciously uniform 16%.


FNS-00 5 Min. Irradiation - P3N5 - TENDL-2019
FNS-00 5 Min. Irradiation - P3N5 - EAF2010
FNS-00 5 Min. Irradiation - P3N5 - JEFF-3.3
FNS-00 5 Min. Irradiation - P3N5 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Si31
N13
P30
Al28
00 Exp

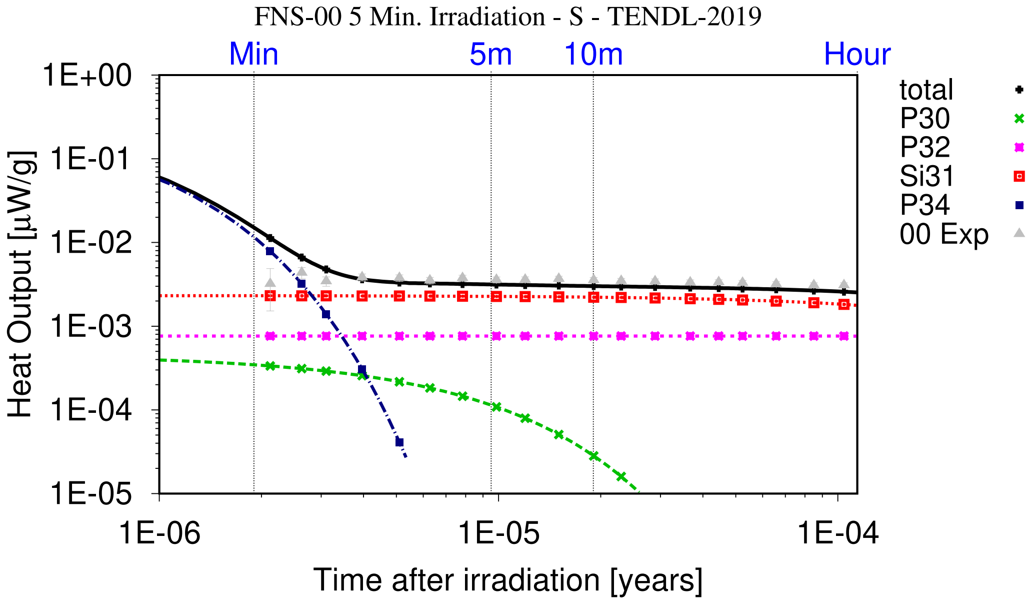

FNS-00 5 Min. Irradiation - P3N5 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
28Al
30P
13N
31Si
Min
Hour
1E-06
1E-05
1E-04
Time after irradiation [years]

Sulphur


FNS-00 5 Min. Irradiation - S
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - S
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
0
10
20
30
40
50
60
Time after irradiation [minutes]

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
1.12	$3.20E{-}03$ +/-52%	$1.13E{-}02$ +/-20%	0.28	0.30	0.25	0.28
1.38	$4.35E{-}03$ +/-15%	$6.62E{-}03$ +/-17%	0.66	0.79	0.48	0.63
1.63	$3.44E{-}03$ +/-13%	$4.77E{-}03$ +/-17%	0.72	1.01	0.46	0.68
2.08	$3.83E{-}03$ +/-10%	$3.64E{-}03$ +/-20%	1.05	1.75	0.59	0.96
2.68	$3.76E{-}03$ +/-9%	$3.32E{-}03$ +/-22%	1.13	1.99	0.62	1.02
3.30	$3.51E{-}03$ +/-9%	$3.24E{-}03$ +/-22%	1.08	1.91	0.61	0.99
4.12	$3.75E{-}03$ +/-8%	$3.20E{-}03$ +/-23%	1.17	2.05	0.67	1.07
5.18	$3.58E{-}03$ +/-8%	$3.15E{-}03$ +/-23%	1.14	1.96	0.67	1.04
6.30	$3.59E{-}03$ +/-8%	$3.10E{-}03$ +/-23%	1.16	1.97	0.70	1.06
7.92	$3.67E{-}03$ +/-8%	$3.06E{-}03$ +/-23%	1.20	2.03	0.74	1.10
10.03	$3.55E{-}03$ +/-8%	$3.01E{-}03$ +/-23%	1.18	1.97	0.74	1.08
12.08	$3.47E{-}03$ +/-7%	$2.98E{-}03$ +/-23%	1.16	1.93	0.74	1.07
15.22	$3.43E{-}03$ +/-7%	$2.94E{-}03$ +/-23%	1.16	1.92	0.75	1.07
19.32	$3.33E{-}03$ +/-7%	$2.90E{-}03$ +/-23%	1.15	1.89	0.74	1.06
23.43	$3.35E{-}03$ +/-7%	$2.86E{-}03$ +/-23%	1.17	1.92	0.76	1.08
27.53	$3.29E{-}03$ +/-7%	$2.82E{-}03$ +/-23%	1.17	1.91	0.76	1.08
34.62	$3.18E{-}03$ +/-7%	$2.76E{-}03$ +/-23%	1.15	1.87	0.75	1.07
44.68	$3.08E{-}03$ +/-7%	$2.67E{-}03$ +/-23%	1.15	1.86	0.75	1.07
54.80	$3.08E{-}03$ +/-7%	$2.59E{-}03$ +/-22%	1.19	1.90	0.78	1.10
mean % diff. from E			29	54	63	24
mean χ^2			4.95	33.60	32.76	3.38

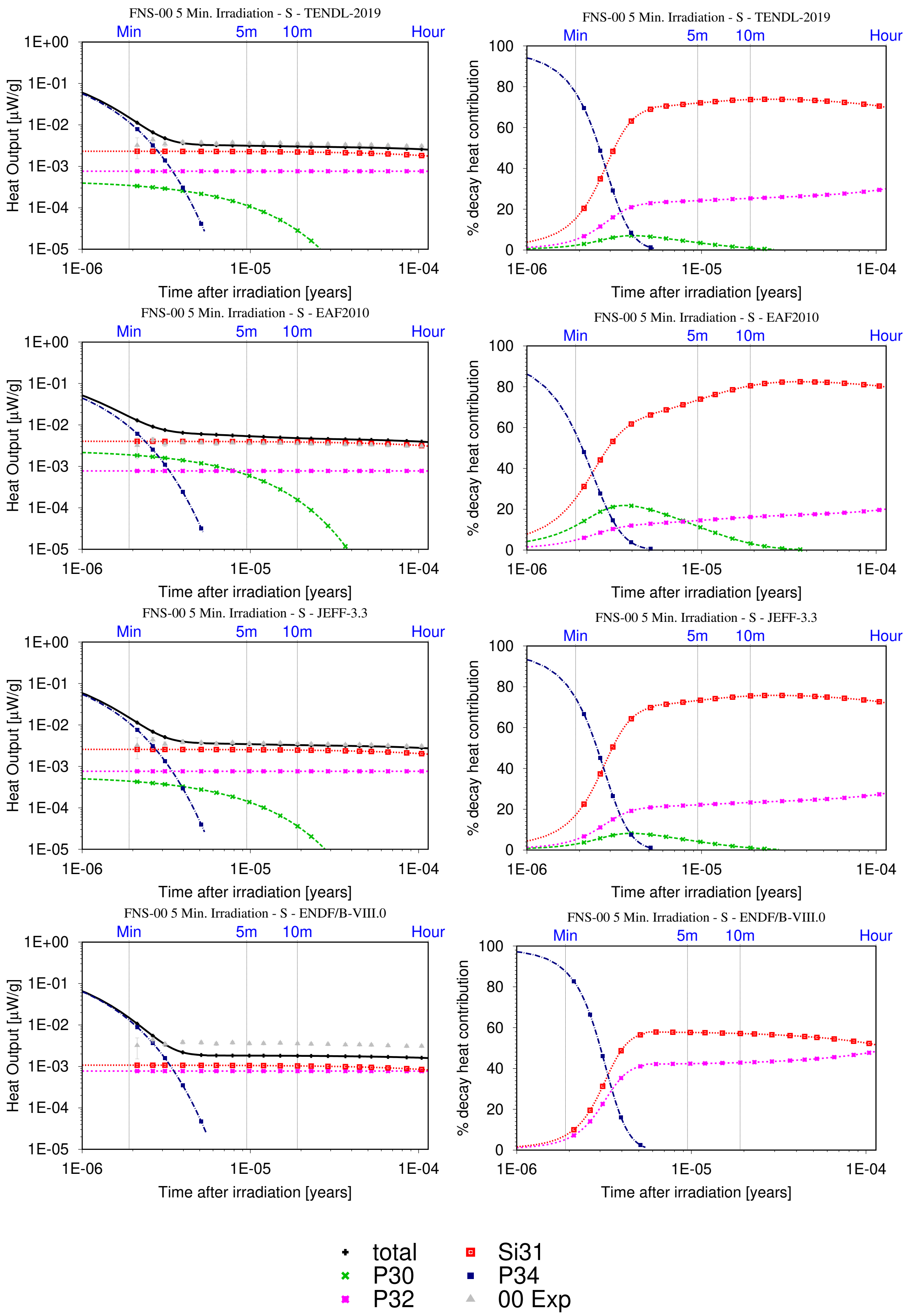


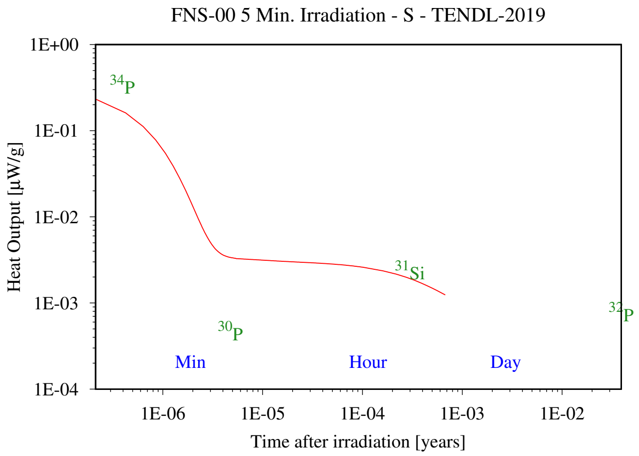
Sulphur, TENDL-2019 5-minute pathway analysis

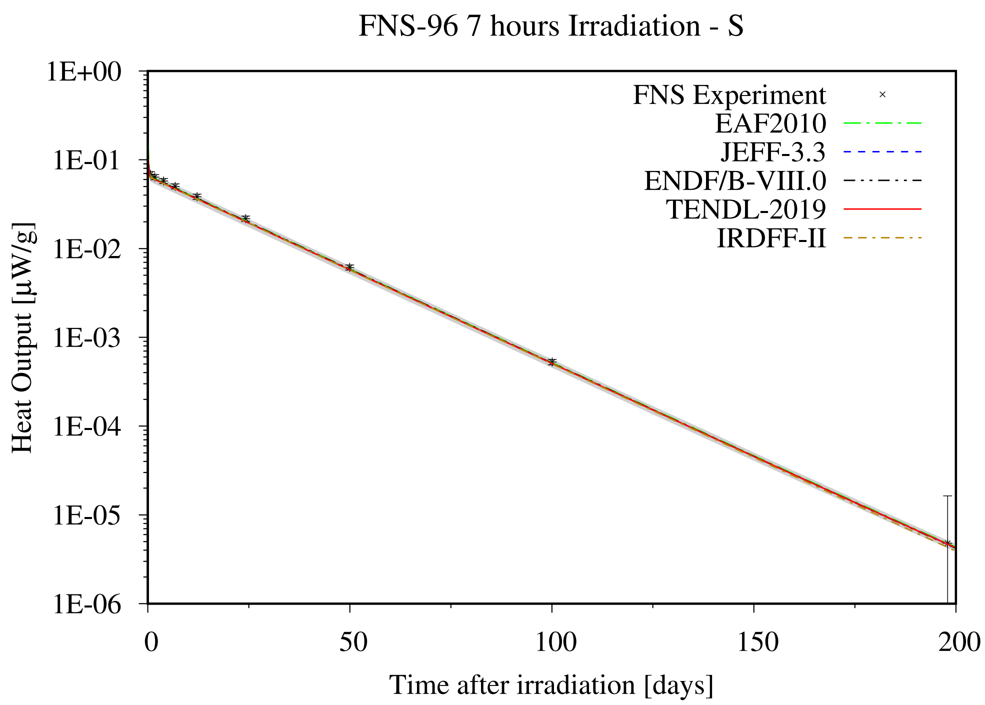
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
P34	12.40s	S34(n,p)P34	100.0
P30	2.50m	S32(n,t)P30	100.0
Si31	2.62h	S34(n,α)Si31	78.2
		S32(n,2p)Si31	21.8
P32	14.27d	S32(n,p)P32	99.5

Comments on Sulphur 5-minute experiments:

The two sets of experimental measurements following 5-minute exposures do not agree, despite the fact that they should have been performed on identical sulphur samples. There is good agreement between TENDL-2019, JEFF-3.3 and the most recent 2000 experiment, while EAF2010 seems to match well with the earlier 1996 experiment. It is difficult to interpret anything more from these results because of such discrepant experimental measurements, although the library simulations all seem to reproduce the time-evolution profile of the experiments well, suggesting that the predicted radionuclide distribution – P34 dominance at first followed by a combination of Si31 and P32 – is a good fit to the experimental reality. Interestingly, ENDF/B-VIII.0 appears to predict a significantly smaller amount of Si31 compared to JEFF, TENDL and EAF because it lacks the (n,2p) production route from S32.


FNS-00 5 Min. Irradiation - S - TENDL-2019
FNS-00 5 Min. Irradiation - S - EAF2010
FNS-00 5 Min. Irradiation - S - JEFF-3.3
FNS-00 5 Min. Irradiation - S - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
P30
P32
Si31
P34
00 Exp

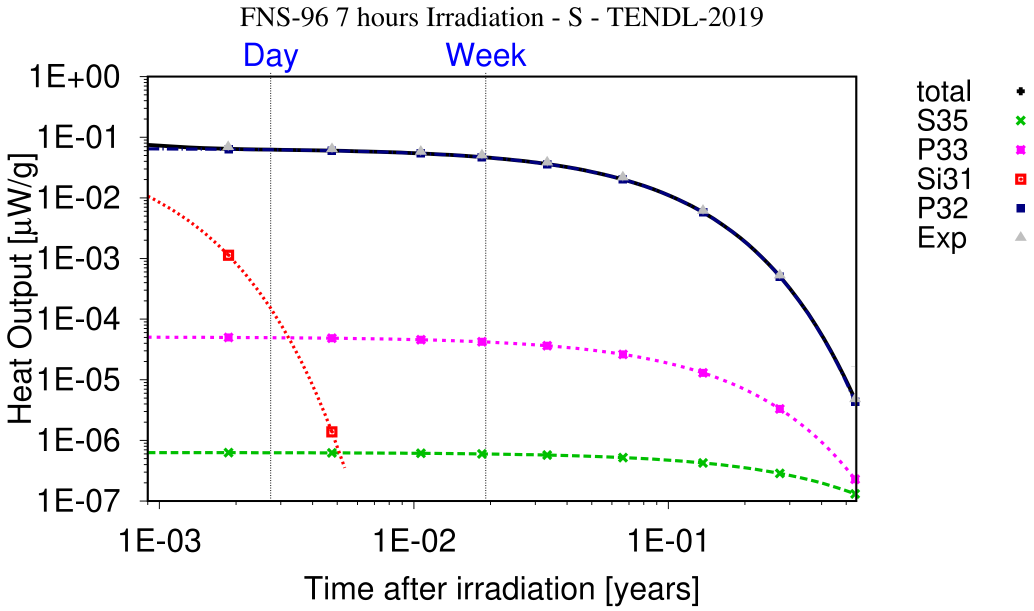

FNS-00 5 Min. Irradiation - S - TENDL-2019
1E+00
1E-01
1E-02
1E-03
1E-04
Heat Output [μW/g]
34P
31Si
30P
32P
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.68	$6.87E{-}02$ +/-7%	$6.43E{-}02$ +/-11%	1.07	1.06	1.04	1.07	1.09
1.74	$6.38E{-}02$ +/-7%	$6.00E{-}02$ +/-11%	1.06	1.05	1.04	1.06	1.07
3.89	$5.77E{-}02$ +/-7%	$5.41E{-}02$ +/-11%	1.07	1.05	1.05	1.07	1.07
6.76	$5.02E{-}02$ +/-7%	$4.71E{-}02$ +/-11%	1.07	1.05	1.05	1.07	1.07
12.20	$3.84E{-}02$ +/-7%	$3.61E{-}02$ +/-11%	1.06	1.05	1.04	1.06	1.07
24.21	$2.17E{-}02$ +/-7%	$2.02E{-}02$ +/-11%	1.08	1.06	1.06	1.08	1.08
49.96	$6.13E{-}03$ +/-7%	$5.78E{-}03$ +/-11%	1.06	1.05	1.04	1.06	1.07
100.09	$5.27E{-}04$ +/-7%	$5.09E{-}04$ +/-11%	1.04	1.03	1.02	1.04	1.05
197.94	$4.79E{-}06$ +/-242%	$4.72E{-}06$ +/-10%	1.02	1.03	1.00	1.02	1.10
mean % diff. from E			5	5	4	5	7
mean χ^2			0.70	0.47	0.34	0.68	0.90

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
P32	14.27d	1.07	7%	11%

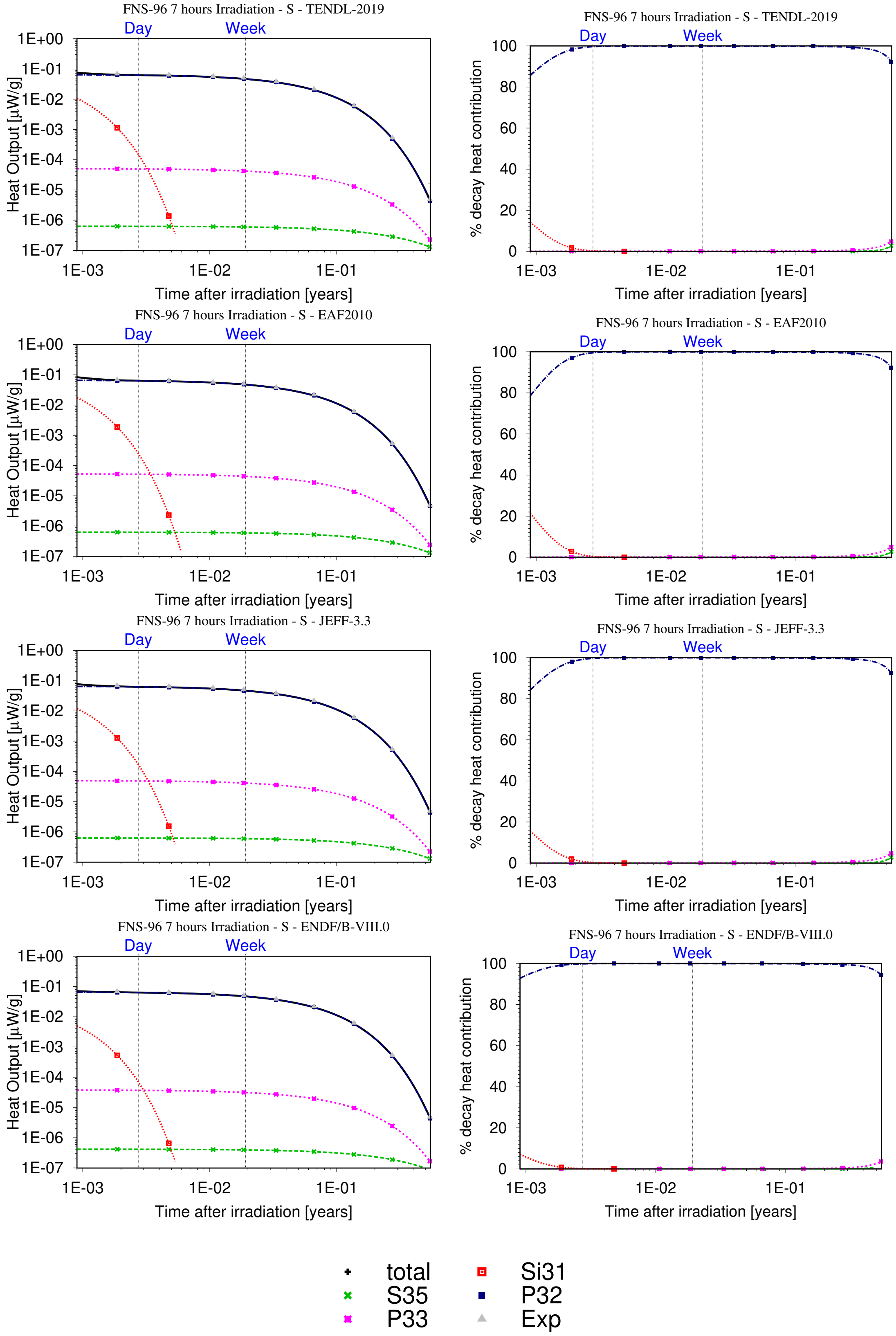


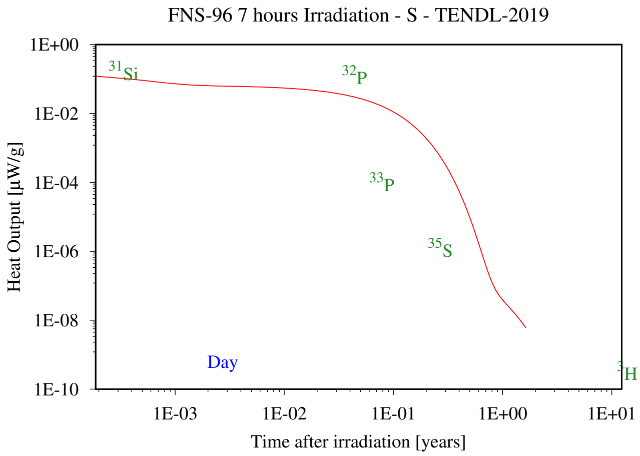
Sulphur,TENDL-2019 7-hours pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Si31	2.62h	S34(n,α)Si31	83.3
		S32(n,2p)Si31	16.7
P32	14.27d	S32(n,p)P32	99.5
P33	25.38d	S34(n,np)P33	52.6
		S33(n,p)P33	35.0
		S34(n,d)P33	12.4
S35	87.32d	S36(n,2n)S35	90.3
		S34(n,γ)S35	9.6

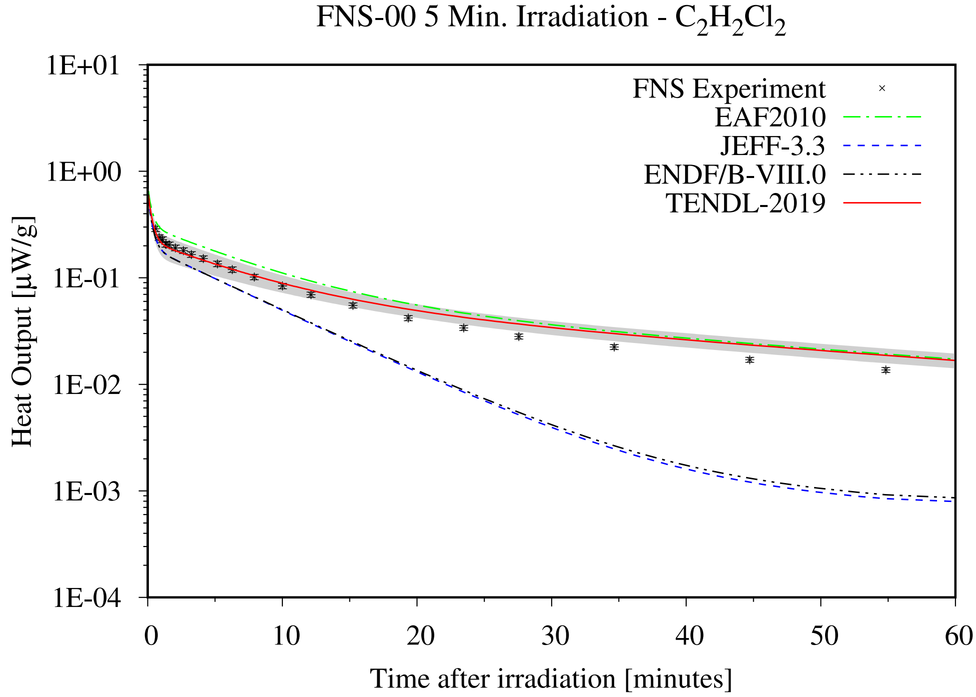
Comments on Sulphur 7-hour experiments:

This is an unambiguous, text-book case of a single important radionuclide (P32) producing all of the measured decay heat. All of the libraries (including IRDFF-II) correctly capture the behaviour both qualitatively and quantitatively, although only TENDL-2019 contains covariance data for the crucial (n,p) channel on S32. A better reproduction of the cross section structure has been achieved in 2-5 MeV region in TENDL-2019, potentially contributing to a slight improvement compared to TENDL-2017.

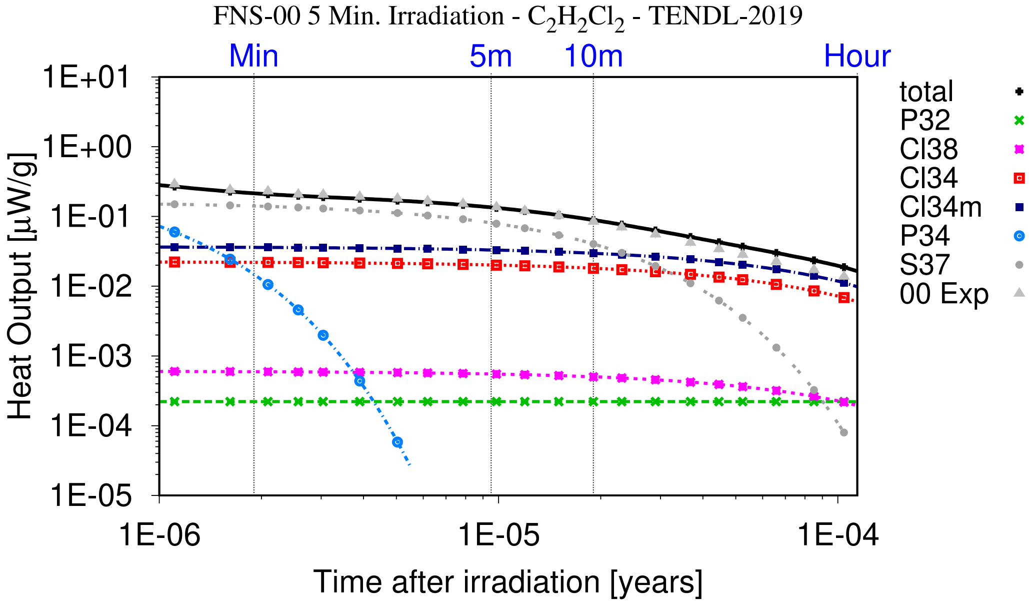

FNS-96 7 hours Irradiation - S - TENDL-2019
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - S - EAF2010
FNS-96 7 hours Irradiation - S - JEFF-3.3
FNS-96 7 hours Irradiation - S - ENDF/B-VIII.0
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
0
20
40
60
80
100
total
S35
P33
Si31
P32
Exp


FNS-96 7 hours Irradiation - S - TENDL-2019
Heat Output [µW/g]
1E+00
1E-02
1E-04
1E-06
1E-08
1E-10
31Si
32P
33P
35S
Day
3H
1E-03
1E-02
1E-01
1E+00
1E+01
Time after irradiation [years]

Chlorine



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	$2.89E{-}01$ +/-6%	$2.69E{-}01$ +/-22%	1.07	1.22	0.84	1.21
0.85	$2.39E{-}01$ +/-6%	$2.28E{-}01$ +/-24%	1.05	1.21	0.79	1.21
1.10	$2.28E{-}01$ +/-6%	$2.08E{-}01$ +/-25%	1.10	1.28	0.81	1.28
1.35	$2.06E{-}01$ +/-6%	$1.97E{-}01$ +/-25%	1.04	1.24	0.77	1.23
1.60	$2.04E{-}01$ +/-6%	$1.90E{-}01$ +/-25%	1.07	1.29	0.79	1.28
2.05	$1.91E{-}01$ +/-6%	$1.80E{-}01$ +/-25%	1.06	1.29	0.78	1.29
2.65	$1.80E{-}01$ +/-6%	$1.69E{-}01$ +/-25%	1.06	1.33	0.79	1.32
3.25	$1.66E{-}01$ +/-6%	$1.59E{-}01$ +/-24%	1.04	1.32	0.77	1.32
4.13	$1.52E{-}01$ +/-6%	$1.46E{-}01$ +/-23%	1.04	1.37	0.78	1.37
5.18	$1.35E{-}01$ +/-6%	$1.33E{-}01$ +/-23%	1.02	1.41	0.77	1.41
6.28	$1.19E{-}01$ +/-6%	$1.20E{-}01$ +/-22%	0.99	1.44	0.76	1.45
7.92	$1.02E{-}01$ +/-6%	$1.05E{-}01$ +/-20%	0.97	1.53	0.76	1.54
10.02	$8.38E{-}02$ +/-6%	$8.89E{-}02$ +/-19%	0.94	1.67	0.76	1.69
12.13	$6.95E{-}02$ +/-6%	$7.64E{-}02$ +/-17%	0.91	1.84	0.75	1.87
15.25	$5.50E{-}02$ +/-6%	$6.29E{-}02$ +/-16%	0.87	2.20	0.74	2.24
19.35	$4.19E{-}02$ +/-6%	$5.08E{-}02$ +/-15%	0.83	2.84	0.73	2.93
23.47	$3.39E{-}02$ +/-6%	$4.26E{-}02$ +/-14%	0.80	3.83	0.72	3.99
27.57	$2.81E{-}02$ +/-5%	$3.69E{-}02$ +/-15%	0.76	5.14	0.71	5.42
34.65	$2.24E{-}02$ +/-5%	$3.00E{-}02$ +/-15%	0.75	8.44	0.71	9.04
44.72	$1.70E{-}02$ +/-5%	$2.34E{-}02$ +/-15%	0.73	12.92	0.70	14.08
54.83	$1.37E{-}02$ +/-5%	$1.87E{-}02$ +/-16%	0.73	14.83	0.71	16.17
mean % diff. from E			13	44	32	44
mean χ^2			10.50	84.53	31.70	86.15

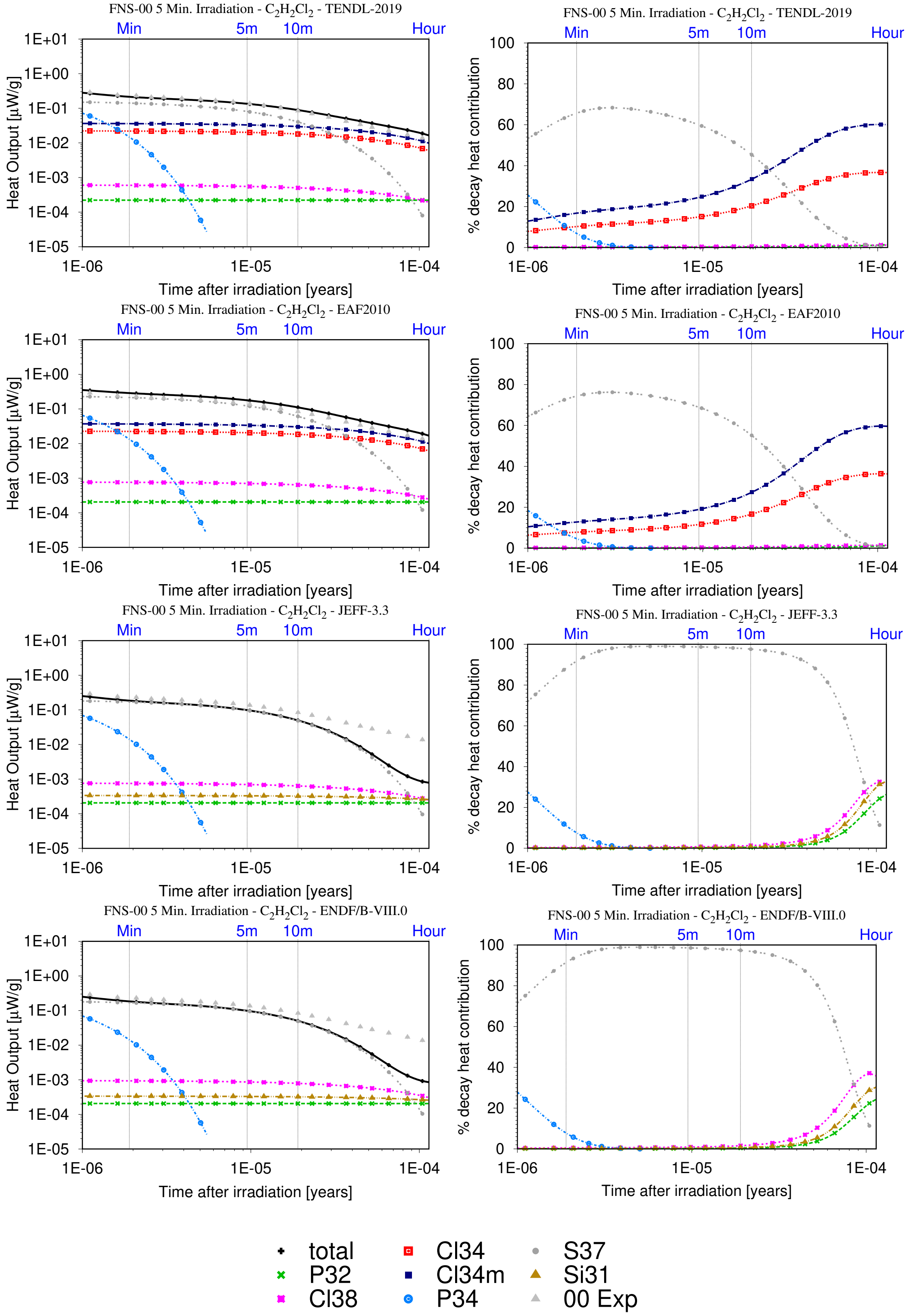


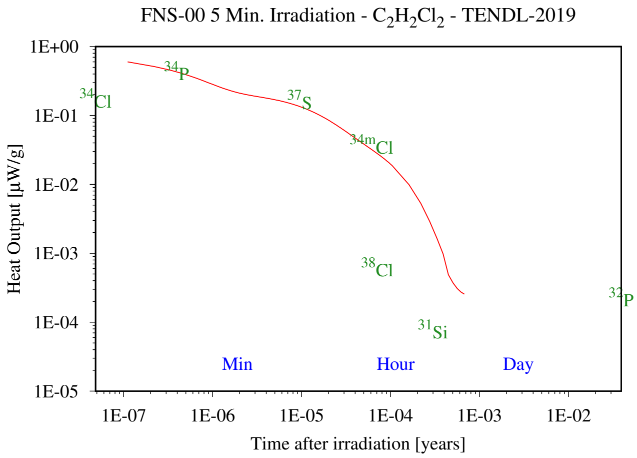
Chlorine, TENDL-2019 5-minute pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Cl34	1.53s	Cl35(n,2n)Cl34	86.9
		Cl35(n,2n)Cl34m(IT)Cl34	13.1
P34	12.40s	Cl37(n,α)P34	99.9
S37	4.99m	Cl37(n,p)S37	100.0
Cl34m	32.10m	Cl35(n,2n)Cl34m	100.0
Cl38	37.21m	Cl37(n,γ)Cl38	73.1
		Cl37(n,γ)Cl38m(IT)Cl38	26.9
Si31	2.62h	Cl35(n,pα)Si31	100.0
P32	14.27d	Cl35(n,α)P32	100.0

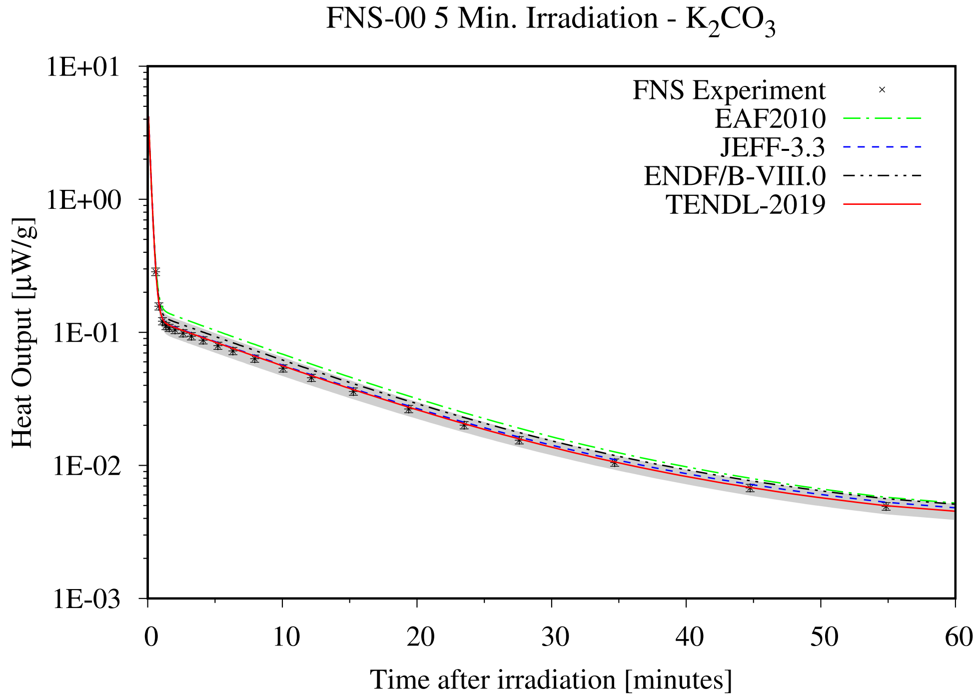
Comments on Chlorine 5-minute experiments:

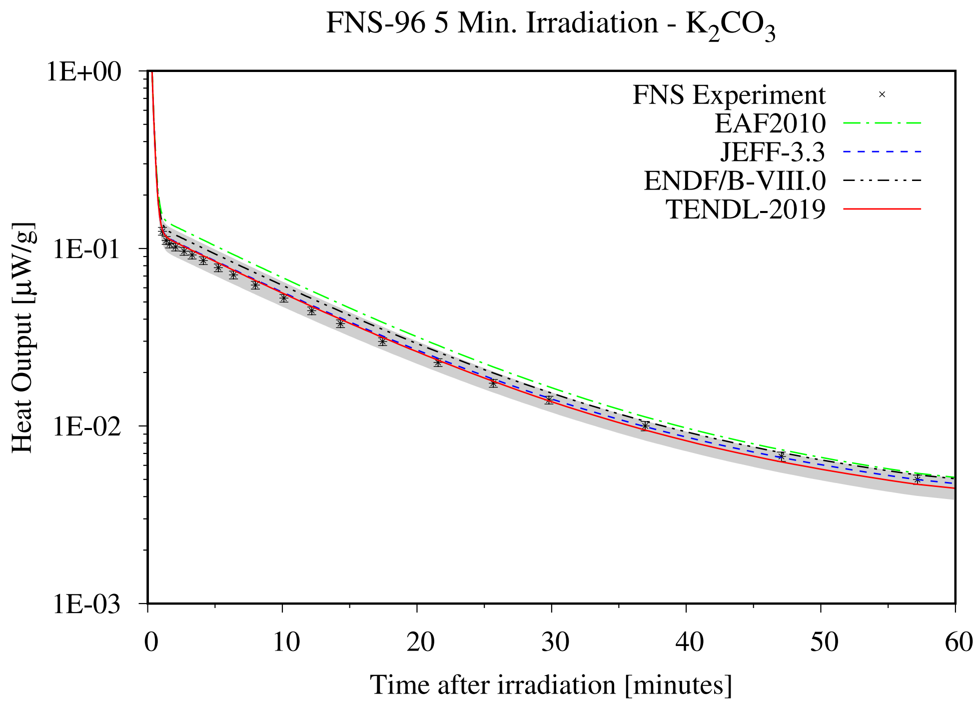
All of the libraries show reasonable agreement with the short-term ($<$ 5 minute) experimental behaviour in Chlorine, which is predominantly from S37. However, JEFF-3.3 and ENDF/B-VIII.0 fail to produce the either Cl34 or Cl34m nuclide (via (n,2n) reactions on Cl35), which predominant in simulations with TENDL-2019 and EAF2010 beyond around 15 minutes of cooling, and so only those latter libraries show some agreement with the experiment beyond this point. However, even in those cases, there is discrepancy (overprediction), which may be a sign of an incorrectly allocated branching ratios or decay-heat contributions for the short-lived metastable and even shorter-lived ground-state that it decays to (which creates the secular equilibrium shown in the plots). Note that the E/C table is omitted here because the simulations predict non-negligible contributions from several radionuclides at all measurement times (see the nuclide contribution graph).


FNS-00 5 Min. Irradiation - $C_2H_2Cl_2$ - TENDL-2019
FNS-00 5 Min. Irradiation - $C_2H_2Cl_2$ - EAF2010
FNS-00 5 Min. Irradiation - $C_2H_2Cl_2$ - JEFF-3.3
FNS-00 5 Min. Irradiation - $C_2H_2Cl_2$ - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
P32
Cl38
Cl34
Cl34m
P34
S37
Si31
00 Exp


FNS-00 5 Min. Irradiation - C2H2Cl2 - TENDL-2019
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
Heat Output [µW/g]
34Cl
34P
37S
34mCl
38Cl
31Si
32P
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

Potassium

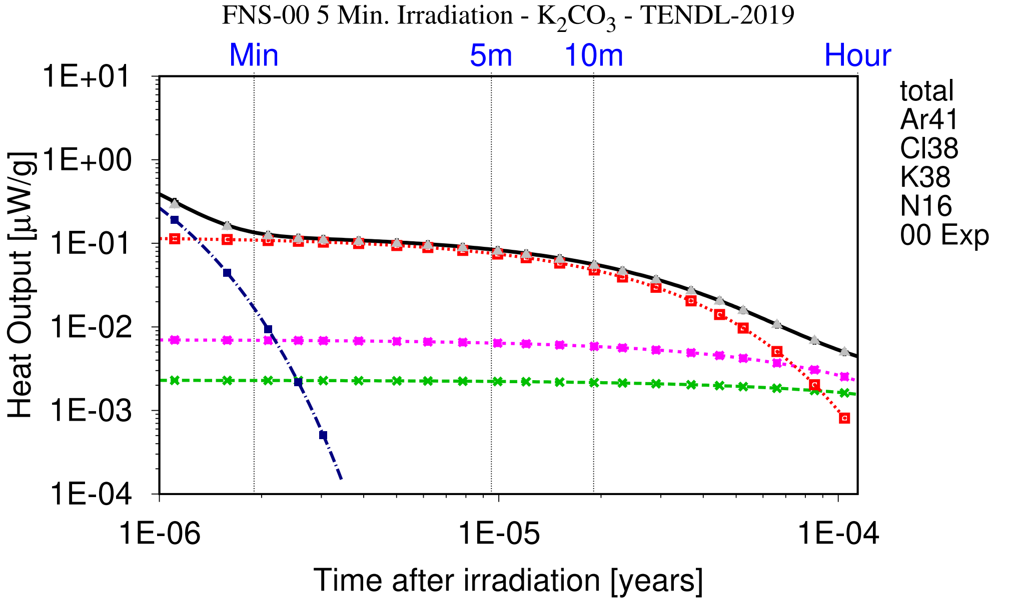

FNS-00 5 Min. Irradiation - K_2CO_3
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - K_2CO_3
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	2.85E−01 +/-7%	3.13E−01 +/-7%	0.91	0.88	0.85	0.91
0.83	1.57E−01 +/-6%	1.64E−01 +/-13%	0.95	0.89	0.82	0.95
1.10	1.21E−01 +/-6%	1.27E−01 +/-16%	0.96	0.88	0.79	0.95
1.35	1.12E−01 +/-6%	1.17E−01 +/-17%	0.95	0.87	0.78	0.95
1.60	1.08E−01 +/-6%	1.13E−01 +/-17%	0.96	0.87	0.78	0.95
2.03	1.04E−01 +/-6%	1.08E−01 +/-17%	0.96	0.87	0.78	0.95
2.63	9.86E−02 +/-6%	1.03E−01 +/-17%	0.96	0.87	0.78	0.95
3.25	9.36E−02 +/-6%	9.79E−02 +/-17%	0.96	0.87	0.78	0.95
4.12	8.72E−02 +/-6%	9.10E−02 +/-17%	0.96	0.87	0.78	0.95
5.22	7.94E−02 +/-6%	8.30E−02 +/-17%	0.96	0.87	0.78	0.95
6.33	7.25E−02 +/-6%	7.57E−02 +/-17%	0.96	0.87	0.78	0.95
7.95	6.35E−02 +/-6%	6.63E−02 +/-16%	0.96	0.87	0.78	0.95
10.05	5.37E−02 +/-6%	5.59E−02 +/-16%	0.96	0.87	0.79	0.95
12.17	4.55E−02 +/-6%	4.72E−02 +/-16%	0.96	0.87	0.79	0.95
15.28	3.59E−02 +/-6%	3.71E−02 +/-15%	0.97	0.87	0.79	0.95
19.38	2.66E−02 +/-6%	2.74E−02 +/-15%	0.97	0.87	0.80	0.95
23.50	2.01E−02 +/-6%	2.06E−02 +/-14%	0.97	0.87	0.81	0.95
27.60	1.55E−02 +/-6%	1.58E−02 +/-13%	0.98	0.88	0.81	0.95
34.68	1.05E−02 +/-6%	1.06E−02 +/-13%	0.99	0.88	0.83	0.95
44.75	6.77E−03 +/-6%	6.83E−03 +/-13%	0.99	0.88	0.85	0.94
54.85	4.93E−03 +/-6%	4.98E−03 +/-14%	0.99	0.88	0.85	0.93
mean % diff. from E			4	15	25	6
mean χ^2			0.46	5.39	16.50	0.85

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$T_{1/2}$	E/C	%ΔE	%ΔC^{nuc}
K38	7.61m	0.96	6%	19%

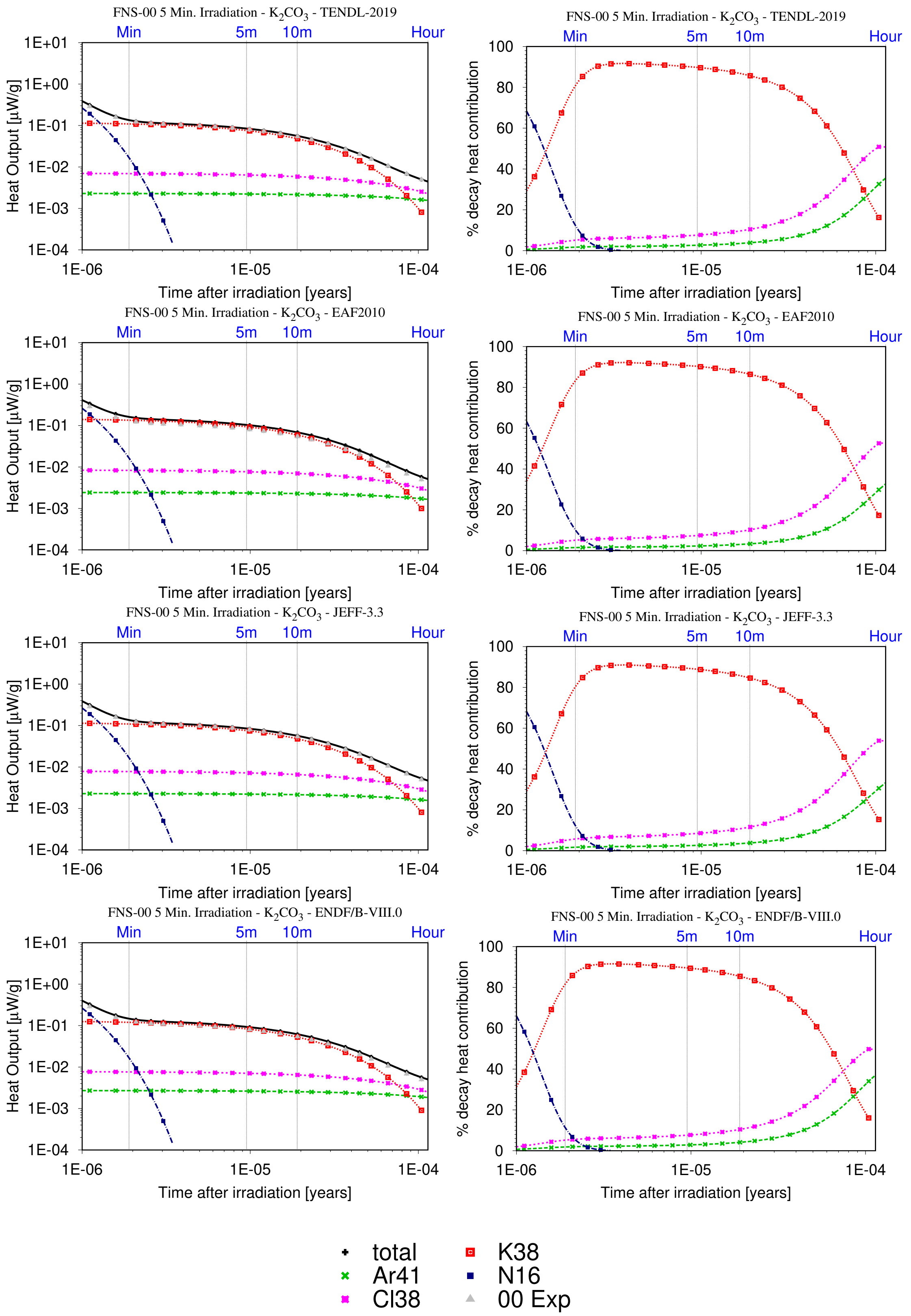


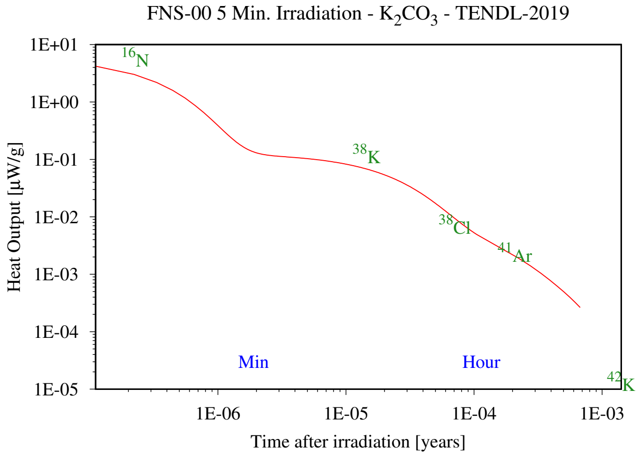
Potassium, TENDL-2019 5-minute pathway analysis

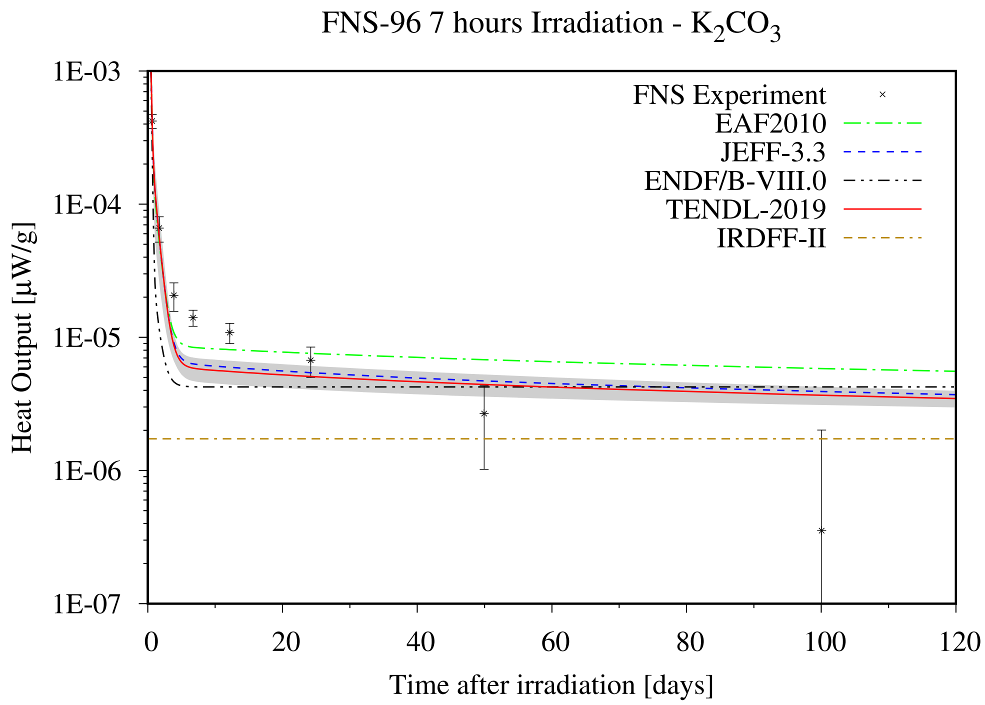
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
K38	7.61m	K39(n,2n)K38	100.0
Cl38	37.21m	K41(n,α)Cl38	71.9
		K41(n,α)Cl38m(IT)Cl38	25.4
		K39(n,2p)Cl38	1.8
Ar41	1.83h	K41(n,p)Ar41	100.0

Comments on Potassium 5-minute experiments:

The extremely rapid measurement – made barely 34 seconds after the irradiation – of the decay heat from the potassium sample with more than 30 wt.% oxygen allows for a glimpse of the contribution of the short-lived N16 isotope. After this has decayed, first K38 and then Cl38 are the predominant contributors to decay heat (the latter is also joined by Ar41 at around 30% at 1 hour of cooling). All included libraries seem to show a some overprediction of production for K38, in particular. TENDL-2019 is the best match (and seems to show less overprediction of Cl38 and Ar41) followed by JEFF-3.3.


FNS-00 5 Min. Irradiation - K2CO3 - TENDL-2019
FNS-00 5 Min. Irradiation - K2CO3 - EAF2010
FNS-00 5 Min. Irradiation - K2CO3 - JEFF-3.3
FNS-00 5 Min. Irradiation - K2CO3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Ar41
Cl38
K38
N16
00 Exp

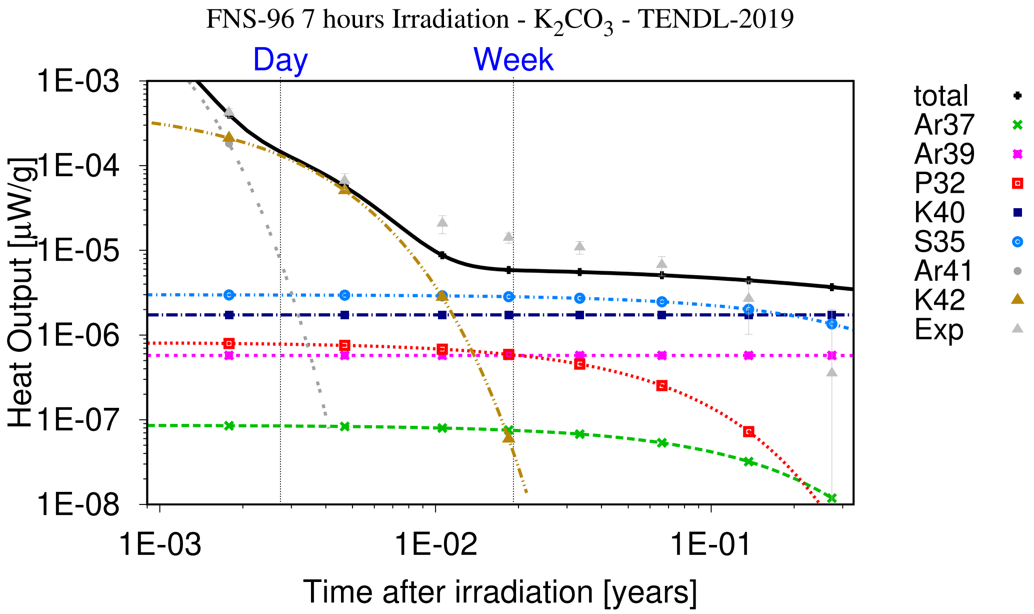

FNS-00 5 Min. Irradiation - K2CO3 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
38K
38Cl
41Ar
42K
Min
Hour
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.65	$4.21E{-}04$ +/-12%	$4.01E{-}04$ +/-33%	1.05	1.72	1.08	1.07	243.55
1.71	$6.62E{-}05$ +/-22%	$5.69E{-}05$ +/-55%	1.16	5.76	1.26	1.18	38.30
3.87	$2.07E{-}05$ +/-24%	$8.76E{-}06$ +/-24%	2.36	4.45	1.89	2.26	11.96
6.73	$1.40E{-}05$ +/-14%	$5.87E{-}06$ +/-20%	2.39	3.30	1.67	2.22	8.12
12.18	$1.09E{-}05$ +/-17%	$5.54E{-}06$ +/-20%	1.96	2.56	1.34	1.82	6.29
24.19	$6.72E{-}06$ +/-26%	$5.08E{-}06$ +/-20%	1.32	1.58	0.89	1.24	3.89
49.94	$2.68E{-}06$ +/-62%	$4.42E{-}06$ +/-19%	0.61	0.63	0.39	0.57	1.55
100.07	$3.53E{-}07$ +/-469%	$3.68E{-}06$ +/-16%	0.10	0.08	0.06	0.09	0.20
mean % diff. from E			152	191	232	160	120
mean χ^2			4.76	10.40	4.13	4.44	21.82

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
K42	12.36h	1.16	22%	61%

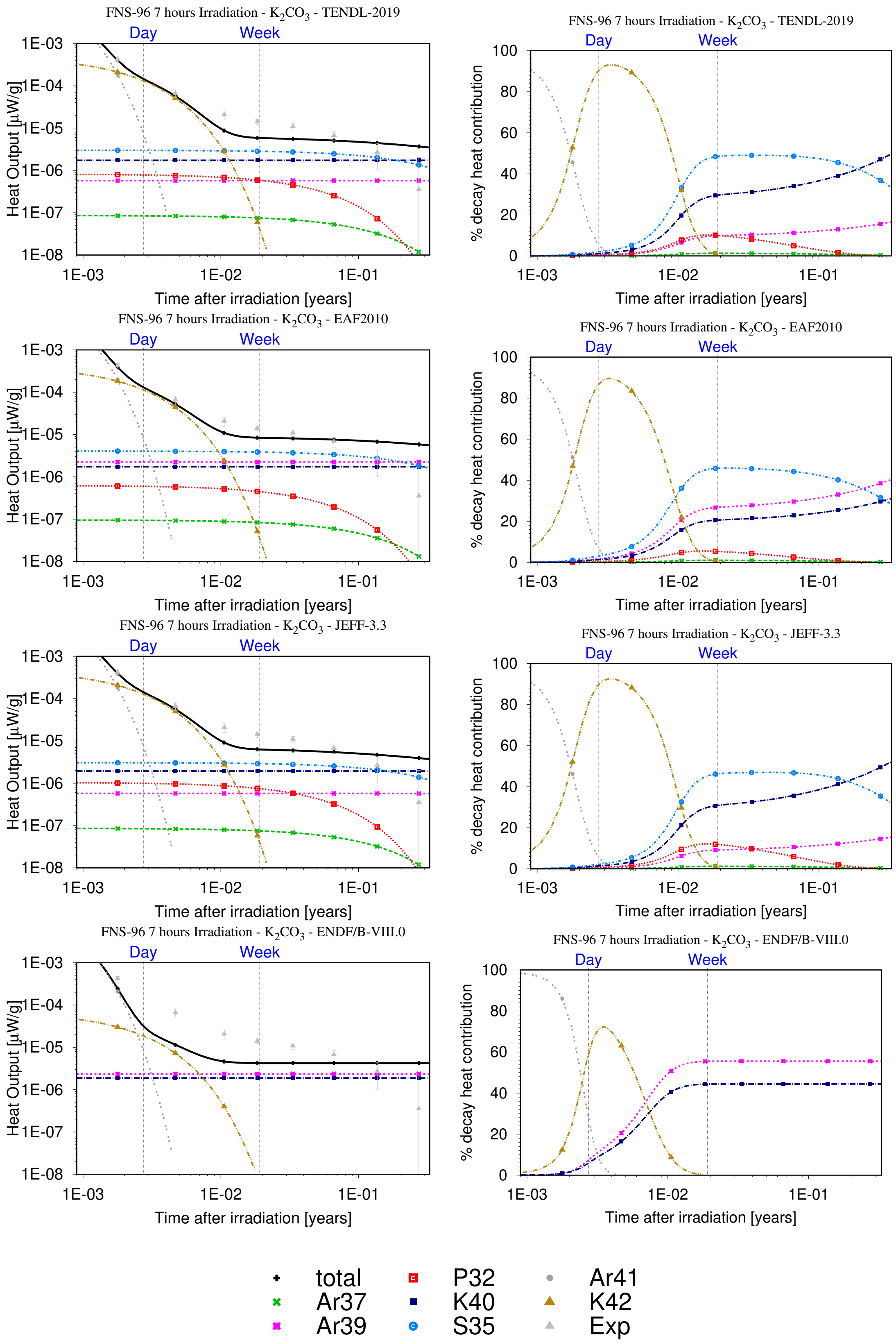


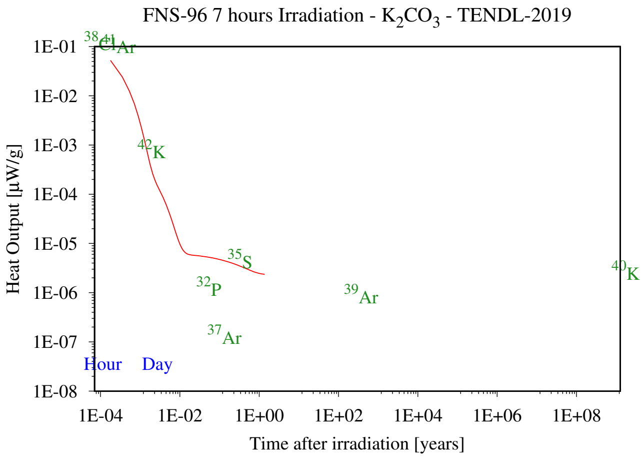
Potassium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Ar41	1.83h	K41(n,p)Ar41	100.0
K42	12.36h	K41(n,γ)K42	100.0
P32	14.27d	K39(n,2α)P32	100.0
Ar37	35.03d	K39(n,t)Ar37	100.0
S35	87.32d	K39(n,pα)S35	100.0
Ar39	269.01y	K39(n,p)Ar39	99.9
K40	1.3 10^9y	no pathways found	

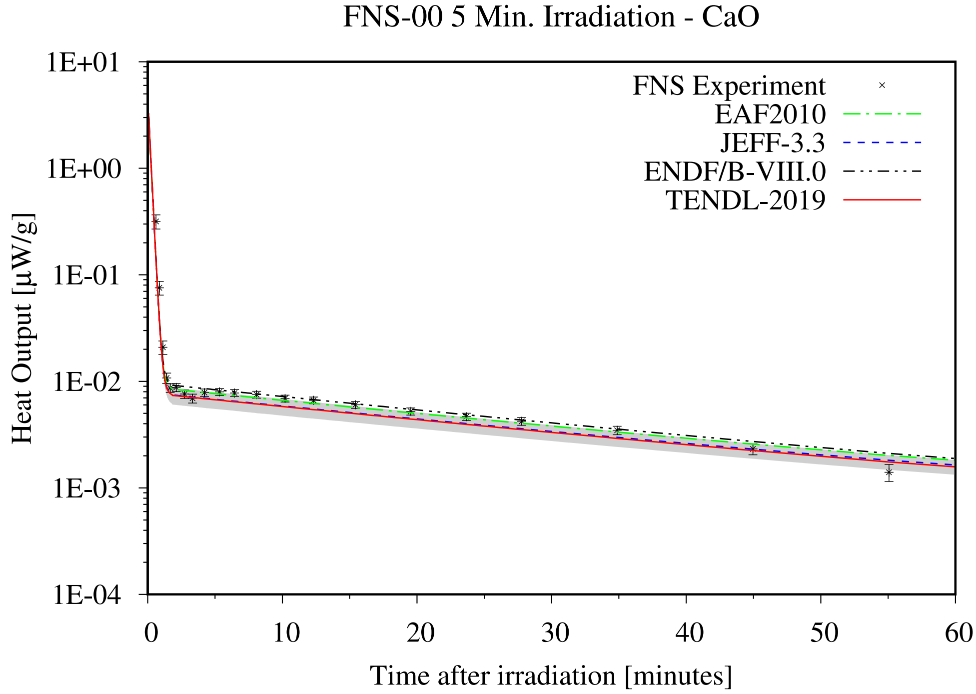
Comments on Potassium 7-hour experiments:

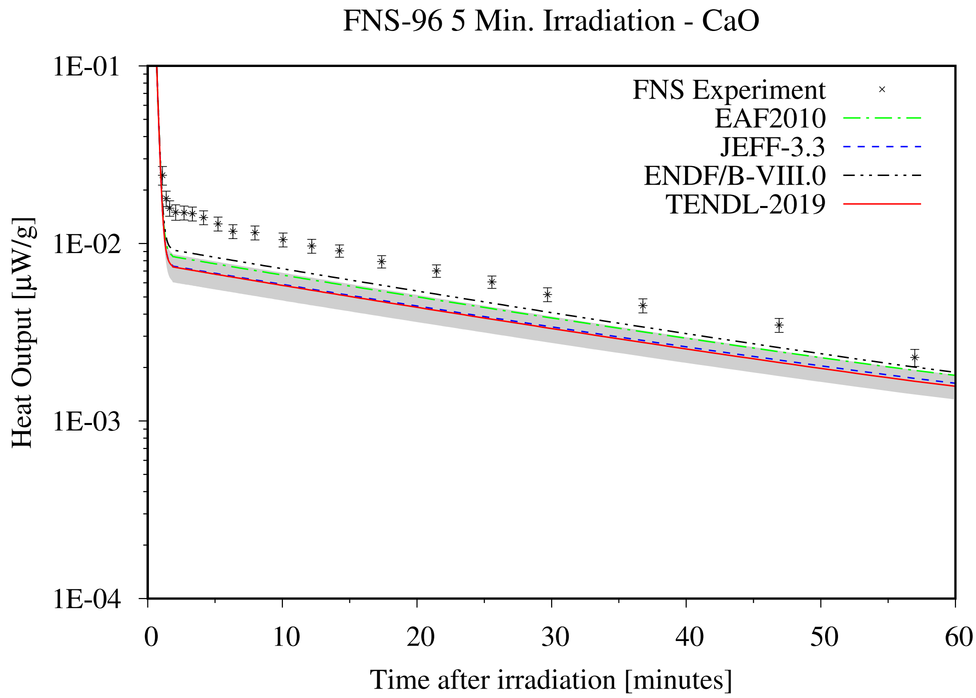
Here the experimental uncertainties are rather high, making a detailed analysis and comparison difficult. The decay-heat profiles appear generally well-shaped with all libraries. Although a better agreement between the experiment and TENDL-2019 results (compared to TENDL-2017) are observed for the experimental measurements at 0.65 and 1.71 days, which could be a sign of an improvement in the evaluation of the (n,γ) channel on K41, producing the K42 radionuclide that dominates the first few cooling times. Notice that K40 is nearly stable on the experimental timescale here.


FNS-96 7 hours Irradiation - K_2CO_3 - TENDL-2019
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - K_2CO_3 - EAF2010
FNS-96 7 hours Irradiation - K_2CO_3 - JEFF-3.3
FNS-96 7 hours Irradiation - K_2CO_3 - ENDF/B-VIII.0
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
1E-02
1E-01
0
20
40
60
80
100
total
Ar37
Ar39
P32
K40
S35
Ar41
K42
Exp


FNS-96 7 hours Irradiation - K2CO3 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
1E-04
1E-02
1E+00
1E+02
1E+04
1E+06
1E+08
38Cl
41Ar
42K
35S
32P
37Ar
39Ar
40K
Hour
Day

Calcium

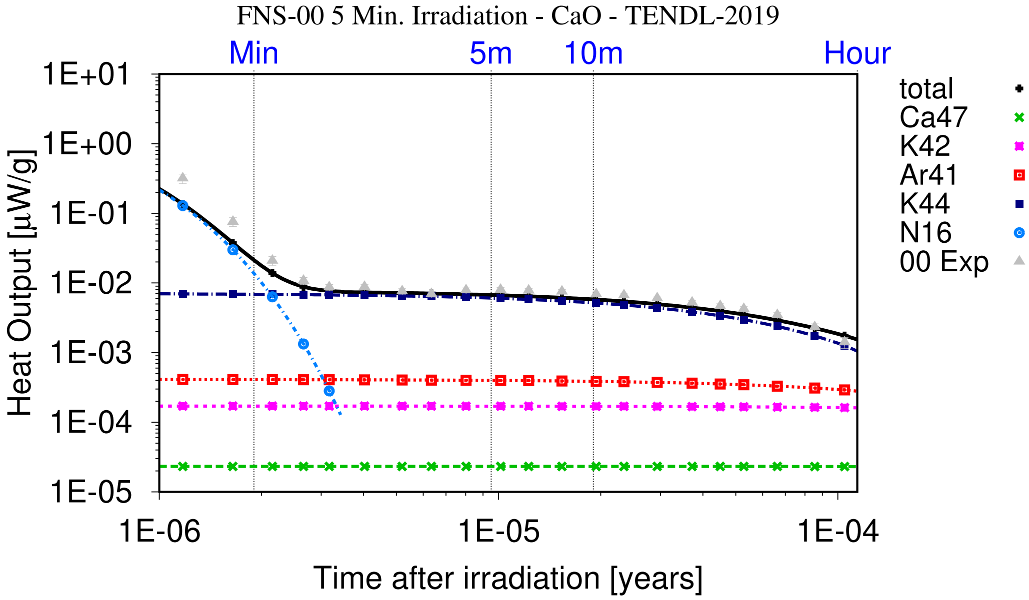

FNS-00 5 Min. Irradiation - CaO
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
Time after irradiation [minutes]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - CaO
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
Time after irradiation [minutes]
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.62	3.17E−01 +/-15%	1.36E−01 +/-1%	2.32	2.30	2.35	2.32
0.87	7.56E−02 +/-15%	3.76E−02 +/-4%	2.01	1.92	1.98	2.01
1.13	2.09E−02 +/-14%	1.39E−02 +/-10%	1.50	1.33	1.41	1.50
1.40	1.07E−02 +/-11%	8.80E−03 +/-15%	1.22	1.01	1.09	1.21
1.67	8.67E−03 +/-9%	7.69E−03 +/-17%	1.13	0.91	0.99	1.11
2.12	8.77E−03 +/-9%	7.32E−03 +/-18%	1.20	0.96	1.05	1.19
2.73	7.60E−03 +/-9%	7.19E−03 +/-18%	1.06	0.85	0.92	1.05
3.33	6.92E−03 +/-9%	7.06E−03 +/-18%	0.98	0.79	0.86	0.97
4.22	7.85E−03 +/-8%	6.87E−03 +/-18%	1.14	0.92	1.00	1.13
5.33	7.97E−03 +/-8%	6.65E−03 +/-18%	1.20	0.96	1.05	1.18
6.45	7.77E−03 +/-8%	6.44E−03 +/-18%	1.21	0.97	1.06	1.19
8.08	7.51E−03 +/-7%	6.14E−03 +/-18%	1.22	0.99	1.07	1.21
10.20	6.91E−03 +/-7%	5.77E−03 +/-18%	1.20	0.96	1.05	1.18
12.32	6.64E−03 +/-7%	5.43E−03 +/-18%	1.22	0.99	1.07	1.21
15.43	6.02E−03 +/-7%	4.97E−03 +/-18%	1.21	0.98	1.06	1.19
19.55	5.22E−03 +/-8%	4.43E−03 +/-17%	1.18	0.95	1.03	1.16
23.67	4.65E−03 +/-8%	3.95E−03 +/-17%	1.18	0.96	1.03	1.16
27.78	4.22E−03 +/-8%	3.53E−03 +/-17%	1.20	0.97	1.05	1.17
34.87	3.47E−03 +/-9%	2.91E−03 +/-17%	1.19	0.97	1.04	1.16
44.95	2.32E−03 +/-12%	2.25E−03 +/-16%	1.03	0.85	0.90	1.00
55.07	1.40E−03 +/-18%	1.75E−03 +/-16%	0.80	0.67	0.70	0.77
mean % diff. from E			19	14	13	18
mean χ^2			4.30	2.54	2.14	3.95

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	**$T_{1/2}$**	**E/C**	**%ΔE**	**%ΔC^{nuc}**
N16	7.13s	2.32	15%	-
K44	22.13m	1.22	11%	20%

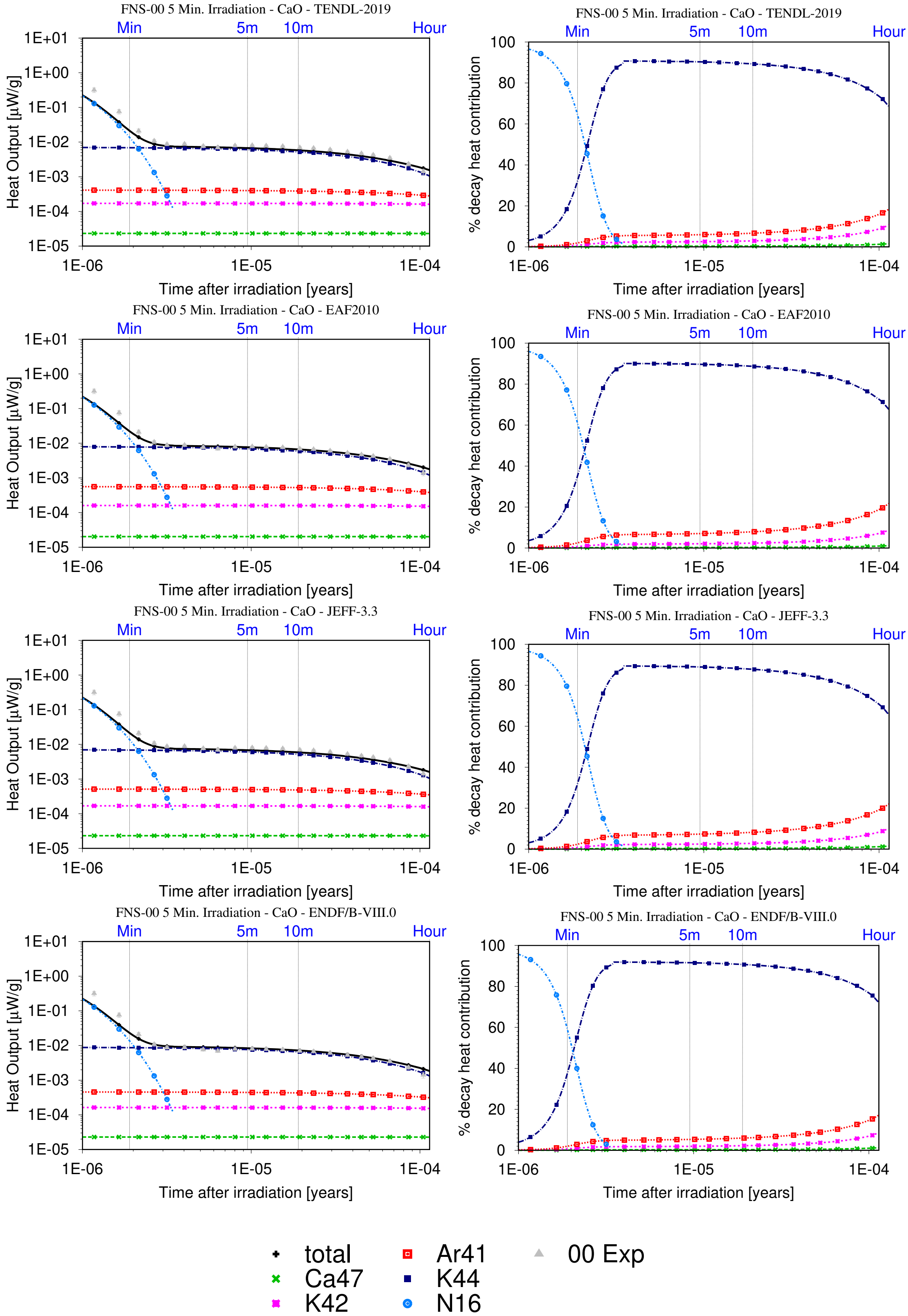


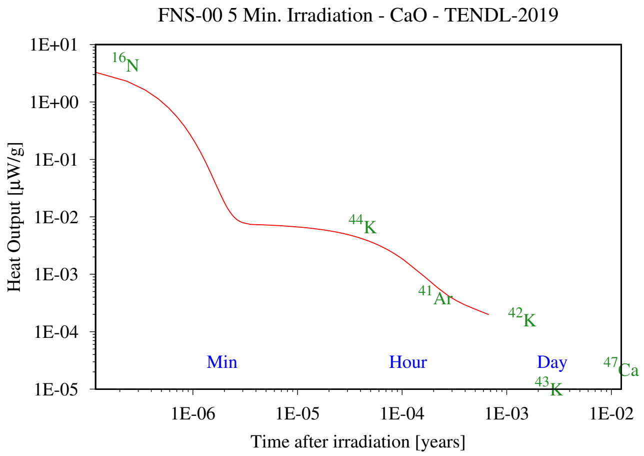
Calcium, TENDL-2019 5-minute pathway analysis

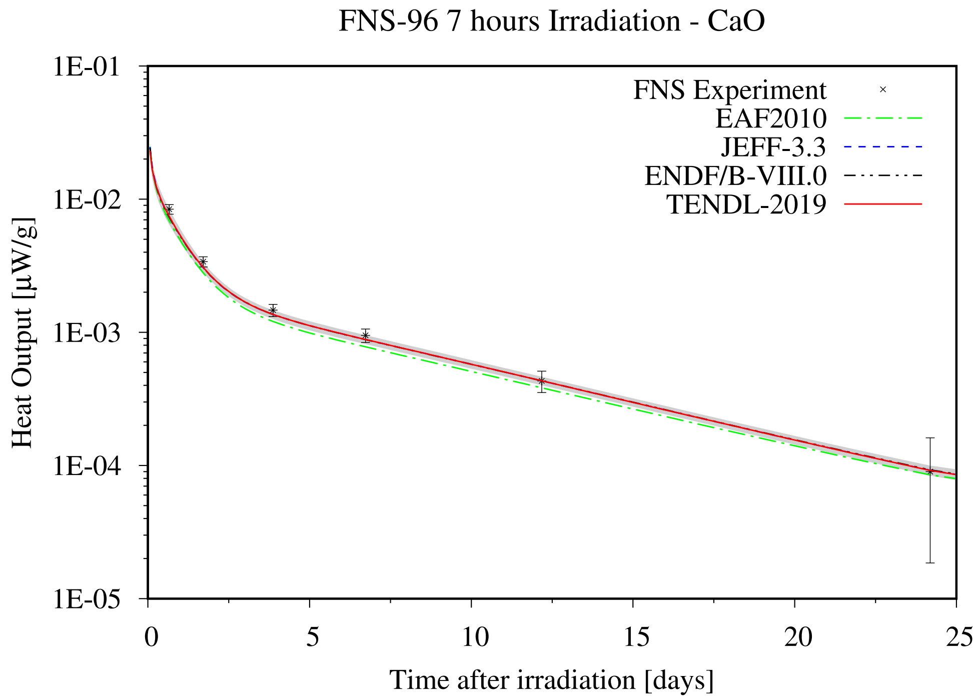
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
K44	22.13m	Ca44(n,p)K44	100.0
Ar41	1.83h	Ca44(n,α)Ar41	100.0
K42	12.36h	Ca42(n,p)K42	97.4
		Ca43(n,np)K42	2.1
Ca47	4.54d	Ca48(n,2n)Ca47	100.0

Comments on Calcium 5-minute experiments:

For the latest, 2000 experiment there is a good agreement for simulations with all included libraries, even at short cooling times, although TENDL-2019 and JEFF-3.3. seem to underpredict K44 slightly (from (n,p) reaction on Ca44) compared to EAF and ENDF/B. For the earlier, 1996 experiment the measurements are systematically higher, resulting in an apparent underprediction in the simulations. One possible explanation for this is that the CaO powder used in the experiment was very fine and was used in very small amounts, sandwiched between plastic tape. The contribution from that tape had to be extracted from the raw measured data, but because it may have been a very significant contribution to the decay heat, the signal-to-noise ratio would have been high and so there may be an unavoidable random variation in the results – a situation that may have also occurred in the SrCO3, Y2O3, and SnO2 samples discussed later. The profile associated with the predominant K44 radionuclide seems to be well-represented by the simulations in all considered cases (despite the aforementioned difference for JEFF and TENDL).


FNS-00 5 Min. Irradiation - CaO - TENDL-2019
FNS-00 5 Min. Irradiation - CaO - EAF2010
FNS-00 5 Min. Irradiation - CaO - JEFF-3.3
FNS-00 5 Min. Irradiation - CaO - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Ca47
K42
Ar41
K44
N16
00 Exp

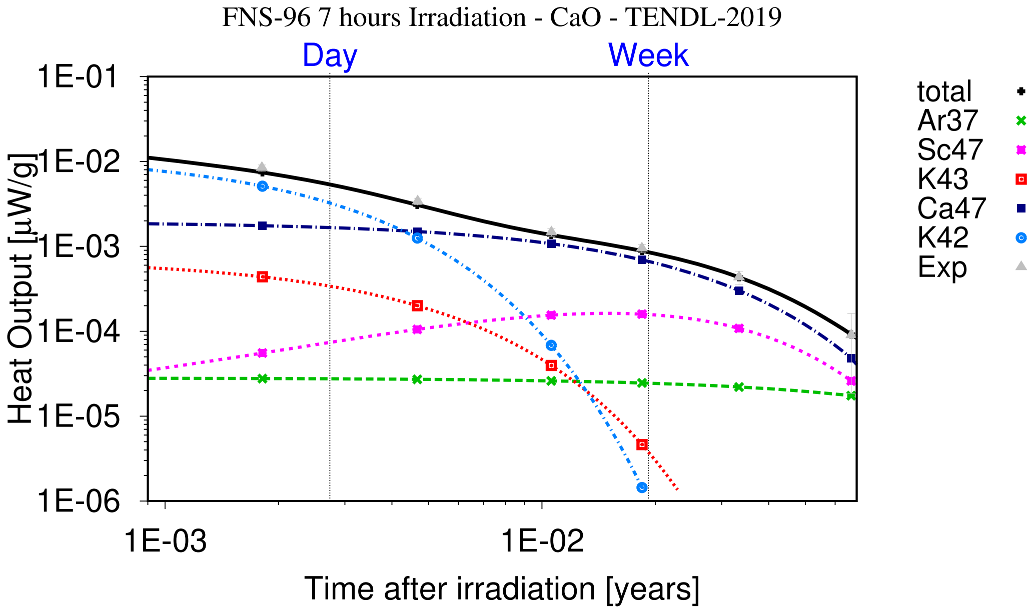

FNS-00 5 Min. Irradiation - CaO - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
16N
44K
41Ar
42K
43K
47Ca
Min
Hour
Day
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.66	$8.41E{-}03$ +/-8%	$7.42E{-}03$ +/-13%	1.13	1.15	1.22	1.14
1.71	$3.40E{-}03$ +/-9%	$3.08E{-}03$ +/-9%	1.10	1.11	1.21	1.11
3.87	$1.47E{-}03$ +/-10%	$1.36E{-}03$ +/-8%	1.08	1.08	1.21	1.08
6.73	$9.49E{-}04$ +/-12%	$8.84E{-}04$ +/-8%	1.07	1.08	1.22	1.07
12.18	$4.32E{-}04$ +/-18%	$4.33E{-}04$ +/-7%	1.00	1.00	1.13	1.00
24.19	$9.00E{-}05$ +/-79%	$9.20E{-}05$ +/-9%	0.98	0.97	1.06	0.98
mean % diff. from E			6	7	15	6
mean χ^2			0.64	0.75	2.39	0.71

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ca47	4.54d	1.08	10%	10%

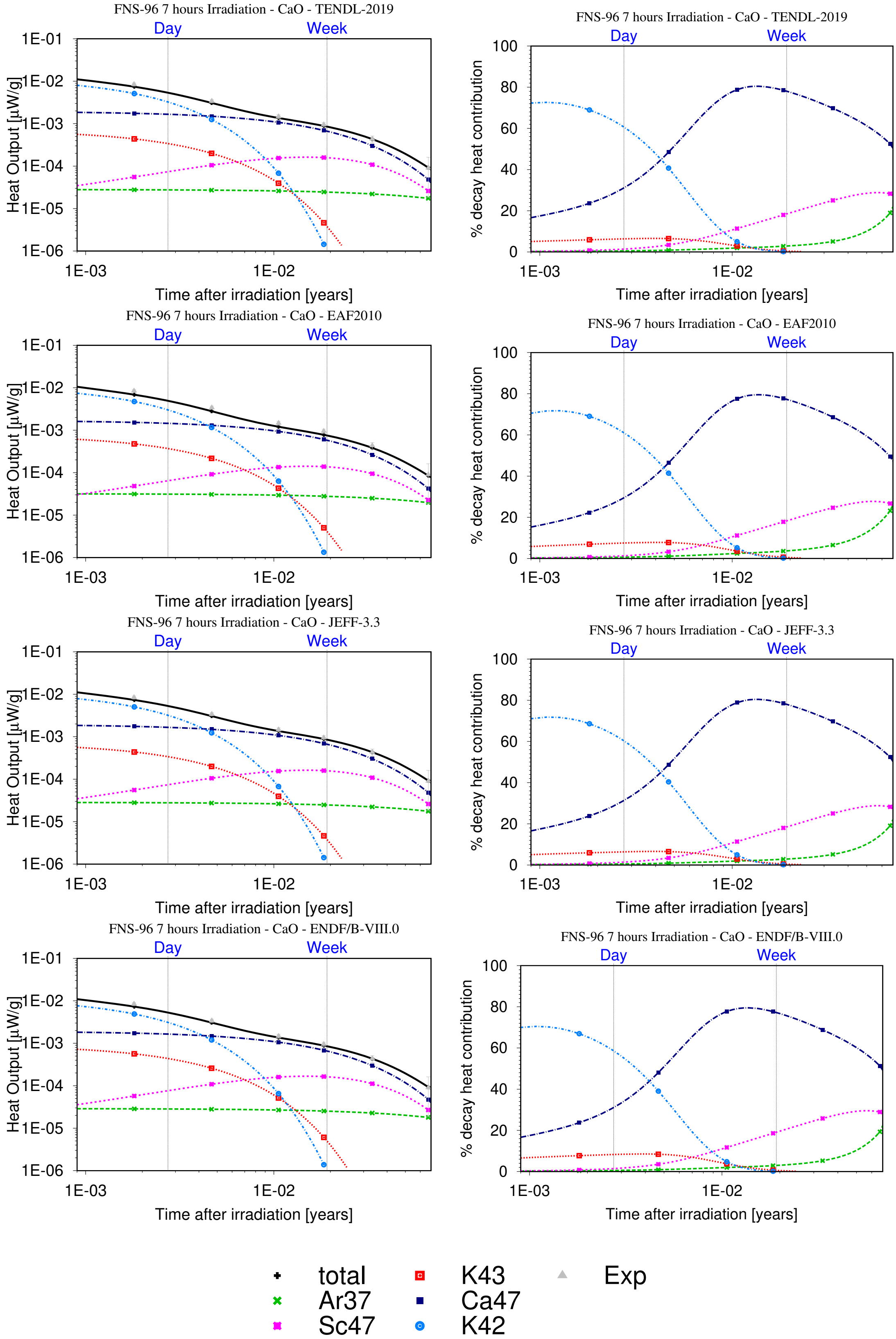


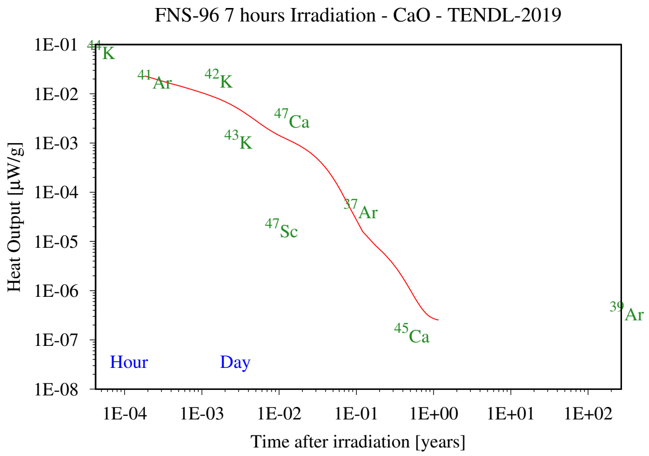
Calcium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
K42	12.36h	Ca42(n,p)K42	98.0
		Ca43(n,np)K42	1.6
K43	22.20h	Ca43(n,p)K43	71.3
		Ca44(n,d)K43	15.2
		Ca44(n,np)K43	13.5
Sc47	3.35d	Ca48(n,2n)Ca47(β^-)Sc47	100.0
Ca47	4.54d	Ca48(n,2n)Ca47	100.0
Ar37	35.03d	Ca40(n,α)Ar37	100.0

Comments on Calcium 7-hour experiments:

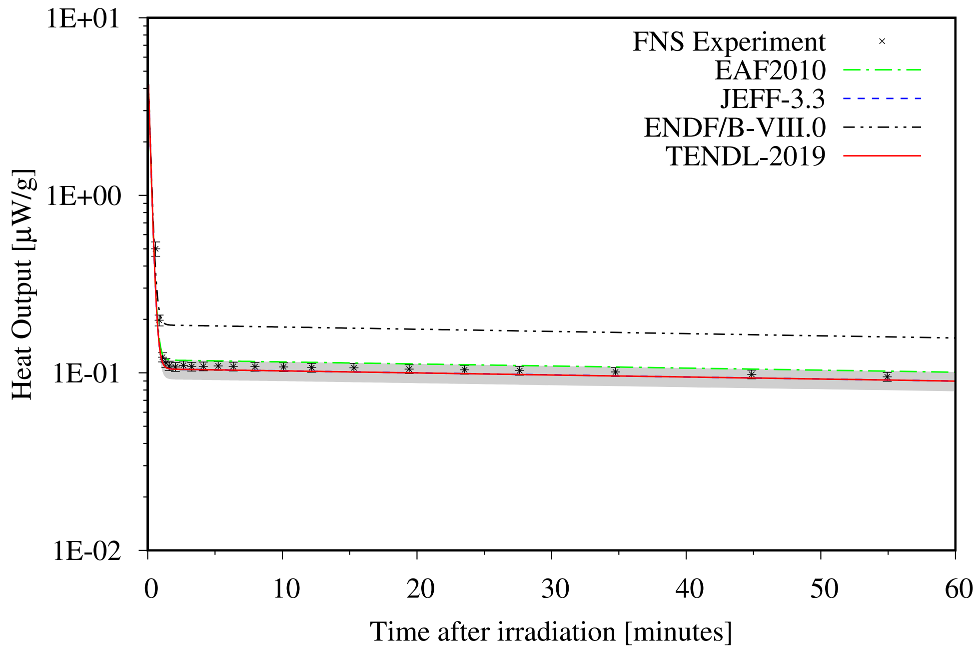
All libraries considered produce a good agreement to the measurements and the data points are all within TENDL-2019's uncertainty band. This is an impressive result given the somewhat complex, multi-nuclide picture, with dominant ($> 50\%$) contributions from K42 and Ca47 at different cooling times, combined with more minor, 10-20% contributions from Sc47, Ar37 and K43.


FNS-96 7 hours Irradiation - CaO - TENDL-2019
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - CaO - EAF2010
FNS-96 7 hours Irradiation - CaO - JEFF-3.3
FNS-96 7 hours Irradiation - CaO - ENDF/B-VIII.0
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
total
Ar37
Sc47
K43
Ca47
K42
Exp


FNS-96 7 hours Irradiation - CaO - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
Hour
Day
44K
41Ar
42K
47Ca
43K
37Ar
47Sc
45Ca
39Ar

Scandium

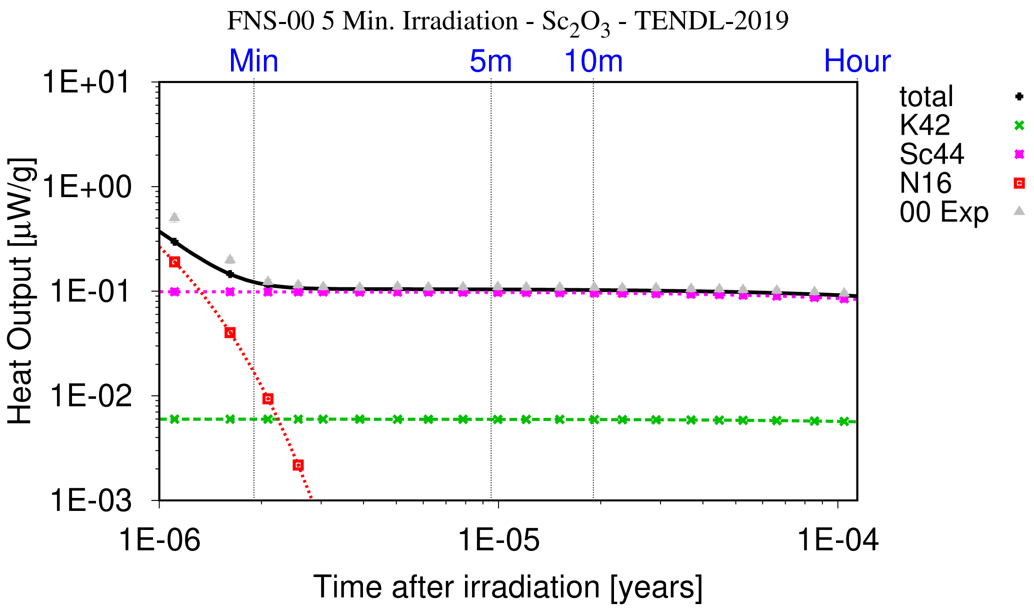
FNS-00 5 Min. Irradiation - Sc_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	$5.00E{-}01$ +/-9%	$2.97E{-}01$ +/-4%	1.69	1.33	1.63	1.69
0.85	$1.98E{-}01$ +/-7%	$1.46E{-}01$ +/-9%	1.36	0.87	1.25	1.36
1.10	$1.23E{-}01$ +/-6%	$1.15E{-}01$ +/-11%	1.07	0.63	0.96	1.07
1.35	$1.14E{-}01$ +/-6%	$1.07E{-}01$ +/-12%	1.06	0.61	0.95	1.06
1.60	$1.09E{-}01$ +/-6%	$1.06E{-}01$ +/-12%	1.04	0.59	0.92	1.04
2.05	$1.08E{-}01$ +/-6%	$1.05E{-}01$ +/-12%	1.03	0.58	0.92	1.03
2.65	$1.10E{-}01$ +/-6%	$1.05E{-}01$ +/-12%	1.05	0.60	0.94	1.05
3.27	$1.08E{-}01$ +/-6%	$1.04E{-}01$ +/-12%	1.04	0.59	0.92	1.04
4.13	$1.09E{-}01$ +/-6%	$1.04E{-}01$ +/-12%	1.04	0.59	0.93	1.04
5.23	$1.10E{-}01$ +/-6%	$1.04E{-}01$ +/-12%	1.05	0.60	0.94	1.05
6.35	$1.09E{-}01$ +/-6%	$1.04E{-}01$ +/-12%	1.05	0.59	0.93	1.05
7.97	$1.08E{-}01$ +/-6%	$1.03E{-}01$ +/-12%	1.05	0.59	0.93	1.05
10.08	$1.08E{-}01$ +/-6%	$1.03E{-}01$ +/-12%	1.05	0.60	0.94	1.05
12.18	$1.07E{-}01$ +/-6%	$1.02E{-}01$ +/-12%	1.05	0.59	0.93	1.05
15.32	$1.07E{-}01$ +/-6%	$1.01E{-}01$ +/-12%	1.06	0.60	0.94	1.06
19.42	$1.05E{-}01$ +/-6%	$1.00E{-}01$ +/-12%	1.05	0.60	0.93	1.05
23.53	$1.04E{-}01$ +/-6%	$9.90E{-}02$ +/-12%	1.05	0.60	0.94	1.05
27.63	$1.03E{-}01$ +/-6%	$9.79E{-}02$ +/-12%	1.05	0.60	0.93	1.05
34.75	$1.01E{-}01$ +/-6%	$9.61E{-}02$ +/-12%	1.05	0.60	0.94	1.05
44.87	$9.81E{-}02$ +/-6%	$9.36E{-}02$ +/-12%	1.05	0.60	0.93	1.05
54.93	$9.50E{-}02$ +/-6%	$9.11E{-}02$ +/-12%	1.04	0.60	0.93	1.04
mean % diff. from E			7	63	9	7
mean χ^2			2.22	129.74	2.64	2.22

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$T_{1/2}$	**E/C**	**%ΔE**	**%Δ**C^{nuc}
Sc44	3.97h	1.07	6%	13%

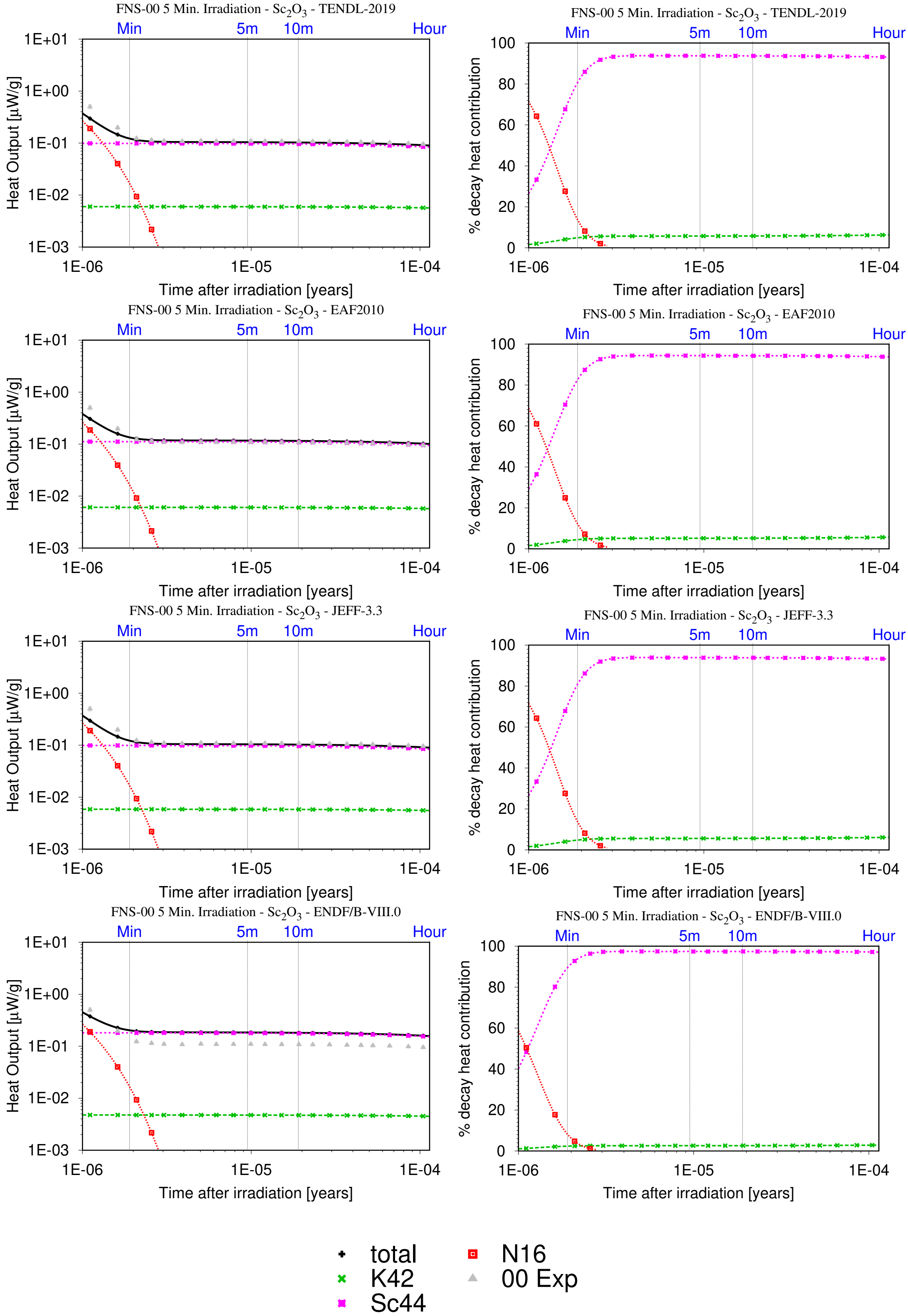


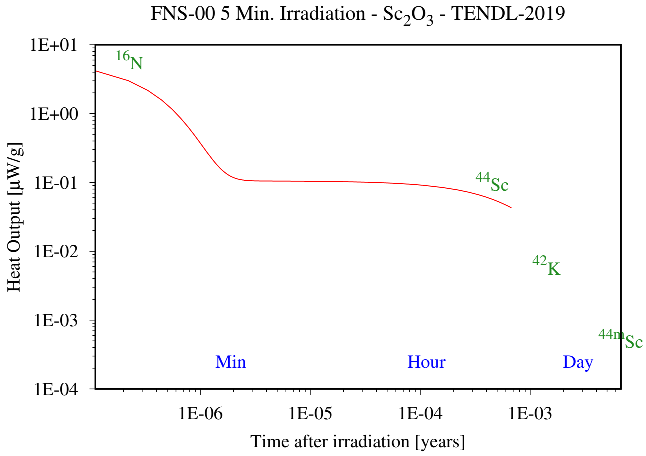
Scandium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Sc44	3.97h	Sc45(n,2n)Sc44	100.0
K42	12.36h	Sc45(n,α)K42	100.0

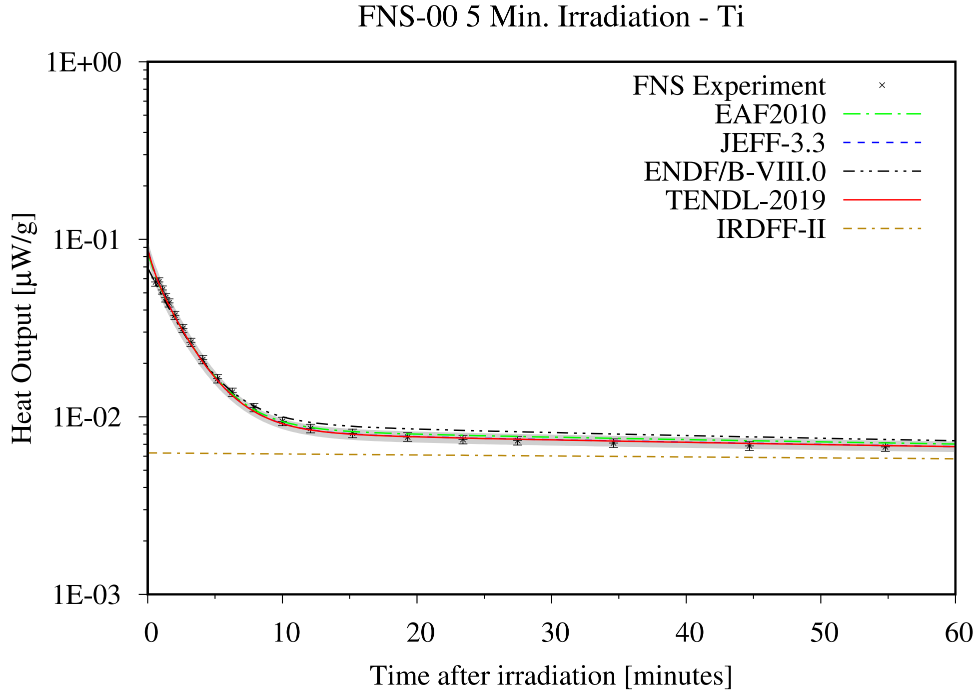
Comments on Scandium 5-minute experiments:

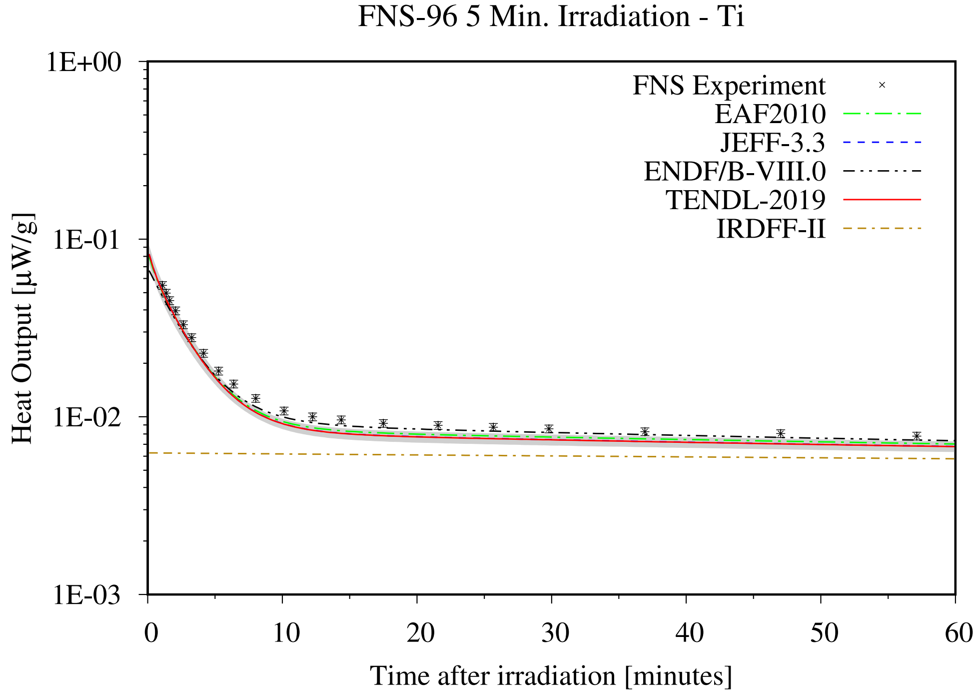
Here the scandium simulations yield good agreement for the production of Sc44, apart from ENDF/B-VIII.0, which overpredicts by a factor of 2. TENDL-2019 shows a particularly excellent agreement for Sc44 production via (n,2n), where the simulated decay-heat beyond 1 minute of cooling is always within the experimental uncertainty (JEFF-3.3 is equally good, suggesting identical underlying data). In principle, this experiment should be used to reduce the cross section uncertainty for Sc45(n,2n), see figure A1 in the appendix. There is more disagreement at cooling times below 1 minute where N16 (from the oxygen in the sample) is important and where there appears to be an underprediction of its production.


FNS-00 5 Min. Irradiation - Sc$_2$O$_3$ - TENDL-2019
Min
5m
10m
Hour
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Sc$_2$O$_3$ - TENDL-2019
% decay heat contribution
100
80
60
40
20
0
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Sc$_2$O$_3$ - EAF2010
FNS-00 5 Min. Irradiation - Sc$_2$O$_3$ - JEFF-3.3
FNS-00 5 Min. Irradiation - Sc$_2$O$_3$ - ENDF/B-VIII.0
total
K42
Sc44
N16
00 Exp


FNS-00 5 Min. Irradiation - Sc2O3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
16N
44Sc
42K
44mSc
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

Titanium


FNS-00 5 Min. Irradiation - Ti
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]

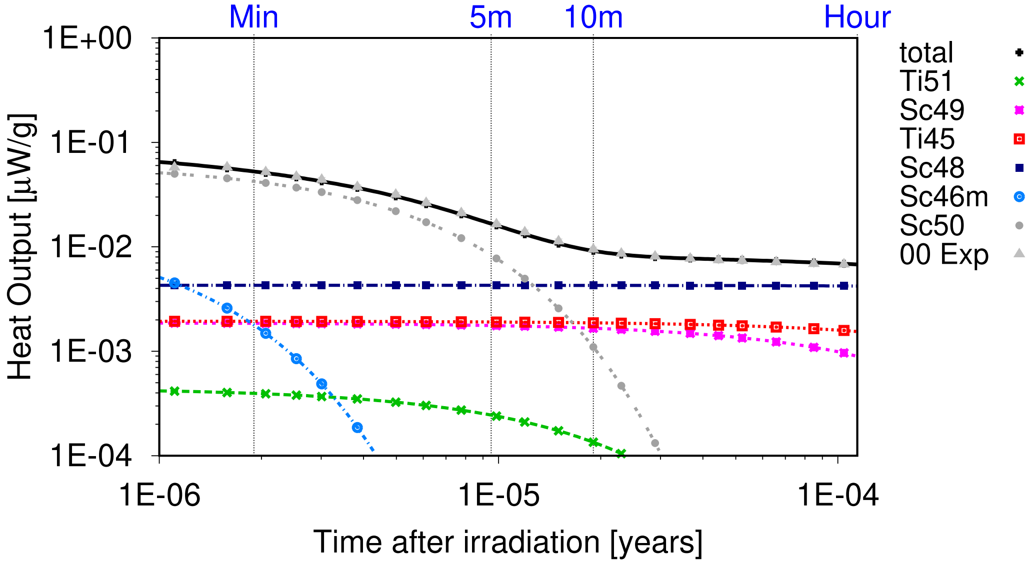

FNS-96 5 Min. Irradiation - Ti
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]

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	5.75$E-$02 +/-5%	6.32$E-$02 +/-13%	0.91	1.02	0.93	0.91	9.19
0.83	5.76$E-$02 +/-5%	5.65$E-$02 +/-13%	1.02	1.11	1.03	1.02	9.20
1.08	5.19$E-$02 +/-5%	5.10$E-$02 +/-13%	1.02	1.08	1.03	1.02	8.29
1.33	4.69$E-$02 +/-5%	4.64$E-$02 +/-13%	1.01	1.06	1.02	1.01	7.50
1.58	4.39$E-$02 +/-5%	4.24$E-$02 +/-12%	1.03	1.08	1.04	1.03	7.02
2.02	3.73$E-$02 +/-5%	3.67$E-$02 +/-12%	1.02	1.04	1.02	1.01	5.97
2.62	3.15$E-$02 +/-5%	3.05$E-$02 +/-12%	1.03	1.05	1.03	1.03	5.05
3.22	2.63$E-$02 +/-5%	2.57$E-$02 +/-11%	1.03	1.03	1.02	1.02	4.22
4.08	2.10$E-$02 +/-5%	2.05$E-$02 +/-10%	1.03	1.02	1.02	1.02	3.37
5.18	1.64$E-$02 +/-5%	1.61$E-$02 +/-9%	1.02	0.99	1.01	1.02	2.64
6.28	1.38$E-$02 +/-5%	1.32$E-$02 +/-7%	1.04	0.99	1.02	1.04	2.22
7.90	1.13$E-$02 +/-5%	1.07$E-$02 +/-7%	1.05	0.98	1.03	1.05	1.82
10.00	9.43$E-$03 +/-5%	9.16$E-$03 +/-7%	1.03	0.94	1.00	1.03	1.53
12.10	8.60$E-$03 +/-6%	8.44$E-$03 +/-7%	1.02	0.92	0.99	1.02	1.40
15.22	8.08$E-$03 +/-6%	7.99$E-$03 +/-7%	1.01	0.91	0.98	1.01	1.32
19.32	7.71$E-$03 +/-6%	7.74$E-$03 +/-7%	1.00	0.90	0.96	0.99	1.26
23.42	7.45$E-$03 +/-6%	7.60$E-$03 +/-7%	0.98	0.89	0.95	0.98	1.23
27.48	7.36$E-$03 +/-6%	7.48$E-$03 +/-7%	0.98	0.89	0.95	0.98	1.22
34.60	7.12$E-$03 +/-6%	7.31$E-$03 +/-7%	0.97	0.89	0.94	0.97	1.19
44.70	6.86$E-$03 +/-6%	7.09$E-$03 +/-7%	0.97	0.89	0.93	0.97	1.16
54.80	6.77$E-$03 +/-6%	6.89$E-$03 +/-7%	0.98	0.91	0.95	0.98	1.16
mean % diff. from E			3	7	3	3	52
mean χ^2			0.38	2.07	0.52	0.37	124.84

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Sc50	1.71m	0.91	5%	16%

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

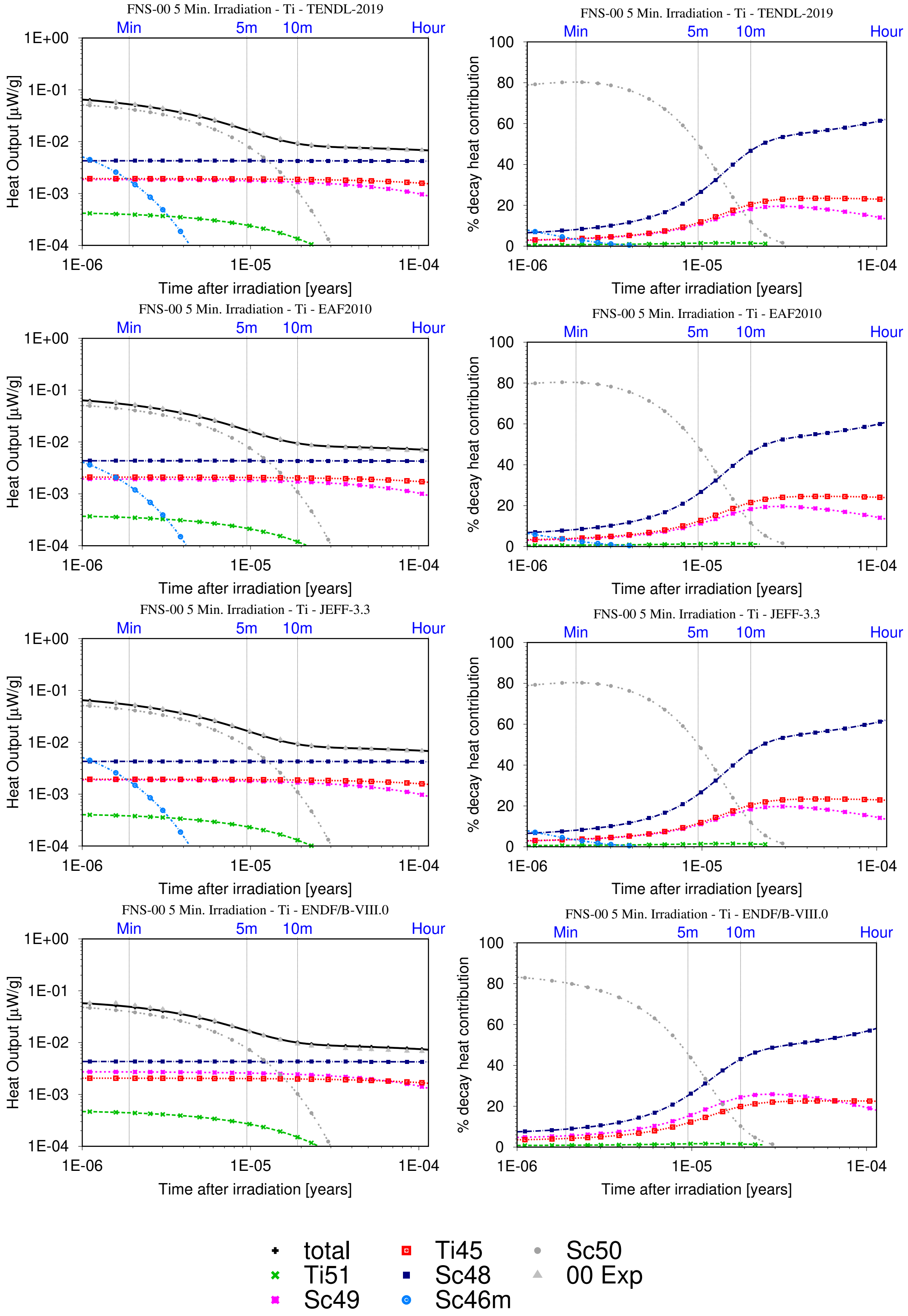


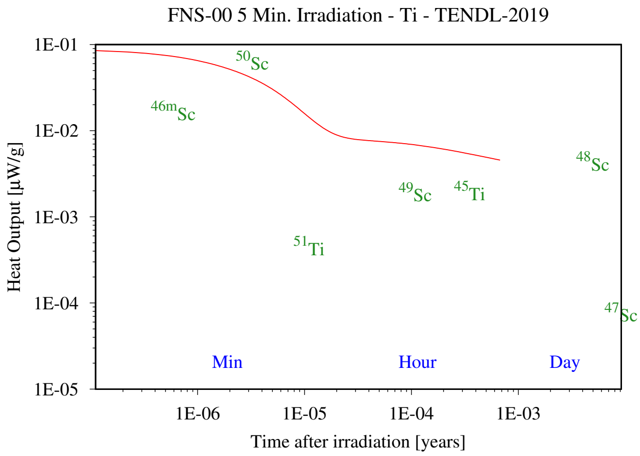
Titanium, TENDL-2019 5-minute pathway analysis

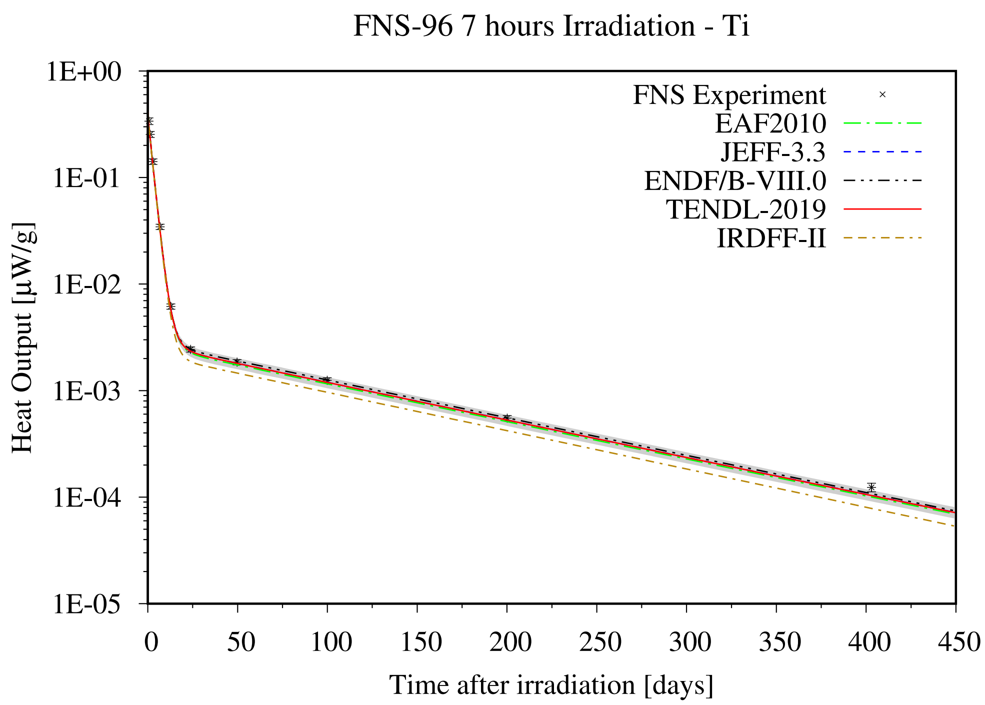
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Sc46m	18.70s	Ti46(n,p)Sc46m	87.9
		Ti47(n,np)Sc46m	10.6
		Ti47(n,d)Sc46m	1.5
Sc50	1.71m	Ti50(n,p)Sc50m(IT)Sc50	57.4
		Ti50(n,p)Sc50	42.6
Ti51	5.80m	Ti50(n,γ)Ti51	100.0
Sc49	57.19m	Ti49(n,p)Sc49	95.7
		Ti50(n,np)Sc49	2.3
		Ti50(n,d)Sc49	2.1
Ti45	3.08h	Ti46(n,2n)Ti45	100.0
Sc48	1.82d	Ti48(n,p)Sc48	99.4

Comments on Titanium 5-minute experiments:

The 5-minute graphs exhibit some unexplained differences between the two experimental batches - reflected in the overprediction by most libraries for the year 2000 experiment, but under prediction of the 1996 case. The routes of production of the identified important isotopes are relatively complex, although the simulations with the four general purpose libraries are in agreement and seem to capture the main profile of the decay heat; it is dominated by first Sc50 ($<$ 5 minutes of cooling) and then Sc48 ($\sim$50% with Sc49+Ti45 (both $\sim$20%) afterwards. IRDFF-II includes the relevant Ti48(n,p)Sc48 channel for this case, but underpredicts due to the absence of the production channels for Sc50 and Sc49.


FNS-00 5 Min. Irradiation - Ti - TENDL-2019
FNS-00 5 Min. Irradiation - Ti - EAF2010
FNS-00 5 Min. Irradiation - Ti - JEFF-3.3
FNS-00 5 Min. Irradiation - Ti - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Ti51
Sc49
Ti45
Sc48
Sc46m
Sc50
00 Exp

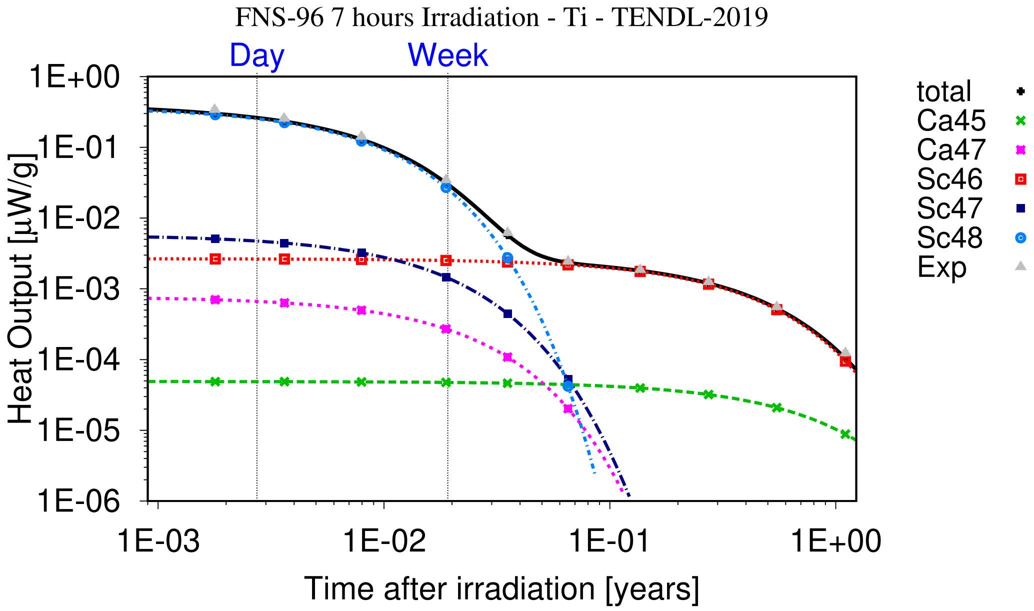

FNS-00 5 Min. Irradiation - Ti - TENDL-2019
Heat Output [μW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
50Sc
46mSc
48Sc
49Sc
45Ti
51Ti
47Sc
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.65	$3.38E{-}01$ +/-7%	$3.00E{-}01$ +/-8%	1.13	1.15	1.12	1.13	1.15
1.32	$2.54E{-}01$ +/-6%	$2.32E{-}01$ +/-8%	1.09	1.11	1.08	1.10	1.11
2.90	$1.41E{-}01$ +/-6%	$1.29E{-}01$ +/-8%	1.09	1.11	1.08	1.09	1.12
6.87	$3.45E{-}02$ +/-6%	$3.14E{-}02$ +/-7%	1.10	1.12	1.08	1.10	1.15
12.87	$6.16E{-}03$ +/-6%	$5.75E{-}03$ +/-7%	1.07	1.07	1.07	1.07	1.24
23.86	$2.43E{-}03$ +/-6%	$2.34E{-}03$ +/-11%	1.04	0.99	1.07	1.04	1.30
49.71	$1.85E{-}03$ +/-6%	$1.80E{-}03$ +/-12%	1.02	0.97	1.06	1.02	1.27
99.90	$1.25E{-}03$ +/-6%	$1.20E{-}03$ +/-12%	1.04	0.99	1.08	1.04	1.29
200.12	$5.51E{-}04$ +/-6%	$5.29E{-}04$ +/-12%	1.04	0.99	1.08	1.04	1.31
402.96	$1.23E{-}04$ +/-9%	$1.04E{-}04$ +/-12%	1.19	1.14	1.23	1.19	1.57
mean % diff. from E			7	7	8	7	19
mean χ^2			1.47	1.49	1.76	1.49	10.47

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Sc48	1.82d	1.13	7%	8%
Sc46	83.79d	1.04	6%	12%

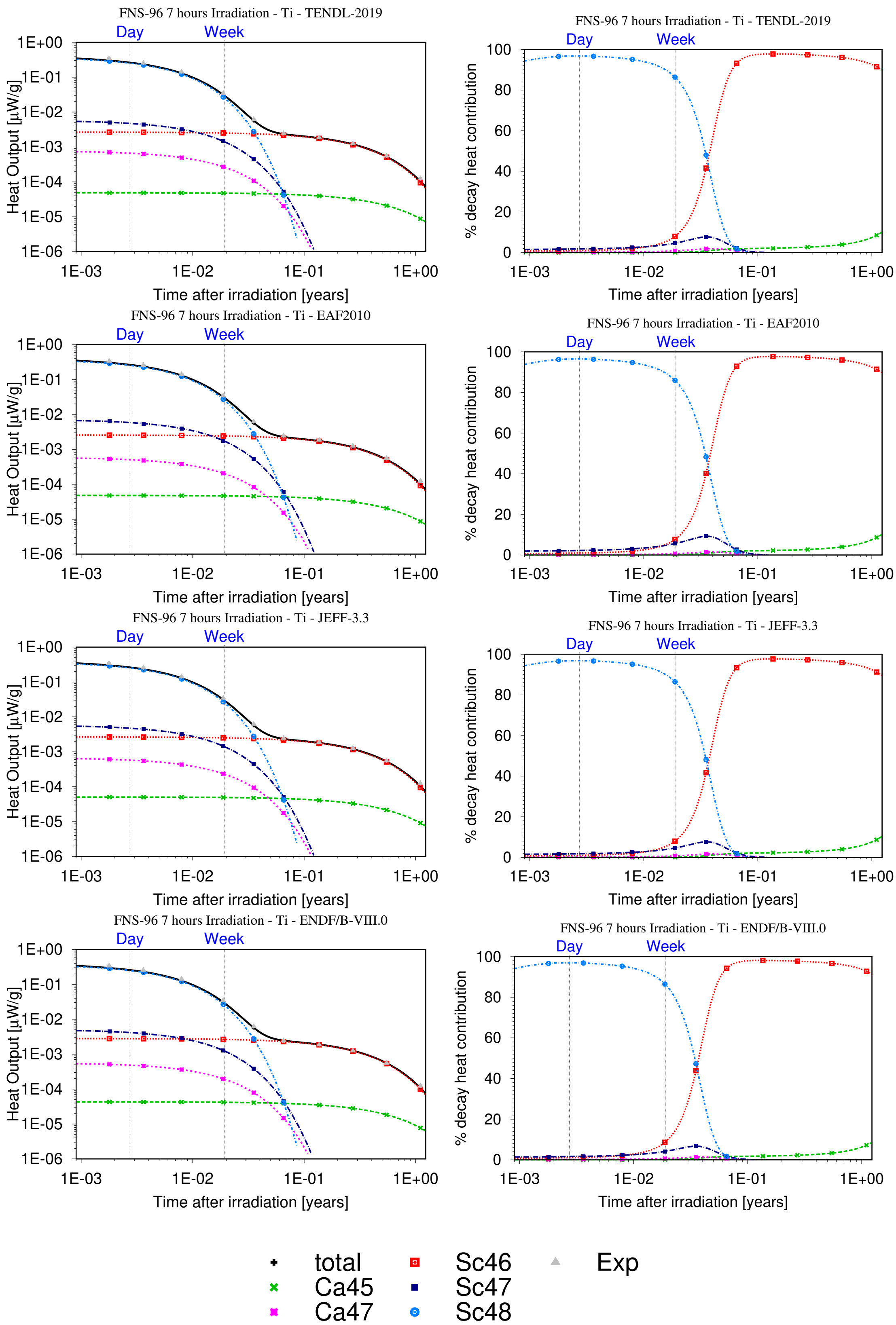


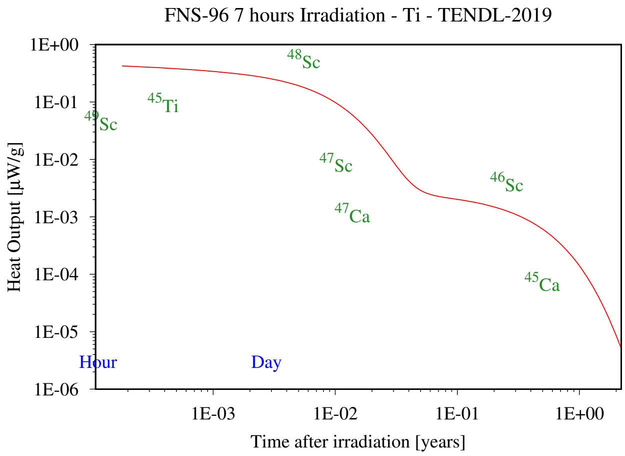
Titanium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Sc48	1.82d	Ti48(n,p)Sc48	99.6
Sc47	3.35d	Ti47(n,p)Sc47	56.1
		Ti48(n,np)Sc47	23.1
		Ti48(n,d)Sc47	20.7
Ca47	4.54d	Ti50(n,α)Ca47	100.0
Sc46	83.79d	Ti46(n,p)Sc46	61.0
		Ti46(n,p)Sc46m(IT)Sc46	21.7
		Ti47(n,np)Sc46	13.8
		Ti47(n,np)Sc46m(IT)Sc46	2.0
		Ti47(n,d)Sc46	1.2
Ca45	162.99d	Ti48(n,α)Ca45	99.9

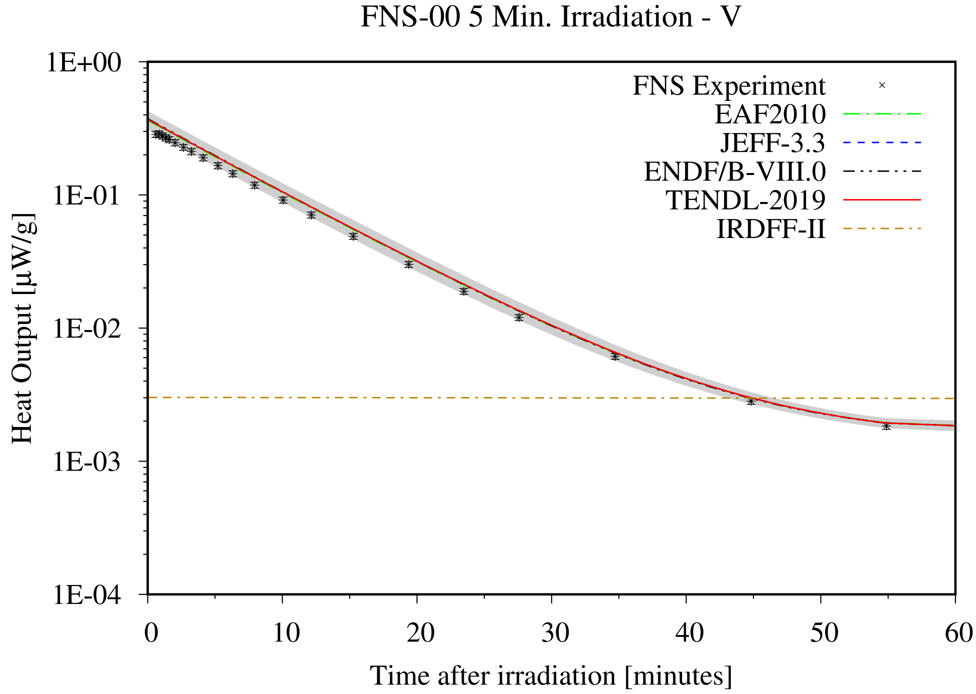
Comments on Titanium 7-hour experiments:

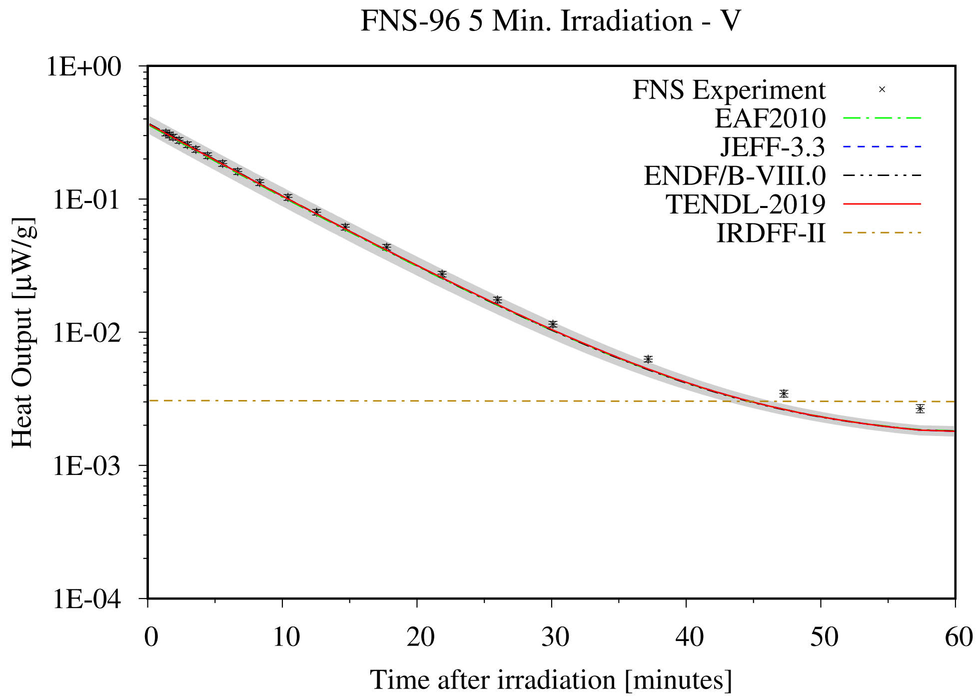
An excellent agreement exists at all cooling times for all libraries (even IRDFF-II, although it is not as good as IRDFF-1.05), even with the relatively complex production routes of Sc46, which dominates at decay times beyond around 14 days and is produced from reaction routes that include (n,p), (n,np) and (n,d) channels.


FNS-96 7 hours Irradiation - Ti - TENDL-2019
FNS-96 7 hours Irradiation - Ti - EAF2010
FNS-96 7 hours Irradiation - Ti - JEFF-3.3
FNS-96 7 hours Irradiation - Ti - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
0
20
40
60
80
100
total
Ca45
Ca47
Sc46
Sc47
Sc48
Exp


FNS-96 7 hours Irradiation - Ti - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-03
1E-02
1E-01
1E+00
Hour
Day
48Sc
45Ti
49Sc
47Sc
46Sc
47Ca
45Ca

Vanadium

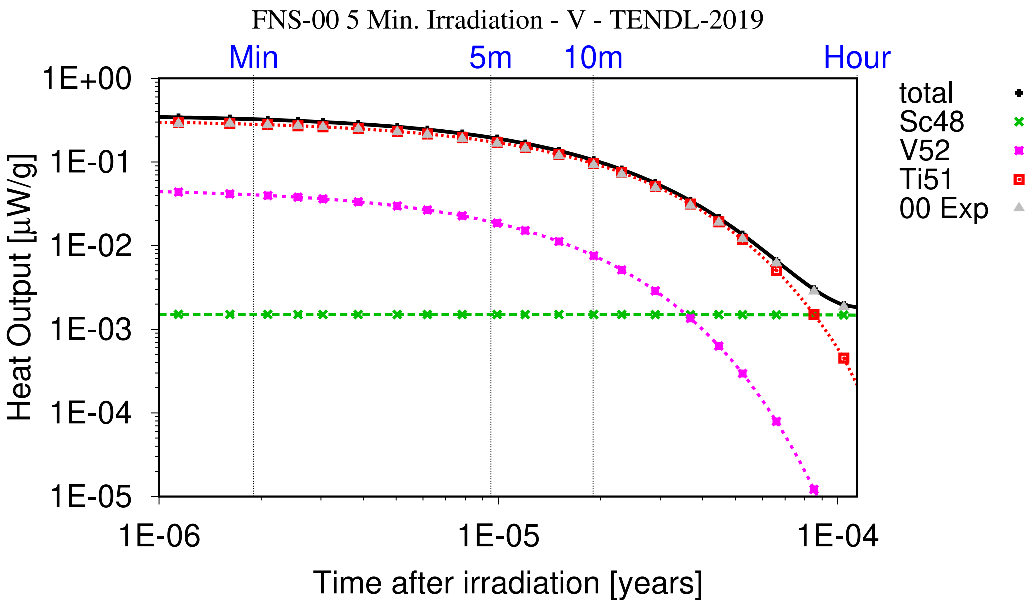

FNS-00 5 Min. Irradiation - V
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - V
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60

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
0.60	2.85E−01 +/-5%	3.42E−01 +/-16%	0.83	0.82	0.85	0.83	94.59
0.85	2.87E−01 +/-5%	3.31E−01 +/-16%	0.87	0.86	0.88	0.87	95.10
1.10	2.77E−01 +/-5%	3.21E−01 +/-16%	0.86	0.85	0.88	0.86	91.92
1.35	2.69E−01 +/-5%	3.11E−01 +/-16%	0.86	0.86	0.88	0.87	89.14
1.60	2.61E−01 +/-5%	3.01E−01 +/-16%	0.87	0.86	0.88	0.87	86.42
2.03	2.47E−01 +/-5%	2.85E−01 +/-16%	0.87	0.86	0.88	0.87	81.86
2.65	2.28E−01 +/-5%	2.64E−01 +/-16%	0.86	0.86	0.88	0.86	75.60
3.25	2.12E−01 +/-5%	2.44E−01 +/-16%	0.87	0.86	0.88	0.87	70.26
4.12	1.90E−01 +/-5%	2.19E−01 +/-16%	0.87	0.86	0.88	0.87	63.04
5.22	1.66E−01 +/-5%	1.91E−01 +/-16%	0.87	0.86	0.88	0.87	55.06
6.32	1.44E−01 +/-5%	1.66E−01 +/-16%	0.87	0.86	0.88	0.87	47.90
7.93	1.18E−01 +/-5%	1.36E−01 +/-16%	0.87	0.86	0.88	0.87	39.31
10.05	9.15E−02 +/-5%	1.05E−01 +/-16%	0.87	0.87	0.88	0.87	30.42
12.15	7.07E−02 +/-5%	8.12E−02 +/-16%	0.87	0.87	0.88	0.87	23.54
15.27	4.89E−02 +/-5%	5.58E−02 +/-16%	0.88	0.88	0.89	0.88	16.29
19.38	3.01E−02 +/-5%	3.43E−02 +/-16%	0.88	0.88	0.89	0.88	10.02
23.48	1.89E−02 +/-5%	2.14E−02 +/-16%	0.88	0.89	0.89	0.88	6.30
27.58	1.20E−02 +/-5%	1.36E−02 +/-16%	0.88	0.89	0.89	0.88	4.01
34.72	6.14E−03 +/-5%	6.60E−03 +/-14%	0.93	0.94	0.94	0.93	2.05
44.82	2.82E−03 +/-6%	3.00E−03 +/-10%	0.94	0.95	0.94	0.94	0.95
54.87	1.84E−03 +/-6%	1.94E−03 +/-9%	0.95	0.95	0.95	0.95	0.62
mean % diff. from E			14	14	13	14	87
mean χ^2			7.17	7.79	5.76	7.12	283.72

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ti51	5.80m	0.83	5%	18%
Sc48	1.82d	0.95	6%	10%

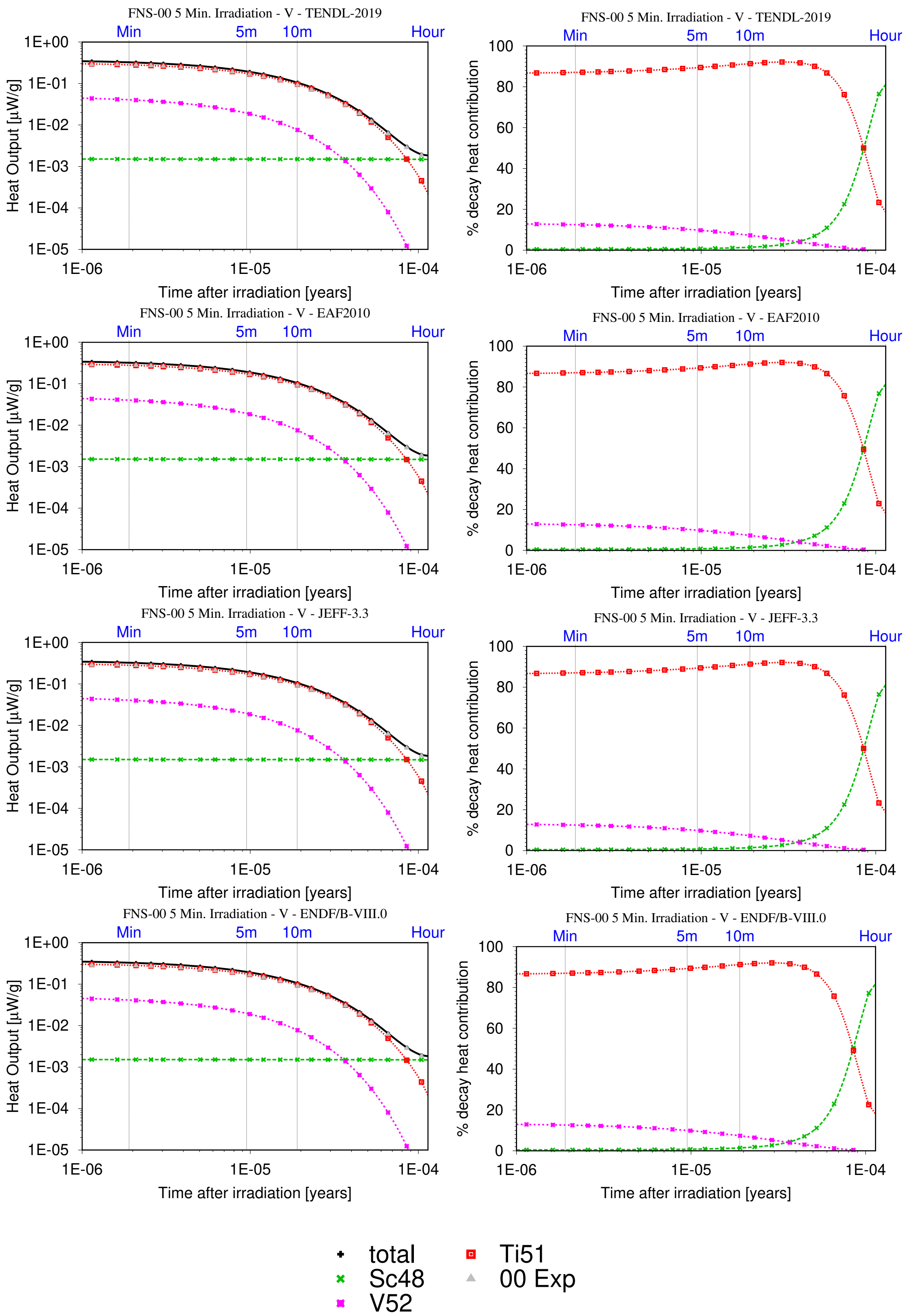


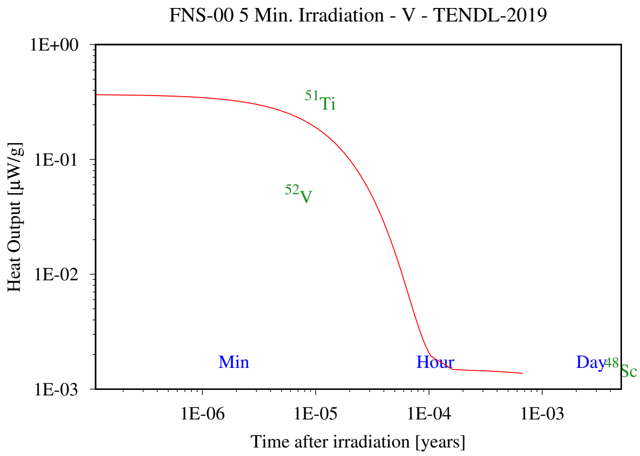
Vanadium, TENDL-2019 5-minute pathway analysis

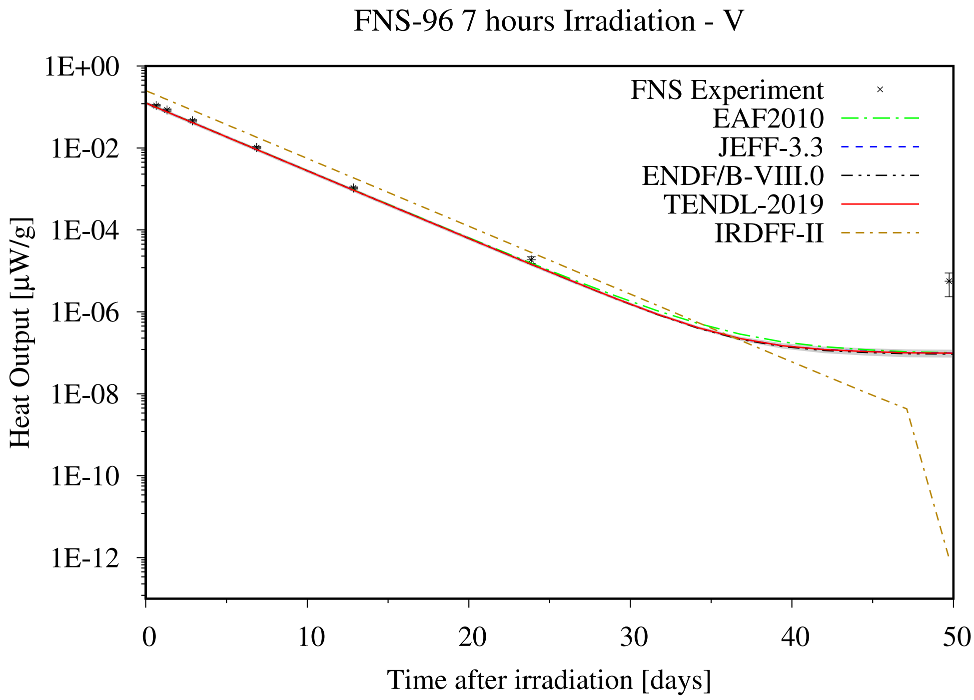
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
V52	3.74m	V51(n,γ)V52	100.0
Ti51	5.80m	V51(n,p)Ti51	100.0
Sc48	1.82d	V51(n,α)Sc48	100.0

Comments on Vanadium 5-minute experiments:

The two sets of experimental measurements here are clearly discrepant with one another – particularly at cooling times beyond 30 minutes, where the identical simulation with all general purpose libraries appear to underpredict the 1996 results but produce very good agreement in the 2000 experiment. IRDFF-II only contains the (n,α) reaction to produce the longer-lived Sc48 radionuclide and even here appears to overestimate the production by a factor of 2 compared to the others. The Ti51 (from (n,p) on V51) profile with JEFF, TENDL, EAF, and ENDF/B nicely captures the experimental profile for all but the last two measurements (where Sc48 becomes important).


FNS-00 5 Min. Irradiation - V - TENDL-2019
FNS-00 5 Min. Irradiation - V - EAF2010
FNS-00 5 Min. Irradiation - V - JEFF-3.3
FNS-00 5 Min. Irradiation - V - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Sc48
V52
Ti51
00 Exp

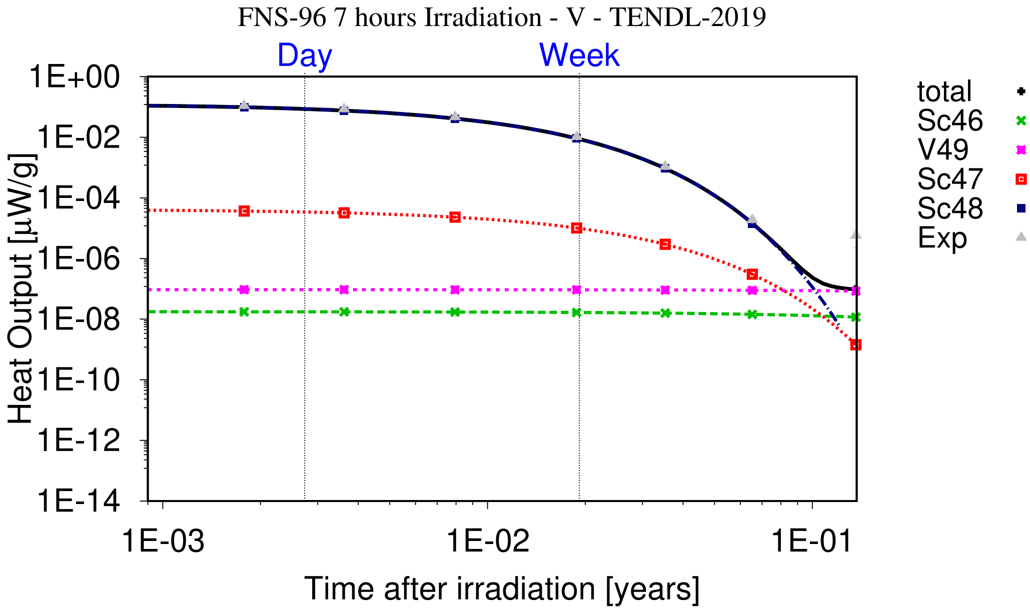

FNS-00 5 Min. Irradiation - V - TENDL-2019
1E+00
1E-01
1E-02
1E-03
Heat Output [µW/g]
51Ti
52V
48Sc
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.65	$1.08E{-}01$ +/-6%	$9.77E{-}02$ +/-10%	1.11	1.10	1.10	1.11	0.55
1.32	$8.42E{-}02$ +/-6%	$7.56E{-}02$ +/-10%	1.11	1.11	1.11	1.11	0.56
2.90	$4.61E{-}02$ +/-6%	$4.14E{-}02$ +/-10%	1.11	1.11	1.10	1.11	0.56
6.87	$1.02E{-}02$ +/-6%	$9.14E{-}03$ +/-10%	1.12	1.11	1.11	1.12	0.56
12.86	$1.06E{-}03$ +/-6%	$9.34E{-}04$ +/-10%	1.13	1.13	1.12	1.13	0.57
23.86	$1.86E{-}05$ +/-18%	$1.45E{-}05$ +/-10%	1.28	1.28	1.20	1.28	0.66
49.73	$5.62E{-}06$ +/-58%	$9.80E{-}08$ +/-22%	57.38	59.82	55.60	56.86	> 1000
mean % diff. from E			25	24	23	25	78
mean χ^2			2.75	2.63	2.35	2.75	125.27

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Sc48	1.82d	1.11	6%	10%
V49	330.01d	57.38	58%	25%

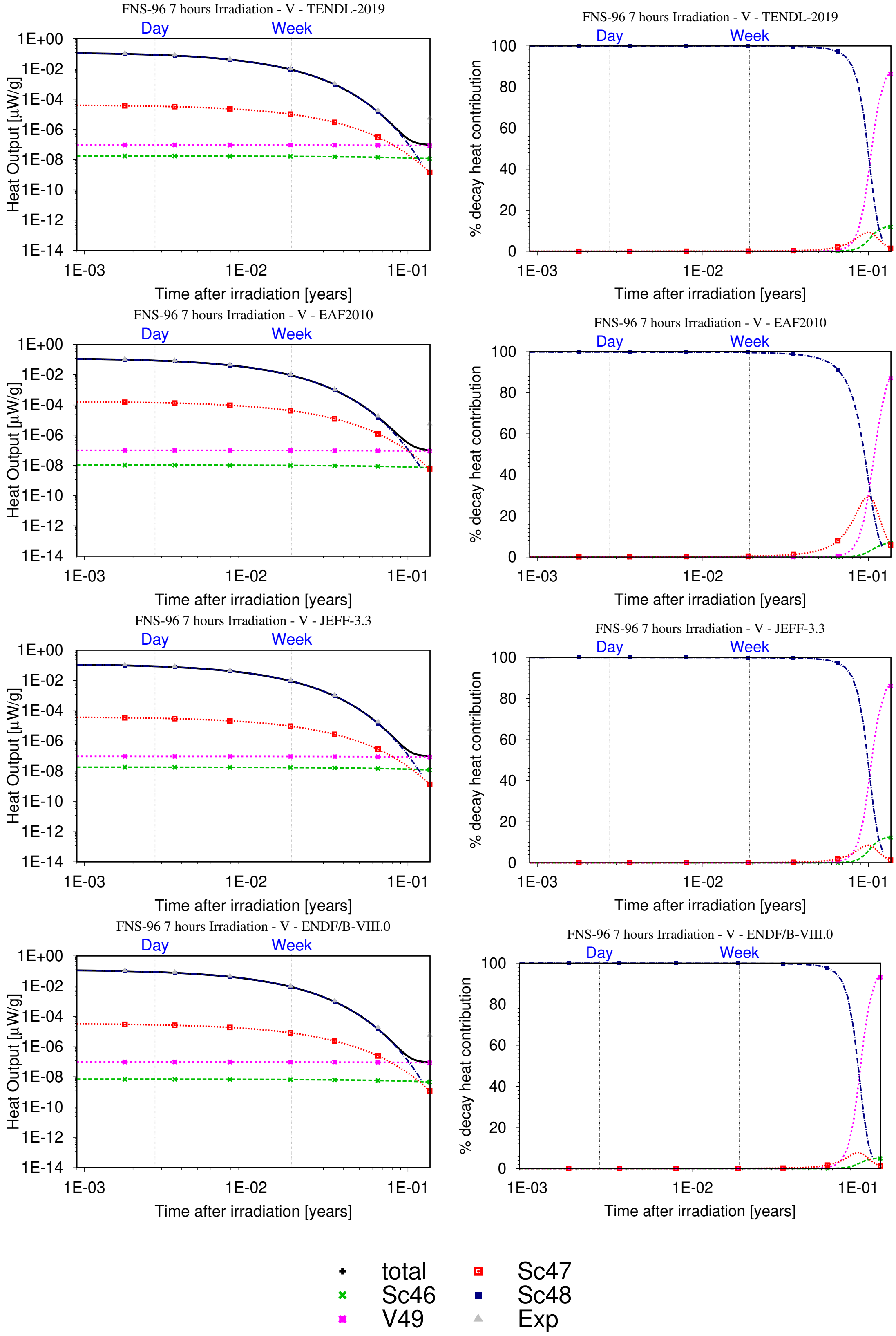


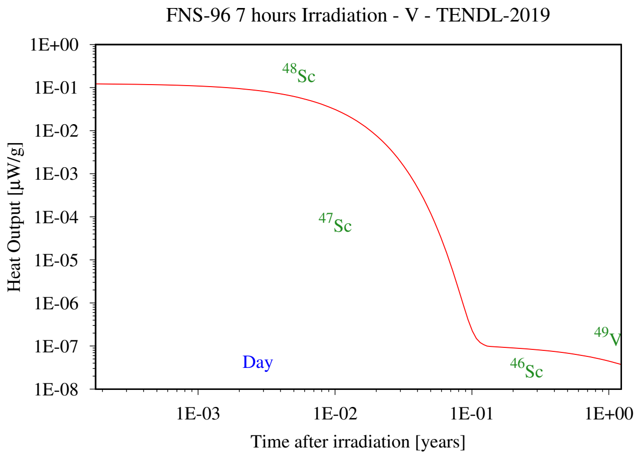
Vanadium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Sc48	1.82d	V51(n,α)Sc48	100.0
Sc47	3.35d	V50(n,α)Sc47	88.9
		V51(n,nα)Sc47	11.1
Sc46	83.79d	V50(n,nα)Sc46	96.3
		V50(n,nα)Sc46m(IT)Sc46	3.7
V49	330.01d	V50(n,2n)V49	100.0

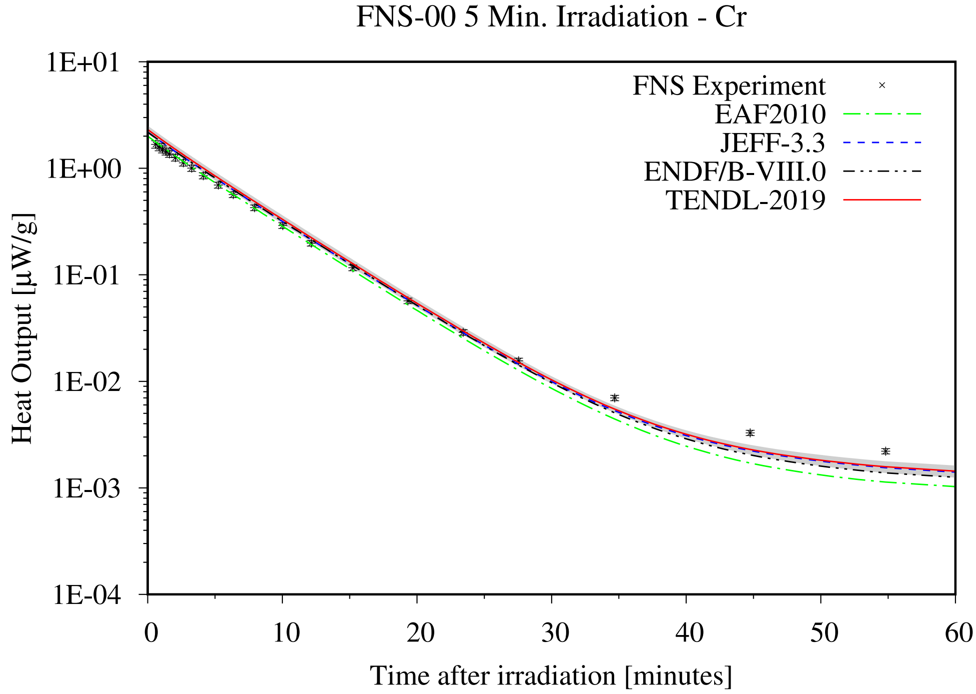
Comments on Vanadium 7-hour experiments:

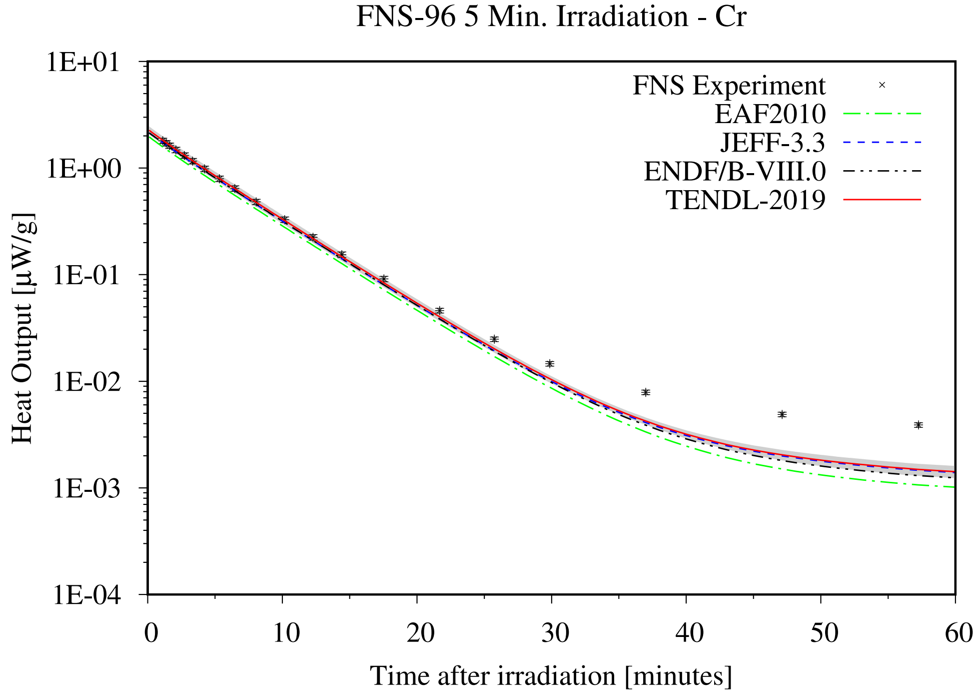
An excellent agreement is seen with TENDL, JEFF, ENDF/B, and EAF libraries at all but the last 50-day cooling step, where the experimental uncertainty is quoted as 58%. IRDFF-II reproduces the simulated profile (dominated in the simulations by Sc48 from (n,α) reactions on V51), but with a twofold overprediction that was not the case with IRDFF-1.05. In the final cooling step, V49 (from (n,2n)) is predicted to contribute around 90% of the decay-heat with all of the general purpose libraries, but the large discrepancy compared to the experiment makes it difficult to draw any definitive conclusions – is it an underpredicted channel in the simulations, or an unaccounted for impurity in the experiment?


FNS-96 7 hours Irradiation - V - TENDL-2019
FNS-96 7 hours Irradiation - V - EAF2010
FNS-96 7 hours Irradiation - V - JEFF-3.3
FNS-96 7 hours Irradiation - V - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-02
1E-04
1E-06
1E-08
1E-10
1E-12
1E-14
1E-03
1E-01
100
80
60
40
20
0
total
Sc46
V49
Sc47
Sc48
Exp


FNS-96 7 hours Irradiation - V - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
48Sc
47Sc
49V
46Sc
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Chromium

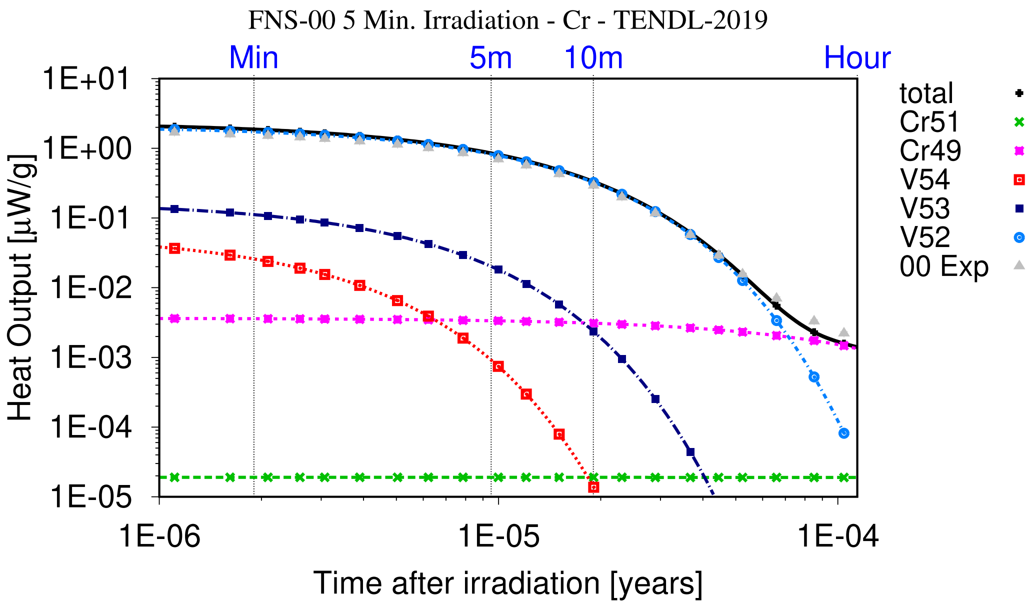

FNS-00 5 Min. Irradiation - Cr
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Cr
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	1.68E+00 +/-8%	2.04E+00 +/-9%	0.82	0.87	0.95	0.87
0.85	1.58E+00 +/-8%	1.93E+00 +/-9%	0.82	0.87	0.95	0.87
1.10	1.51E+00 +/-8%	1.83E+00 +/-9%	0.82	0.87	0.95	0.87
1.37	1.44E+00 +/-8%	1.73E+00 +/-9%	0.83	0.87	0.96	0.87
1.62	1.37E+00 +/-7%	1.65E+00 +/-9%	0.83	0.87	0.96	0.87
2.05	1.26E+00 +/-7%	1.51E+00 +/-9%	0.83	0.88	0.96	0.88
2.65	1.13E+00 +/-7%	1.34E+00 +/-9%	0.84	0.88	0.97	0.88
3.27	1.00E+00 +/-7%	1.19E+00 +/-9%	0.85	0.89	0.98	0.89
4.13	8.53$E-$01 +/-7%	1.00E+00 +/-9%	0.85	0.89	0.98	0.89
5.25	6.95$E-$01 +/-6%	8.10$E-$01 +/-9%	0.86	0.90	0.99	0.90
6.35	5.67$E-$01 +/-6%	6.57$E-$01 +/-9%	0.86	0.90	1.00	0.90
7.93	4.26$E-$01 +/-6%	4.88$E-$01 +/-9%	0.87	0.91	1.01	0.91
10.03	2.90$E-$01 +/-6%	3.31$E-$01 +/-9%	0.88	0.92	1.02	0.92
12.15	1.98$E-$01 +/-6%	2.24$E-$01 +/-9%	0.88	0.92	1.02	0.92
15.23	1.16$E-$01 +/-6%	1.27$E-$01 +/-9%	0.91	0.95	1.06	0.95
19.33	5.70$E-$02 +/-6%	6.10$E-$02 +/-9%	0.93	0.98	1.09	0.98
23.43	2.88$E-$02 +/-6%	2.98$E-$02 +/-9%	0.97	1.02	1.13	1.01
27.55	1.56$E-$02 +/-6%	1.51$E-$02 +/-8%	1.03	1.09	1.22	1.07
34.68	6.98$E-$03 +/-6%	5.51$E-$03 +/-8%	1.27	1.37	1.57	1.31
44.75	3.28$E-$03 +/-6%	2.30$E-$03 +/-10%	1.43	1.60	1.91	1.46
54.82	2.21$E-$03 +/-6%	1.58$E-$03 +/-13%	1.40	1.60	1.95	1.43
mean % diff. from E			17	14	10	13
mean χ^2			7.86	7.45	9.49	5.80

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
V52	3.74m	0.82	8%	9%
Cr49	41.90m	1.43	6%	14%

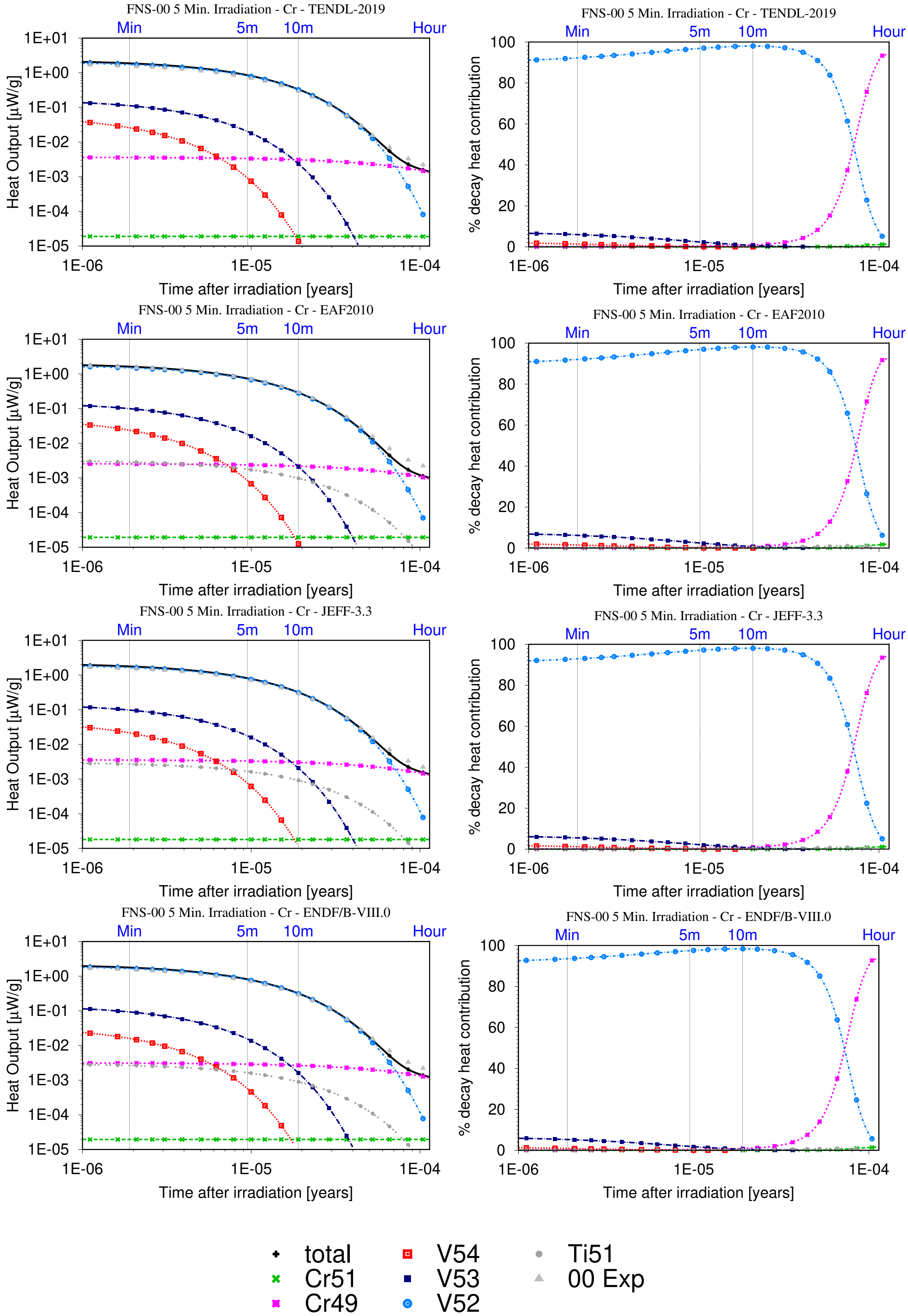


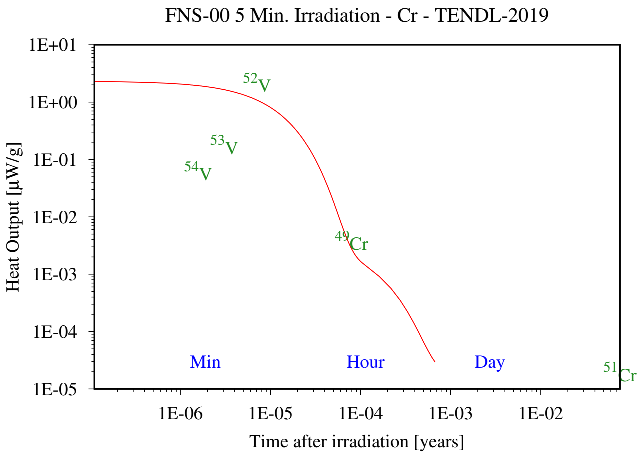
Chromium, TENDL-2019 5-minute pathway analysis

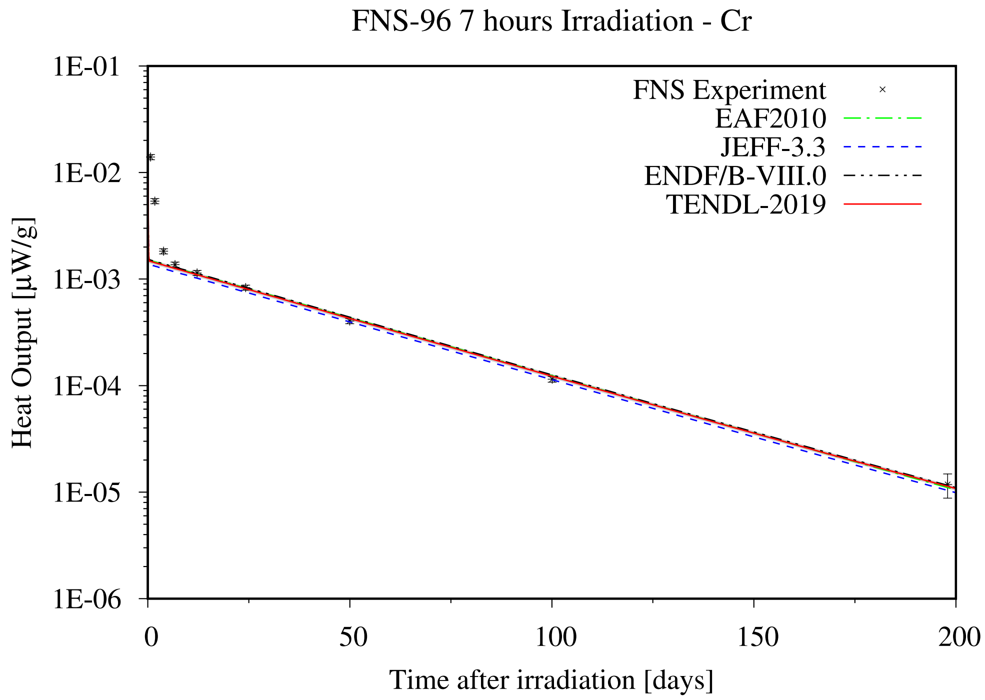
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
V54	49.80s	Cr54(n,p)V54	100.0
V53	1.62m	Cr53(n,p)V53	99.3
V52	3.74m	Cr52(n,p)V52	98.0
		Cr53(n,np)V52	1.6
Ti51	5.80m	Cr54(n,α)Ti51	100.0
Cr49	41.90m	Cr50(n,2n)Cr49	100.0
Cr51	27.70d	Cr52(n,2n)Cr51	100.0

Comments on Chromium 5-minute experiments:

There is a good simulation.vs.experiment agreement up to around 30 minutes of cooling with all of the included libraries, which is precisely the timescale over which V52 dominates. V52 is primarily produced via (n,p) reactions on Cr52 (see the pathways table), but this reaction is missing from IRDFF (V52 is too short lived to be of interest for a dosimetry file) and so that library is not included here. At longer times there is deviation from the experiment, which could come from Al and Fe impurities. These may have been present in the sample at levels of up to 2000 and 6000 ppm, respectively (such levels of impurities have been measured in similar samples). Else there is an underprediction in the Cr50(n,2n)Cr49 channel, but further experiments would be needed to confirm this.


FNS-00 5 Min. Irradiation - Cr - TENDL-2019
FNS-00 5 Min. Irradiation - Cr - EAF2010
FNS-00 5 Min. Irradiation - Cr - JEFF-3.3
FNS-00 5 Min. Irradiation - Cr - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Cr51
Cr49
V54
V53
V52
Ti51
00 Exp

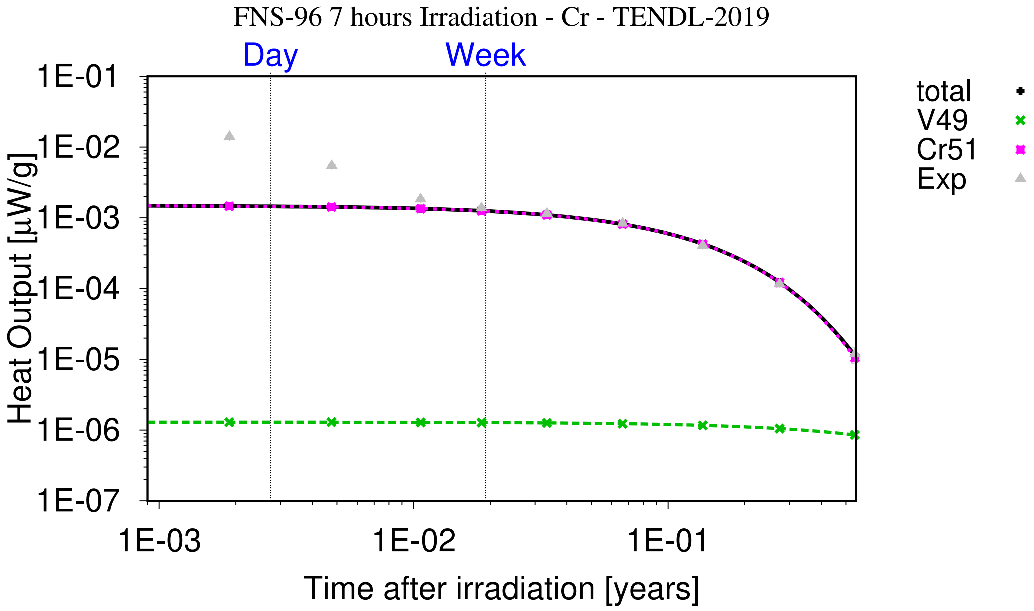

FNS-00 5 Min. Irradiation - Cr - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
52V
53V
54V
49Cr
51Cr
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.69	$1.40E{-}02$ +/-6%	$1.46E{-}03$ +/-4%	9.54	9.28	9.39	10.28
1.74	$5.39E{-}03$ +/-6%	$1.43E{-}03$ +/-4%	3.78	3.68	3.72	4.07
3.89	$1.83E{-}03$ +/-6%	$1.35E{-}03$ +/-4%	1.35	1.31	1.33	1.46
6.75	$1.37E{-}03$ +/-6%	$1.26E{-}03$ +/-4%	1.09	1.06	1.07	1.17
12.20	$1.14E{-}03$ +/-6%	$1.10E{-}03$ +/-4%	1.04	1.01	1.02	1.12
24.21	$8.31E{-}04$ +/-6%	$8.13E{-}04$ +/-4%	1.02	0.99	1.01	1.10
49.96	$4.03E{-}04$ +/-6%	$4.28E{-}04$ +/-4%	0.94	0.92	0.93	1.02
100.09	$1.15E{-}04$ +/-6%	$1.23E{-}04$ +/-4%	0.93	0.91	0.92	1.01
197.96	$1.18E{-}05$ +/-26%	$1.14E{-}05$ +/-4%	1.04	1.02	1.06	1.13
mean % diff. from E			24	24	24	27
mean χ^2			51.98	51.12	51.44	55.61

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Cr51	27.70d	9.54	6%	4%

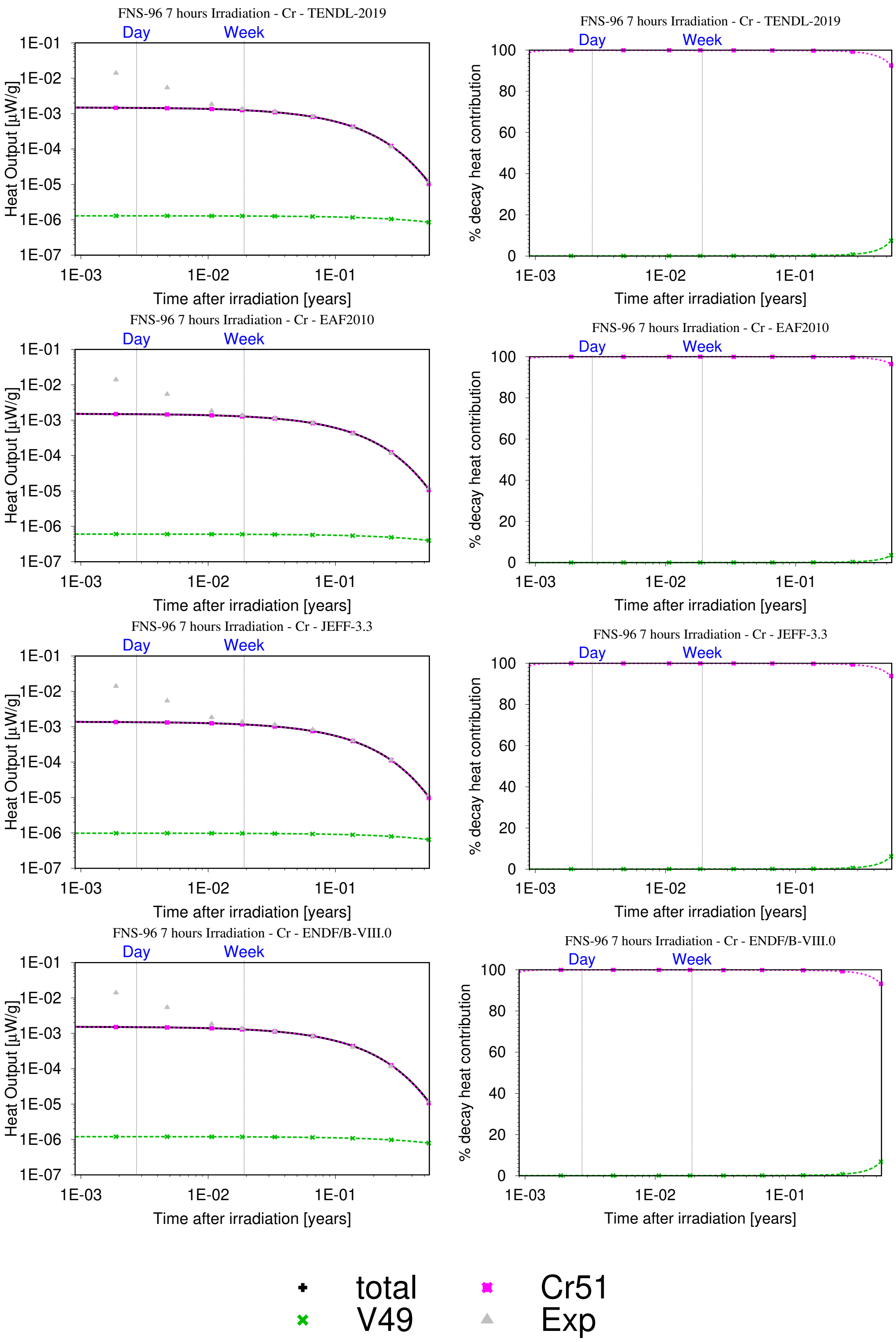


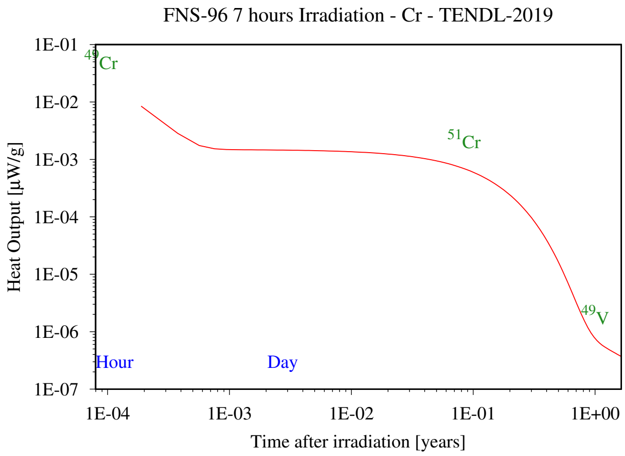
Chromium,TENDL-2019 7-hours pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Cr51	27.70d	Cr52(n,2n)Cr51	100.0
V49	330.01d	Cr50(n,np)V49	93.7
		Cr50(n,2n)Cr49(β^+)V49	4.2
		Cr50(n,d)V49	2.1

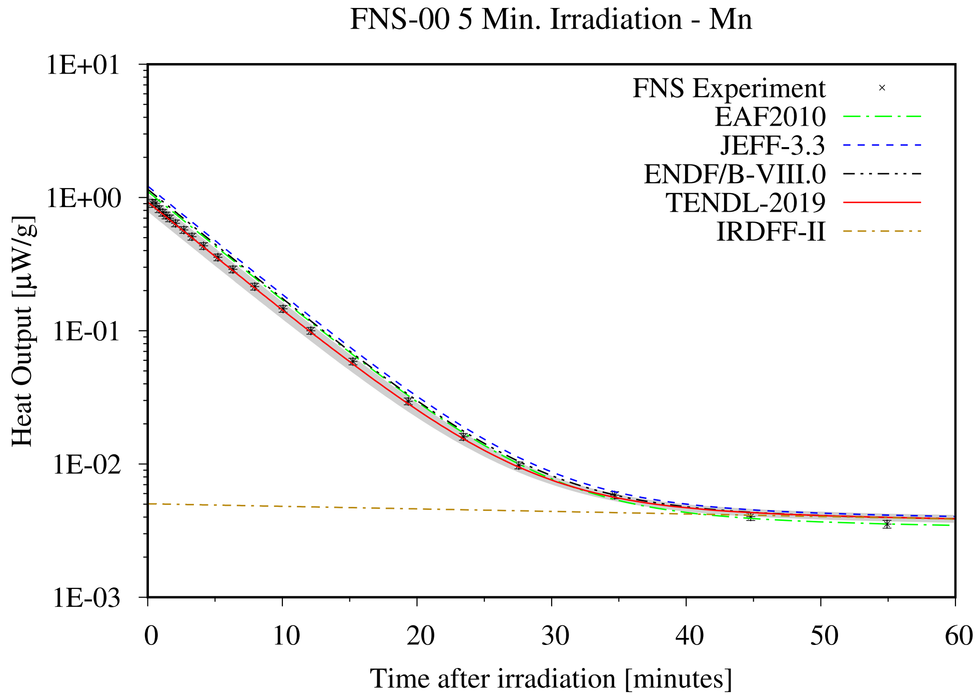
Comments on Chromium 7-hour experiments:

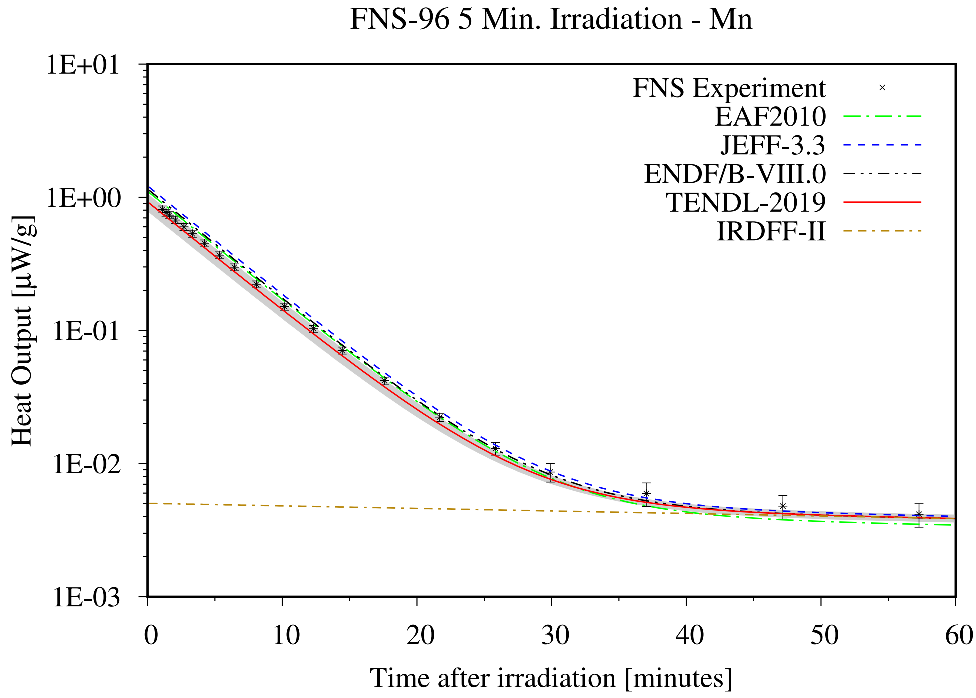
Some short-lived isotopes seem to be missing in all the simulations, almost certainly produced from impurities within the sample (as discussed for the 5 minute experiments earlier where only production of the very short-lived V52 nuclide was seen to follow the decay cooling in the experiment), but the overall agreement, completely dominated by Cr52(n,2n)Cr51, remains excellent. Note that IRDFF-1.05 included this important channel, but IRDFF-II misses it (due to shift to natural Cr data files?) and is omitted from the plots.


FNS-96 7 hours Irradiation - Cr - TENDL-2019
Day
Week
Heat Output [µW/g]
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - TENDL-2019
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - EAF2010
Heat Output [µW/g]
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - EAF2010
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - JEFF-3.3
Heat Output [µW/g]
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - JEFF-3.3
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - ENDF/B-VIII.0
Heat Output [µW/g]
Time after irradiation [years]
FNS-96 7 hours Irradiation - Cr - ENDF/B-VIII.0
% decay heat contribution
Time after irradiation [years]
total
Cr51
V49
Exp


FNS-96 7 hours Irradiation - Cr - TENDL-2019
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
49Cr
51Cr
49V
Hour
Day
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Manganese

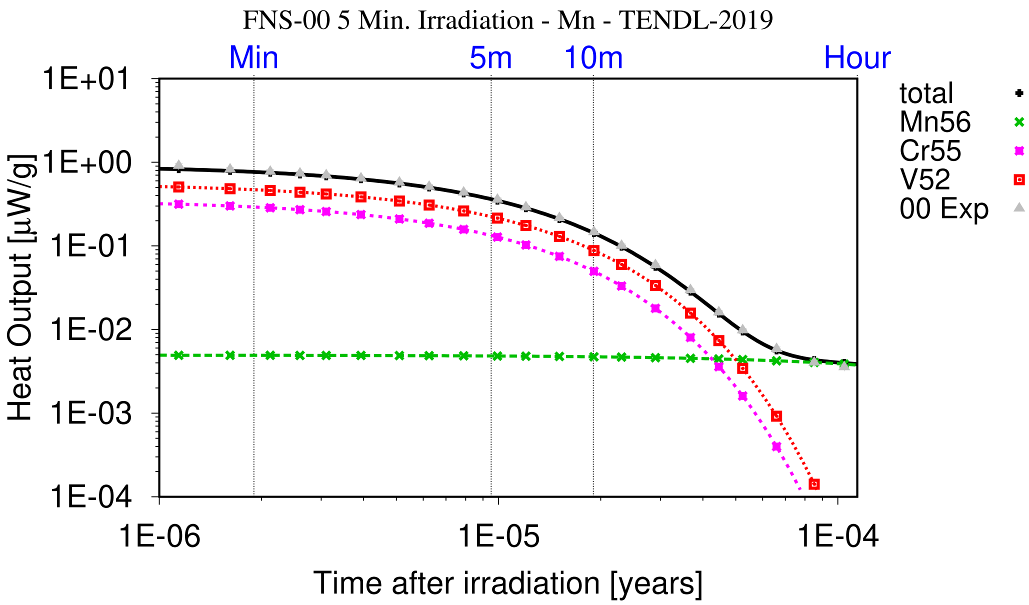

FNS-00 5 Min. Irradiation - Mn
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - Mn
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

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
0.33	9.06E−01 +/-7%	8.69E−01 +/-15%	1.04	0.84	0.87	0.79	180.50
0.60	9.06E−01 +/-6%	8.26E−01 +/-15%	1.10	0.88	0.91	0.83	180.55
0.85	8.18E−01 +/-6%	7.88E−01 +/-15%	1.04	0.83	0.87	0.79	163.28
1.12	7.70E−01 +/-6%	7.50E−01 +/-15%	1.03	0.83	0.86	0.78	153.86
1.37	7.34E−01 +/-6%	7.15E−01 +/-15%	1.03	0.82	0.85	0.78	146.73
1.63	6.98E−01 +/-6%	6.80E−01 +/-15%	1.03	0.83	0.86	0.78	139.83
2.07	6.41E−01 +/-6%	6.27E−01 +/-15%	1.02	0.82	0.85	0.78	128.54
2.68	5.71E−01 +/-6%	5.59E−01 +/-15%	1.02	0.82	0.85	0.78	114.93
3.28	5.09E−01 +/-6%	4.99E−01 +/-15%	1.02	0.82	0.85	0.78	102.66
4.15	4.33E−01 +/-6%	4.24E−01 +/-15%	1.02	0.82	0.85	0.78	87.74
5.22	3.56E−01 +/-6%	3.48E−01 +/-15%	1.02	0.83	0.85	0.78	72.45
6.33	2.89E−01 +/-6%	2.83E−01 +/-15%	1.02	0.83	0.86	0.78	59.13
7.95	2.15E−01 +/-6%	2.09E−01 +/-15%	1.03	0.84	0.86	0.78	44.21
10.05	1.46E−01 +/-6%	1.42E−01 +/-15%	1.03	0.84	0.86	0.79	30.36
12.12	1.00E−01 +/-6%	9.78E−02 +/-14%	1.02	0.84	0.86	0.79	20.99
15.25	5.88E−02 +/-6%	5.62E−02 +/-14%	1.05	0.87	0.89	0.81	12.50
19.35	2.95E−02 +/-6%	2.84E−02 +/-13%	1.04	0.88	0.90	0.82	6.39
23.45	1.60E−02 +/-6%	1.55E−02 +/-11%	1.03	0.90	0.93	0.84	3.53
27.57	9.76E−03 +/-6%	9.49E−03 +/-9%	1.03	0.93	0.97	0.87	2.19
34.68	5.85E−03 +/-6%	5.63E−03 +/-6%	1.04	1.00	1.08	0.94	1.35
44.80	4.02E−03 +/-7%	4.32E−03 +/-7%	0.93	0.93	1.03	0.89	0.97
54.92	3.54E−03 +/-7%	3.98E−03 +/-7%	0.89	0.89	1.00	0.86	0.90
mean % diff. from E			4	17	13	24	83
mean χ^2			0.52	8.98	5.79	17.52	223.86

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Mn56	2.58h	1.04	6%	7%

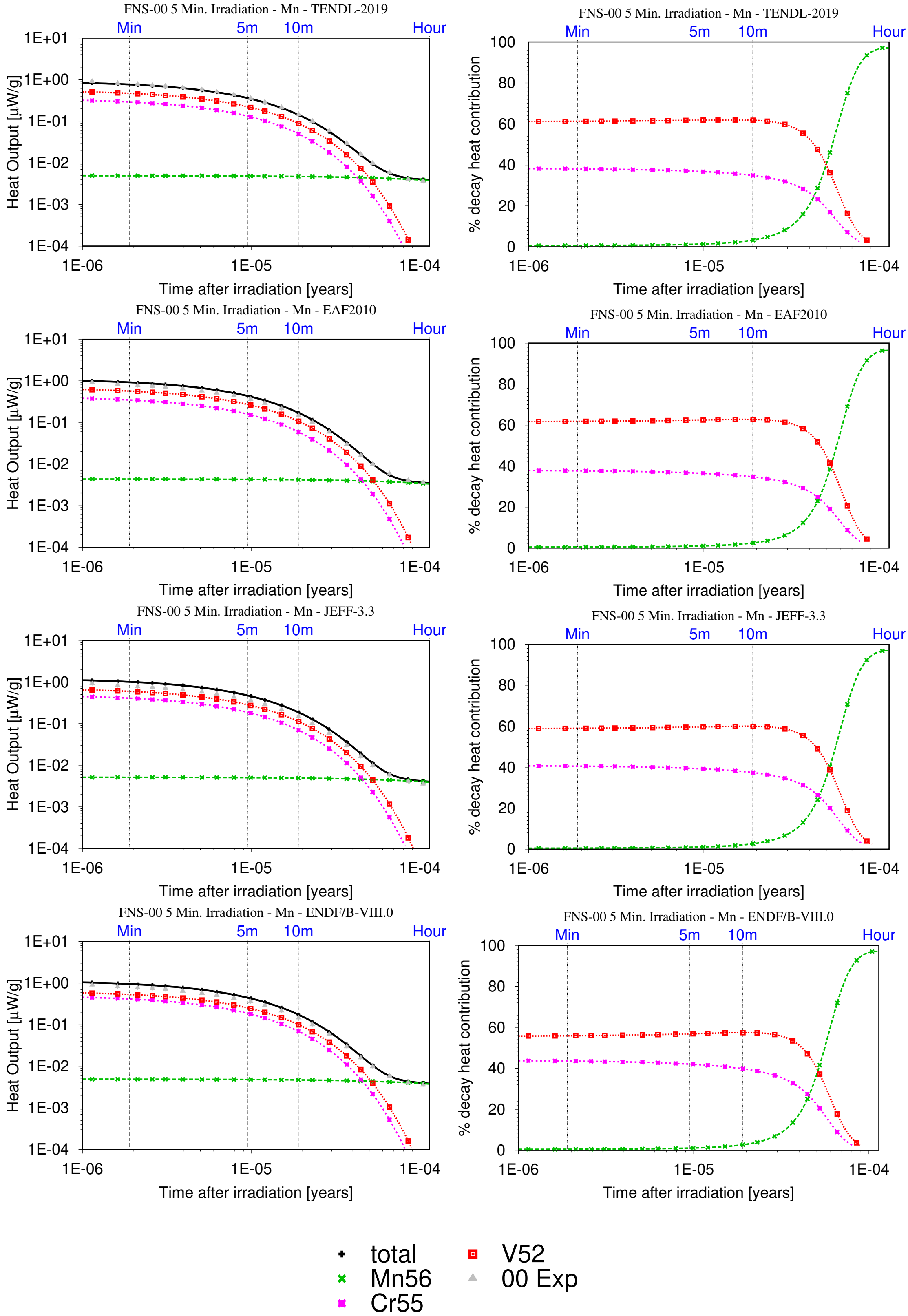


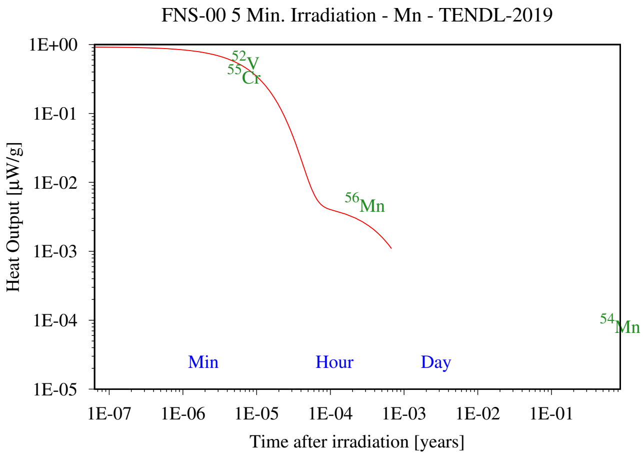
Manganese, TENDL-2019 5-minute pathway analysis

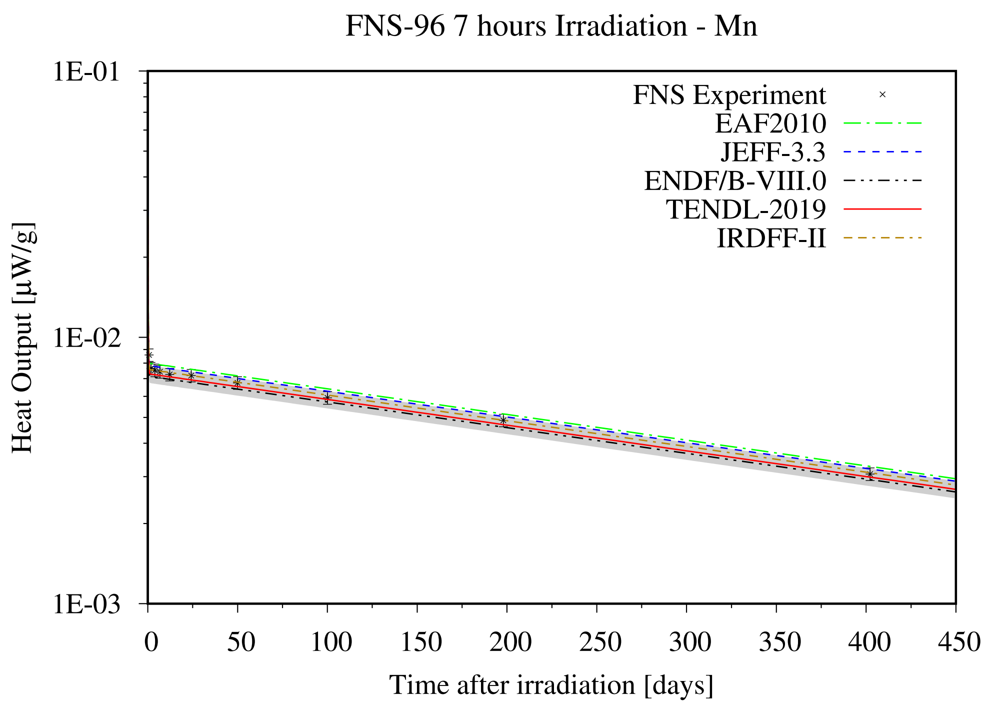
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Cr55	3.54m	Mn55(n,p)Cr55	100.0
V52	3.74m	Mn55(n,α)V52	100.0
Mn56	2.58h	Mn55(n,γ)Mn56	100.0

Comments on Manganese 5-minute experiments:

For Manganese, there is a good agreement at short cooling times for both batches with all general purpose libraries (IRDFF-II misses the Cr55 and V52 production). A slightly improved overall agreement with the experiment is noted for TENDL-2019 results compared to those with TENDL-2017, seemingly due a reduction in the cross section of the (n,α) channel that produces V52 (this is the dominant nuclide below 30 minutes).


FNS-00 5 Min. Irradiation - Mn - TENDL-2019
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Mn - EAF2010
FNS-00 5 Min. Irradiation - Mn - JEFF-3.3
FNS-00 5 Min. Irradiation - Mn - ENDF/B-VIII.0
total
Mn56
Cr55
V52
00 Exp

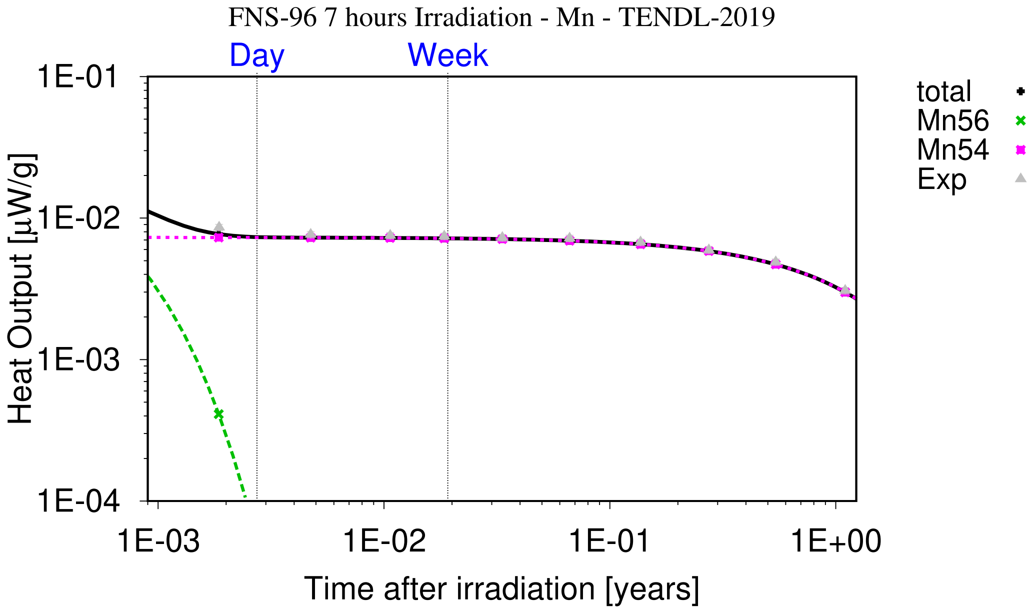

FNS-00 5 Min. Irradiation - Mn - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
52V
55Cr
56Mn
54Mn
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.68	8.58E−03 +/-5%	7.70E−03 +/-7%	1.11	1.14	1.02	1.04	1.08
1.73	7.64E−03 +/-5%	7.27E−03 +/-8%	1.05	1.07	0.96	0.98	1.01
3.89	7.52E−03 +/-5%	7.24E−03 +/-8%	1.04	1.06	0.95	0.97	1.00
6.75	7.43E−03 +/-5%	7.19E−03 +/-8%	1.03	1.06	0.94	0.96	0.99
12.20	7.25E−03 +/-5%	7.11E−03 +/-8%	1.02	1.04	0.93	0.95	0.98
24.21	7.19E−03 +/-5%	6.92E−03 +/-8%	1.04	1.06	0.95	0.97	1.00
49.96	6.74E−03 +/-5%	6.53E−03 +/-8%	1.03	1.05	0.94	0.96	0.99
100.10	5.93E−03 +/-5%	5.85E−03 +/-8%	1.01	1.04	0.93	0.95	0.98
197.97	4.88E−03 +/-5%	4.70E−03 +/-8%	1.04	1.06	0.95	0.97	1.00
402.18	3.07E−03 +/-5%	2.99E−03 +/-8%	1.03	1.05	0.94	0.96	0.99
mean % diff. from E			4	6	6	4	1
mean χ^2			0.69	1.36	1.23	0.56	0.21

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Mn54	312.16d	1.11	5%	8%

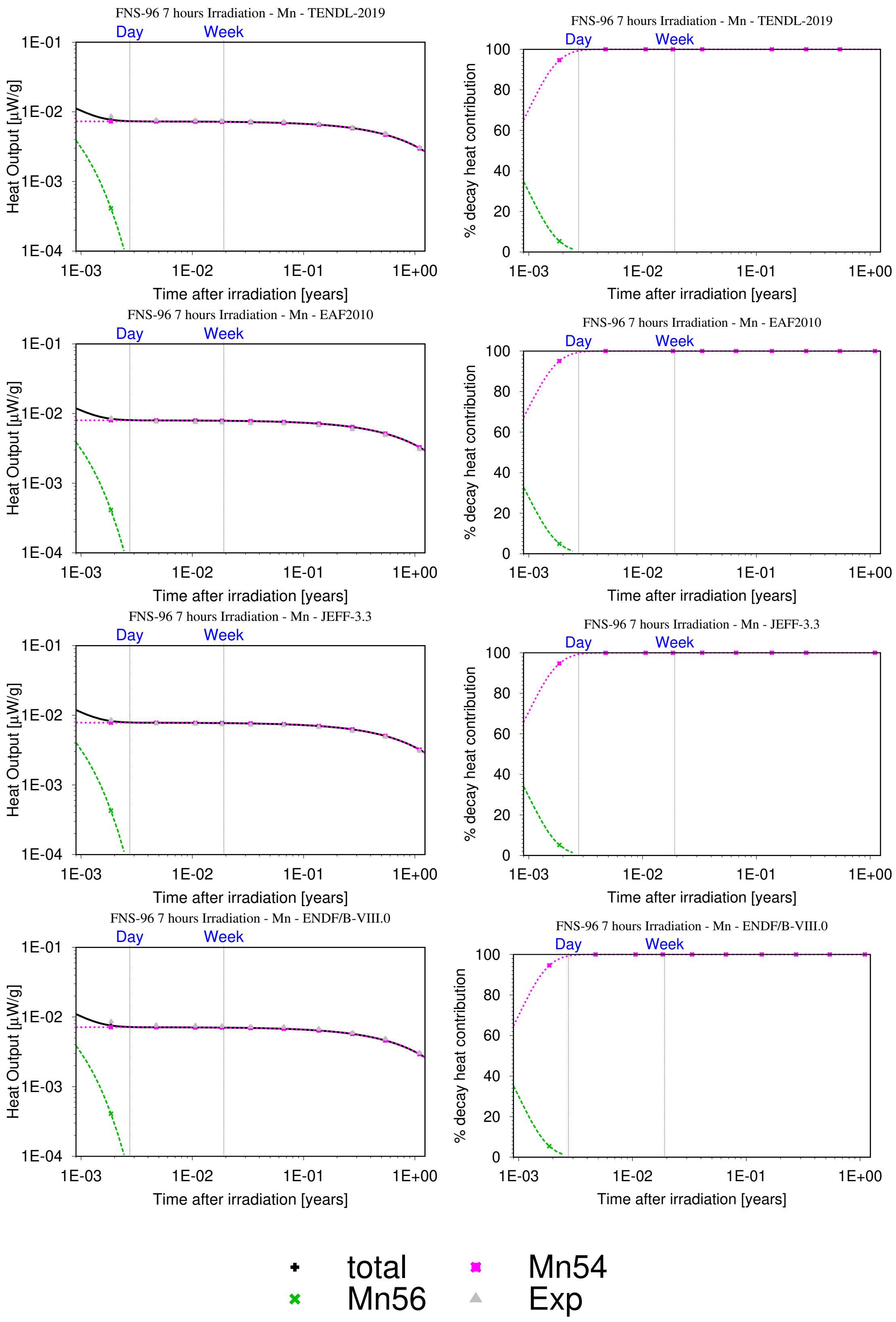


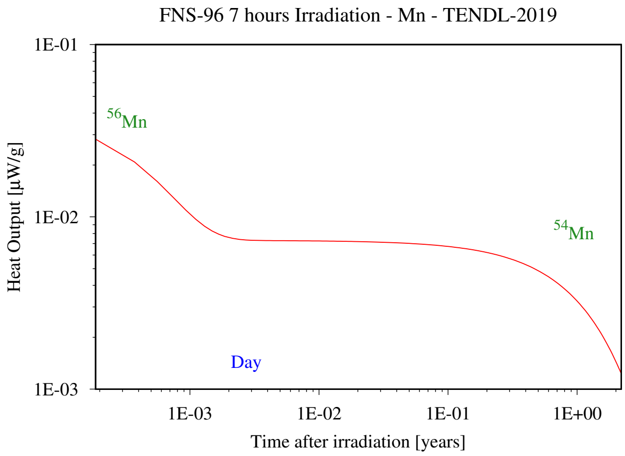
Manganese,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Mn56	2.58h	Mn55(n,γ)Mn56	100.0
Mn54	312.16d	Mn55(n,2n)Mn54	100.0

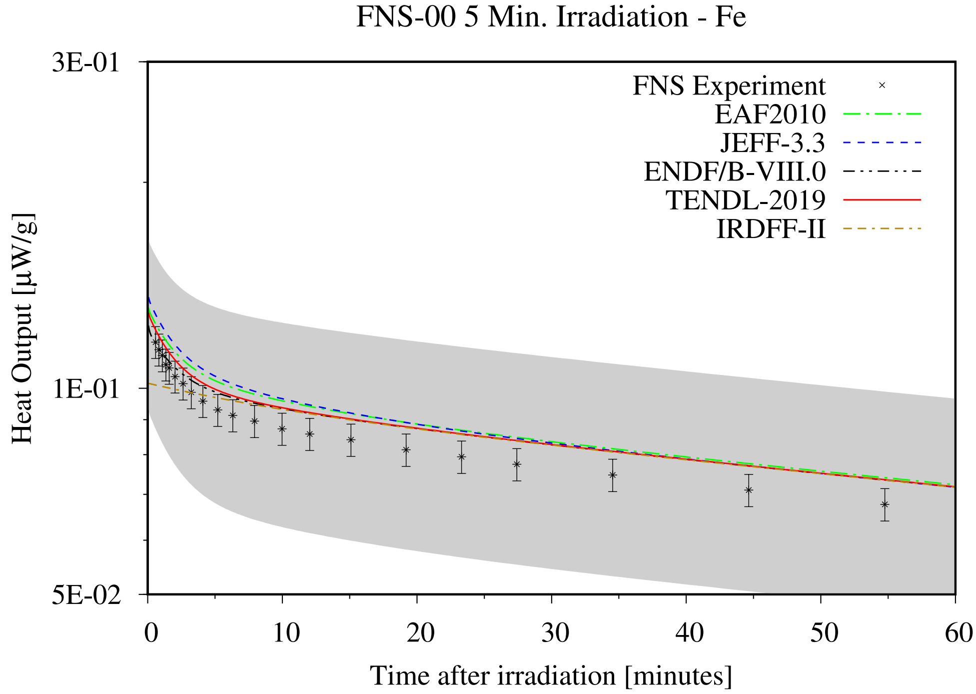
Comments on Manganese 7-hour experiments:

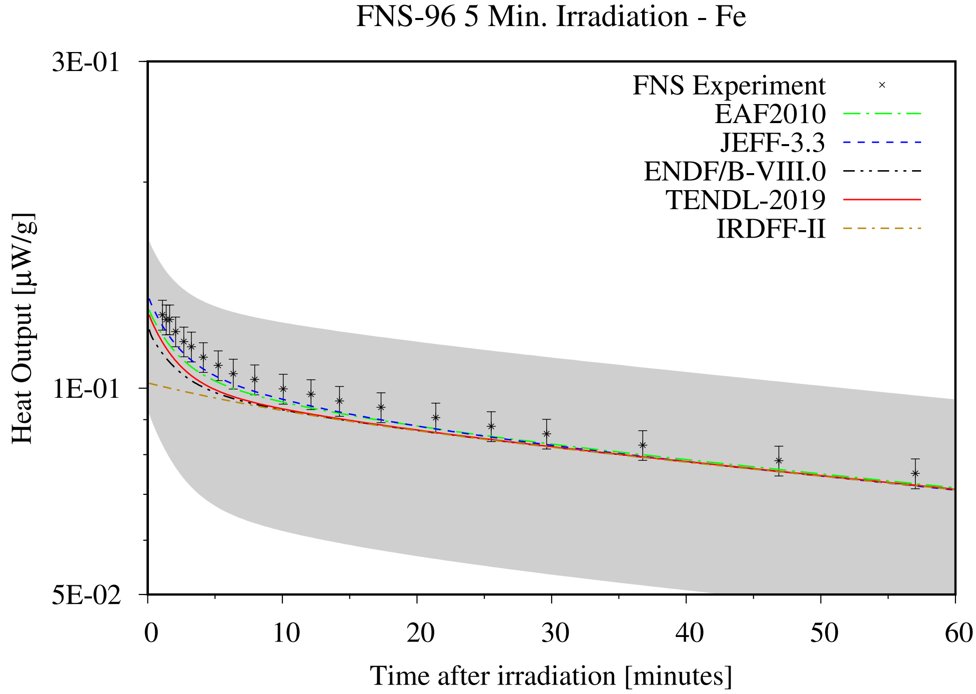
All of the simulations are in good agreement with the experimental measurements (generally within the experimental uncertainty) for this simple case dominated by the Mn55(n,2n)Mn54 reaction path (also part of IRDFF-II).


FNS-96 7 hours Irradiation - Mn - TENDL-2019
FNS-96 7 hours Irradiation - Mn - EAF2010
FNS-96 7 hours Irradiation - Mn - JEFF-3.3
FNS-96 7 hours Irradiation - Mn - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E+00
100
80
60
40
20
0
total
Mn54
Mn56
Exp


FNS-96 7 hours Irradiation - Mn - TENDL-2019
Heat Output [µW/g]
1E-01
1E-02
1E-03
56Mn
54Mn
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Iron

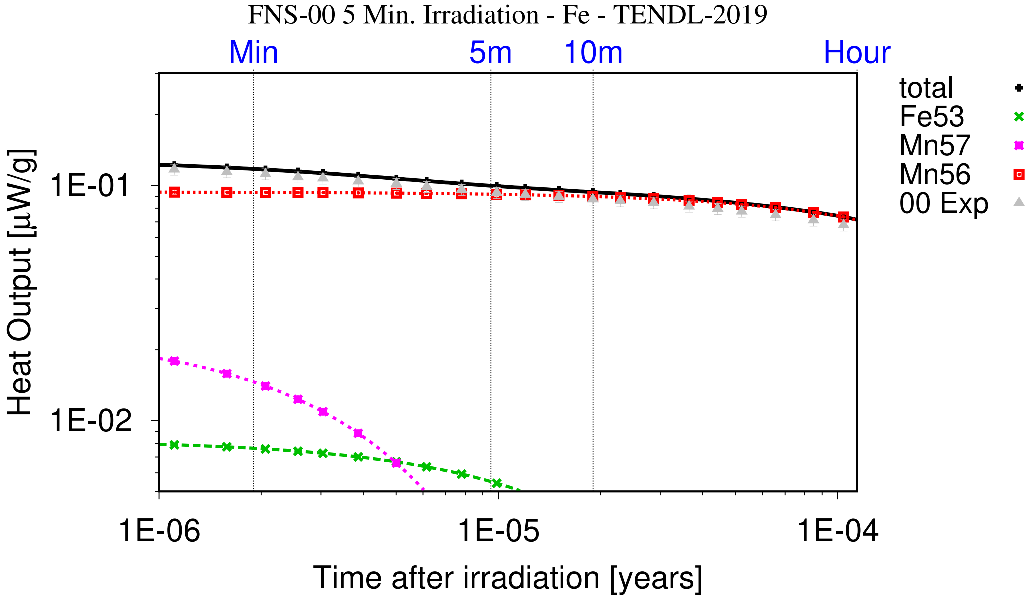

FNS-00 5 Min. Irradiation - Fe
Heat Output [µW/g]
3E-01
1E-01
5E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II


FNS-96 5 Min. Irradiation - Fe
Heat Output [µW/g]
3E-01
1E-01
5E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II

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

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

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

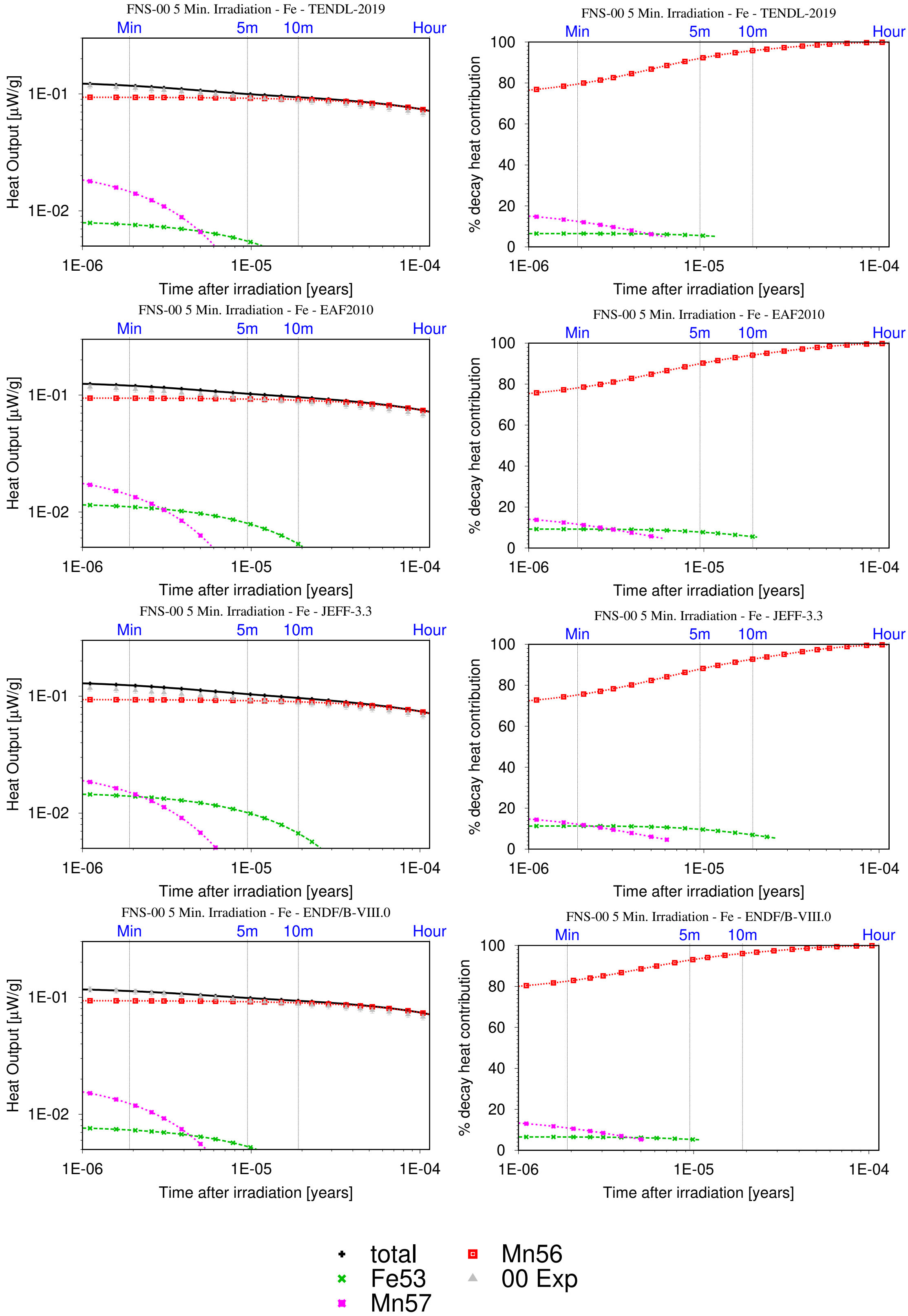


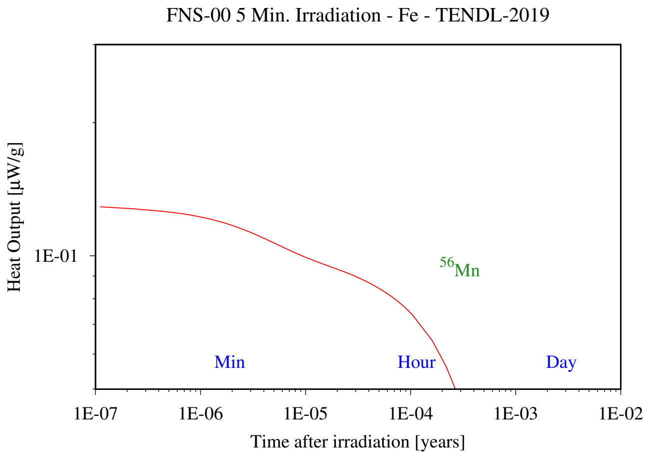
Iron, TENDL-2019 5-minute pathway analysis

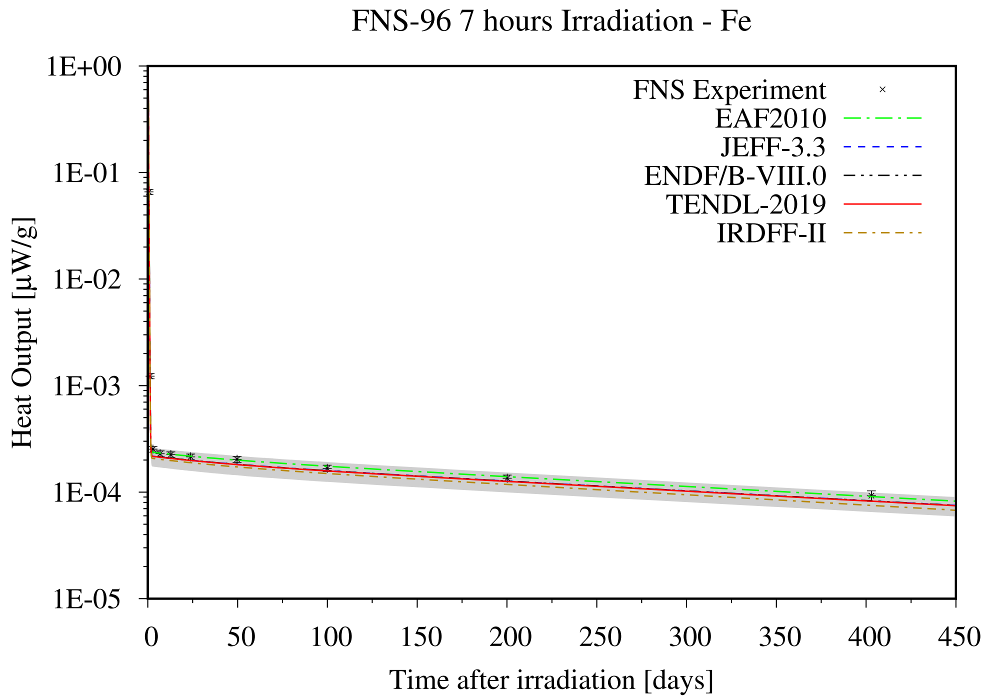
Product	$T_{1/2}$	Pathways	Path %
Mn57	1.42m	Fe57(n,p)Mn57	99.5
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Mn56	2.58h	Fe56(n,p)Mn56	99.7

Comments on Iron 5-minute experiments:

The two sets of calculated decay-heat curves, one for the experiment in 2000 and one for 1996, are in exact agreement (with some differences in the distribution of measured cooling times), as would be expected. However, the experimental decay results in the two batches disagree; one is just below the simulation curves (which are virtually identical with all libraries) and one above. This is suspicious and there is even more cause for concern with the reported data because the quoted uncertainty appears to be a simple, fixed standard deviation value, rather than an actual experimental error. IRDFF-II does not include the necessary reaction paths for the two short-lived radionuclides, Fe53 and Mn57, which the general purpose libraries predict (correctly) to be important in the first few minutes of cooling – for example, the dominant Mn56 contributes less than 80% of the decay-heat during the first minute of cooling (but is 100% after round 20 minutes and which IRDFF captures).


FNS-00 5 Min. Irradiation - Fe - TENDL-2019
Min
5m
10m
Hour
Heat Output [µW/g]
1E-01
1E-02
1E-06
1E-05
1E-04
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Fe - TENDL-2019
% decay heat contribution
100
80
60
40
20
0
FNS-00 5 Min. Irradiation - Fe - EAF2010
FNS-00 5 Min. Irradiation - Fe - EAF2010
FNS-00 5 Min. Irradiation - Fe - JEFF-3.3
FNS-00 5 Min. Irradiation - Fe - JEFF-3.3
FNS-00 5 Min. Irradiation - Fe - ENDF/B-VIII.0
FNS-00 5 Min. Irradiation - Fe - ENDF/B-VIII.0
total
Fe53
Mn57
Mn56
00 Exp

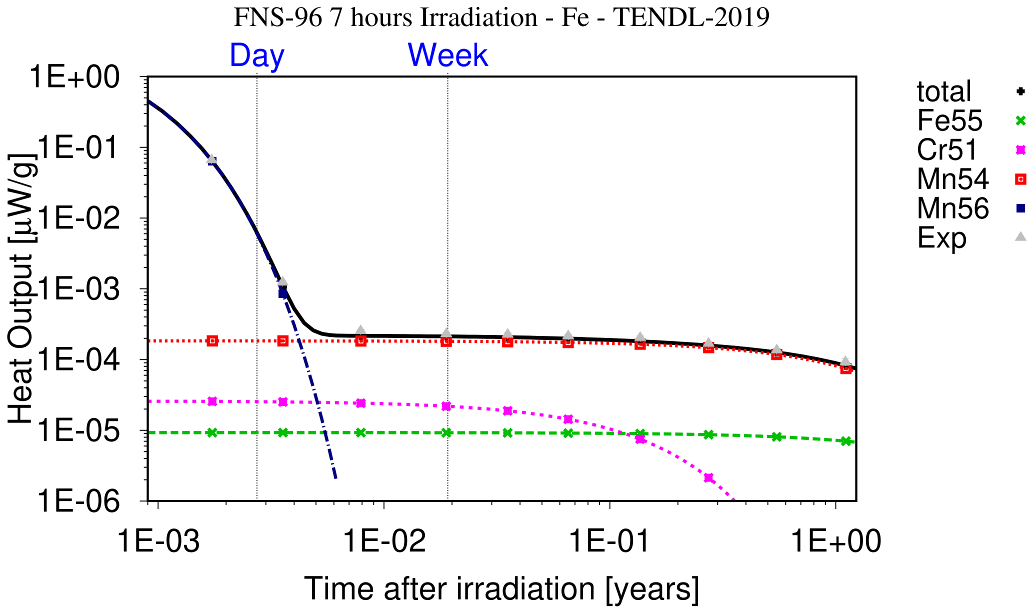

FNS-00 5 Min. Irradiation - Fe - TENDL-2019
Heat Output [µW/g]
1E-01
56Mn
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.63	6.58E−02 +/-5%	6.35E−02 +/-31%	1.04	1.04	1.03	1.04	1.04
1.30	1.23E−03 +/-5%	1.07E−03 +/-25%	1.15	1.16	1.12	1.16	1.16
2.88	2.53E−04 +/-6%	2.17E−04 +/-20%	1.17	1.16	1.07	1.17	1.22
6.89	2.30E−04 +/-6%	2.13E−04 +/-20%	1.08	1.08	0.99	1.08	1.13
12.88	2.25E−04 +/-6%	2.07E−04 +/-20%	1.09	1.08	0.99	1.08	1.14
23.89	2.14E−04 +/-6%	1.98E−04 +/-20%	1.08	1.08	0.99	1.08	1.13
49.72	2.03E−04 +/-6%	1.81E−04 +/-21%	1.12	1.11	1.01	1.11	1.18
99.91	1.67E−04 +/-7%	1.58E−04 +/-21%	1.06	1.05	0.96	1.05	1.12
200.13	1.35E−04 +/-7%	1.26E−04 +/-21%	1.07	1.06	0.97	1.06	1.14
402.95	9.24E−05 +/-11%	8.18E−05 +/-21%	1.13	1.12	1.02	1.12	1.24
mean % diff. from E			9	9	3	9	13
mean χ^2			2.14	2.10	0.60	2.13	4.02

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Mn56	2.58h	1.04	6%	31%
Mn54	312.16d	1.17	6%	23%

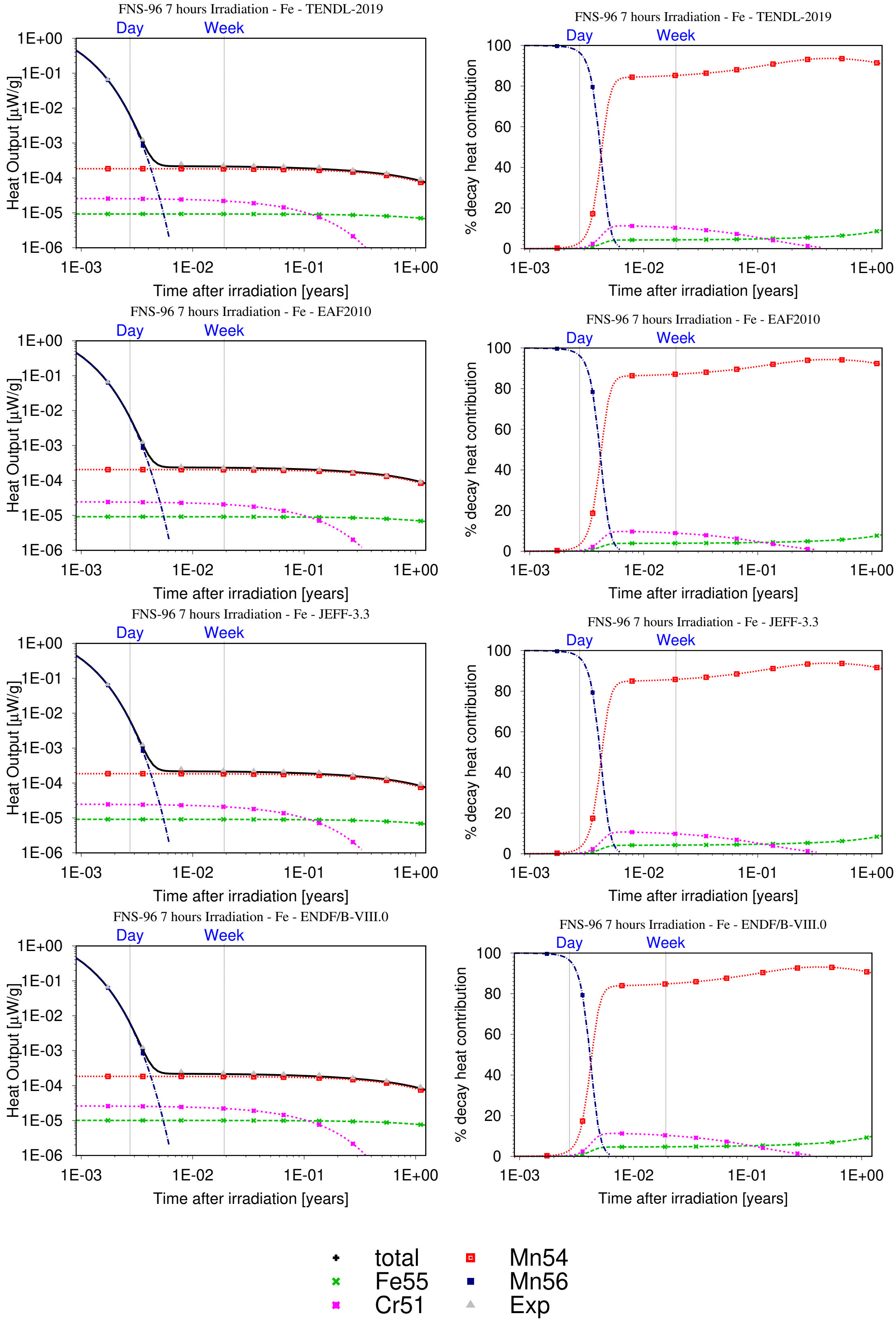


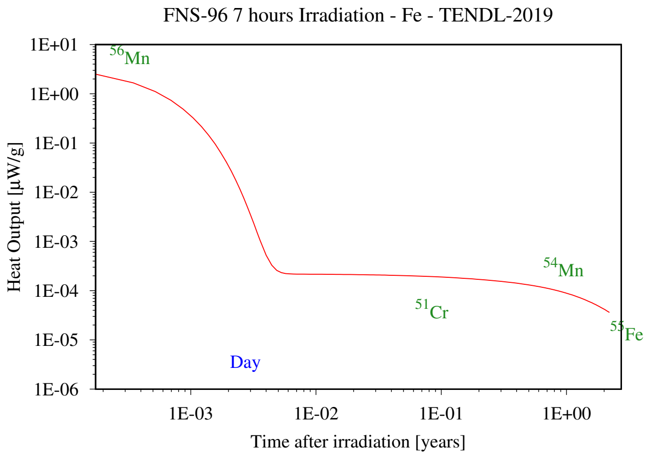
Iron,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Mn56	2.58h	Fe56(n,p)Mn56	99.7
Cr51	27.70d	Fe54(n,α)Cr51	100.0
Mn54	312.16d	Fe54(n,p)Mn54	100.0
Fe55	2.73y	Fe56(n,2n)Fe55	100.0

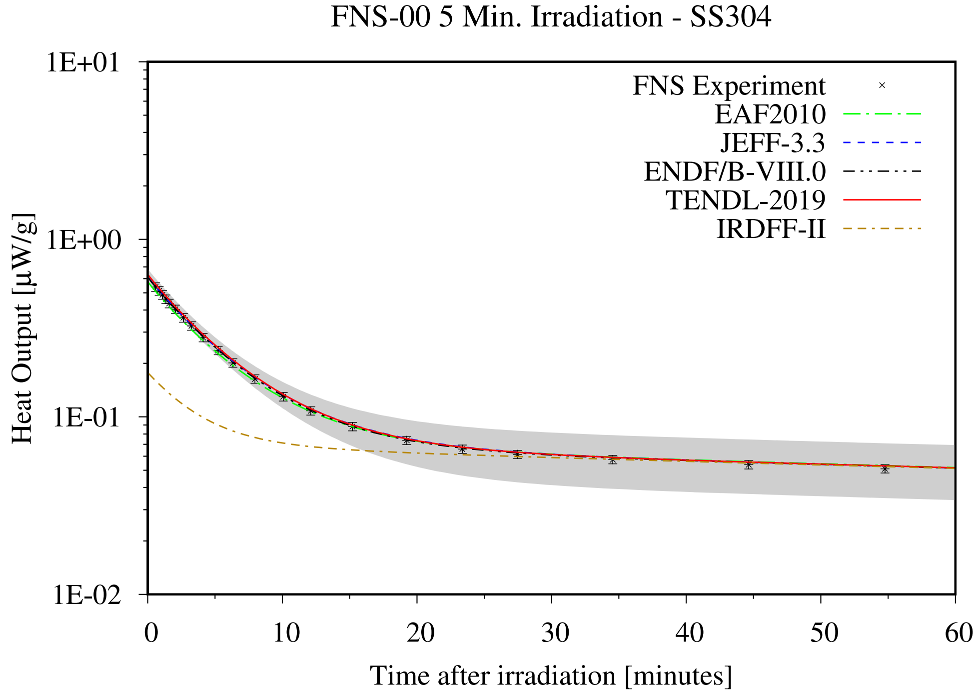
Comments on Iron 7-hour experiments:

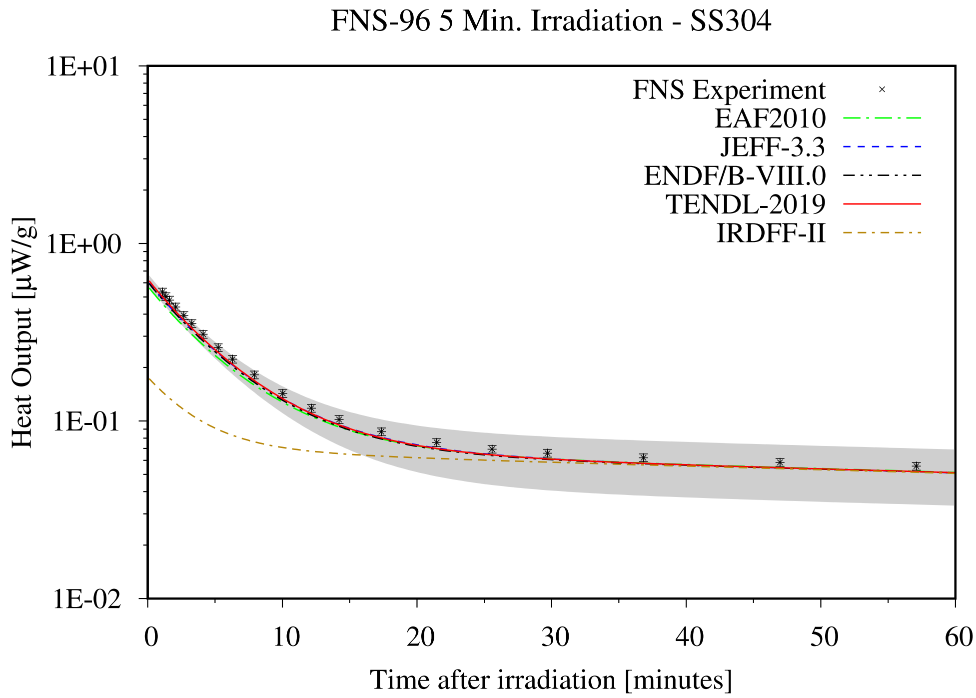
As with the 5-minute experiments, there is generally good agreement for iron between the simulation and experiment, with the decay profiles associated with the dominant Mn56 and Mn54 nuclides (both produced via (n,p) reactions) appearing to well-capture the experimental profile. The simulated curves are generally within the experimental uncertainty.


FNS-96 7 hours Irradiation - Fe - TENDL-2019
Day
Week
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]
FNS-96 7 hours Irradiation - Fe - TENDL-2019
% decay heat contribution
100
80
60
40
20
0
FNS-96 7 hours Irradiation - Fe - EAF2010
FNS-96 7 hours Irradiation - Fe - JEFF-3.3
FNS-96 7 hours Irradiation - Fe - ENDF/B-VIII.0
total
Fe55
Cr51
Mn54
Mn56
Exp


FNS-96 7 hours Irradiation - Fe - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-03
1E-02
1E-01
1E+00
56Mn
54Mn
51Cr
55Fe
Day

SS304

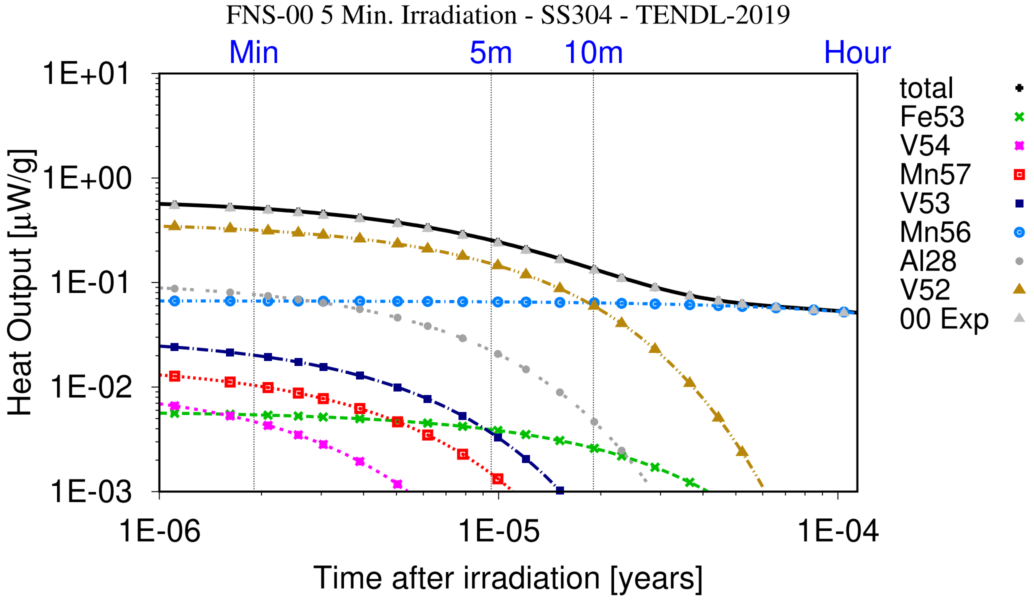

FNS-00 5 Min. Irradiation - SS304
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+01
1E+00
1E-01
1E-02
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - SS304
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+01
1E+00
1E-01
1E-02
0
10
20
30
40
50
60

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	5.39E−01 +/-6%	5.60E−01 +/-8%	0.96	1.00	1.06	0.99	3.37
0.85	5.12E−01 +/-6%	5.30E−01 +/-8%	0.97	1.00	1.06	1.00	3.35
1.10	4.86E−01 +/-6%	5.04E−01 +/-8%	0.97	1.00	1.06	0.99	3.32
1.35	4.60E−01 +/-6%	4.79E−01 +/-8%	0.96	0.99	1.05	0.99	3.27
1.60	4.35E−01 +/-6%	4.56E−01 +/-8%	0.95	0.98	1.04	0.98	3.21
2.05	4.04E−01 +/-6%	4.19E−01 +/-8%	0.96	0.99	1.05	0.99	3.18
2.65	3.61E−01 +/-6%	3.75E−01 +/-9%	0.96	0.99	1.05	0.98	3.09
3.25	3.25E−01 +/-6%	3.38E−01 +/-9%	0.96	0.99	1.05	0.98	2.99
4.12	2.80E−01 +/-6%	2.92E−01 +/-10%	0.96	0.99	1.04	0.98	2.82
5.23	2.37E−01 +/-5%	2.45E−01 +/-11%	0.96	0.99	1.04	0.98	2.63
6.33	2.01E−01 +/-5%	2.09E−01 +/-12%	0.96	0.99	1.03	0.97	2.42
7.97	1.64E−01 +/-5%	1.69E−01 +/-14%	0.97	0.99	1.03	0.97	2.14
10.07	1.30E−01 +/-5%	1.34E−01 +/-17%	0.97	0.99	1.02	0.97	1.83
12.12	1.08E−01 +/-5%	1.11E−01 +/-20%	0.97	0.99	1.01	0.97	1.59
15.20	8.82E−02 +/-5%	9.01E−02 +/-24%	0.98	1.00	1.00	0.98	1.35
19.25	7.37E−02 +/-5%	7.52E−02 +/-28%	0.98	0.99	0.99	0.98	1.17
23.37	6.59E−02 +/-5%	6.75E−02 +/-31%	0.98	0.99	0.98	0.97	1.08
27.47	6.15E−02 +/-5%	6.32E−02 +/-32%	0.97	0.98	0.97	0.97	1.03
34.55	5.74E−02 +/-5%	5.91E−02 +/-33%	0.97	0.98	0.97	0.97	1.00
44.65	5.38E−02 +/-5%	5.57E−02 +/-34%	0.97	0.97	0.96	0.97	0.98
54.77	5.10E−02 +/-5%	5.29E−02 +/-34%	0.96	0.97	0.96	0.96	0.97
mean % diff. from E			3	1	4	2	44
mean χ^2			0.41	0.07	0.52	0.20	88.79

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Mn56	2.58h	0.98	5%	34%

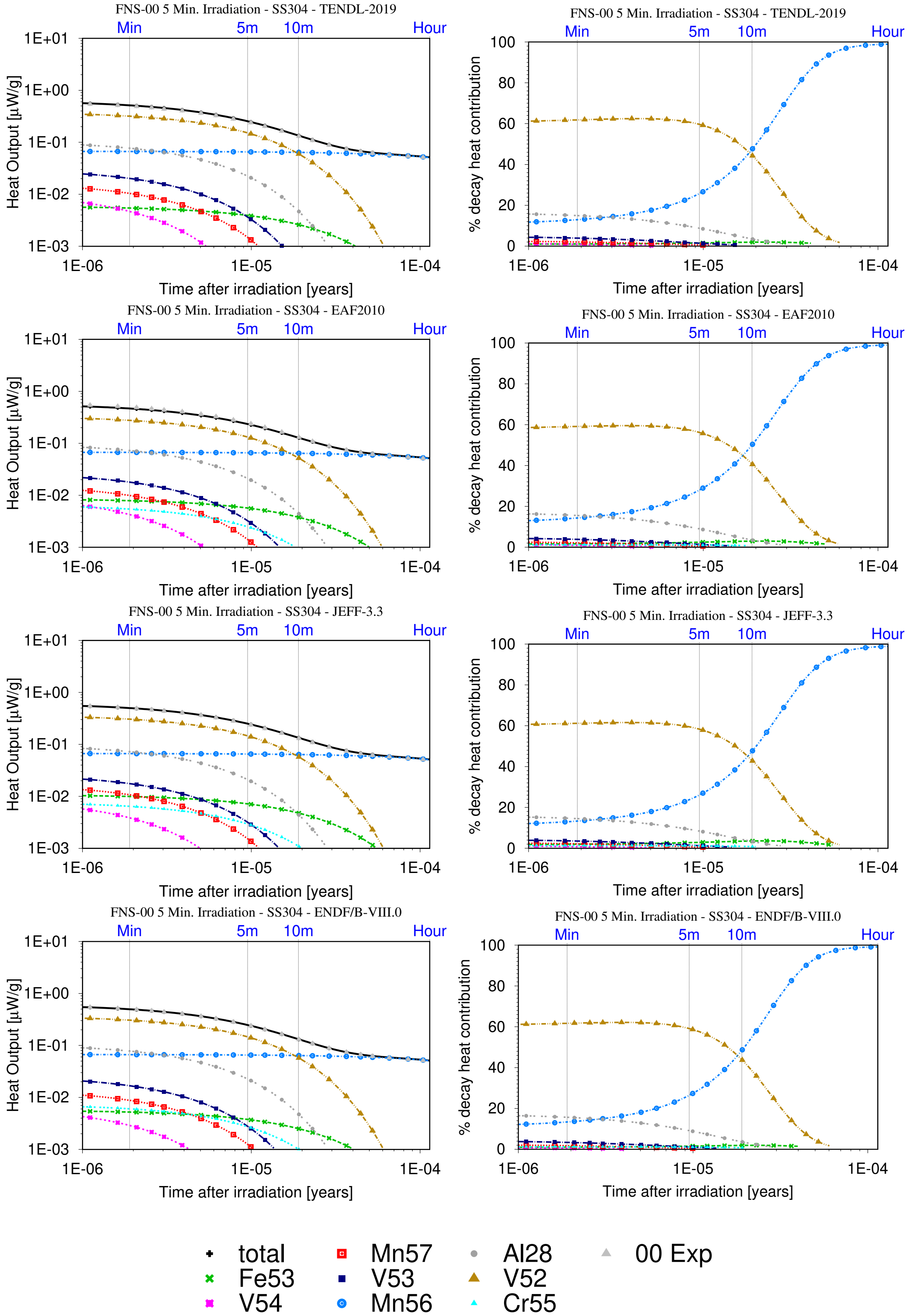


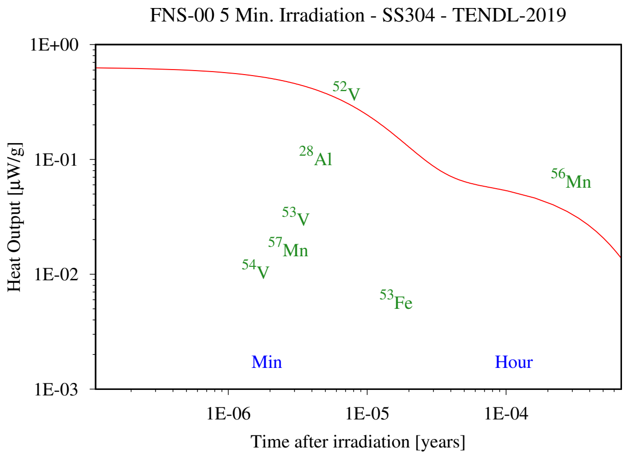
SS304, TENDL-2019 5-minute pathway analysis

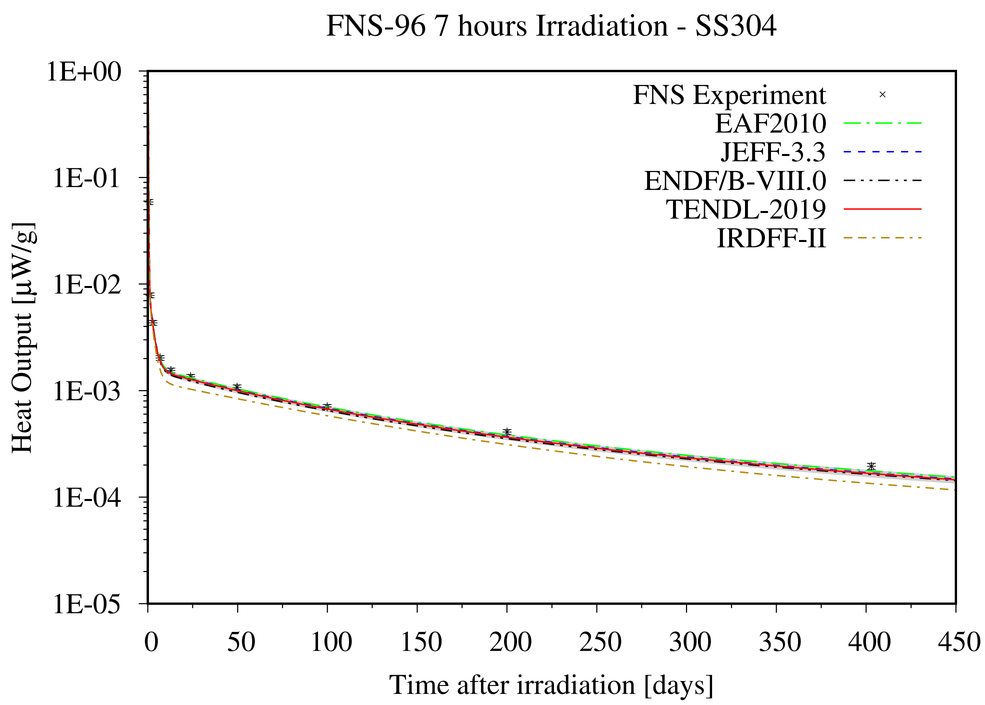
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
V54	49.80s	Cr54(n,p)V54	100.0
Mn57	1.42m	Fe57(n,p)Mn57	99.5
V53	1.62m	Cr53(n,p)V53	99.3
Al28	2.24m	Si28(n,p)Al28	99.7
Cr55	3.54m	Mn55(n,p)Cr55	90.4
		Fe58(n,α)Cr55	8.5
		Cr54(n,γ)Cr55	1.0
V52	3.74m	Cr52(n,p)V52	95.9
		Mn55(n,α)V52	2.1
		Cr53(n,np)V52	1.6
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Mn56	2.58h	Fe56(n,p)Mn56	99.6

Comments on SS304 5-minute experiments:

Remarkable agreement between experiment and simulation (with TENDL-2019, JEFF-3.3, EAF2010 and ENDF/B-VIII.0) for cooling times of up to 1 hour (IRDFF-II is discrepant below 20 minutes because it doesn't include the Cr52(n,p)V52 channel). All libraries capture the profile associated with the important Mn56 nuclide, which dominates beyond 10 minutes.


FNS-00 5 Min. Irradiation - SS304 - TENDL-2019
FNS-00 5 Min. Irradiation - SS304 - EAF2010
FNS-00 5 Min. Irradiation - SS304 - JEFF-3.3
FNS-00 5 Min. Irradiation - SS304 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Fe53
V54
Mn57
V53
Mn56
Al28
V52
Cr55
00 Exp

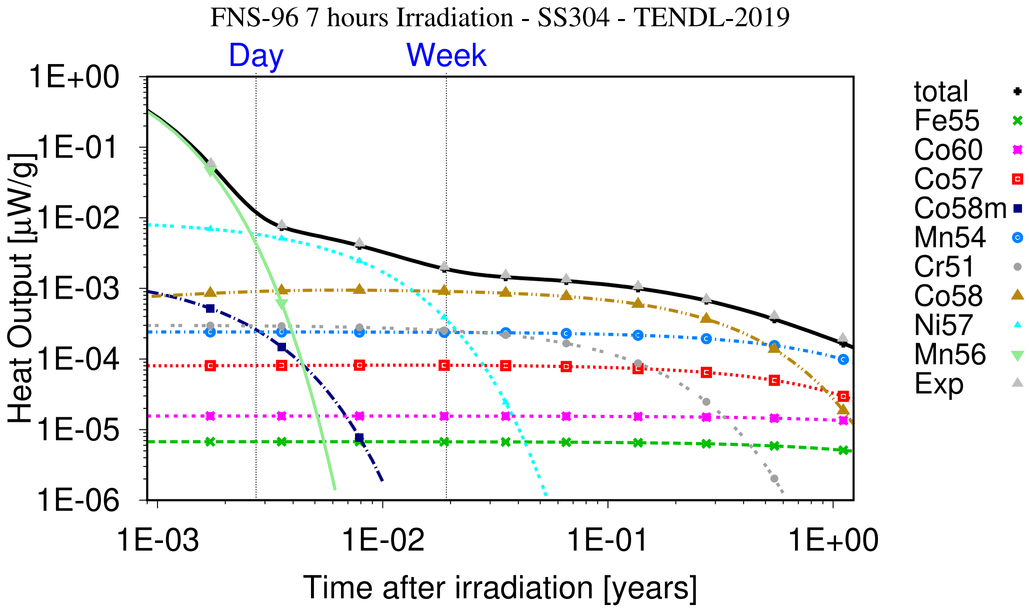

FNS-00 5 Min. Irradiation - SS304 - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
52V
28Al
53V
57Mn
54V
53Fe
56Mn
Min
Hour
1E-06
1E-05
1E-04
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.63	5.90E−02 +/-6%	5.64E−02 +/-26%	1.05	1.05	1.03	1.04	1.06
1.30	7.85E−03 +/-5%	7.43E−03 +/-7%	1.06	1.05	1.01	1.02	1.13
2.88	4.32E−03 +/-5%	4.03E−03 +/-6%	1.07	1.06	1.03	1.04	1.18
6.85	2.02E−03 +/-5%	1.90E−03 +/-5%	1.06	1.09	1.02	1.05	1.29
12.84	1.54E−03 +/-5%	1.45E−03 +/-6%	1.07	1.10	1.03	1.06	1.34
23.84	1.35E−03 +/-5%	1.27E−03 +/-6%	1.06	1.10	1.02	1.05	1.31
49.69	1.07E−03 +/-5%	1.00E−03 +/-6%	1.07	1.11	1.03	1.06	1.28
99.88	7.03E−04 +/-5%	6.72E−04 +/-6%	1.04	1.08	1.00	1.03	1.21
200.10	4.08E−04 +/-5%	3.65E−04 +/-6%	1.12	1.15	1.06	1.10	1.31
402.93	1.94E−04 +/-7%	1.65E−04 +/-8%	1.18	1.20	1.11	1.16	1.46
mean % diff. from E			7	9	3	6	20
mean χ^2			1.86	2.93	0.51	1.29	14.84

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Mn56	2.58h	1.05	6%	31%

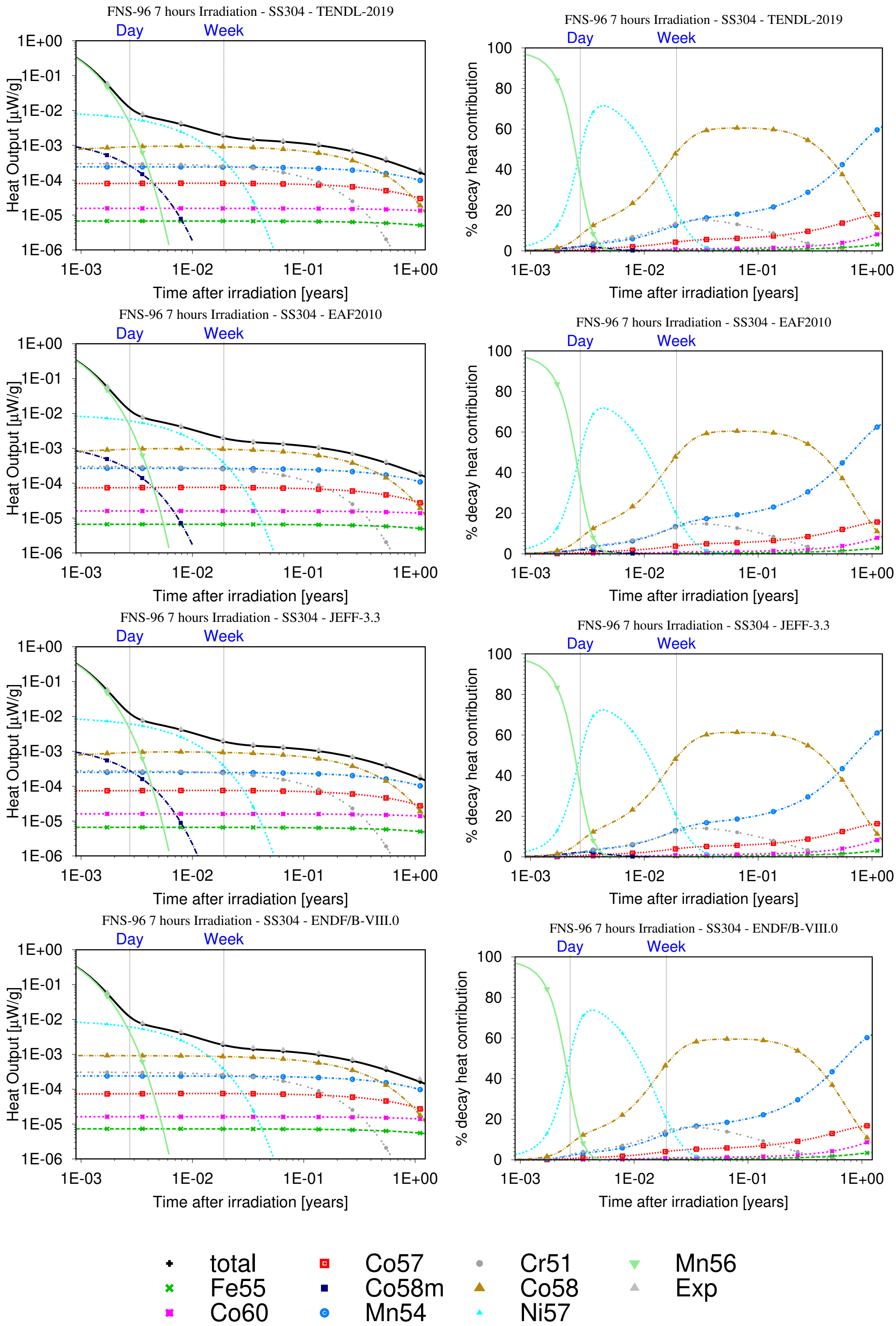


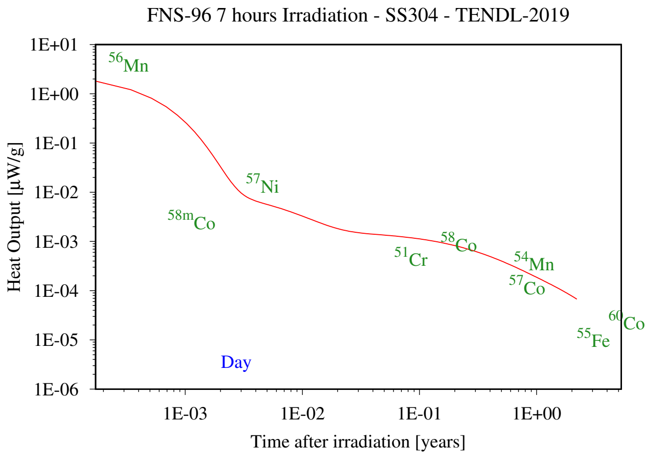
SS304,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Mn56	2.58h	Fe56(n,p)Mn56	99.7
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Cr51	27.70d	Cr52(n,2n)Cr51	93.8
		Fe54(n,α)Cr51	6.1
Co58	70.87d	Ni58(n,p)Co58	80.0
		Ni58(n,p)Co58m(IT)Co58	20.0
Co57	271.77d	Ni58(n,np)Co57	97.5
		Ni58(n,d)Co57	2.1
Mn54	312.16d	Fe54(n,p)Mn54	54.0
		Mn55(n,2n)Mn54	45.9
Fe55	2.73y	Fe56(n,2n)Fe55	98.0
		Ni58(n,α)Fe55	2.0
Co60	5.27y	Ni60(n,p)Co60m(IT)Co60	56.3
		Ni60(n,p)Co60	42.4

Comments on SS304 7-hour experiments:

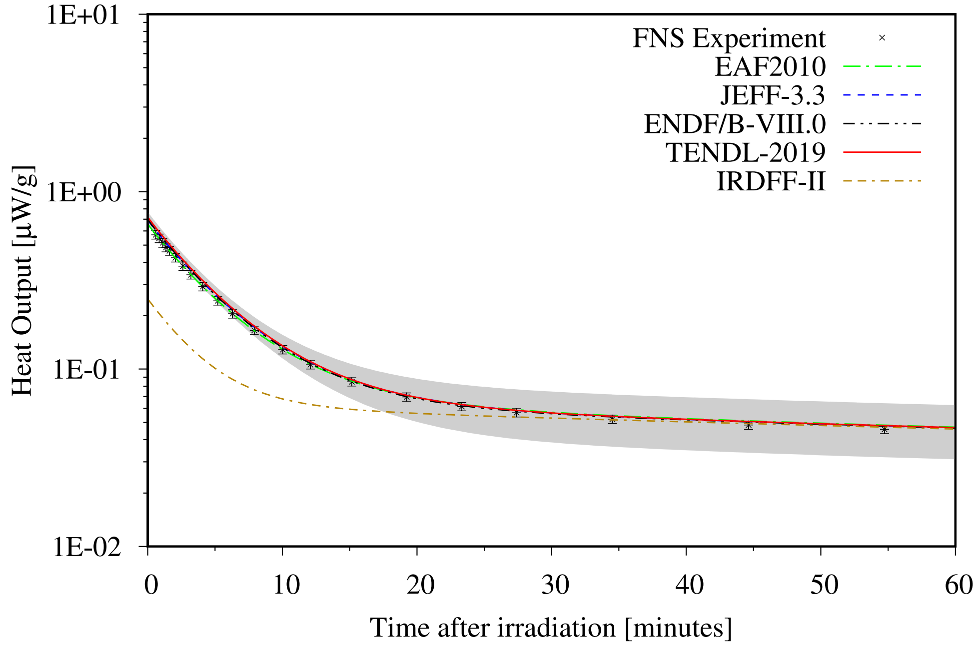
A very clean and well defined agreement despite the complexity of the system, with many nuclides providing non-negligible contributions, and four-overlapping plateau regions where different predominant nuclides (see the % contribution plots). IRDFF-II only misses the channels for Co57 (from Ni58), which provides a 20% contribution towards the ends of the measurement time, but otherwise captures the important nuclides and production routes identified by TENDL-2019.


FNS-96 7 hours Irradiation - SS304 - TENDL-2019
FNS-96 7 hours Irradiation - SS304 - EAF2010
FNS-96 7 hours Irradiation - SS304 - JEFF-3.3
FNS-96 7 hours Irradiation - SS304 - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
0
20
40
60
80
100
total
Fe55
Co60
Co57
Co58m
Mn54
Cr51
Co58
Ni57
Mn56
Exp

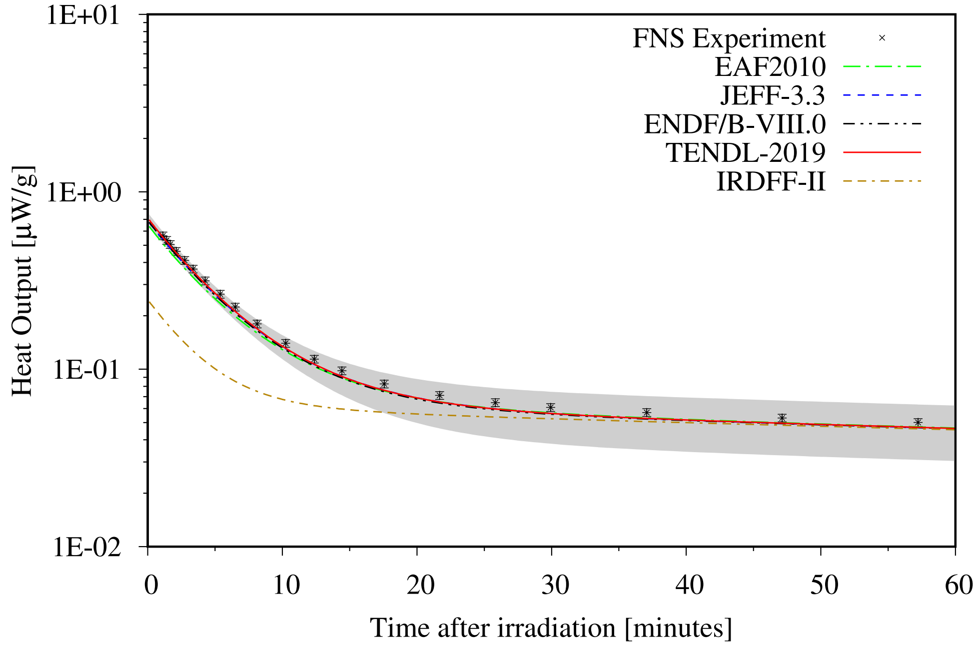

FNS-96 7 hours Irradiation - SS304 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
56Mn
57Ni
58mCo
51Cr
58Co
54Mn
57Co
60Co
55Fe
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

SS316

FNS-00 5 Min. Irradiation - SS316



FNS-96 5 Min. Irradiation - SS316

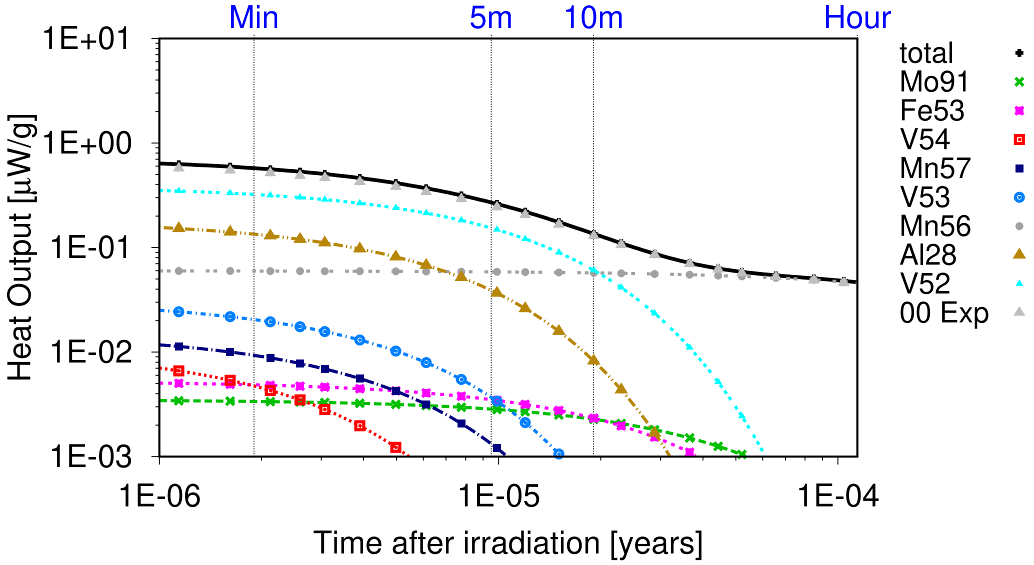


Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.60	5.72E−01 +/-6%	6.27E−01 +/-7%	0.91	0.94	1.00	0.95	2.63
0.85	5.46E−01 +/-6%	5.94E−01 +/-7%	0.92	0.95	1.00	0.95	2.65
1.12	5.15E−01 +/-6%	5.61E−01 +/-7%	0.92	0.94	1.00	0.95	2.65
1.37	4.85E−01 +/-6%	5.32E−01 +/-7%	0.91	0.94	0.99	0.94	2.63
1.62	4.64E−01 +/-6%	5.05E−01 +/-7%	0.92	0.94	1.00	0.95	2.64
2.05	4.24E−01 +/-6%	4.62E−01 +/-8%	0.92	0.94	1.00	0.95	2.63
2.62	3.80E−01 +/-6%	4.14E−01 +/-8%	0.92	0.94	1.00	0.95	2.62
3.22	3.40E−01 +/-6%	3.69E−01 +/-8%	0.92	0.95	1.00	0.95	2.60
4.08	2.91E−01 +/-6%	3.16E−01 +/-9%	0.92	0.95	1.00	0.95	2.55
5.20	2.43E−01 +/-5%	2.61E−01 +/-10%	0.93	0.95	1.00	0.95	2.46
6.30	2.05E−01 +/-5%	2.20E−01 +/-11%	0.93	0.96	1.00	0.95	2.34
7.92	1.65E−01 +/-5%	1.75E−01 +/-12%	0.95	0.97	1.00	0.96	2.16
10.03	1.29E−01 +/-5%	1.35E−01 +/-15%	0.95	0.97	1.00	0.96	1.90
12.08	1.06E−01 +/-5%	1.10E−01 +/-18%	0.96	0.98	0.99	0.97	1.68
15.17	8.48E−02 +/-5%	8.72E−02 +/-22%	0.97	0.99	0.99	0.97	1.43
19.23	6.96E−02 +/-5%	7.13E−02 +/-27%	0.98	0.99	0.98	0.98	1.23
23.33	6.15E−02 +/-5%	6.31E−02 +/-29%	0.98	0.99	0.97	0.97	1.12
27.40	5.68E−02 +/-5%	5.86E−02 +/-31%	0.97	0.98	0.96	0.97	1.06
34.52	5.22E−02 +/-5%	5.42E−02 +/-33%	0.96	0.97	0.95	0.96	1.01
44.63	4.84E−02 +/-5%	5.07E−02 +/-33%	0.95	0.96	0.95	0.96	0.98
54.73	4.57E−02 +/-5%	4.80E−02 +/-34%	0.95	0.96	0.95	0.95	0.97
mean % diff. from E			6	4	1	5	42
mean χ^2			1.58	0.69	0.19	0.75	77.26

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	$\mathbf{\%\Delta C^{nuc}}$
Mn56	2.58h	0.98	5%	34%

FNS-00 5 Min. Irradiation - SS316 - TENDL-2019

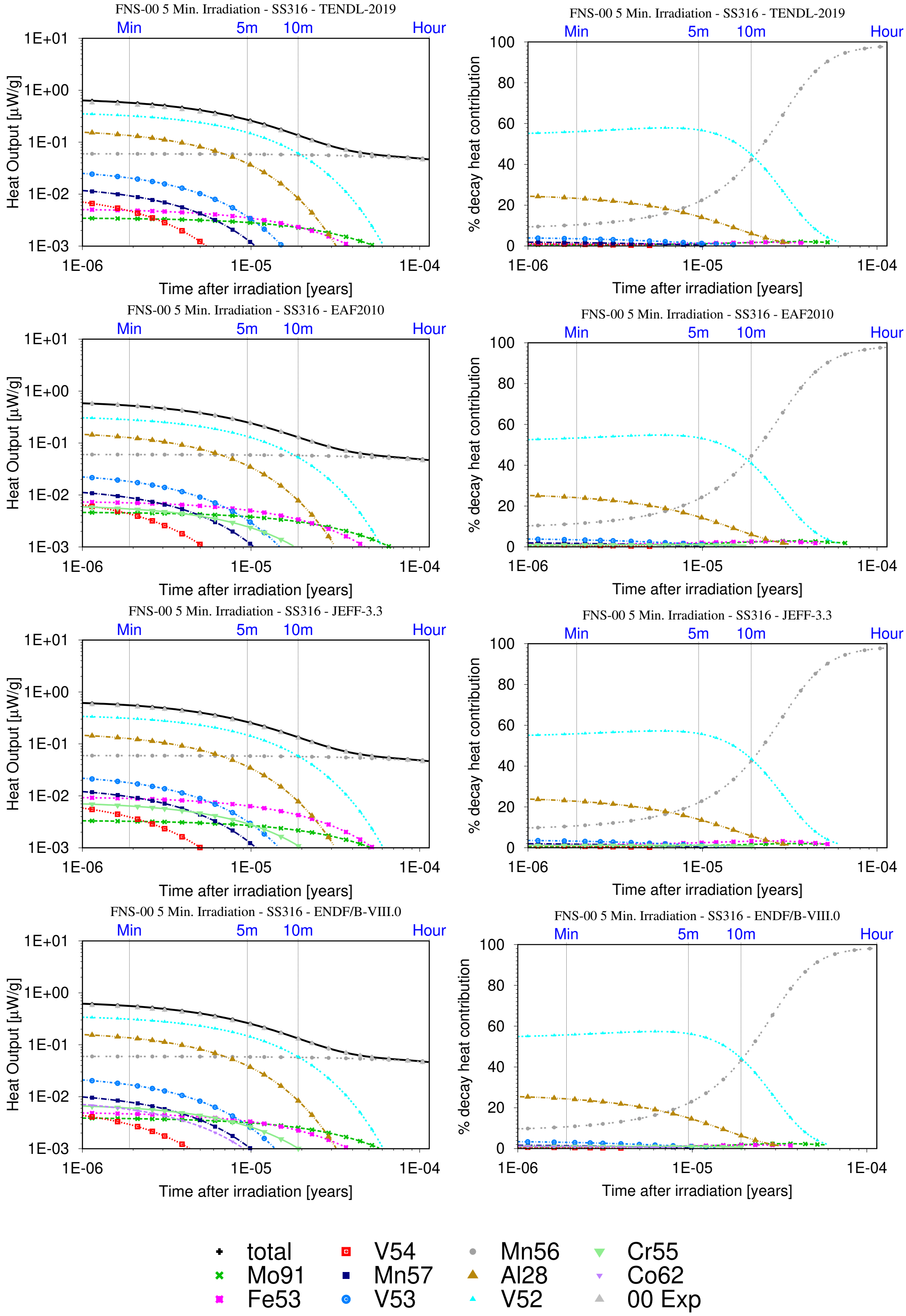


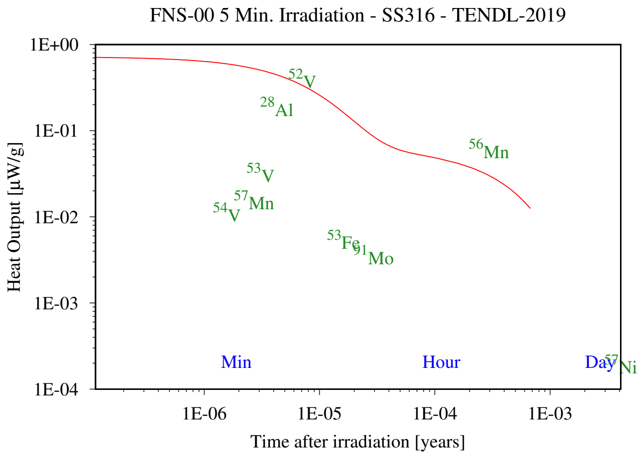
SS316, TENDL-2019 5-minute pathway analysis

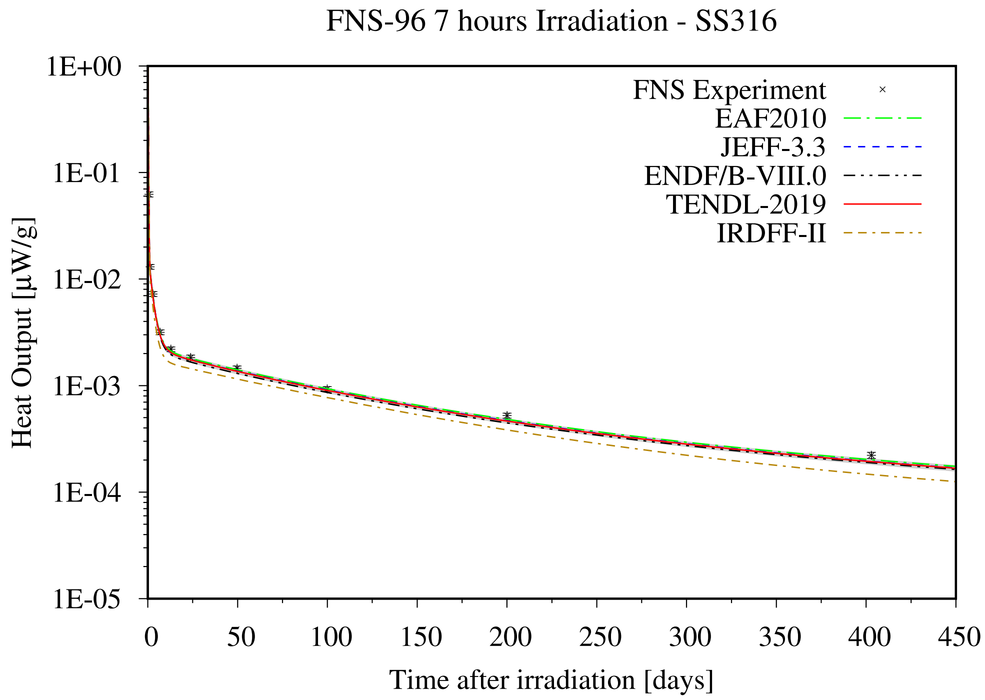
Product	$T_{1/2}$	Pathways	Path %
V54	49.80s	Cr54(n,p)V54	100.0
Mn57	1.42m	Fe57(n,p)Mn57	99.5
Co62	1.50m	Ni62(n,p)Co62	99.9
V53	1.62m	Cr53(n,p)V53	99.3
Al28	2.24m	Si28(n,p)Al28	99.7
Cr55	3.54m	Mn55(n,p)Cr55	91.2
		Fe58(n,α)Cr55	7.7
		Cr54(n,γ)Cr55	1.1
V52	3.74m	Cr52(n,p)V52	96.0
		Mn55(n,α)V52	2.1
		Cr53(n,np)V52	1.6
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Mo91	15.49m	Mo92(n,2n)Mo91	95.7
		Mo92(n,2n)Mo91m(IT)Mo91	4.3
Mn56	2.58h	Fe56(n,p)Mn56	99.5

Comments on SS316 5-minute experiments:

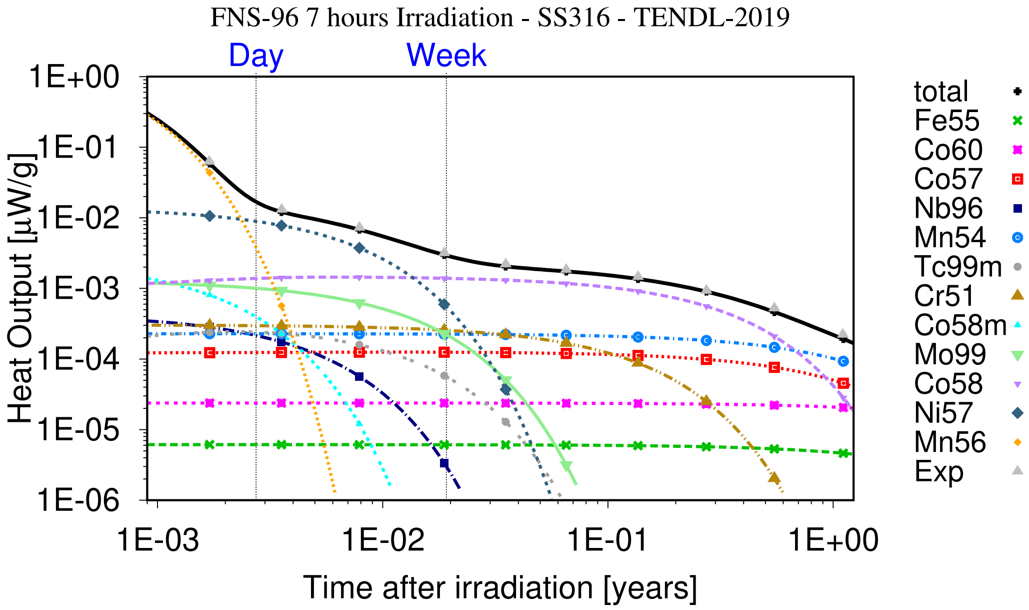
Identically to SS304: Remarkable agreement between experiment and simulation (with TENDL-2019, JEFF-3.3, EAF2010 and ENDF/B-VIII.0) for cooling times of up to 1 hour (IRDFF-II is discrepant below 20 minutes because it doesn't include the Cr52(n,p)V52 channel). All libraries capture the profile associated with the important Mn56 nuclide, which dominates beyond 10 minutes.


FNS-00 5 Min. Irradiation - SS316 - TENDL-2019
FNS-00 5 Min. Irradiation - SS316 - EAF2010
FNS-00 5 Min. Irradiation - SS316 - JEFF-3.3
FNS-00 5 Min. Irradiation - SS316 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Mo91
Fe53
V54
Mn57
V53
Mn56
Al28
V52
Cr55
Co62
00 Exp


FNS-00 5 Min. Irradiation - SS316 - TENDL-2019
1E+00
1E-01
1E-02
1E-03
1E-04
Heat Output [µW/g]
52V
28Al
56Mn
53V
57Mn
54V
53Fe
91Mo
Min
Hour
Day
57Ni
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.62	6.24$E-$02 +/-6%	5.88$E-$02 +/-23%	1.06	1.07	1.04	1.06	1.12
1.30	1.30$E-$02 +/-5%	1.21$E-$02 +/-7%	1.07	1.07	1.04	1.05	1.28
2.88	7.24$E-$03 +/-5%	6.80$E-$03 +/-6%	1.06	1.06	1.03	1.05	1.31
6.85	3.17$E-$03 +/-5%	2.98$E-$03 +/-5%	1.06	1.10	1.03	1.07	1.39
12.84	2.19$E-$03 +/-5%	2.05$E-$03 +/-6%	1.07	1.12	1.04	1.08	1.35
23.83	1.84$E-$03 +/-5%	1.74$E-$03 +/-6%	1.05	1.10	1.02	1.05	1.27
49.69	1.45$E-$03 +/-5%	1.36$E-$03 +/-6%	1.07	1.11	1.03	1.06	1.26
99.88	9.31$E-$04 +/-5%	9.02$E-$04 +/-6%	1.03	1.08	1.00	1.02	1.20
200.10	5.23$E-$04 +/-5%	4.64$E-$04 +/-6%	1.13	1.17	1.08	1.12	1.36
402.93	2.22$E-$04 +/-7%	1.92$E-$04 +/-7%	1.15	1.18	1.11	1.15	1.53
mean % diff. from E			7	10	4	6	23
mean χ^2			1.85	3.39	0.69	1.59	19.48

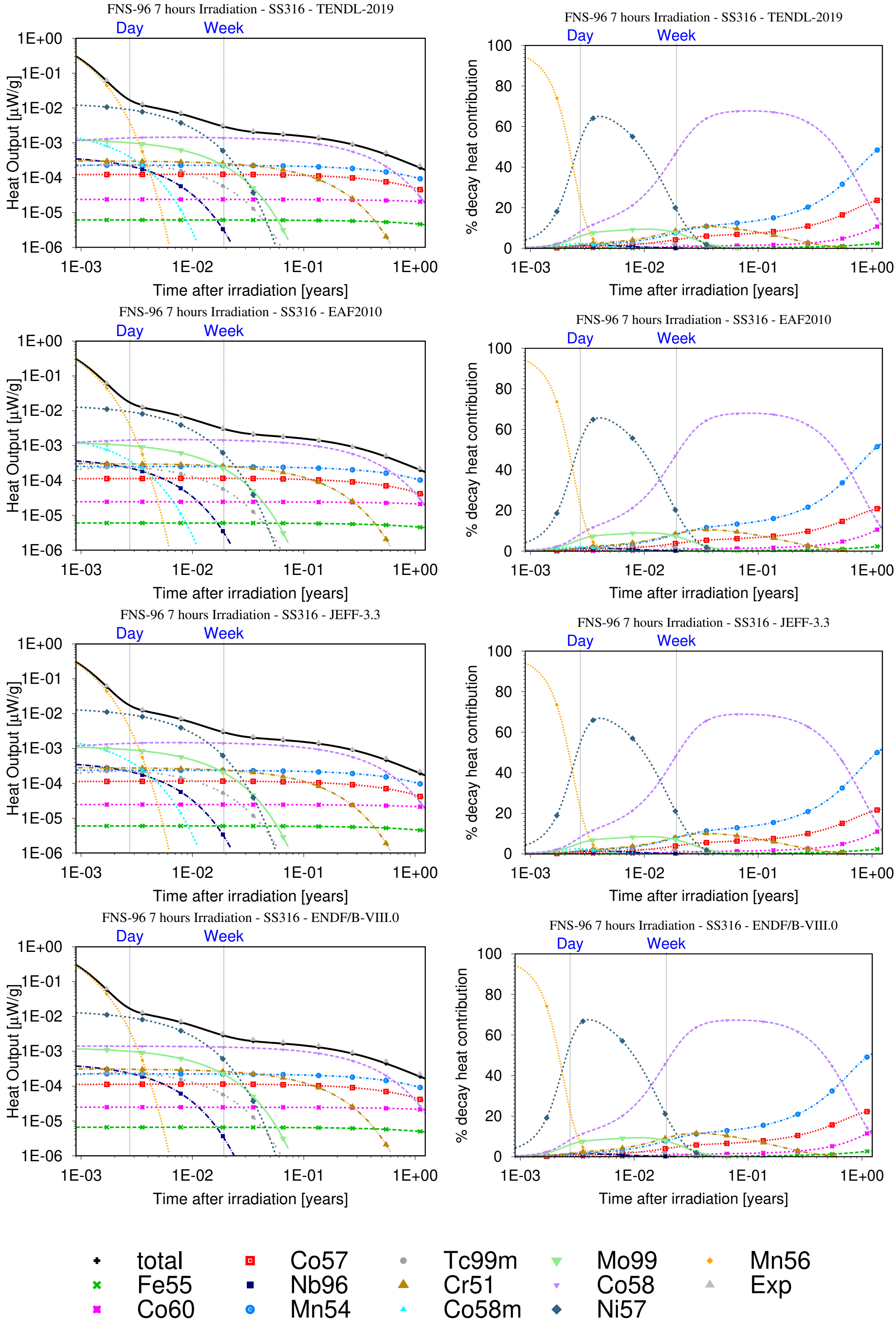


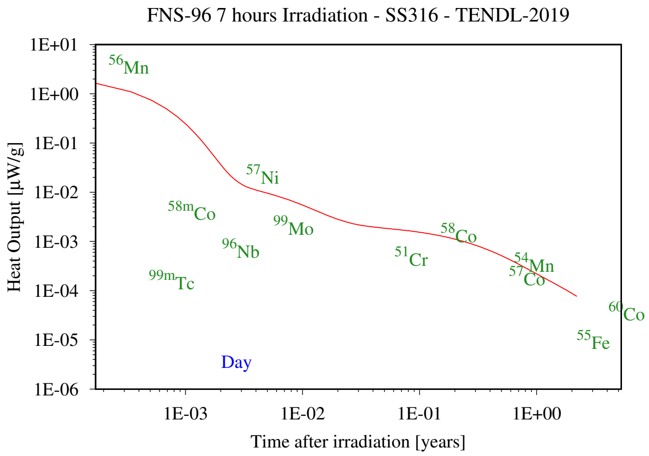
SS316,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Mn56	2.58h	Fe56(n,p)Mn56	99.7
Tc99m	6.01h	no pathways found	
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Nb96	23.35h	Mo96(n,p)Nb96	93.8
		Mo97(n,d)Nb96	3.1
		Mo97(n,np)Nb96	3.1
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Mo99	2.75d	Mo100(n,2n)Mo99	99.6
Cr51	27.70d	Cr52(n,2n)Cr51	94.5
		Fe54(n,α)Cr51	5.5
Co58	70.87d	Ni58(n,p)Co58	80.0
		Ni58(n,p)Co58m(IT)Co58	20.0
Co57	271.77d	Ni58(n,np)Co57	97.5
		Ni58(n,d)Co57	2.1
Mn54	312.16d	Fe54(n,p)Mn54	51.3
		Mn55(n,2n)Mn54	48.6
Fe55	2.73y	Fe56(n,2n)Fe55	96.7
		Ni58(n,α)Fe55	3.3
Co60	5.27y	Ni60(n,p)Co60m(IT)Co60	56.3
		Ni60(n,p)Co60	42.4

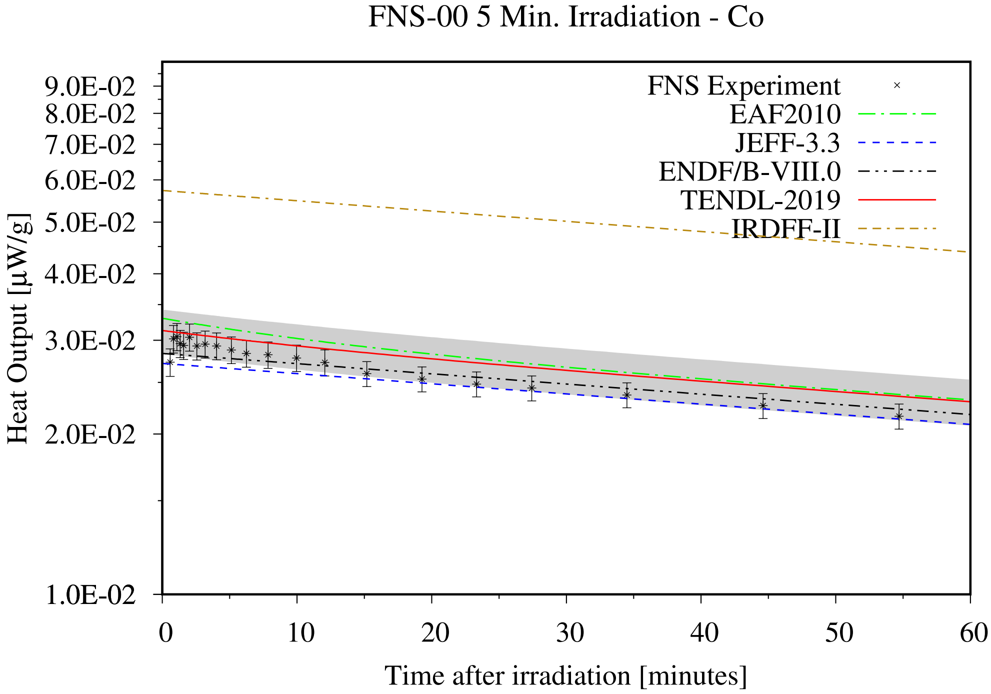
Comments on SS316 7-hour experiments:

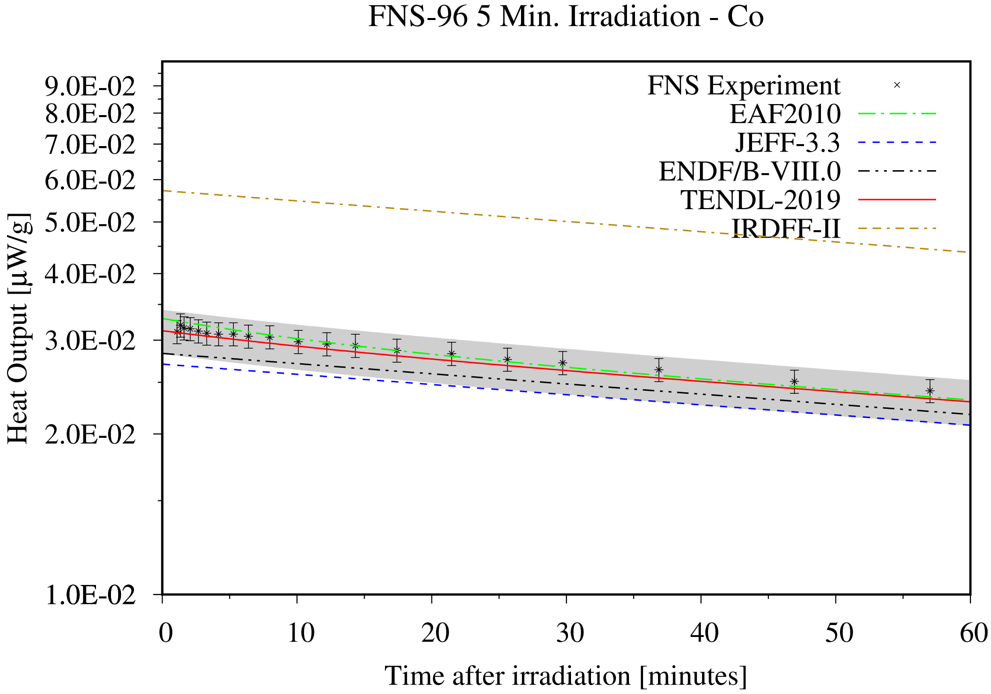
Virtually identical to the SS304 results and comparison: A very clean and well defined agreement despite the complexity of the system, with many nuclides providing non-negligible contributions, and four-overlapping plateau regions where different predominant nuclides (see the % contribution plots). IRDFF-II only misses the channels for Co57 (from Ni58), which provides a 20% contribution towards the ends of the measurement time, but otherwise captures the important nuclides and production routes identified by TENDL-2019.


FNS-96 7 hours Irradiation - SS316 - TENDL-2019
FNS-96 7 hours Irradiation - SS316 - EAF2010
FNS-96 7 hours Irradiation - SS316 - JEFF-3.3
FNS-96 7 hours Irradiation - SS316 - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
0
20
40
60
80
100
total
Fe55
Co60
Co57
Nb96
Mn54
Tc99m
Cr51
Co58m
Mo99
Co58
Ni57
Mn56
Exp


FNS-96 7 hours Irradiation - SS316 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
56Mn
57Ni
58mCo
99Mo
96Nb
99mTc
51Cr
58Co
54Mn
57Co
60Co
55Fe
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Cobalt


FNS-00 5 Min. Irradiation - Co
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
9.0E-02
8.0E-02
7.0E-02
6.0E-02
5.0E-02
4.0E-02
3.0E-02
2.0E-02
1.0E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]

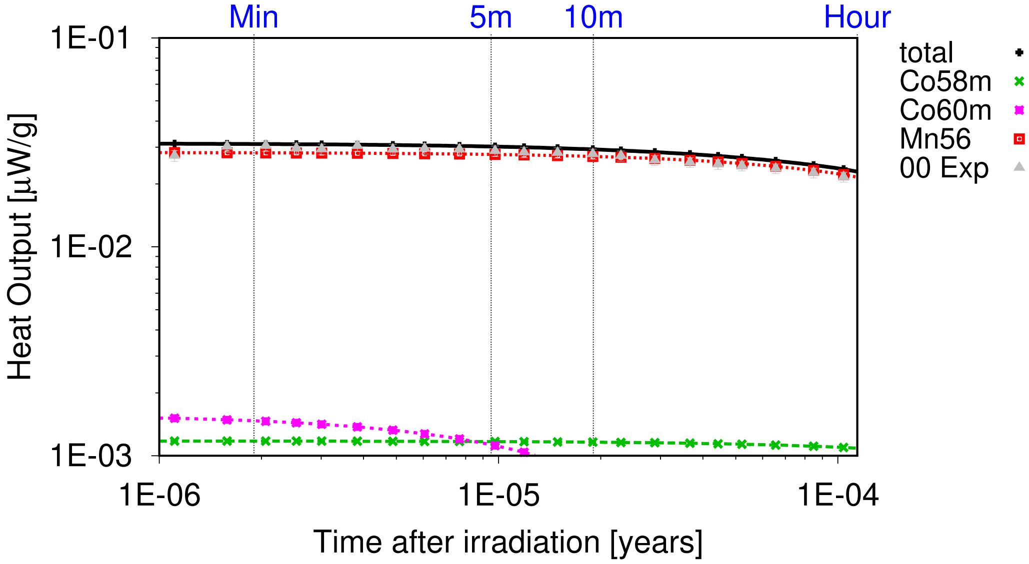

FNS-96 5 Min. Irradiation - Co
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
9.0E-02
8.0E-02
7.0E-02
6.0E-02
5.0E-02
4.0E-02
3.0E-02
2.0E-02
1.0E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]

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	2.73E−02 +/-6%	3.12E−02 +/-10%	0.88	0.97	0.83	1.01	0.48
0.83	3.02E−02 +/-6%	3.11E−02 +/-10%	0.97	1.07	0.92	1.12	0.53
1.08	3.05E−02 +/-6%	3.10E−02 +/-10%	0.98	1.08	0.93	1.13	0.53
1.33	2.96E−02 +/-6%	3.10E−02 +/-10%	0.95	1.05	0.91	1.10	0.52
1.58	2.93E−02 +/-6%	3.09E−02 +/-10%	0.95	1.04	0.90	1.09	0.52
2.02	3.04E−02 +/-6%	3.08E−02 +/-10%	0.99	1.08	0.94	1.13	0.54
2.57	2.93E−02 +/-6%	3.07E−02 +/-10%	0.95	1.04	0.91	1.09	0.52
3.18	2.95E−02 +/-6%	3.06E−02 +/-10%	0.96	1.06	0.92	1.10	0.52
4.03	2.93E−02 +/-6%	3.04E−02 +/-10%	0.96	1.05	0.92	1.10	0.52
5.13	2.88E−02 +/-6%	3.02E−02 +/-10%	0.95	1.04	0.91	1.08	0.51
6.25	2.83E−02 +/-6%	3.00E−02 +/-10%	0.95	1.03	0.91	1.07	0.51
7.85	2.82E−02 +/-6%	2.97E−02 +/-10%	0.95	1.03	0.92	1.07	0.51
9.97	2.78E−02 +/-6%	2.93E−02 +/-10%	0.95	1.02	0.92	1.07	0.51
12.07	2.72E−02 +/-6%	2.89E−02 +/-10%	0.94	1.01	0.92	1.06	0.50
15.18	2.60E−02 +/-5%	2.84E−02 +/-10%	0.91	0.98	0.89	1.02	0.48
19.28	2.54E−02 +/-5%	2.78E−02 +/-10%	0.91	0.97	0.89	1.02	0.48
23.33	2.48E−02 +/-5%	2.72E−02 +/-10%	0.91	0.97	0.90	1.01	0.48
27.43	2.44E−02 +/-5%	2.67E−02 +/-10%	0.91	0.97	0.90	1.01	0.48
34.50	2.37E−02 +/-5%	2.58E−02 +/-10%	0.92	0.97	0.91	1.02	0.48
44.60	2.26E−02 +/-5%	2.46E−02 +/-10%	0.92	0.97	0.91	1.01	0.48
54.70	2.16E−02 +/-5%	2.36E−02 +/-10%	0.92	0.97	0.91	1.01	0.48
mean % diff. from E			6	4	10	6	99
mean χ^2			1.65	0.53	3.43	1.39	309.77

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Mn56	2.58h	0.88	6%	10%

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

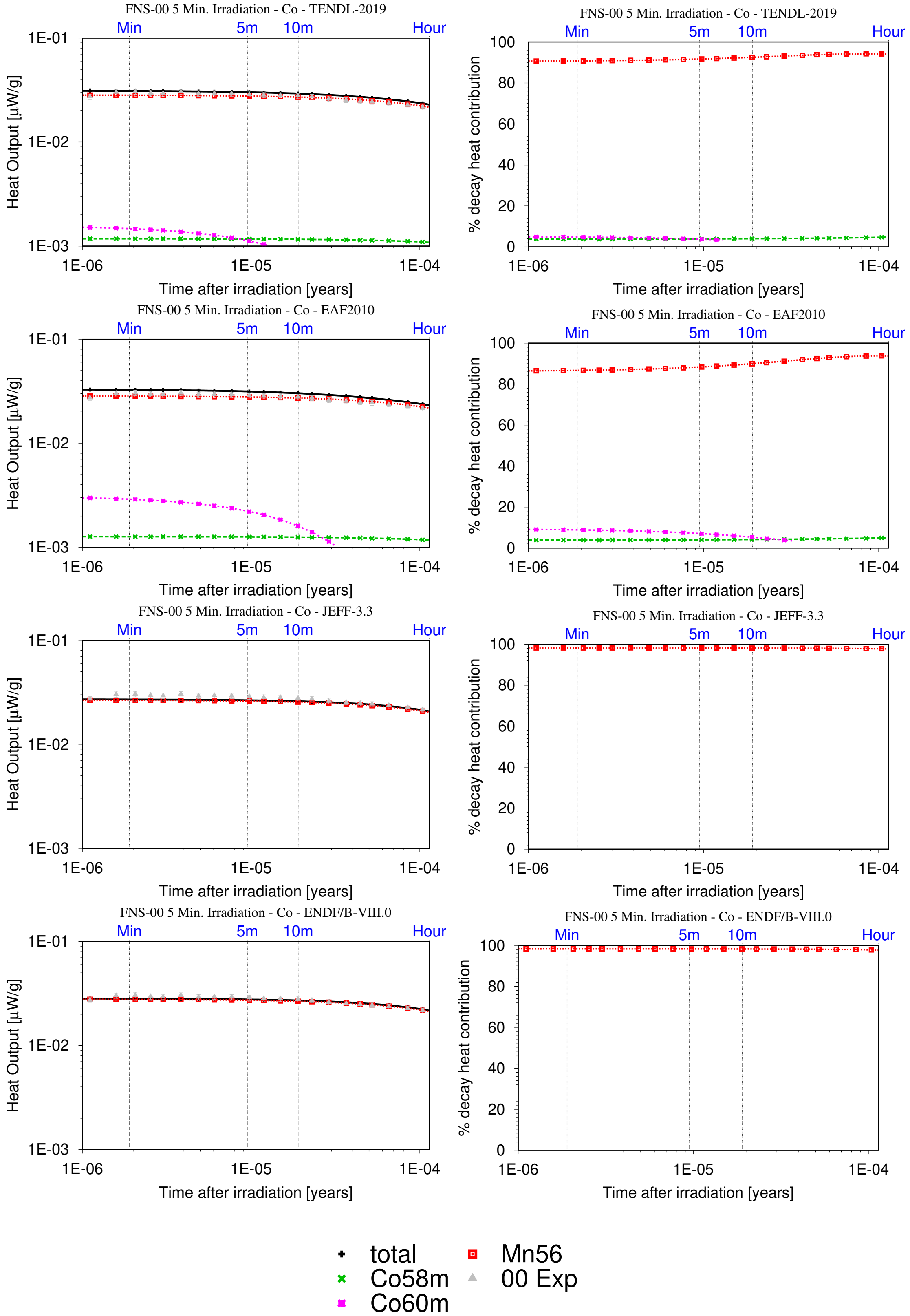


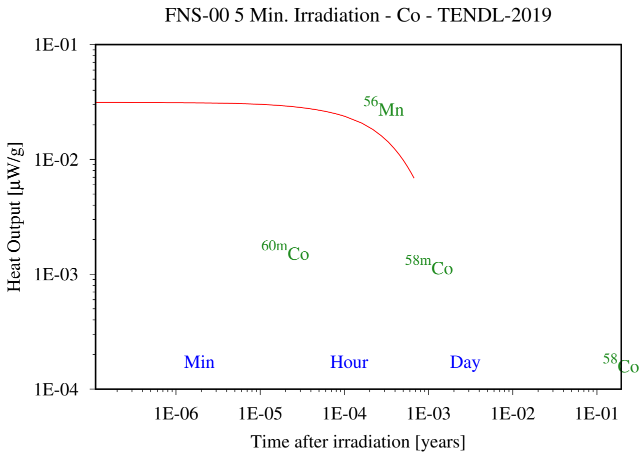
Cobalt, TENDL-2019 5-minute pathway analysis

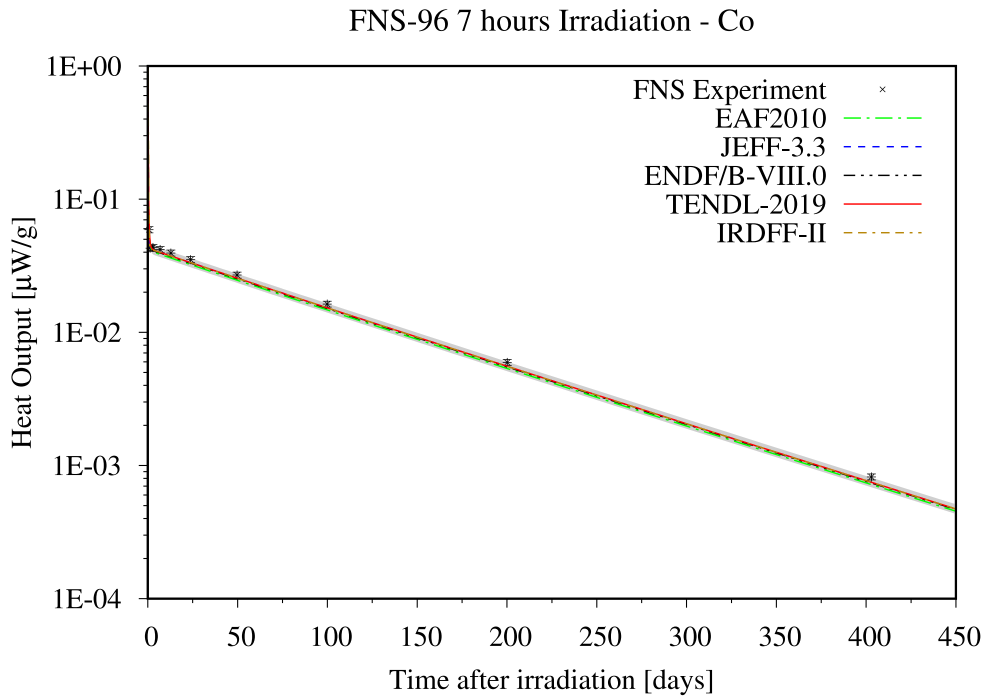
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Co60m	10.47m	Co59(n,γ)Co60m	100.0
Mn56	2.58h	Co59(n,α)Mn56	100.0
Co58m	8.90h	Co59(n,2n)Co58m	100.0

Comments on Cobalt 5-minute experiments:

The two batches of measured experimental data sets are different when there is no reason for them to be (the simulated predictions are identical for the two batches – apart from some minor variations in the [measured] cooling times), and, furthermore, these unexplained differences lie outside of the quoted experimental uncertainty. Despite the obvious issues with the experimental results (it is not even clear that this is impurity related), simulations with the general purpose libraries nicely capture the decay profile measured in the experiments. Both TENDL-2019 and EAF2010 predict some minor contributions from Co60m at cooling times below 5 minutes, which JEFF-3.3 and ENDF/B-VIII.0 miss, but the contribution is too small for its inclusion (or not) to have any significant impact on the quality of predictions (especially given the experimental abnormalities). IRDFF-II is worse than IRDFF-1.05; seemingly overpredicting the production of the completely dominant Mn56 (via (n,α) on Co59) by a factor of two (2).


FNS-00 5 Min. Irradiation - Co - TENDL-2019
FNS-00 5 Min. Irradiation - Co - EAF2010
FNS-00 5 Min. Irradiation - Co - JEFF-3.3
FNS-00 5 Min. Irradiation - Co - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
1E-01
1E-02
1E-03
% decay heat contribution
100
80
60
40
20
0
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Co58m
Co60m
Mn56
00 Exp

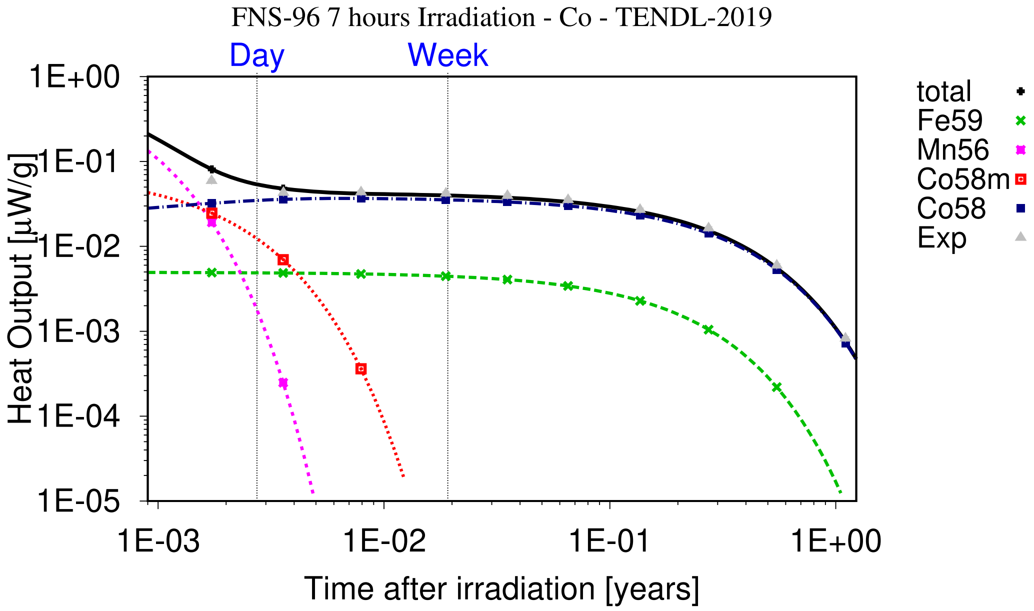

FNS-00 5 Min. Irradiation - Co - TENDL-2019
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
56Mn
60mCo
58mCo
58Co
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.63	$5.90E{-}02$ +/-5%	$8.08E{-}02$ +/-5%	0.73	0.97	0.73	0.97	0.73
1.31	$4.28E{-}02$ +/-5%	$4.79E{-}02$ +/-7%	0.89	1.02	0.91	1.01	1.00
2.89	$4.33E{-}02$ +/-5%	$4.18E{-}02$ +/-8%	1.04	1.05	1.07	1.04	1.04
6.86	$4.19E{-}02$ +/-5%	$3.98E{-}02$ +/-8%	1.05	1.06	1.09	1.05	1.05
12.85	$3.94E{-}02$ +/-5%	$3.74E{-}02$ +/-8%	1.05	1.06	1.09	1.05	1.05
23.84	$3.52E{-}02$ +/-5%	$3.34E{-}02$ +/-8%	1.05	1.06	1.09	1.05	1.05
49.70	$2.69E{-}02$ +/-5%	$2.56E{-}02$ +/-8%	1.05	1.06	1.09	1.05	1.05
99.89	$1.63E{-}02$ +/-5%	$1.53E{-}02$ +/-8%	1.07	1.08	1.10	1.07	1.07
200.11	$5.95E{-}03$ +/-5%	$5.57E{-}03$ +/-8%	1.07	1.08	1.11	1.07	1.07
402.95	$8.21E{-}04$ +/-5%	$7.35E{-}04$ +/-8%	1.12	1.13	1.16	1.12	1.12
mean % diff. from E			10	6	12	5	9
mean χ^2			6.41	1.52	7.65	1.18	5.99

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Co58	70.87d	1.04	5%	8%

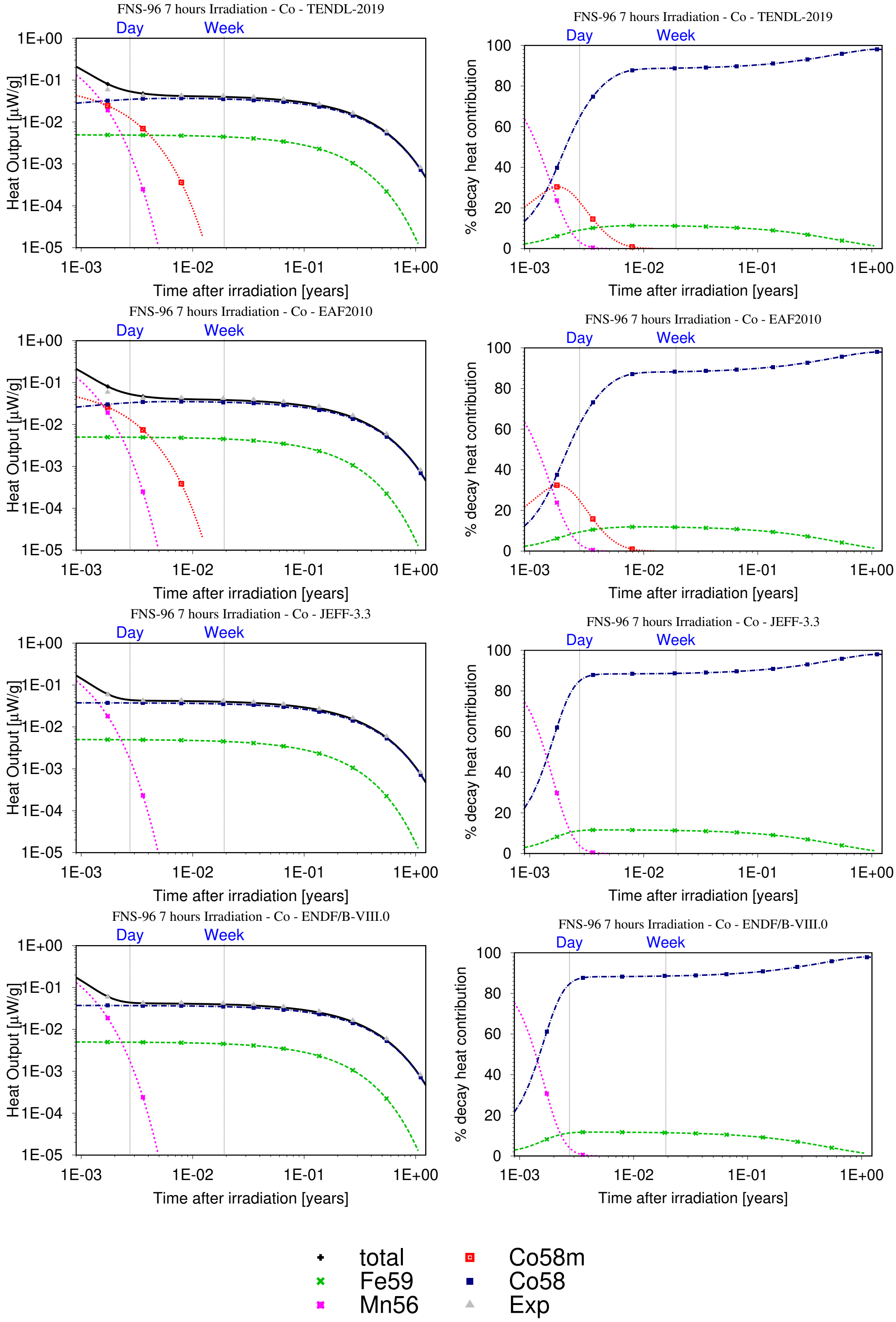


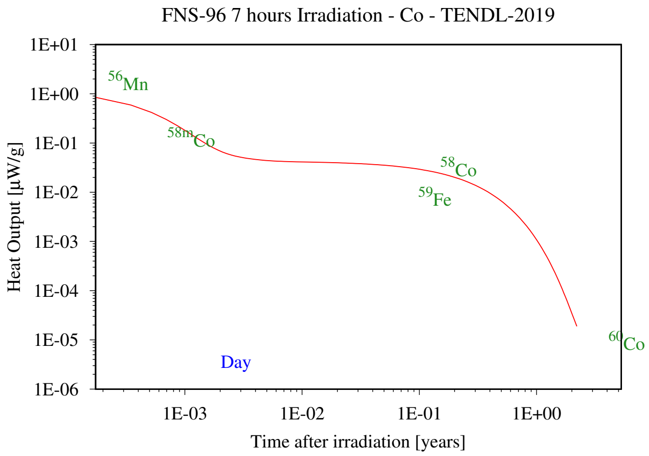
Cobalt,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Mn56	2.58h	Co59(n,α)Mn56	100.0
Co58m	8.90h	Co59(n,2n)Co58m	100.0
Fe59	44.50d	Co59(n,p)Fe59	100.0
Co58	70.87d	Co59(n,2n)Co58	71.8
		Co59(n,2n)Co58m(IT)Co58	28.2

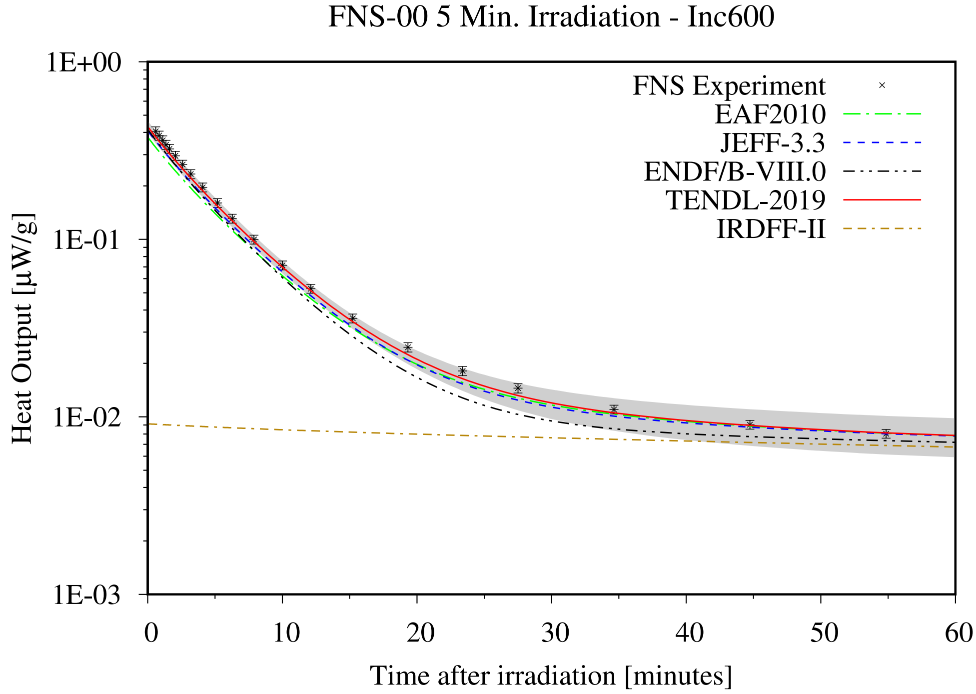
Comments on Cobalt 7-hour experiments:

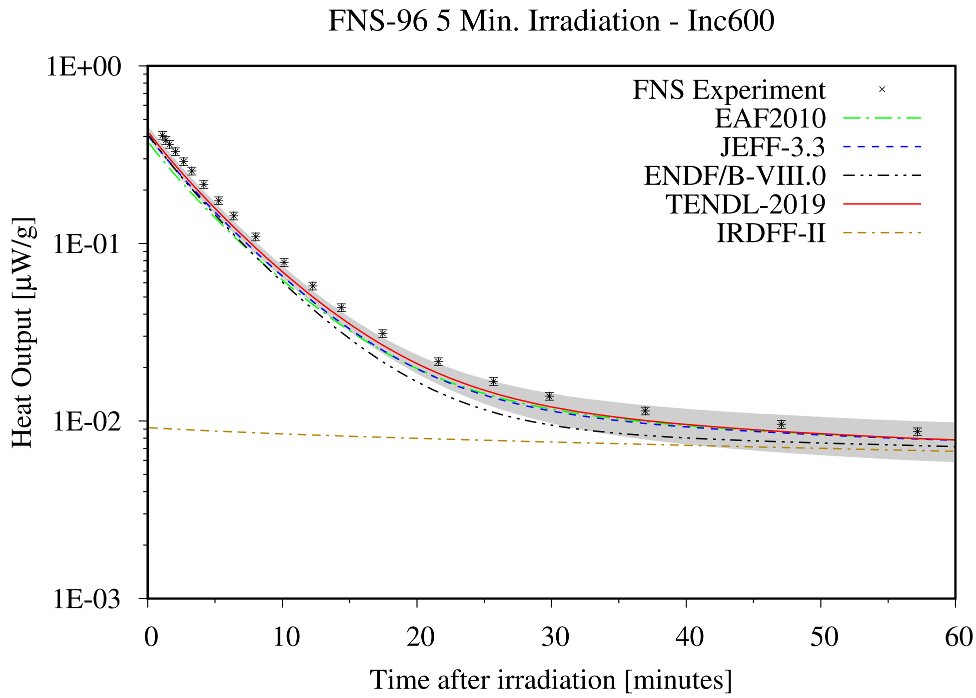
Good agreement with all libraries for this relatively simple case, which is dominated by Co58 decay heat (produced via Co59(n,2n)Co58) at all cooling times greater than 1 day (see the % contribution plots). All simulation curves fall almost within the experimental uncertainties when this nuclide is dominant. At shorter cooling times, associated with the experimental measurements at 0.63 and 1.31 days, JEFF and ENDF/B seem to do better than either TENDL-2019 or EAF2010 (or IRDFF-II). For these first two cooling times, TENDL and EAF results seem to overpredict the experiment by around 20%, which almost exactly corresponds to the % contribution from Co58m predicted in the simulations with these two libraries. JEFF-3.3 and ENDF/B-VIII.0 on the other hand, only predict the production of Mn56 (via (n,α) on Co59), and at a level that EAF2010 and TENDL-2019 agree with – it appears that the Co58m contribution is unnecessary (and thus overpredicted) and doesn't reflect reality. The IRDFF-II issue at these first two cooling times appears, once again (as in the 5 minute experiment), more related to the overprediction of Mn56 compared to IRDFF-1.05.


FNS-96 7 hours Irradiation - Co - TENDL-2019
Day
Week
Heat Output [µW/g]
Time after irradiation [years]
% decay heat contribution
FNS-96 7 hours Irradiation - Co - EAF2010
FNS-96 7 hours Irradiation - Co - JEFF-3.3
FNS-96 7 hours Irradiation - Co - ENDF/B-VIII.0
total
Fe59
Mn56
Co58m
Co58
Exp


FNS-96 7 hours Irradiation - Co - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
56Mn
58mCo
58Co
59Fe
60Co
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Inconel-600

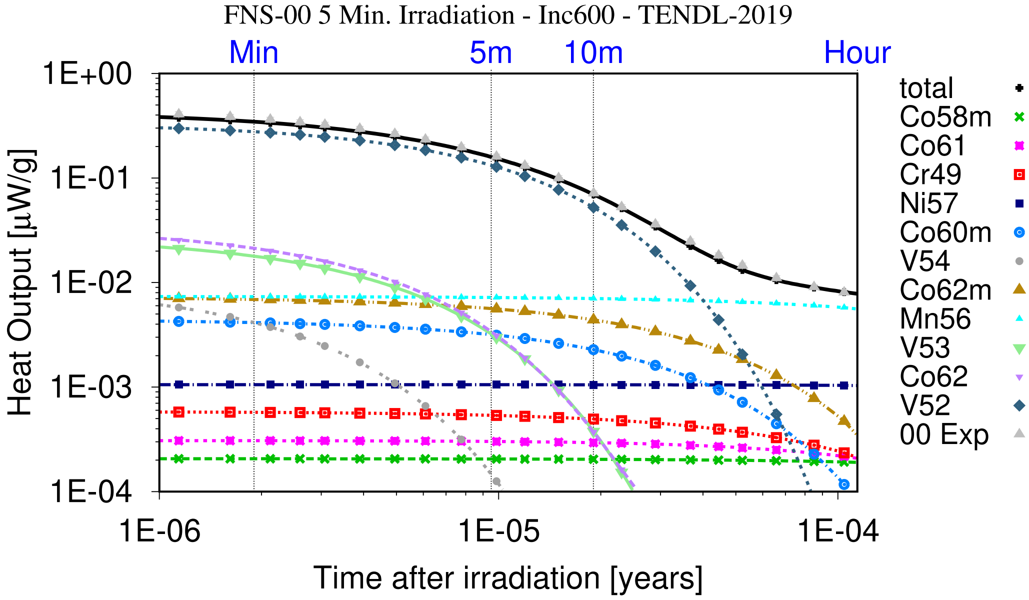

FNS-00 5 Min. Irradiation - Inc600
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Inc600
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]

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
0.60	4.06$E-$01 +/-6%	3.77$E-$01 +/-8%	1.08	1.12	1.23	1.14	44.69
0.85	3.84$E-$01 +/-6%	3.57$E-$01 +/-8%	1.08	1.12	1.23	1.13	42.36
1.12	3.61$E-$01 +/-6%	3.37$E-$01 +/-8%	1.07	1.12	1.23	1.13	39.93
1.37	3.41$E-$01 +/-6%	3.20$E-$01 +/-8%	1.07	1.12	1.22	1.12	37.79
1.62	3.23$E-$01 +/-6%	3.03$E-$01 +/-8%	1.06	1.12	1.22	1.12	35.89
2.05	2.95$E-$01 +/-6%	2.78$E-$01 +/-8%	1.06	1.13	1.21	1.12	32.93
2.60	2.64$E-$01 +/-6%	2.49$E-$01 +/-8%	1.06	1.13	1.21	1.12	29.52
3.20	2.33$E-$01 +/-6%	2.22$E-$01 +/-8%	1.05	1.13	1.20	1.11	26.24
4.08	1.96$E-$01 +/-6%	1.88$E-$01 +/-8%	1.04	1.13	1.19	1.10	22.25
5.18	1.60$E-$01 +/-6%	1.54$E-$01 +/-8%	1.04	1.14	1.18	1.10	18.30
6.28	1.31$E-$01 +/-6%	1.27$E-$01 +/-8%	1.03	1.14	1.17	1.09	15.09
7.90	9.98$E-$02 +/-6%	9.71$E-$02 +/-8%	1.03	1.15	1.16	1.09	11.63
10.02	7.14$E-$02 +/-6%	6.97$E-$02 +/-8%	1.02	1.17	1.15	1.09	8.44
12.12	5.27$E-$02 +/-6%	5.14$E-$02 +/-8%	1.02	1.20	1.14	1.09	6.31
15.23	3.59$E-$02 +/-6%	3.44$E-$02 +/-9%	1.04	1.26	1.14	1.12	4.38
19.33	2.47$E-$02 +/-6%	2.24$E-$02 +/-12%	1.10	1.39	1.18	1.18	3.07
23.40	1.81$E-$02 +/-6%	1.64$E-$02 +/-15%	1.11	1.42	1.16	1.18	2.31
27.50	1.45$E-$02 +/-6%	1.32$E-$02 +/-17%	1.10	1.40	1.14	1.17	1.88
34.63	1.10$E-$02 +/-6%	1.05$E-$02 +/-21%	1.04	1.28	1.06	1.09	1.47
44.73	9.03$E-$03 +/-6%	8.96$E-$03 +/-23%	1.01	1.17	1.02	1.03	1.26
54.85	8.03$E-$03 +/-6%	8.12$E-$03 +/-24%	0.99	1.09	0.99	1.00	1.16
mean % diff. from E			5	15	14	10	78
mean χ^2			0.91	7.97	6.31	3.18	201.23

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
V52	3.74m	1.08	6%	9%

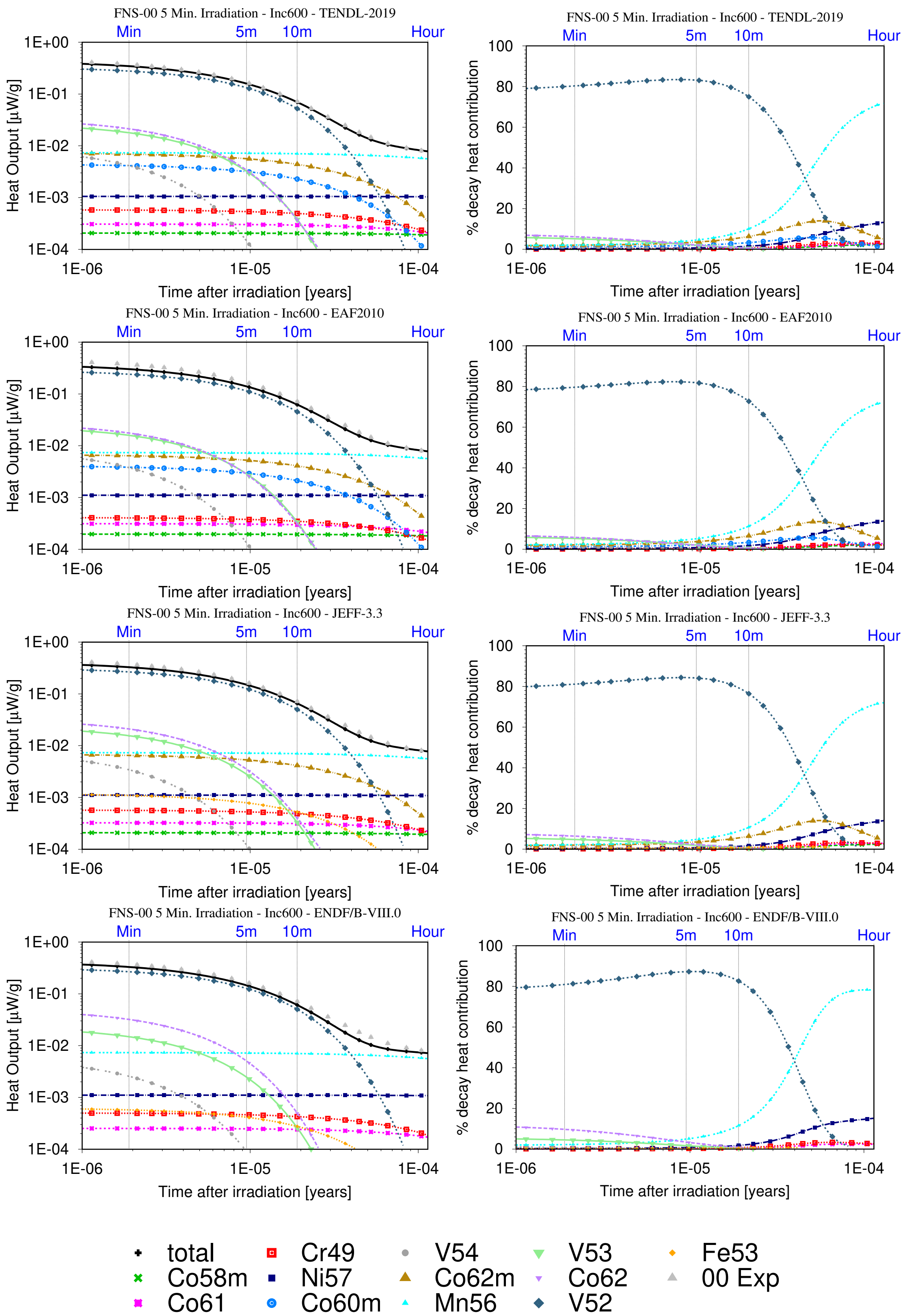


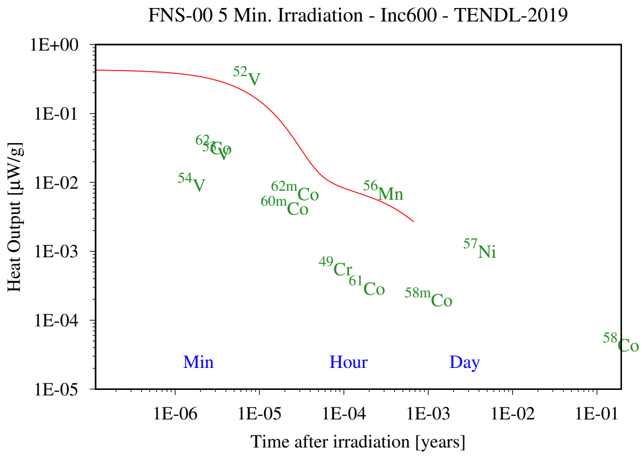
Inconel-600, TENDL-2019 5-minute pathway analysis

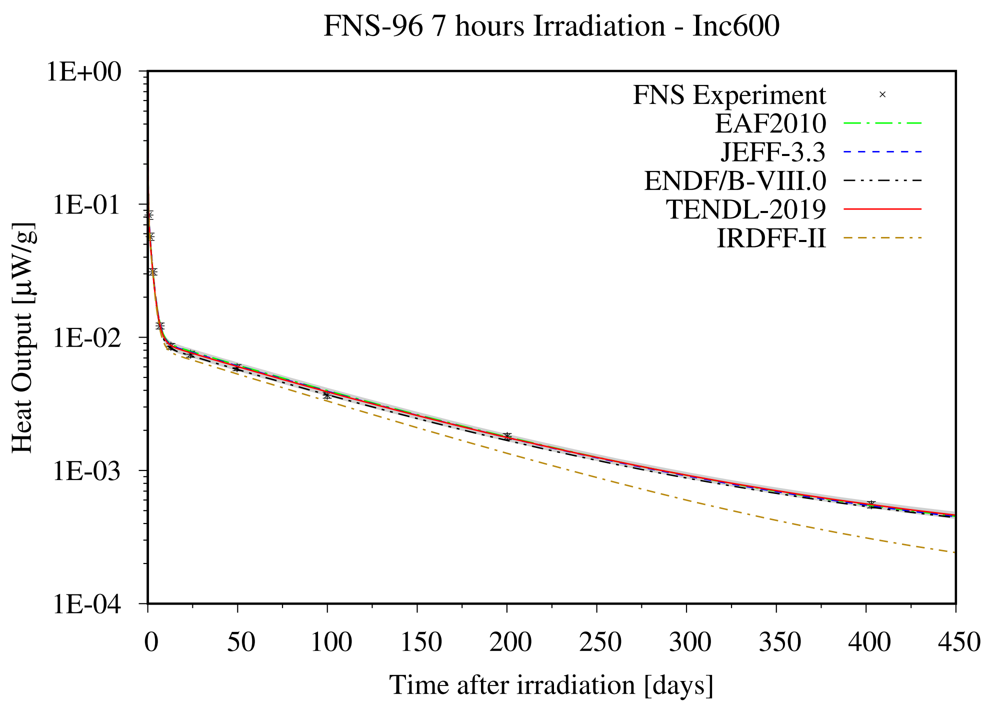
Product	$T_{1/2}$	Pathways	Path %
V54	49.80s	Cr54(n,p)V54	100.0
Co62	1.50m	Ni62(n,p)Co62	99.9
V53	1.62m	Cr53(n,p)V53	99.3
V52	3.74m	Cr52(n,p)V52	97.4
		Cr53(n,np)V52	1.6
Fe53	8.51m	Fe54(n,2n)Fe53	100.0
Co60m	10.47m	Ni60(n,p)Co60m	98.9
Co62m	13.91m	Ni62(n,p)Co62m	100.0
Cr49	41.90m	Cr50(n,2n)Cr49	100.0
Co61	1.65h	Ni61(n,p)Co61	76.8
		Ni62(n,np)Co61	15.3
		Ni62(n,d)Co61	6.8
		Ni64(n,α)Fe61(β^-)Co61	1.1
Mn56	2.58h	Fe56(n,p)Mn56	99.4
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0

Comments on Inconel-600 5-minute experiments:

Two main radionuclides are predicted (by the general purpose libraries) to dominate: V52 (mainly from Cr52(n,p)) during the first 20 minutes of cooling and then Mn56 (via Fe56(n,p)) for the remainder, up to 1-hour of cooling. The combined profile of these two nuclides seems to well capture the experimental profile, although the simulations all give a slight, systematic underprediction. As with the Cr experiment, IRDFF-II misses the production of V52, but does capture the production of Mn56. TENDL-2019 performs better than all other libraries, with the experimental points mostly within the simulation uncertainty. It is difficult to attribute the underestimation to anything specific in this complex material – certainly it is unlikely to be an issue with Cr52(n,p)V52 because that produced an overprediction in the Cr 5-minute experiments.


FNS-00 5 Min. Irradiation - Inc600 - TENDL-2019
FNS-00 5 Min. Irradiation - Inc600 - EAF2010
FNS-00 5 Min. Irradiation - Inc600 - JEFF-3.3
FNS-00 5 Min. Irradiation - Inc600 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Cr49
V54
V53
Fe53
Co58m
Ni57
Co62m
Co62
00 Exp
Co61
Co60m
Mn56
V52

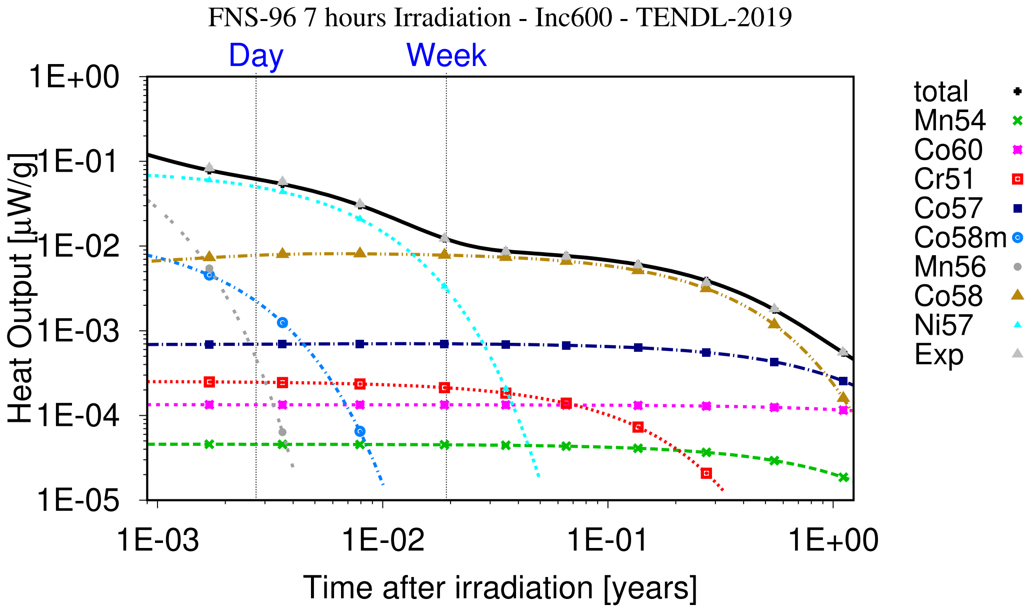

FNS-00 5 Min. Irradiation - Inc600 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
52V
54V
62mCo
60mCo
56Mn
57Ni
49Cr
61Co
58mCo
58Co
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.62	8.29E−02 +/-7%	7.84E−02 +/-8%	1.06	1.07	1.02	1.02	1.12
1.31	5.70E−02 +/-6%	5.39E−02 +/-8%	1.06	1.05	1.01	1.01	1.09
2.89	3.11E−02 +/-6%	3.02E−02 +/-7%	1.03	1.02	0.99	0.99	1.06
6.86	1.22E−02 +/-5%	1.23E−02 +/-6%	0.99	1.02	0.96	0.97	1.07
12.86	8.55E−03 +/-5%	8.69E−03 +/-7%	0.98	1.03	0.96	0.97	1.10
23.84	7.47E−03 +/-5%	7.66E−03 +/-8%	0.98	1.03	0.95	0.96	1.10
49.69	5.92E−03 +/-5%	6.05E−03 +/-7%	0.98	1.03	0.95	0.97	1.11
99.88	3.68E−03 +/-5%	3.90E−03 +/-7%	0.94	0.99	0.92	0.93	1.11
200.11	1.80E−03 +/-5%	1.77E−03 +/-6%	1.02	1.07	1.01	1.02	1.34
402.94	5.53E−04 +/-6%	5.50E−04 +/-6%	1.01	1.05	1.02	1.03	1.82
mean % diff. from E			3	4	3	3	14
mean χ^2			0.36	0.49	0.63	0.40	10.95

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ni57	1.50d	1.06	7%	10%
Co58	70.87d	0.98	5%	9%

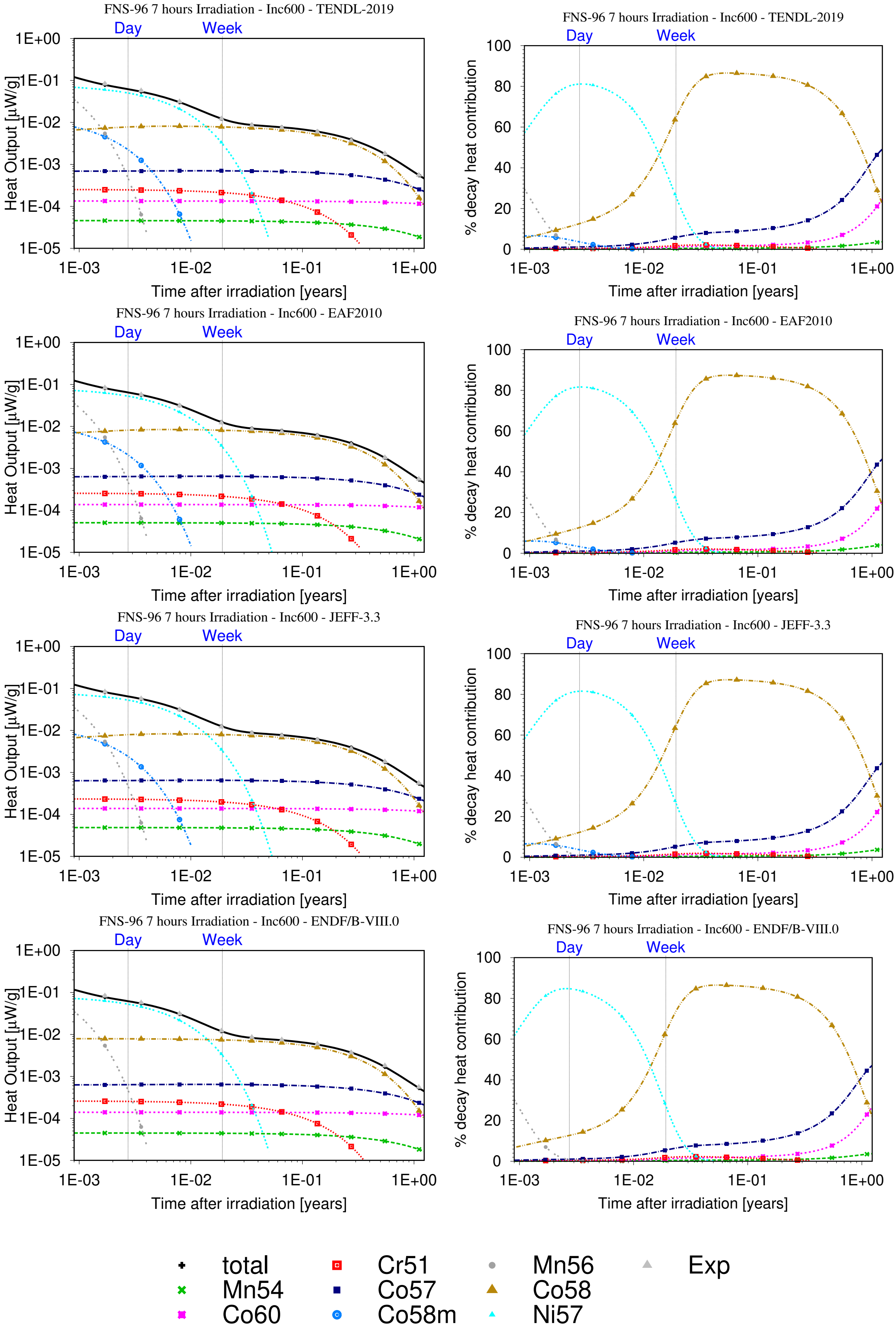


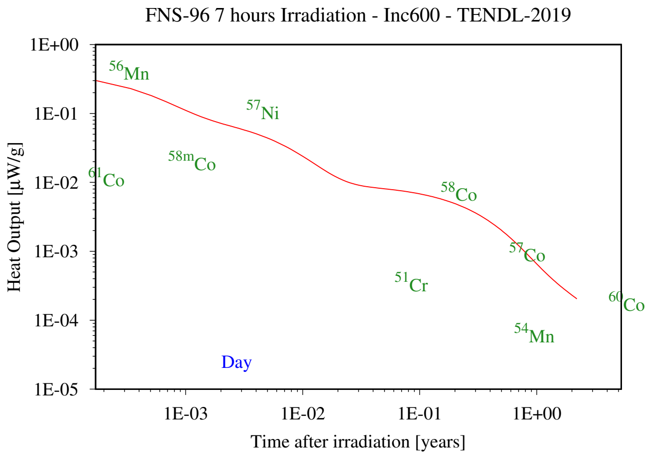
Inconel-600,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Mn56	2.58h	Fe56(n,p)Mn56	99.7
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Cr51	27.70d	Cr52(n,2n)Cr51	99.2
Co58	70.87d	Ni58(n,p)Co58	80.0
		Ni58(n,p)Co58m(IT)Co58	20.0
Co57	271.77d	Ni58(n,np)Co57	97.5
		Ni58(n,d)Co57	2.1
Mn54	312.16d	Mn55(n,2n)Mn54	65.8
		Fe54(n,p)Mn54	31.4
		Ni58(n,pα)Mn54	2.8
Co60	5.27y	Ni60(n,p)Co60m(IT)Co60	56.3
		Ni60(n,p)Co60	42.4

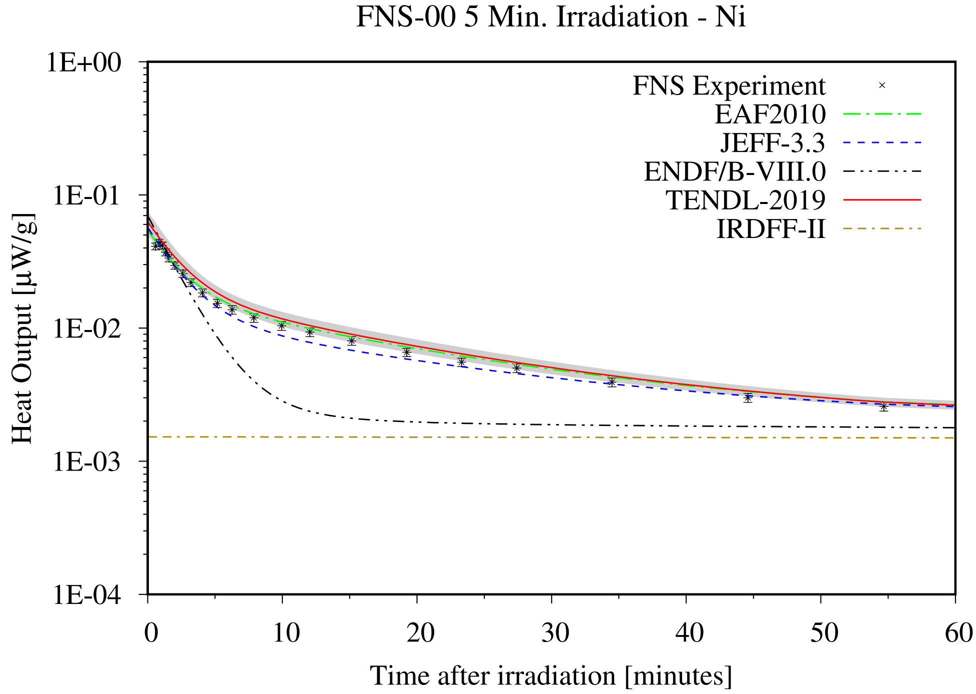
Comments on Inconel-600 7-hour experiments:

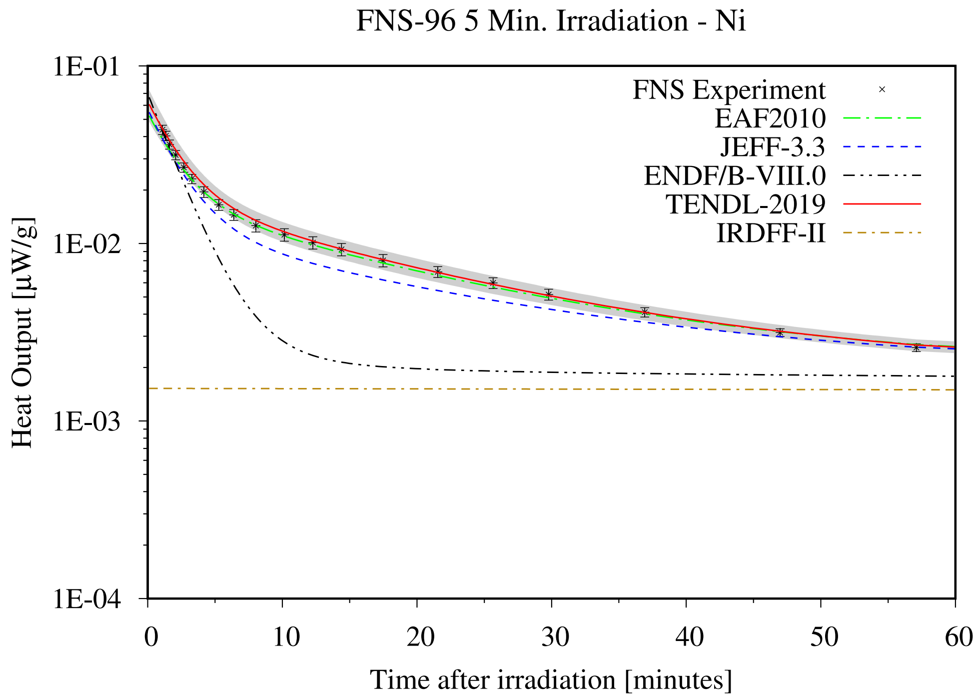
There is a very good agreement between the TENDL, JEFF, EAF, and ENDF/B libraries and experiment for this Inconel-600 alloy, with these libraries within a few % of the measurements at all decay times. IRDFF-II captures well the profile when first Ni57 and then Co58 dominate the decay heat, but misses the production of Co57 and Co60, which become important (along with Co58) in for the final 2 experimental measurements (or beyond around 100 days of cooling).


FNS-96 7 hours Irradiation - Inc600 - TENDL-2019
FNS-96 7 hours Irradiation - Inc600 - EAF2010
FNS-96 7 hours Irradiation - Inc600 - JEFF-3.3
FNS-96 7 hours Irradiation - Inc600 - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
total
Mn54
Co60
Cr51
Co57
Co58m
Mn56
Co58
Ni57
Exp

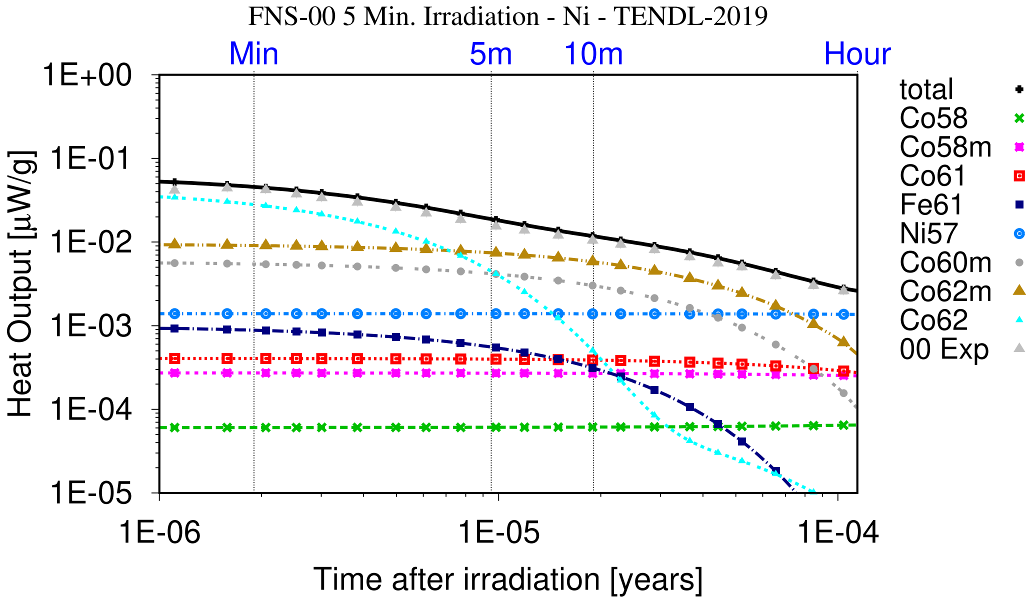

FNS-96 7 hours Irradiation - Inc600 - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
56Mn
57Ni
58mCo
61Co
58Co
57Co
51Cr
60Co
54Mn
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Nickel


FNS-00 5 Min. Irradiation - Ni
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - Ni
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60

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	4.11E−02 +/-6%	5.20E−02 +/-19%	0.79	0.76	0.91	0.89	26.94
0.83	4.38E−02 +/-6%	4.80E−02 +/-19%	0.91	0.91	1.05	1.03	28.71
1.08	4.18E−02 +/-6%	4.45E−02 +/-18%	0.94	0.96	1.07	1.07	27.37
1.33	3.71E−02 +/-6%	4.13E−02 +/-17%	0.90	0.95	1.03	1.03	24.33
1.58	3.35E−02 +/-6%	3.85E−02 +/-17%	0.87	0.96	0.99	1.00	21.95
2.02	2.95E−02 +/-6%	3.42E−02 +/-16%	0.86	1.02	0.98	1.01	19.38
2.62	2.56E−02 +/-6%	2.95E−02 +/-15%	0.87	1.14	0.97	1.03	16.82
3.22	2.20E−02 +/-7%	2.58E−02 +/-14%	0.85	1.24	0.95	1.03	14.42
4.07	1.84E−02 +/-7%	2.19E−02 +/-13%	0.84	1.45	0.93	1.04	12.09
5.17	1.53E−02 +/-7%	1.84E−02 +/-12%	0.83	1.79	0.91	1.06	10.05
6.27	1.37E−02 +/-7%	1.60E−02 +/-12%	0.86	2.27	0.92	1.12	9.01
7.88	1.19E−02 +/-7%	1.37E−02 +/-12%	0.87	2.97	0.93	1.16	7.84
9.95	1.04E−02 +/-8%	1.18E−02 +/-13%	0.88	3.64	0.93	1.19	6.84
12.05	9.32E−03 +/-8%	1.04E−02 +/-13%	0.89	3.93	0.94	1.19	6.13
15.15	8.02E−03 +/-7%	8.99E−03 +/-13%	0.89	3.81	0.93	1.18	5.28
19.25	6.58E−03 +/-7%	7.53E−03 +/-12%	0.87	3.32	0.91	1.12	4.34
23.32	5.54E−03 +/-7%	6.41E−03 +/-12%	0.86	2.87	0.90	1.08	3.66
27.42	5.00E−03 +/-7%	5.52E−03 +/-11%	0.91	2.64	0.94	1.10	3.31
34.48	3.92E−03 +/-8%	4.39E−03 +/-10%	0.89	2.11	0.91	1.03	2.59
44.58	3.00E−03 +/-8%	3.38E−03 +/-9%	0.89	1.64	0.90	0.97	1.99
54.68	2.58E−03 +/-8%	2.78E−03 +/-8%	0.93	1.44	0.93	0.96	1.72
mean % diff. from E			14	39	7	7	83
mean χ^2			4.82	41.17	1.16	1.51	159.13

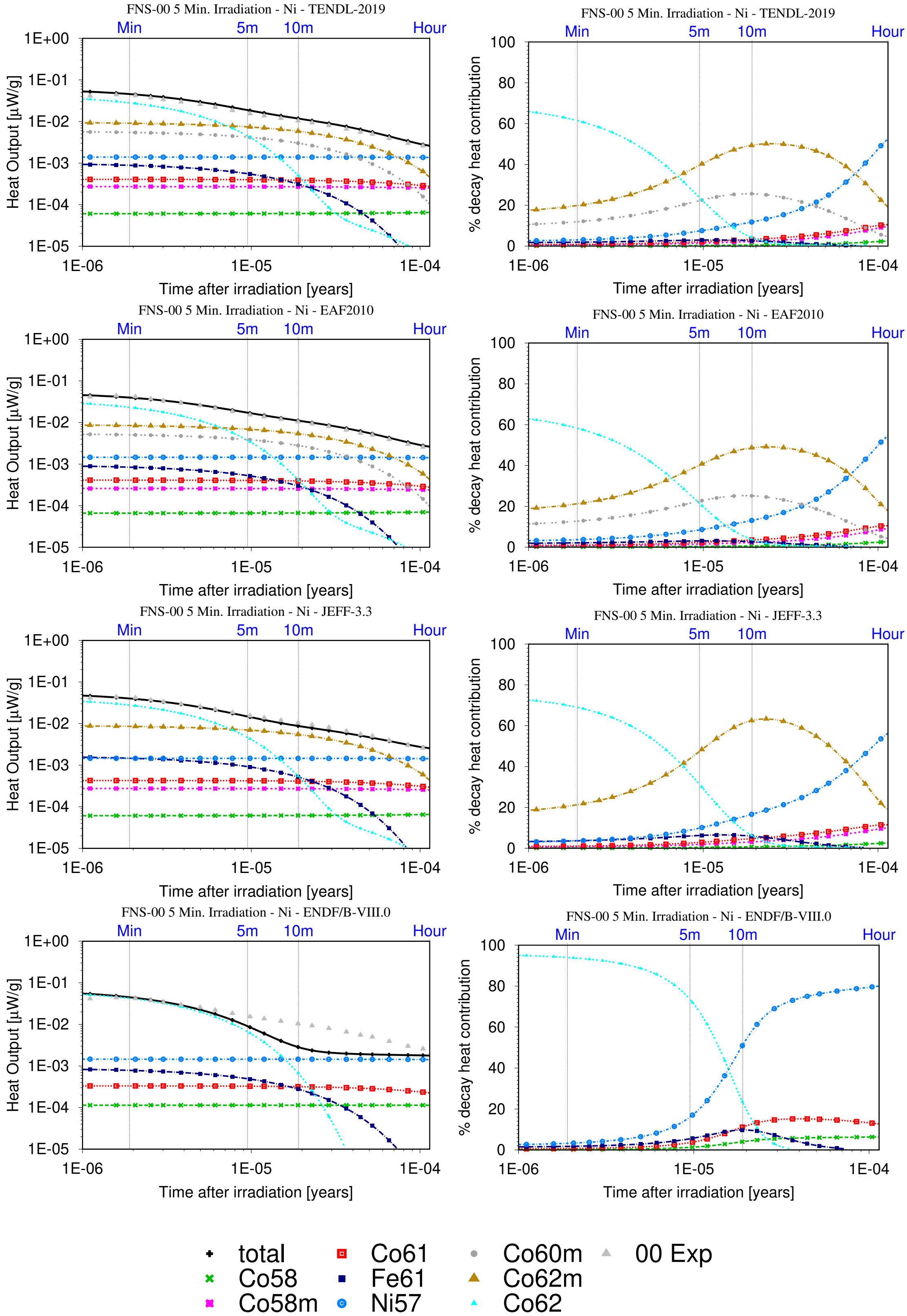


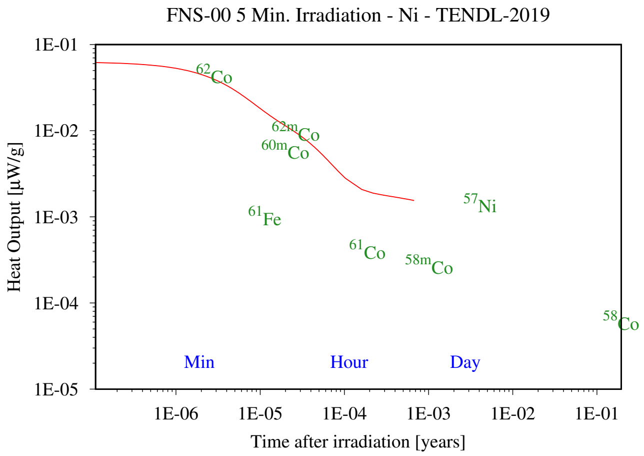
Nickel, TENDL-2019 5-minute pathway analysis

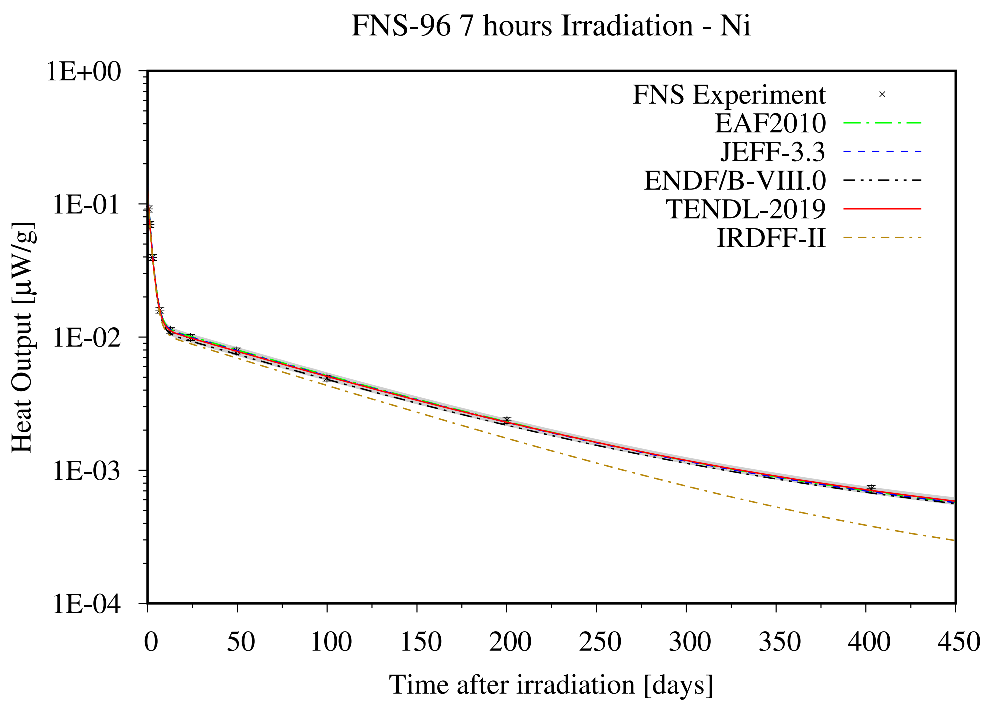
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Co62	1.50m	Ni62(n,p)Co62	99.9
Fe61	5.98m	Ni64(n,α)Fe61	100.0
Co60m	10.47m	Ni60(n,p)Co60m	98.9
Co62m	13.91m	Ni62(n,p)Co62m	100.0
Co61	1.65h	Ni61(n,p)Co61	76.8
		Ni62(n,np)Co61	15.3
		Ni62(n,d)Co61	6.8
		Ni64(n,α)Fe61(β^-)Co61	1.1
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Co58	70.87d	Ni58(n,p)Co58	99.7

Comments on Nickel 5-minute experiments:

Here the two 5-minutes data-sets of experimental measurements differ (without explanation), but the predictions stay within 15% of the measurements at all cooling times for simulations with TENDL-2019 or EAF2010, and within 20% for JEFF-3.3. ENDF/B-VIII.0 performs badly as it lacks the metastable isomer production pathways, particularly Co60m and Co62m (both from (n,p) reactions on Ni isotopes according to the TENDL-2019 simulations). IRDFF-II also misses the production of these metastables, as well as the production of the short-lived Co62 (via (n,p) on Ni62)) and only has the simple decay-profile associated with the longer-lived Ni57.


FNS-00 5 Min. Irradiation - Ni - TENDL-2019
FNS-00 5 Min. Irradiation - Ni - EAF2010
FNS-00 5 Min. Irradiation - Ni - JEFF-3.3
FNS-00 5 Min. Irradiation - Ni - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Co58
Co58m
Co61
Fe61
Ni57
Co60m
Co62m
Co62
00 Exp

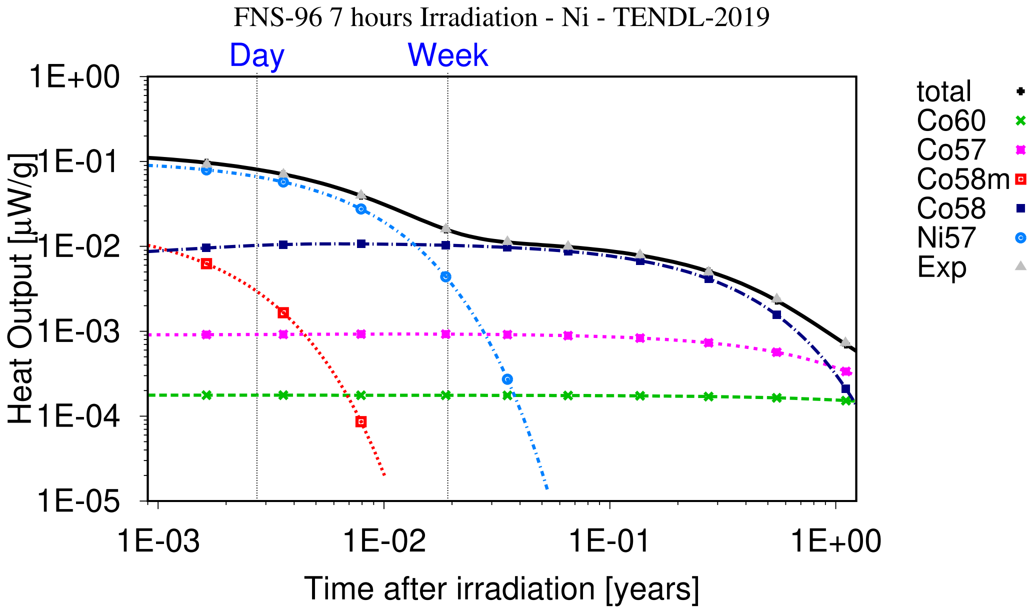

FNS-00 5 Min. Irradiation - Ni - TENDL-2019
Heat Output [μW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
62Co
62mCo
60mCo
61Fe
61Co
58mCo
57Ni
58Co
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.60	$9.17E{-}02$ +/-5%	$9.68E{-}02$ +/-8%	0.95	0.96	0.91	0.91	1.01
1.31	$7.01E{-}02$ +/-5%	$7.07E{-}02$ +/-8%	0.99	0.98	0.95	0.95	1.02
2.89	$3.96E{-}02$ +/-5%	$3.95E{-}02$ +/-7%	1.00	0.99	0.96	0.96	1.03
6.86	$1.59E{-}02$ +/-5%	$1.59E{-}02$ +/-6%	1.00	1.03	0.97	0.98	1.07
12.85	$1.13E{-}02$ +/-5%	$1.12E{-}02$ +/-8%	1.01	1.06	0.98	0.99	1.11
23.85	$9.92E{-}03$ +/-5%	$9.86E{-}03$ +/-8%	1.01	1.06	0.98	0.99	1.11
49.70	$7.87E{-}03$ +/-5%	$7.83E{-}03$ +/-8%	1.01	1.06	0.98	0.99	1.13
99.89	$4.92E{-}03$ +/-5%	$5.07E{-}03$ +/-7%	0.97	1.02	0.95	0.96	1.14
200.11	$2.37E{-}03$ +/-5%	$2.29E{-}03$ +/-6%	1.04	1.09	1.03	1.04	1.37
402.94	$7.27E{-}04$ +/-6%	$7.00E{-}04$ +/-6%	1.04	1.09	1.06	1.06	1.94
mean % diff. from E			2	5	4	4	13
mean χ^2			0.24	0.95	0.79	0.78	11.96

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Ni57	1.50d	0.95	5%	10%
Co58	70.87d	1.01	5%	9%

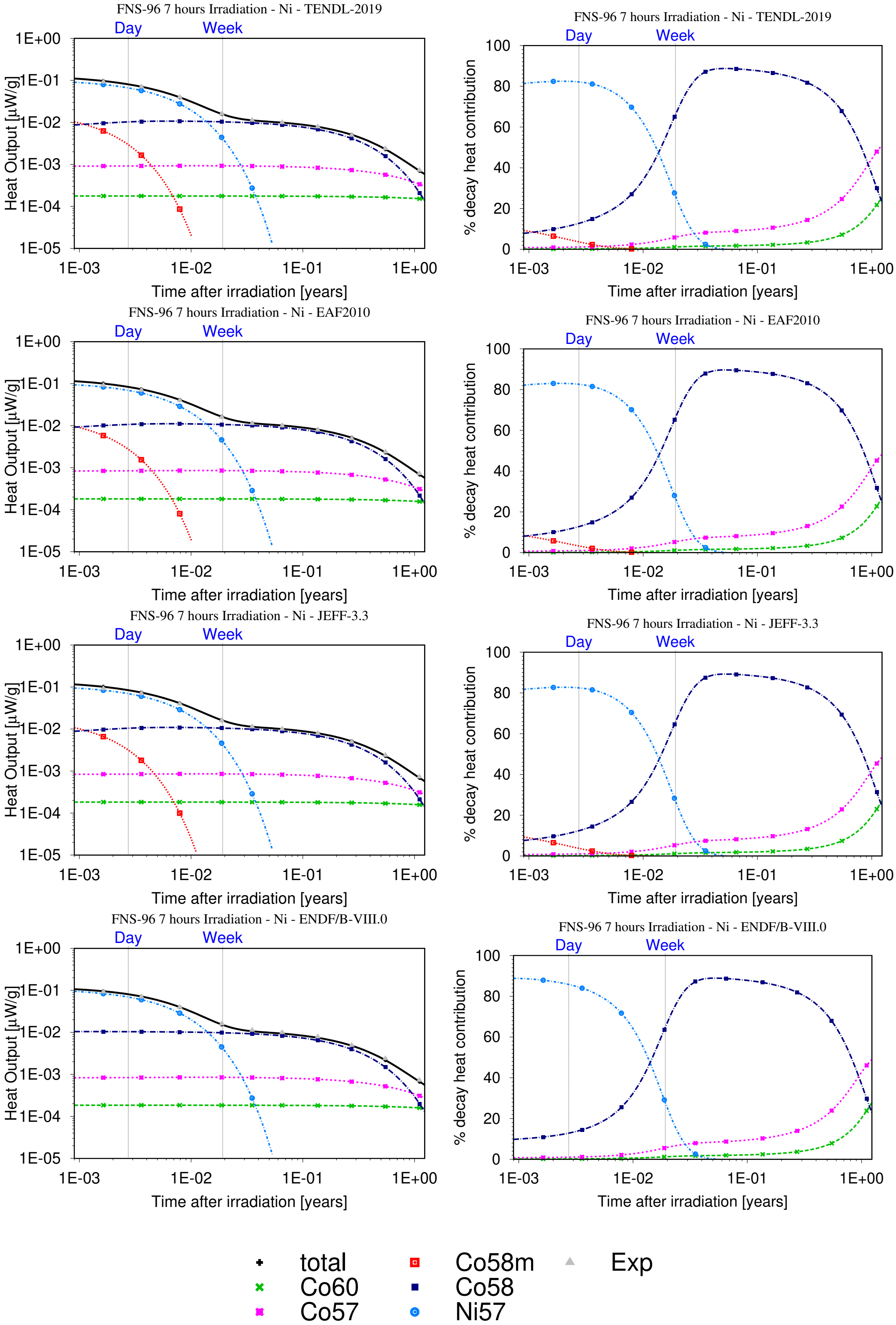


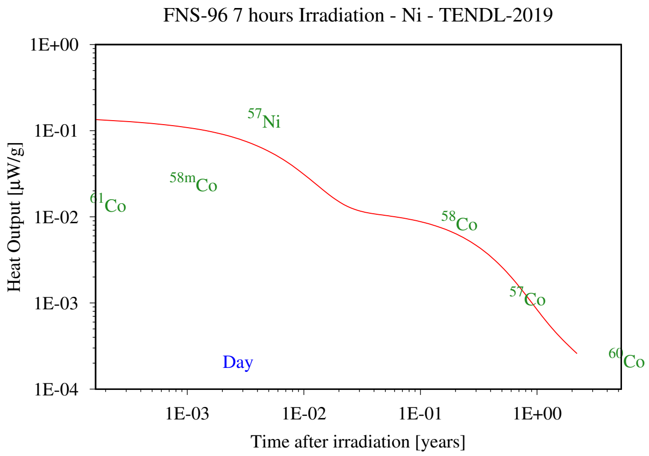
Nickel,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Co58m	8.90h	Ni58(n,p)Co58m	100.0
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
Co57	271.77d	Ni58(n,np)Co57	97.5
		Ni58(n,d)Co57	2.1
Co60	5.27y	Ni60(n,p)Co60m(IT)Co60	56.3
		Ni60(n,p)Co60	42.4

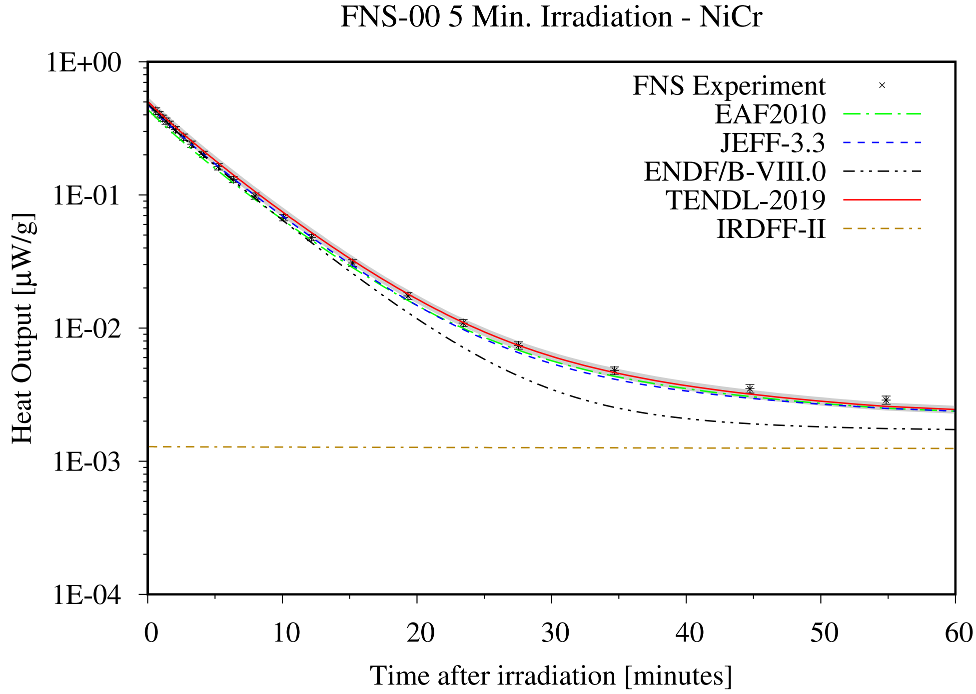
Comments on Nickel 7-hour experiments:

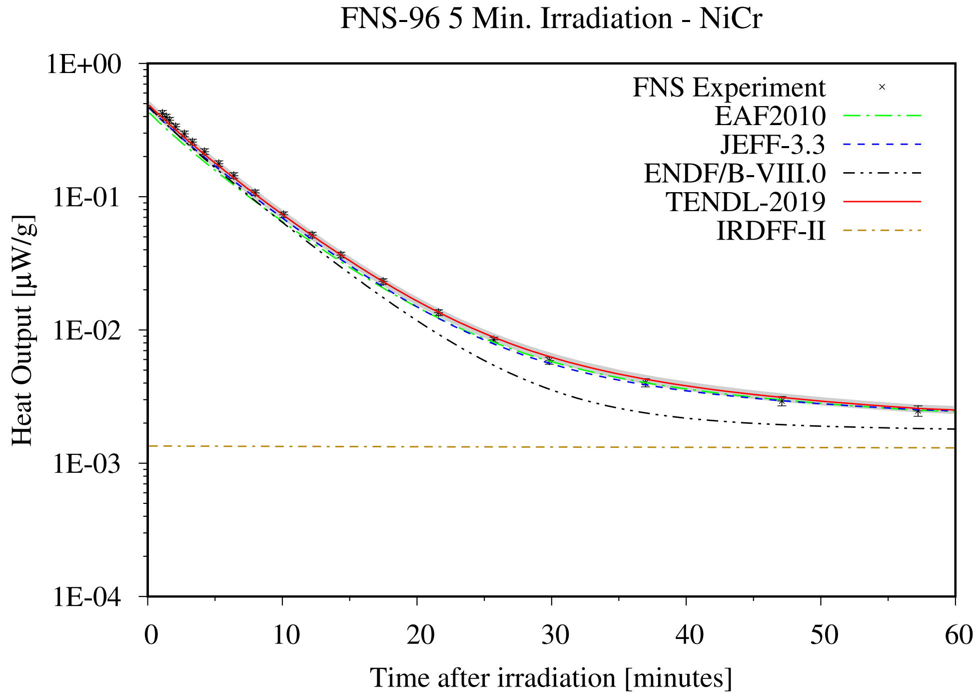
Excellent agreement between experiment and simulation for the 4 general purpose libraries considered. Predictions show (correctly) that the decay-heat is dominated by Ni57 during the first few days of cooling and then by Co58. As with the Inconel 7-hour experiment, Co57 and Co60 join Co58 to contribute significantly in the final two cooling steps (IRDFF-II misses these two nuclides, but, as before, captures the profile associated with Co58 and Ni57).


FNS-96 7 hours Irradiation - Ni - TENDL-2019
FNS-96 7 hours Irradiation - Ni - EAF2010
FNS-96 7 hours Irradiation - Ni - JEFF-3.3
FNS-96 7 hours Irradiation - Ni - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-03
1E-02
1E-01
1E+00
0
20
40
60
80
100
total
Co60
Co57
Co58m
Co58
Ni57
Exp


FNS-96 7 hours Irradiation - Ni - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
57Ni
58mCo
61Co
58Co
57Co
60Co
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Nickel-chrome

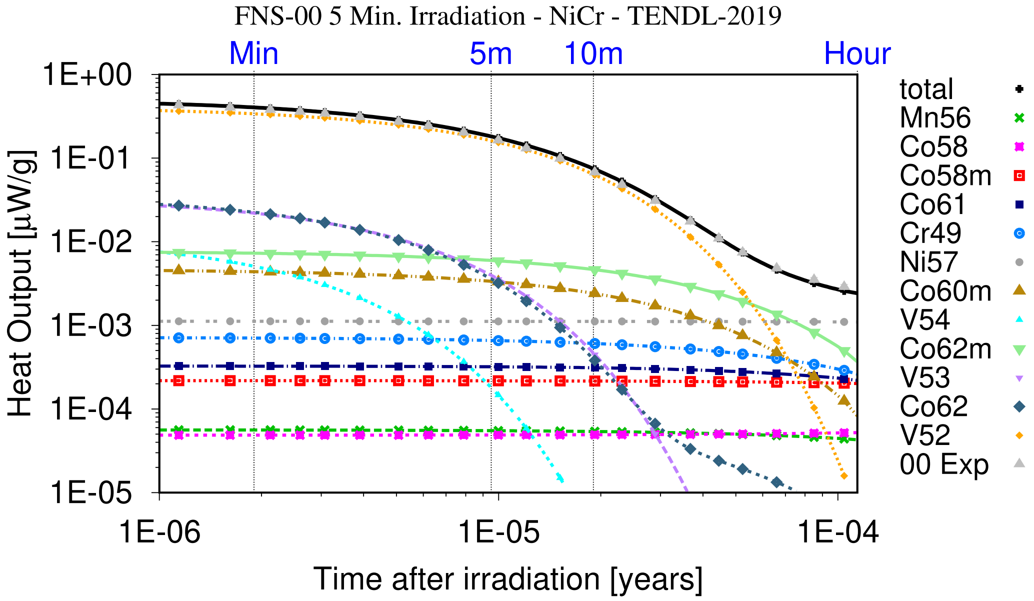




Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.60	4.27E−01 +/-5%	4.41E−01 +/-8%	0.97	1.01	1.12	1.03	332.46
0.85	4.01E−01 +/-5%	4.17E−01 +/-8%	0.96	1.01	1.11	1.02	312.06
1.12	3.77E−01 +/-5%	3.94E−01 +/-8%	0.96	1.01	1.10	1.02	293.46
1.37	3.59E−01 +/-5%	3.73E−01 +/-8%	0.96	1.01	1.11	1.02	279.20
1.62	3.40E−01 +/-5%	3.54E−01 +/-8%	0.96	1.01	1.11	1.02	264.69
2.05	3.10E−01 +/-5%	3.24E−01 +/-8%	0.96	1.01	1.10	1.01	241.03
2.67	2.72E−01 +/-5%	2.86E−01 +/-8%	0.95	1.02	1.10	1.01	211.93
3.27	2.40E−01 +/-5%	2.54E−01 +/-8%	0.95	1.02	1.09	1.01	187.40
4.15	2.02E−01 +/-5%	2.14E−01 +/-8%	0.94	1.02	1.09	1.00	157.27
5.25	1.63E−01 +/-5%	1.74E−01 +/-8%	0.94	1.03	1.08	1.00	127.03
6.35	1.31E−01 +/-5%	1.42E−01 +/-8%	0.92	1.02	1.06	0.98	101.98
7.98	9.83E−02 +/-5%	1.06E−01 +/-8%	0.93	1.04	1.06	0.99	76.81
10.10	6.75E−02 +/-5%	7.36E−02 +/-8%	0.92	1.06	1.05	0.99	52.85
12.15	4.78E−02 +/-5%	5.24E−02 +/-8%	0.91	1.09	1.04	0.99	37.48
15.22	3.08E−02 +/-6%	3.24E−02 +/-8%	0.95	1.20	1.08	1.04	24.21
19.33	1.74E−02 +/-6%	1.81E−02 +/-7%	0.96	1.33	1.08	1.07	13.71
23.43	1.09E−02 +/-6%	1.10E−02 +/-7%	0.99	1.52	1.09	1.12	8.60
27.55	7.42E−03 +/-6%	7.43E−03 +/-7%	1.00	1.69	1.09	1.13	5.86
34.68	4.80E−03 +/-6%	4.64E−03 +/-8%	1.04	1.89	1.10	1.16	3.81
44.73	3.50E−03 +/-7%	3.20E−03 +/-8%	1.10	1.83	1.14	1.18	2.79
54.85	2.88E−03 +/-7%	2.58E−03 +/-7%	1.12	1.64	1.15	1.16	2.31
mean % diff. from E			5	13	8	4	93
mean χ^2			1.09	10.92	2.24	1.06	274.41

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
V52	3.74m	0.97	5%	9%

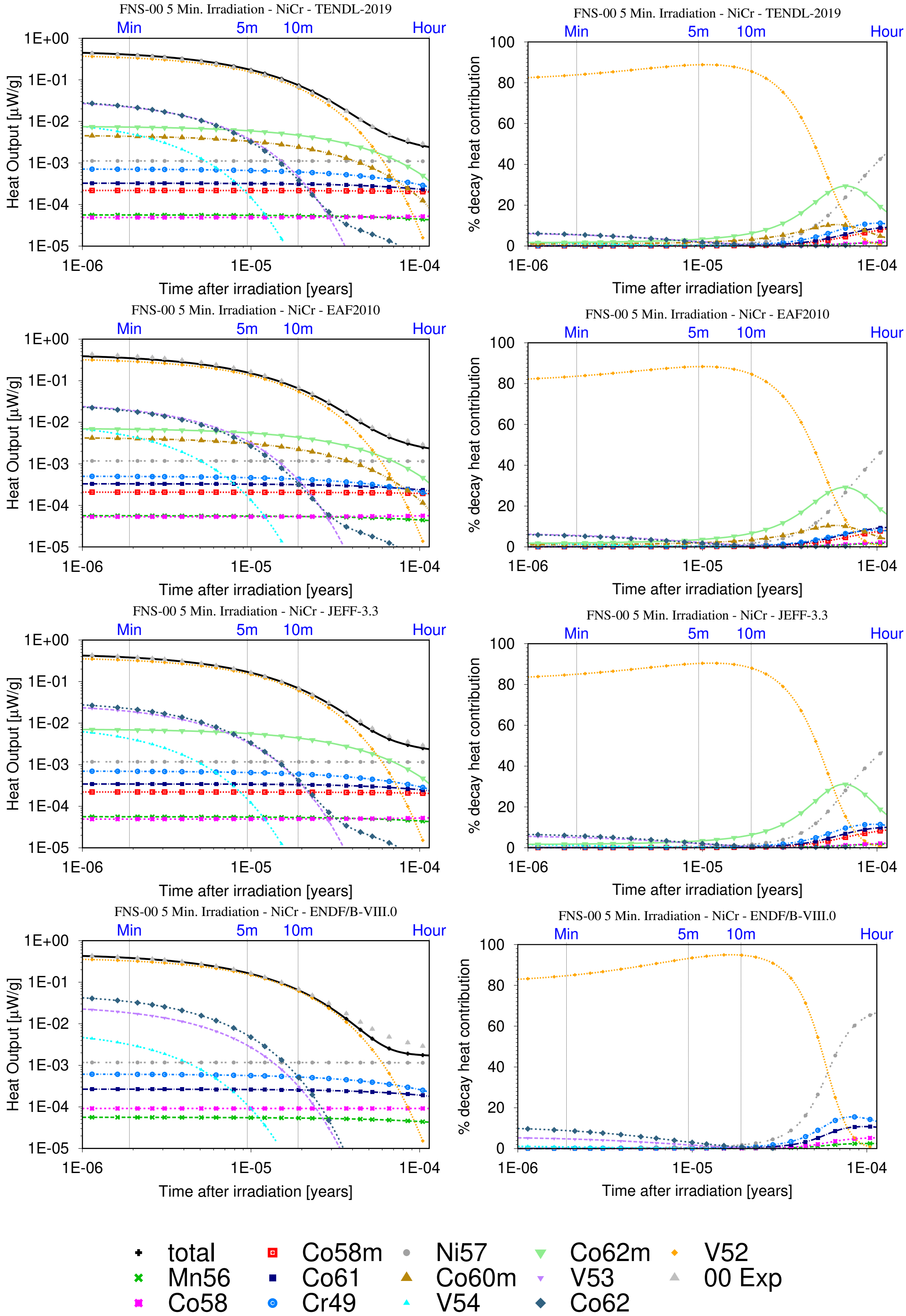


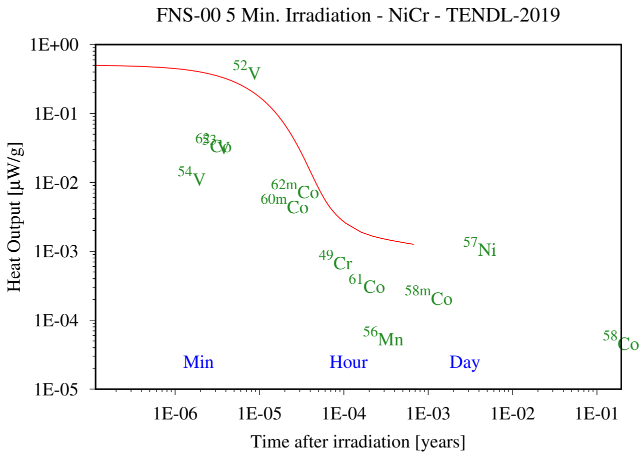
Nickel-chrome, TENDL-2019 5-minute pathway analysis

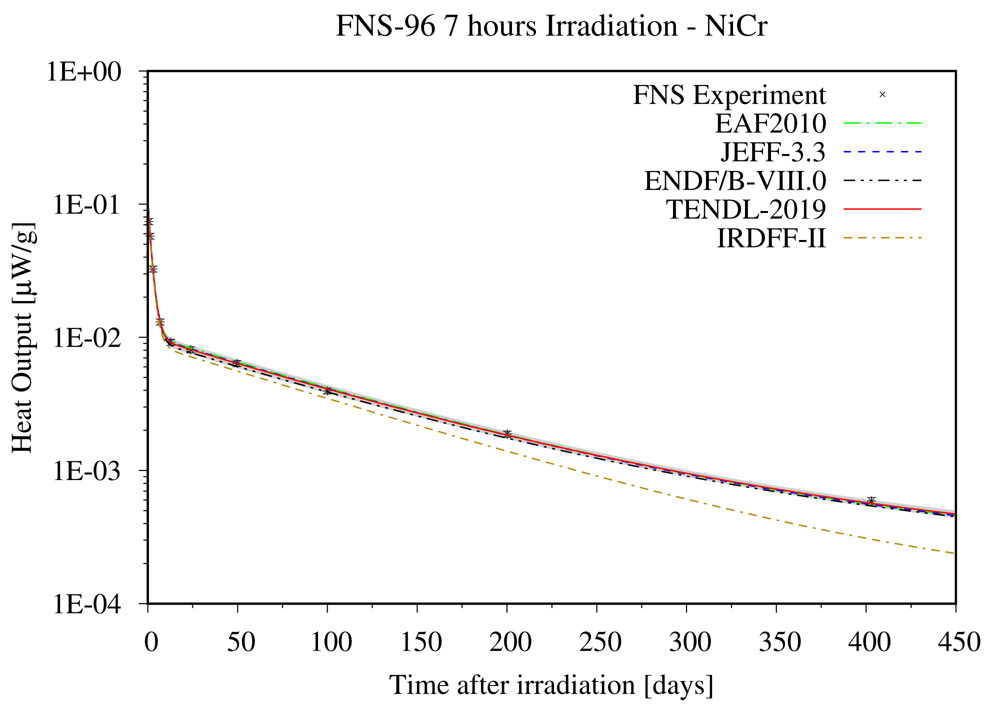
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
V54	49.80s	Cr54(n,p)V54	100.0
Co62	1.50m	Ni62(n,p)Co62	99.9
V53	1.62m	Cr53(n,p)V53	99.3
V52	3.74m	Cr52(n,p)V52	98.0
		Cr53(n,np)V52	1.6
Co60m	10.47m	Ni60(n,p)Co60m	98.9
Co62m	13.91m	Ni62(n,p)Co62m	100.0
Cr49	41.90m	Cr50(n,2n)Cr49	100.0
Co61	1.65h	Ni61(n,p)Co61	76.8
		Ni62(n,np)Co61	15.3
		Ni62(n,d)Co61	6.8
		Ni64(n,α)Fe61(β^-)Co61	1.1
Mn56	2.58h	Fe56(n,p)Mn56	99.7
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Co58	70.87d	Ni58(n,p)Co58	99.7

Comments on Nickel-chrome 5-minute experiments:

The first 15 minutes of cooling time are dominated by the Cr-isotope produced V-52; a trend that was also seen in the Cr experiments. This early, chromium-dominated behaviour is well-captured by all the general purpose libraries. However, at later cooling time, ENDF/B-VIII.0 suffers (as it did in predictions for Ni) because it omits, in particular, the metastable Co62m isotope produced via (n,p) reactions on Ni62. As already noted (for Cr and Ni), IRDFF-II lacks the reaction channel to produce either the short-lived V52 from Cr or the Co isotopes from Ni – only the longer-lived Ni57 is produced, which TENDL-2019, JEFF-3.3 and EAF2010 predict contributes 50% at 1-hour of cooling – those three libraries all perform almost identically and well-match the experiment.


FNS-00 5 Min. Irradiation - NiCr - TENDL-2019
FNS-00 5 Min. Irradiation - NiCr - EAF2010
FNS-00 5 Min. Irradiation - NiCr - JEFF-3.3
FNS-00 5 Min. Irradiation - NiCr - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Mn56
Co58
Co58m
Co61
Cr49
Ni57
Co60m
V54
Co62m
V53
Co62
V52
00 Exp

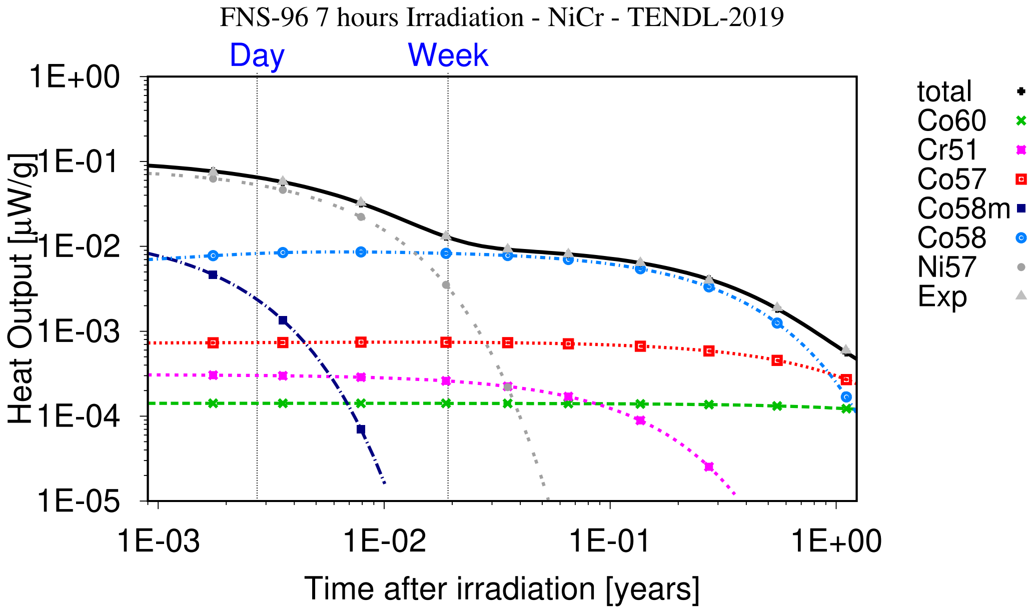

FNS-00 5 Min. Irradiation - NiCr - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
Time after irradiation [years]
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Min
Hour
Day
52V
54V
62mCo
60mCo
49Cr
61Co
58mCo
56Mn
57Ni
58Co



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.64	7.40$E-$02 +/-5%	7.66$E-$02 +/-8%	0.97	0.98	0.93	0.92	1.03
1.30	5.75$E-$02 +/-5%	5.73$E-$02 +/-8%	1.00	0.99	0.96	0.96	1.04
2.88	3.26$E-$02 +/-5%	3.21$E-$02 +/-7%	1.01	1.00	0.97	0.98	1.05
6.85	1.31$E-$02 +/-5%	1.30$E-$02 +/-6%	1.00	1.03	0.97	0.98	1.09
12.85	9.18$E-$03 +/-5%	9.18$E-$03 +/-7%	1.00	1.05	0.97	0.99	1.12
23.85	8.07$E-$03 +/-5%	8.09$E-$03 +/-8%	1.00	1.05	0.97	0.99	1.13
49.70	6.36$E-$03 +/-5%	6.37$E-$03 +/-7%	1.00	1.05	0.97	0.99	1.14
99.89	3.96$E-$03 +/-5%	4.10$E-$03 +/-7%	0.97	1.02	0.95	0.96	1.14
200.12	1.88$E-$03 +/-5%	1.84$E-$03 +/-6%	1.02	1.07	1.01	1.02	1.34
402.94	5.92$E-$04 +/-6%	5.63$E-$04 +/-6%	1.05	1.10	1.07	1.08	1.96
mean % diff. from E			2	4	4	3	14
mean χ^2			0.19	0.73	0.68	0.60	11.84

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ni57	1.50d	0.97	5%	10%
Co58	70.87d	1.00	5%	9%

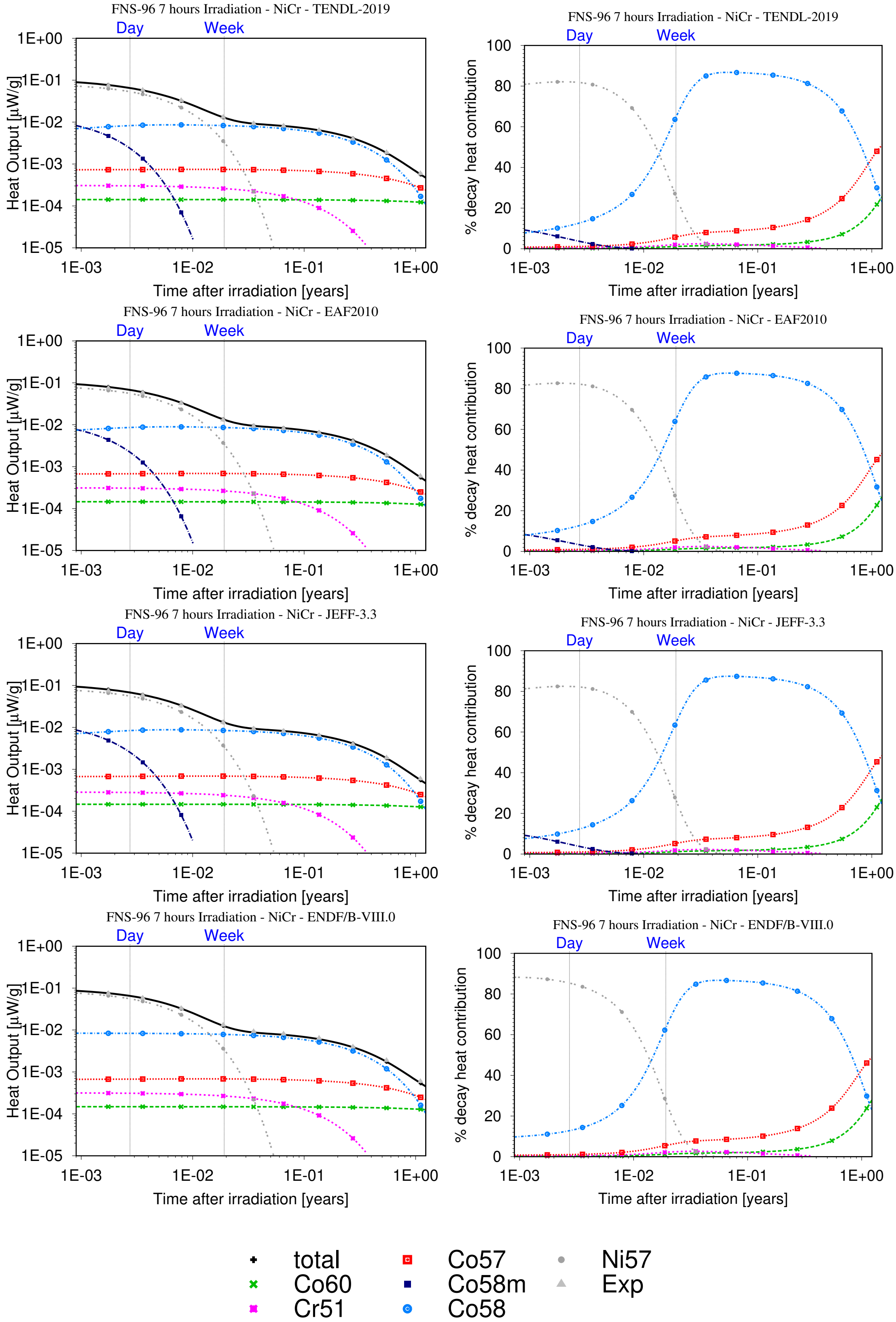


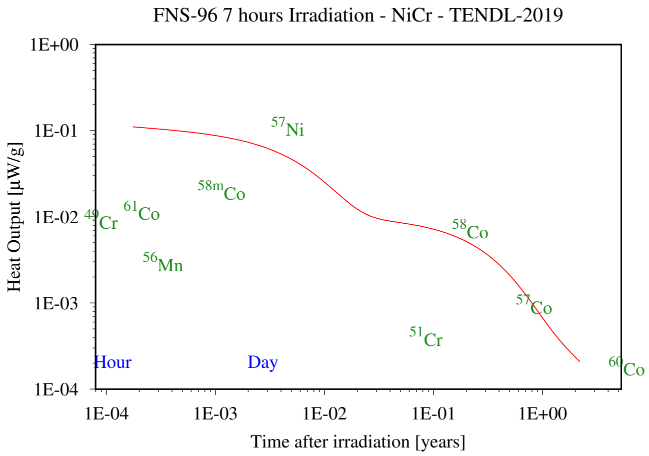
Nickel-chrome,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Co58m	8.90h	Ni58(n,p)Co58m	100.0
Ni57	1.50d	Ni58(n,2n)Ni57	100.0
Cr51	27.70d	Cr52(n,2n)Cr51	100.0
Co58	70.87d	Ni58(n,p)Co58	80.0
		Ni58(n,p)Co58m(IT)Co58	20.0
Co57	271.77d	Ni58(n,np)Co57	97.5
		Ni58(n,d)Co57	2.1
Co60	5.27y	Ni60(n,p)Co60m(IT)Co60	56.3
		Ni60(n,p)Co60	42.4

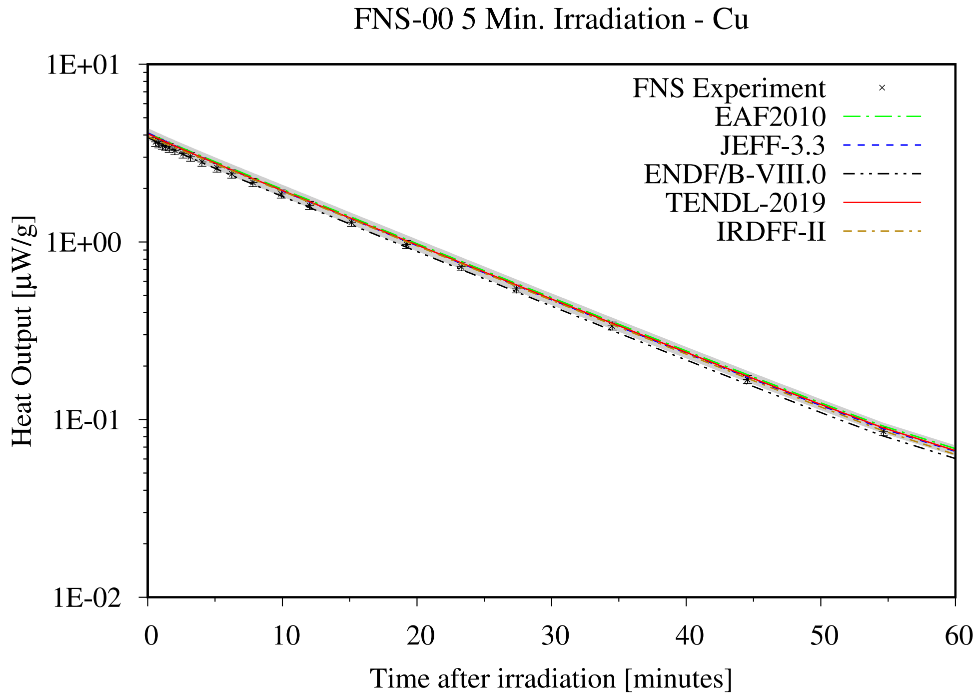
Comments on Nickel-chrome 7-hour experiments:

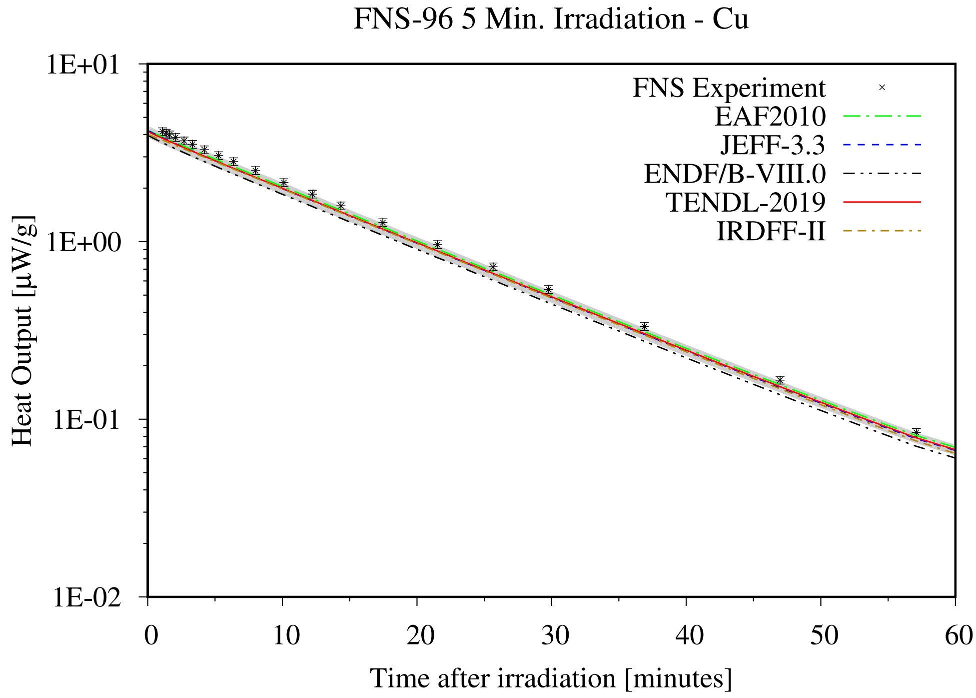
The Cr makes up around 20 weight % of the samples and the main radionuclides produced from Cr only have impact at shorter times (see the discussion of the 5-minute experiment), and so, unsurprisingly, the observations for this longer experiment are identical to those of pure Ni. Excellent agreement exits for simulations with TENDL, JEFF, EAF, and ENDF/B, while IRDFF-II misses the Co57 and Co60 that are important at 1-year of cooling.


FNS-96 7 hours Irradiation - NiCr - TENDL-2019
FNS-96 7 hours Irradiation - NiCr - TENDL-2019
FNS-96 7 hours Irradiation - NiCr - EAF2010
FNS-96 7 hours Irradiation - NiCr - EAF2010
FNS-96 7 hours Irradiation - NiCr - JEFF-3.3
FNS-96 7 hours Irradiation - NiCr - JEFF-3.3
FNS-96 7 hours Irradiation - NiCr - ENDF/B-VIII.0
FNS-96 7 hours Irradiation - NiCr - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-03
1E-02
1E-01
1E+00
0
20
40
60
80
100
total
Co60
Cr51
Co57
Co58m
Co58
Ni57
Exp


FNS-96 7 hours Irradiation - NiCr - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-04
1E-03
1E-02
1E-01
1E+00
57Ni
58mCo
49Cr
61Co
56Mn
58Co
57Co
51Cr
60Co
Hour
Day

Copper

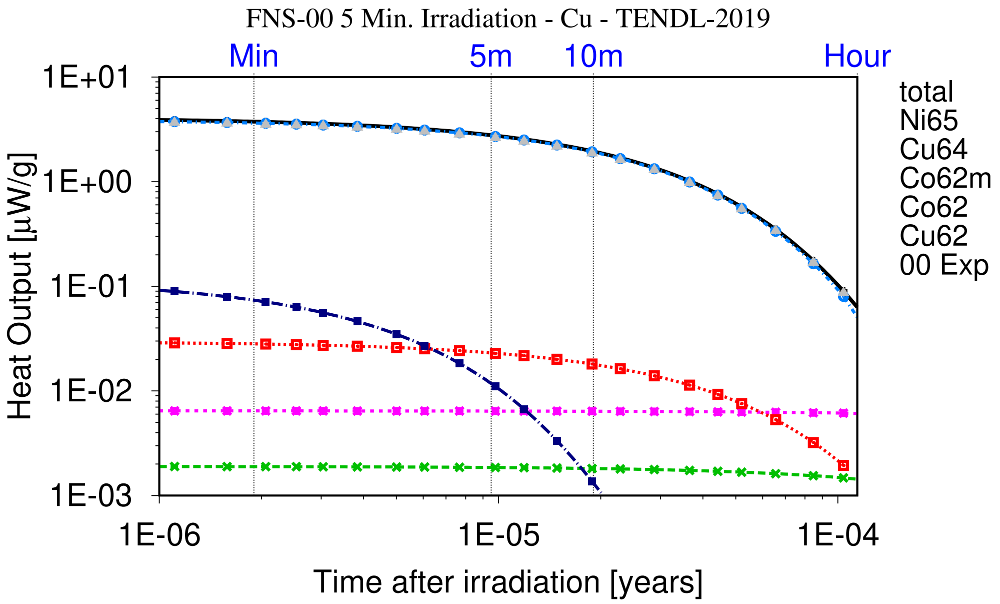

FNS-00 5 Min. Irradiation - Cu
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II


FNS-96 5 Min. Irradiation - Cu
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II

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	3.66E+00 +/-6%	3.88E+00 +/-8%	0.94	0.99	0.93	0.93	0.97
0.83	3.59E+00 +/-6%	3.80E+00 +/-8%	0.94	1.00	0.93	0.94	0.97
1.08	3.50E+00 +/-6%	3.73E+00 +/-8%	0.94	0.99	0.93	0.93	0.96
1.33	3.45E+00 +/-6%	3.66E+00 +/-8%	0.94	1.00	0.93	0.94	0.97
1.60	3.38E+00 +/-6%	3.58E+00 +/-8%	0.94	1.00	0.93	0.94	0.97
2.02	3.28E+00 +/-6%	3.47E+00 +/-8%	0.95	1.00	0.93	0.94	0.96
2.63	3.14E+00 +/-6%	3.31E+00 +/-8%	0.95	1.01	0.93	0.95	0.97
3.18	3.01E+00 +/-6%	3.18E+00 +/-8%	0.95	1.01	0.93	0.95	0.96
4.03	2.82E+00 +/-6%	2.99E+00 +/-8%	0.95	1.01	0.93	0.95	0.96
5.15	2.61E+00 +/-5%	2.75E+00 +/-8%	0.95	1.02	0.93	0.95	0.96
6.25	2.42E+00 +/-5%	2.54E+00 +/-8%	0.95	1.02	0.93	0.95	0.96
7.82	2.16E+00 +/-5%	2.27E+00 +/-8%	0.95	1.02	0.93	0.95	0.96
9.92	1.86E+00 +/-5%	1.96E+00 +/-8%	0.95	1.03	0.93	0.96	0.96
12.02	1.61E+00 +/-5%	1.69E+00 +/-8%	0.95	1.03	0.94	0.96	0.96
15.13	1.29E+00 +/-5%	1.35E+00 +/-8%	0.95	1.03	0.94	0.96	0.96
19.23	9.68$E-$01 +/-5%	1.02E+00 +/-8%	0.95	1.04	0.94	0.96	0.96
23.28	7.26$E-$01 +/-5%	7.64$E-$01 +/-8%	0.95	1.04	0.93	0.96	0.96
27.38	5.44$E-$01 +/-5%	5.73$E-$01 +/-8%	0.95	1.04	0.93	0.96	0.96
34.50	3.37$E-$01 +/-5%	3.50$E-$01 +/-7%	0.96	1.06	0.95	0.97	0.98
44.55	1.68$E-$01 +/-5%	1.76$E-$01 +/-7%	0.96	1.06	0.94	0.97	0.98
54.65	8.60$E-$02 +/-5%	9.00$E-$02 +/-7%	0.96	1.06	0.93	0.97	0.99
mean % diff. from E			5	2	7	5	3
mean χ^2			0.97	0.31	1.70	0.93	0.42

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Cu62	9.75m	0.94	6%	8%

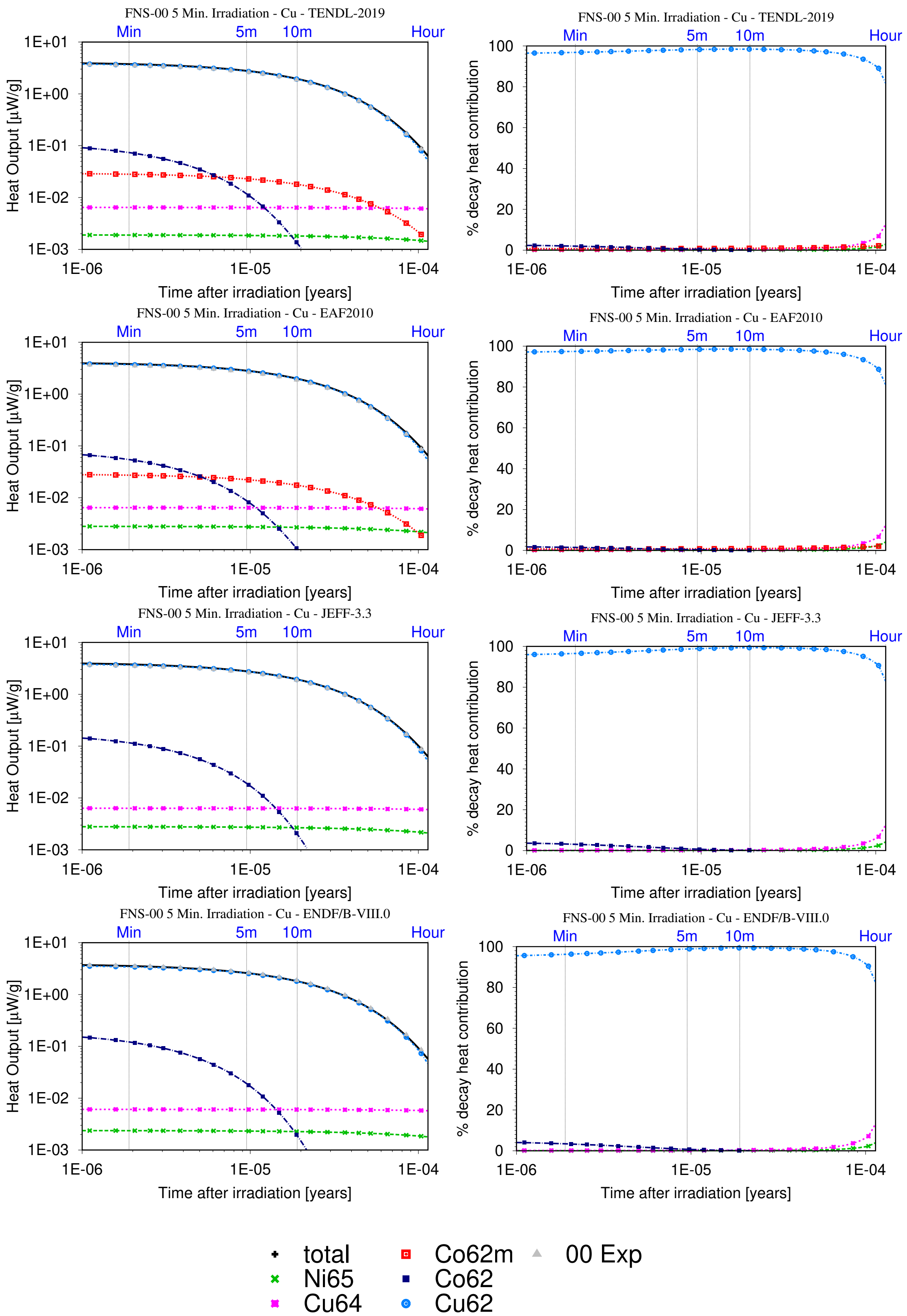


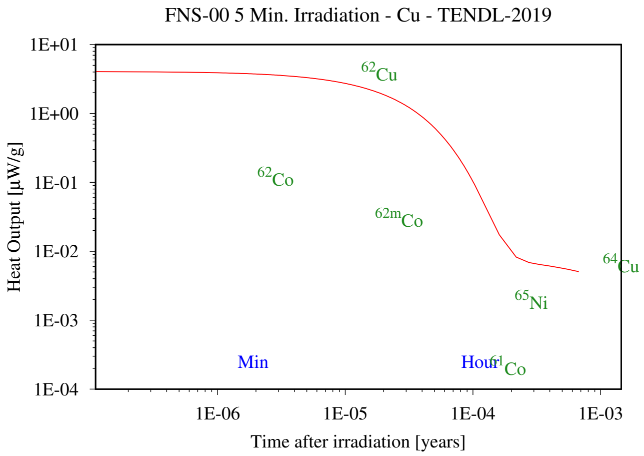
Copper, TENDL-2019 5-minute pathway analysis

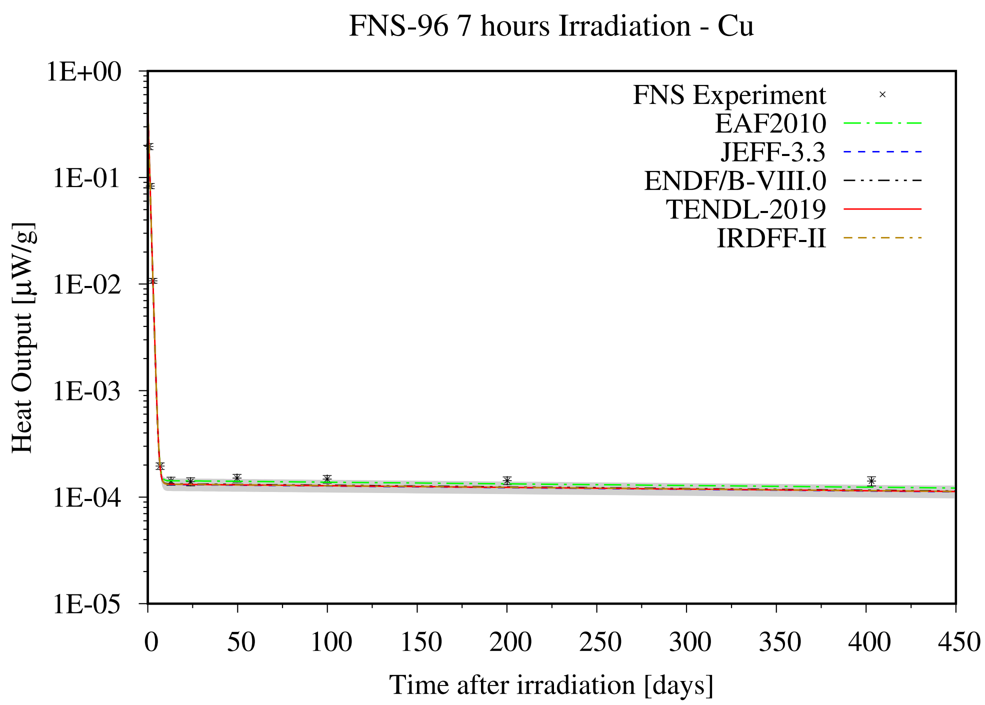
Product	$T_{1/2}$	Pathways	Path %
Co62	1.50m	Cu65(n,α)Co62	99.9
Cu62	9.75m	Cu63(n,2n)Cu62	100.0
Co62m	13.91m	Cu65(n,α)Co62m	100.0
Ni65	2.52h	Cu65(n,p)Ni65	100.0
Cu64	12.70h	Cu65(n,2n)Cu64	99.2

Comments on Copper 5-minute experiments:

A good agreement between experiment and simulation (with all libraries) for both sample-runs for this straightforward case of (n,2n)-generated Cu62 decay-heat dominance at all cooling times. However, the experimental uncertainties seem rather uniform at 5 or 6%, which seems questionable given that the two experiments themselves differ by more than this amount.


FNS-00 5 Min. Irradiation - Cu - TENDL-2019
FNS-00 5 Min. Irradiation - Cu - EAF2010
FNS-00 5 Min. Irradiation - Cu - JEFF-3.3
FNS-00 5 Min. Irradiation - Cu - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
1E+01
1E+00
1E-01
1E-02
1E-03
100
80
60
40
20
0
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Ni65
Cu64
Co62m
Co62
Cu62
00 Exp

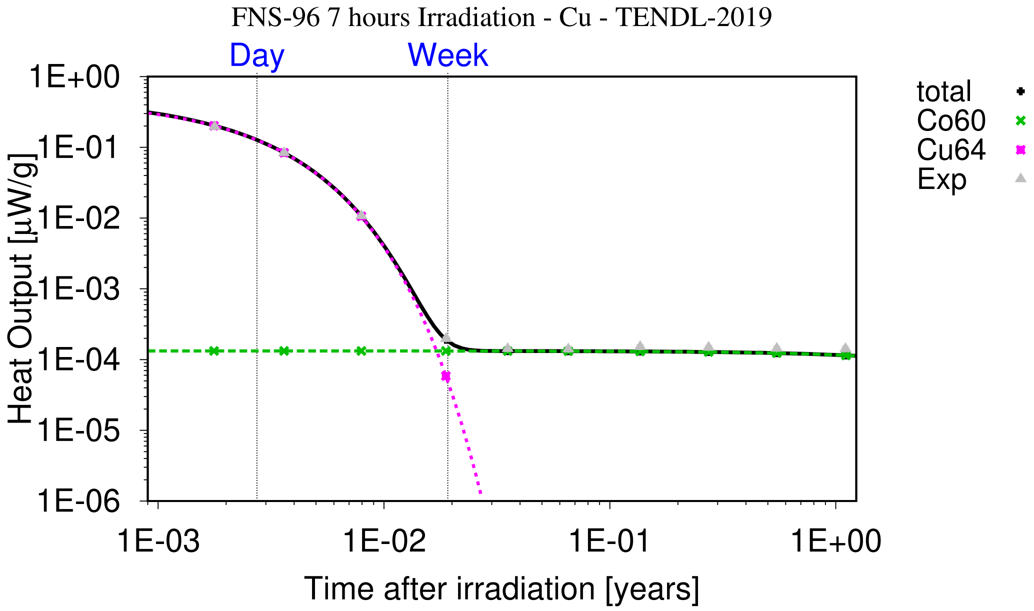

FNS-00 5 Min. Irradiation - Cu - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
62Cu
62Co
62mCo
64Cu
65Ni
61Co
Min
Hour
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.65	1.95$E-$01 +/-7%	2.03$E-$01 +/-6%	0.96	1.02	0.96	0.98	0.96
1.32	8.31$E-$02 +/-6%	8.38$E-$02 +/-7%	0.99	1.05	0.99	1.01	0.99
2.90	1.07$E-$02 +/-5%	1.07$E-$02 +/-6%	1.00	1.06	1.00	1.02	1.00
6.87	1.96$E-$04 +/-7%	1.91$E-$04 +/-10%	1.03	1.04	0.97	1.04	1.02
12.89	1.42$E-$04 +/-9%	1.32$E-$04 +/-14%	1.07	1.06	0.99	1.08	1.07
23.90	1.40$E-$04 +/-9%	1.31$E-$04 +/-14%	1.06	1.05	0.98	1.07	1.06
49.72	1.51$E-$04 +/-8%	1.30$E-$04 +/-14%	1.16	1.15	1.07	1.17	1.16
99.92	1.48$E-$04 +/-8%	1.28$E-$04 +/-14%	1.15	1.14	1.07	1.16	1.15
200.14	1.43$E-$04 +/-8%	1.23$E-$04 +/-14%	1.16	1.15	1.07	1.16	1.16
402.97	1.41$E-$04 +/-10%	1.15$E-$04 +/-14%	1.23	1.22	1.14	1.24	1.23
mean % diff. from E			8	8	4	8	8
mean χ^2			1.35	1.36	0.42	1.45	1.31

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Cu64	12.70h	0.96	7%	7%
Co60	5.27y	1.07	9%	14%

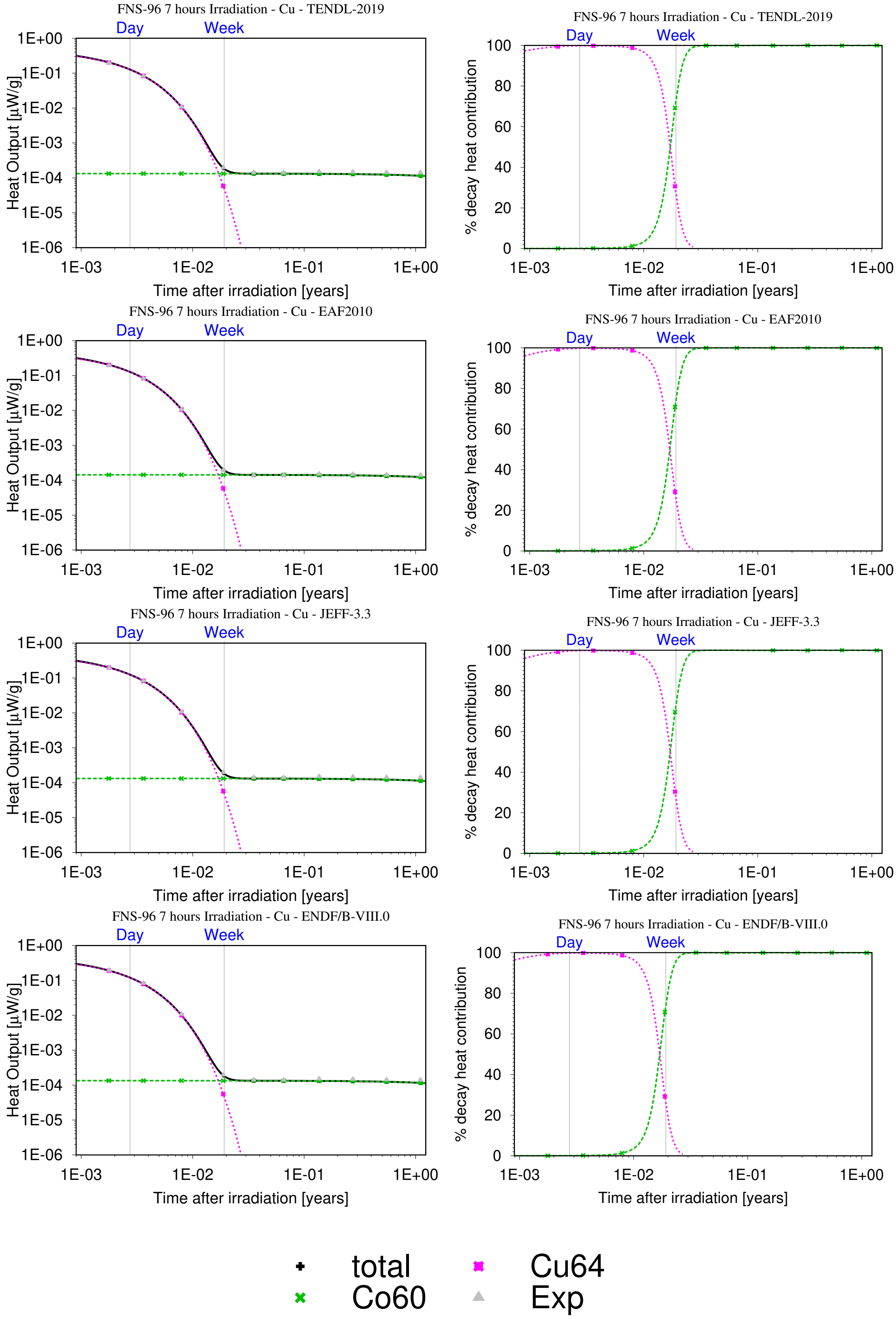


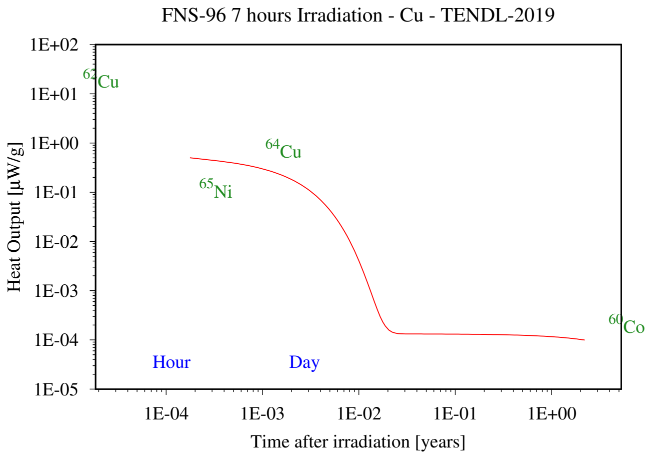
Copper,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Cu64	12.70h	Cu65(n,2n)Cu64	99.7
Co60	5.27y	Cu63(n,α)Co60m(IT)Co60	53.0
		Cu63(n,α)Co60	47.0

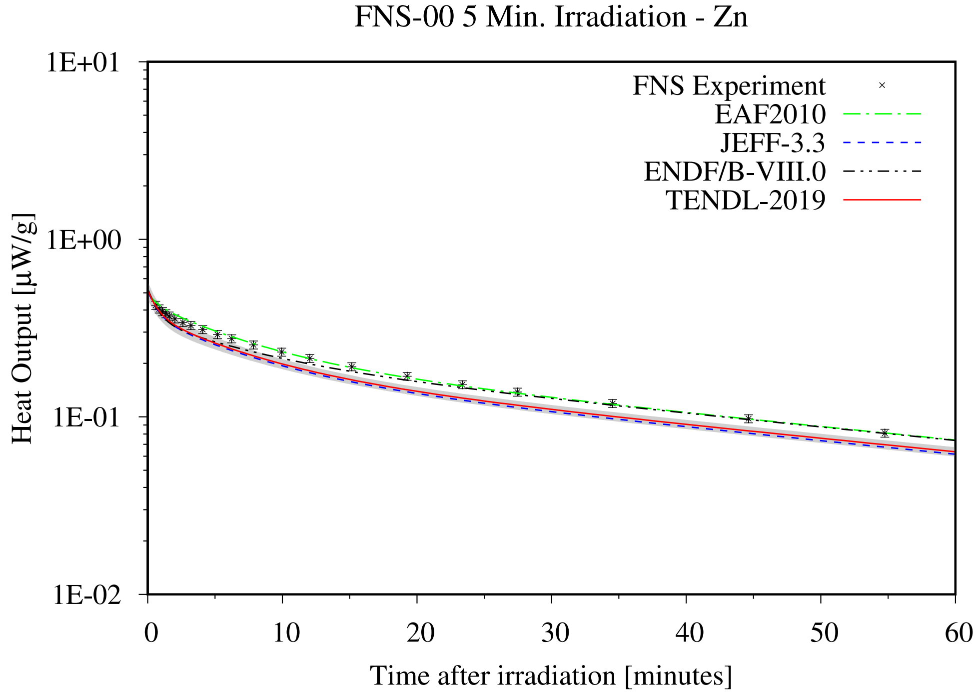
Comments on Copper 7-hour experiments:

A simple, two-nuclide contribution profile – Cu64 during the first week and Co60 afterward – captures well the experimental result, with the simulated decay-heat values often within the experimental uncertainty for all libraries.


FNS-96 7 hours Irradiation - Cu - TENDL-2019
FNS-96 7 hours Irradiation - Cu - EAF2010
FNS-96 7 hours Irradiation - Cu - JEFF-3.3
FNS-96 7 hours Irradiation - Cu - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
0
20
40
60
80
100
total
Cu64
Co60
Exp


FNS-96 7 hours Irradiation - Cu - TENDL-2019
Heat Output [μW/g]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
62Cu
64Cu
65Ni
60Co
Hour
Day
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

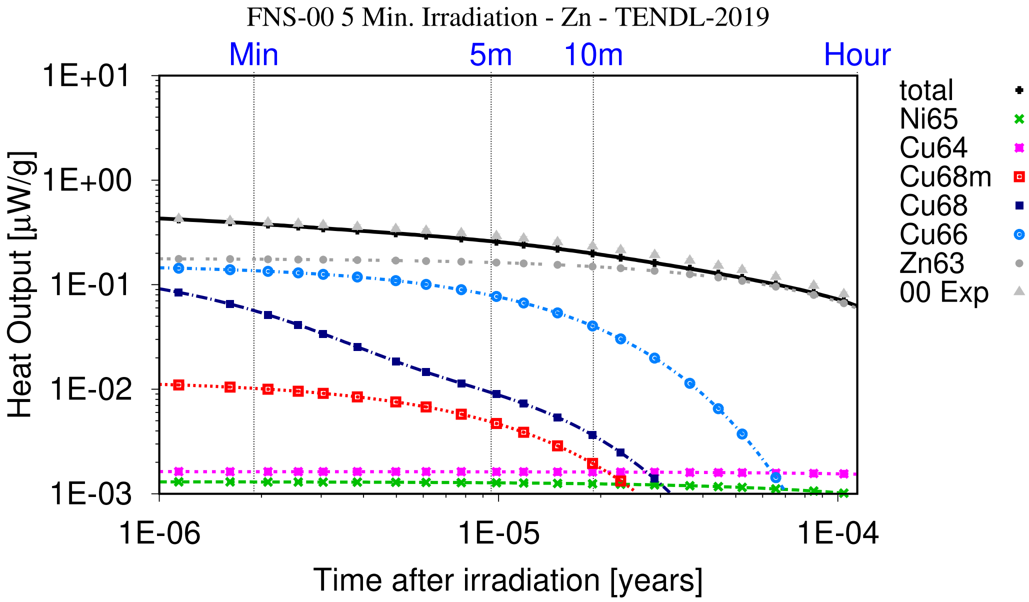
Zinc



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	$4.25E{-}01$ +/-5%	$4.22E{-}01$ +/-10%	1.01	1.02	0.96	1.02
0.85	$4.06E{-}01$ +/-5%	$3.96E{-}01$ +/-10%	1.02	1.04	0.95	1.04
1.10	$3.92E{-}01$ +/-5%	$3.76E{-}01$ +/-10%	1.04	1.06	0.95	1.06
1.35	$3.81E{-}01$ +/-5%	$3.60E{-}01$ +/-9%	1.06	1.08	0.95	1.08
1.60	$3.70E{-}01$ +/-5%	$3.47E{-}01$ +/-9%	1.07	1.09	0.94	1.09
2.02	$3.57E{-}01$ +/-5%	$3.29E{-}01$ +/-9%	1.08	1.11	0.94	1.10
2.62	$3.40E{-}01$ +/-5%	$3.10E{-}01$ +/-9%	1.10	1.11	0.94	1.12
3.22	$3.27E{-}01$ +/-5%	$2.95E{-}01$ +/-9%	1.11	1.12	0.95	1.13
4.08	$3.10E{-}01$ +/-5%	$2.77E{-}01$ +/-8%	1.12	1.12	0.96	1.14
5.18	$2.91E{-}01$ +/-5%	$2.58E{-}01$ +/-8%	1.13	1.11	0.96	1.15
6.23	$2.76E{-}01$ +/-5%	$2.42E{-}01$ +/-8%	1.14	1.10	0.97	1.16
7.85	$2.55E{-}01$ +/-5%	$2.21E{-}01$ +/-7%	1.15	1.09	0.98	1.18
9.95	$2.32E{-}01$ +/-5%	$1.99E{-}01$ +/-7%	1.16	1.08	0.99	1.19
12.05	$2.13E{-}01$ +/-5%	$1.82E{-}01$ +/-6%	1.18	1.08	1.00	1.20
15.17	$1.92E{-}01$ +/-5%	$1.62E{-}01$ +/-6%	1.19	1.06	1.01	1.22
19.27	$1.69E{-}01$ +/-5%	$1.42E{-}01$ +/-6%	1.19	1.05	1.02	1.22
23.37	$1.52E{-}01$ +/-5%	$1.28E{-}01$ +/-6%	1.19	1.04	1.02	1.22
27.47	$1.38E{-}01$ +/-5%	$1.16E{-}01$ +/-6%	1.19	1.03	1.01	1.22
34.53	$1.19E{-}01$ +/-5%	$1.01E{-}01$ +/-6%	1.18	1.02	1.01	1.22
44.63	$9.77E{-}02$ +/-5%	$8.35E{-}02$ +/-6%	1.17	1.01	1.00	1.21
54.75	$8.10E{-}02$ +/-5%	$6.98E{-}02$ +/-6%	1.16	1.00	1.00	1.20
mean % diff. from E			11	6	3	13
mean χ^2			5.23	1.83	0.53	7.07

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	$\mathbf{\%\Delta C^{nuc}}$
Zn63	38.41m	1.18	5%	6%

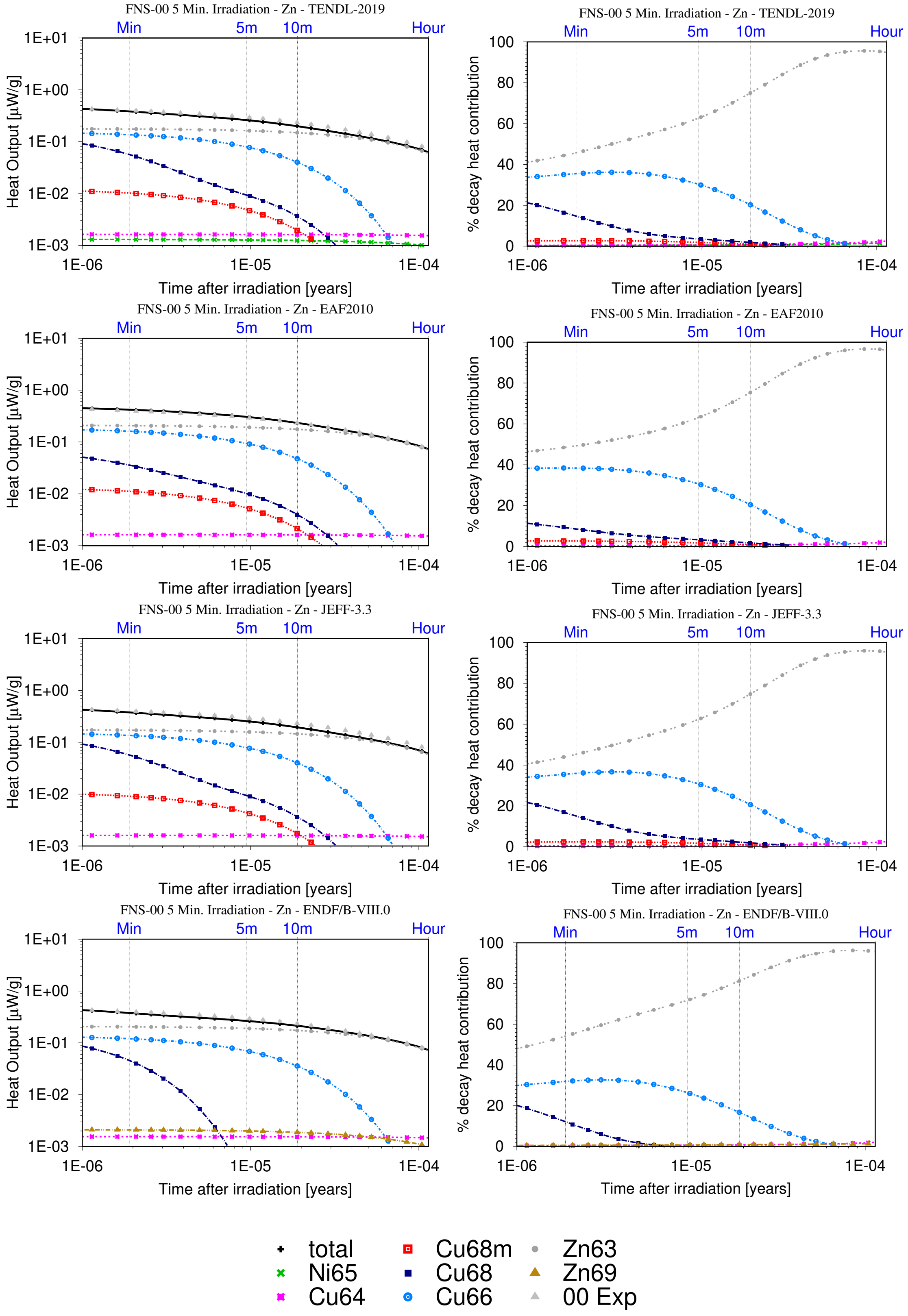


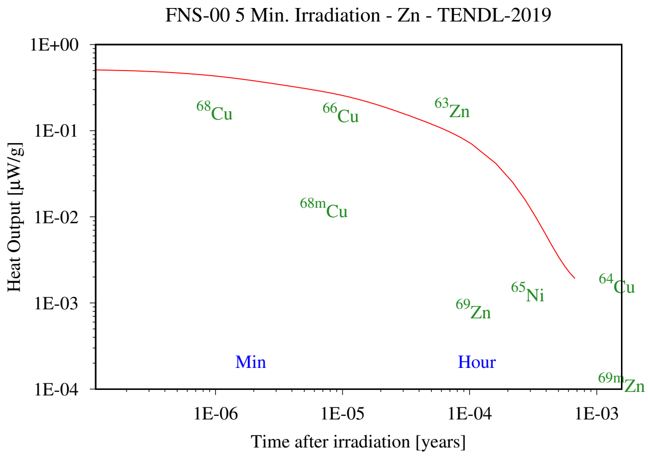
Zinc, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Cu68	31.10s	Zn68(n,p)Cu68	89.3
		Zn68(n,p)Cu68m(IT)Cu68	10.7
Cu68m	3.75m	Zn68(n,p)Cu68m	100.0
Cu66	5.10m	Zn66(n,p)Cu66	95.1
		Zn67(n,np)Cu66	3.6
		Zn67(n,d)Cu66	1.3
Zn63	38.41m	Zn64(n,2n)Zn63	100.0
Zn69	56.41m	Zn70(n,2n)Zn69	88.0
		Zn68(n,γ)Zn69	11.5
Ni65	2.52h	Zn68(n,α)Ni65	100.0
Cu64	12.70h	Zn64(n,p)Cu64	100.0

Comments on Zinc 5-minute experiments:

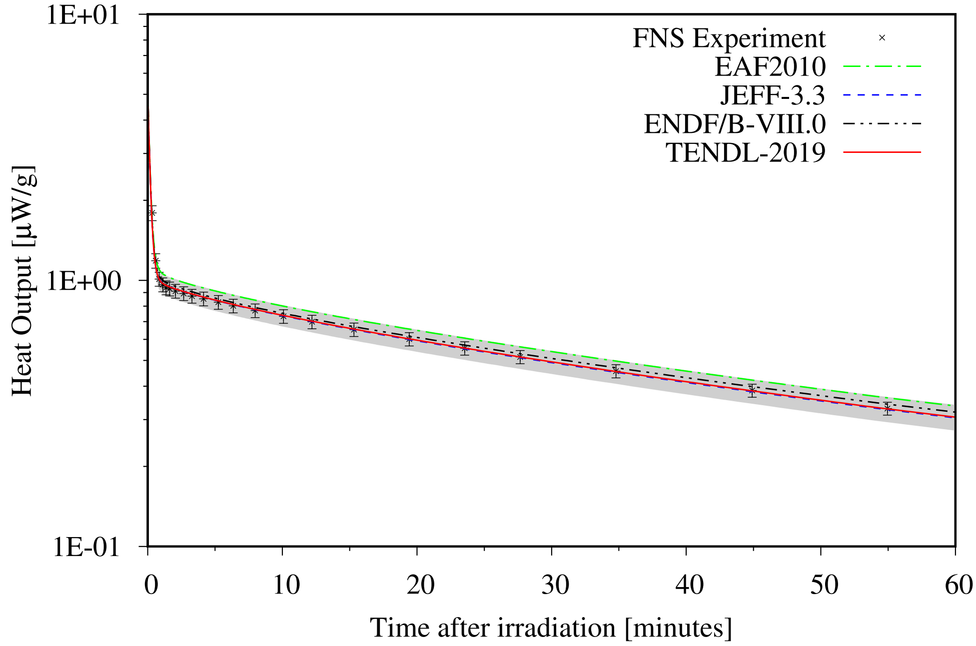
Both ENDF/B-VIII.0 and EAF2010 show remarkable agreement with the experiment, especially at cooling time beyond around 20 minutes where Zn63 (via (n,2n) reactions on Zn64) is particularly dominant. However, all libraries considered show very good agreement, with the short-term contribution from Cu66 ($\sim$30%) also well captured.


FNS-00 5 Min. Irradiation - Zn - TENDL-2019
FNS-00 5 Min. Irradiation - Zn - EAF2010
FNS-00 5 Min. Irradiation - Zn - JEFF-3.3
FNS-00 5 Min. Irradiation - Zn - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Ni65
Cu64
Cu68m
Cu68
Cu66
Zn63
Zn69
00 Exp


FNS-00 5 Min. Irradiation - Zn - TENDL-2019
1E+00
1E-01
1E-02
1E-03
1E-04
Heat Output [µW/g]
68Cu
66Cu
63Zn
68mCu
64Cu
65Ni
69Zn
69mZn
Min
Hour
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

Gallium

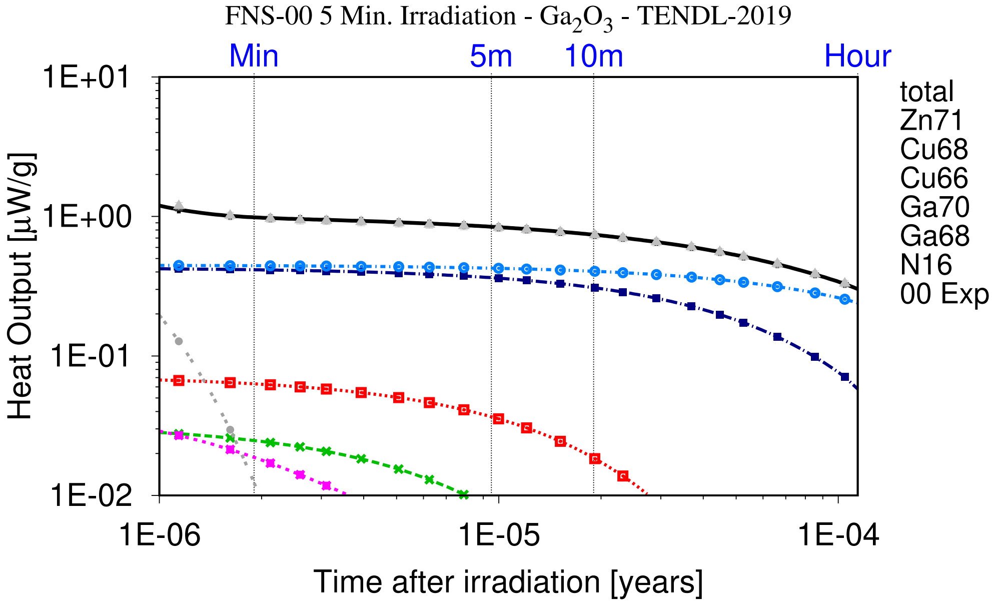
FNS-00 5 Min. Irradiation - Ga_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	µW/g	µW/g	E/C	E/C	E/C	E/C
0.33	1.79E+00 +/-6%	1.62E+00 +/-5%	1.11	1.08	1.05	1.11
0.60	1.19E+00 +/-6%	1.12E+00 +/-8%	1.06	1.02	0.97	1.05
0.85	1.01E+00 +/-6%	1.01E+00 +/-8%	1.00	0.97	0.92	1.00
1.12	9.63E−01 +/-6%	9.74E−01 +/-9%	0.99	0.96	0.91	0.99
1.37	9.39E−01 +/-6%	9.57E−01 +/-9%	0.98	0.96	0.90	0.98
1.63	9.29E−01 +/-6%	9.45E−01 +/-9%	0.98	0.96	0.91	0.98
2.07	9.12E−01 +/-6%	9.29E−01 +/-9%	0.98	0.96	0.91	0.98
2.67	8.92E−01 +/-6%	9.09E−01 +/-9%	0.98	0.96	0.91	0.98
3.28	8.73E−01 +/-6%	8.90E−01 +/-9%	0.98	0.96	0.91	0.98
4.15	8.53E−01 +/-6%	8.66E−01 +/-9%	0.99	0.97	0.91	0.99
5.25	8.28E−01 +/-6%	8.38E−01 +/-9%	0.99	0.97	0.91	0.99
6.35	8.02E−01 +/-6%	8.12E−01 +/-9%	0.99	0.97	0.91	0.99
7.98	7.70E−01 +/-6%	7.78E−01 +/-9%	0.99	0.97	0.91	0.99
10.08	7.33E−01 +/-6%	7.38E−01 +/-9%	0.99	0.97	0.92	1.00
12.20	6.99E−01 +/-6%	7.03E−01 +/-9%	0.99	0.98	0.92	1.00
15.32	6.53E−01 +/-6%	6.56E−01 +/-9%	0.99	0.97	0.92	1.00
19.43	6.02E−01 +/-6%	6.03E−01 +/-10%	1.00	0.97	0.92	1.00
23.55	5.56E−01 +/-6%	5.57E−01 +/-10%	1.00	0.97	0.92	1.00
27.67	5.15E−01 +/-6%	5.16E−01 +/-10%	1.00	0.97	0.92	1.01
34.78	4.56E−01 +/-6%	4.55E−01 +/-10%	1.00	0.97	0.92	1.01
44.90	3.85E−01 +/-6%	3.84E−01 +/-11%	1.00	0.97	0.91	1.01
54.95	3.30E−01 +/-6%	3.29E−01 +/-11%	1.00	0.96	0.91	1.01
mean % diff. from E			2	3	9	2
mean χ^2			0.17	0.37	2.48	0.16

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$T_{1/2}$	E/C	%ΔE	%ΔC^{nuc}
Ga68	1.13h	1.00	6%	14%

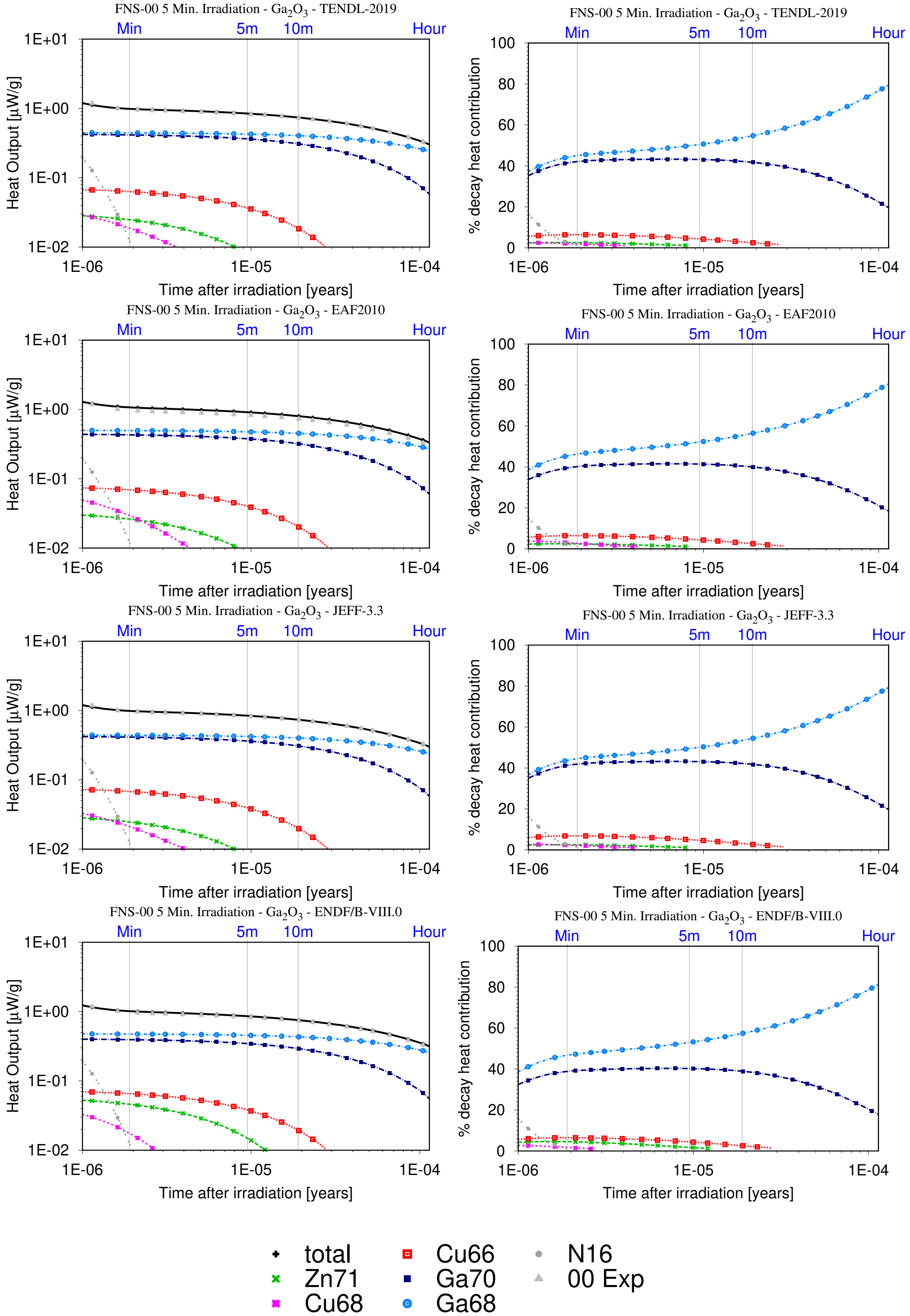


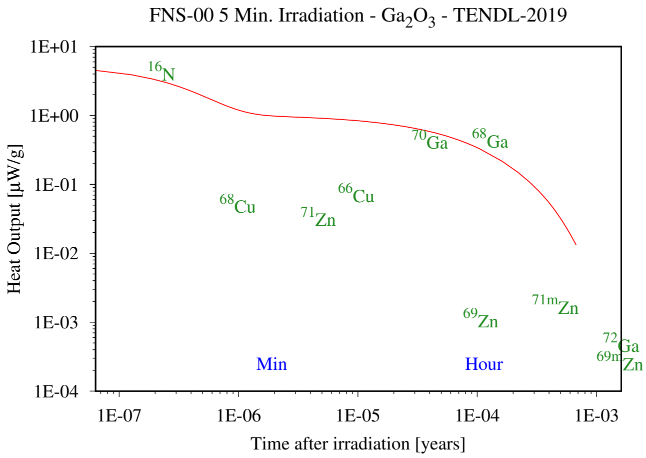
Gallium, TENDL-2019 5-minute pathway analysis

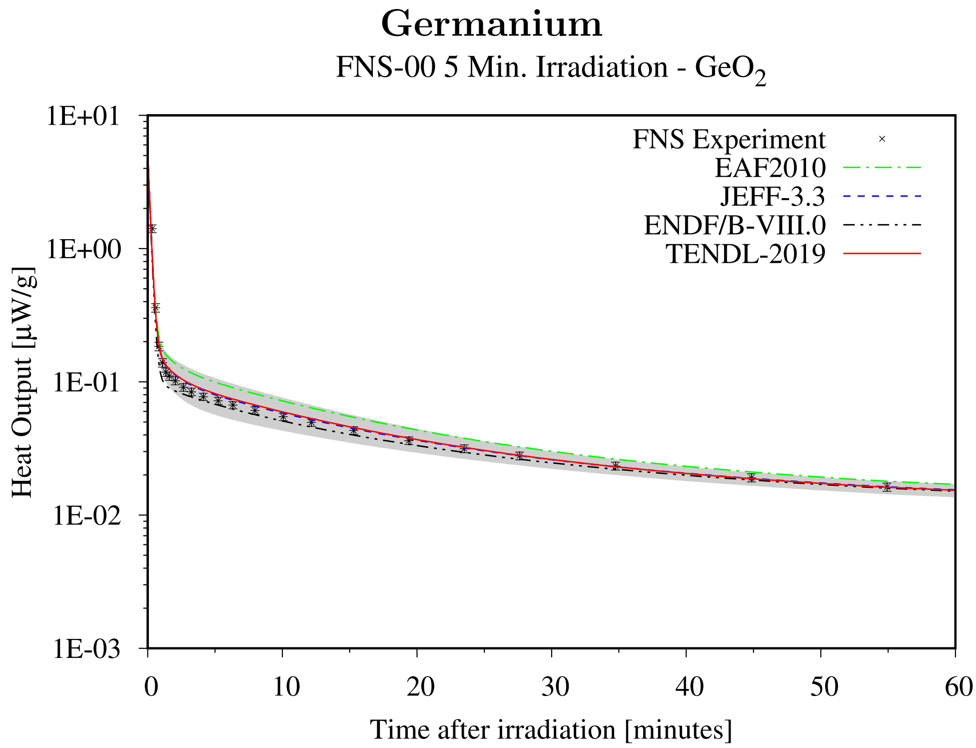
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Cu68	31.10s	Ga71(n,α)Cu68	85.1
		Ga71(n,α)Cu68m(IT)Cu68	14.9
Zn71	2.45m	Ga71(n,p)Zn71	100.0
Cu66	5.10m	Ga69(n,α)Cu66	100.0
Ga70	21.14m	Ga71(n,2n)Ga70	98.9
		Ga69(n,γ)Ga70	1.1
Ga68	1.13h	Ga69(n,2n)Ga68	100.0

Comments on Gallium 5-minute experiments:

All included libraries produce a very good simulation agreement to the experimental measurements, mostly within the experimental uncertainty, demonstrating that the (n,2n) reactions involved in producing the two equally dominant Ga70 and Ga68 nuclides are well evaluated in the libraries.


FNS-00 5 Min. Irradiation - Ga2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Ga2O3 - EAF2010
FNS-00 5 Min. Irradiation - Ga2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Ga2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Zn71
Cu68
Cu66
Ga70
Ga68
N16
00 Exp

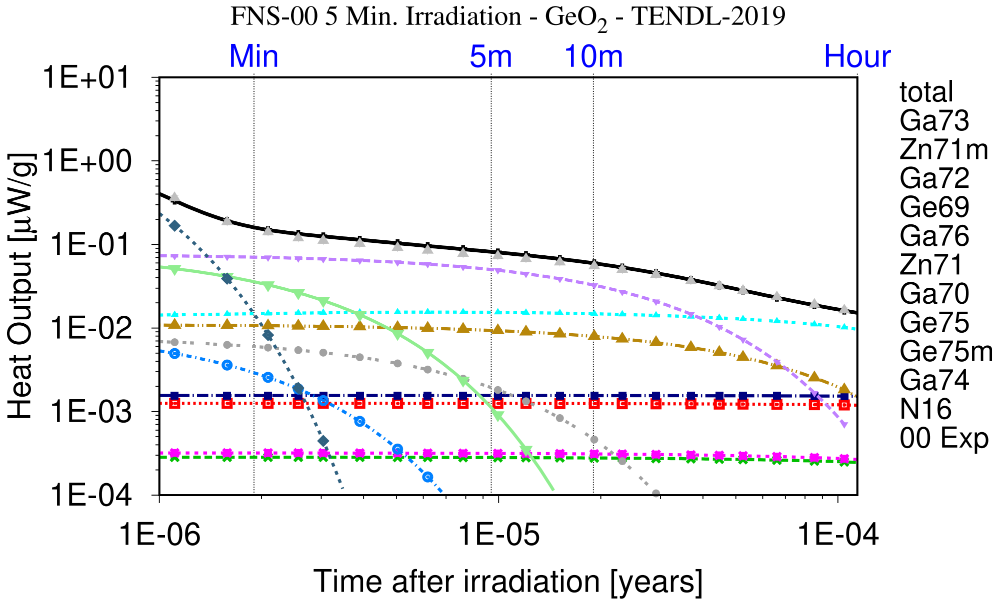

FNS-00 5 Min. Irradiation - Ga2O3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
16N
70Ga
68Ga
68Cu
66Cu
71Zn
69Zn
71mZn
72Ga
69mZn
Min
Hour
1E-07
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.33	1.41E+00 +/-7%	9.04E−01 +/-4%	1.56	1.71	1.53	1.56
0.58	3.60E−01 +/-7%	3.34E−01 +/-11%	1.08	1.34	1.00	1.08
0.83	1.84E−01 +/-7%	1.92E−01 +/-19%	0.96	1.34	0.84	0.97
1.10	1.39E−01 +/-7%	1.49E−01 +/-24%	0.93	1.35	0.79	0.94
1.35	1.18E−01 +/-7%	1.34E−01 +/-26%	0.88	1.26	0.74	0.89
1.60	1.11E−01 +/-7%	1.25E−01 +/-27%	0.89	1.23	0.74	0.89
2.05	1.02E−01 +/-7%	1.14E−01 +/-28%	0.90	1.19	0.74	0.91
2.65	9.09E−02 +/-7%	1.03E−01 +/-30%	0.88	1.12	0.72	0.89
3.25	8.42E−02 +/-6%	9.58E−02 +/-30%	0.88	1.09	0.72	0.89
4.13	7.73E−02 +/-6%	8.77E−02 +/-31%	0.88	1.07	0.72	0.90
5.23	7.21E−02 +/-6%	8.02E−02 +/-31%	0.90	1.08	0.74	0.92
6.33	6.69E−02 +/-6%	7.43E−02 +/-30%	0.90	1.07	0.74	0.92
7.97	6.09E−02 +/-6%	6.71E−02 +/-29%	0.91	1.07	0.75	0.93
10.07	5.47E−02 +/-6%	5.94E−02 +/-28%	0.92	1.08	0.76	0.94
12.17	4.96E−02 +/-6%	5.30E−02 +/-26%	0.93	1.08	0.78	0.95
15.30	4.32E−02 +/-7%	4.54E−02 +/-24%	0.95	1.08	0.80	0.97
19.40	3.62E−02 +/-7%	3.78E−02 +/-21%	0.96	1.07	0.81	0.97
23.50	3.15E−02 +/-7%	3.23E−02 +/-18%	0.98	1.06	0.83	0.99
27.62	2.78E−02 +/-7%	2.81E−02 +/-16%	0.99	1.06	0.85	1.00
34.75	2.34E−02 +/-7%	2.31E−02 +/-13%	1.01	1.06	0.89	1.01
44.85	1.91E−02 +/-7%	1.88E−02 +/-12%	1.02	1.04	0.90	1.01
54.92	1.63E−02 +/-7%	1.62E−02 +/-11%	1.01	1.02	0.91	1.00
mean % diff. from E			9	12	27	8
mean χ^2			3.09	5.20	19.02	2.59

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	**$T_{1/2}$**	**E/C**	**%ΔE**	**%ΔC^{nuc}**
N16	7.13s	1.56	7%	-

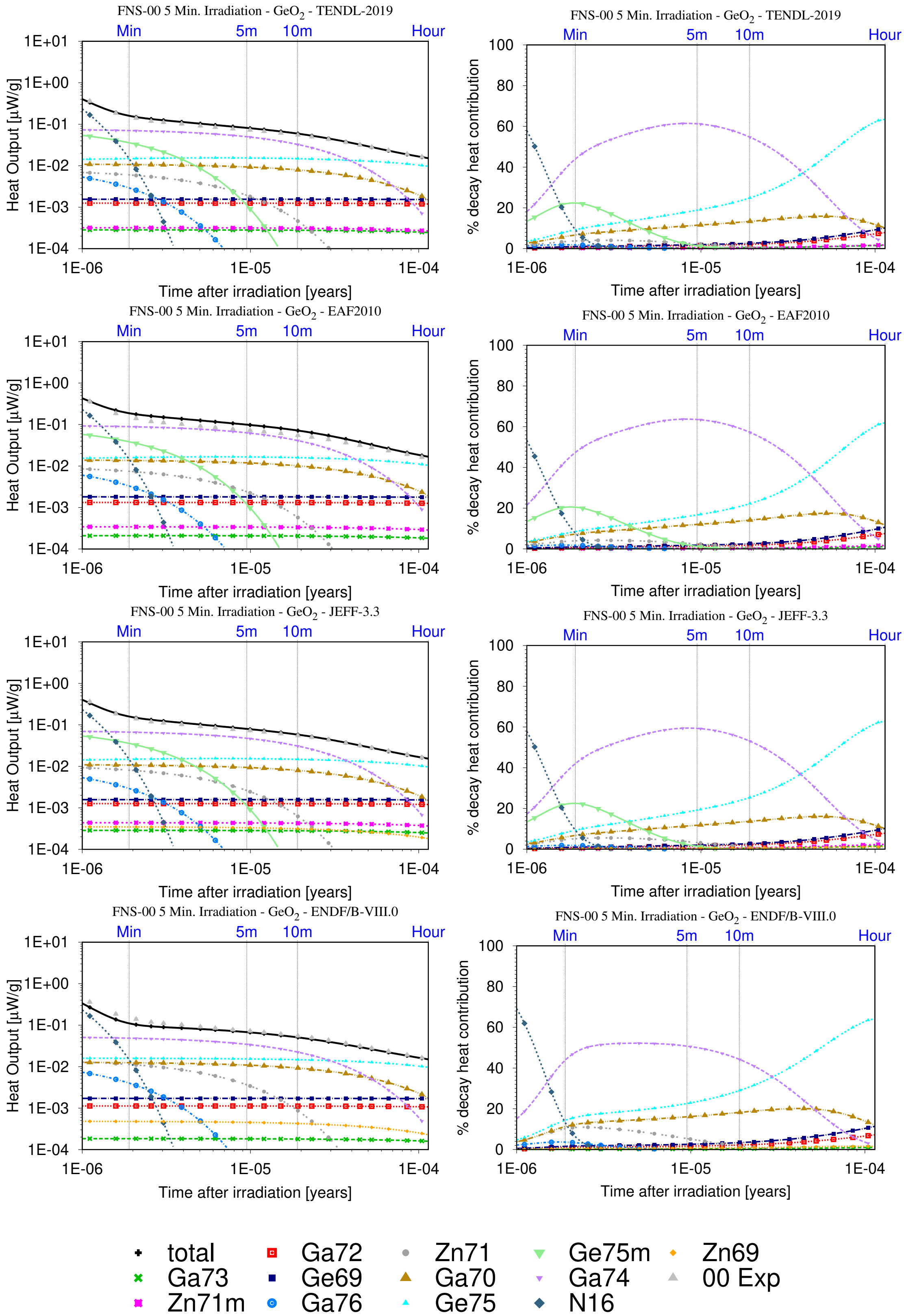


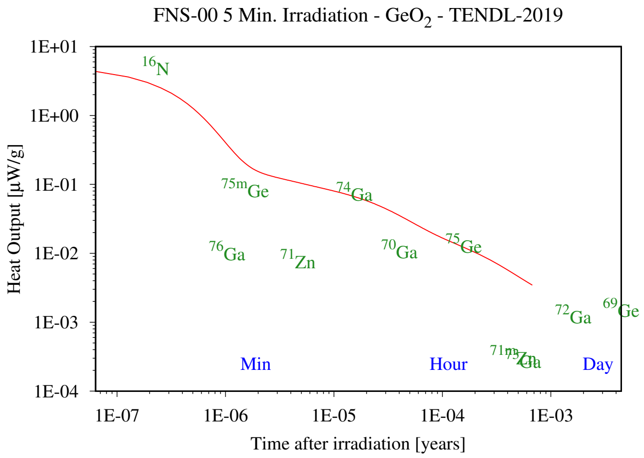
Germanium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ga76	32.60s	Ge76(n,p)Ga76	100.0
Ge75m	48.00s	Ge76(n,2n)Ge75m	99.6
Zn71	2.45m	Ge74(n,α)Zn71	100.0
Ga74	8.12m	Ge74(n,p)Ga74	81.0
		Ge74(n,p)Ga74m(IT)Ga74	19.0
Ga70	21.14m	Ge70(n,p)Ga70	100.0
Zn69	56.41m	Ge72(n,α)Zn69	93.7
		Ge73(n,nα)Zn69	6.1
Ge75	1.38h	Ge76(n,2n)Ge75m(IT)Ge75	66.1
		Ge76(n,2n)Ge75	33.1
Zn71m	3.96h	Ge74(n,α)Zn71m	100.0
Ga73	4.86h	Ge73(n,p)Ga73	67.8
		Ge74(n,np)Ga73	14.4
		Ge74(n,d)Ga73	13.6
		Ge76(n,α)Zn73(β^-)Ga73	4.0
Ga72	14.10h	Ge72(n,p)Ga72	94.7
		Ge73(n,np)Ga72	3.6
		Ge73(n,d)Ga72	1.7
Ge69	1.63d	Ge70(n,2n)Ge69	100.0

Comments on Germanium 5-minute experiments:

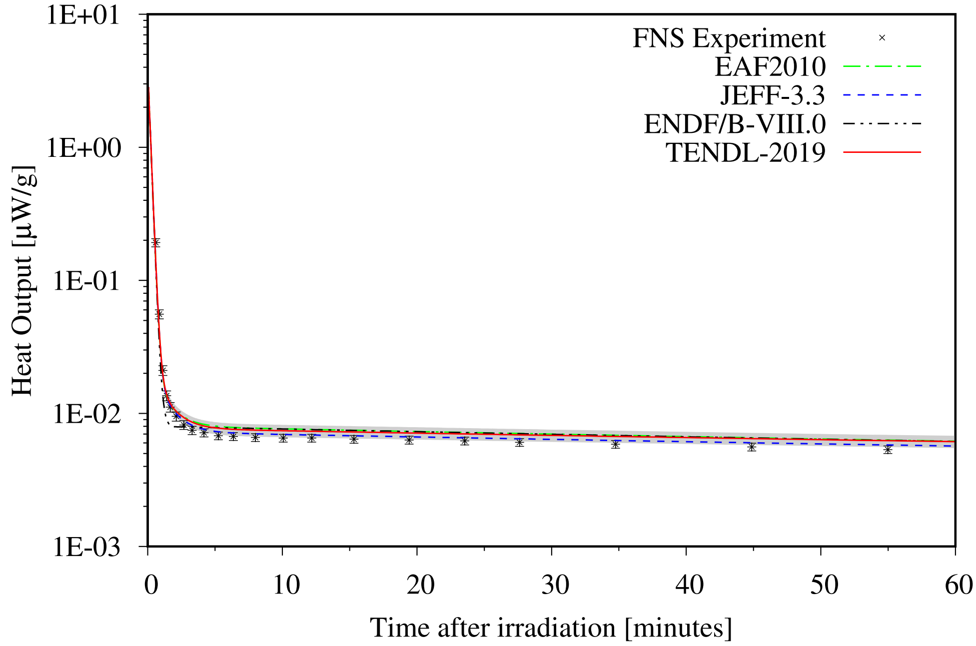
A good agreement for most libraries, although there appears to be an underprediction of the short-lived N16 nuclide from O16, which dominates the very first cooling step. EAF2010 predictions seem to be too high in general, despite showing a near-identical nuclide contribution profile to the others. TENDL-2019 nicely follows the profile, particularly beyond 20 minutes of cooling where Ge75 (from (n,2n) reactions on Ge76) dominates.


FNS-00 5 Min. Irradiation - GeO2 - TENDL-2019
FNS-00 5 Min. Irradiation - GeO2 - EAF2010
FNS-00 5 Min. Irradiation - GeO2 - JEFF-3.3
FNS-00 5 Min. Irradiation - GeO2 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Ga73
Zn71m
Ga72
Ge69
Ga76
Zn71
Ga70
Ge75
Ge75m
Ga74
N16
Zn69
00 Exp


FNS-00 5 Min. Irradiation - GeO2 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
Time after irradiation [years]
1E-07
1E-06
1E-05
1E-04
1E-03
16N
75mGe
74Ga
76Ga
71Zn
70Ga
75Ge
72Ga
69Ge
Min
Hour
Day

Arsenic

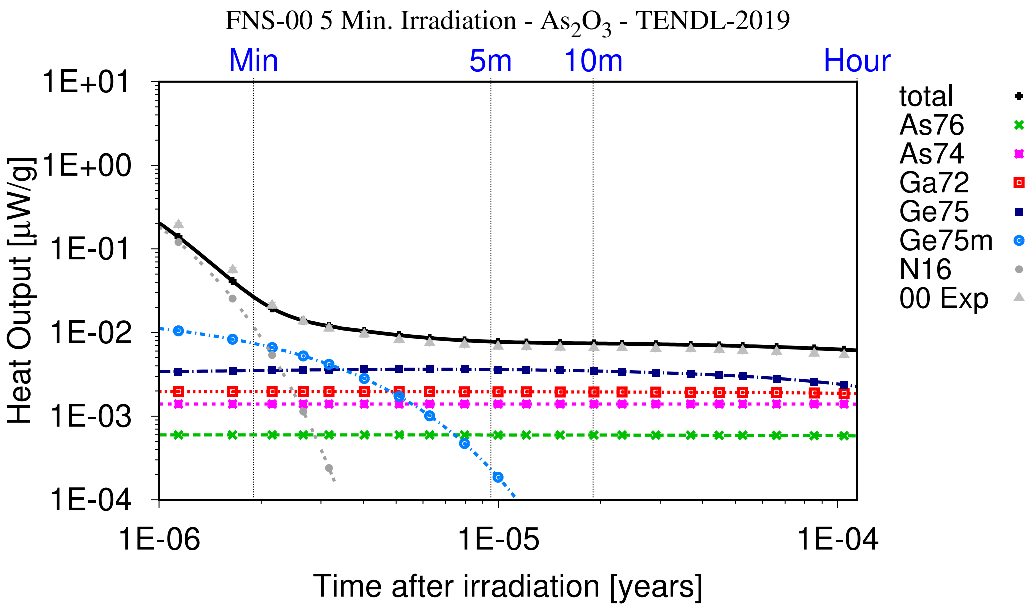
FNS-00 5 Min. Irradiation - As_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	1.92$E-$01 +/-7%	1.39$E-$01 +/-2%	1.39	1.50	1.42	1.39
0.87	5.56$E-$02 +/-8%	4.13$E-$02 +/-4%	1.35	1.67	1.39	1.36
1.13	2.11$E-$02 +/-8%	1.94$E-$02 +/-8%	1.08	1.58	1.11	1.11
1.40	1.36$E-$02 +/-9%	1.39$E-$02 +/-9%	0.98	1.50	1.00	1.01
1.67	1.12$E-$02 +/-8%	1.19$E-$02 +/-9%	0.93	1.36	0.95	0.97
2.12	9.50$E-$03 +/-8%	1.04$E-$02 +/-9%	0.91	1.20	0.92	0.96
2.68	8.19$E-$03 +/-8%	9.31$E-$03 +/-9%	0.88	1.04	0.87	0.92
3.30	7.47$E-$03 +/-7%	8.60$E-$03 +/-10%	0.87	0.95	0.85	0.92
4.18	7.16$E-$03 +/-7%	8.05$E-$03 +/-10%	0.89	0.91	0.87	0.94
5.25	6.79$E-$03 +/-7%	7.74$E-$03 +/-11%	0.88	0.87	0.85	0.93
6.37	6.71$E-$03 +/-7%	7.59$E-$03 +/-11%	0.88	0.86	0.86	0.94
8.00	6.60$E-$03 +/-7%	7.49$E-$03 +/-11%	0.88	0.86	0.85	0.94
10.07	6.53$E-$03 +/-7%	7.41$E-$03 +/-11%	0.88	0.85	0.85	0.94
12.18	6.52$E-$03 +/-7%	7.34$E-$03 +/-11%	0.89	0.86	0.86	0.95
15.32	6.40$E-$03 +/-7%	7.25$E-$03 +/-11%	0.88	0.86	0.86	0.94
19.42	6.31$E-$03 +/-7%	7.13$E-$03 +/-11%	0.89	0.86	0.86	0.95
23.55	6.21$E-$03 +/-7%	7.01$E-$03 +/-11%	0.89	0.87	0.86	0.95
27.62	6.06$E-$03 +/-7%	6.90$E-$03 +/-11%	0.88	0.86	0.86	0.94
34.75	5.87$E-$03 +/-7%	6.71$E-$03 +/-11%	0.87	0.86	0.86	0.94
44.87	5.60$E-$03 +/-7%	6.47$E-$03 +/-10%	0.87	0.86	0.85	0.93
54.98	5.34$E-$03 +/-7%	6.24$E-$03 +/-10%	0.86	0.85	0.85	0.92
mean % diff. from E			14	19	16	8
mean χ^2			4.40	8.14	5.94	2.12

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	1.39	7%	-

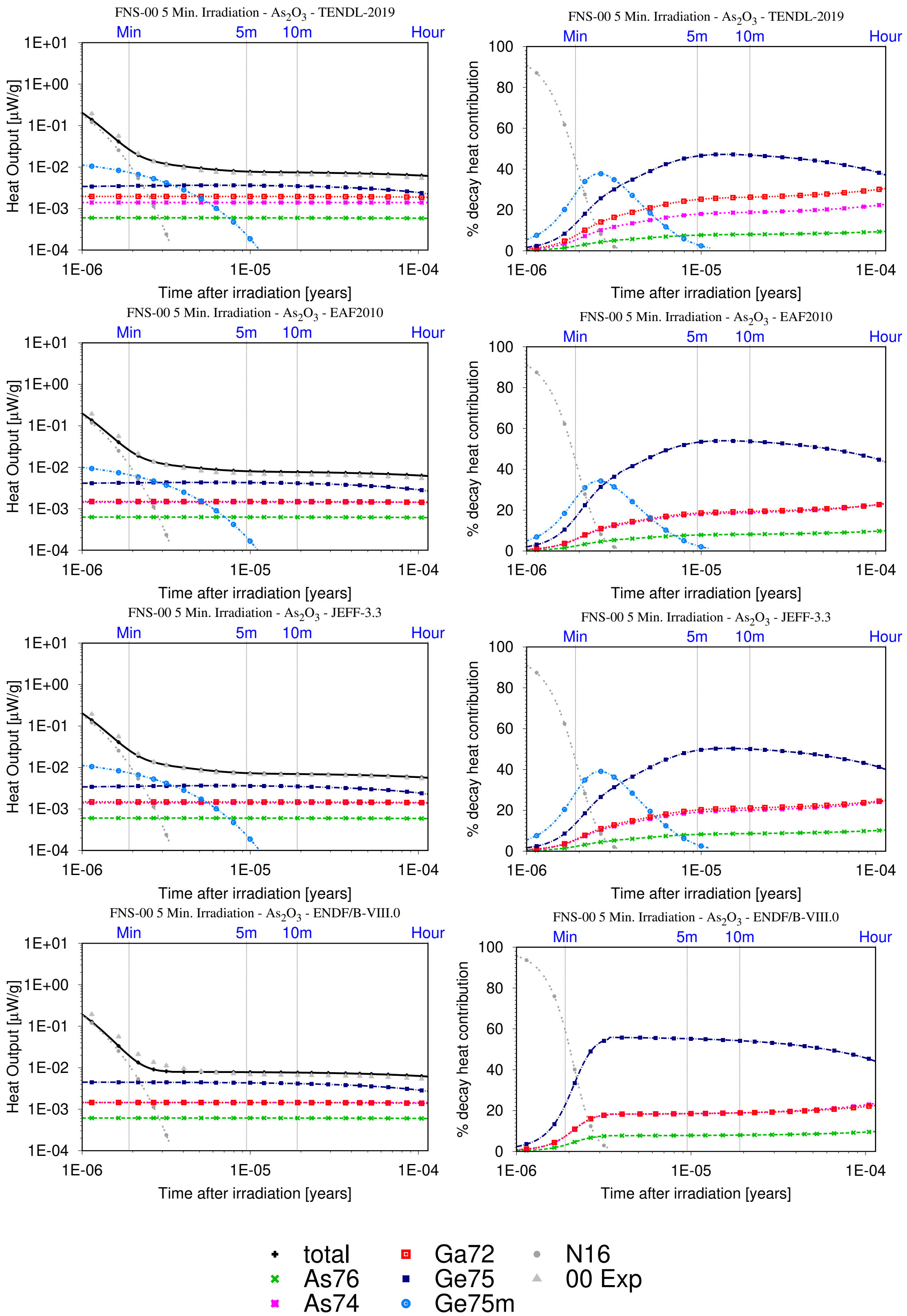


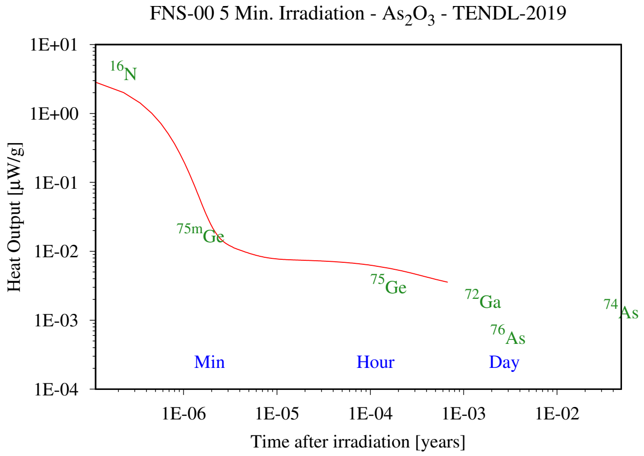
Arsenic, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ge75m	48.00s	As75(n,p)Ge75m	100.0
Ge75	1.38h	As75(n,p)Ge75m(IT)Ge75	57.3
		As75(n,p)Ge75	42.7
Ga72	14.10h	As75(n,α)Ga72	100.0
As76	1.09d	As75(n,γ)As76	100.0
As74	17.78d	As75(n,2n)As74	100.0

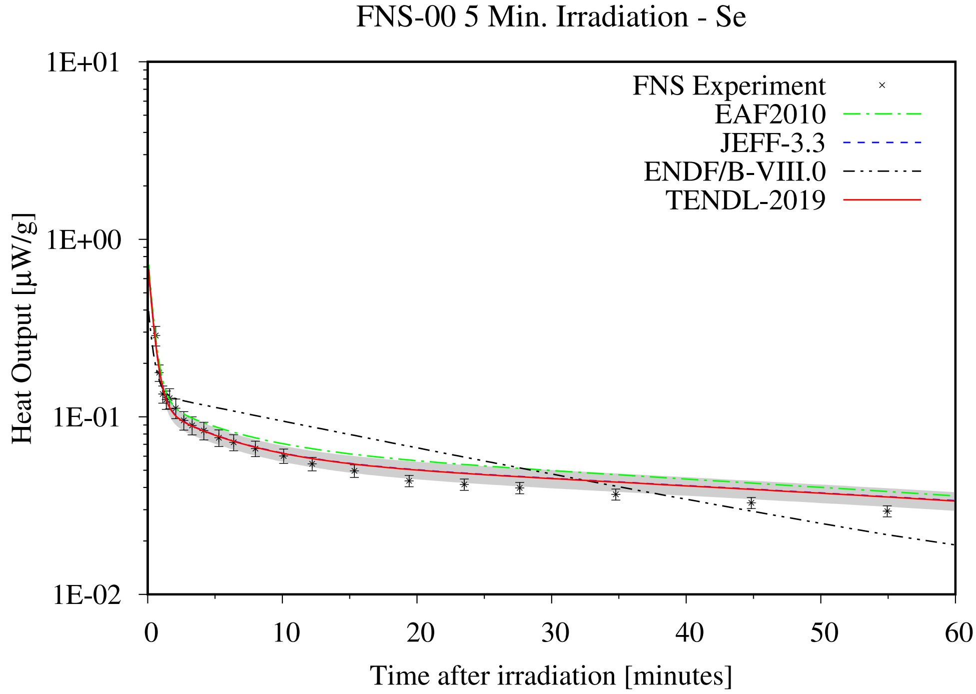
Comments on Arsenic 5-minute experiments:

There is good agreement with all libraries, although there is an apparent and systematic overprediction once the short-lived N16 from oxygen has faded away (after about 1 minute of cooling). Since the quoted experimental uncertainties are relatively small – smaller than the overprediction by the libraries – it could indicate a need for slight revision of the (n,p) channel cross section that produces the Ge75 nuclide from As75 – this nuclides contributes 40-50% of the predicted decay-heat with all libraries. However, it is difficult to be definitive about this need as there are also several minor contributing nuclides: Ga72, As74, and As76.

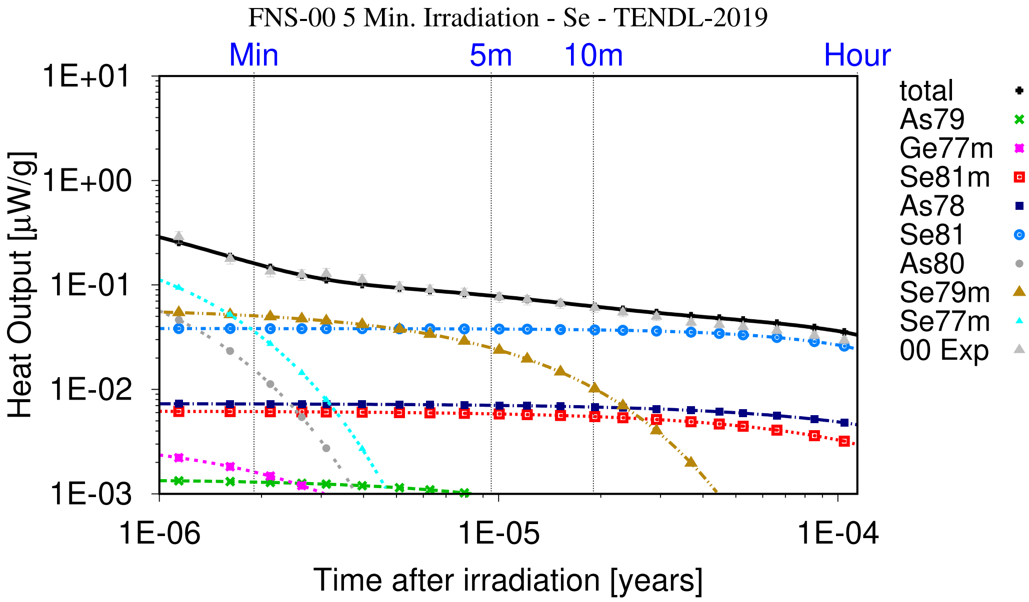

FNS-00 5 Min. Irradiation - As2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - As2O3 - EAF2010
FNS-00 5 Min. Irradiation - As2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - As2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
As76
As74
Ga72
Ge75
Ge75m
N16
00 Exp


FNS-00 5 Min. Irradiation - As2O3 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
16N
75mGe
75Ge
72Ga
76As
74As
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

Selenium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	2.87E−01 +/-13%	2.56E−01 +/-10%	1.12	1.49	1.03	1.11
0.85	1.77E−01 +/-11%	1.87E−01 +/-9%	0.95	1.10	0.87	0.94
1.12	1.34E−01 +/-11%	1.47E−01 +/-9%	0.92	0.93	0.83	0.91
1.38	1.25E−01 +/-12%	1.25E−01 +/-10%	1.00	0.92	0.91	0.99
1.63	1.28E−01 +/-13%	1.13E−01 +/-11%	1.13	0.97	1.02	1.12
2.08	1.12E−01 +/-13%	1.01E−01 +/-11%	1.10	0.88	1.00	1.10
2.68	9.56E−02 +/-12%	9.37E−02 +/-11%	1.02	0.78	0.92	1.02
3.30	8.95E−02 +/-12%	8.87E−02 +/-11%	1.01	0.74	0.91	1.01
4.17	8.37E−02 +/-11%	8.32E−02 +/-11%	1.01	0.72	0.90	1.00
5.28	7.63E−02 +/-11%	7.75E−02 +/-10%	0.98	0.68	0.88	0.98
6.38	7.18E−02 +/-10%	7.29E−02 +/-10%	0.99	0.67	0.88	0.98
8.00	6.63E−02 +/-10%	6.74E−02 +/-10%	0.98	0.65	0.87	0.98
10.10	6.03E−02 +/-9%	6.21E−02 +/-10%	0.97	0.64	0.85	0.97
12.22	5.44E−02 +/-9%	5.82E−02 +/-11%	0.93	0.62	0.82	0.93
15.35	4.96E−02 +/-8%	5.41E−02 +/-11%	0.92	0.63	0.81	0.91
19.42	4.36E−02 +/-7%	5.06E−02 +/-11%	0.86	0.64	0.76	0.86
23.52	4.16E−02 +/-7%	4.80E−02 +/-12%	0.87	0.70	0.77	0.86
27.63	3.98E−02 +/-7%	4.60E−02 +/-12%	0.87	0.77	0.78	0.86
34.77	3.66E−02 +/-7%	4.29E−02 +/-12%	0.85	0.90	0.77	0.85
44.83	3.28E−02 +/-7%	3.90E−02 +/-12%	0.84	1.11	0.77	0.84
54.93	2.95E−02 +/-7%	3.54E−02 +/-12%	0.83	1.36	0.77	0.83
mean % diff. from E			8	32	17	9
mean χ^2			1.90	17.87	6.28	1.99

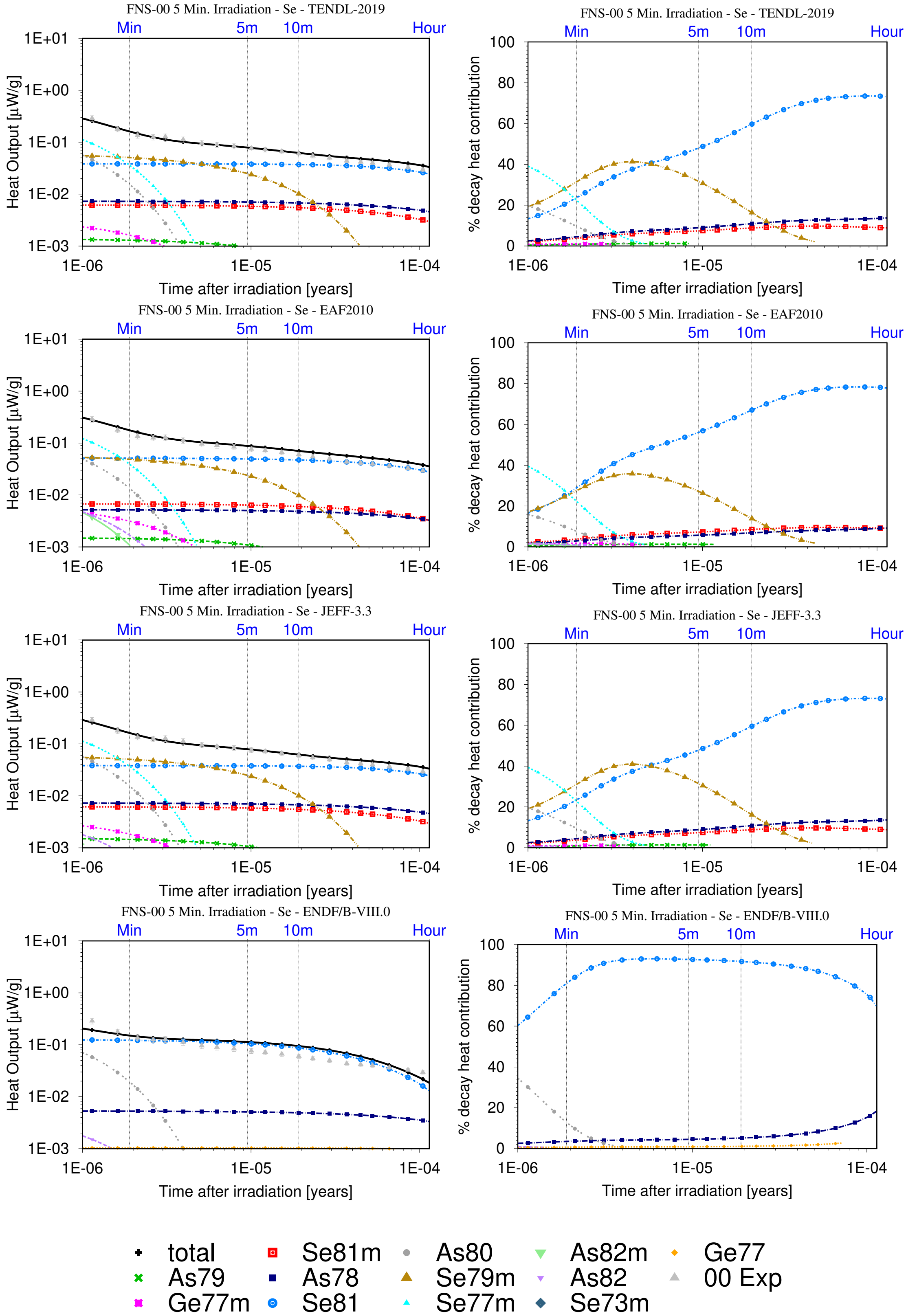


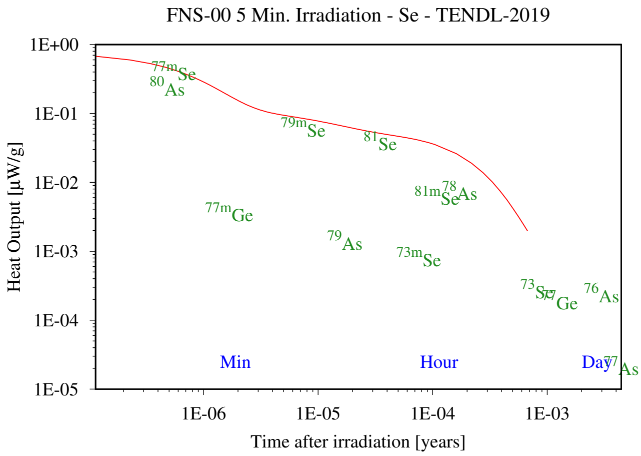
Selenium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
As82m	13.60s	Se82(n,p)As82m	100.0
As80	15.20s	Se80(n,p)As80	100.0
Se77m	17.36s	Se78(n,2n)Se77m	87.2
		Se77(n,n′)Se77m	12.6
As82	19.10s	Se82(n,p)As82	100.0
Ge77m	52.91s	Se80(n,α)Ge77m	100.0
Se79m	3.90m	Se80(n,2n)Se79m	99.5
As79	9.01m	Se80(n,d)As79	75.5
		Se80(n,np)As79	14.6
		Se82(n,α)Ge79(β^-)As79	5.8
		Se82(n,α)Ge79m(β^-)As79	3.9
Se81	18.39m	Se82(n,2n)Se81	88.9
		Se82(n,2n)Se81m(IT)Se81	8.6
		Se80(n,γ)Se81	2.5
Se73m	39.79m	Se74(n,2n)Se73m	100.0
Se81m	57.28m	Se82(n,2n)Se81m	99.0
		Se80(n,γ)Se81m	1.0
As78	1.51h	Se78(n,p)As78	100.0
Ge77	11.30h	Se80(n,α)Ge77	97.7
		Se80(n,α)Ge77m(IT)Ge77	2.3

Comments on Selenium 5-minute experiments:

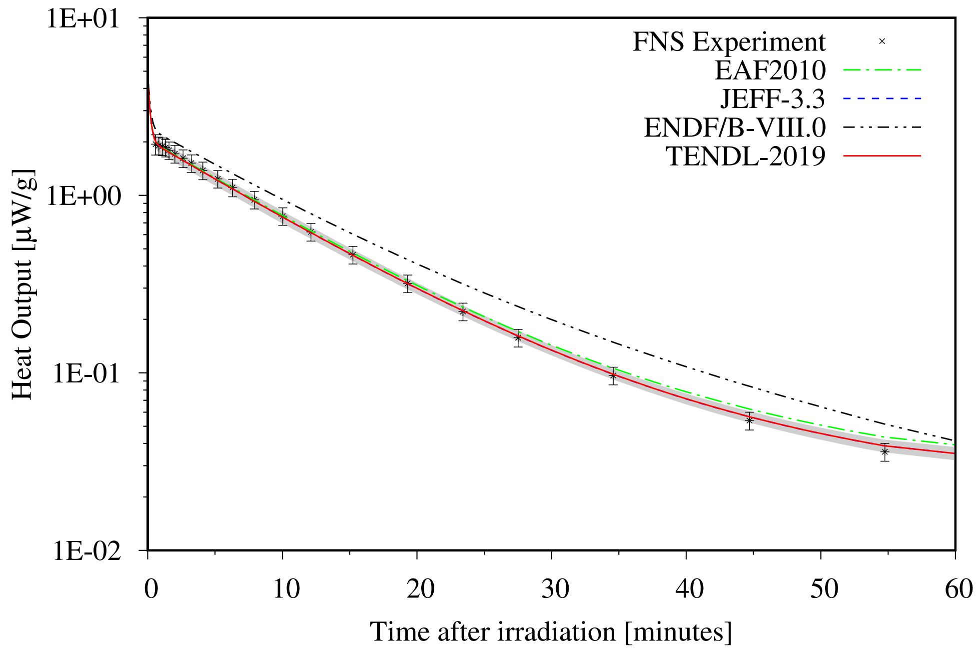
A good agreement between simulation and experiment for TENDL-2019, JEFF-3.3 and EAF2010. TENDL-2019 is almost within the experimental uncertainties, JEFF-3.3 is slightly more outside, and EAF2010 produces the correct decay profile, but generally overpredicts by 15-30% (of the experiment). At short cooling times (less than around 1 minute) there are a complex set of important radionuclides and associated reaction pathways, but the majority of the decay cooling is dominated by Se81 (via (n,2n) reactions on Se82). ENDF/B-VIII.0 completely omits the various metastable nuclides that are predicted by the other libraries to be important during the first few minutes of cooling – particularly the Se79m whose decay profile is required to properly match the experimental shape between 1 and 10 minutes of cooling. Furthermore, ENDF/B-VIII/0 omits Se81m production and instead appears to combine its contribution via (n,2n) on Se82 into the Se81 production leading to an overprediction of that ground state nuclide and a complete misrepresentation of the profile.


FNS-00 5 Min. Irradiation - Se - TENDL-2019
FNS-00 5 Min. Irradiation - Se - EAF2010
FNS-00 5 Min. Irradiation - Se - JEFF-3.3
FNS-00 5 Min. Irradiation - Se - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Se81m
As80
As82m
Ge77
As79
As78
Se79m
As82
00 Exp
Ge77m
Se81
Se77m
Se73m


FNS-00 5 Min. Irradiation - Se - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
Min
Hour
Day
77mSe
80As
79mSe
81Se
81mSe
78As
77mGe
79As
73mSe
73Se
77Ge
76As
77As

Bromine

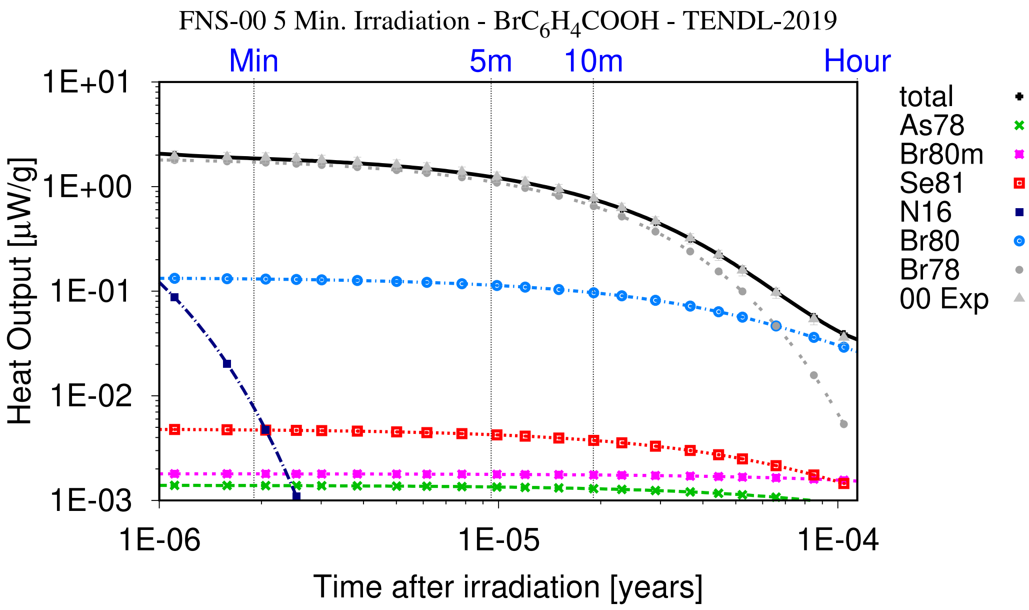
FNS-00 5 Min. Irradiation - BrC_6H_4COOH



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	$1.94E{+}00$ +/-13%	$2.02E{+}00$ +/-8%	0.96	0.82	0.95	0.96
0.83	$1.91E{+}00$ +/-11%	$1.90E{+}00$ +/-8%	1.00	0.85	0.99	1.00
1.08	$1.89E{+}00$ +/-11%	$1.84E{+}00$ +/-8%	1.03	0.87	1.02	1.02
1.33	$1.85E{+}00$ +/-11%	$1.79E{+}00$ +/-8%	1.04	0.88	1.03	1.03
1.58	$1.79E{+}00$ +/-11%	$1.75E{+}00$ +/-8%	1.03	0.87	1.02	1.03
2.02	$1.71E{+}00$ +/-11%	$1.67E{+}00$ +/-8%	1.03	0.86	1.01	1.02
2.63	$1.62E{+}00$ +/-11%	$1.57E{+}00$ +/-8%	1.03	0.87	1.02	1.03
3.23	$1.52E{+}00$ +/-11%	$1.48E{+}00$ +/-8%	1.03	0.86	1.01	1.03
4.10	$1.38E{+}00$ +/-11%	$1.35E{+}00$ +/-8%	1.02	0.85	1.01	1.02
5.20	$1.24E{+}00$ +/-11%	$1.21E{+}00$ +/-8%	1.02	0.84	1.01	1.02
6.30	$1.11E{+}00$ +/-11%	$1.09E{+}00$ +/-8%	1.02	0.83	1.00	1.02
7.92	$9.44E{-}01$ +/-11%	$9.27E{-}01$ +/-8%	1.02	0.82	1.00	1.02
10.03	$7.64E{-}01$ +/-11%	$7.54E{-}01$ +/-8%	1.01	0.81	0.99	1.01
12.13	$6.23E{-}01$ +/-11%	$6.16E{-}01$ +/-8%	1.01	0.79	0.99	1.01
15.25	$4.63E{-}01$ +/-11%	$4.60E{-}01$ +/-8%	1.01	0.77	0.98	1.01
19.32	$3.19E{-}01$ +/-11%	$3.18E{-}01$ +/-7%	1.00	0.73	0.97	1.00
23.42	$2.22E{-}01$ +/-11%	$2.24E{-}01$ +/-7%	0.99	0.70	0.94	0.99
27.52	$1.58E{-}01$ +/-11%	$1.62E{-}01$ +/-7%	0.97	0.67	0.92	0.98
34.58	$9.66E{-}02$ +/-11%	$9.84E{-}02$ +/-7%	0.98	0.65	0.91	0.98
44.70	$5.39E{-}02$ +/-11%	$5.67E{-}02$ +/-7%	0.95	0.64	0.86	0.95
54.75	$3.59E{-}02$ +/-11%	$3.89E{-}02$ +/-8%	0.92	0.70	0.82	0.92
mean % diff. from E			2	27	4	2
mean χ^2			0.07	7.15	0.36	0.07

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Br78	6.46m	0.96	13%	9%
Br80	17.60m	0.92	11%	11%

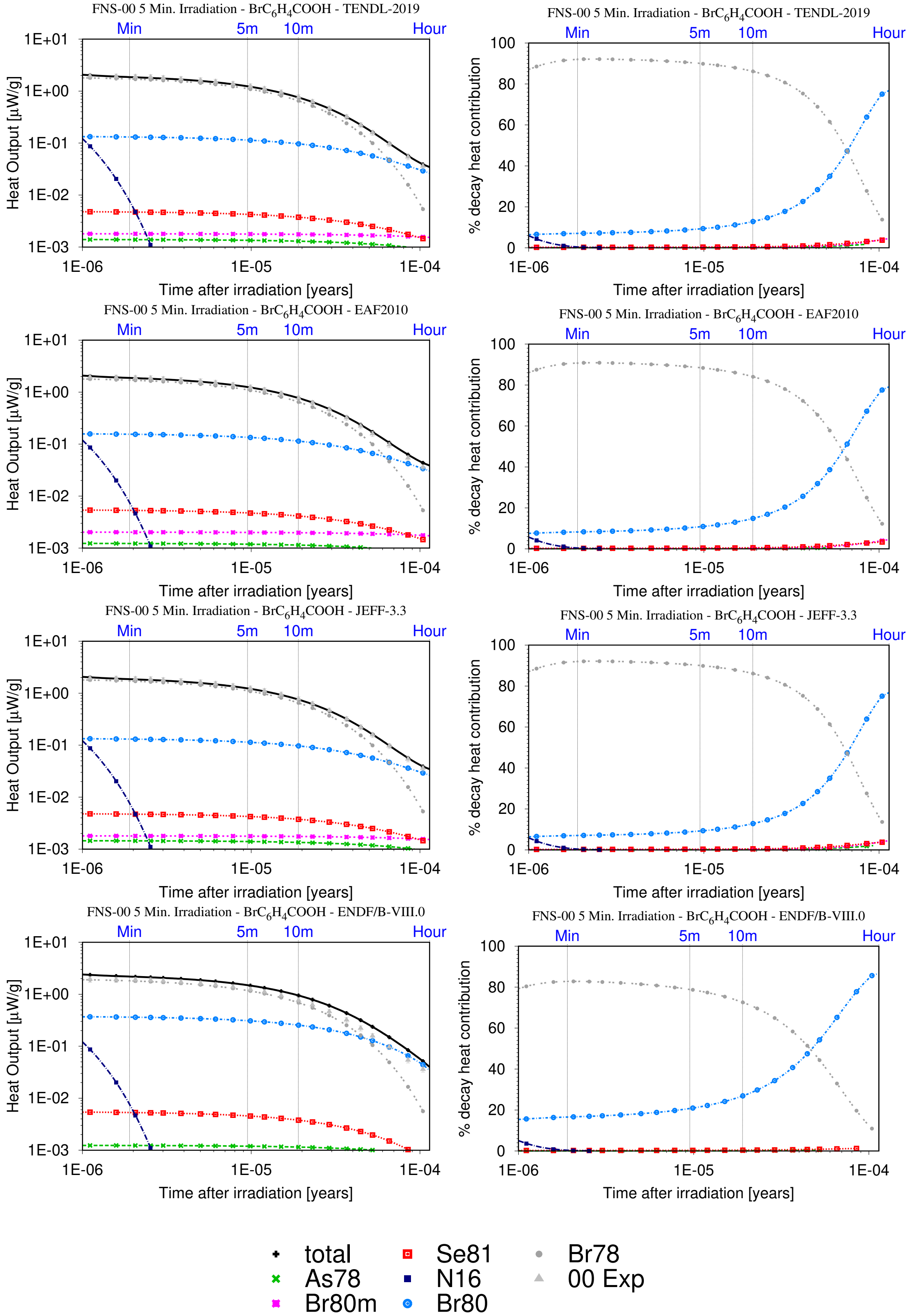


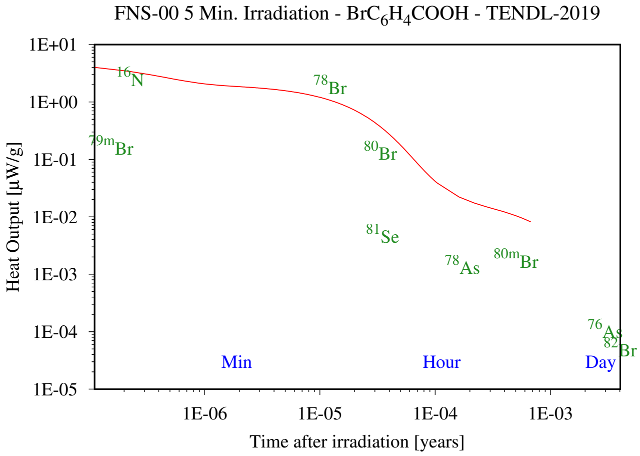
Bromine, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Br78	6.46m	Br79(n,2n)Br78	100.0
Br80	17.60m	Br81(n,2n)Br80	92.2
		Br79(n,γ)Br80	6.6
		Br81(n,2n)Br80m(IT)Br80	1.1
Se81	18.39m	Br81(n,p)Se81	97.3
		Br81(n,p)Se81m(IT)Se81	2.7
As78	1.51h	Br81(n,α)As78	100.0
Br80m	4.41h	Br81(n,2n)Br80m	99.0
		Br79(n,γ)Br80m	1.0

Comments on Bromine 5-minute experiments:

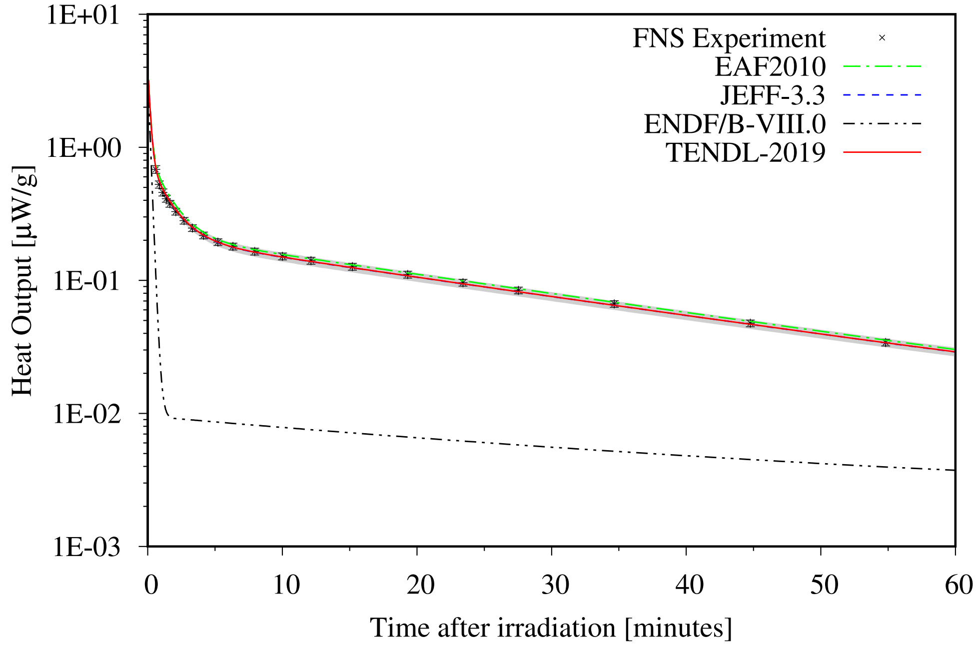
Similarly, to the case with selenium, for bromine, ENDF/B-VIII.0 combines the contributions from Br81(n,2n) to both Br80 and Br80m into simply the production of Br80, which has a much shorter half-life than its metastable and thus a completely different decay profile. This leads to a significant overprediction of Br80 with that library and, even though it contributes only around 10% of the decay heat before 10 minutes of cooling (only becoming dominant at around 1-hour of cooling), this leads to a dramatic and obvious overprediction of the decay heat by the ENDF/B-VIII.0 library calculations. The predictions get worse for that library at later cooling after the previously dominant Br78 (also from (n,2n) reactions) falls away leaving Br80 to dominate. The other libraries considered produce excellent agreement to the experiment (particularly TENDL-2019 and JEFF-3.3) – well within the experimental uncertainties. This result demonstrates again the need to populate all reaction channel cross sections to create a truly general purpose library.


FNS-00 5 Min. Irradiation - BrC6H4COOH - TENDL-2019
FNS-00 5 Min. Irradiation - BrC6H4COOH - EAF2010
FNS-00 5 Min. Irradiation - BrC6H4COOH - JEFF-3.3
FNS-00 5 Min. Irradiation - BrC6H4COOH - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
As78
Br80m
Se81
N16
Br80
Br78
00 Exp


FNS-00 5 Min. Irradiation - BrC6H4COOH - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
78Br
79mBr
80Br
81Se
78As
80mBr
76As
82Br
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

Rubidium

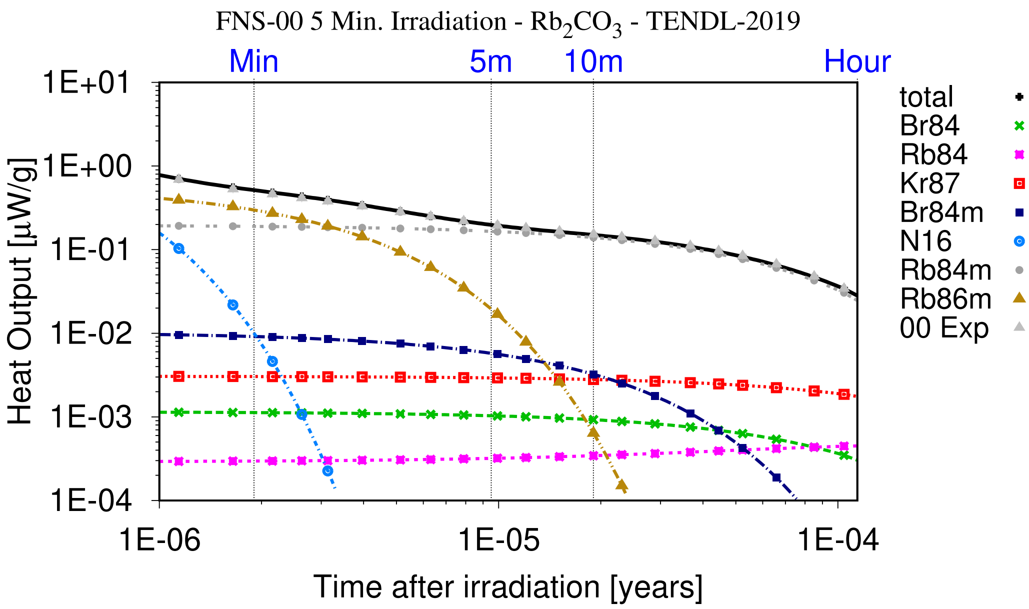
FNS-00 5 Min. Irradiation - Rb_2CO_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	6.83E−01 +/-7%	7.04E−01 +/-5%	0.97	6.09	0.89	0.97
0.87	5.26E−01 +/-6%	5.56E−01 +/-6%	0.95	16.92	0.86	0.95
1.13	4.58E−01 +/-6%	4.82E−01 +/-6%	0.95	32.97	0.87	0.95
1.38	4.11E−01 +/-6%	4.34E−01 +/-6%	0.95	39.74	0.87	0.95
1.65	3.77E−01 +/-6%	3.93E−01 +/-6%	0.96	39.82	0.88	0.96
2.08	3.29E−01 +/-6%	3.41E−01 +/-6%	0.97	35.95	0.90	0.97
2.70	2.81E−01 +/-6%	2.87E−01 +/-6%	0.98	31.08	0.91	0.98
3.32	2.47E−01 +/-6%	2.51E−01 +/-6%	0.99	27.70	0.93	0.99
4.15	2.18E−01 +/-6%	2.19E−01 +/-7%	1.00	24.80	0.95	1.00
5.22	1.94E−01 +/-6%	1.94E−01 +/-7%	1.00	22.53	0.96	1.00
6.33	1.80E−01 +/-6%	1.78E−01 +/-8%	1.01	21.38	0.97	1.02
7.95	1.65E−01 +/-6%	1.63E−01 +/-8%	1.01	20.21	0.97	1.01
10.02	1.52E−01 +/-6%	1.50E−01 +/-8%	1.01	19.32	0.97	1.01
12.13	1.41E−01 +/-6%	1.39E−01 +/-8%	1.01	18.65	0.97	1.02
15.20	1.27E−01 +/-6%	1.25E−01 +/-8%	1.02	17.76	0.97	1.02
19.32	1.11E−01 +/-6%	1.08E−01 +/-8%	1.02	16.65	0.97	1.02
23.42	9.62E−02 +/-6%	9.43E−02 +/-8%	1.02	15.52	0.97	1.02
27.53	8.40E−02 +/-6%	8.22E−02 +/-8%	1.02	14.49	0.97	1.02
34.65	6.65E−02 +/-6%	6.50E−02 +/-8%	1.02	12.81	0.97	1.02
44.77	4.76E−02 +/-6%	4.68E−02 +/-8%	1.02	10.57	0.97	1.02
54.82	3.41E−02 +/-6%	3.40E−02 +/-8%	1.00	8.62	0.96	1.00
mean % diff. from E			2	94	7	2
mean χ^2			0.23	256.24	1.97	0.21

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$T_{1/2}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Rb84m	20.40m	1.00	6%	8%

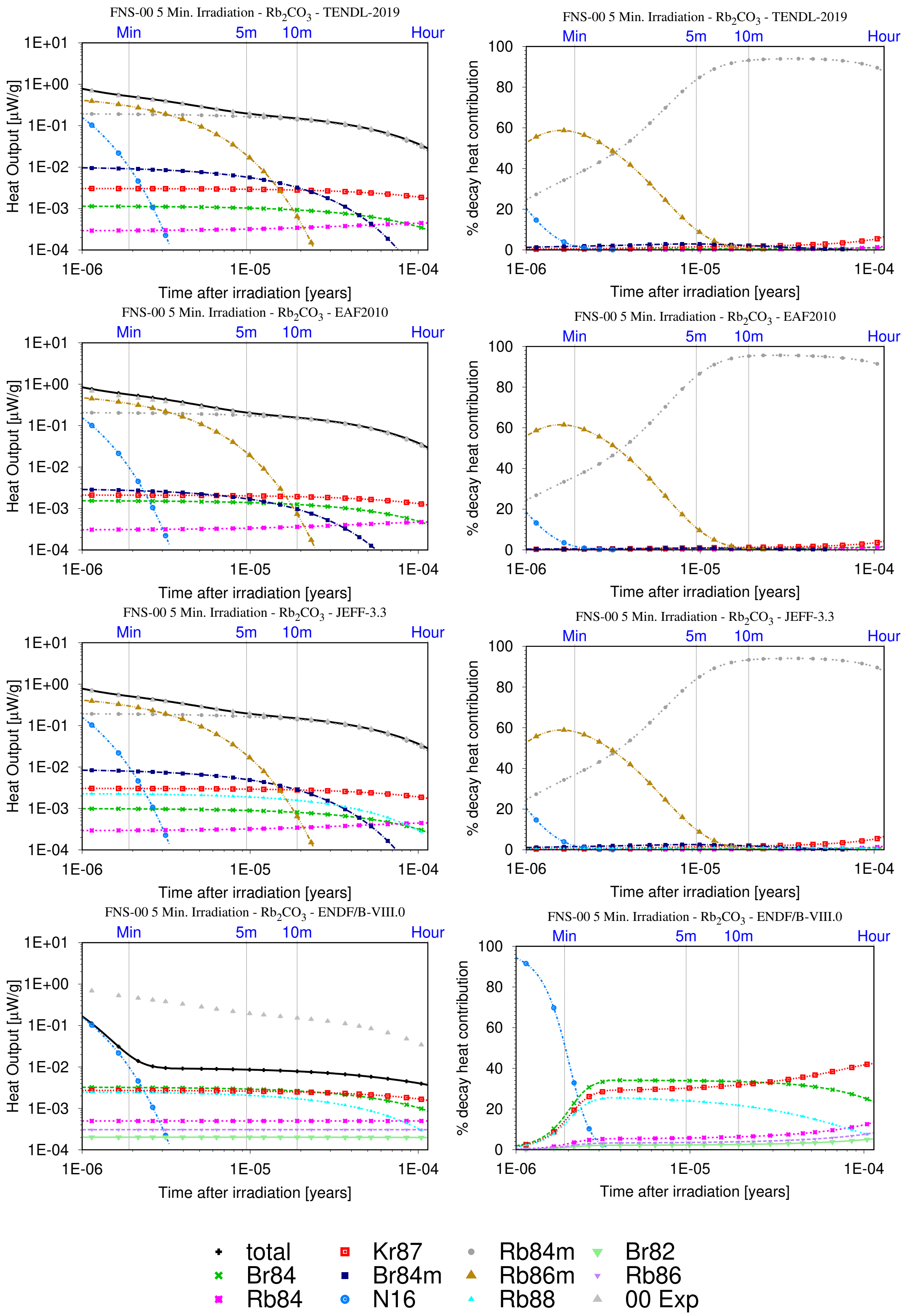


Rubidium, TENDL-2019 5-minute pathway analysis

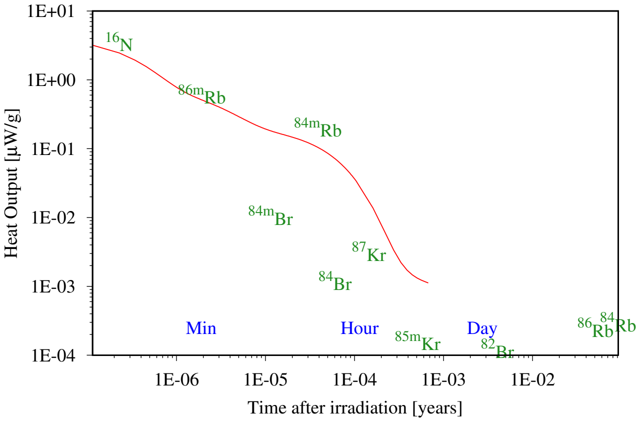
Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Rb86m	1.02m	Rb87(n,2n)Rb86m	99.5
Br84m	6.00m	Rb87(n,α)Br84m	100.0
Rb88	17.80m	Rb87(n,γ)Rb88	100.0
Rb84m	20.40m	Rb85(n,2n)Rb84m	100.0
Br84	31.80m	Rb87(n,α)Br84	100.0
Kr87	1.27h	Rb87(n,p)Kr87	100.0
Br82	1.47d	Rb85(n,α)Br82	76.5
		Rb85(n,α)Br82m(IT)Br82	23.5
Rb86	18.64d	Rb87(n,2n)Rb86	67.0
		Rb87(n,2n)Rb86m(IT)Rb86	31.4
		Rb85(n,γ)Rb86	1.4
Rb84	33.50d	Rb85(n,2n)Rb84	94.4
		Rb85(n,2n)Rb84m(IT)Rb84	5.6

Comments on Rubidium 5-minute experiments:

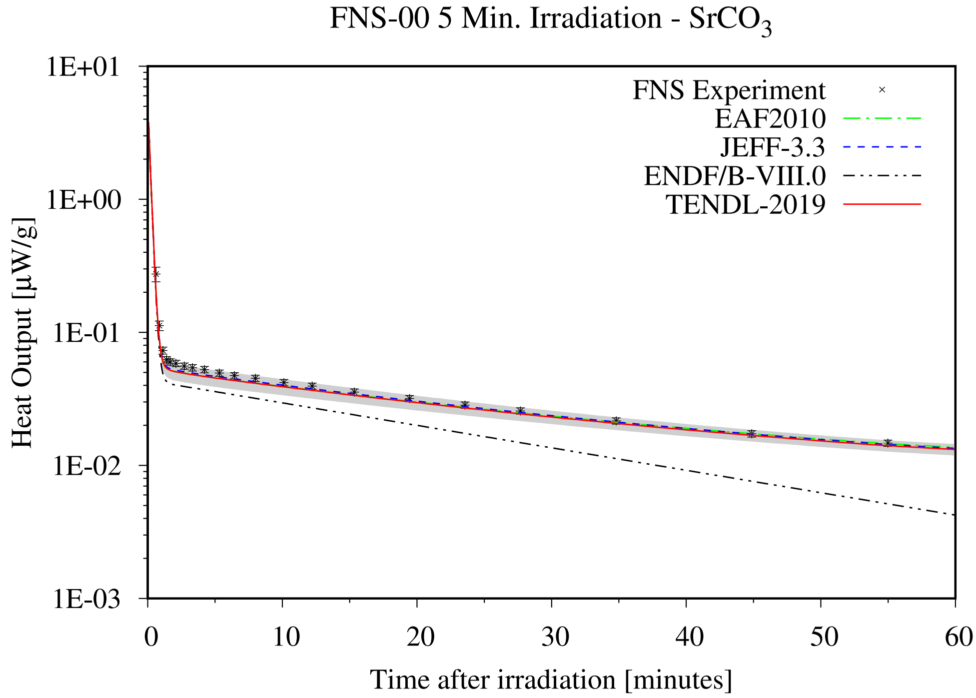
TENDL-2019 properly matches this experiment, JEFF-3.3 and EAF2010 also perform well, but ENDF/B-VIII.0 does not capture the various channels to metastable nuclides – particularly the dominant Rb86m (at times less than 1.5 minutes) and Rb84 (dominant throughout the remainder of the experimental timescale) from (n,2n) reactions. This leads to a massive underprediction of the experiment by ENDF/B-VIII.0 in a situation where the pathways to the metastable nuclides are clearly validated by the C/E values obtained with the other libraries.

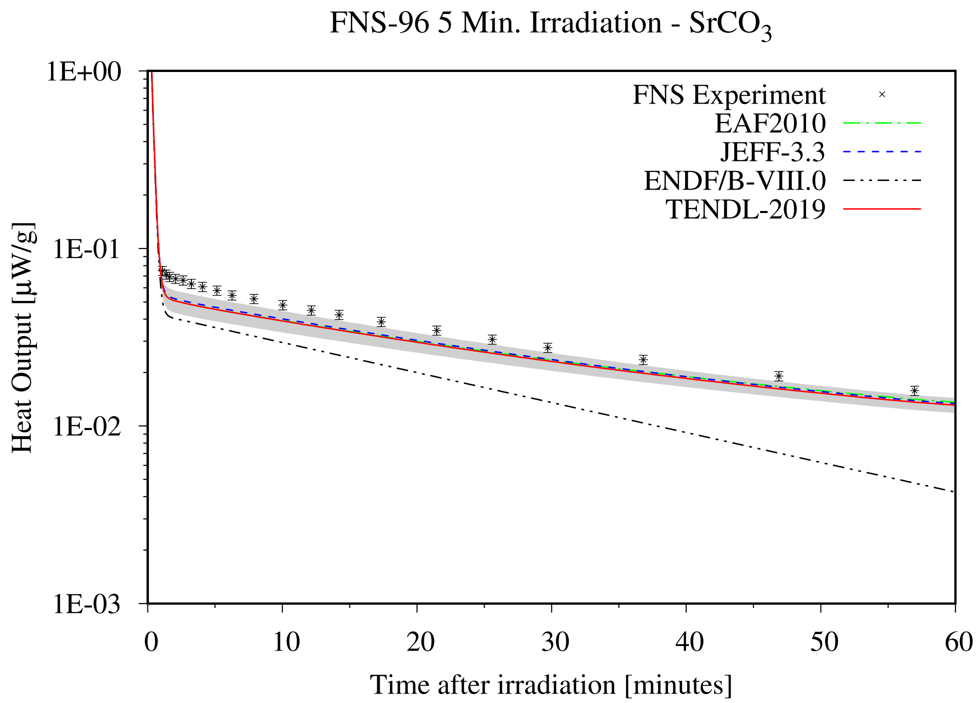

FNS-00 5 Min. Irradiation - Rb$_2$CO$_3$ - TENDL-2019
FNS-00 5 Min. Irradiation - Rb$_2$CO$_3$ - EAF2010
FNS-00 5 Min. Irradiation - Rb$_2$CO$_3$ - JEFF-3.3
FNS-00 5 Min. Irradiation - Rb$_2$CO$_3$ - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Kr87
Rb84m
Br82
Br84
Br84m
Rb86m
Rb86
Rb84
N16
Rb88
00 Exp

FNS-00 5 Min. Irradiation - Rb_2CO_3 - TENDL-2019

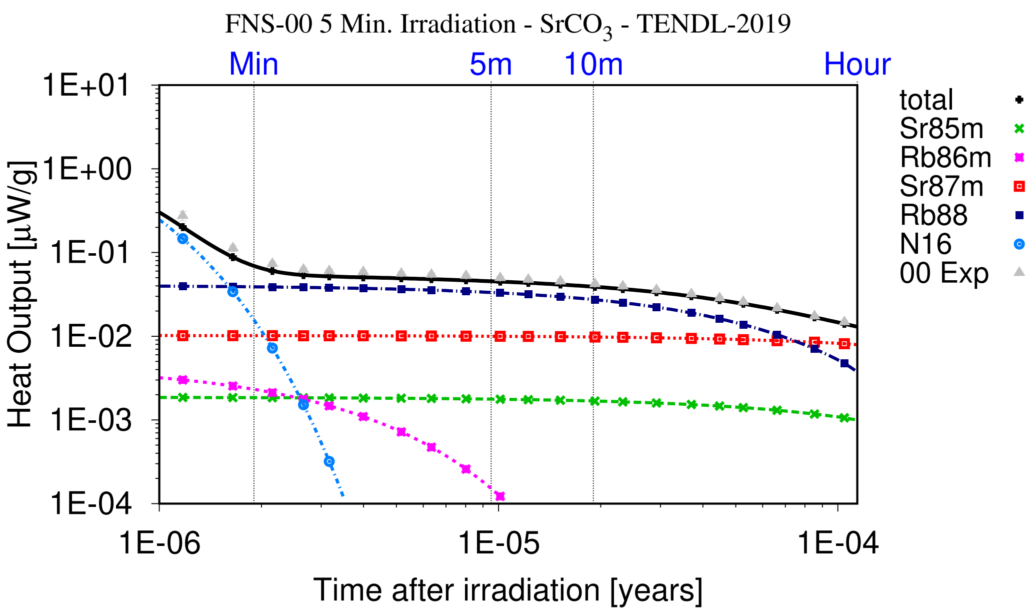


Strontium


FNS-00 5 Min. Irradiation - SrCO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
Time after irradiation [minutes]
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - SrCO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
Time after irradiation [minutes]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.62	2.74E−01 +/-13%	2.02E−01 +/-4%	1.36	1.45	1.38	1.35
0.87	1.12E−01 +/-8%	8.82E−02 +/-9%	1.27	1.48	1.28	1.26
1.13	7.30E−02 +/-6%	6.03E−02 +/-13%	1.21	1.49	1.21	1.18
1.40	6.23E−02 +/-6%	5.39E−02 +/-14%	1.16	1.46	1.16	1.13
1.67	6.00E−02 +/-6%	5.19E−02 +/-14%	1.16	1.46	1.15	1.13
2.10	5.85E−02 +/-6%	5.05E−02 +/-14%	1.16	1.46	1.16	1.13
2.72	5.58E−02 +/-6%	4.92E−02 +/-14%	1.13	1.42	1.13	1.10
3.33	5.42E−02 +/-6%	4.81E−02 +/-14%	1.13	1.42	1.13	1.10
4.22	5.25E−02 +/-6%	4.66E−02 +/-14%	1.13	1.42	1.12	1.10
5.32	4.94E−02 +/-6%	4.50E−02 +/-14%	1.10	1.39	1.10	1.07
6.43	4.73E−02 +/-6%	4.34E−02 +/-14%	1.09	1.39	1.09	1.06
8.00	4.51E−02 +/-5%	4.14E−02 +/-14%	1.09	1.41	1.09	1.06
10.12	4.19E−02 +/-5%	3.89E−02 +/-14%	1.08	1.43	1.07	1.05
12.22	3.94E−02 +/-5%	3.67E−02 +/-14%	1.08	1.46	1.07	1.05
15.35	3.56E−02 +/-5%	3.36E−02 +/-13%	1.06	1.48	1.05	1.03
19.45	3.18E−02 +/-5%	3.01E−02 +/-13%	1.06	1.56	1.05	1.03
23.57	2.84E−02 +/-5%	2.70E−02 +/-12%	1.05	1.63	1.04	1.03
27.68	2.57E−02 +/-5%	2.44E−02 +/-12%	1.05	1.73	1.03	1.03
34.80	2.16E−02 +/-5%	2.07E−02 +/-11%	1.04	1.92	1.02	1.02
44.87	1.73E−02 +/-5%	1.68E−02 +/-10%	1.03	2.27	1.00	1.01
54.98	1.47E−02 +/-5%	1.41E−02 +/-10%	1.05	2.86	1.01	1.02
mean % diff. from E			10	35	9	8
mean χ^2			3.12	42.02	2.98	2.07

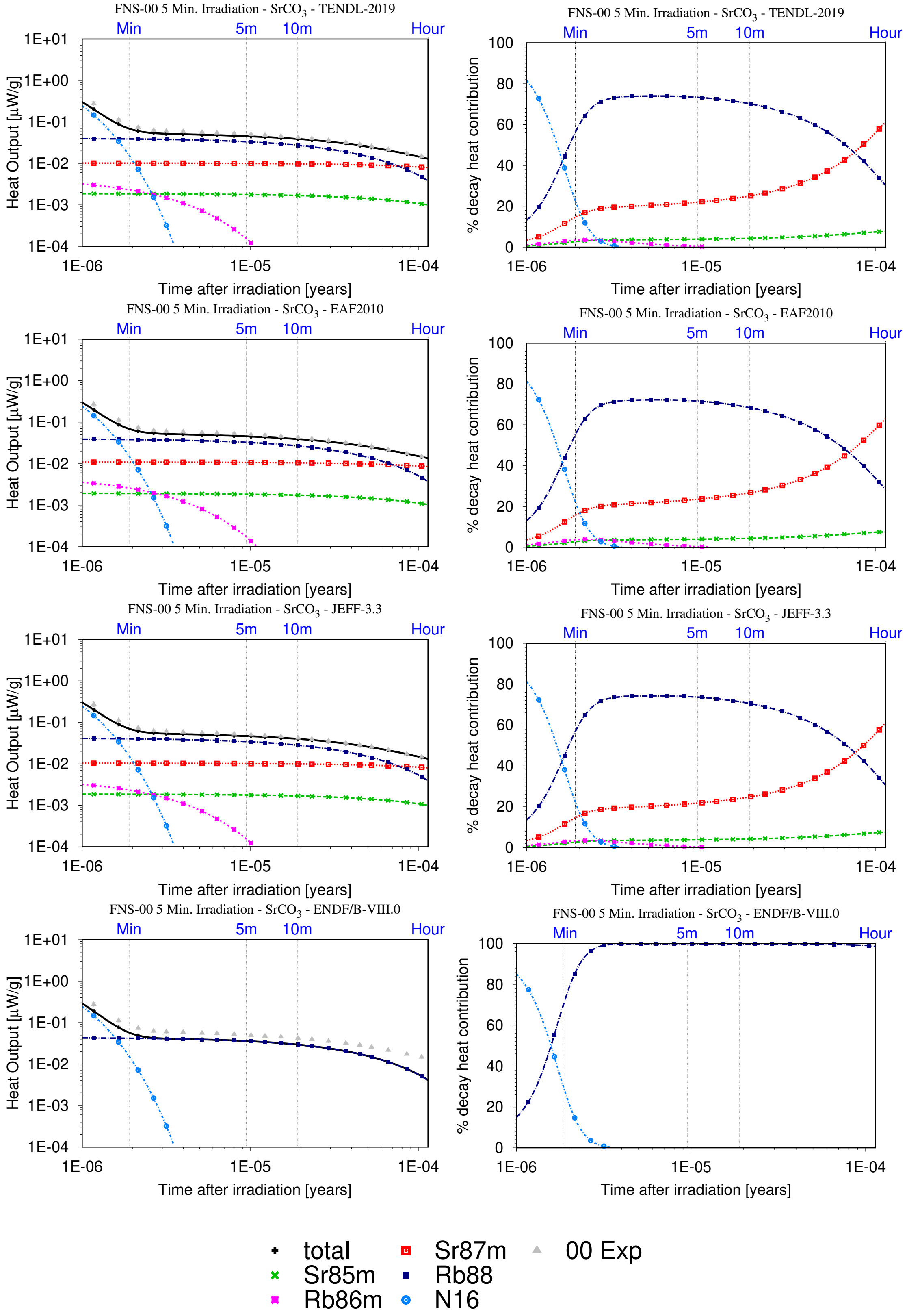


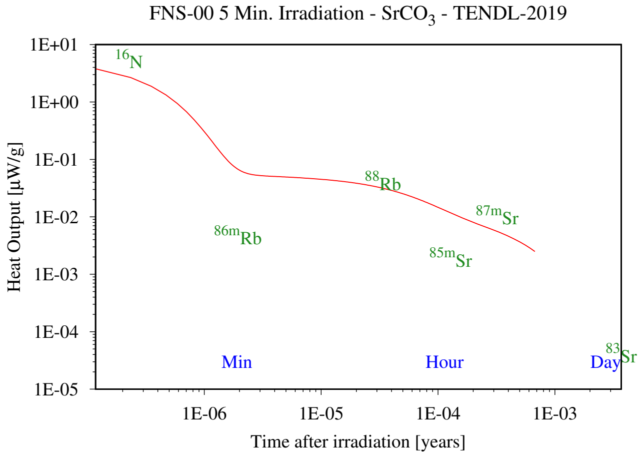
Strontium, TENDL-2019 5-minute pathway analysis

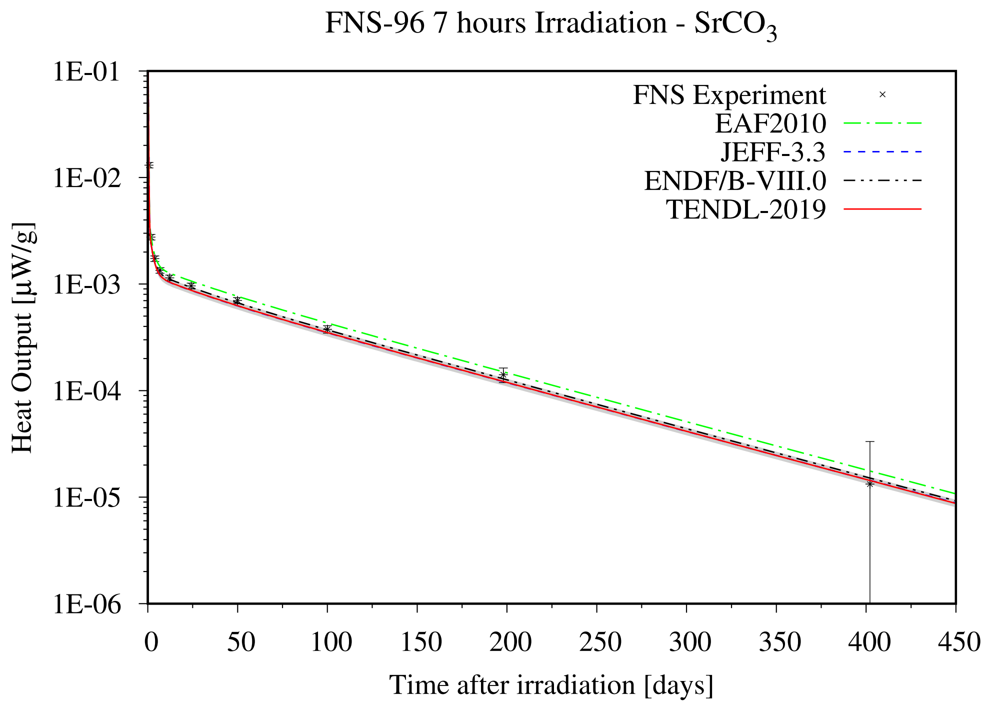
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Rb86m	1.02m	Sr86(n,p)Rb86m	88.3
		Sr87(n,np)Rb86m	8.1
		Sr87(n,d)Rb86m	3.6
Rb88	17.80m	Sr88(n,p)Rb88	100.0
Sr85m	1.13h	Sr86(n,2n)Sr85m	99.8
Sr87m	2.82h	Sr88(n,2n)Sr87m	96.9
		Sr87(n,n′)Sr87m	2.9

Comments on Strontium 5-minute experiments:

An interesting case where a metastable isomer (Sr87m) becomes dominant at the end of the measurement while a ground state nuclide (Rb88) contributes the most decay heat during the first 20-30 minutes (after the short-lived contribution of N16 produced from oxygen has disappeared). TENDL-2019, JEFF-3.3 and EAF2010 also show excellent agreement to both experimental batches (even though there are some unexplained differences between the experiments). ENDF/B-VIII.0 underpredicts significantly at all times due to the missing contribution from Sr87m. Note that the N16 contribution appears underpredicted with all libraries, but this is more likely an experimental artefact than a problem with the well-characterised (n,p) channel on O16.


FNS-00 5 Min. Irradiation - SrCO3 - TENDL-2019
FNS-00 5 Min. Irradiation - SrCO3 - EAF2010
FNS-00 5 Min. Irradiation - SrCO3 - JEFF-3.3
FNS-00 5 Min. Irradiation - SrCO3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Sr85m
Rb86m
Sr87m
Rb88
N16
00 Exp

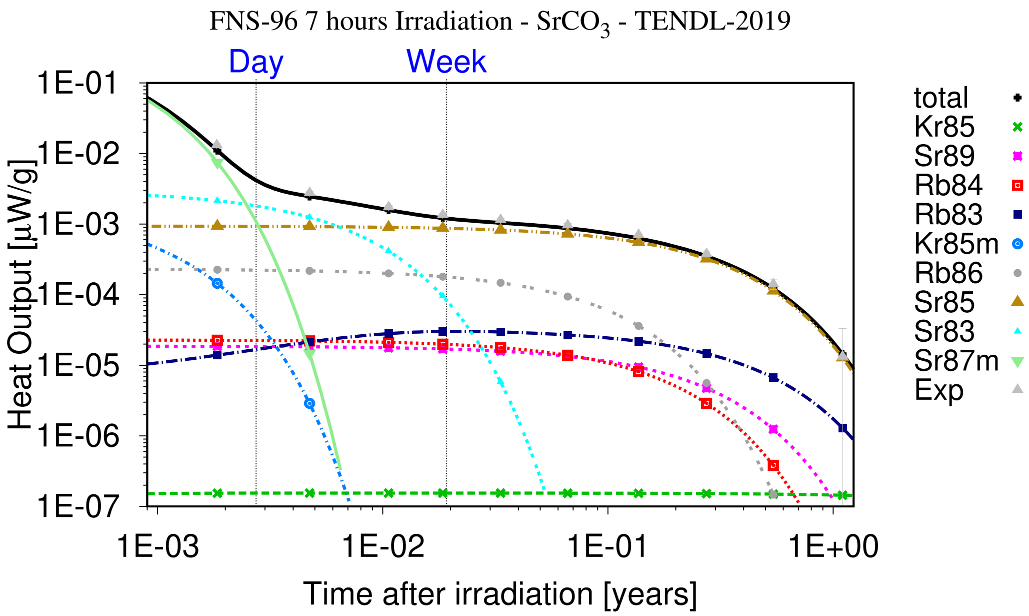

FNS-00 5 Min. Irradiation - SrCO3 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
16N
88Rb
87mSr
86mRb
85mSr
83Sr
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.67	$1.31E{-}02$ +/-6%	$1.10E{-}02$ +/-9%	1.19	4.05	1.10	1.16
1.73	$2.76E{-}03$ +/-6%	$2.47E{-}03$ +/-7%	1.12	1.14	0.97	1.12
3.88	$1.73E{-}03$ +/-6%	$1.58E{-}03$ +/-7%	1.09	1.07	0.93	1.09
6.75	$1.34E{-}03$ +/-6%	$1.22E{-}03$ +/-7%	1.10	1.05	0.92	1.11
12.19	$1.14E{-}03$ +/-6%	$1.04E{-}03$ +/-8%	1.10	1.03	0.90	1.10
24.20	$9.61E{-}04$ +/-6%	$8.75E{-}04$ +/-8%	1.10	1.03	0.90	1.10
49.95	$7.01E{-}04$ +/-6%	$6.27E{-}04$ +/-8%	1.12	1.05	0.91	1.12
100.08	$3.76E{-}04$ +/-8%	$3.51E{-}04$ +/-8%	1.07	1.01	0.87	1.08
197.95	$1.41E{-}04$ +/-16%	$1.22E{-}04$ +/-8%	1.16	1.09	0.94	1.16
402.15	$1.33E{-}05$ +/-151%	$1.43E{-}05$ +/-8%	0.92	0.87	0.75	0.92
mean % diff. from E			10	13	11	10
mean χ^2			2.33	17.23	1.90	2.25

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Sr85	64.85d	1.10	6%	9%

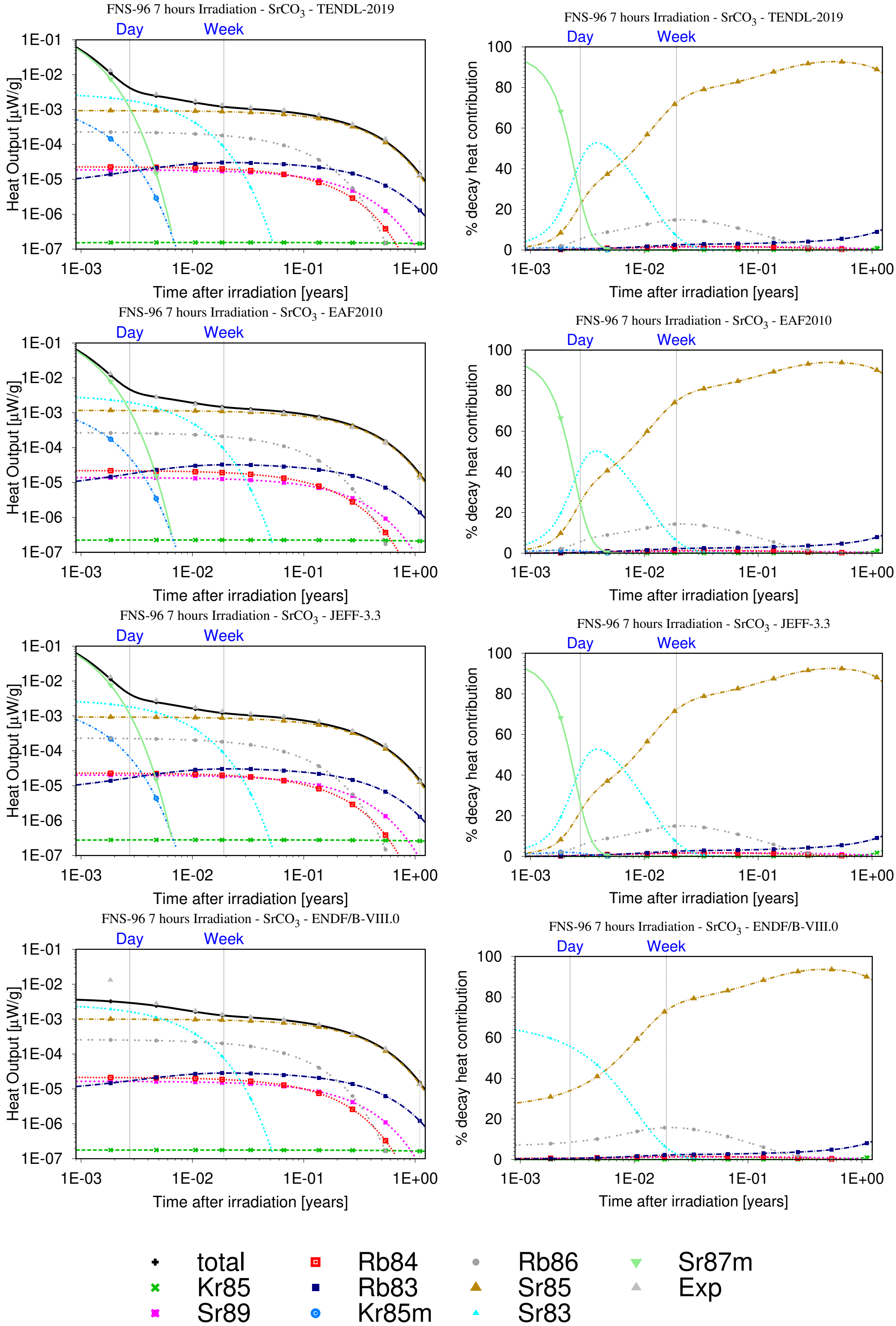


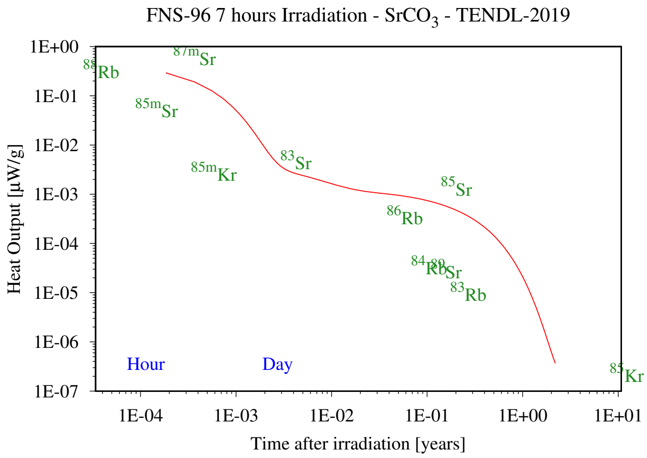
Strontium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Sr87m	2.82h	Sr88(n,2n)Sr87m	97.4
		Sr87(n,n′)Sr87m	2.6
Kr85m	4.48h	Sr88(n,α)Kr85m	100.0
Sr83	1.35d	Sr84(n,2n)Sr83	84.1
		Sr84(n,2n)Sr83m(IT)Sr83	15.9
Rb86	18.64d	Sr86(n,p)Rb86	67.0
		Sr86(n,p)Rb86m(IT)Rb86	26.2
		Sr87(n,d)Rb86	2.1
		Sr87(n,np)Rb86	2.0
		Sr87(n,np)Rb86m(IT)Rb86	1.9
Rb84	33.50d	Sr84(n,p)Rb84	58.7
		Sr84(n,p)Rb84m(IT)Rb84	41.3
Sr89	50.58d	Sr88(n,γ)Sr89	100.0
Sr85	64.85d	Sr86(n,2n)Sr85	80.6
		Sr86(n,2n)Sr85m(IT)Sr85	19.4
Rb83	86.20d	Sr84(n,np)Rb83	66.1
		Sr84(n,2n)Sr83(β^+)Rb83	26.7
		Sr84(n,2n)Sr83m(IT)Sr83(β^+)Rb83	5.0
		Sr84(n,d)Rb83	2.1
Kr85	10.75y	Sr88(n,α)Kr85	95.5
		Sr88(n,α)Kr85m(IT)Kr85	4.5

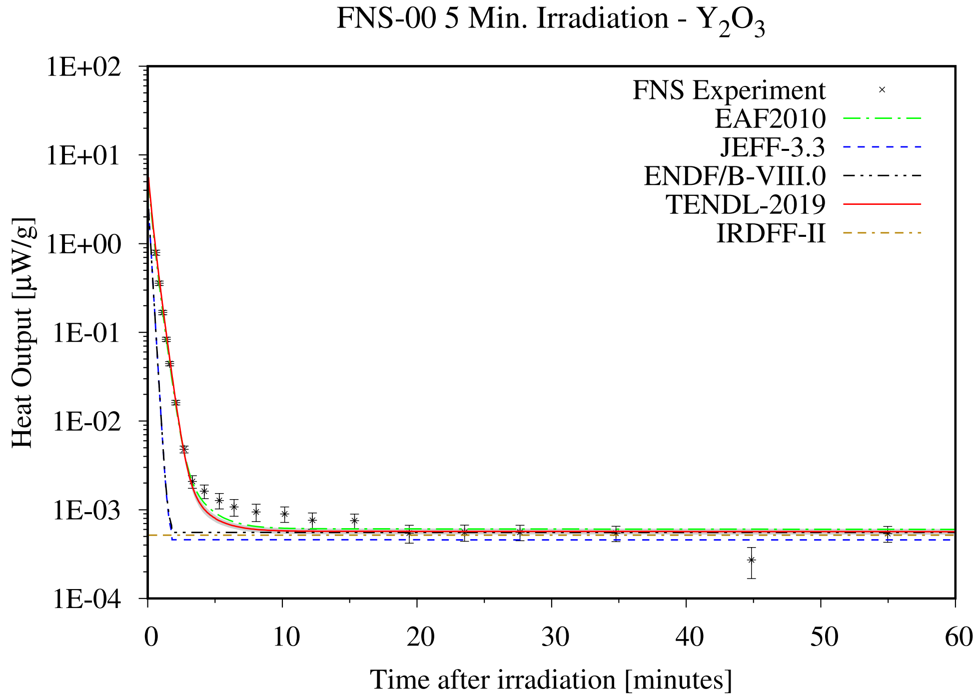
Comments on Strontium 7-hour experiments:

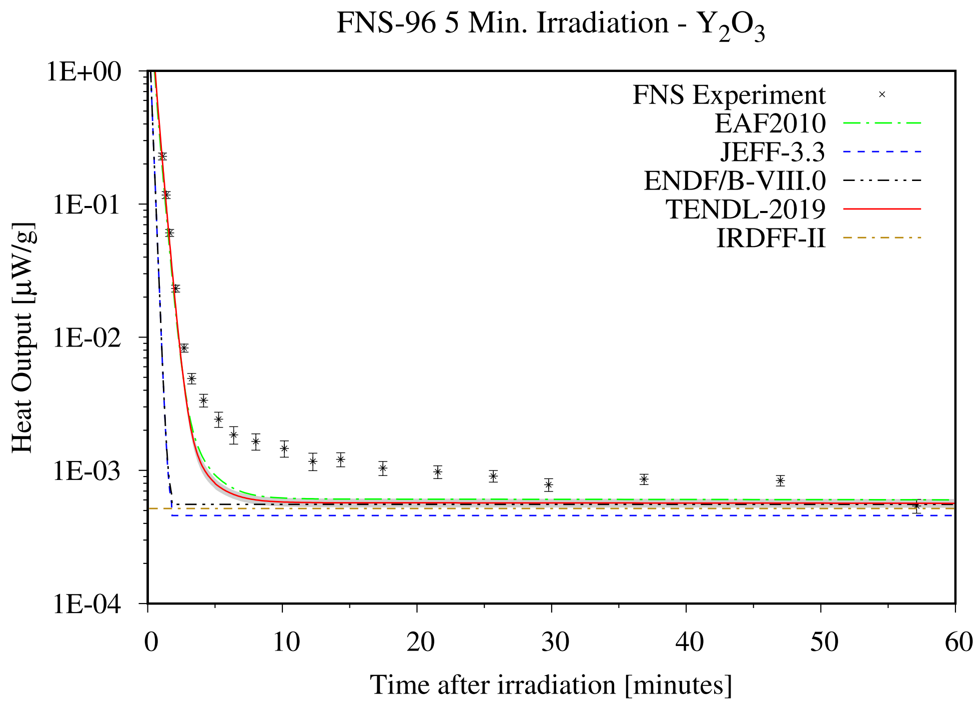
A good agreement with all libraries, except for the first cooling step with ENDF/B-VIII.0 where there is an underprediction due to the missing Sr87m metastable. A relatively complex picture, with three different overlapping nuclide contributions (Sr87m, Sr83, and then Sr85 as a function of time according to TENDL, JEFF, and EAF), so the level of agreement is very pleasing.


FNS-96 7 hours Irradiation - $SrCO_3$ - TENDL-2019
FNS-96 7 hours Irradiation - $SrCO_3$ - EAF2010
FNS-96 7 hours Irradiation - $SrCO_3$ - JEFF-3.3
FNS-96 7 hours Irradiation - $SrCO_3$ - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E+00
0
20
40
60
80
100
total
Kr85
Sr89
Rb84
Rb83
Kr85m
Rb86
Sr85
Sr83
Sr87m
Exp


FNS-96 7 hours Irradiation - SrCO3 - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-04
1E-03
1E-02
1E-01
1E+00
1E+01
Hour
Day
87mSr
85mSr
85mKr
83Sr
85Sr
86Rb
83Rb
85Kr

Yttrium

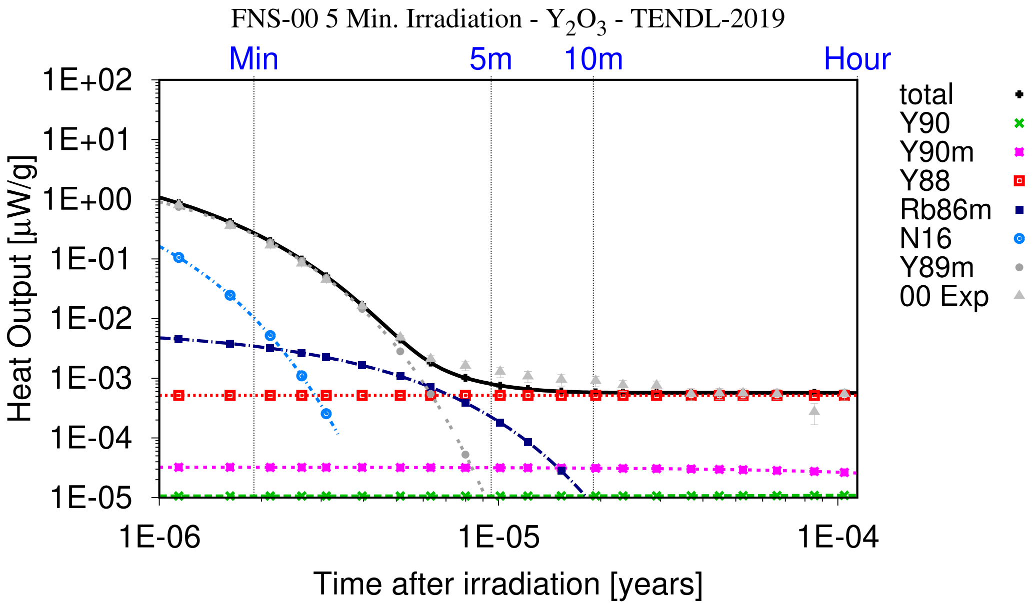

FNS-00 5 Min. Irradiation - Y_2O_3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Y_2O_3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]

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
0.60	7.92$E-01$ +/-7%	8.55$E-01$ +/-11%	0.93	7.50	1.06	7.46	> 1000
0.85	3.58$E-01$ +/-6%	4.12$E-01$ +/-12%	0.87	14.29	1.00	14.29	692.34
1.12	1.68$E-01$ +/-6%	1.98$E-01$ +/-12%	0.85	29.21	0.98	29.63	324.02
1.38	8.35$E-02$ +/-6%	9.73$E-02$ +/-12%	0.86	51.10	0.99	53.46	161.51
1.63	4.44$E-02$ +/-6%	5.10$E-02$ +/-12%	0.87	55.10	0.99	62.13	85.97
2.08	1.61$E-02$ +/-6%	1.67$E-02$ +/-11%	0.96	29.00	1.06	35.16	31.18
2.70	4.80$E-03$ +/-9%	4.47$E-03$ +/-10%	1.07	8.63	1.06	10.47	9.28
3.32	2.08$E-03$ +/-16%	1.83$E-03$ +/-11%	1.14	3.75	1.01	4.54	4.03
4.20	1.62$E-03$ +/-17%	1.01$E-03$ +/-11%	1.60	2.91	1.35	3.53	3.13
5.32	1.27$E-03$ +/-20%	7.54$E-04$ +/-8%	1.69	2.29	1.48	2.78	2.46
6.42	1.07$E-03$ +/-21%	6.58$E-04$ +/-7%	1.63	1.93	1.47	2.34	2.08
8.05	9.46$E-04$ +/-22%	6.01$E-04$ +/-7%	1.57	1.70	1.46	2.06	1.83
10.17	8.98$E-04$ +/-20%	5.78$E-04$ +/-7%	1.55	1.62	1.45	1.96	1.74
12.23	7.62$E-04$ +/-21%	5.73$E-04$ +/-8%	1.33	1.37	1.25	1.66	1.47
15.37	7.54$E-04$ +/-19%	5.71$E-04$ +/-8%	1.32	1.36	1.24	1.64	1.46
19.43	5.45$E-04$ +/-23%	5.71$E-04$ +/-8%	0.95	0.98	0.90	1.19	1.05
23.53	5.56$E-04$ +/-21%	5.70$E-04$ +/-8%	0.98	1.00	0.92	1.21	1.08
27.65	5.57$E-04$ +/-20%	5.70$E-04$ +/-8%	0.98	1.00	0.92	1.22	1.08
34.78	5.45$E-04$ +/-20%	5.69$E-04$ +/-8%	0.96	0.98	0.90	1.19	1.05
44.85	2.72$E-04$ +/-38%	5.68$E-04$ +/-7%	0.48	0.49	0.45	0.59	0.53
54.97	5.39$E-04$ +/-20%	5.67$E-04$ +/-7%	0.95	0.97	0.89	1.18	1.04
mean % diff. from E			22	55	19	60	58
mean χ^2			3.11	83.73	1.30	85.04	90.03

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Y89m	15.66s	0.93	7%	13%
Y88	106.63d	1.63	21%	8%

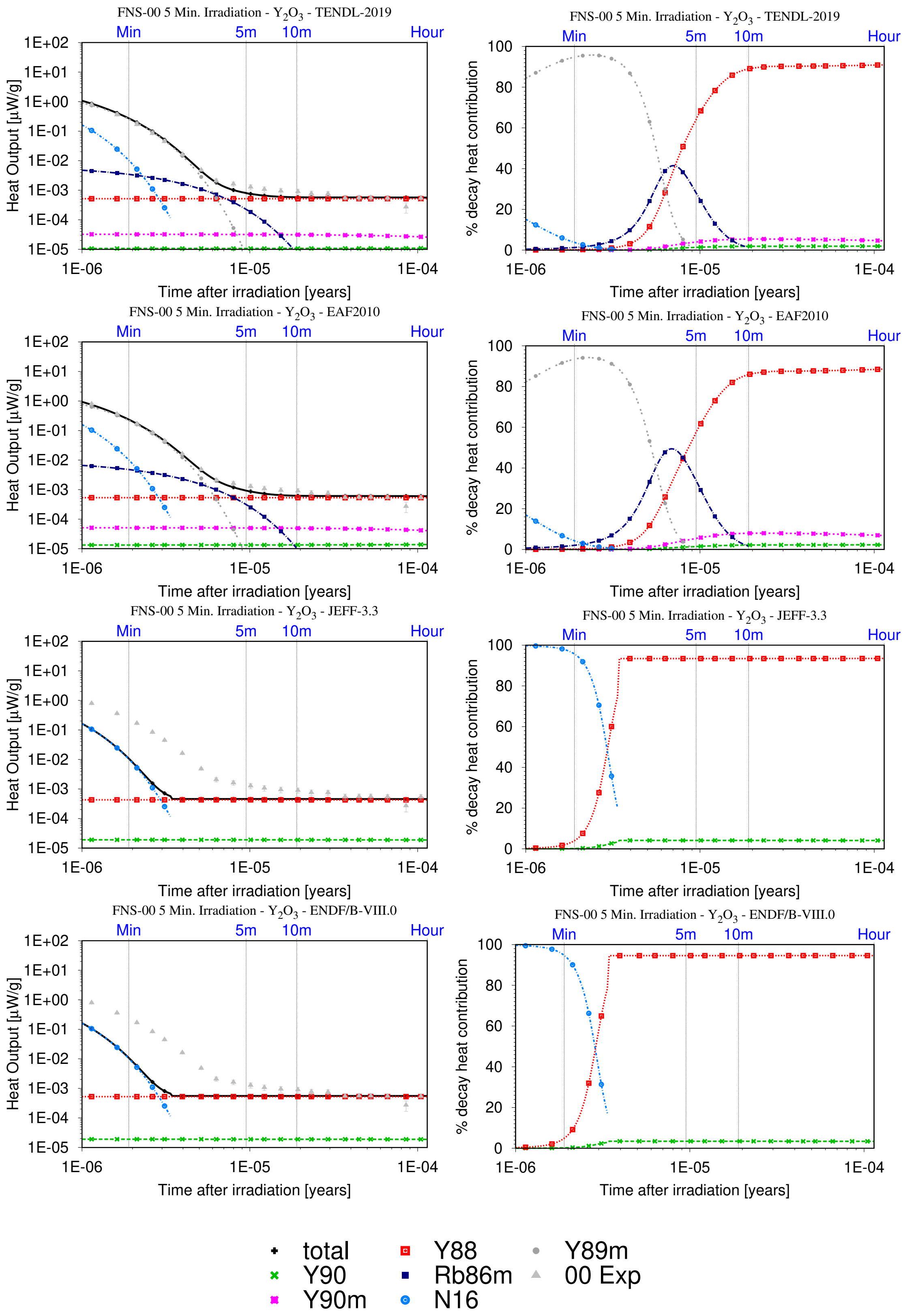


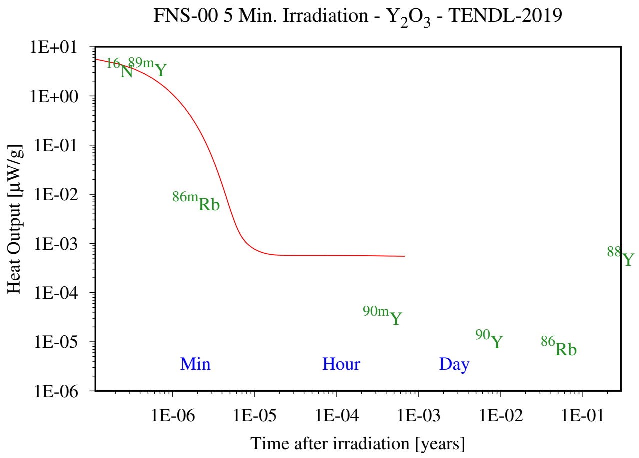
Yttrium, TENDL-2019 5-minute pathway analysis

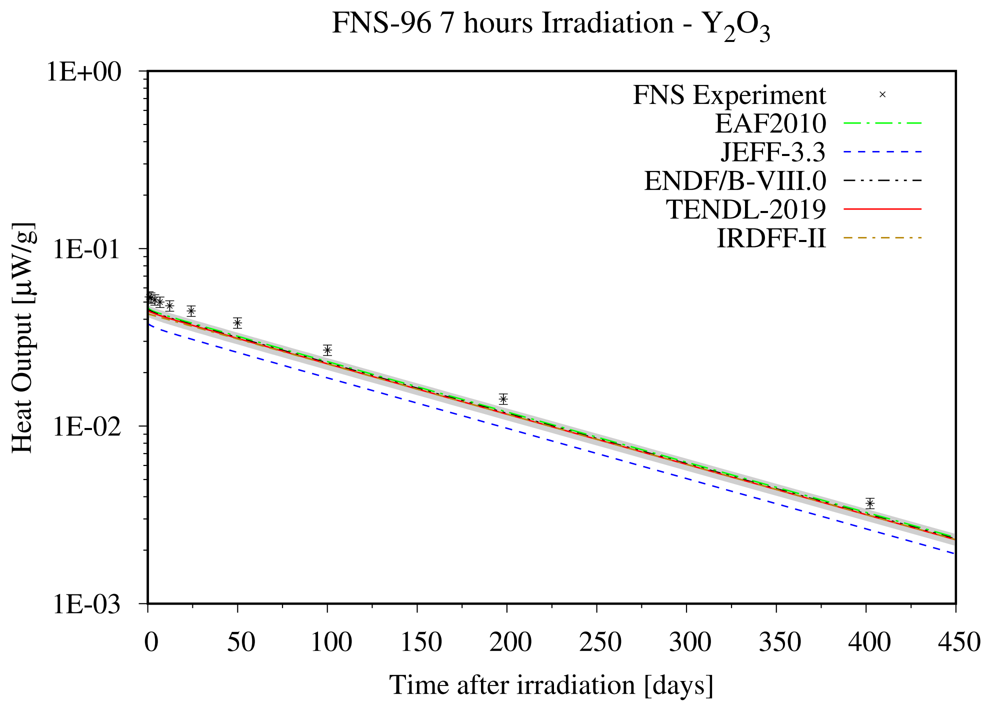
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Y89m	15.66s	Y89(n,n′)Y89m	100.0
Rb86m	1.02m	Y89(n,α)Rb86m	100.0
Y90m	3.19h	Y89(n,γ)Y90m	100.0
Y90	2.67d	Y89(n,γ)Y90	99.8
Y88	106.63d	Y89(n,2n)Y88	100.0

Comments on Yttrium 5-minute experiments:

Some large experimental uncertainties in the 2000 batch experiment for yttrium and the two batches (1996 vs. 2000) disagree significantly. Only TENDL-2019 and EAF2010 capture the dominance of Y89m at cooling times below around 3 minutes of cooling (JEFF and ENDF/B miss this nuclide). None of the libraries give very good agreement at intermediate cooling times (∼3-10 minutes of cooling), but all give better agreement at longer times where the single ground-state nuclide Y88 (from (n,2n) on Y89) is completely dominant. Rb86m seems to be the underpredicted nuclide that would properly match the experiment profile at the intermediate times, and so its production via (n,α) on Y89 should be reviewed.


FNS-00 5 Min. Irradiation - Y_2O_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Y_2O_3 - EAF2010
FNS-00 5 Min. Irradiation - Y_2O_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Y_2O_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Y90
Y90m
Y88
Rb86m
N16
Y89m
00 Exp

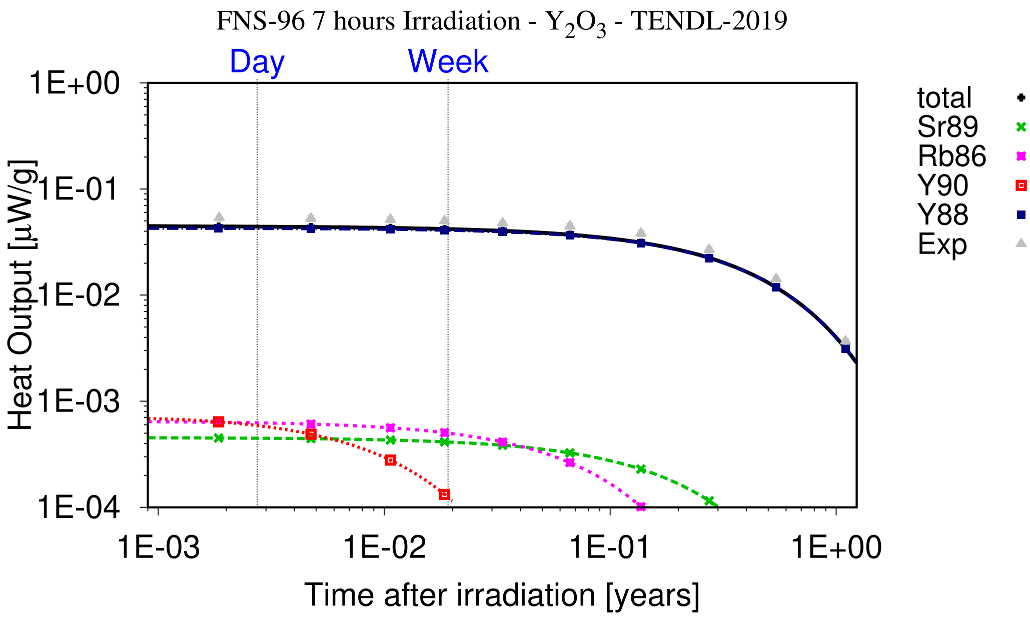

FNS-00 5 Min. Irradiation - Y2O3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
16N
89mY
86mRb
90mY
90Y
86Rb
88Y
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.68	5.35E−02 +/-7%	4.43E−02 +/-7%	1.21	1.19	1.17	1.43	1.25
1.73	5.27E−02 +/-7%	4.38E−02 +/-7%	1.20	1.19	1.17	1.43	1.24
3.89	5.14E−02 +/-7%	4.30E−02 +/-8%	1.20	1.18	1.17	1.43	1.23
6.76	5.00E−02 +/-7%	4.20E−02 +/-8%	1.19	1.18	1.16	1.43	1.22
12.20	4.76E−02 +/-7%	4.03E−02 +/-8%	1.18	1.17	1.15	1.42	1.20
24.21	4.45E−02 +/-7%	3.71E−02 +/-8%	1.20	1.19	1.17	1.44	1.22
49.96	3.81E−02 +/-7%	3.12E−02 +/-8%	1.22	1.21	1.19	1.47	1.23
100.09	2.68E−02 +/-7%	2.24E−02 +/-8%	1.19	1.18	1.16	1.43	1.20
197.96	1.42E−02 +/-7%	1.18E−02 +/-8%	1.20	1.19	1.17	1.44	1.20
402.17	3.67E−03 +/-7%	3.13E−03 +/-8%	1.17	1.16	1.14	1.41	1.17
mean % diff. from E			16	15	14	30	18
mean χ^2			5.88	5.25	4.35	19.88	6.92

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Y88	106.63d	1.21	7%	8%

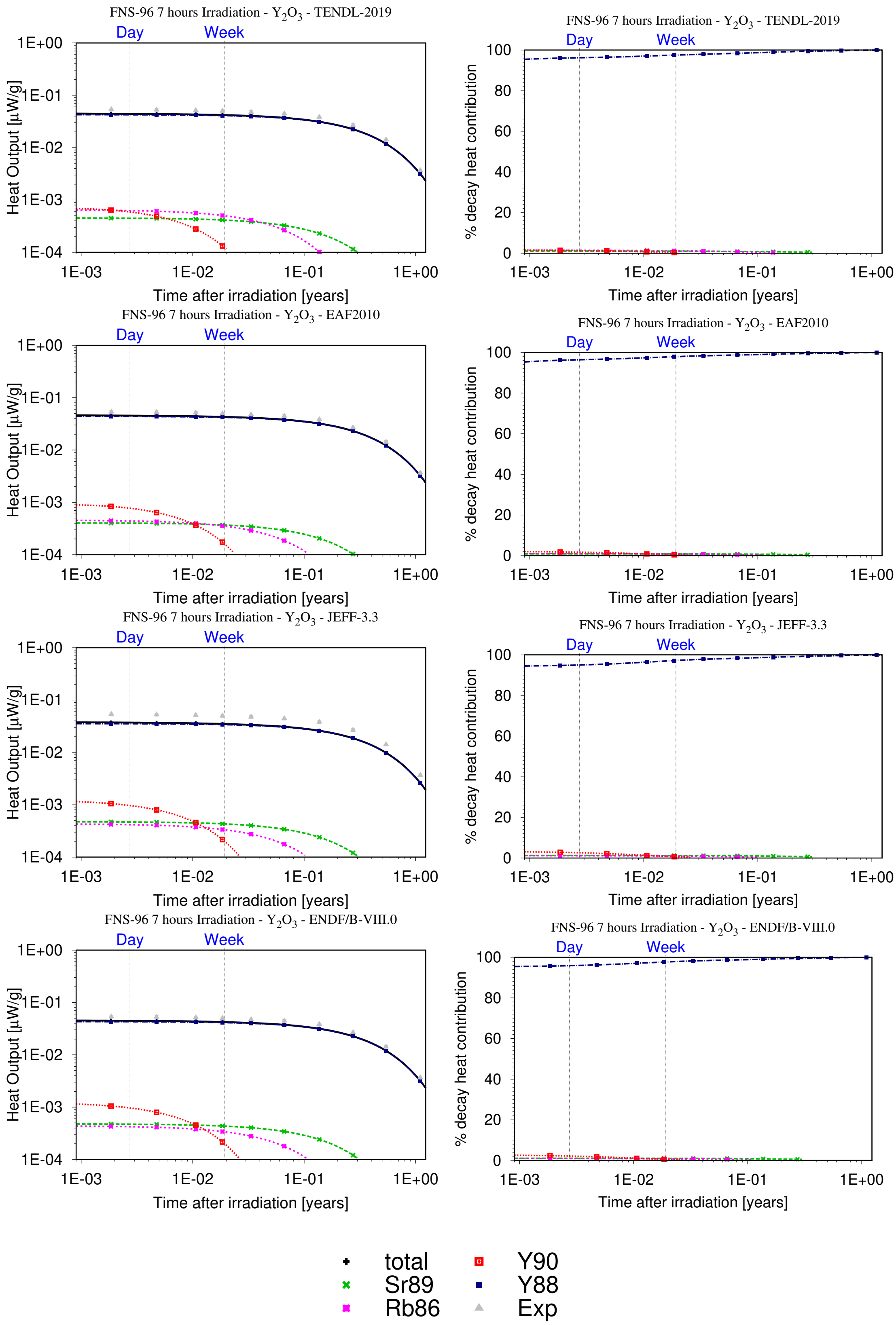


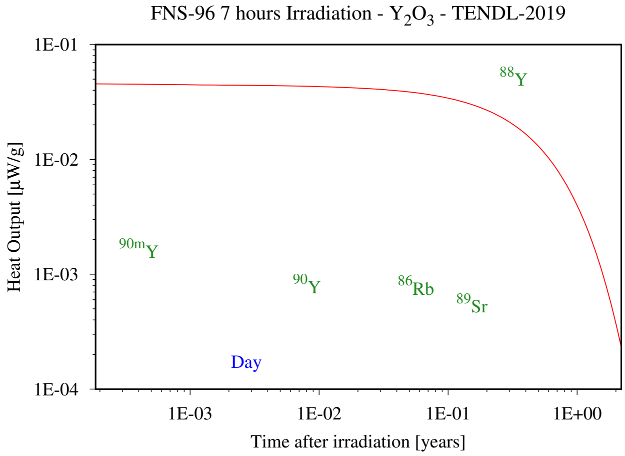
Yttrium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Y90	2.67d	Y89(n,γ)Y90	86.9
		Y89(n,γ)Y90m(IT)Y90	13.1
Rb86	18.64d	Y89(n,α)Rb86	85.0
		Y89(n,α)Rb86m(IT)Rb86	15.0
Sr89	50.58d	Y89(n,p)Sr89	100.0
Y88	106.63d	Y89(n,2n)Y88	100.0

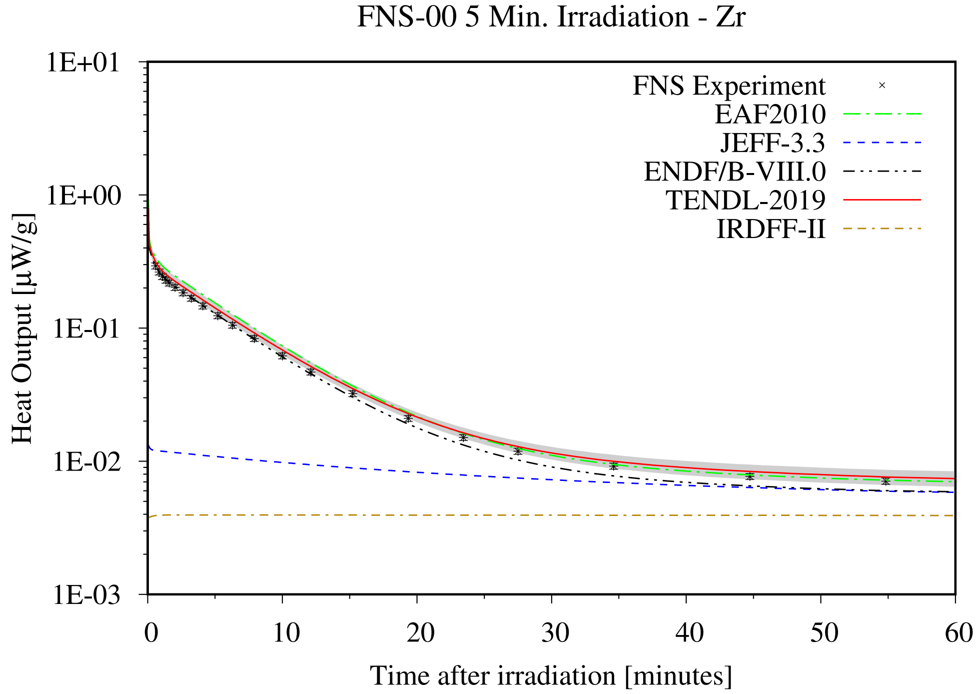
Comments on Yttrium 7-hour experiments:

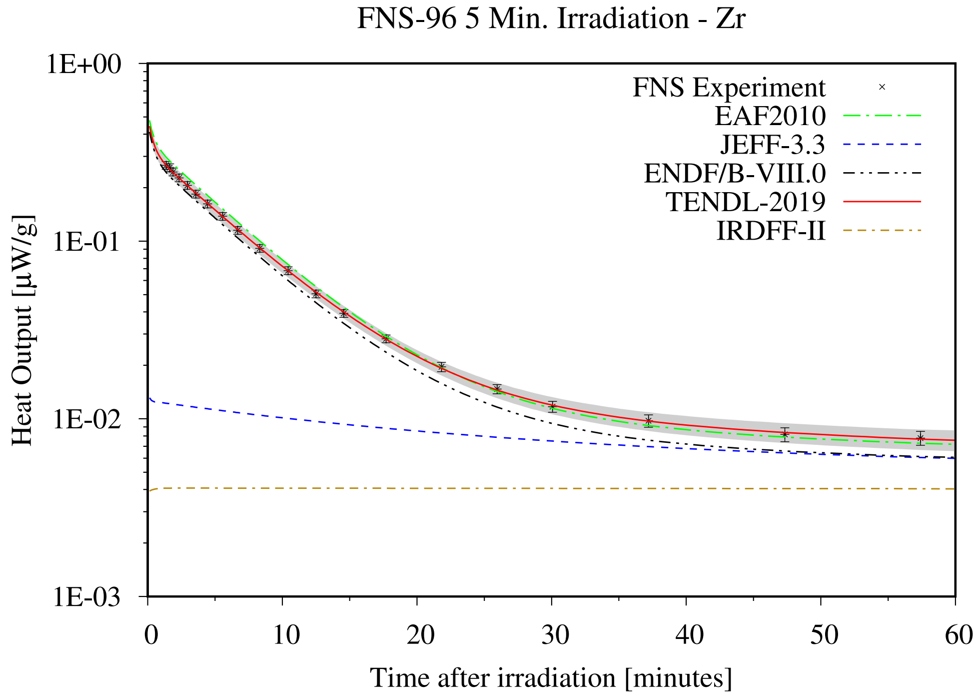
All of the code predictions seem to underestimate the experimental measurement consistently and evenly to differing degrees up to 400 days of cooling, with EAF2010 the closest and JEFF-3.3 the worst. The response is predicted to be entirely due to the production of Y88 via Y89(n,2n), so this seems to suggest a need to re-evaluate the cross section for this reaction or the decay data associated with Y88 (if not backed up by differential measurements).


FNS-96 7 hours Irradiation - Y_2O_3 - TENDL-2019
Day
Week
Heat Output [µW/g]
Time after irradiation [years]
% decay heat contribution
FNS-96 7 hours Irradiation - Y_2O_3 - EAF2010
FNS-96 7 hours Irradiation - Y_2O_3 - JEFF-3.3
FNS-96 7 hours Irradiation - Y_2O_3 - ENDF/B-VIII.0
1E+00
1E-01
1E-02
1E-03
1E-04
0
20
40
60
80
100
total
Sr89
Rb86
Y90
Y88
Exp


FNS-96 7 hours Irradiation - Y2O3 - TENDL-2019
Heat Output [μW/g]
1E-01
1E-02
1E-03
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]
88Y
90mY
90Y
86Rb
89Sr
Day

Zirconium

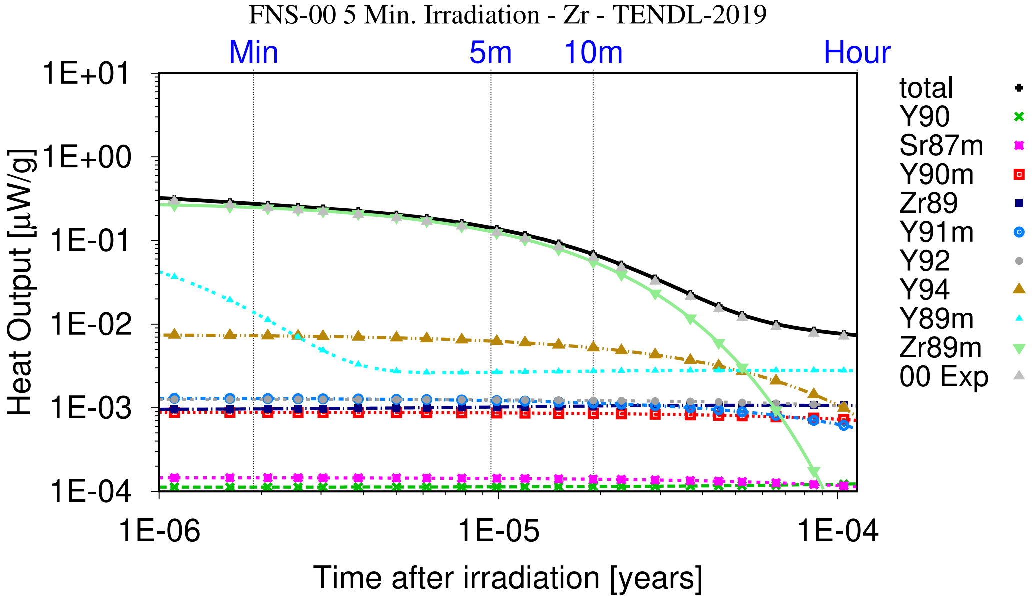

FNS-00 5 Min. Irradiation - Zr
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - Zr
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

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	2.93E−01 +/-5%	3.15E−01 +/-9%	0.93	1.00	0.86	24.42	75.09
0.85	2.64E−01 +/-5%	2.86E−01 +/-9%	0.92	1.00	0.84	22.07	67.12
1.10	2.44E−01 +/-5%	2.68E−01 +/-9%	0.91	0.99	0.83	20.51	61.88
1.35	2.29E−01 +/-5%	2.54E−01 +/-9%	0.90	0.98	0.82	19.37	58.04
1.60	2.18E−01 +/-5%	2.42E−01 +/-9%	0.90	0.98	0.82	18.56	55.24
2.03	2.02E−01 +/-5%	2.25E−01 +/-9%	0.90	0.98	0.82	17.37	51.14
2.63	1.84E−01 +/-5%	2.04E−01 +/-9%	0.90	0.99	0.82	16.05	46.58
3.23	1.68E−01 +/-5%	1.86E−01 +/-9%	0.90	0.99	0.82	14.82	42.41
4.10	1.47E−01 +/-5%	1.63E−01 +/-9%	0.90	0.99	0.83	13.25	37.17
5.20	1.24E−01 +/-5%	1.38E−01 +/-9%	0.90	0.99	0.83	11.46	31.38
6.30	1.05E−01 +/-5%	1.17E−01 +/-9%	0.90	1.00	0.83	9.95	26.62
7.92	8.35E−02 +/-5%	9.21E−02 +/-9%	0.91	1.01	0.84	8.18	21.15
10.02	6.19E−02 +/-5%	6.84E−02 +/-8%	0.90	1.02	0.84	6.32	15.68
12.12	4.67E−02 +/-5%	5.16E−02 +/-8%	0.91	1.03	0.85	4.97	11.85
15.23	3.22E−02 +/-5%	3.51E−02 +/-8%	0.92	1.06	0.88	3.61	8.16
19.35	2.10E−02 +/-5%	2.28E−02 +/-8%	0.92	1.10	0.90	2.51	5.32
23.45	1.51E−02 +/-5%	1.64E−02 +/-9%	0.92	1.13	0.93	1.91	3.82
27.50	1.19E−02 +/-5%	1.29E−02 +/-10%	0.92	1.16	0.95	1.59	3.02
34.62	9.20E−03 +/-5%	9.99E−03 +/-12%	0.92	1.18	0.97	1.33	2.34
44.73	7.69E−03 +/-5%	8.38E−03 +/-13%	0.92	1.18	0.97	1.21	1.96
54.83	7.09E−03 +/-5%	7.62E−03 +/-13%	0.93	1.18	0.98	1.19	1.81
mean % diff. from E			10	5	16	74	87
mean χ^2			3.57	2.02	10.82	232.50	288.11

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Zr89m	4.18m	0.93	5%	10%

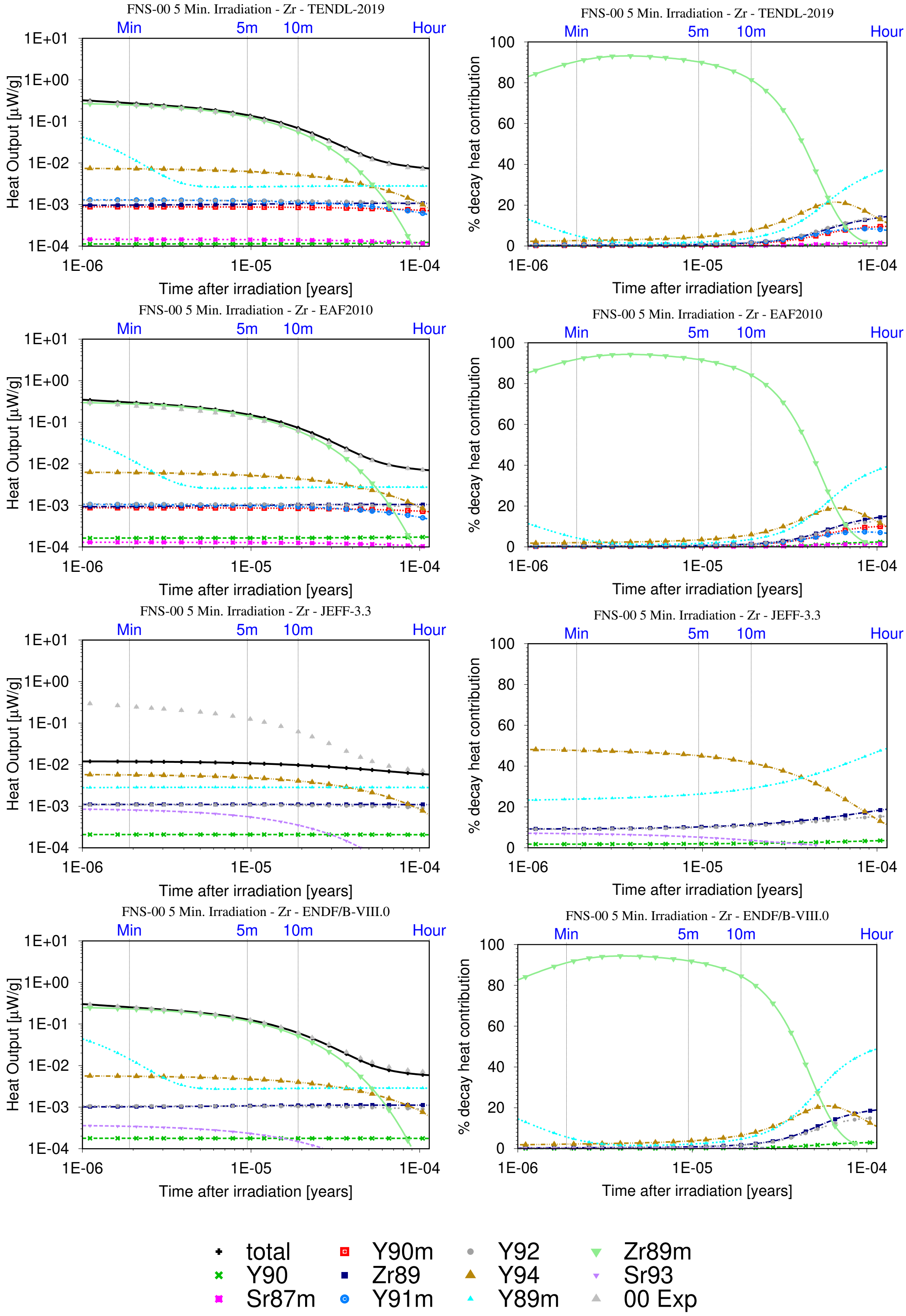


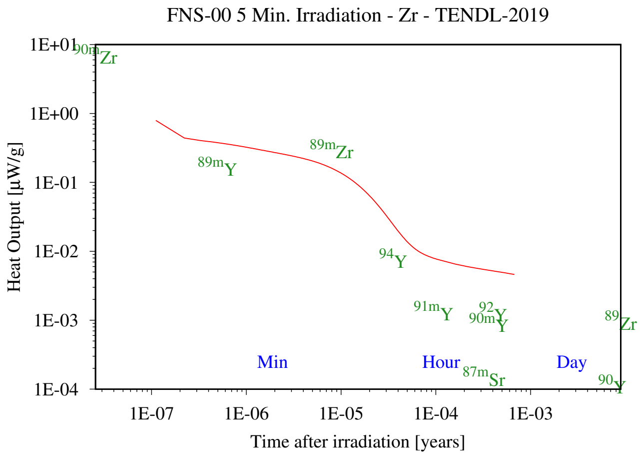
Zirconium, TENDL-2019 5-minute pathway analysis

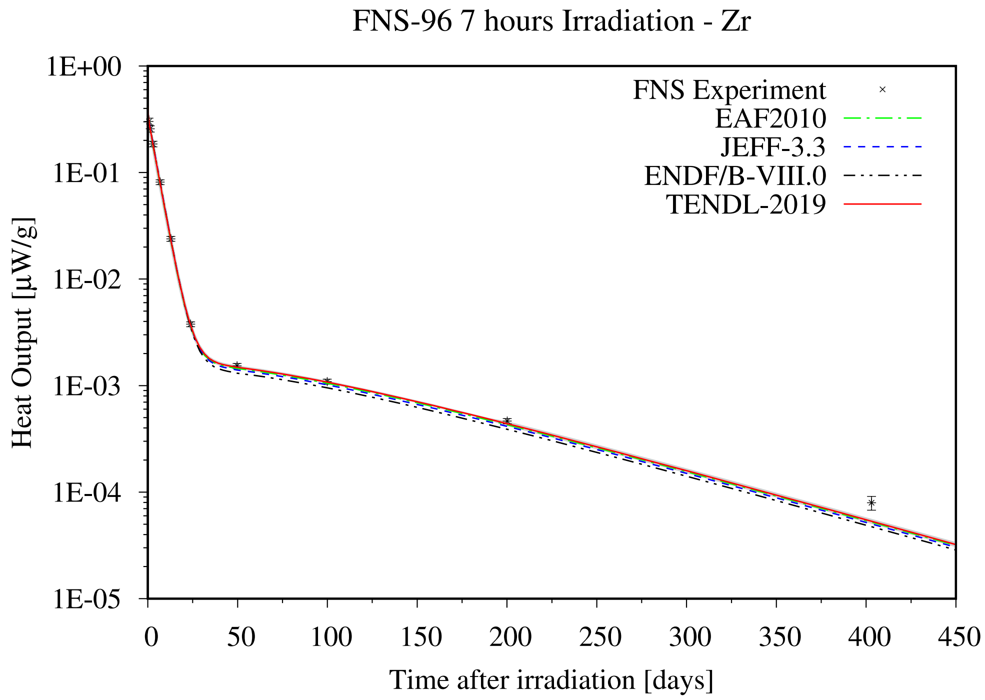
Product	$T_{1/2}$	Pathways	Path %
Y89m	15.66s	Zr90(n,np)Y89m	91.8
		Zr90(n,d)Y89m	6.5
		Zr90(n,2n)Zr89(β^+)Y89m	1.3
Zr89m	4.18m	Zr90(n,2n)Zr89m	100.0
Sr93	7.42m	Zr96(n,α)Sr93	100.0
Y94	18.70m	Zr94(n,p)Y94	100.0
Y91m	49.71m	Zr91(n,p)Y91m	83.7
		Zr92(n,np)Y91m	11.8
		Zr92(n,d)Y91m	4.5
Sr87m	2.82h	Zr90(n,α)Sr87m	99.8
Y90m	3.19h	Zr90(n,p)Y90m	90.8
		Zr91(n,np)Y90m	6.6
		Zr91(n,d)Y90m	2.5
Y92	3.54h	Zr92(n,p)Y92	99.9
Y90	2.67d	Zr90(n,p)Y90	90.0
		Zr91(n,np)Y90	7.3
		Zr91(n,d)Y90	2.1
Zr89	3.27d	Zr90(n,2n)Zr89	93.8
		Zr90(n,2n)Zr89m(IT)Zr89	6.2

Comments on Zirconium 5-minute experiments:

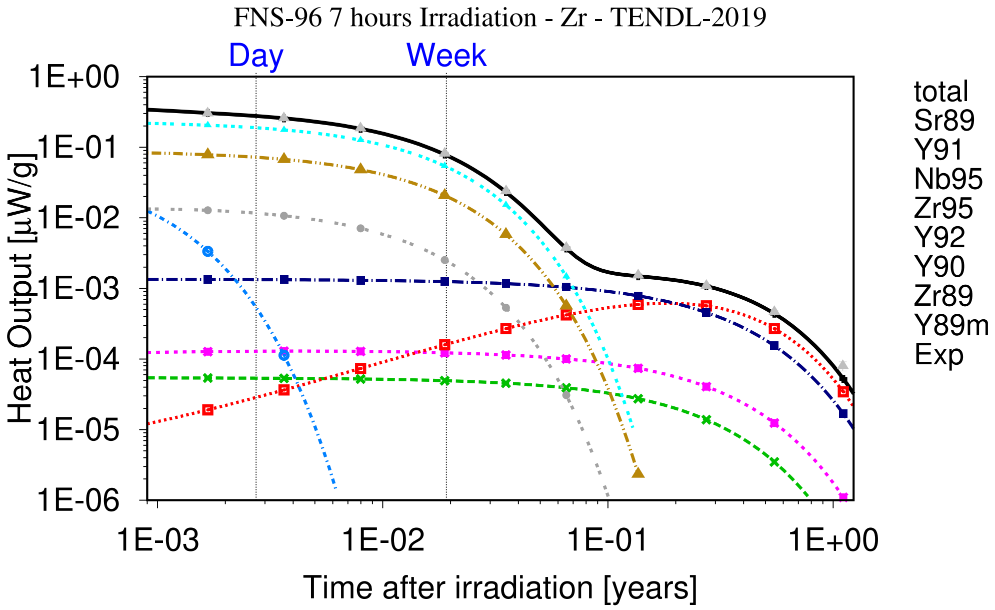
As this element is part of fission fuel cladding and is this very important, unusually, ENDF/B-VIII.0 includes the necessary production of the metastable Zr89m nuclide, which dominates the decay-heat below 10 minutes of cooling. This nuclide is also produced (via (n,2n) reactions on Zr90) in simulations with TENDL-2019 and EAF2010, but JEFF-3.3 omits it (also unexpected because it was included in JEFF-3.2 – see [7]). In fact, ENDF/B-VIII.0 gives the best agreement to the early phase of the decay profile in the two 5-minute experiments and has the best (lowest) average deviation from the 2000 experiment. However, TENDL-2019 gives the best visual agreement to the experimental decay profile, with a fairly uniform 5-10% over-prediction, while ENDF/B-VIII.0 seems to underestimate the decay heat at longer cooling times (after Zr89m falls away) despite also predicting the Y89m metastable (TENDL-2019 and EAF2010 also have this), which dominates after around 20 minutes of cooling. IRDFF-II is included here, but it is only suitable to observe the small, constant (on the experimental timescale) contribution from Zr89 (from (n,2n) on Zr90).


FNS-00 5 Min. Irradiation - Zr - TENDL-2019
FNS-00 5 Min. Irradiation - Zr - EAF2010
FNS-00 5 Min. Irradiation - Zr - JEFF-3.3
FNS-00 5 Min. Irradiation - Zr - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Y90
Sr87m
Y90m
Zr89
Y91m
Y92
Y94
Y89m
Zr89m
Sr93
00 Exp


FNS-00 5 Min. Irradiation - Zr - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-07
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]
90mZr
89mY
89mZr
94Y
91mY
92Y
90mY
89Zr
87mSr
90Y
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.61	3.02E−01 +/-7%	3.06E−01 +/-20%	0.99	0.97	1.00	0.97
1.33	2.57E−01 +/-7%	2.57E−01 +/-21%	1.00	0.98	1.02	0.98
2.91	1.85E−01 +/-6%	1.83E−01 +/-21%	1.01	0.99	1.03	0.99
6.88	8.12E−02 +/-5%	7.91E−02 +/-21%	1.03	1.01	1.04	1.01
12.88	2.39E−02 +/-5%	2.31E−02 +/-20%	1.03	1.02	1.05	1.02
23.85	3.77E−03 +/-5%	3.68E−03 +/-12%	1.02	1.07	1.05	1.04
49.71	1.53E−03 +/-5%	1.48E−03 +/-4%	1.03	1.17	1.06	1.09
99.90	1.09E−03 +/-5%	1.08E−03 +/-3%	1.01	1.14	1.03	1.07
200.12	4.64E−04 +/-6%	4.40E−04 +/-5%	1.06	1.19	1.08	1.12
402.96	7.94E−05 +/-15%	5.24E−05 +/-5%	1.52	1.71	1.55	1.61
mean % diff. from E			5	10	7	7
mean χ^2			0.74	3.01	1.13	1.49

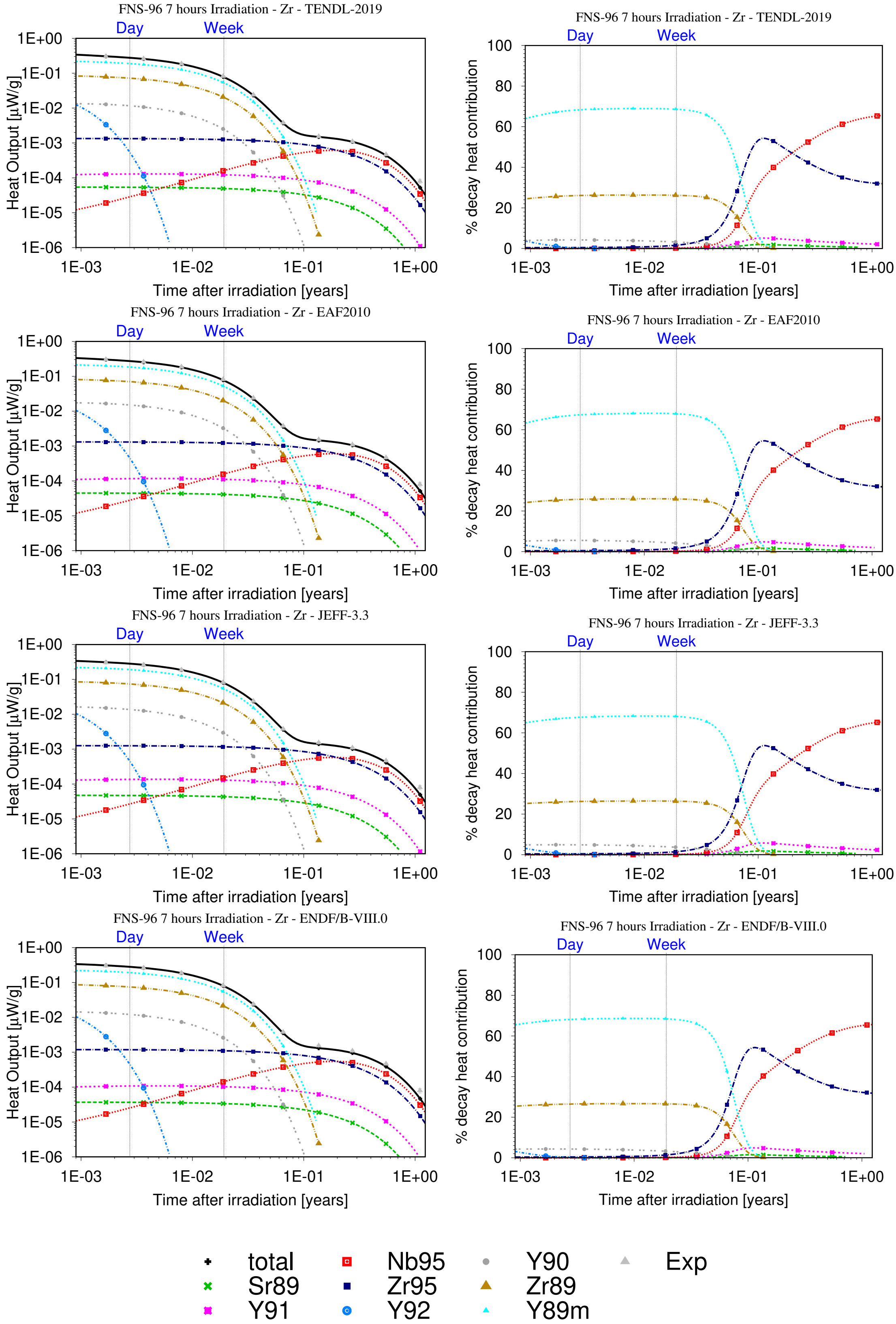


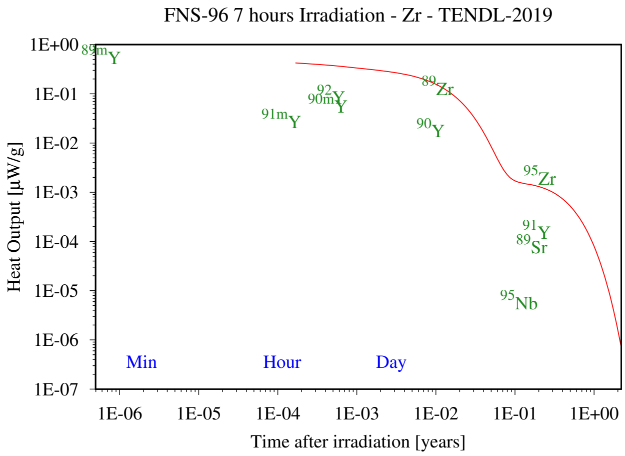
Zirconium,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Y89m	15.66s	Zr90(n,2n)Zr89(β^+)Y89m	51.4
		Zr90(n,np)Y89m	36.4
		Zr90(n,2n)Zr89m(IT)Zr89(β^+)Y89m	9.6
		Zr90(n,d)Y89m	2.5
Y92	3.54h	Zr92(n,p)Y92	99.9
Y90	2.67d	Zr90(n,p)Y90	71.8
		Zr90(n,p)Y90m(IT)Y90	19.9
		Zr91(n,np)Y90	5.1
		Zr91(n,d)Y90	1.5
		Zr91(n,np)Y90m(IT)Y90	1.2
Zr89	3.27d	Zr90(n,2n)Zr89	84.2
		Zr90(n,2n)Zr89m(IT)Zr89	15.8
Nb95	34.99d	Zr96(n,2n)Zr95(β^-)Nb95	98.4
		Zr96(n,2n)Zr95(β^-)Nb95m(IT)Nb95	1.1
Sr89	50.58d	Zr92(n,α)Sr89	100.0
Y91	58.52d	Zr91(n,p)Y91m(IT)Y91	51.1
		Zr91(n,p)Y91	29.5
		Zr92(n,np)Y91	5.8
		Zr92(n,np)Y91m(IT)Y91	5.3
		Zr92(n,d)Y91	2.9
		Zr92(n,d)Y91m(IT)Y91	2.3
		Zr94(n,α)Sr91(β^-)Y91m(IT)Y91	1.7
		Zr94(n,α)Sr91(β^-)Y91	1.5
Zr95	64.03d	Zr96(n,2n)Zr95	99.5

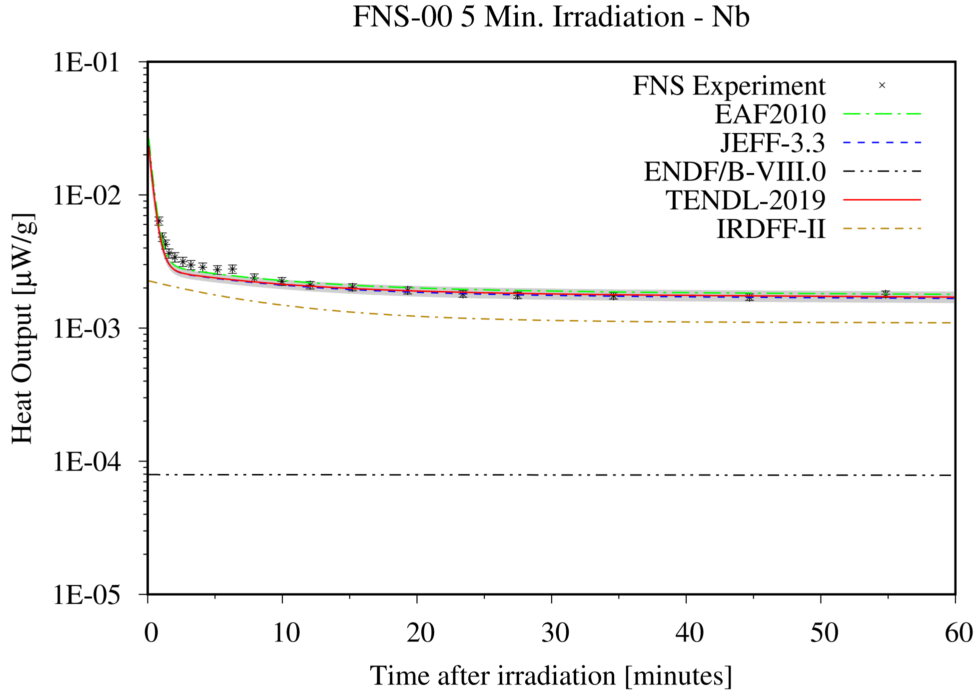
Comments on Zirconium 7-hour experiments:

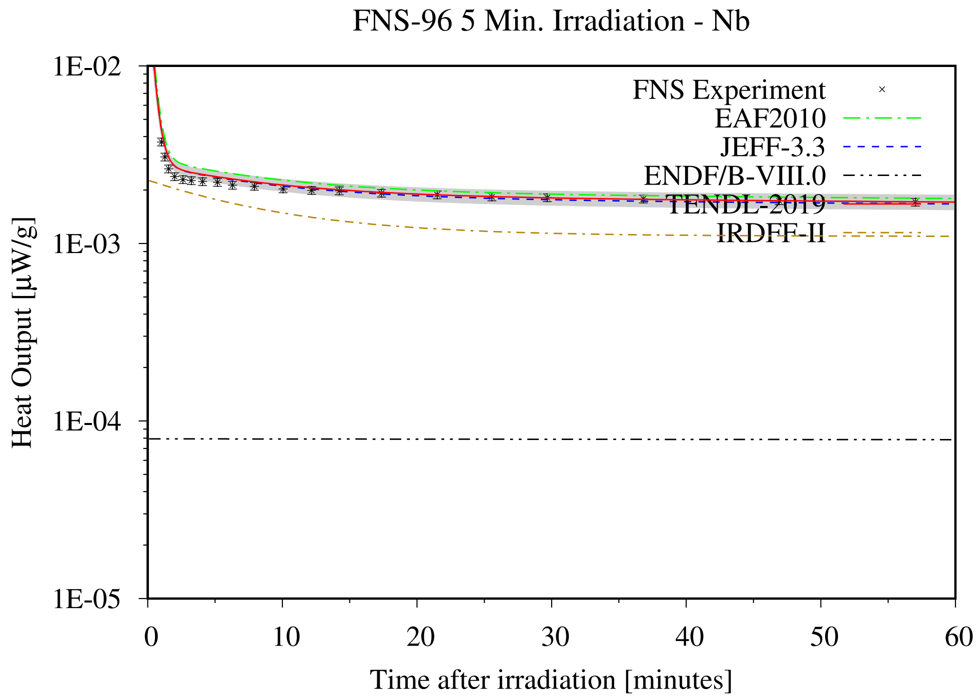
A complex simulation picture, with four different radionuclides contributing at least 20% of the decay-heat at some point during the simulations with all libraries considered, but excellent agreement exists between experiment and simulation (almost within experimental uncertainty in the case of TENDL-2019). Only in the last cooling step there is significant deviation, with all of the libraries underpredicting the experimental result. It is difficult to assess the cause of this – the Zn95 radionuclide and the Nb95 produced from it (via decay) follow the experimental profile at cooling times below 1-year, so their production seems properly simulated – perhaps an unknown impurity in the experimental sample? Alternatively, the decay properties of one or other of these nuclides may need adjustment.


FNS-96 7 hours Irradiation - Zr - TENDL-2019
Day
Week
Heat Output [µW/g]
Time after irradiation [years]
% decay heat contribution
FNS-96 7 hours Irradiation - Zr - EAF2010
FNS-96 7 hours Irradiation - Zr - JEFF-3.3
FNS-96 7 hours Irradiation - Zr - ENDF/B-VIII.0
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
total
Sr89
Y91
Nb95
Zr95
Y92
Y90
Zr89
Y89m
Exp

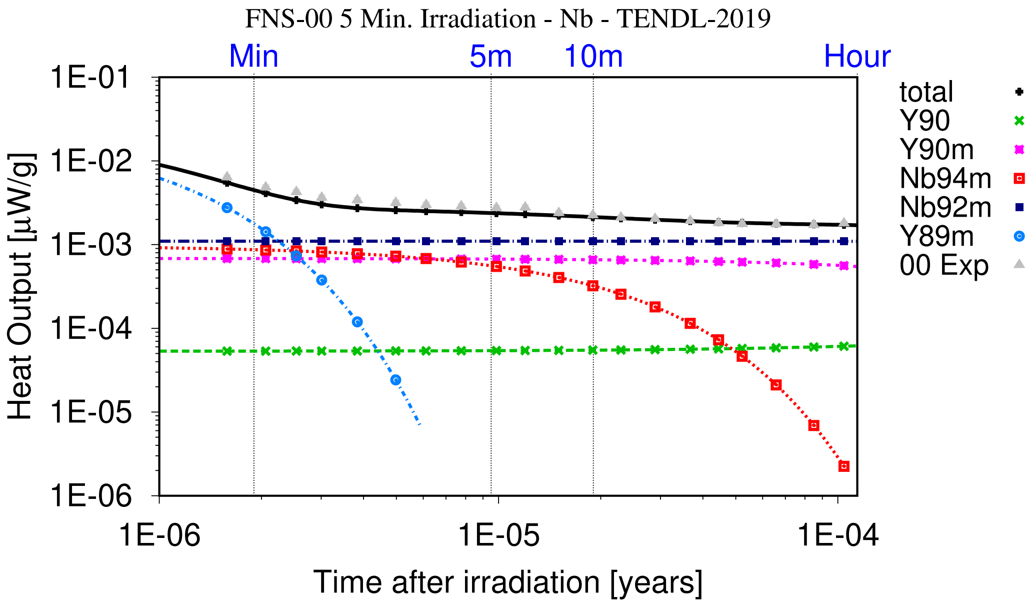

FNS-96 7 hours Irradiation - Zr - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
89mY
92Y
90mY
91mY
89Zr
90Y
95Zr
91Y
89Sr
95Nb
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Niobium


FNS-00 5 Min. Irradiation - Nb
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - Nb
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E-02
1E-03
1E-04
1E-05
0
10
20
30
40
50
60
Time after irradiation [minutes]

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
0.83	6.37E−03 +/-7%	5.49E−03 +/-14%	1.16	80.35	1.04	1.16	2.94
1.08	4.83E−03 +/-7%	4.12E−03 +/-11%	1.17	60.91	1.06	1.17	2.26
1.33	4.25E−03 +/-8%	3.41E−03 +/-8%	1.25	53.60	1.14	1.25	2.01
1.58	3.64E−03 +/-8%	3.03E−03 +/-7%	1.20	45.85	1.10	1.20	1.74
2.02	3.40E−03 +/-8%	2.73E−03 +/-7%	1.25	42.90	1.15	1.25	1.67
2.62	3.15E−03 +/-8%	2.58E−03 +/-7%	1.22	39.74	1.13	1.22	1.59
3.22	2.98E−03 +/-8%	2.51E−03 +/-7%	1.18	37.54	1.10	1.19	1.55
4.08	2.86E−03 +/-8%	2.45E−03 +/-8%	1.17	36.07	1.09	1.18	1.55
5.18	2.74E−03 +/-7%	2.37E−03 +/-8%	1.15	34.56	1.07	1.16	1.56
6.30	2.78E−03 +/-7%	2.31E−03 +/-8%	1.20	35.02	1.12	1.21	1.65
7.92	2.38E−03 +/-7%	2.22E−03 +/-8%	1.07	30.08	1.00	1.08	1.50
9.97	2.24E−03 +/-7%	2.14E−03 +/-8%	1.05	28.31	0.98	1.06	1.51
12.07	2.10E−03 +/-6%	2.07E−03 +/-9%	1.02	26.56	0.96	1.03	1.49
15.22	2.03E−03 +/-6%	1.98E−03 +/-9%	1.02	25.64	0.97	1.04	1.54
19.32	1.92E−03 +/-6%	1.91E−03 +/-9%	1.01	24.29	0.95	1.03	1.55
23.42	1.81E−03 +/-6%	1.86E−03 +/-9%	0.97	22.86	0.92	0.99	1.52
27.48	1.76E−03 +/-6%	1.82E−03 +/-10%	0.97	22.32	0.92	0.99	1.53
34.60	1.75E−03 +/-6%	1.78E−03 +/-10%	0.98	22.17	0.94	1.01	1.56
44.70	1.71E−03 +/-6%	1.75E−03 +/-10%	0.98	21.73	0.93	1.00	1.55
54.82	1.80E−03 +/-6%	1.72E−03 +/-10%	1.04	22.88	1.00	1.07	1.63
mean % diff. from E			10	97	7	10	39
mean χ^2			2.45	210.79	1.18	2.58	35.05

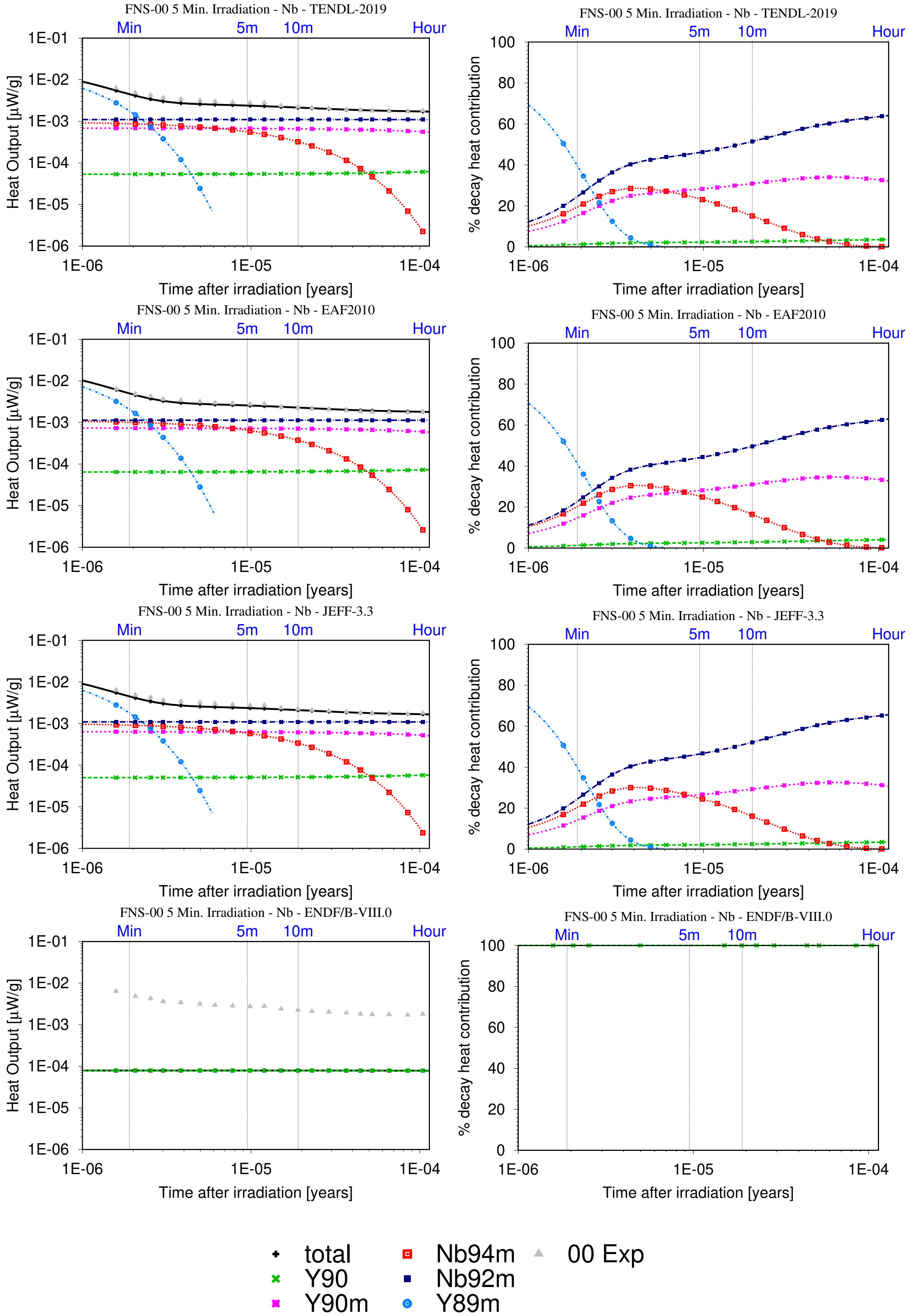


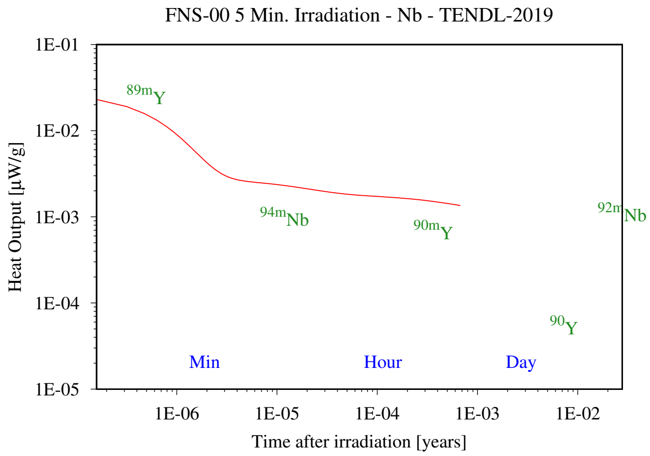
Niobium, TENDL-2019 5-minute pathway analysis

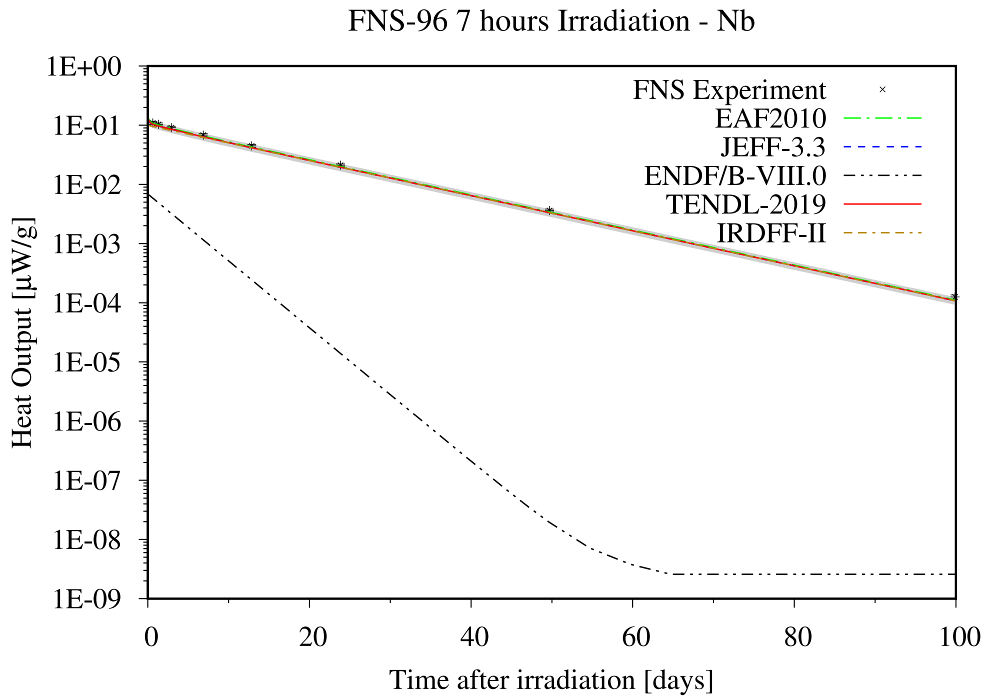
Product	**$T_{1/2}$**	**Pathways**	**Path %**
Y89m	15.66s	Nb93(n,nα)Y89m	100.0
Nb94m	6.26m	Nb93(n,γ)Nb94m	100.0
Y90m	3.19h	Nb93(n,α)Y90m	100.0
Y90	2.67d	Nb93(n,α)Y90	99.2
Nb92m	10.15d	Nb93(n,2n)Nb92m	100.0

Comments on Niobium 5-minute experiments:

ENDF/B-VIII.0 does very badly here, completely missing the production of metastables Nb94m, Nb92m, Y90m, and Y89m, which all provide contributions of at least 20% to the decay-heat at some time in the simulations with the other libraries. That library only contains the reaction channel to produce Y90 and thus dramatically underpredicts the measurements. All other libraries considered give a good agreement to both experimental batches and clearly well represent this relatively complex picture dominated by four competing metastable nuclides. JEFF-3.3, in particular, has improved relative to earlier versions of that library (see the JEFF-3.2 results in [7]). In IRDFF-II, Nb93(n,2n)Nb92m is the only reaction pathway that is relevant for this experiment, contributing more than 60% after around 30 minutes of cooling, and so this library performs better than ENDF/B-VIII.0 for this case.


FNS-00 5 Min. Irradiation - Nb - TENDL-2019
FNS-00 5 Min. Irradiation - Nb - EAF2010
FNS-00 5 Min. Irradiation - Nb - JEFF-3.3
FNS-00 5 Min. Irradiation - Nb - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
1E-06
1E-05
1E-04
total
Y90
Y90m
Nb94m
Nb92m
Y89m
00 Exp

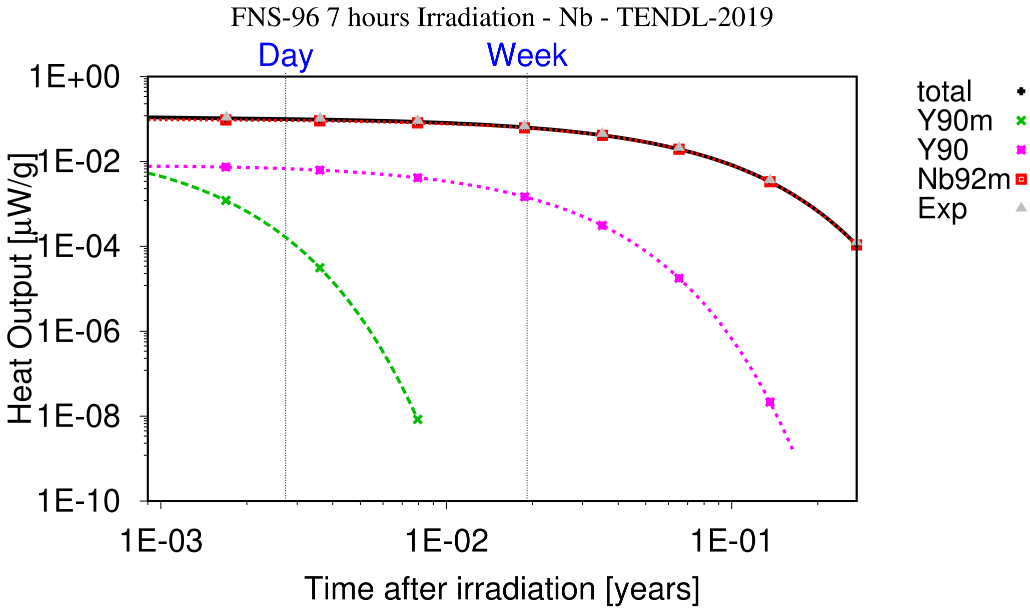

FNS-00 5 Min. Irradiation - Nb - TENDL-2019
1E-01
1E-02
1E-03
1E-04
1E-05
Heat Output [μW/g]
89mY
94mNb
90mY
92mNb
90Y
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.62	1.09$E-$01 +/-6%	1.04$E-$01 +/-13%	1.05	18.68	1.01	1.06	1.15
1.32	1.03$E-$01 +/-6%	9.70$E-$02 +/-14%	1.06	21.11	1.02	1.07	1.14
2.90	9.08$E-$02 +/-6%	8.56$E-$02 +/-14%	1.06	28.02	1.02	1.06	1.11
6.86	6.81$E-$02 +/-6%	6.36$E-$02 +/-14%	1.07	58.94	1.04	1.07	1.10
12.86	4.48$E-$02 +/-5%	4.16$E-$02 +/-15%	1.08	184.46	1.05	1.08	1.09
23.85	2.10$E-$02 +/-5%	1.95$E-$02 +/-15%	1.08	$>$ 1000	1.05	1.08	1.08
49.70	3.62$E-$03 +/-5%	3.33$E-$03 +/-15%	1.09	$>$ 1000	1.06	1.09	1.09
99.89	1.25$E-$04 +/-8%	1.09$E-$04 +/-15%	1.15	$>$ 1000	1.12	1.15	1.15
mean % diff. from E			7	98	4	8	10
mean χ^2			1.60	290.06	0.63	1.67	2.99

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Nb92m	10.15d	1.05	6%	15%

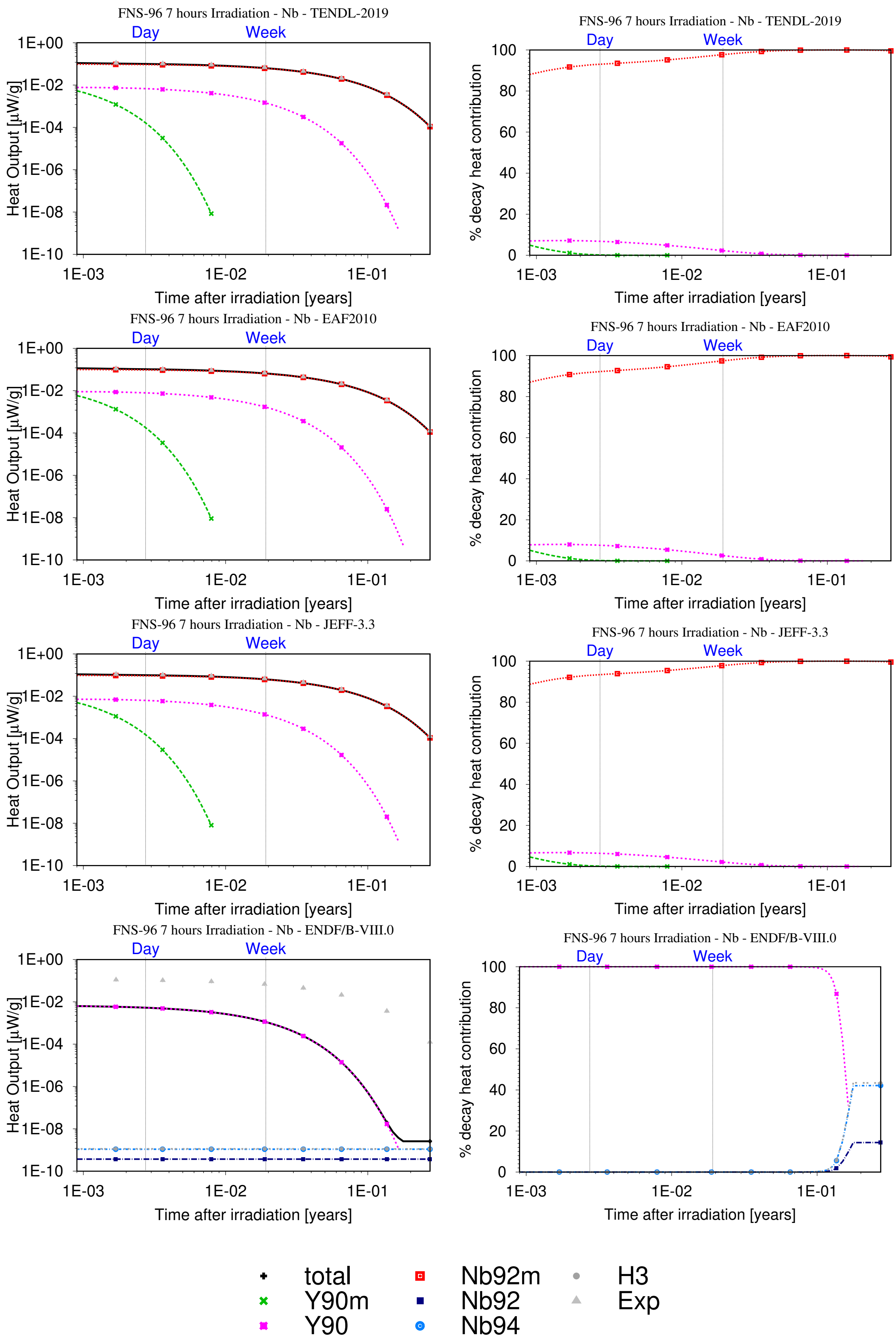


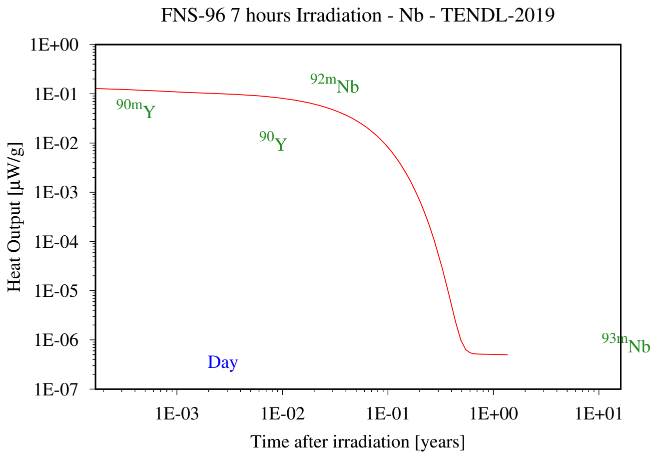
Niobium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Y90m	3.19h	Nb93(n,α)Y90m	100.0
Y90	2.67d	Nb93(n,α)Y90	68.9
		Nb93(n,α)Y90m(IT)Y90	31.1
Nb92m	10.15d	Nb93(n,2n)Nb92m	100.0
H3	12.33y	Nb93(n,t)H3	100.0
Nb94	2.0 10^4y	Nb93(n,γ)Nb94m(IT)Nb94	55.9
		Nb93(n,γ)Nb94	44.1
Nb92	3.5 10^7y	Nb93(n,2n)Nb92	100.0

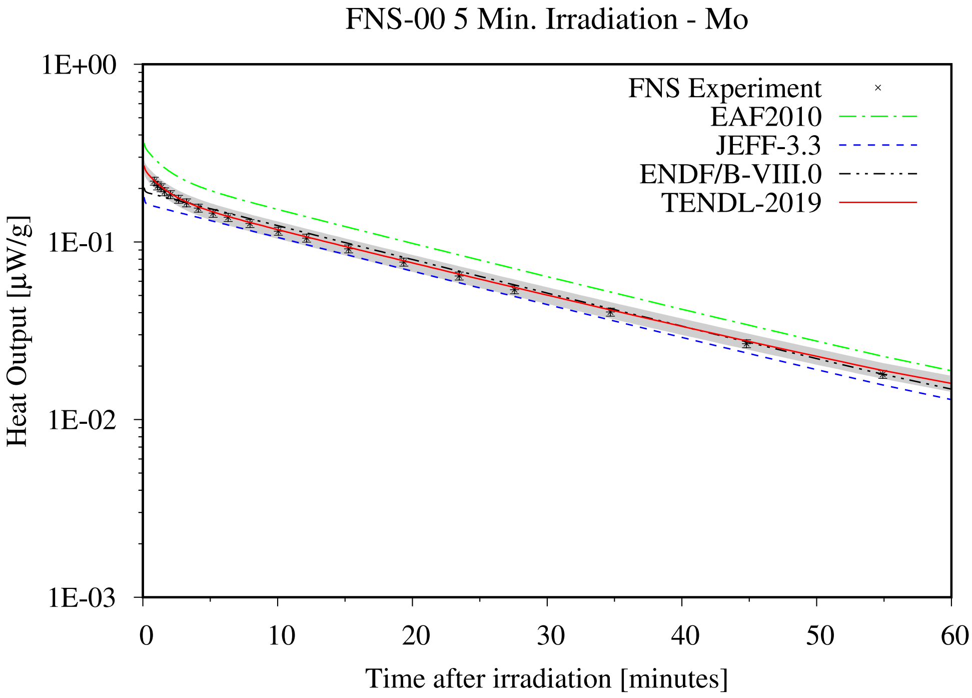
Comments on Niobium 7-hour experiments:

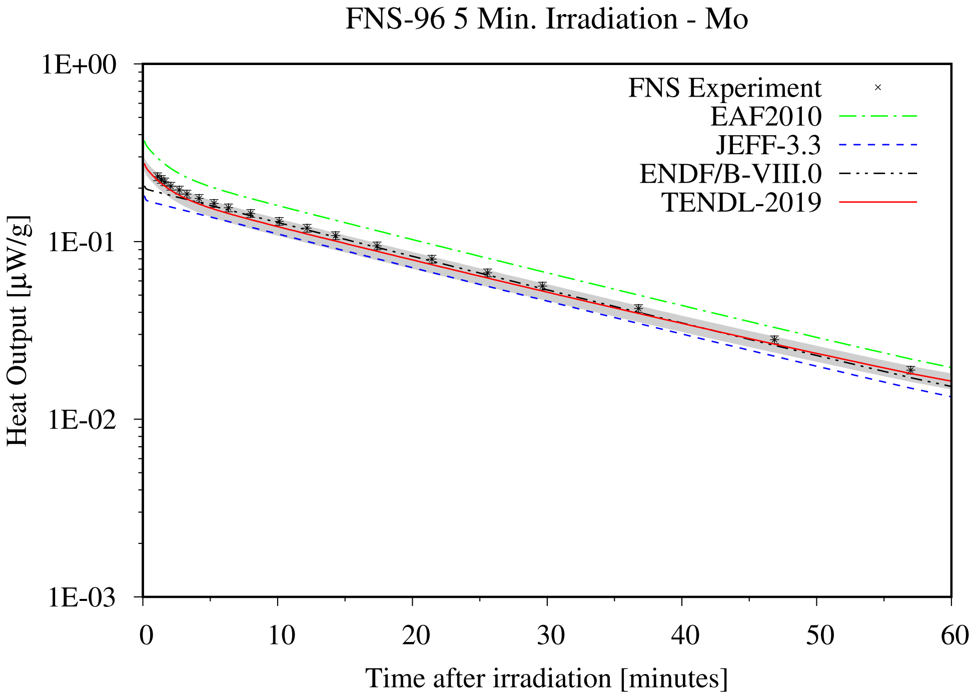
A superb agreement is seen here for predictions with TENDL-2019, JEFF-3.3, EAF2010, and IRDFF-II, due to the correct production of Nb92m via (n,2n) reactions. As in the 5-minute experiments, ENDF/B-VIII.0 is severely discrepant because it misses the production of that metastable, instead producing a completely different, and obviously erroneous, profile of contributing nuclides.


FNS-96 7 hours Irradiation - Nb - TENDL-2019
FNS-96 7 hours Irradiation - Nb - EAF2010
FNS-96 7 hours Irradiation - Nb - JEFF-3.3
FNS-96 7 hours Irradiation - Nb - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-02
1E-04
1E-06
1E-08
1E-10
1E-03
1E-01
0
20
40
60
80
100
total
Y90m
Y90
Nb92m
Nb92
Nb94
H3
Exp


FNS-96 7 hours Irradiation - Nb - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-03
1E-02
1E-01
1E+00
1E+01
Time after irradiation [years]
92mNb
90mY
90Y
93mNb
Day

Molybdenum


FNS-00 5 Min. Irradiation - Mo
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

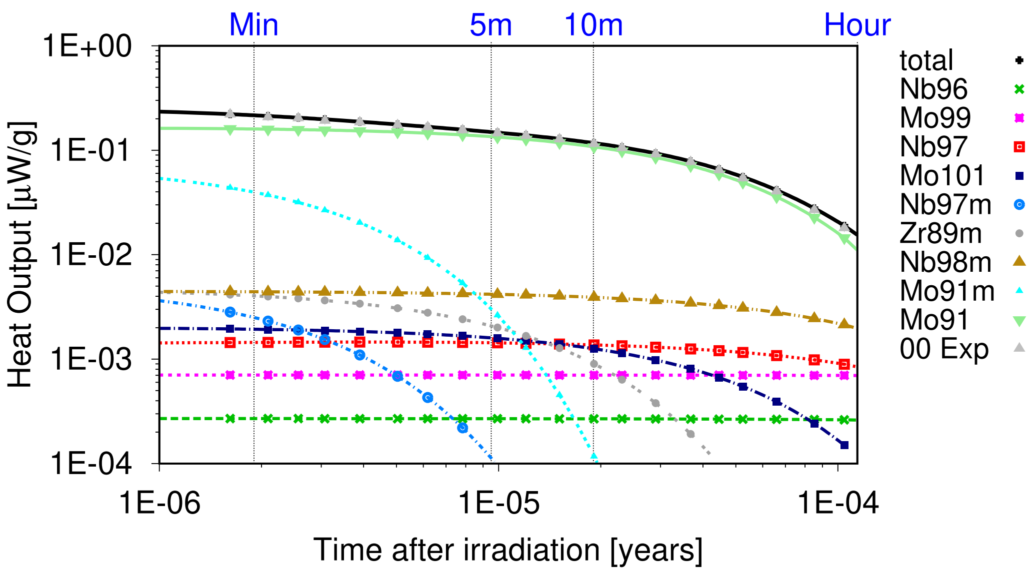

FNS-96 5 Min. Irradiation - Mo
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	2.20$E-$01 +/-5%	2.21$E-$01 +/-9%	0.99	1.19	0.75	1.39
1.10	2.07$E-$01 +/-5%	2.13$E-$01 +/-9%	0.97	1.13	0.73	1.32
1.35	2.02$E-$01 +/-5%	2.05$E-$01 +/-9%	0.99	1.12	0.74	1.30
1.62	1.92$E-$01 +/-5%	1.98$E-$01 +/-10%	0.97	1.07	0.73	1.25
2.05	1.85$E-$01 +/-5%	1.88$E-$01 +/-10%	0.98	1.05	0.75	1.23
2.65	1.74$E-$01 +/-5%	1.77$E-$01 +/-10%	0.98	1.02	0.75	1.19
3.25	1.66$E-$01 +/-5%	1.68$E-$01 +/-10%	0.99	1.00	0.76	1.16
4.12	1.55$E-$01 +/-5%	1.58$E-$01 +/-11%	0.98	0.97	0.75	1.13
5.22	1.45$E-$01 +/-5%	1.48$E-$01 +/-11%	0.98	0.95	0.75	1.11
6.33	1.38$E-$01 +/-5%	1.39$E-$01 +/-11%	0.99	0.95	0.76	1.10
7.95	1.27$E-$01 +/-5%	1.29$E-$01 +/-11%	0.99	0.94	0.76	1.10
10.05	1.15$E-$01 +/-5%	1.17$E-$01 +/-11%	0.98	0.93	0.76	1.09
12.15	1.05$E-$01 +/-5%	1.07$E-$01 +/-11%	0.98	0.94	0.76	1.09
15.27	9.15$E-$02 +/-5%	9.33$E-$02 +/-11%	0.98	0.93	0.76	1.09
19.37	7.70$E-$02 +/-5%	7.83$E-$02 +/-11%	0.98	0.94	0.76	1.09
23.47	6.44$E-$02 +/-5%	6.59$E-$02 +/-11%	0.98	0.94	0.76	1.09
27.58	5.38$E-$02 +/-5%	5.55$E-$02 +/-11%	0.97	0.94	0.76	1.09
34.70	4.03$E-$02 +/-5%	4.15$E-$02 +/-11%	0.97	0.96	0.77	1.11
44.80	2.67$E-$02 +/-5%	2.78$E-$02 +/-10%	0.96	0.98	0.78	1.13
54.90	1.80$E-$02 +/-5%	1.89$E-$02 +/-10%	0.95	1.00	0.79	1.15
mean % diff. from E			2	6	32	13
mean χ^2			0.22	1.87	39.81	8.13

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	**$T_{1/2}$**	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Mo91	15.49m	0.99	5%	12%

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

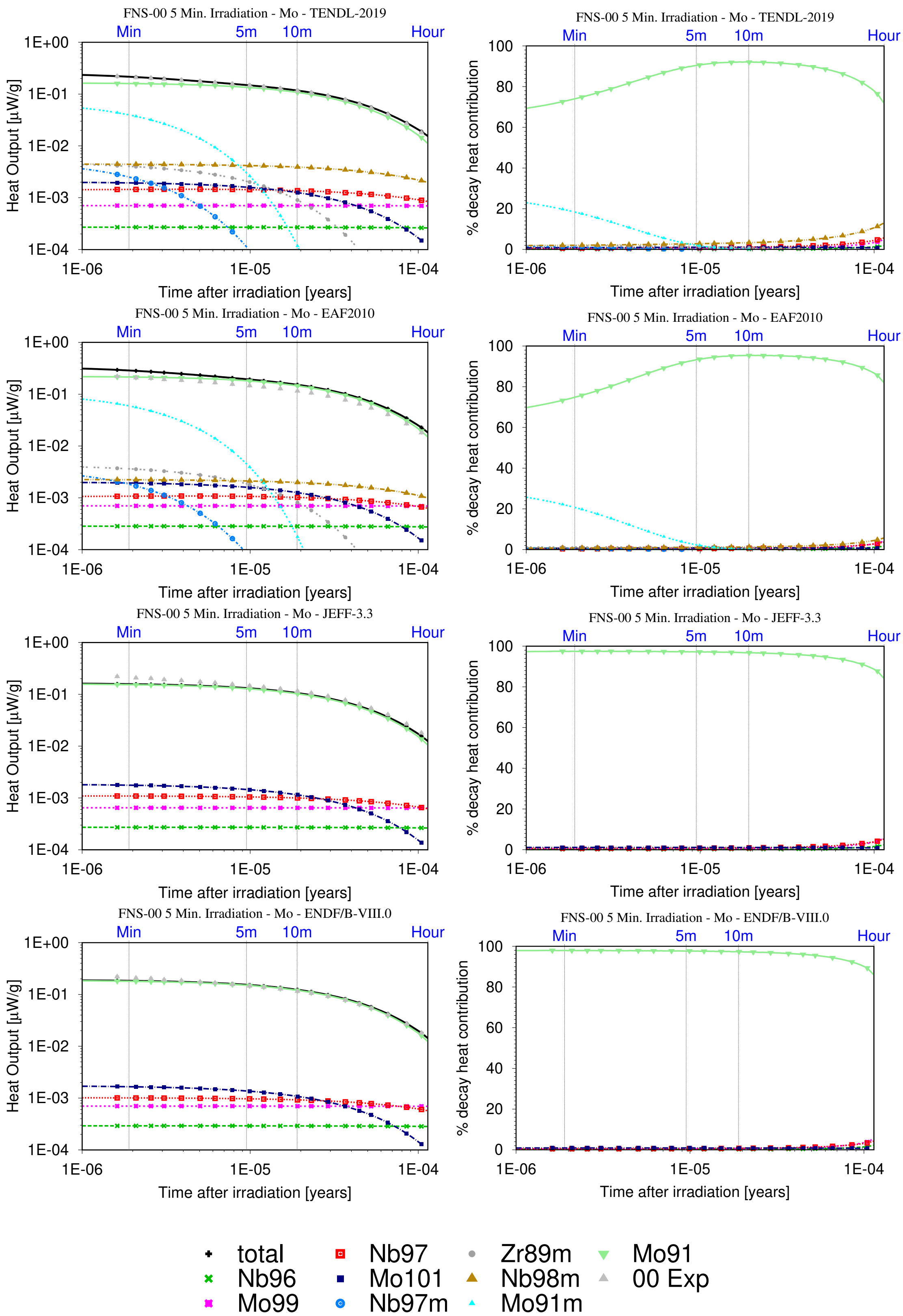


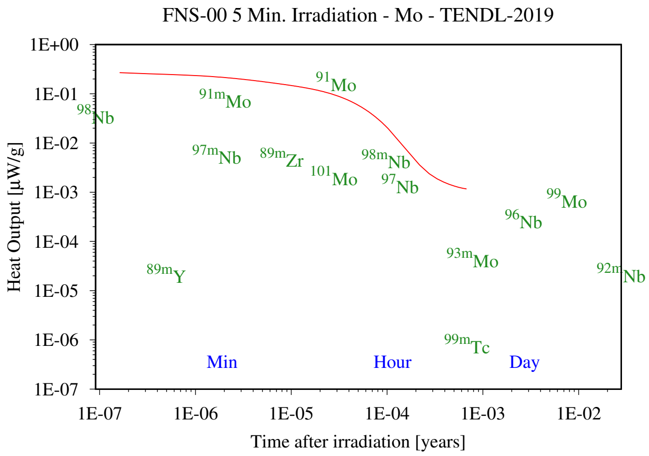
Molybdenum, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Nb97m	52.71s	Mo97(n,p)Nb97m	79.8
		Mo98(n,d)Nb97m	17.1
		Mo98(n,np)Nb97m	3.0
Mo91m	1.08m	Mo92(n,2n)Mo91m	100.0
Zr89m	4.18m	Mo92(n,α)Zr89m	100.0
Mo101	14.61m	Mo100(n,γ)Mo101	100.0
Mo91	15.49m	Mo92(n,2n)Mo91	95.7
		Mo92(n,2n)Mo91m(IT)Mo91	4.3
Nb98m	51.30m	Mo98(n,p)Nb98m	100.0
Nb97	1.20h	Mo97(n,p)Nb97	61.0
		Mo97(n,p)Nb97m(IT)Nb97	17.3
		Mo98(n,np)Nb97	13.4
		Mo98(n,d)Nb97	4.0
		Mo98(n,d)Nb97m(IT)Nb97	3.7
Nb96	23.35h	Mo96(n,p)Nb96	92.3
		Mo97(n,np)Nb96	4.0
		Mo97(n,d)Nb96	3.7
Mo99	2.75d	Mo100(n,2n)Mo99	99.1

Comments on Molybdenum 5-minute experiments:

There is slight, unexplained difference between the two otherwise identical experimental batches for molybdenum. However, TENDL-2019, JEFF-3.3, and ENDF/B-VIII.0 give good agreement to the experiments. TENDL-2019, in particular, produces a remarkably close match to the 2000 experiment, well within the experimental uncertainty, while ENDF/B-VIII.0 does the same when compared to the 1996 experiment. Unusually, EAF2010 seems to consistently overpredict, which suggests that an error in the Mo92(n,2n)Mo91 cross section has been corrected in the nuclear data field since the generation of that legacy-style library. There is a minor contribution (max. 20%) from Mo91m during the first 5-minutes of cooling in the TENDL-2019 (and EAF2010) simulations, which could explain why that library, in particular, produces a good, uniform match at all cooling times – JEFF-3.3. and ENDF/B-VIII.0 miss that metastable isomer and show a varying agreement profile, which is worse at shorter cooling times.


FNS-00 5 Min. Irradiation - Mo - TENDL-2019
Min
5m
10m
Hour
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Mo - TENDL-2019
% decay heat contribution
100
80
60
40
20
0
FNS-00 5 Min. Irradiation - Mo - EAF2010
FNS-00 5 Min. Irradiation - Mo - JEFF-3.3
FNS-00 5 Min. Irradiation - Mo - ENDF/B-VIII.0
total
Nb97
Zr89m
Mo91
Nb96
Mo101
Nb98m
00 Exp
Mo99
Nb97m
Mo91m


FNS-00 5 Min. Irradiation - Mo - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
91Mo
91mMo
98Nb
97mNb
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97Nb
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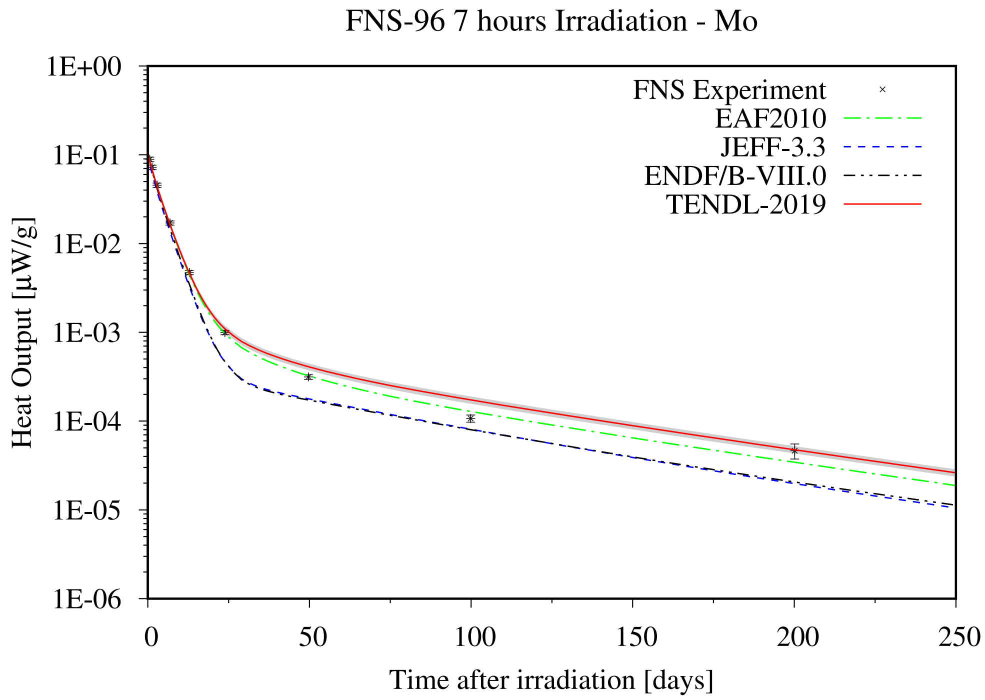
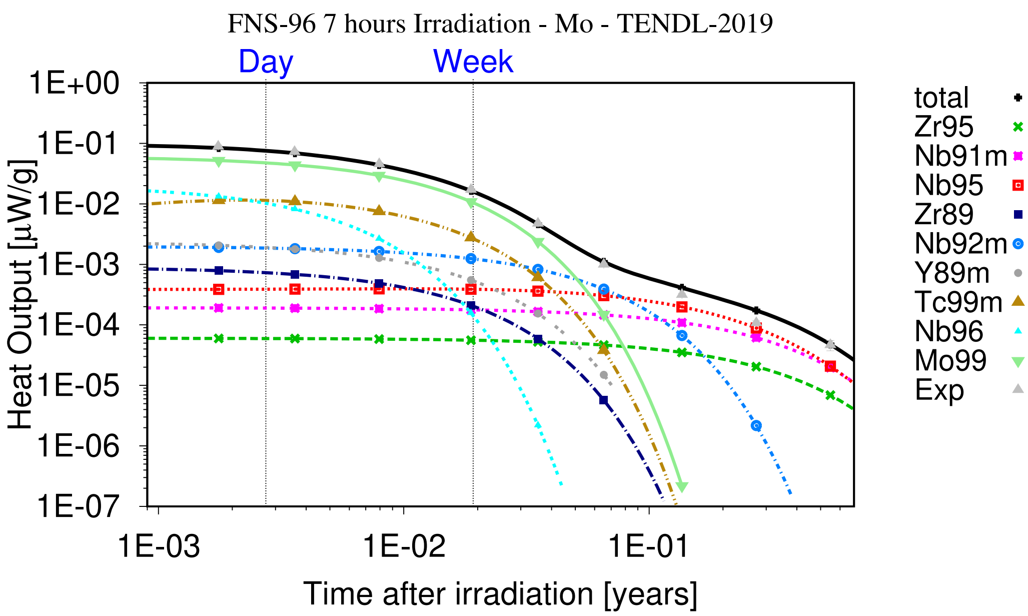
89mY
92mNb
99mTc
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.64	8.87$E-$02 +/-6%	8.38$E-$02 +/-8%	1.06	1.09	1.05	1.18
1.31	7.23$E-$02 +/-6%	6.87$E-$02 +/-8%	1.05	1.09	1.05	1.17
2.90	4.54$E-$02 +/-5%	4.39$E-$02 +/-8%	1.03	1.09	1.04	1.17
6.86	1.70$E-$02 +/-5%	1.64$E-$02 +/-8%	1.04	1.16	1.06	1.24
12.86	4.71$E-$03 +/-5%	4.64$E-$03 +/-7%	1.02	1.35	1.06	1.44
23.86	9.95$E-$04 +/-5%	1.10$E-$03 +/-9%	0.91	2.14	1.02	2.14
49.71	3.14$E-$04 +/-6%	4.10$E-$04 +/-9%	0.77	1.82	0.97	1.76
99.90	1.07$E-$04 +/-9%	1.73$E-$04 +/-10%	0.62	1.34	0.83	1.32
200.14	4.64$E-$05 +/-19%	4.77$E-$05 +/-9%	0.97	2.25	1.35	2.35
mean % diff. from E			14	27	8	30
mean χ^2			8.44	22.64	1.22	25.56

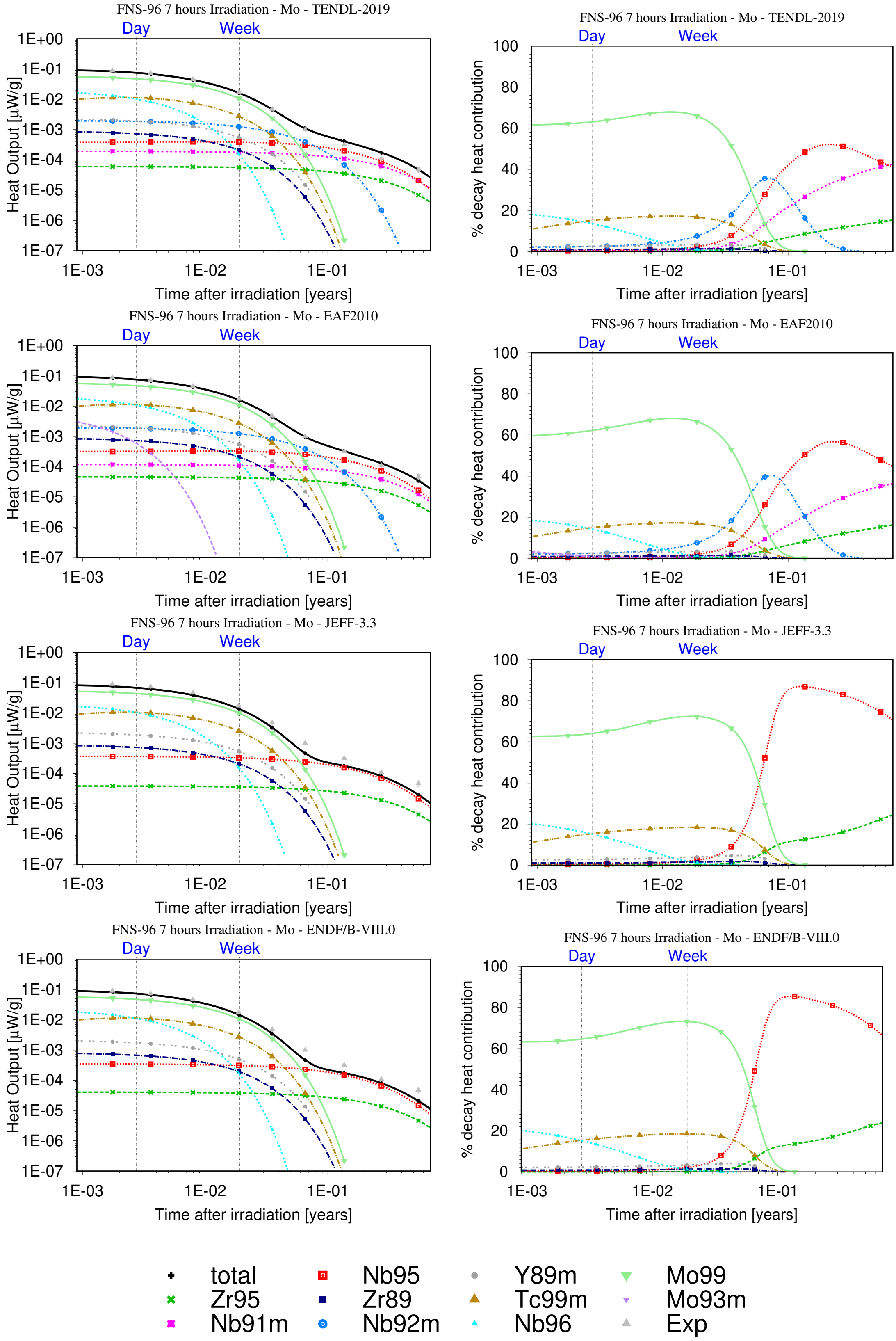


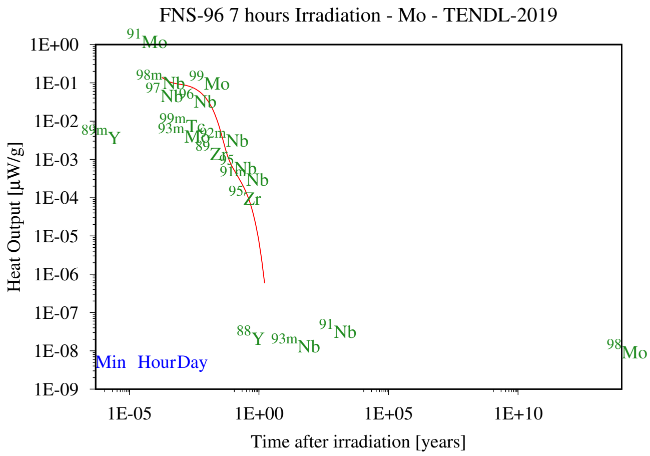
Molybdenum,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Y89m	15.66s	Mo92(n,α)Zr89(β^+)Y89m	71.7
		Mo92(n,α)Zr89m(IT)Zr89(β^+)Y89m	28.3
Tc99m	6.01h	Mo100(n,2n)Mo99(β^-)Tc99m	99.6
Mo93m	6.85h	Mo94(n,2n)Mo93m	97.7
		Mo92(n,γ)Mo93m	2.3
Nb96	23.35h	Mo96(n,p)Nb96	93.8
		Mo97(n,d)Nb96	3.1
		Mo97(n,np)Nb96	3.1
Mo99	2.75d	Mo100(n,2n)Mo99	99.6
Zr89	3.27d	Mo92(n,α)Zr89	71.7
		Mo92(n,α)Zr89m(IT)Zr89	28.3
Nb92m	10.15d	Mo92(n,p)Nb92m	100.0
Nb95	34.99d	Mo95(n,p)Nb95	86.8
		Mo96(n,d)Nb95	6.9
		Mo96(n,np)Nb95	5.6
Nb91m	60.92d	Mo92(n,np)Nb91m	94.0
		Mo92(n,2n)Mo91m(β^+)Nb91m	3.7
		Mo92(n,d)Nb91m	2.3
Zr95	64.03d	Mo98(n,α)Zr95	100.0

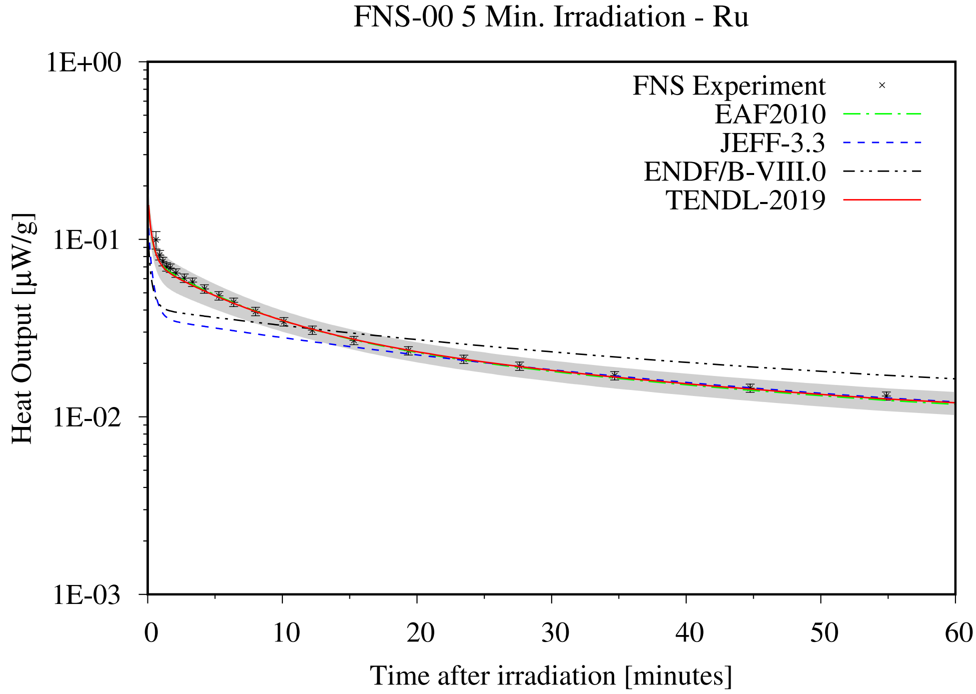
Comments on Molybdenum 7-hour experiments:

The complex decay heat picture predicted by TENDL-2019 (and EAF2010) – with many contributing nuclides, particularly beyond 10 days of cooling – reproduces the experimentally measured profile for 200 days of cooling. ENDF/B-VIII.0 and JEFF-3.3 begin to underestimate the decay heat from around 10 days of cooling, primarily because of the absence of two metastable radionuclides: Nb92m via Mo92(n,p) and Nb91m via Mo92(n,np), which provide important contributions in the simulations with EAF2010 and TENDL-2019 (Nb92m is actually dominant at the 24-minute measurement time).


FNS-96 7 hours Irradiation - Mo - TENDL-2019
FNS-96 7 hours Irradiation - Mo - EAF2010
FNS-96 7 hours Irradiation - Mo - JEFF-3.3
FNS-96 7 hours Irradiation - Mo - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
100
80
60
40
20
0
total
Zr95
Nb91m
Nb95
Zr89
Nb92m
Y89m
Tc99m
Nb96
Mo99
Mo93m
Exp


FNS-96 7 hours Irradiation - Mo - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
1E-09
1E-05
1E+00
1E+05
1E+10
Min
Hour
Day
91Mo
98mNb
97Nb
96Nb
99Mo
99mTc
93mMo
92mNb
89Zr
95Nb
91mNb
95Zr
89mY
88Y
93mNb
91Nb
98Mo

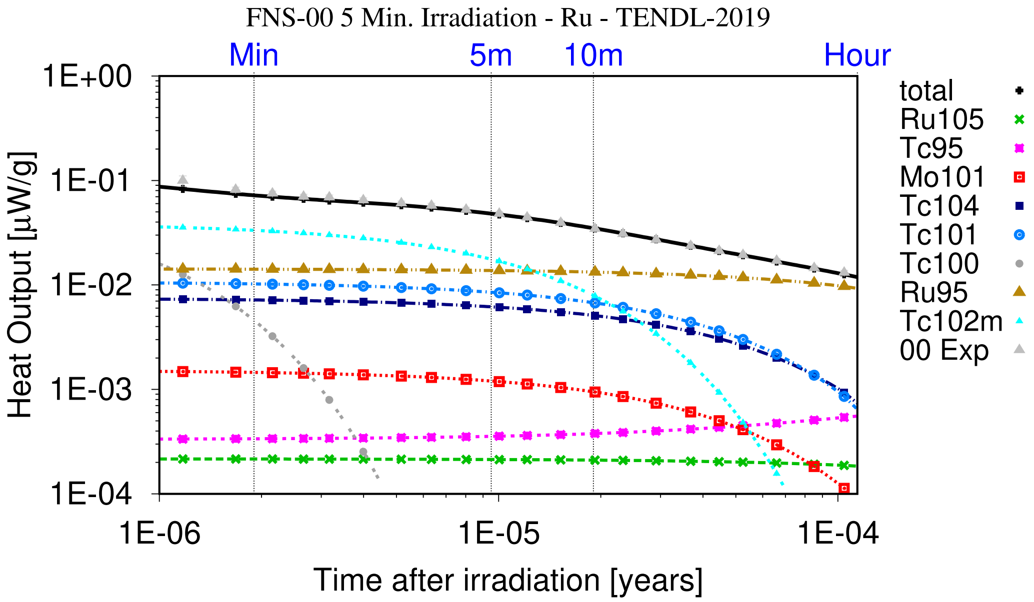
Ruthenium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.62	9.93E−02 +/-11%	8.30E−02 +/-18%	1.20	2.14	1.20	2.06
0.88	8.15E−02 +/-6%	7.46E−02 +/-19%	1.09	1.90	1.09	1.97
1.13	7.50E−02 +/-6%	6.99E−02 +/-19%	1.07	1.82	1.06	1.96
1.40	7.00E−02 +/-5%	6.67E−02 +/-19%	1.05	1.74	1.03	1.92
1.67	6.89E−02 +/-5%	6.43E−02 +/-19%	1.07	1.74	1.05	1.95
2.10	6.46E−02 +/-5%	6.13E−02 +/-19%	1.05	1.66	1.04	1.88
2.72	6.04E−02 +/-5%	5.79E−02 +/-18%	1.04	1.58	1.03	1.79
3.33	5.74E−02 +/-5%	5.49E−02 +/-18%	1.05	1.52	1.03	1.74
4.22	5.25E−02 +/-5%	5.12E−02 +/-17%	1.03	1.42	1.01	1.63
5.28	4.81E−02 +/-5%	4.72E−02 +/-16%	1.02	1.33	1.01	1.53
6.38	4.42E−02 +/-5%	4.36E−02 +/-15%	1.01	1.25	1.01	1.45
8.02	3.93E−02 +/-5%	3.92E−02 +/-14%	1.00	1.15	1.00	1.34
10.12	3.43E−02 +/-5%	3.47E−02 +/-14%	0.99	1.05	0.99	1.23
12.23	3.08E−02 +/-5%	3.12E−02 +/-13%	0.99	0.98	0.99	1.16
15.32	2.69E−02 +/-5%	2.73E−02 +/-13%	0.99	0.91	0.99	1.09
19.37	2.36E−02 +/-5%	2.37E−02 +/-13%	0.99	0.86	1.00	1.04
23.48	2.11E−02 +/-5%	2.12E−02 +/-13%	1.00	0.82	1.01	1.01
27.62	1.93E−02 +/-5%	1.92E−02 +/-13%	1.01	0.80	1.02	1.00
34.68	1.70E−02 +/-5%	1.68E−02 +/-14%	1.02	0.78	1.03	1.00
44.75	1.45E−02 +/-5%	1.44E−02 +/-14%	1.01	0.76	1.03	1.00
54.87	1.31E−02 +/-5%	1.26E−02 +/-15%	1.04	0.76	1.06	1.02
mean % diff. from E			4	29	3	27
mean χ^2			0.52	29.72	0.42	32.41

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ru95	1.64h	1.04	5%	19%

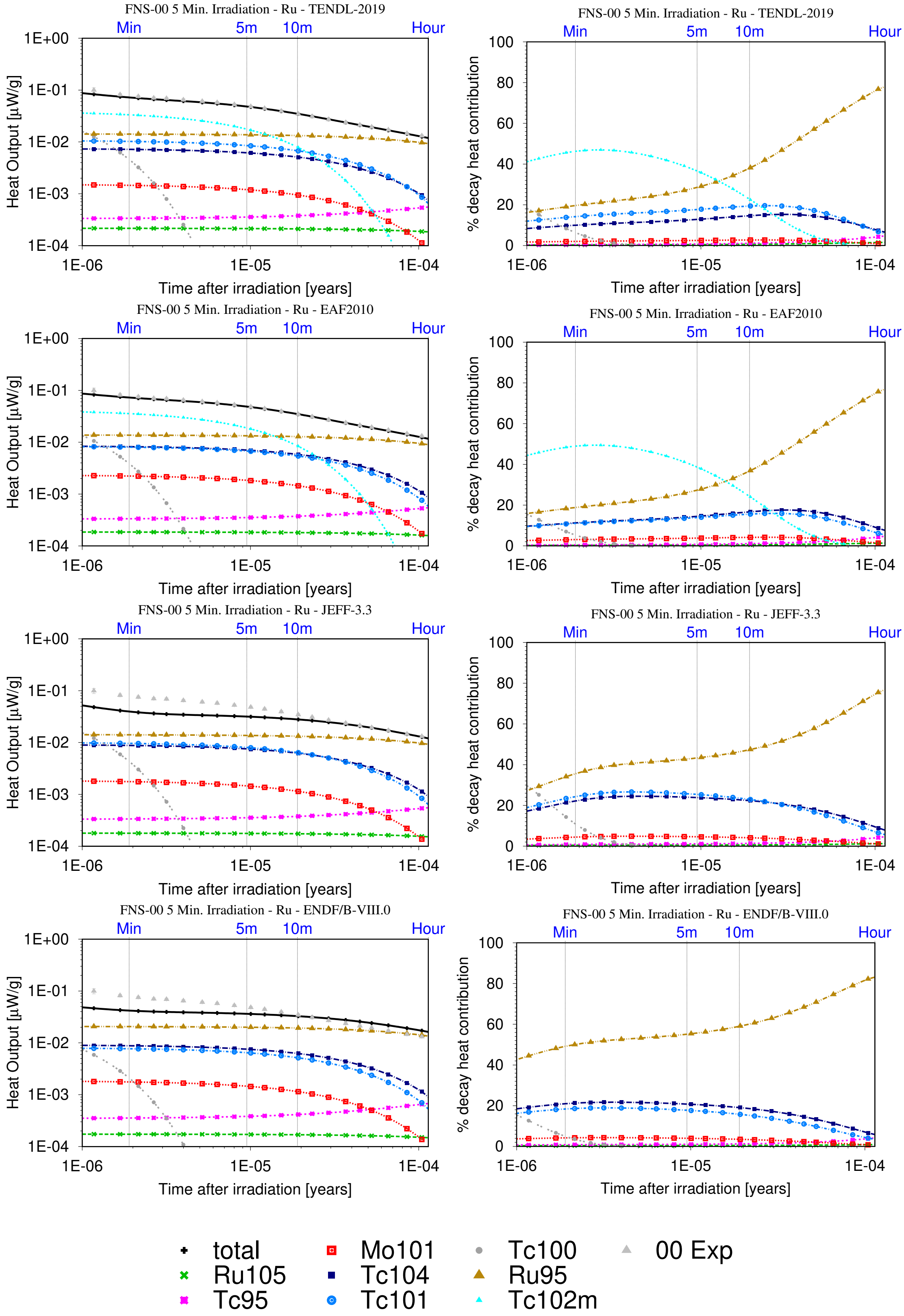


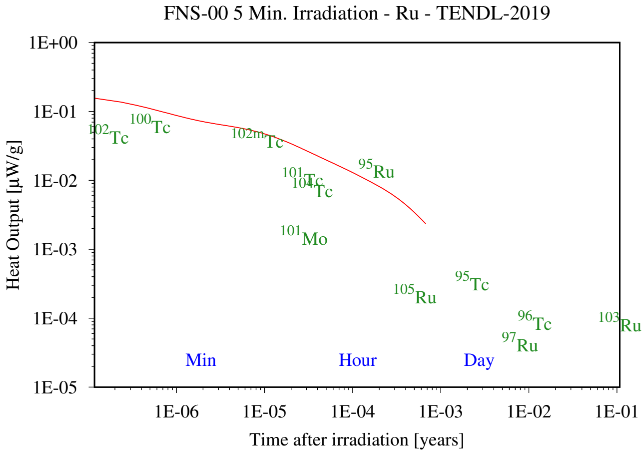
Ruthenium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Tc100	15.80s	Ru100(n,p)Tc100	76.2
		Ru101(n,np)Tc100	18.1
		Ru101(n,d)Tc100	5.7
Tc102m	4.35m	Ru102(n,p)Tc102m	100.0
Tc101	14.20m	Ru101(n,p)Tc101	90.3
		Ru102(n,d)Tc101	5.6
		Ru102(n,np)Tc101	3.5
Mo101	14.61m	Ru104(n,α)Mo101	100.0
Tc104	18.30m	Ru104(n,p)Tc104	100.0
Ru95	1.64h	Ru96(n,2n)Ru95	100.0
Ru105	4.44h	Ru104(n,γ)Ru105	100.0
Tc95	20.00h	Ru96(n,np)Tc95	94.2
		Ru96(n,2n)Ru95(β^+)Tc95	3.7
		Ru96(n,d)Tc95	2.2

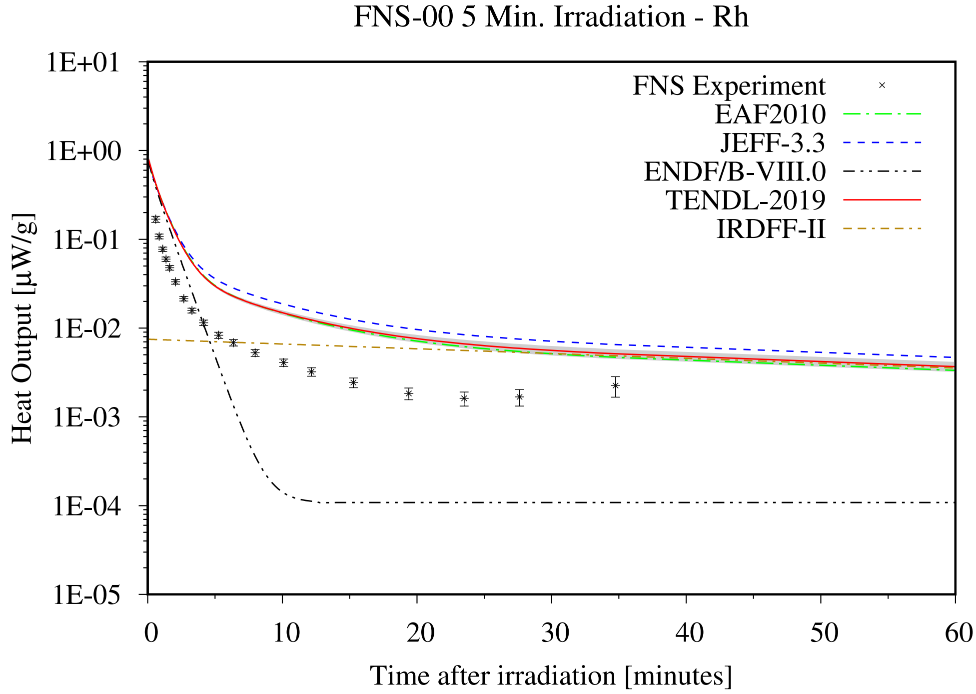
Comments on Ruthenium 5-minute experiments:

A superb fit to the experiment can be seen in the predictions with both TENDL-2019 and EAF2010, even at short cooling times of less than around 10 minutes where the Tc102m metastable is seen to dominate (although not sufficiently for its reaction channel [(n,p) reactions on Ru102] to be fully-validated by the experiment) – Ru95 from (n,2n) reactions on Ru96 dominates at all later cooling times. The combined and overlapping profile from these two nuclides perfectly captures the experimental profile and the two libraries are within the experimental uncertainties at almost all cooling times. ENDF/B-VIII.0 and JEFF-3.3 both miss the production of the metastable and thus produce the wrong decay profile, while ENDF/B-VIII.0 also overpredicts the contribution from Ru95.


FNS-00 5 Min. Irradiation - Ru - TENDL-2019
FNS-00 5 Min. Irradiation - Ru - EAF2010
FNS-00 5 Min. Irradiation - Ru - JEFF-3.3
FNS-00 5 Min. Irradiation - Ru - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
% decay heat contribution
100
80
60
40
20
0
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Ru105
Tc95
Mo101
Tc104
Tc101
Tc100
Ru95
Tc102m
00 Exp


FNS-00 5 Min. Irradiation - Ru - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
102Tc
100Tc
102mTc
95Ru
101Tc
104Tc
101Mo
105Ru
95Tc
96Tc
97Ru
103Ru
Min
Hour
Day

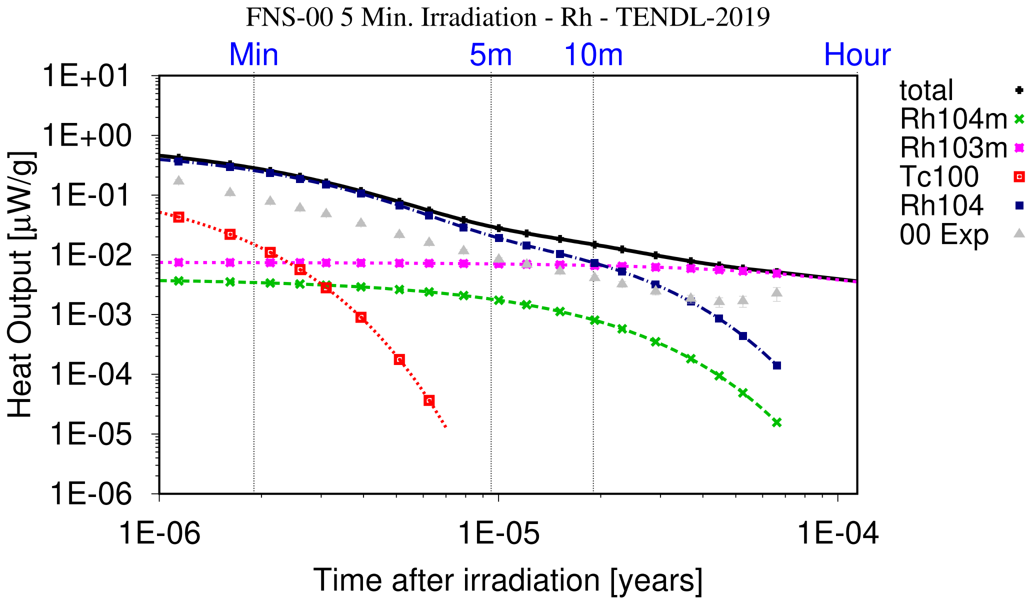
Rhodium



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
0.60	1.69E−01 +/-8%	4.23E−01 +/-6%	0.40	0.43	0.40	0.41	22.67
0.85	1.08E−01 +/-6%	3.28E−01 +/-4%	0.33	0.36	0.33	0.33	14.55
1.12	7.72E−02 +/-6%	2.55E−01 +/-3%	0.30	0.35	0.30	0.30	10.46
1.37	5.97E−02 +/-6%	2.04E−01 +/-3%	0.29	0.35	0.29	0.29	8.11
1.63	4.78E−02 +/-6%	1.63E−01 +/-2%	0.29	0.36	0.29	0.28	6.51
2.07	3.32E−02 +/-6%	1.17E−01 +/-2%	0.28	0.39	0.28	0.27	4.54
2.68	2.15E−02 +/-6%	7.72E−02 +/-2%	0.28	0.46	0.27	0.25	2.96
3.28	1.58E−02 +/-6%	5.53E−02 +/-3%	0.29	0.61	0.28	0.25	2.19
4.15	1.15E−02 +/-7%	3.83E−02 +/-3%	0.30	1.04	0.29	0.25	1.62
5.27	8.31E−03 +/-8%	2.80E−02 +/-4%	0.30	2.22	0.29	0.24	1.18
6.37	6.85E−03 +/-8%	2.28E−02 +/-4%	0.30	5.10	0.30	0.24	0.99
7.98	5.27E−03 +/-9%	1.84E−02 +/-5%	0.29	14.62	0.29	0.23	0.78
10.10	4.08E−03 +/-10%	1.48E−02 +/-6%	0.28	29.24	0.28	0.22	0.62
12.17	3.22E−03 +/-11%	1.23E−02 +/-7%	0.26	28.71	0.27	0.21	0.50
15.28	2.44E−03 +/-13%	9.82E−03 +/-8%	0.25	22.54	0.26	0.20	0.39
19.40	1.83E−03 +/-15%	7.82E−03 +/-10%	0.23	16.94	0.25	0.19	0.31
23.50	1.61E−03 +/-18%	6.65E−03 +/-11%	0.24	14.92	0.26	0.19	0.29
27.62	1.68E−03 +/-21%	5.92E−03 +/-12%	0.28	15.48	0.31	0.22	0.31
34.75	2.25E−03 +/-26%	5.13E−03 +/-13%	0.44	20.80	0.48	0.35	0.46
mean % diff. from E			245	110	240	302	97
mean χ^2			952.57	307.51	972.04	1296.34	119.28

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Rh104	42.29s	0.40	8%	2%
Rh103m	56.11m	0.23	15%	13%

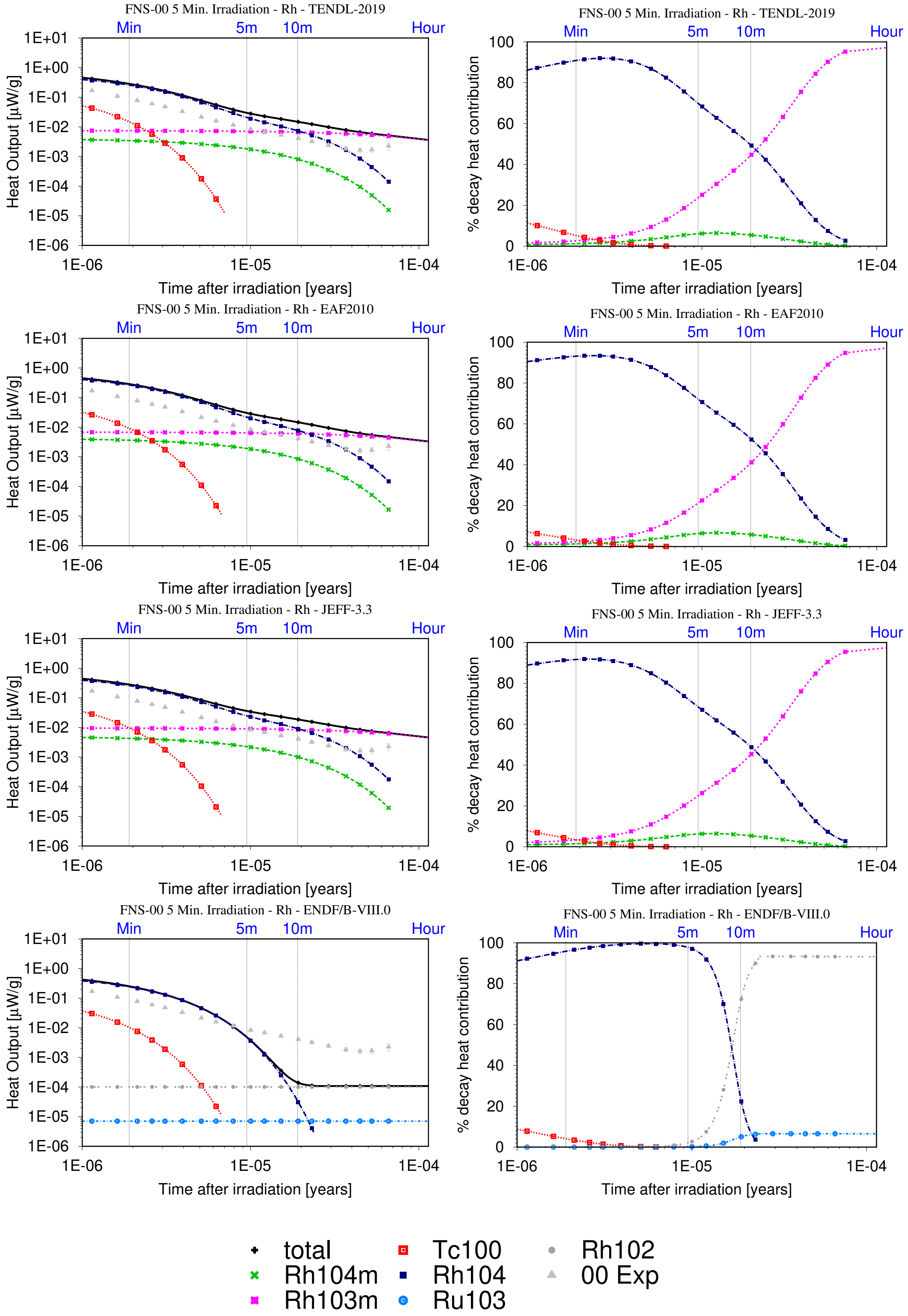


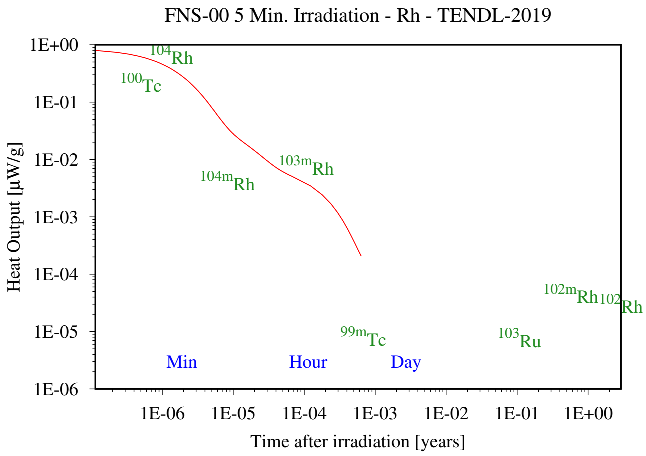
Rhodium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Tc100	15.80s	Rh103(n,α)Tc100	100.0
Rh104	42.29s	Rh103(n,γ)Rh104	96.0
		Rh103(n,γ)Rh104m(IT)Rh104	4.0
Rh104m	4.34m	Rh103(n,γ)Rh104m	100.0
Rh103m	56.11m	Rh103(n,n$'$)Rh103m	100.0
Ru103	39.27d	Rh103(n,p)Ru103	100.0
Rh102	2.90y	Rh103(n,2n)Rh102	100.0

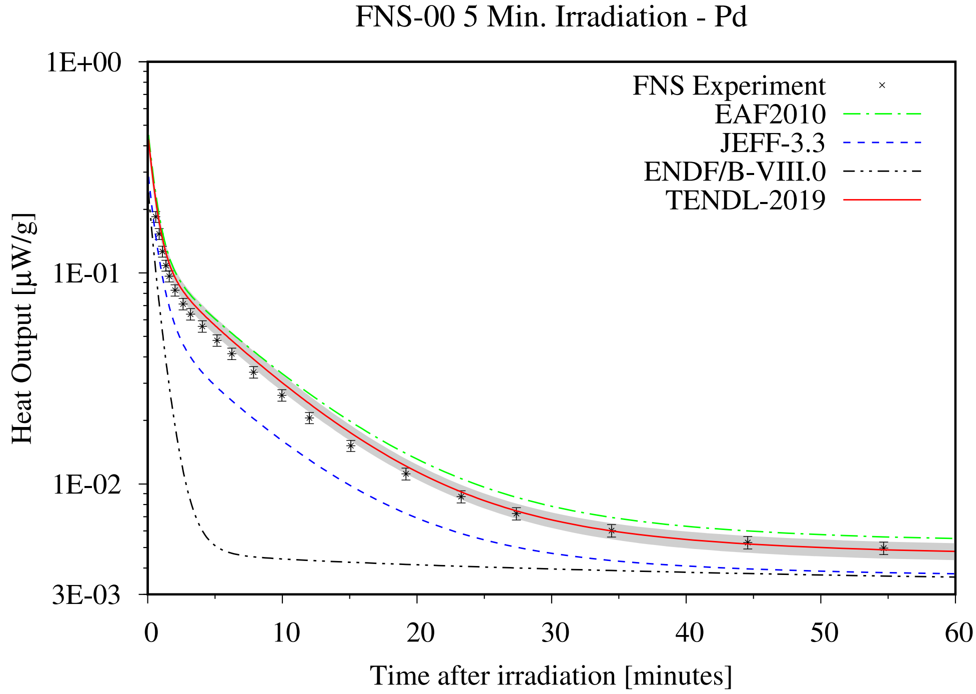
Comments on Rhodium 5-minute experiments:

The fit to the experimental measurement is poor with all libraries for this important element. The two predominant radionuclides are: Rh104, whose production route involves a branched capture channel (on Rh103), which cannot be well characterised in the FNS neutron spectrum; and, at least in simulations with TENDL-2019, EAF2010 JEFF-3.3, Rh103m, whose production is via a super-inelastic reaction. Despite the overprediction, the combination of these two nuclides, which are completely dominant (no other nuclide contributes more than 10% with TENDL, EAF, or JEFF), produces a profile that is a good match to the experimental profile. The predominance of non-threshold reactions in the simulations make it difficult to make any definitive conclusions or recommendations regarding the quality of the agreement (or lack of). ENDF/B-VIII.0 misses the production of Rh103m completely and produces a decay-profile that is not a good match to the experiment, despite having a seemingly lower average deviation from the measurements. IRDFF-II includes the channel to Rh103m and shows the same overprediction as TENDL-2019 (and others).

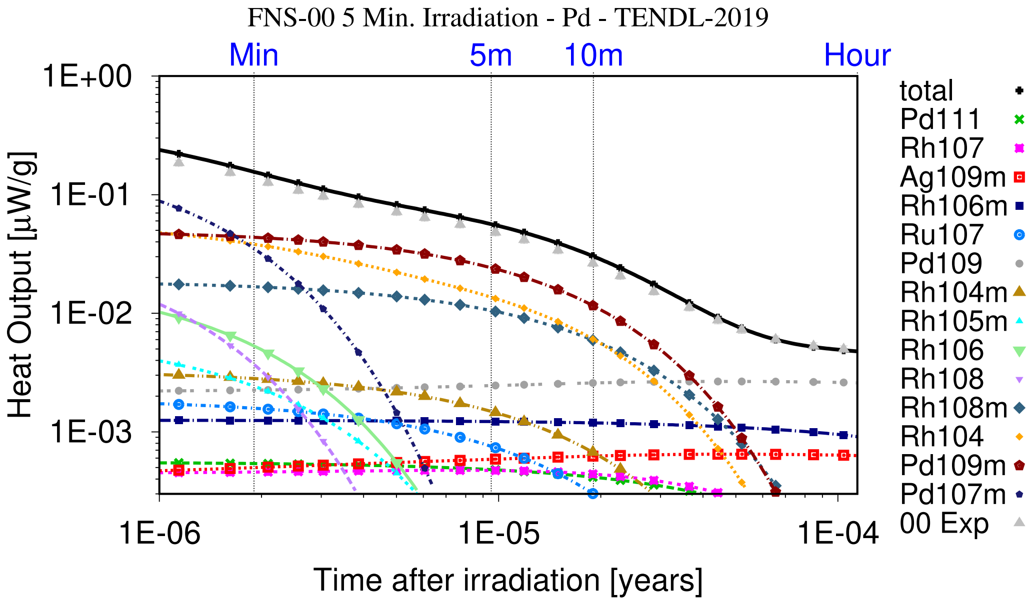

FNS-00 5 Min. Irradiation - Rh - TENDL-2019
FNS-00 5 Min. Irradiation - Rh - EAF2010
FNS-00 5 Min. Irradiation - Rh - JEFF-3.3
FNS-00 5 Min. Irradiation - Rh - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Rh104m
Rh103m
Tc100
Rh104
Ru103
Rh102
00 Exp


FNS-00 5 Min. Irradiation - Rh - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
104Rh
100Tc
104mRh
103mRh
99mTc
103Ru
102mRh
102Rh
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Palladium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	1.84$E-$01 +/-6%	2.21$E-$01 +/-10%	0.84	1.81	0.78	1.24
0.85	1.53$E-$01 +/-6%	1.75$E-$01 +/-9%	0.87	2.12	0.81	1.30
1.10	1.26$E-$01 +/-6%	1.45$E-$01 +/-9%	0.87	2.42	0.81	1.32
1.35	1.08$E-$01 +/-6%	1.25$E-$01 +/-9%	0.87	2.81	0.81	1.35
1.60	9.64$E-$02 +/-6%	1.11$E-$01 +/-9%	0.87	3.31	0.81	1.39
2.03	8.27$E-$02 +/-6%	9.50$E-$02 +/-10%	0.87	4.39	0.82	1.47
2.63	7.13$E-$02 +/-6%	8.18$E-$02 +/-10%	0.87	6.17	0.82	1.55
3.18	6.38$E-$02 +/-6%	7.38$E-$02 +/-10%	0.86	7.68	0.81	1.60
4.05	5.58$E-$02 +/-6%	6.44$E-$02 +/-10%	0.87	9.27	0.81	1.65
5.15	4.79$E-$02 +/-6%	5.53$E-$02 +/-10%	0.87	9.51	0.81	1.67
6.25	4.14$E-$02 +/-6%	4.78$E-$02 +/-9%	0.87	8.82	0.80	1.67
7.87	3.38$E-$02 +/-6%	3.90$E-$02 +/-9%	0.87	7.49	0.79	1.66
9.97	2.63$E-$02 +/-6%	3.03$E-$02 +/-9%	0.87	5.96	0.79	1.64
12.02	2.06$E-$02 +/-6%	2.40$E-$02 +/-9%	0.86	4.73	0.77	1.58
15.08	1.52$E-$02 +/-6%	1.75$E-$02 +/-9%	0.87	3.56	0.77	1.54
19.18	1.12$E-$02 +/-6%	1.22$E-$02 +/-8%	0.92	2.68	0.80	1.54
23.28	8.71$E-$03 +/-7%	9.19$E-$03 +/-8%	0.95	2.14	0.82	1.49
27.38	7.24$E-$03 +/-7%	7.47$E-$03 +/-8%	0.97	1.81	0.84	1.44
34.45	6.02$E-$03 +/-7%	6.00$E-$03 +/-9%	1.00	1.55	0.87	1.39
44.57	5.28$E-$03 +/-7%	5.20$E-$03 +/-9%	1.02	1.40	0.88	1.33
54.67	4.97$E-$03 +/-7%	4.88$E-$03 +/-9%	1.02	1.36	0.89	1.31
mean % diff. from E			12	66	23	32
mean χ^2			4.77	121.59	14.31	26.91

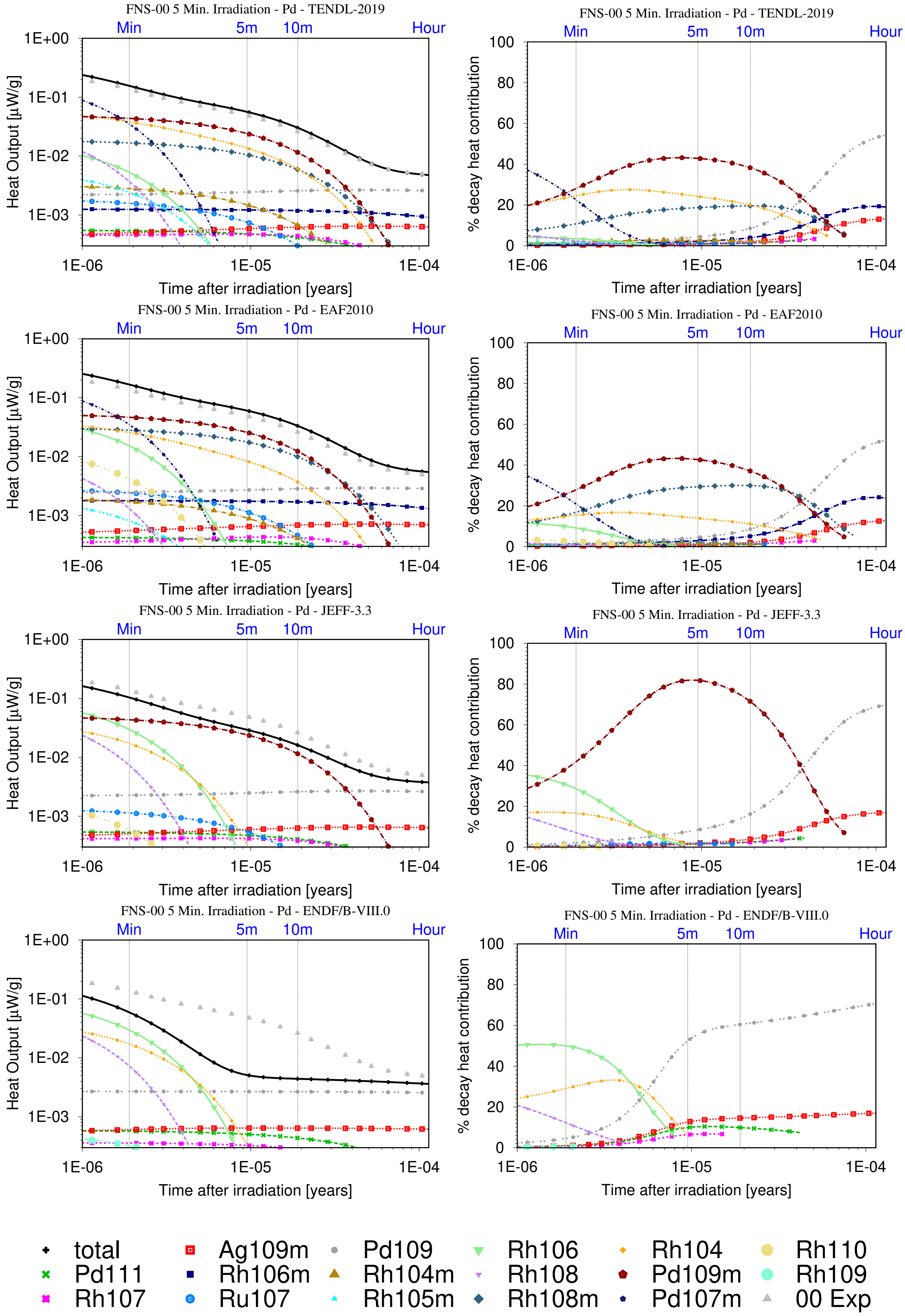


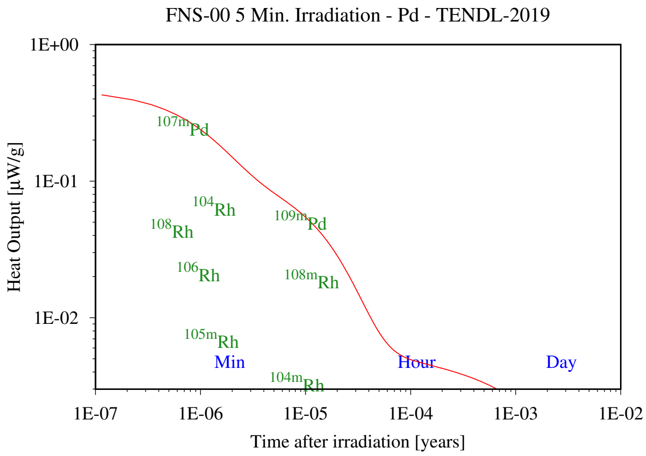
Palladium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Rh108	16.80s	Pd108(n,p)Rh108	100.0
Pd107m	21.30s	Pd108(n,2n)Pd107m	99.8
Rh110	28.50s	Pd110(n,p)Rh110	100.0
Rh106	30.01s	Pd106(n,p)Rh106	100.0
Ag109m	39.70s	Pd110(n,2n)Pd109(β^-)Ag109m	84.5
		Pd110(n,2n)Pd109m(IT)Pd109(β^-)Ag109m	9.3
		Pd108(n,γ)Pd109(β^-)Ag109m	6.1
Rh105m	40.00s	Pd105(n,p)Rh105m	97.3
		Pd106(n,d)Rh105m	2.1
Rh104	42.29s	Pd104(n,p)Rh104	35.7
		Pd105(n,np)Rh104	28.8
		Pd105(n,np)Rh104m(IT)Rh104	17.8
		Pd104(n,p)Rh104m(IT)Rh104	13.6
		Pd105(n,d)Rh104	2.6
		Pd105(n,d)Rh104m(IT)Rh104	1.5
Rh109	1.33m	Pd110(n,d)Rh109	93.5
		Pd110(n,np)Rh109	6.5
Ru107	3.75m	Pd110(n,α)Ru107	100.0
Rh104m	4.34m	Pd105(n,np)Rh104m	54.2
		Pd104(n,p)Rh104m	41.3
		Pd105(n,d)Rh104m	4.6
Pd109m	4.69m	Pd110(n,2n)Pd109m	99.1
Rh108m	6.00m	Pd108(n,p)Rh108m	100.0
Rh107	21.70m	Pd108(n,d)Rh107	52.0
		Pd108(n,np)Rh107	28.6
		Pd110(n,α)Ru107(β^-)Rh107	19.4
Pd111	23.40m	Pd110(n,γ)Pd111	100.0
Rh106m	2.20h	Pd106(n,p)Rh106m	100.0
Pd109	13.70h	Pd110(n,2n)Pd109	83.4
		Pd110(n,2n)Pd109m(IT)Pd109	10.5
		Pd108(n,γ)Pd109	6.0

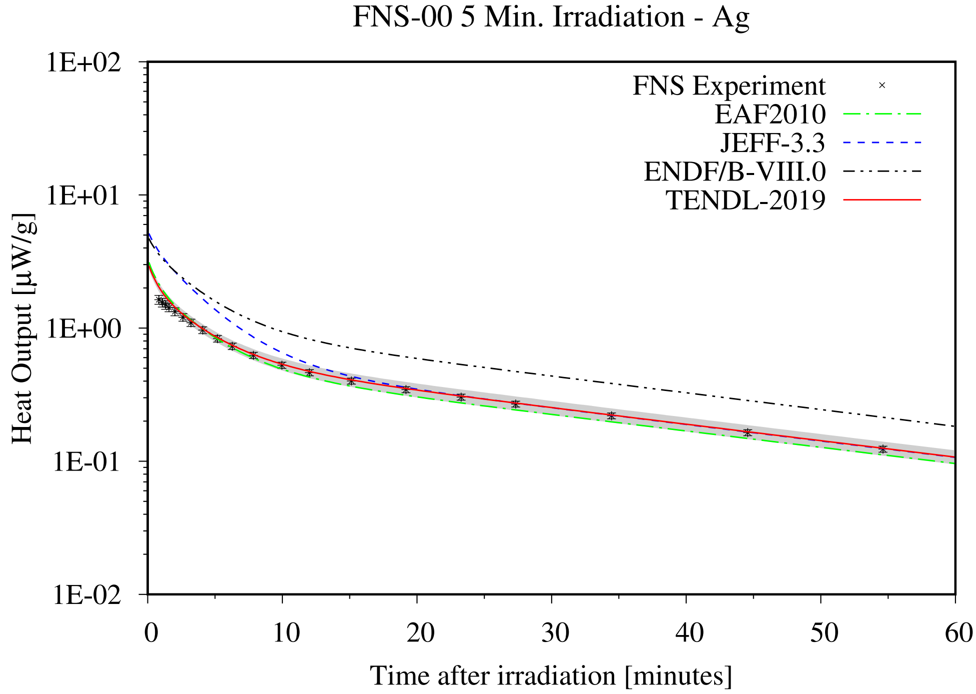
Comments on Palladium 5-minute experiments:

A nice agreement between experiment and simulations with TENDL-2019 – fairly remarkable given the complexity of the case (a large number of contributing nuclides with multiple production pathways). Shorter cooling times are dominated by metastable isomers, particularly Pd109m and Pd107m produced via (n,2n) reactions and Rh108m from (n,p). ENDF/B-VIII.0 misses all of these nuclides, while JEFF-3.3 does slightly better by including the channel to Pd109m but misses the others. Additionally, TENDL-2019 and EAF-2010 predict that Rh106m is important at longer cooling times underneath the predominant Pd109 (all libraries predict this), but JEFF and ENDF/B miss this (via (n,p) on Pd106). There have been some minor changes in TENDL-2019 compared to TENDL-2017; agreement to the experiment beyond 20 minutes of cooling has improved, while deviation has increased at very short cooling times (possibly due to a new overprediction of Rh104). EAF2010 includes the production of all the necessary metastables, but overpredicts the production of Rh108m, leading to a significant (25%) overprediction at cooling times less than around 20 minutes. This proves once again the strength of the TALYS modelling processes to produce a truly general purpose library with proper inclusion of all reaction channels.


FNS-00 5 Min. Irradiation - Pd - TENDL-2019
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-00 5 Min. Irradiation - Pd - EAF2010
FNS-00 5 Min. Irradiation - Pd - JEFF-3.3
FNS-00 5 Min. Irradiation - Pd - ENDF/B-VIII.0
total
Ag109m
Pd109
Rh106
Rh104
Rh110
Pd111
Rh106m
Rh104m
Rh108
Pd109m
Rh109
Rh107
Ru107
Rh105m
Rh108m
Pd107m
00 Exp


FNS-00 5 Min. Irradiation - Pd - TENDL-2019
1E+00
1E-01
1E-02
Heat Output [µW/g]
107mPd
104Rh
108Rh
109mPd
106Rh
108mRh
105mRh
104mRh
Min
Hour
Day
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

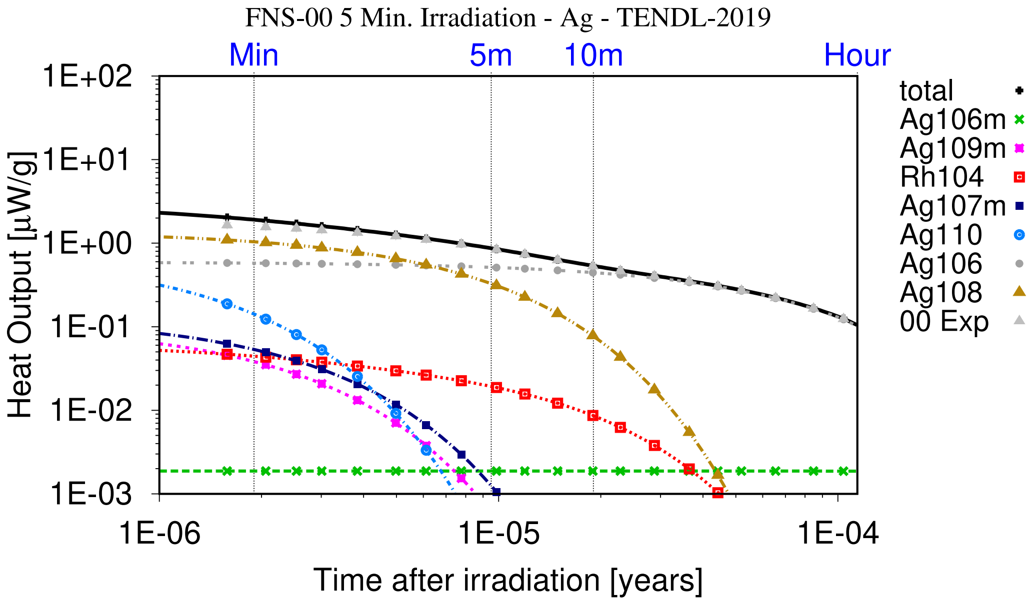
Silver



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.83	$1.64E{+}00$ +/-8%	$2.03E{+}00$ +/-7%	0.80	0.46	0.76	0.43
1.08	$1.55E{+}00$ +/-7%	$1.86E{+}00$ +/-8%	0.84	0.47	0.80	0.45
1.33	$1.49E{+}00$ +/-7%	$1.72E{+}00$ +/-8%	0.87	0.48	0.83	0.47
1.58	$1.43E{+}00$ +/-7%	$1.60E{+}00$ +/-8%	0.89	0.49	0.86	0.48
2.02	$1.33E{+}00$ +/-7%	$1.44E{+}00$ +/-8%	0.92	0.50	0.89	0.50
2.62	$1.21E{+}00$ +/-7%	$1.27E{+}00$ +/-8%	0.95	0.51	0.93	0.53
3.22	$1.10E{+}00$ +/-6%	$1.14E{+}00$ +/-8%	0.96	0.52	0.95	0.55
4.08	$9.65E{-}01$ +/-6%	$9.90E{-}01$ +/-8%	0.98	0.53	0.98	0.58
5.18	$8.33E{-}01$ +/-6%	$8.49E{-}01$ +/-9%	0.98	0.54	1.01	0.62
6.28	$7.30E{-}01$ +/-6%	$7.43E{-}01$ +/-9%	0.98	0.54	1.02	0.67
7.85	$6.24E{-}01$ +/-5%	$6.35E{-}01$ +/-10%	0.98	0.55	1.05	0.73
9.97	$5.26E{-}01$ +/-5%	$5.37E{-}01$ +/-10%	0.98	0.56	1.07	0.80
12.02	$4.63E{-}01$ +/-5%	$4.73E{-}01$ +/-11%	0.98	0.56	1.08	0.86
15.13	$4.00E{-}01$ +/-5%	$4.09E{-}01$ +/-12%	0.98	0.57	1.09	0.92
19.18	$3.45E{-}01$ +/-5%	$3.52E{-}01$ +/-12%	0.98	0.57	1.10	0.96
23.28	$3.03E{-}01$ +/-5%	$3.09E{-}01$ +/-12%	0.98	0.57	1.10	0.98
27.33	$2.69E{-}01$ +/-5%	$2.74E{-}01$ +/-12%	0.98	0.57	1.11	0.98
34.45	$2.19E{-}01$ +/-5%	$2.23E{-}01$ +/-12%	0.99	0.57	1.11	0.99
44.57	$1.64E{-}01$ +/-5%	$1.67E{-}01$ +/-12%	0.98	0.57	1.11	0.99
54.62	$1.23E{-}01$ +/-5%	$1.25E{-}01$ +/-12%	0.98	0.58	1.10	0.99
mean % diff. from E			6	88	10	51
mean χ^2			1.39	219.42	3.68	101.01

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ag106	24.00m	0.98	5%	12%

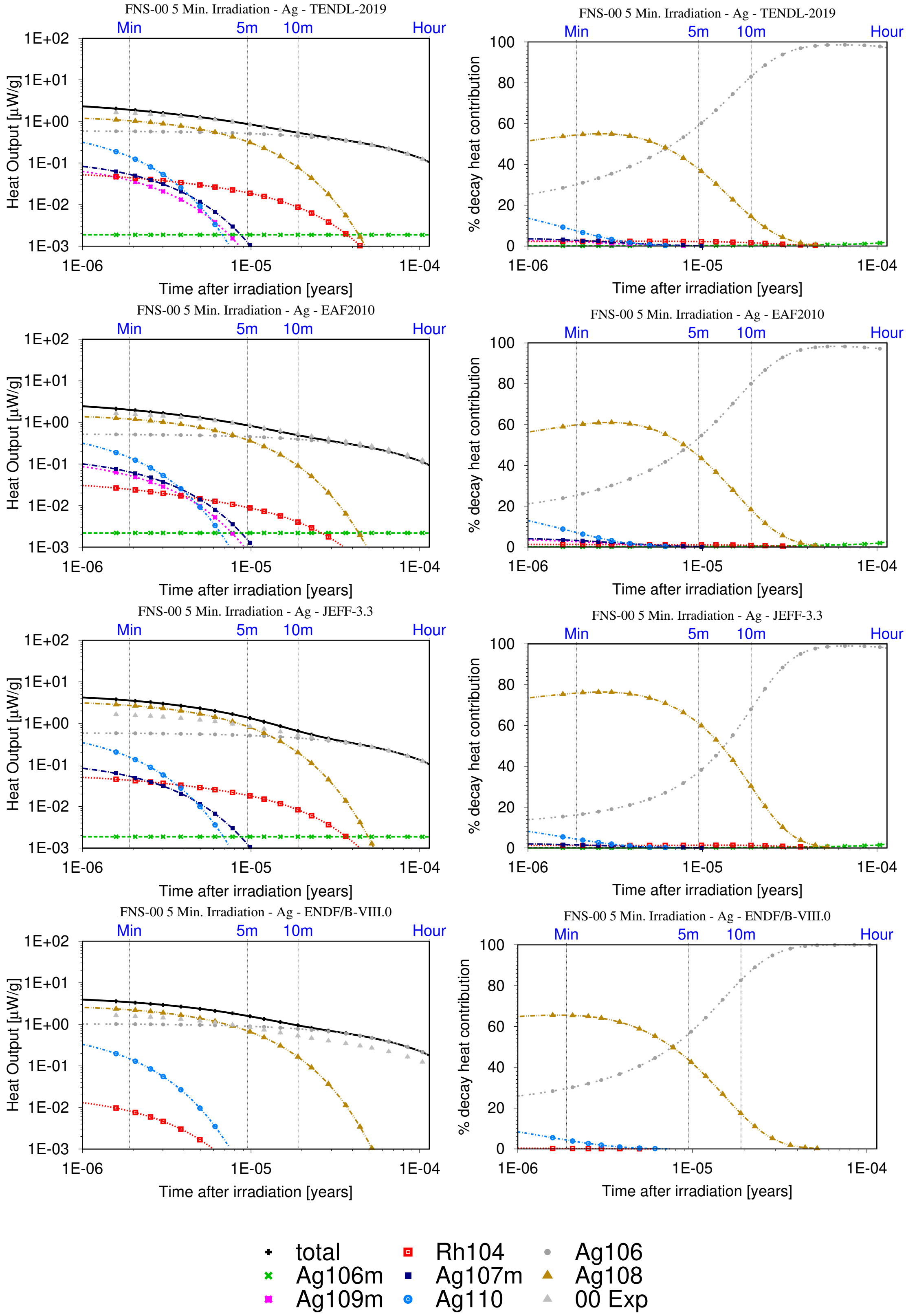


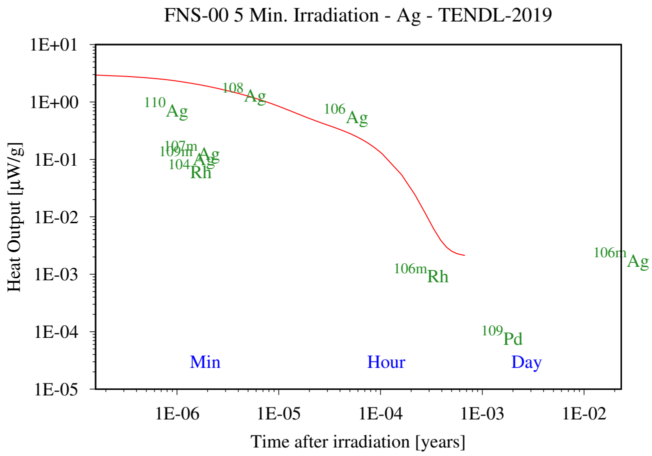
Silver, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Ag110	24.56s	Ag109(n,γ)Ag110	100.0
Ag109m	39.70s	Ag109(n,n′)Ag109m	100.0
Rh104	42.29s	Ag107(n,α)Rh104	53.3
		Ag107(n,α)Rh104m(IT)Rh104	46.7
Ag107m	44.29s	Ag107(n,n′)Ag107m	100.0
Ag108	2.40m	Ag109(n,2n)Ag108	95.7
		Ag107(n,γ)Ag108	4.3
Ag106	24.00m	Ag107(n,2n)Ag106	100.0
Ag106m	8.46d	Ag107(n,2n)Ag106m	100.0

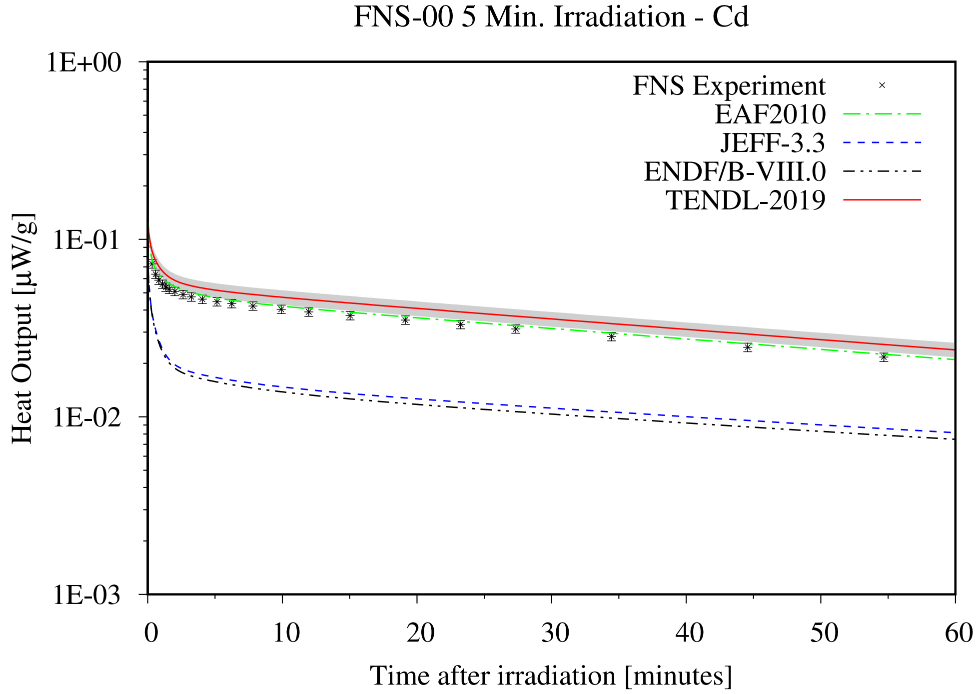
Comments on Silver 5-minute experiments:

TENDL-2019 and EAF2010 both overpredict slightly at cooling times less than 5 minutes, while at longer cooling times EAF2010 underpredicts quite significantly. Overall, TENDL-2019 does very well in capturing the experimental profile, which is dominated by the decay of nuclides from two different (n,2n) production channels – to produce Ag108 and Ag106, which are both important during the initial cooling phase, while Ag106 is completely dominant beyond 10 minutes of cooling. JEFF-3.3 overpredicts the production of Ag108 and so performs badly during the first 10 minutes, while ENDF/B-VIII.0 overpredicts both (n,2n) channels and hence the decay-heat dramatically (by a factor of 2 at all cooling times).


FNS-00 5 Min. Irradiation - Ag - TENDL-2019
FNS-00 5 Min. Irradiation - Ag - EAF2010
FNS-00 5 Min. Irradiation - Ag - JEFF-3.3
FNS-00 5 Min. Irradiation - Ag - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Rh104
Ag106
Ag106m
Ag107m
Ag108
Ag109m
Ag110
00 Exp


FNS-00 5 Min. Irradiation - Ag - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02
110Ag
108Ag
106Ag
107mAg
109mAg
104Rh
106mRh
106mAg
109Pd
Min
Hour
Day

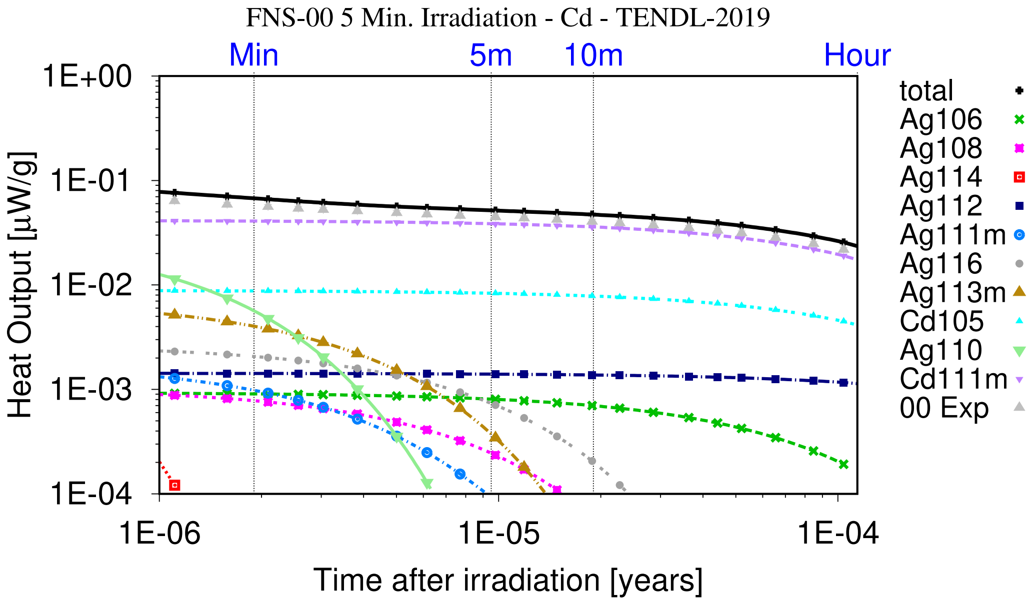
Cadmium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.33	7.28E−02 +/-5%	8.55E−02 +/-9%	0.85	1.96	0.95	1.90
0.58	6.36E−02 +/-5%	7.62E−02 +/-9%	0.83	2.11	0.94	2.04
0.83	5.88E−02 +/-5%	7.04E−02 +/-8%	0.84	2.26	0.93	2.18
1.10	5.59E−02 +/-5%	6.62E−02 +/-8%	0.85	2.41	0.93	2.32
1.35	5.38E−02 +/-5%	6.33E−02 +/-8%	0.85	2.52	0.93	2.41
1.60	5.24E−02 +/-5%	6.12E−02 +/-9%	0.86	2.60	0.93	2.49
2.02	5.09E−02 +/-5%	5.87E−02 +/-9%	0.87	2.71	0.94	2.59
2.63	4.89E−02 +/-5%	5.63E−02 +/-9%	0.87	2.77	0.94	2.63
3.23	4.74E−02 +/-5%	5.47E−02 +/-9%	0.87	2.79	0.94	2.65
4.05	4.60E−02 +/-5%	5.32E−02 +/-9%	0.86	2.81	0.95	2.66
5.15	4.45E−02 +/-5%	5.16E−02 +/-9%	0.86	2.84	0.95	2.68
6.25	4.35E−02 +/-5%	5.04E−02 +/-9%	0.86	2.87	0.96	2.70
7.82	4.21E−02 +/-5%	4.89E−02 +/-9%	0.86	2.90	0.96	2.73
9.92	4.03E−02 +/-5%	4.72E−02 +/-9%	0.85	2.91	0.96	2.73
11.97	3.90E−02 +/-5%	4.58E−02 +/-9%	0.85	2.93	0.96	2.74
15.03	3.72E−02 +/-5%	4.38E−02 +/-9%	0.85	2.95	0.96	2.75
19.13	3.51E−02 +/-5%	4.13E−02 +/-9%	0.85	2.95	0.96	2.75
23.25	3.32E−02 +/-5%	3.90E−02 +/-9%	0.85	2.95	0.96	2.73
27.35	3.13E−02 +/-5%	3.69E−02 +/-9%	0.85	2.92	0.96	2.71
34.47	2.83E−02 +/-5%	3.35E−02 +/-9%	0.84	2.88	0.96	2.66
44.57	2.46E−02 +/-5%	2.93E−02 +/-9%	0.84	2.80	0.95	2.58
54.68	2.17E−02 +/-5%	2.56E−02 +/-9%	0.85	2.75	0.96	2.53
mean % diff. from E			17	63	5	60
mean χ^2			10.12	132.44	1.06	123.47

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Cd111m	48.74m	0.86	5%	12%

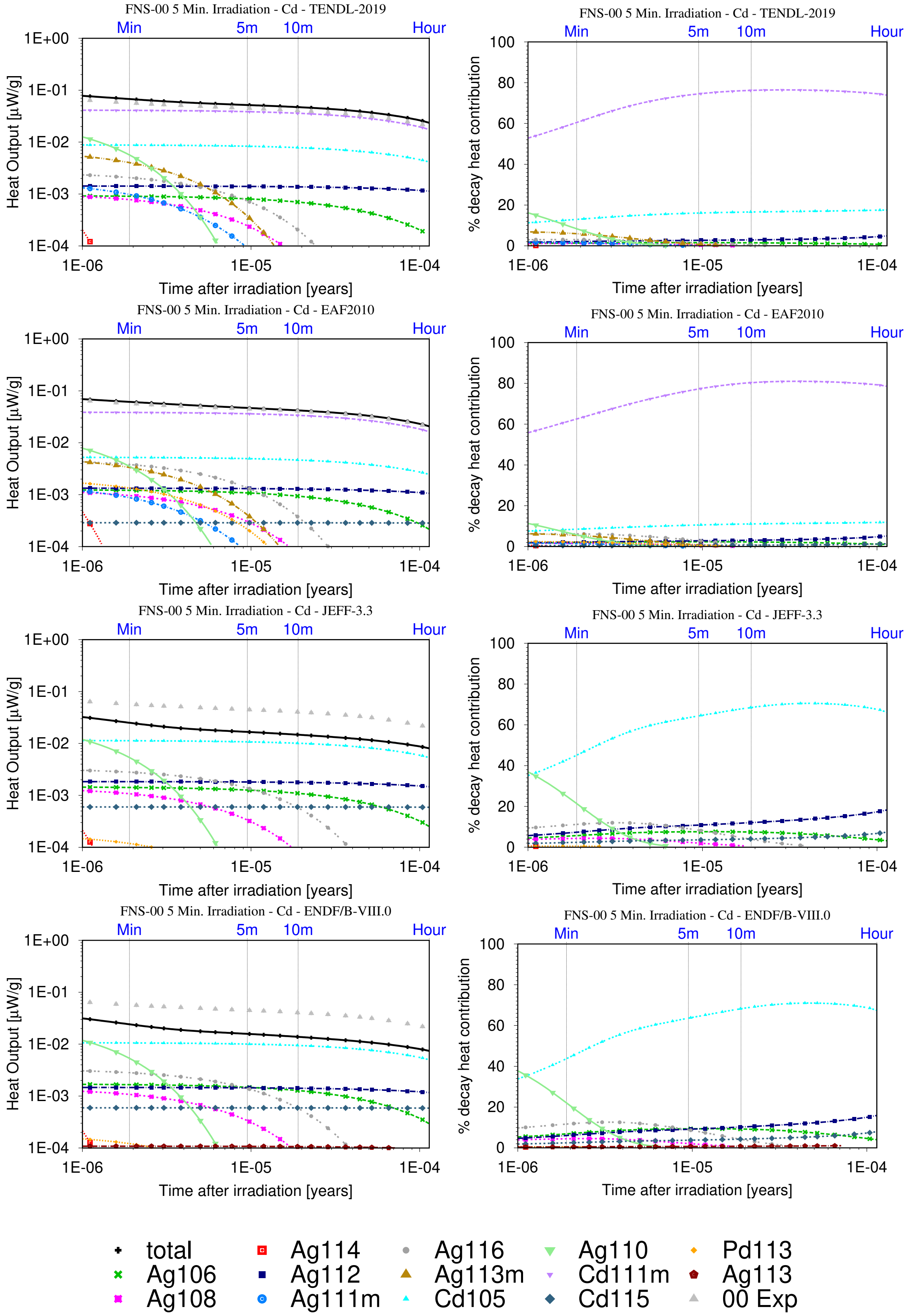


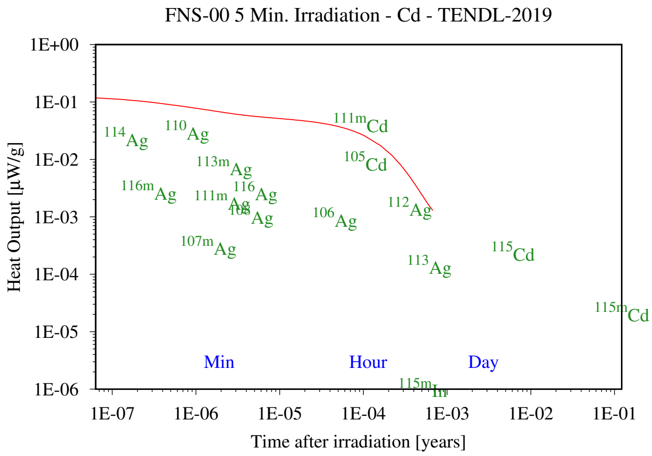
Cadmium, TENDL-2019 5-minute pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Ag114	4.60s	Cd114(n,p)Ag114	100.0
Ag110	24.56s	Cd110(n,p)Ag110	85.0
		Cd111(n,np)Ag110	11.1
		Cd111(n,d)Ag110	3.8
Ag111m	1.08m	Cd111(n,p)Ag111m	91.4
		Cd112(n,d)Ag111m	4.6
		Cd112(n,np)Ag111m	3.1
Ag113m	1.14m	Cd113(n,p)Ag113m	96.2
		Cd114(n,d)Ag113m	1.7
		Cd114(n,np)Ag113m	1.0
Pd113	1.52m	Cd116(n,α)Pd113m(IT)Pd113	51.4
		Cd116(n,α)Pd113	48.6
Ag108	2.40m	Cd108(n,p)Ag108	100.0
Ag116	2.68m	Cd116(n,p)Ag116	95.0
		Cd116(n,p)Ag116m(IT)Ag116	5.0
Ag106	24.00m	Cd106(n,p)Ag106	100.0
Cd111m	48.74m	Cd112(n,2n)Cd111m	84.7
		Cd111(n,n′)Cd111m	15.2
Cd105	55.49m	Cd106(n,2n)Cd105	100.0
Ag112	3.13h	Cd112(n,p)Ag112	96.8
		Cd113(n,d)Ag112	1.7
		Cd113(n,np)Ag112	1.5
Ag113	5.37h	Cd113(n,p)Ag113	49.2
		Cd113(n,p)Ag113m(IT)Ag113	48.0
Cd115	2.23d	Cd116(n,2n)Cd115	96.7
		Cd114(n,γ)Cd115	3.2

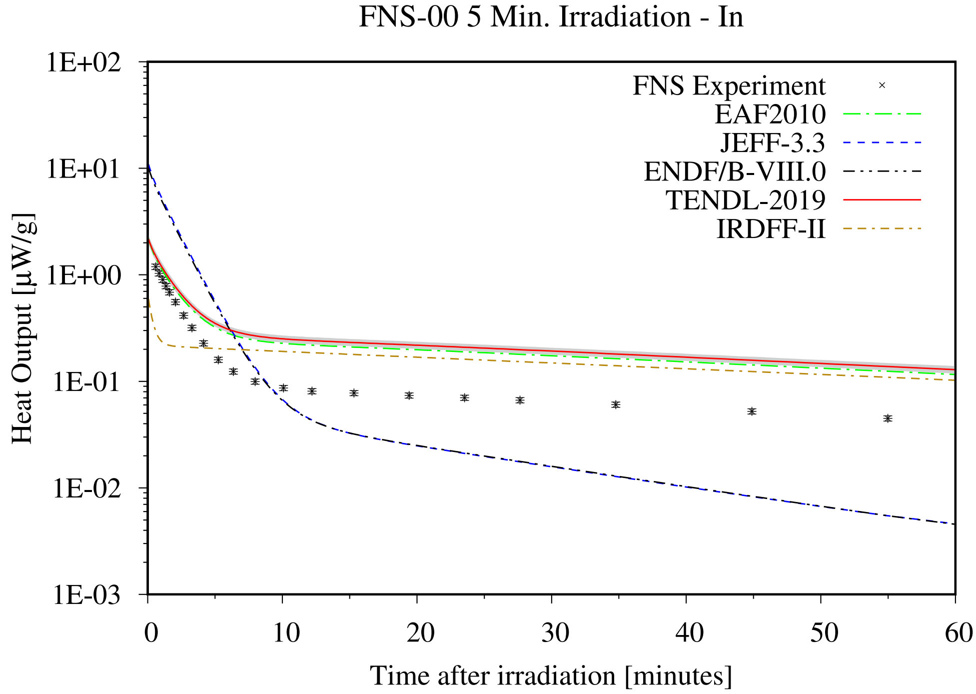
Comments on Cadmium 5-minute experiments:

EAF2010 performs very well here, almost within the experimental uncertainty, while TENDL-2019 seems to overpredict by between 10 and 20% at all cooling times. Examining the simulations in detail, one notes that TENDL-2019 predicts significantly more decay heat from Cd105, which contributes around 10-20% of the decay-heat at all cooling times. Indeed, the total cross section for the (n,2n) reaction on Cd106 producing this nuclide is roughly twice as high with TENDL-2019 compared to EAF2010 – suggesting that the TENDL evaluation should be reassessed in this case. There may also be a need to adjust the production channels for Cd111m, which dominates the decay heat at all cooling times – it is produced primarily via (n,2n) reactions on Cd112 and TENDL-2017 and EAF2010 are nearly in agreement for that total cross section. However, an inelastic scattering channel on Cd111 also provides a non-negligible contribution and has a somewhat higher total cross section with TENDL-2019. At the same time, TENDL-2019 clearly outperforms both ENDF/B-VIII.0 and JEFF-3.3, which massively underpredict the experiment because they do not include either of the Cd111m production routes – they only capture the contribution from Cd105.


FNS-00 5 Min. Irradiation - Cd - TENDL-2019
FNS-00 5 Min. Irradiation - Cd - EAF2010
FNS-00 5 Min. Irradiation - Cd - JEFF-3.3
FNS-00 5 Min. Irradiation - Cd - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Ag114
Ag116
Ag110
Pd113
Ag106
Ag112
Ag113m
Cd111m
Ag113
Ag108
Ag111m
Cd105
Cd115
00 Exp


FNS-00 5 Min. Irradiation - Cd - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
Time after irradiation [years]
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Min
Hour
Day
114Ag
110Ag
113mAg
116mAg
111mAg
116Ag
108Ag
107mAg
106Ag
111mCd
105Cd
112Ag
113Ag
115Cd
115mCd
115mIn

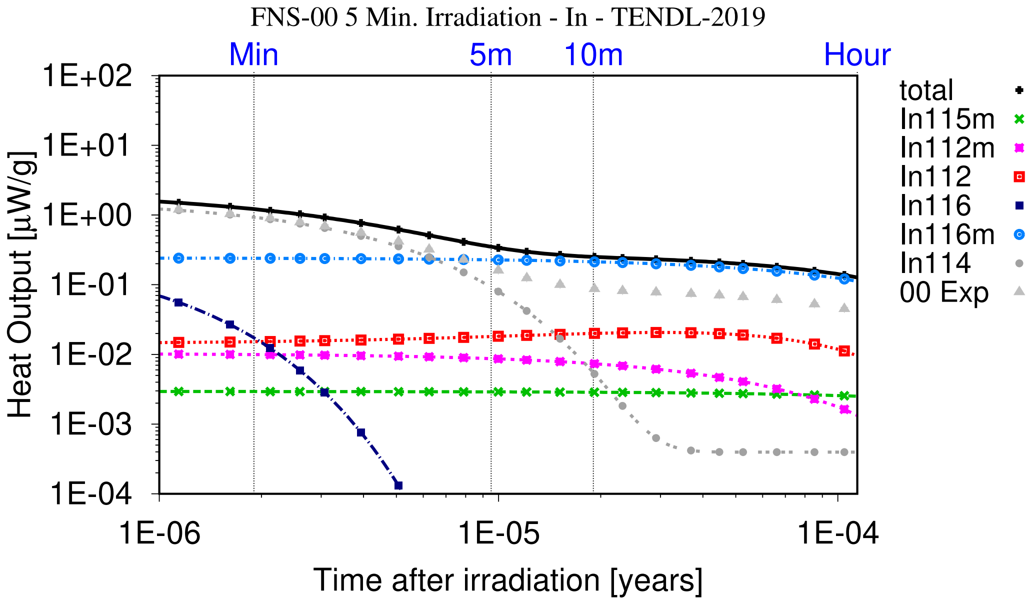
Indium



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
0.60	1.19E+00 +/-6%	1.50E+00 +/-10%	0.80	0.18	0.83	0.17	4.05
0.85	1.03E+00 +/-6%	1.31E+00 +/-10%	0.79	0.18	0.83	0.17	4.07
1.12	9.00E−01 +/-6%	1.15E+00 +/-10%	0.78	0.19	0.83	0.18	3.87
1.37	7.85E−01 +/-6%	1.03E+00 +/-10%	0.77	0.19	0.81	0.18	3.52
1.62	6.87E−01 +/-6%	9.21E−01 +/-10%	0.75	0.19	0.79	0.18	3.16
2.07	5.56E−01 +/-6%	7.69E−01 +/-9%	0.72	0.20	0.77	0.19	2.61
2.67	4.15E−01 +/-6%	6.20E−01 +/-8%	0.67	0.21	0.72	0.20	1.97
3.28	3.19E−01 +/-6%	5.12E−01 +/-8%	0.62	0.23	0.67	0.22	1.53
4.15	2.28E−01 +/-6%	4.12E−01 +/-7%	0.55	0.27	0.60	0.25	1.11
5.25	1.59E−01 +/-6%	3.38E−01 +/-7%	0.47	0.34	0.51	0.32	0.79
6.37	1.24E−01 +/-6%	2.97E−01 +/-7%	0.42	0.46	0.46	0.44	0.62
7.98	9.95E−02 +/-6%	2.68E−01 +/-7%	0.37	0.76	0.41	0.74	0.51
10.08	8.65E−02 +/-6%	2.50E−01 +/-8%	0.35	1.33	0.38	1.31	0.45
12.20	8.10E−02 +/-6%	2.41E−01 +/-8%	0.34	1.88	0.37	1.87	0.44
15.32	7.76E−02 +/-6%	2.31E−01 +/-8%	0.34	2.42	0.37	2.43	0.43
19.42	7.37E−02 +/-6%	2.20E−01 +/-8%	0.33	2.87	0.37	2.89	0.43
23.53	7.01E−02 +/-6%	2.09E−01 +/-8%	0.34	3.29	0.37	3.32	0.43
27.65	6.66E−02 +/-6%	1.98E−01 +/-8%	0.34	3.76	0.37	3.80	0.43
34.77	6.05E−02 +/-6%	1.81E−01 +/-8%	0.33	4.68	0.37	4.73	0.43
44.88	5.23E−02 +/-6%	1.58E−01 +/-8%	0.33	6.26	0.37	6.31	0.42
54.98	4.49E−02 +/-6%	1.38E−01 +/-8%	0.33	8.18	0.36	8.18	0.41
mean % diff. from E			123	213	104	226	90
mean χ^2			634.53	2148.44	463.19	2465.79	295.92

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
In114	1.20m	0.80	6%	13%
In116m	54.60m	0.42	6%	9%



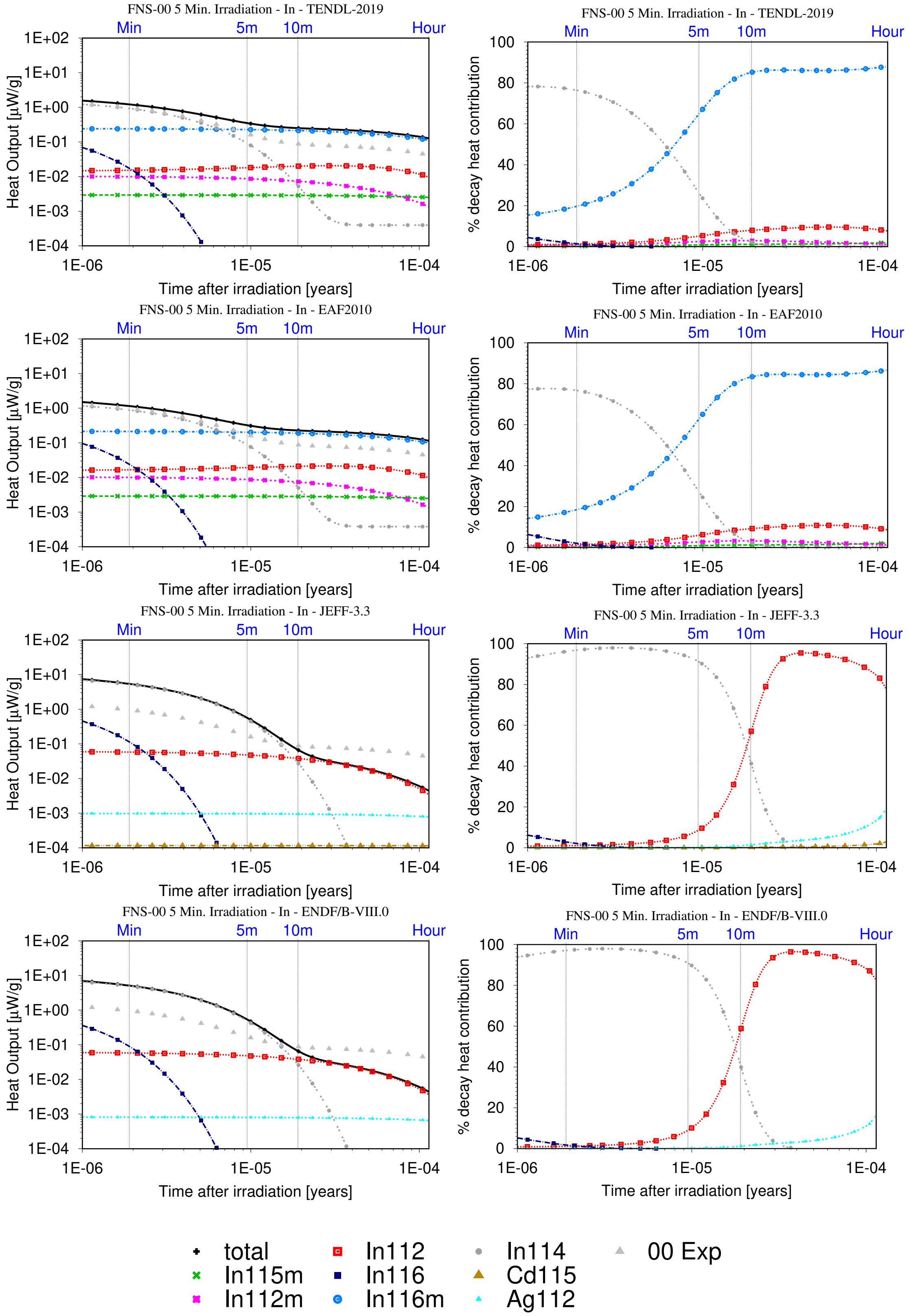
Indium, TENDL-2019 5-minute pathway analysis

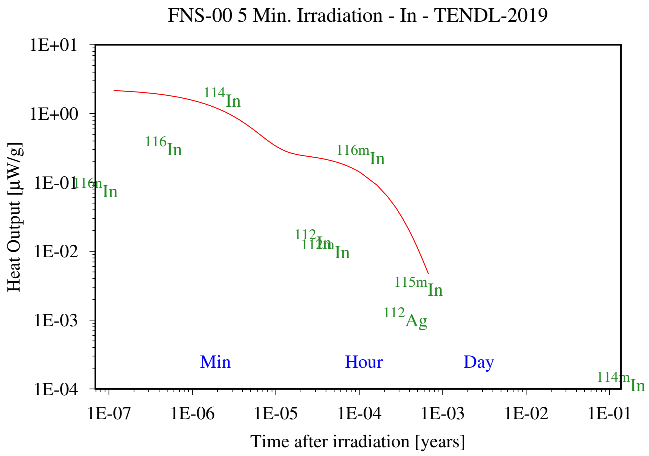
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
In116	14.20s	In115(n,γ)In116	100.0
In114	1.20m	In115(n,2n)In114	99.8
In112	14.70m	In113(n,2n)In112	72.4
		In113(n,2n)In112m(IT)In112	27.6
In112m	20.70m	In113(n,2n)In112m	100.0
In116m	54.60m	In115(n,γ)In116m	65.3
		In115(n,γ)In116n(IT)In116m	34.7
Ag112	3.13h	In115(n,α)Ag112	100.0
In115m	4.49h	In115(n,n′)In115m	100.0
Cd115	2.23d	In115(n,p)Cd115	100.0

Comments on Indium 5-minute experiments:

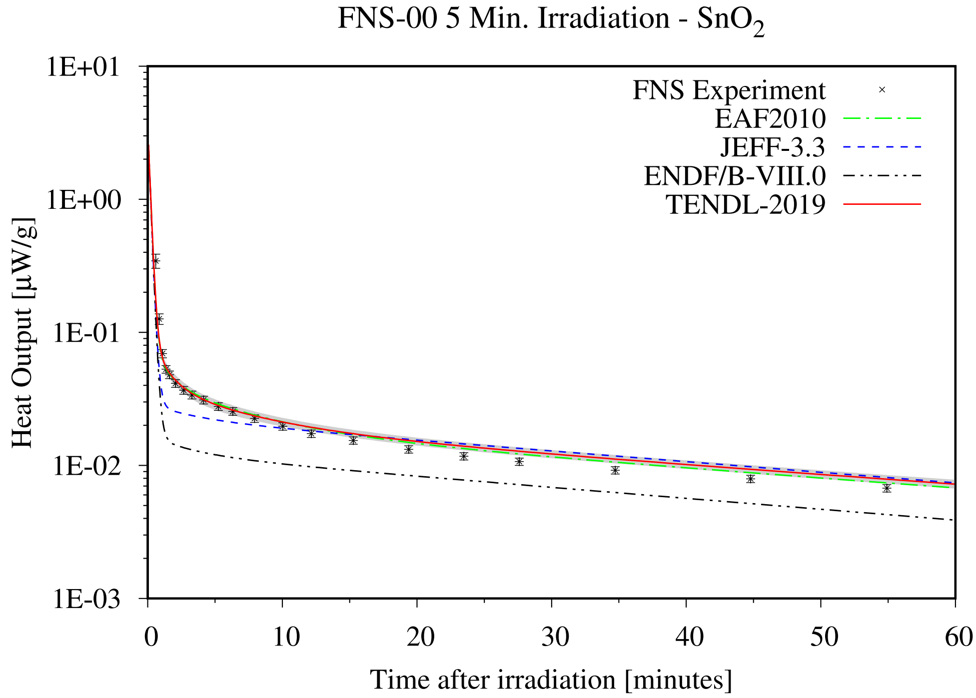
TENDL-2019 and EAF2010 produce an overprediction for this element, particularly at cooling times greater than 5 minutes, when In116m becomes dominant. However, the overall decay-profile is a reasonably good match to the experimental profile (unlike the IRDFF-II result, which only represents the In116m and In116 contributions, and misses the In114 production). TENDL-2019 does much better than TENDL-2017 (see [6]) for this element, reflecting the adjustment in the In115(n,γ) channel to the different isomeric states, but there is evidence from this experiment for further adjustment. The In114 profile is the correct match for the measurements during the first 5-minutes of cooling, but there is still potentially some issue with the branching ratio to In116m (and In116n and In116), because its contribution and dominance at later cooling times is too high. An alternative explanation to the overprediction of In116m could be poor characterisation of the thermal profile in the FNS neutron spectrum, but this is not observed in experiments on other materials (in general).
JEFF-3.3 and ENDF/B-VIII.0 fail to predict In116m at all, and also get the In114 contribution wrong, so those libraries have even greater issues for this case. The overprediction of In114 with those two libraries is due to incorrect summing of the In115(n,2n) contributions into one channel for In114 production, instead of including the correct (dominant) branching to In114m – a very longer-lived metastable. A rare case where IRDFF-II has multiple relevant reactions channels on the same element, but the profile and decay-heat

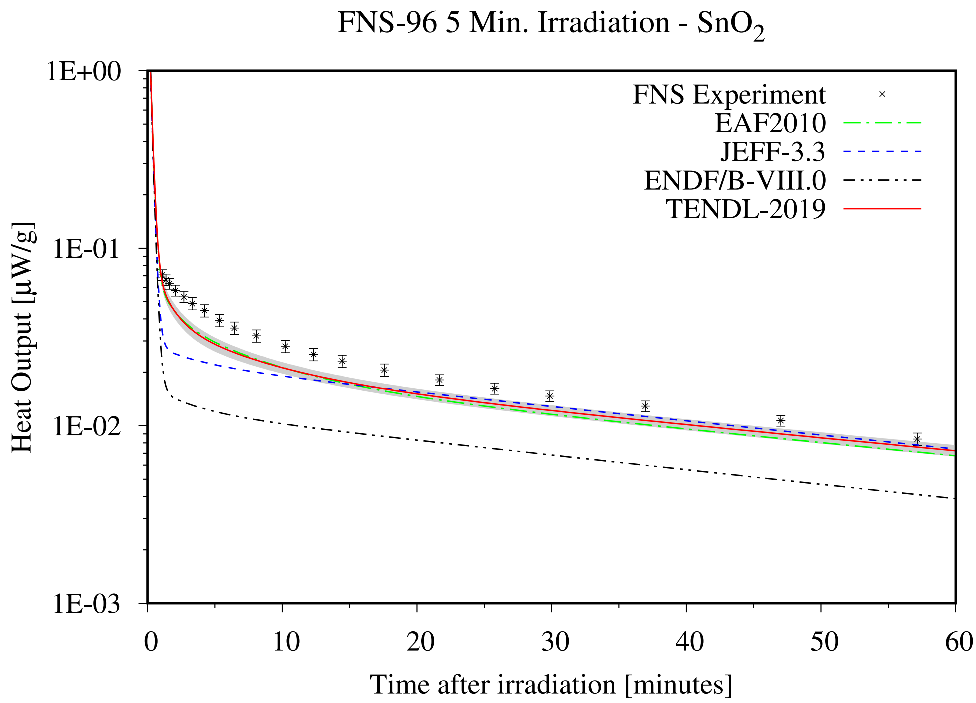
level are not a good match to the experiment.


FNS-00 5 Min. Irradiation - In - TENDL-2019
FNS-00 5 Min. Irradiation - In - EAF2010
FNS-00 5 Min. Irradiation - In - JEFF-3.3
FNS-00 5 Min. Irradiation - In - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
In115m
In112m
In112
In116
In116m
In114
Cd115
Ag112
00 Exp

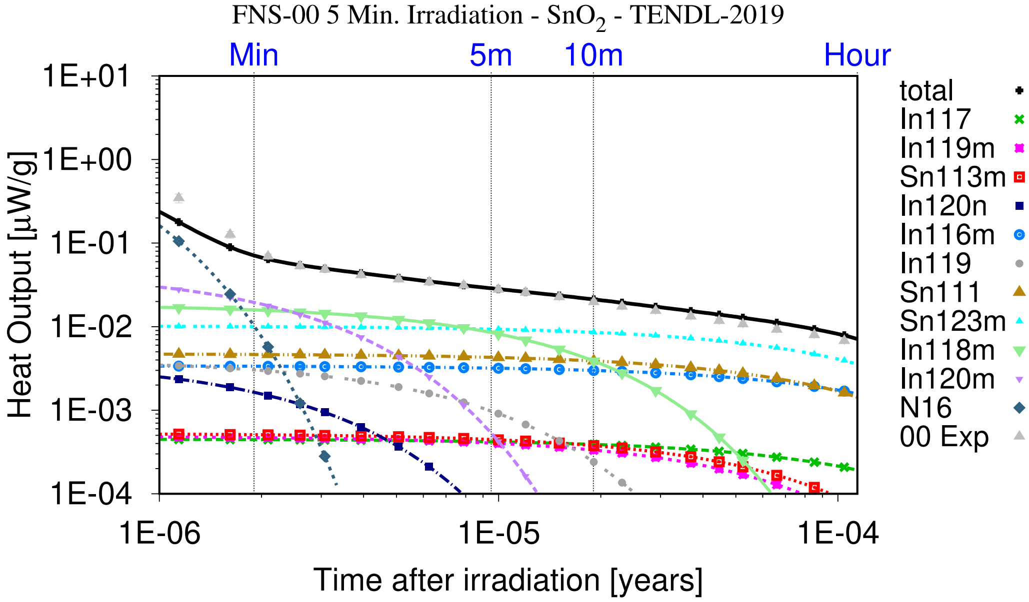

FNS-00 5 Min. Irradiation - In - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
114In
116In
116mIn
112In
112mIn
115mIn
112Ag
114mIn
Min
Hour
Day

Tin


FNS-00 5 Min. Irradiation - SnO_2
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - SnO_2
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
0
10
20
30
40
50
60
Time after irradiation [minutes]

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	3.45E−01 +/-12%	1.78E−01 +/-4%	1.93	2.73	1.99	2.50
0.85	1.26E−01 +/-9%	8.94E−02 +/-6%	1.41	2.97	1.47	2.34
1.10	6.93E−02 +/-7%	6.43E−02 +/-8%	1.08	3.12	1.12	2.06
1.37	5.28E−02 +/-7%	5.45E−02 +/-9%	0.97	3.16	1.00	1.88
1.62	4.81E−02 +/-7%	4.95E−02 +/-9%	0.97	3.16	0.99	1.81
2.07	4.14E−02 +/-7%	4.37E−02 +/-9%	0.95	2.91	0.95	1.63
2.67	3.67E−02 +/-7%	3.85E−02 +/-9%	0.96	2.70	0.94	1.50
3.28	3.39E−02 +/-7%	3.48E−02 +/-9%	0.97	2.59	0.95	1.43
4.15	3.10E−02 +/-7%	3.12E−02 +/-9%	0.99	2.48	0.97	1.36
5.25	2.77E−02 +/-7%	2.82E−02 +/-9%	0.98	2.33	0.96	1.27
6.32	2.55E−02 +/-7%	2.60E−02 +/-9%	0.98	2.23	0.96	1.21
7.93	2.25E−02 +/-7%	2.36E−02 +/-8%	0.96	2.07	0.94	1.12
10.03	1.97E−02 +/-6%	2.12E−02 +/-7%	0.93	1.92	0.93	1.03
12.15	1.73E−02 +/-6%	1.94E−02 +/-7%	0.90	1.78	0.90	0.96
15.27	1.54E−02 +/-6%	1.73E−02 +/-7%	0.89	1.69	0.91	0.91
19.38	1.32E−02 +/-6%	1.54E−02 +/-7%	0.86	1.57	0.89	0.84
23.48	1.17E−02 +/-6%	1.39E−02 +/-7%	0.84	1.51	0.88	0.81
27.60	1.07E−02 +/-6%	1.28E−02 +/-7%	0.84	1.49	0.88	0.79
34.73	9.20E−03 +/-6%	1.12E−02 +/-7%	0.82	1.47	0.87	0.78
44.78	7.92E−03 +/-6%	9.36E−03 +/-7%	0.85	1.53	0.90	0.81
54.90	6.74E−03 +/-6%	7.88E−03 +/-7%	0.86	1.58	0.91	0.83
mean % diff. from E			12	52	11	28
mean χ^2			4.29	59.93	3.21	19.64

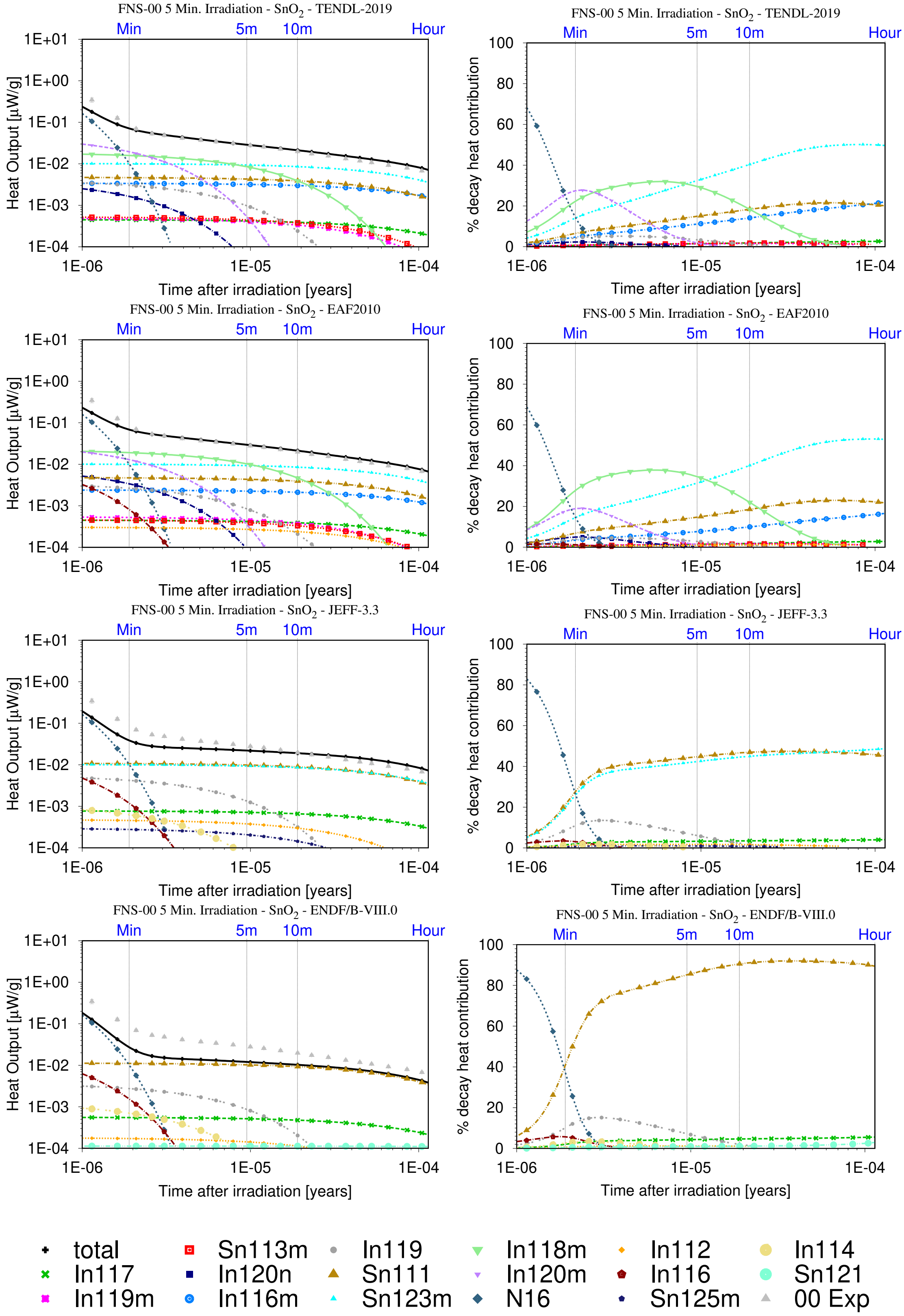


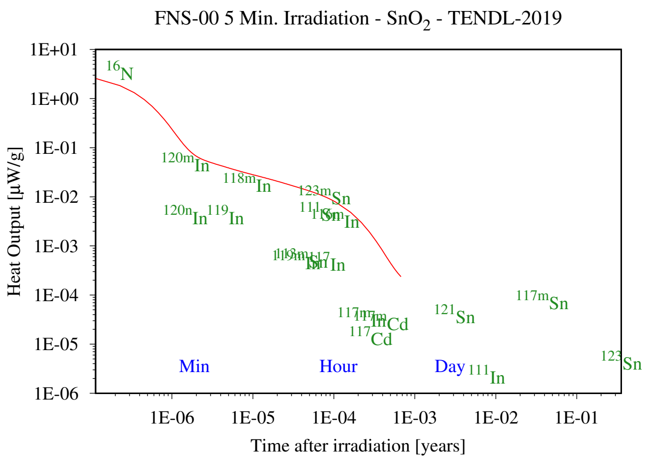
Tin, TENDL-2019 5-minute pathway analysis

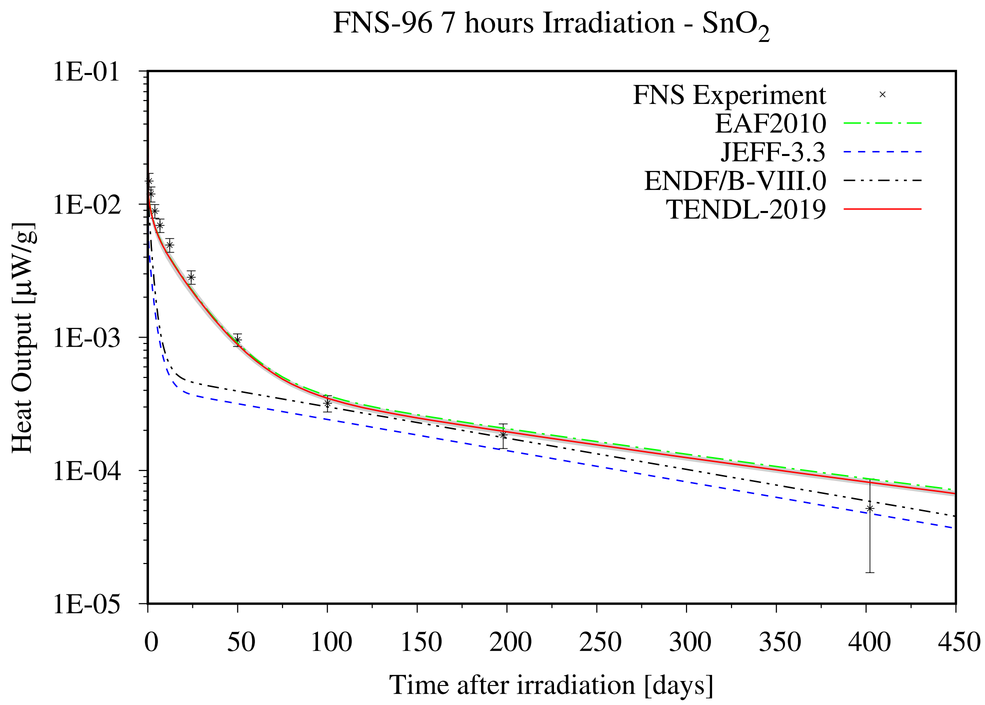
Product	**$T_{1/2}$**	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
In116	14.20s	Sn116(n,p)In116	97.0
		Sn117(n,np)In116	2.0
		Sn117(n,d)In116	1.1
In120n	46.21s	Sn120(n,p)In120n	100.0
In120m	46.21s	Sn120(n,p)In120m	100.0
In114	1.20m	Sn114(n,p)In114	83.3
		Sn115(n,np)In114	14.3
		Sn115(n,d)In114	2.3
In119	2.40m	Sn119(n,p)In119	91.3
		Sn120(n,np)In119	4.2
		Sn120(n,d)In119	3.8
In118m	4.45m	Sn118(n,p)In118m	88.2
		Sn118(n,p)In118n(IT)In118m	10.6
Sn125m	9.53m	Sn124(n,γ)Sn125m	100.0
In112	14.70m	Sn112(n,p)In112	84.6
		Sn112(n,p)In112m(IT)In112	15.4
In119m	18.00m	Sn119(n,p)In119m	92.1
		Sn120(n,d)In119m	6.5
Sn113m	20.90m	Sn114(n,2n)Sn113m	98.8
		Sn112(n,γ)Sn113m	1.2
Sn111	35.30m	Sn112(n,2n)Sn111	100.0
Sn123m	40.06m	Sn124(n,2n)Sn123m	99.9
In117	43.20m	Sn117(n,p)In117	89.5
		Sn118(n,np)In117	6.9
		Sn118(n,d)In117	3.1
In116m	54.60m	Sn116(n,p)In116m	59.0
		Sn116(n,p)In116n(IT)In116m	38.5
		Sn117(n,np)In116m	1.4
Sn121	1.12d	Sn122(n,2n)Sn121	97.2
		Sn120(n,γ)Sn121	2.8

Comments on Tin 5-minute experiments:

The two experimental result sets differ, although the simulation with TENDL, JEFF, and EAF produce a much better agreement with the most recent, year-2000 one. TENDL-2019 and EAF2010 seem to match the decay profile the best. JEFF-3.3 has the wrong shape at cooling times of less than 10 minutes, apparently because of missing (n,p) channels to metastable In118m and In120m. An improvement of the agreement for the TENDL-2019 (compared to TENDL-2017) with the experiment is observed for cooling times between 1 and 10 minutes when In118m is important – the overprediction of that nuclide with TENDL-2017 has been corrected. ENDF/B-VIII.0 misses not only the short-term metastables, but also the longer-lived Sn123m (from (n,2n) on Sn124) whose contribution is predicted to be dominant with TENDL-2019 after around 10 minutes. This latter point actually disagrees with JEFF-3.3, where Sn111 is shown to be just as important; demonstrating that there is general uncertainty in certain aspects of this complex picture for a material with so many naturally occurring isotopes, although TENDL and EAF perform best, suggesting that the picture they predict is more likely to be correct.


FNS-00 5 Min. Irradiation - SnO2 - TENDL-2019
FNS-00 5 Min. Irradiation - SnO2 - EAF2010
FNS-00 5 Min. Irradiation - SnO2 - JEFF-3.3
FNS-00 5 Min. Irradiation - SnO2 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Sn113m
In119
In118m
In112
In114
In117
In120n
Sn111
In120m
In116
Sn121
In119m
In116m
Sn123m
N16
Sn125m
00 Exp

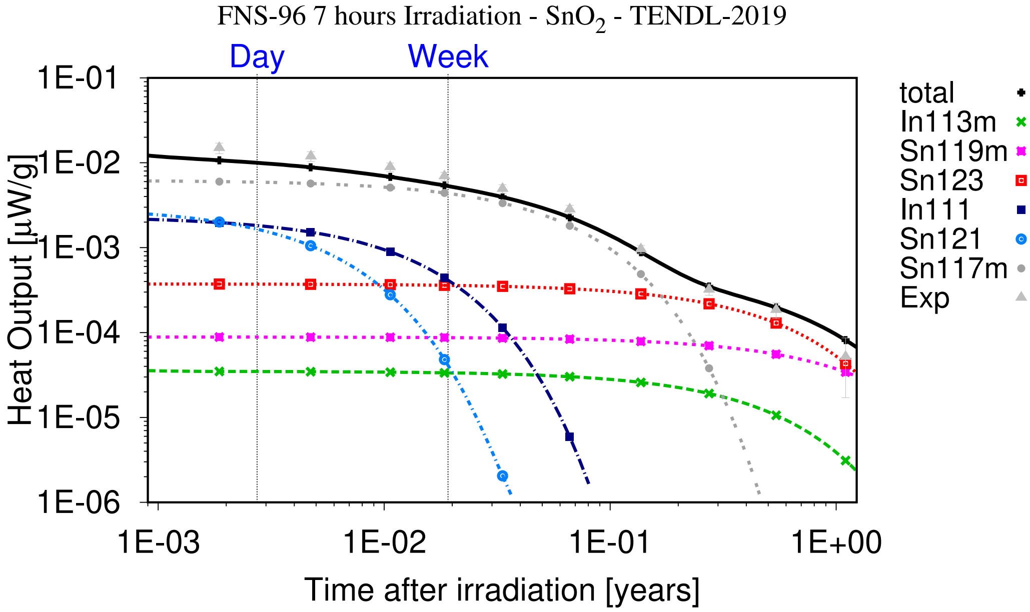

FNS-00 5 Min. Irradiation - SnO2 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
Min
Hour
Day
16N
120mIn
118mIn
123mSn
120nIn
119In
121Sn
117mSn
117Cd
111In
123Sn



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.68	1.49E−02 +/-14%	1.07E−02 +/-9%	1.40	1.72	1.38	3.24
1.73	1.19E−02 +/-13%	8.84E−03 +/-10%	1.35	2.22	1.33	3.85
3.88	8.88E−03 +/-12%	6.81E−03 +/-10%	1.30	3.77	1.29	5.44
6.75	6.93E−03 +/-12%	5.40E−03 +/-10%	1.28	6.03	1.27	7.60
12.20	4.94E−03 +/-12%	3.94E−03 +/-10%	1.25	7.91	1.24	9.66
24.20	2.83E−03 +/-12%	2.27E−03 +/-9%	1.25	6.12	1.23	7.61
49.95	9.57E−04 +/-11%	8.85E−04 +/-7%	1.08	2.42	1.05	3.01
100.08	3.20E−04 +/-14%	3.49E−04 +/-5%	0.92	1.06	0.88	1.32
197.93	1.85E−04 +/-21%	1.97E−04 +/-5%	0.94	1.04	0.89	1.30
402.13	5.18E−05 +/-67%	8.14E−05 +/-5%	0.64	0.88	0.60	1.09
mean % diff. from E			22	51	23	61
mean χ^2			2.29	25.28	2.21	31.51

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Sn117m	13.60d	1.28	12%	12%

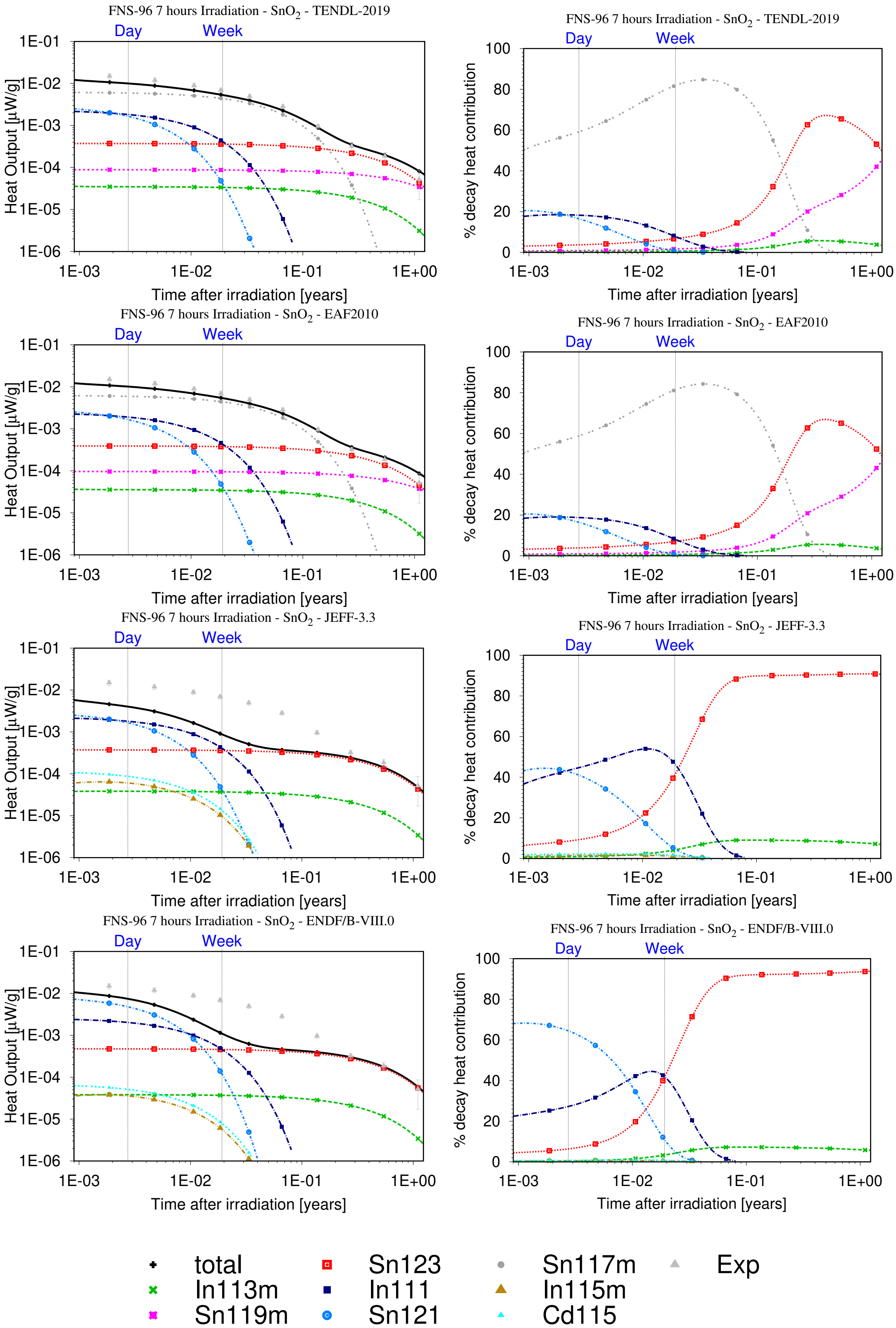


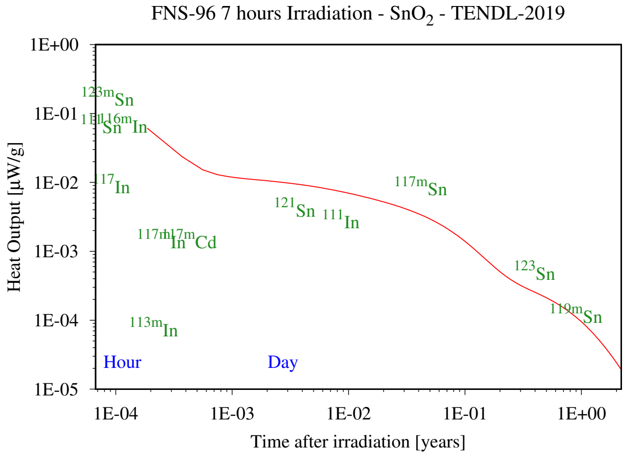
Tin,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
In113m	1.66h	no pathways found	
In115m	4.49h	no pathways found	
Sn121	1.12d	Sn122(n,2n)Sn121	98.4
		Sn120(n,γ)Sn121	1.5
Cd115	2.23d	Sn118(n,α)Cd115	99.9
In111	2.81d	Sn112(n,2n)Sn111(β^+)In111	95.9
		Sn112(n,np)In111	3.3
Sn117m	13.60d	Sn118(n,2n)Sn117m	94.0
		Sn117(n,n')Sn117m	5.9
Sn123	129.21d	Sn124(n,2n)Sn123	99.9
Sn119m	293.01d	Sn120(n,2n)Sn119m	93.9
		Sn119(n,n')Sn119m	6.0

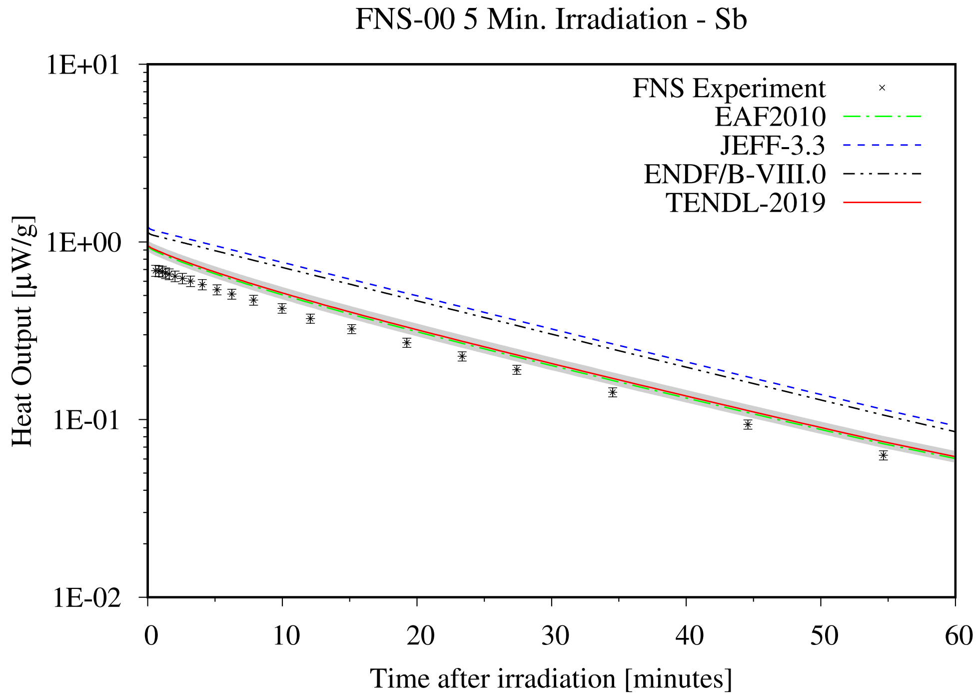
Comments on Tin 7-hour experiments:

Only TENDL-2019 and EAF2010 properly capture (to within around 20%) the experimentally measured decay profile for this longer tin experiment. JEFF-3.3 and ENDF/B-VIII.0 both miss the production of the Sn117m metastable that is important out to 50 days of cooling. This case also shows the limit of the experimental measurement technique, with the large uncertainty after 13 months of cooling reflecting the fact that the heat output is approaching the pico-watt limit of sensitivity.


FNS-96 7 hours Irradiation - SnO_2 - TENDL-2019
FNS-96 7 hours Irradiation - SnO_2 - EAF2010
FNS-96 7 hours Irradiation - SnO_2 - JEFF-3.3
FNS-96 7 hours Irradiation - SnO_2 - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E+00
0
20
40
60
80
100
total
Sn123
Sn117m
Exp
In113m
In111
In115m
Sn119m
Sn121
Cd115


FNS-96 7 hours Irradiation - SnO2 - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-04
1E-03
1E-02
1E-01
1E+00
Hour
Day
123mSn
116mIn
117In
117mIn
117mCd
113mIn
121Sn
111In
117mSn
123Sn
119mSn

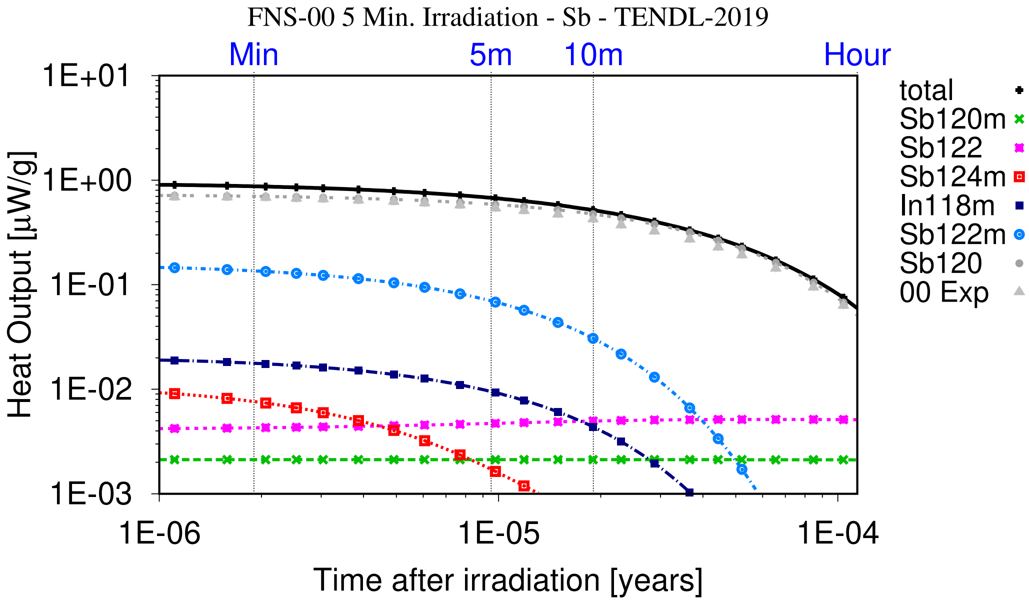
Antimony



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	6.89E−01 +/-7%	9.02E−01 +/-7%	0.76	0.64	0.78	0.60
0.83	6.86E−01 +/-7%	8.85E−01 +/-7%	0.78	0.64	0.79	0.60
1.08	6.81E−01 +/-7%	8.69E−01 +/-7%	0.78	0.64	0.80	0.60
1.33	6.68E−01 +/-7%	8.54E−01 +/-7%	0.78	0.64	0.80	0.60
1.60	6.59E−01 +/-7%	8.38E−01 +/-7%	0.79	0.64	0.80	0.60
2.03	6.41E−01 +/-7%	8.14E−01 +/-7%	0.79	0.63	0.80	0.59
2.58	6.23E−01 +/-7%	7.85E−01 +/-7%	0.79	0.63	0.81	0.59
3.18	6.02E−01 +/-7%	7.56E−01 +/-7%	0.80	0.62	0.81	0.58
4.05	5.75E−01 +/-7%	7.17E−01 +/-7%	0.80	0.62	0.82	0.58
5.15	5.38E−01 +/-7%	6.72E−01 +/-8%	0.80	0.61	0.82	0.57
6.25	5.09E−01 +/-6%	6.31E−01 +/-8%	0.81	0.60	0.83	0.56
7.87	4.70E−01 +/-6%	5.78E−01 +/-8%	0.81	0.60	0.83	0.56
9.98	4.23E−01 +/-6%	5.17E−01 +/-8%	0.82	0.59	0.84	0.55
12.08	3.70E−01 +/-6%	4.65E−01 +/-8%	0.80	0.56	0.82	0.53
15.15	3.24E−01 +/-6%	4.01E−01 +/-8%	0.81	0.56	0.83	0.53
19.25	2.71E−01 +/-6%	3.32E−01 +/-8%	0.82	0.56	0.84	0.53
23.35	2.27E−01 +/-6%	2.76E−01 +/-8%	0.82	0.56	0.84	0.53
27.42	1.91E−01 +/-6%	2.31E−01 +/-8%	0.83	0.56	0.85	0.53
34.53	1.42E−01 +/-6%	1.71E−01 +/-8%	0.83	0.57	0.86	0.53
44.58	9.39E−02 +/-6%	1.13E−01 +/-8%	0.83	0.58	0.86	0.54
54.65	6.30E−02 +/-6%	7.52E−02 +/-8%	0.84	0.59	0.86	0.55
mean % diff. from E			24	66	22	78
mean χ^2			14.48	114.21	11.33	156.11

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Sb120	15.90m	0.76	7%	9%

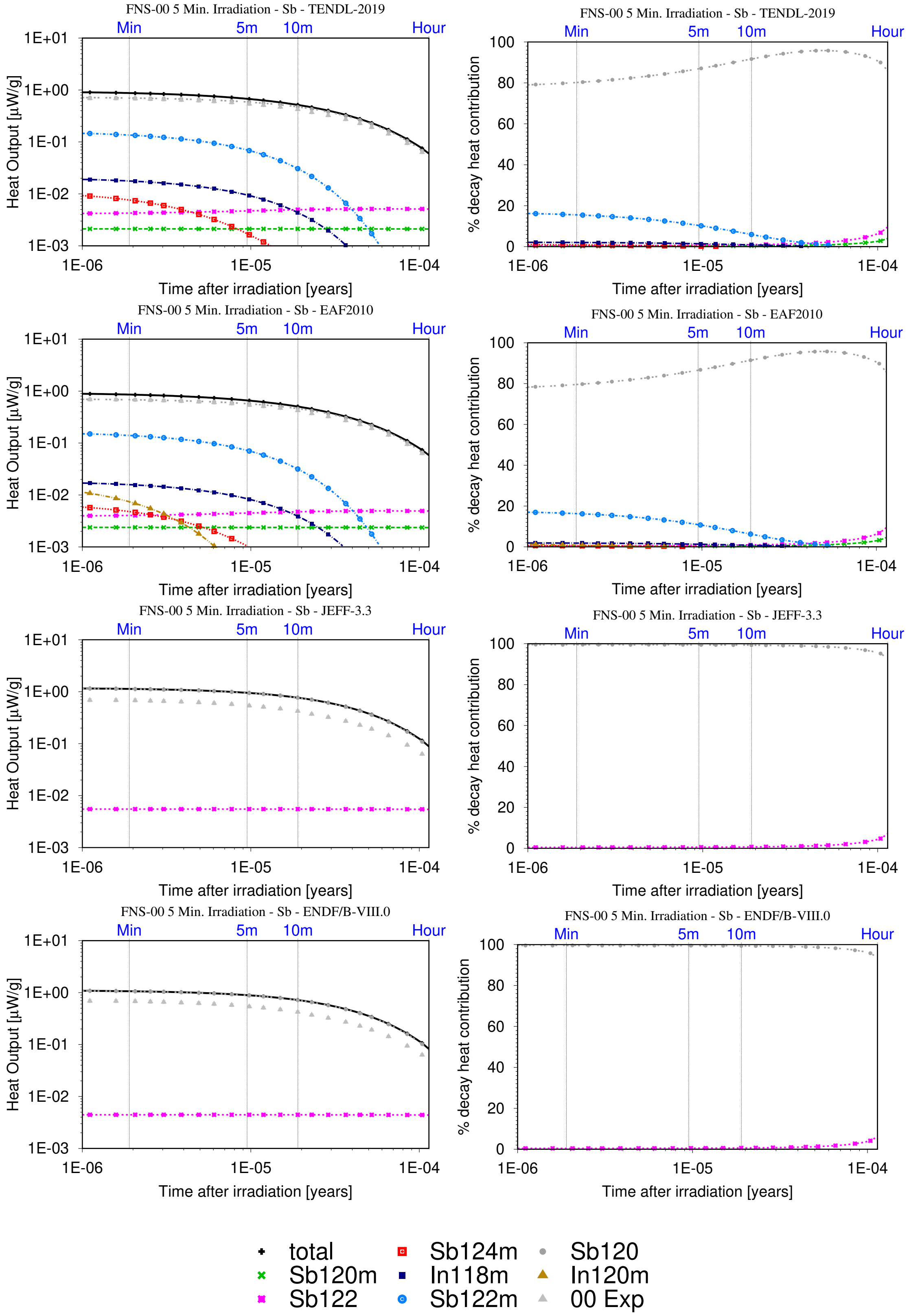


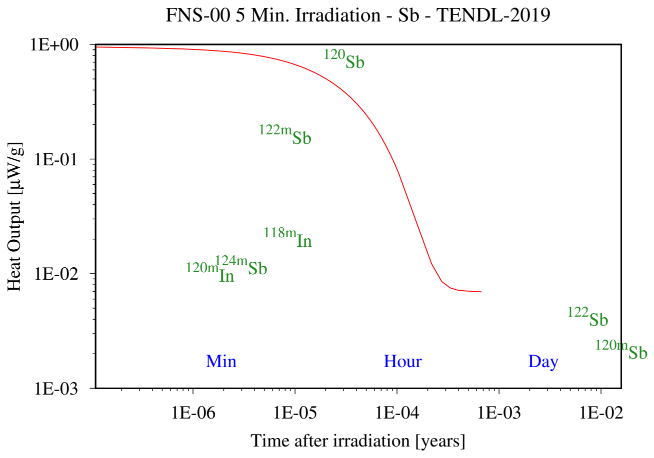
Antimony, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
In120m	46.21s	Sb123(n,α)In120m	100.0
Sb124m	1.55m	Sb123(n,γ)Sb124m	96.8
		Sb123(n,γ)Sb124n(IT)Sb124m	3.1
Sb122m	4.19m	Sb123(n,2n)Sb122m	99.8
In118m	4.45m	Sb121(n,α)In118m	65.5
		Sb121(n,α)In118n(IT)In118m	34.5
Sb120	15.90m	Sb121(n,2n)Sb120	100.0
Sb122	2.70d	Sb123(n,2n)Sb122	84.5
		Sb123(n,2n)Sb122m(IT)Sb122	12.1
		Sb121(n,γ)Sb122	3.4
Sb120m	5.76d	Sb121(n,2n)Sb120m	100.0

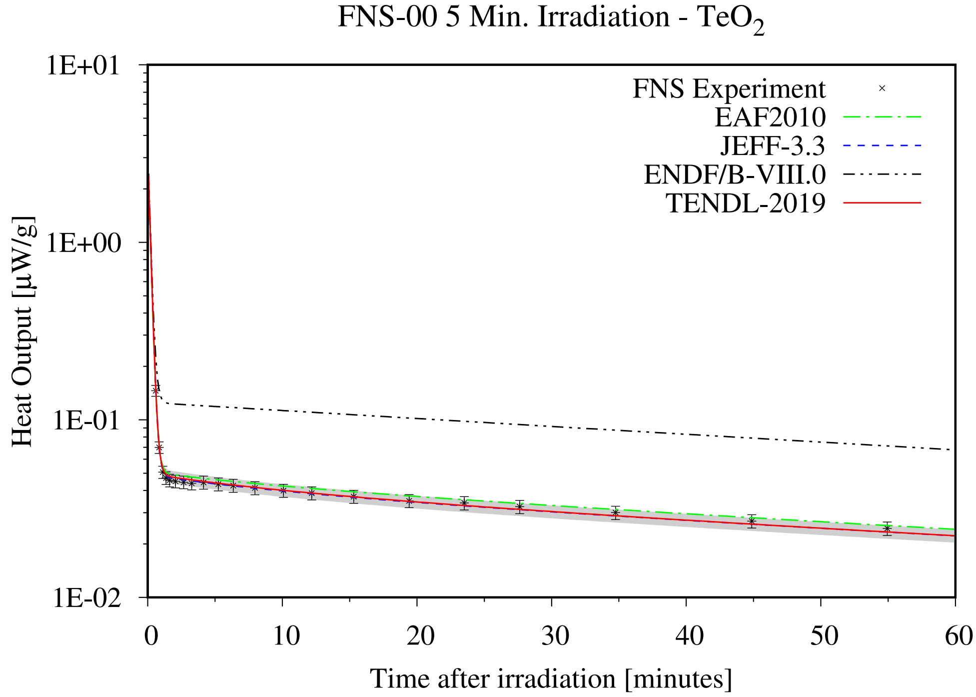
Comments on Antimony 5-minute experiments:

TENDL-2019 results are very similar to EAF2010, but both over-predict by around 20-30% at all cooling times, suggesting that there may need to be some re-evaluation of the (n,2n) channel on Sb121, which is responsible for the production of the Sb120 nuclide that is predicted to dominate at all cooling times measured. Still, these two libraries are performing better than either ENDF/B-VIII.0 or JEFF-3.3, which seem to get this reaction channel very wrong.


FNS-00 5 Min. Irradiation - Sb - TENDL-2019
FNS-00 5 Min. Irradiation - Sb - EAF2010
FNS-00 5 Min. Irradiation - Sb - JEFF-3.3
FNS-00 5 Min. Irradiation - Sb - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Sb120m
Sb122
Sb124m
In118m
Sb122m
Sb120
In120m
00 Exp


FNS-00 5 Min. Irradiation - Sb - TENDL-2019
1E+00
1E-01
1E-02
1E-03
Heat Output [µW/g]
120Sb
122mSb
118mIn
120mIn
124mSb
122Sb
120mSb
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

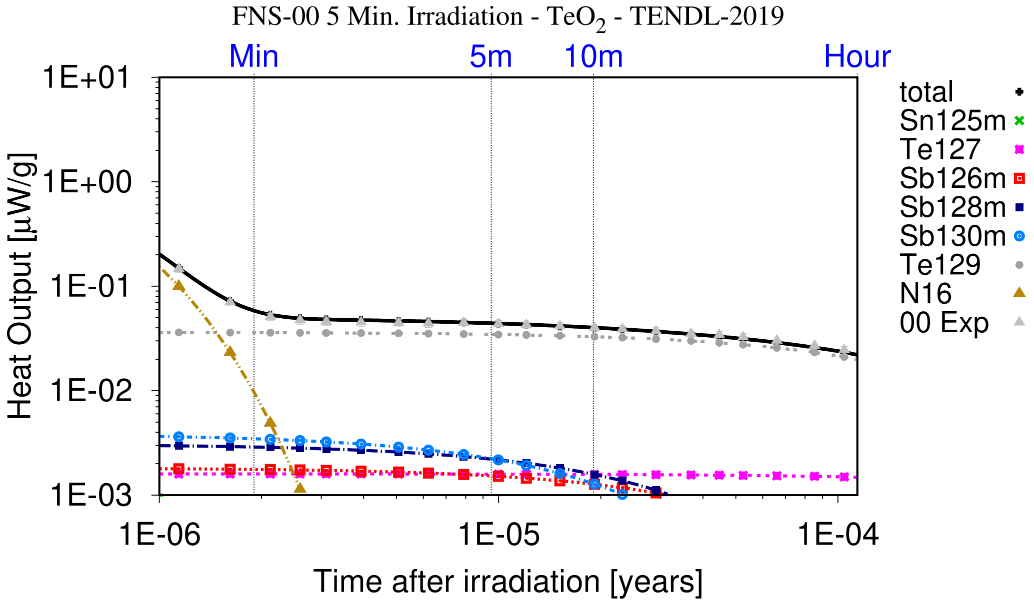
Tellurium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	1.46E−01 +/-7%	1.49E−01 +/-3%	0.98	0.65	0.98	0.99
0.85	6.99E−02 +/-7%	7.20E−02 +/-6%	0.97	0.47	0.96	0.98
1.12	5.08E−02 +/-8%	5.34E−02 +/-8%	0.95	0.39	0.93	0.96
1.37	4.71E−02 +/-8%	4.93E−02 +/-8%	0.96	0.38	0.93	0.97
1.63	4.56E−02 +/-8%	4.81E−02 +/-8%	0.95	0.37	0.92	0.96
2.07	4.51E−02 +/-8%	4.73E−02 +/-8%	0.95	0.37	0.92	0.97
2.67	4.45E−02 +/-8%	4.66E−02 +/-8%	0.96	0.37	0.92	0.97
3.27	4.39E−02 +/-8%	4.59E−02 +/-8%	0.96	0.36	0.92	0.97
4.15	4.44E−02 +/-8%	4.50E−02 +/-8%	0.99	0.37	0.95	1.00
5.25	4.34E−02 +/-8%	4.40E−02 +/-8%	0.99	0.37	0.95	1.00
6.35	4.27E−02 +/-8%	4.30E−02 +/-8%	0.99	0.36	0.95	1.00
7.97	4.13E−02 +/-8%	4.17E−02 +/-8%	0.99	0.36	0.94	1.00
10.08	4.00E−02 +/-8%	4.01E−02 +/-8%	1.00	0.35	0.94	1.01
12.18	3.86E−02 +/-8%	3.87E−02 +/-8%	1.00	0.35	0.94	1.01
15.30	3.70E−02 +/-8%	3.69E−02 +/-8%	1.00	0.35	0.94	1.01
19.42	3.50E−02 +/-8%	3.48E−02 +/-8%	1.01	0.34	0.94	1.01
23.52	3.40E−02 +/-9%	3.29E−02 +/-8%	1.03	0.35	0.96	1.04
27.63	3.24E−02 +/-9%	3.13E−02 +/-8%	1.03	0.34	0.96	1.04
34.75	3.00E−02 +/-9%	2.89E−02 +/-8%	1.04	0.34	0.96	1.04
44.87	2.69E−02 +/-9%	2.59E−02 +/-8%	1.04	0.34	0.96	1.04
54.93	2.44E−02 +/-9%	2.34E−02 +/-8%	1.05	0.34	0.96	1.05
mean % diff. from E			3	170	6	2
mean χ^2			0.16	429.22	0.58	0.11

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Te129	1.16h	0.95	8%	9%

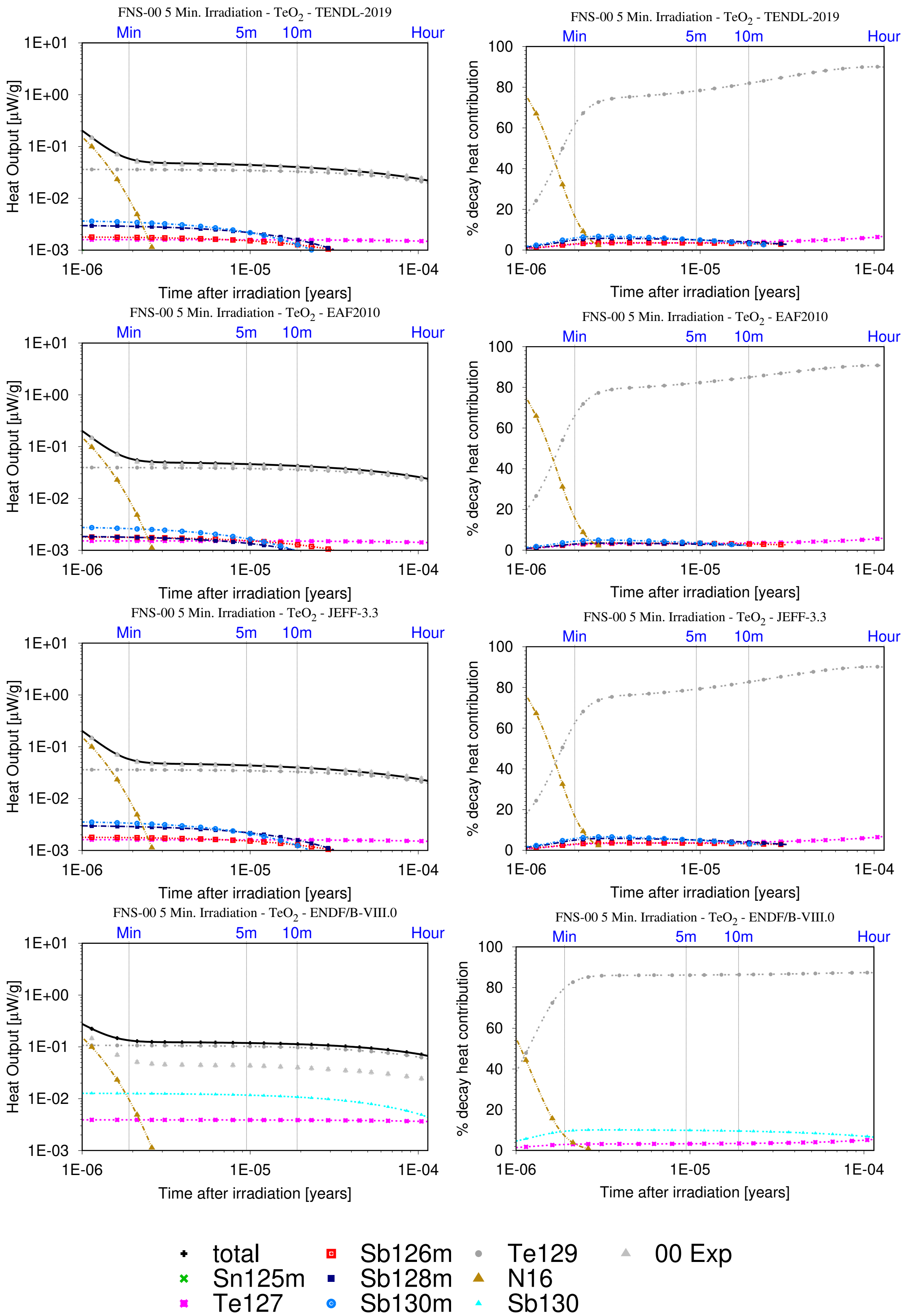


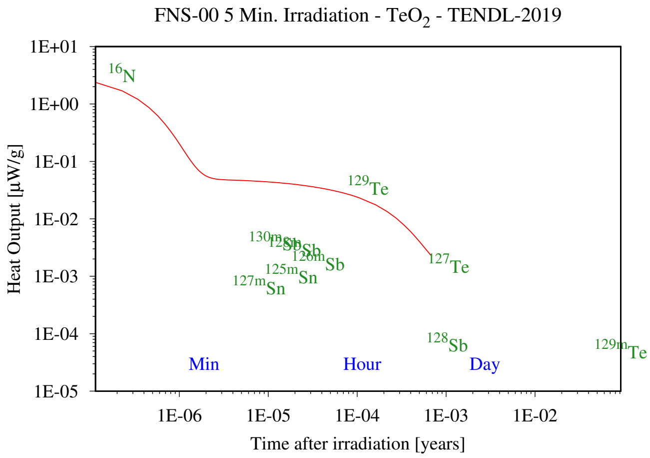
Tellurium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Sb130m	6.30m	Te130(n,p)Sb130m	100.0
Sn125m	9.53m	Te128(n,α)Sn125m	100.0
Sb128m	10.40m	Te128(n,p)Sb128m	100.0
Sb126m	19.10m	Te126(n,p)Sb126n(IT)Sb126m	58.6
		Te126(n,p)Sb126m	41.4
Sb130	39.50m	Te130(n,p)Sb130	100.0
Te129	1.16h	Te130(n,2n)Te129	99.6
Te127	9.35h	Te128(n,2n)Te127	99.6

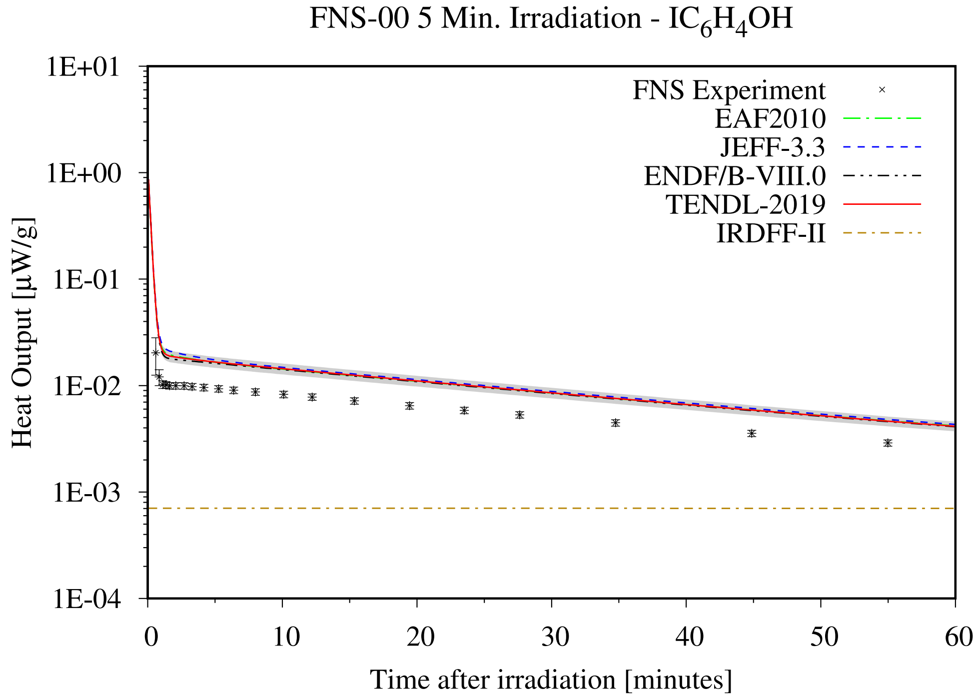
Comments on Tellurium 5-minute experiments:

An excellent simulation versus experiment comparison for TENDL-2019, JEFF-3.3 and EAF2010, even for the prediction of N16 from oxygen at very short cooling time. ENDF/B-VIII.0 seems to massively overpredict the production of the dominant Te129, which is almost certainly due to the incorrect summing of contributions from Te130(n,2n)Te129 and Te130(n,2n)Te129m into a single channel producing Te129. Te129m has a much longer half-life than its ground-state daughter (33.6 days versus 1.16 hours) and so does not contribute measurably to the decay-heat when properly accounted for.


FNS-00 5 Min. Irradiation - TeO_2 - TENDL-2019
FNS-00 5 Min. Irradiation - TeO_2 - EAF2010
FNS-00 5 Min. Irradiation - TeO_2 - JEFF-3.3
FNS-00 5 Min. Irradiation - TeO_2 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Sn125m
Te127
Sb126m
Sb128m
Sb130m
Te129
N16
Sb130
00 Exp


FNS-00 5 Min. Irradiation - TeO2 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02
16N
129Te
127Te
128Sb
129mTe
130mSb
125Sb
126Sb
126mSb
125mSn
127mSn
Min
Hour
Day

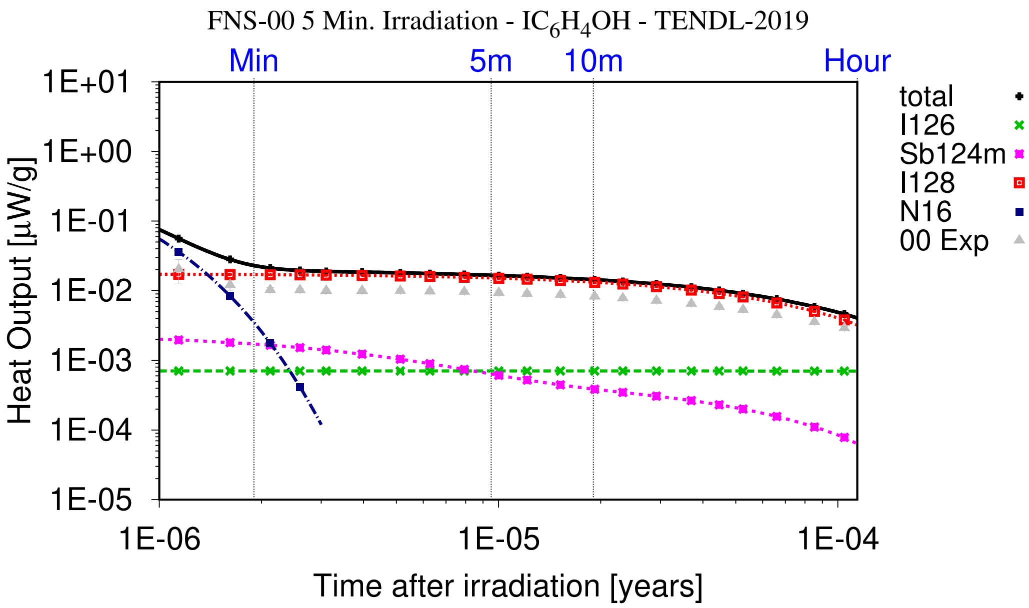
Iodine



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
0.60	$2.03E{-}02$ +/-38%	$5.61E{-}02$ +/-5%	0.36	0.37	0.36	0.34	28.83
0.85	$1.20E{-}02$ +/-17%	$2.81E{-}02$ +/-9%	0.43	0.45	0.42	0.39	17.12
1.12	$1.03E{-}02$ +/-8%	$2.12E{-}02$ +/-11%	0.48	0.52	0.47	0.43	14.56
1.37	$1.02E{-}02$ +/-7%	$1.96E{-}02$ +/-12%	0.52	0.55	0.50	0.46	14.45
1.63	$9.97E{-}03$ +/-7%	$1.89E{-}02$ +/-12%	0.53	0.56	0.51	0.47	14.16
2.08	$9.98E{-}03$ +/-7%	$1.85E{-}02$ +/-12%	0.54	0.57	0.53	0.49	14.17
2.70	$9.95E{-}03$ +/-7%	$1.81E{-}02$ +/-12%	0.55	0.58	0.54	0.51	14.13
3.30	$9.78E{-}03$ +/-7%	$1.76E{-}02$ +/-12%	0.55	0.58	0.55	0.52	13.90
4.17	$9.59E{-}03$ +/-7%	$1.71E{-}02$ +/-12%	0.56	0.58	0.56	0.53	13.63
5.27	$9.34E{-}03$ +/-7%	$1.65E{-}02$ +/-12%	0.57	0.58	0.57	0.54	13.27
6.38	$9.04E{-}03$ +/-7%	$1.60E{-}02$ +/-12%	0.57	0.58	0.57	0.55	12.84
8.00	$8.71E{-}03$ +/-7%	$1.52E{-}02$ +/-12%	0.57	0.58	0.58	0.55	12.38
10.10	$8.26E{-}03$ +/-7%	$1.44E{-}02$ +/-12%	0.57	0.59	0.58	0.56	11.74
12.22	$7.80E{-}03$ +/-7%	$1.36E{-}02$ +/-12%	0.57	0.58	0.58	0.56	11.08
15.35	$7.18E{-}03$ +/-7%	$1.25E{-}02$ +/-12%	0.57	0.58	0.58	0.56	10.21
19.45	$6.47E{-}03$ +/-7%	$1.12E{-}02$ +/-12%	0.58	0.58	0.58	0.56	9.19
23.52	$5.84E{-}03$ +/-7%	$1.01E{-}02$ +/-11%	0.58	0.59	0.58	0.56	8.30
27.63	$5.31E{-}03$ +/-7%	$9.09E{-}03$ +/-11%	0.58	0.59	0.59	0.57	7.56
34.75	$4.47E{-}03$ +/-7%	$7.58E{-}03$ +/-11%	0.59	0.60	0.59	0.57	6.36
44.87	$3.56E{-}03$ +/-7%	$5.90E{-}03$ +/-11%	0.60	0.61	0.60	0.58	5.06
54.98	$2.89E{-}03$ +/-7%	$4.63E{-}03$ +/-11%	0.62	0.63	0.62	0.60	4.11
mean % diff. from E			85	79	86	96	90
mean χ^2			113.61	98.20	116.51	147.15	147.35

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
I128	24.99m	0.48	8%	13%

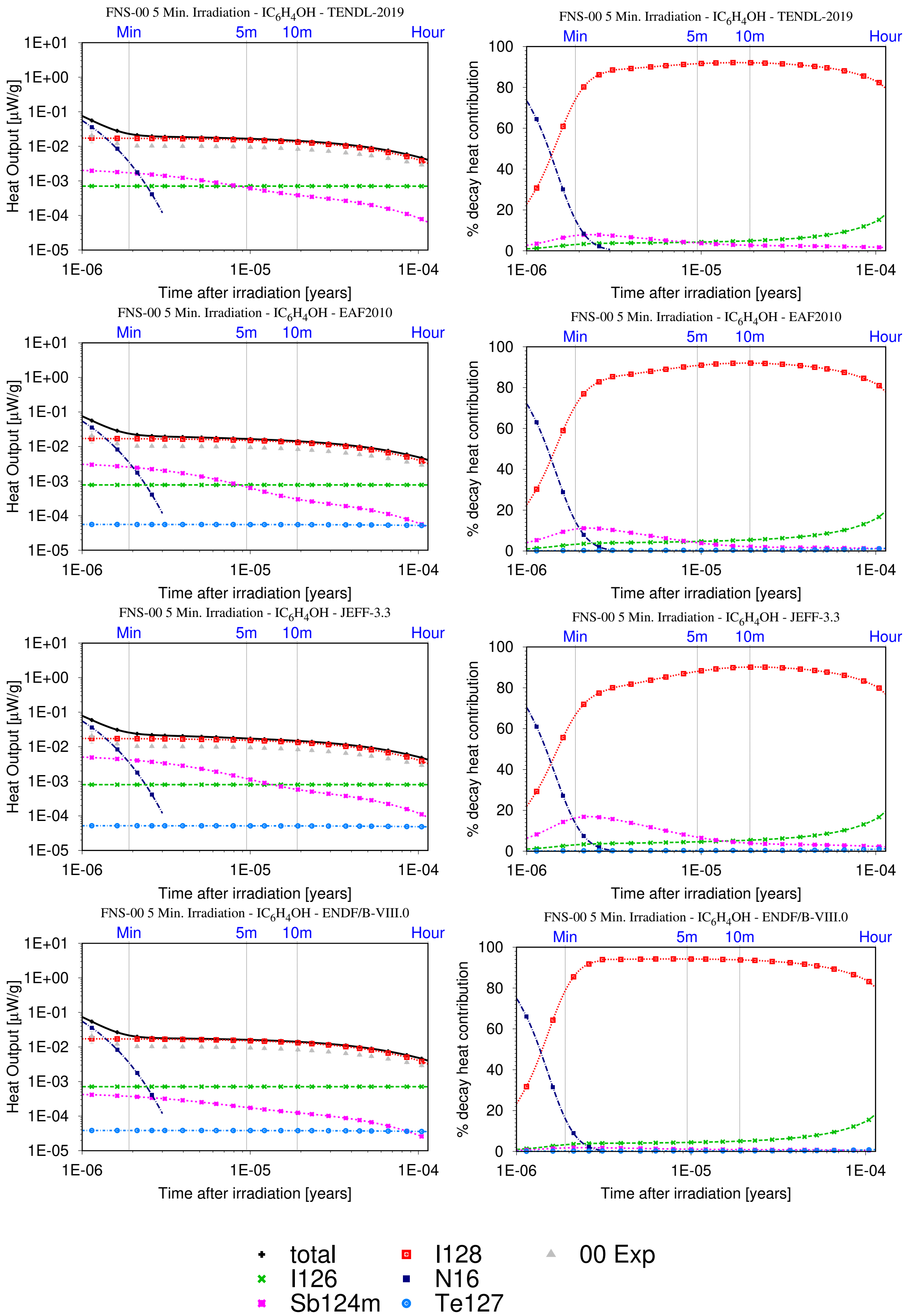


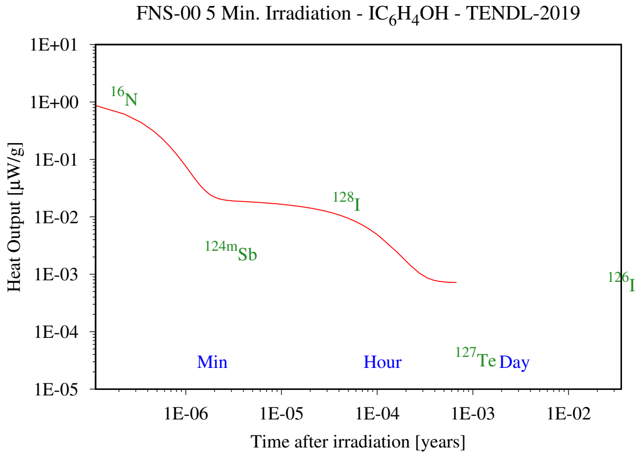
Iodine, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Sb124m	1.55m	I127(n,α)Sb124m	88.0
		I127(n,α)Sb124n(IT)Sb124m	12.0
I128	24.99m	I127(n,γ)I128	100.0
Te127	9.35h	I127(n,p)Te127	100.0
I126	12.98d	I127(n,2n)I126	100.0

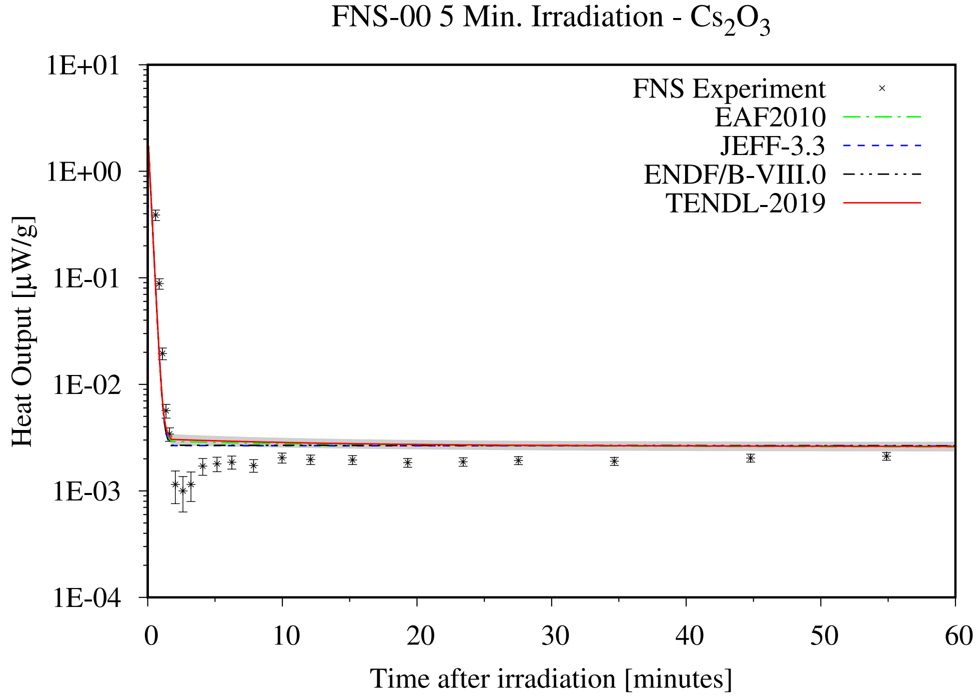
Comments on Iodine 5-minute experiments:

A systematic overprediction with all of the general purpose libraries. At cooling times less than 1 minute N16 from oxygen dominates the decay heat, but this seems overpredicted by a factor of 2 in the simulations. Beyond 1-minute of cooling the (n,γ) reaction on I127 to produce the dominant I128 seems to have been overpredicted with all general libraries suggesting that the thermal part of that cross section may not be correct (or there is a problem in the characterisation of the neutron spectrum). IRDFF-II only contains the (n,2n) channel to produce the long-lived I126 from I127 and so shows a massive underprediction but is included here to illustrate the underlying decay-heat that will become dominant at longer cooling times.


FNS-00 5 Min. Irradiation - IC_6H_4OH - TENDL-2019
FNS-00 5 Min. Irradiation - IC_6H_4OH - EAF2010
FNS-00 5 Min. Irradiation - IC_6H_4OH - JEFF-3.3
FNS-00 5 Min. Irradiation - IC_6H_4OH - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
I128
00 Exp
I126
N16
Sb124m
Te127


FNS-00 5 Min. Irradiation - IC6H4OH - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
128I
124mSb
126I
127Te
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

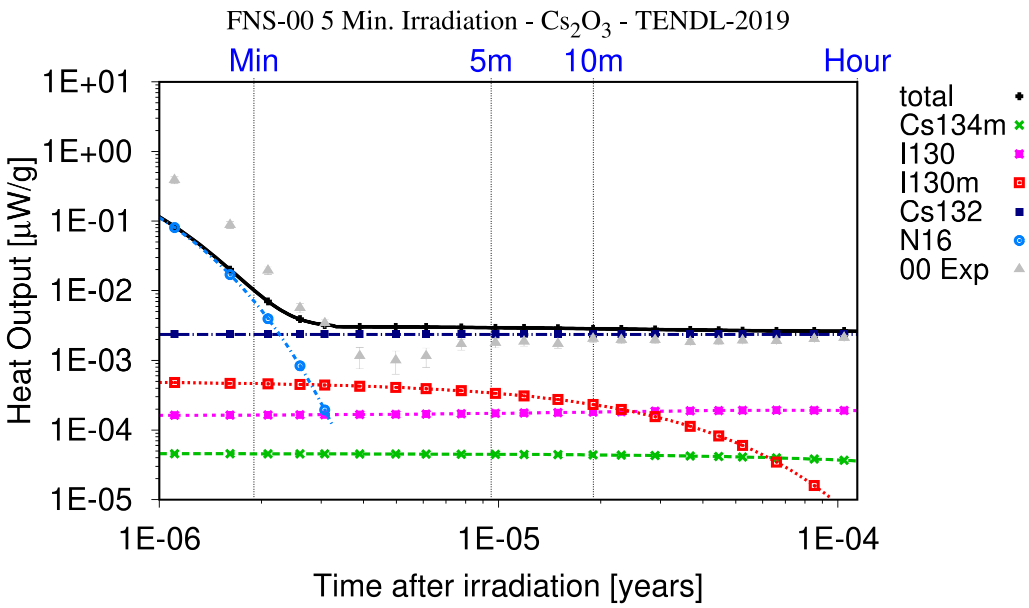
Caesium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	3.89$E-$01 +/-11%	8.38$E-$02 +/-0%	4.64	4.68	4.73	4.66
0.85	8.81$E-$02 +/-11%	2.01$E-$02 +/-2%	4.38	4.49	4.49	4.47
1.10	1.95$E-$02 +/-13%	7.02$E-$03 +/-5%	2.78	2.95	2.86	2.95
1.37	5.66$E-$03 +/-15%	3.88$E-$03 +/-10%	1.46	1.61	1.52	1.62
1.62	3.42$E-$03 +/-15%	3.24$E-$03 +/-11%	1.05	1.19	1.10	1.20
2.05	1.15$E-$03 +/-34%	3.03$E-$03 +/-12%	0.38	0.43	0.40	0.43
2.62	9.98$E-$04 +/-37%	3.02$E-$03 +/-12%	0.33	0.37	0.35	0.38
3.22	1.15$E-$03 +/-31%	3.00$E-$03 +/-12%	0.38	0.43	0.40	0.43
4.08	1.71$E-$03 +/-18%	2.98$E-$03 +/-11%	0.57	0.64	0.60	0.64
5.15	1.79$E-$03 +/-16%	2.95$E-$03 +/-11%	0.61	0.67	0.63	0.67
6.25	1.86$E-$03 +/-14%	2.92$E-$03 +/-11%	0.64	0.70	0.66	0.70
7.87	1.73$E-$03 +/-14%	2.89$E-$03 +/-11%	0.60	0.65	0.62	0.65
9.98	2.04$E-$03 +/-11%	2.85$E-$03 +/-11%	0.72	0.76	0.74	0.77
12.10	1.97$E-$03 +/-10%	2.82$E-$03 +/-10%	0.70	0.74	0.71	0.74
15.22	1.95$E-$03 +/-10%	2.78$E-$03 +/-10%	0.70	0.73	0.72	0.74
19.32	1.84$E-$03 +/-9%	2.74$E-$03 +/-10%	0.67	0.69	0.68	0.69
23.43	1.87$E-$03 +/-9%	2.71$E-$03 +/-10%	0.69	0.70	0.70	0.71
27.53	1.93$E-$03 +/-9%	2.68$E-$03 +/-10%	0.72	0.72	0.73	0.73
34.67	1.90$E-$03 +/-9%	2.66$E-$03 +/-10%	0.72	0.71	0.72	0.72
44.78	2.03$E-$03 +/-9%	2.63$E-$03 +/-10%	0.77	0.76	0.78	0.77
54.88	2.12$E-$03 +/-8%	2.62$E-$03 +/-10%	0.81	0.80	0.81	0.80
mean % diff. from E			67	59	63	58
mean χ^2			21.05	17.80	19.41	17.36

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
N16	7.13s	4.64	11%	-
Cs132	6.53d	0.38	34%	11%

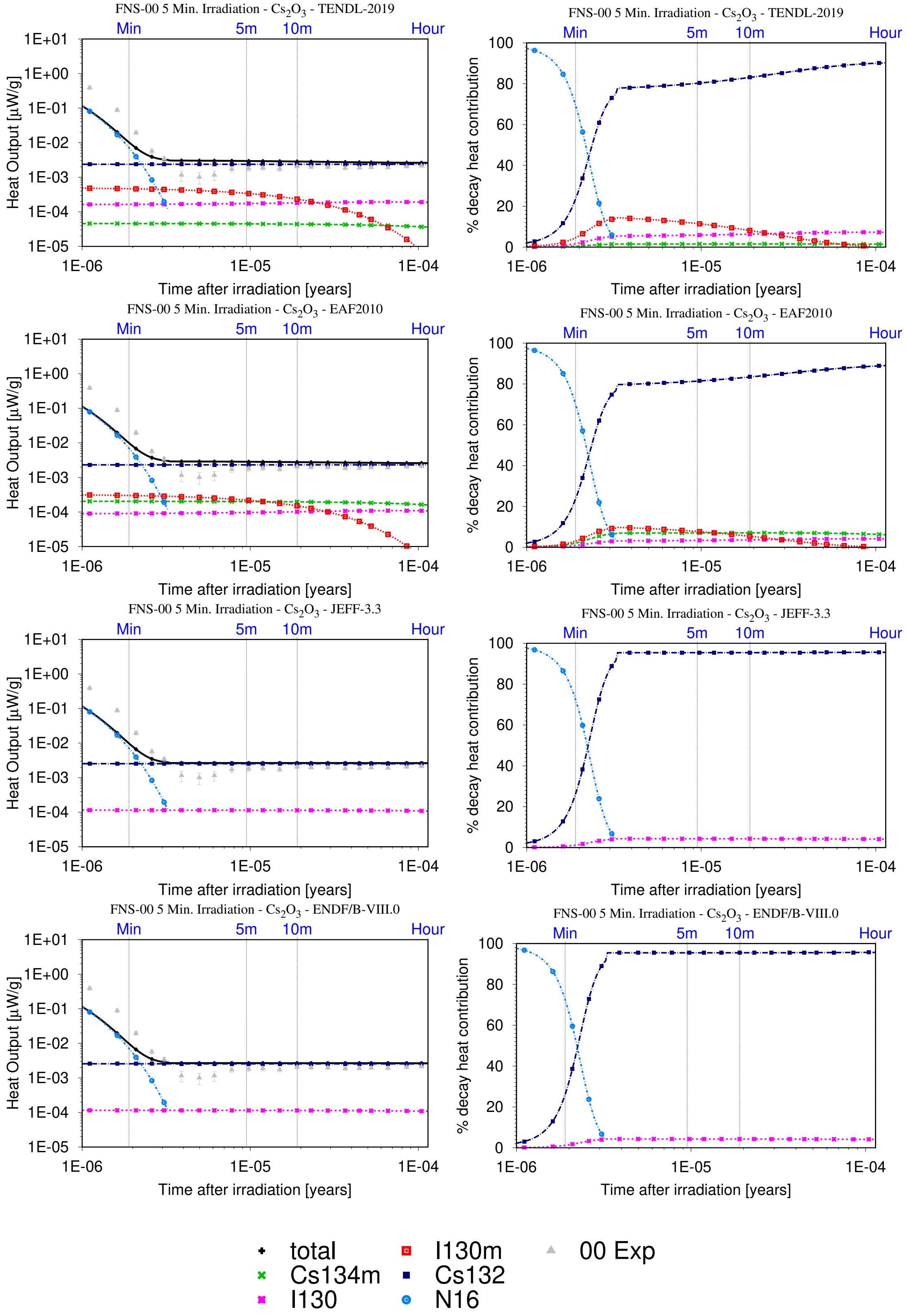


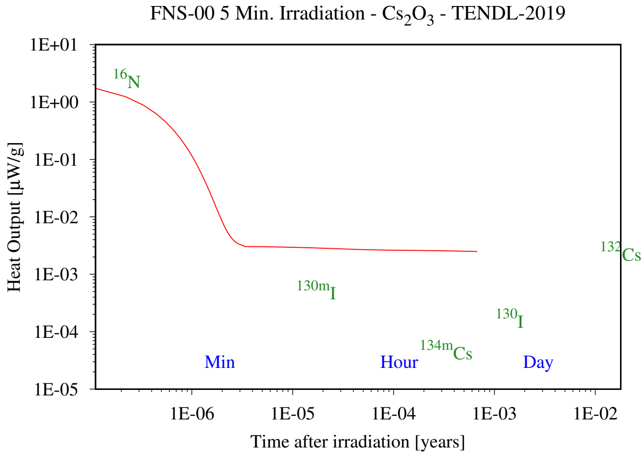
Caesium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
I130m	9.00m	Cs133(n,α)I130m	100.0
Cs134m	2.91h	Cs133(n,γ)Cs134m	100.0
I130	12.36h	Cs133(n,α)I130	95.0
		Cs133(n,α)I130m(IT)I130	5.0
Cs132	6.53d	Cs133(n,2n)Cs132	100.0

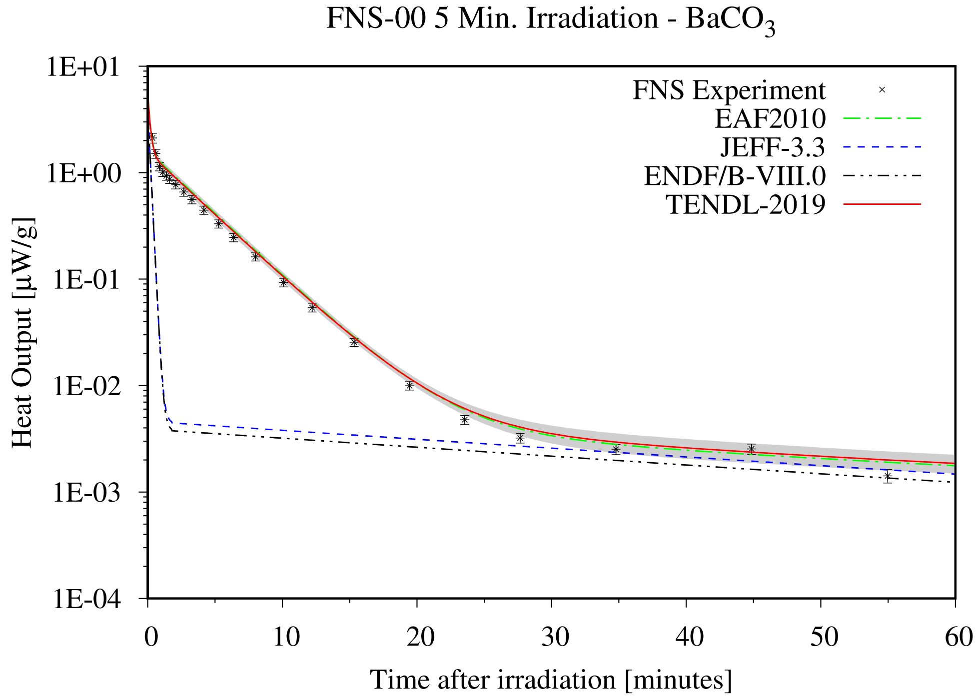
Comments on Caesium 5-minute experiments:

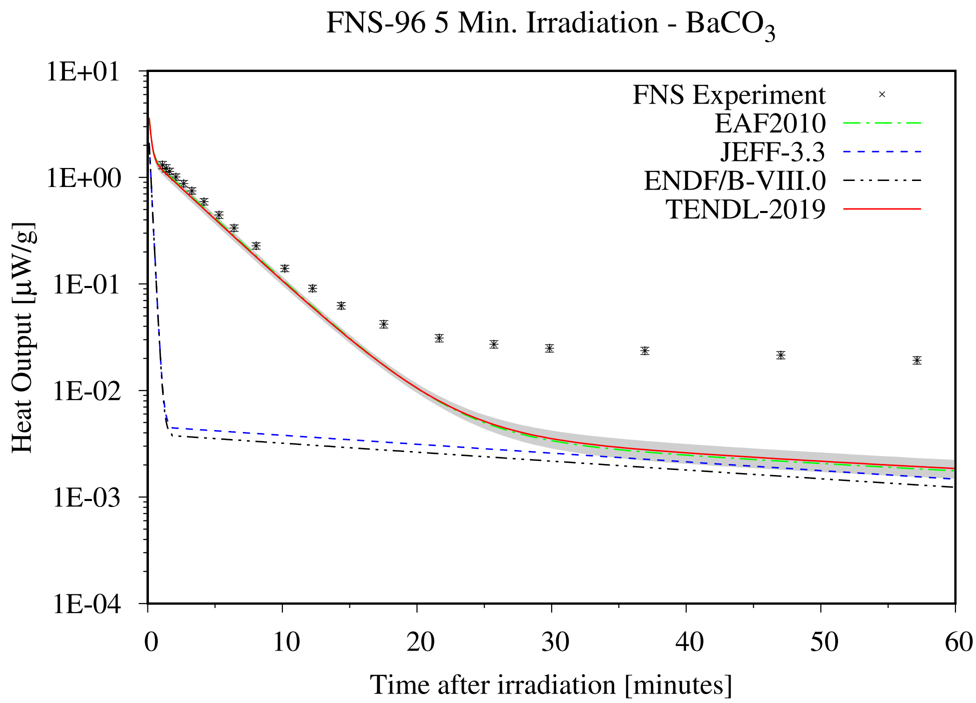
A surprising, but not necessarily un-physical upward trend in the experimental heat measurements during the first 1.5 minutes of cooling is observed, which may be caused by a larger than expected subtraction of the tape contribution, or unidentified isomeric states (although there is nothing obvious missing). The simulations do not capture this part of the profile, showing, instead a simple two-nuclide profile from first N16 ad then Cs132 for all remaining decay times. The simulations and experiment all seem to agree on the longer term (10-60 minutes) dominance of the Cs132 nuclide from (n,2n) reactions, although the simulations seem to overpredict its contribution slightly.


FNS-00 5 Min. Irradiation - Cs2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Cs2O3 - EAF2010
FNS-00 5 Min. Irradiation - Cs2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Cs2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Cs134m
I130
I130m
Cs132
N16
00 Exp


FNS-00 5 Min. Irradiation - Cs_2O_3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
^{16}N
^{130m}I
^{134m}Cs
^{130}I
^{132}Cs
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

Barium

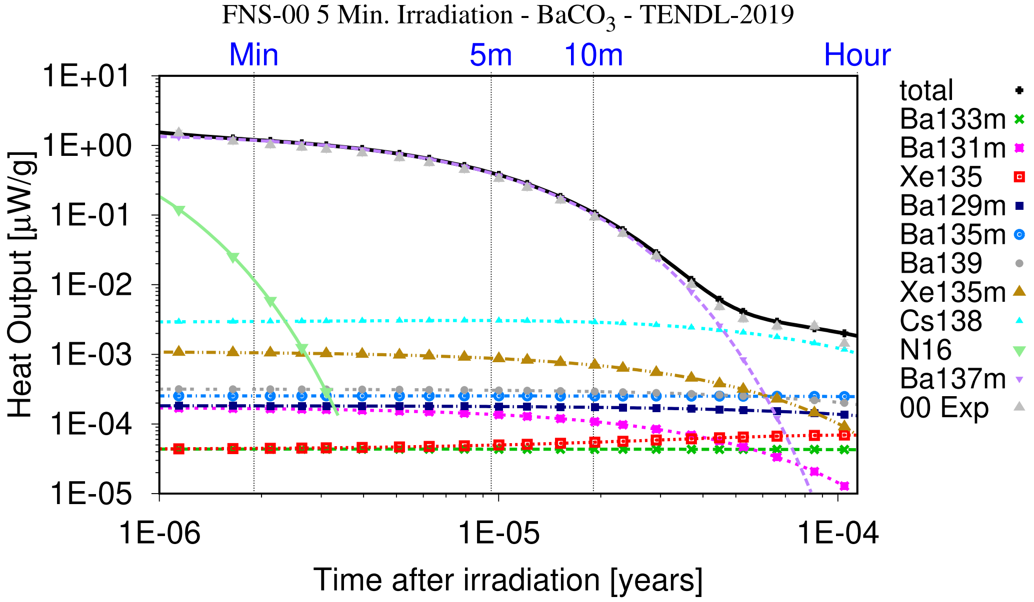

FNS-00 5 Min. Irradiation - BaCO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]


FNS-96 5 Min. Irradiation - BaCO3
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.35	2.12E+00 +/-11%	1.94E+00 +/-7%	1.09	4.07	1.08	4.04
0.60	1.51E+00 +/-10%	1.45E+00 +/-9%	1.04	12.17	1.02	12.04
0.87	1.14E+00 +/-9%	1.26E+00 +/-10%	0.90	38.99	0.88	37.97
1.12	1.01E+00 +/-9%	1.16E+00 +/-10%	0.87	103.77	0.85	96.79
1.38	9.32$E-$01 +/-9%	1.08E+00 +/-10%	0.87	185.15	0.84	162.49
1.63	8.69$E-$01 +/-9%	1.00E+00 +/-10%	0.86	213.73	0.84	181.35
2.08	7.72$E-$01 +/-9%	8.90$E-$01 +/-10%	0.87	206.27	0.84	174.12
2.68	6.58$E-$01 +/-9%	7.57$E-$01 +/-10%	0.87	177.90	0.85	150.16
3.28	5.59$E-$01 +/-9%	6.44$E-$01 +/-10%	0.87	152.94	0.85	129.08
4.17	4.45$E-$01 +/-9%	5.07$E-$01 +/-10%	0.88	123.88	0.85	104.55
5.27	3.31$E-$01 +/-9%	3.78$E-$01 +/-10%	0.88	94.16	0.85	79.45
6.38	2.46$E-$01 +/-9%	2.80$E-$01 +/-10%	0.88	71.54	0.86	60.35
8.00	1.62$E-$01 +/-9%	1.82$E-$01 +/-10%	0.89	48.63	0.87	41.02
10.10	9.27$E-$02 +/-9%	1.05$E-$01 +/-9%	0.88	29.00	0.86	24.45
12.22	5.38$E-$02 +/-9%	6.08$E-$02 +/-9%	0.88	17.54	0.87	14.79
15.33	2.55$E-$02 +/-9%	2.83$E-$02 +/-9%	0.90	8.84	0.89	7.45
19.45	9.97$E-$03 +/-9%	1.17$E-$02 +/-10%	0.85	3.74	0.85	3.15
23.55	4.78$E-$03 +/-9%	6.10$E-$03 +/-13%	0.78	1.94	0.80	1.64
27.67	3.21$E-$03 +/-10%	4.08$E-$03 +/-18%	0.79	1.41	0.82	1.19
34.78	2.52$E-$03 +/-11%	2.95$E-$03 +/-21%	0.86	1.27	0.90	1.07
44.85	2.54$E-$03 +/-11%	2.37$E-$03 +/-21%	1.07	1.55	1.13	1.30
54.97	1.42$E-$03 +/-14%	2.00$E-$03 +/-20%	0.71	1.05	0.75	0.88
mean % diff. from E			16	79	17	77
mean χ^2			2.99	89.04	3.36	86.93

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ba137m	2.55m	1.04	10%	10%

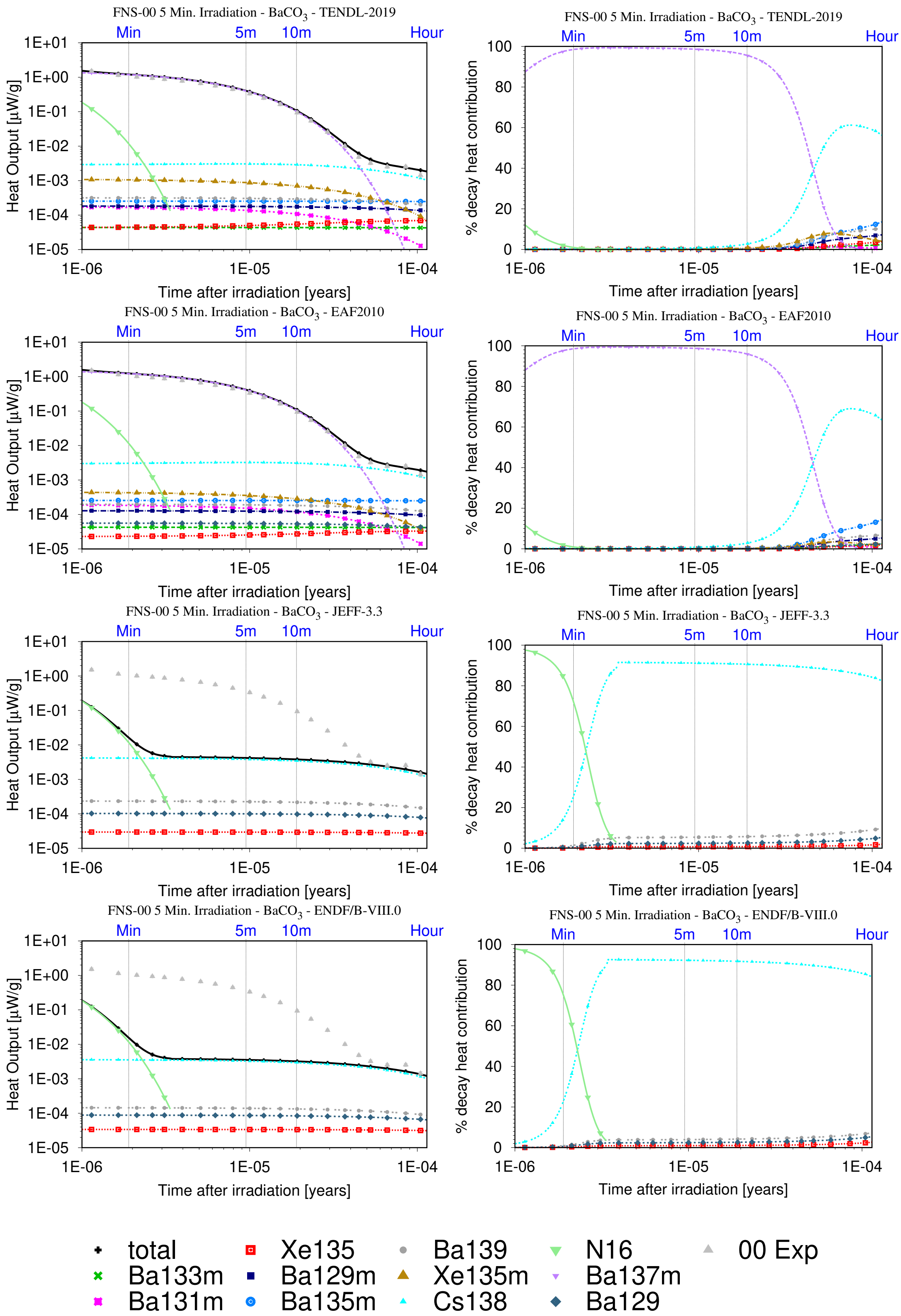


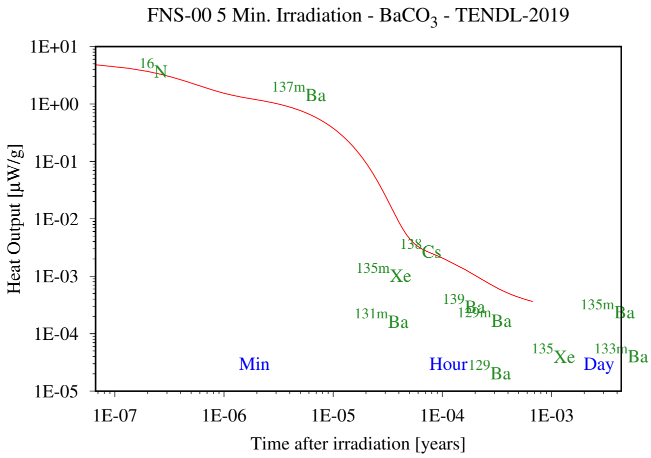
Barium, TENDL-2019 5-minute pathway analysis

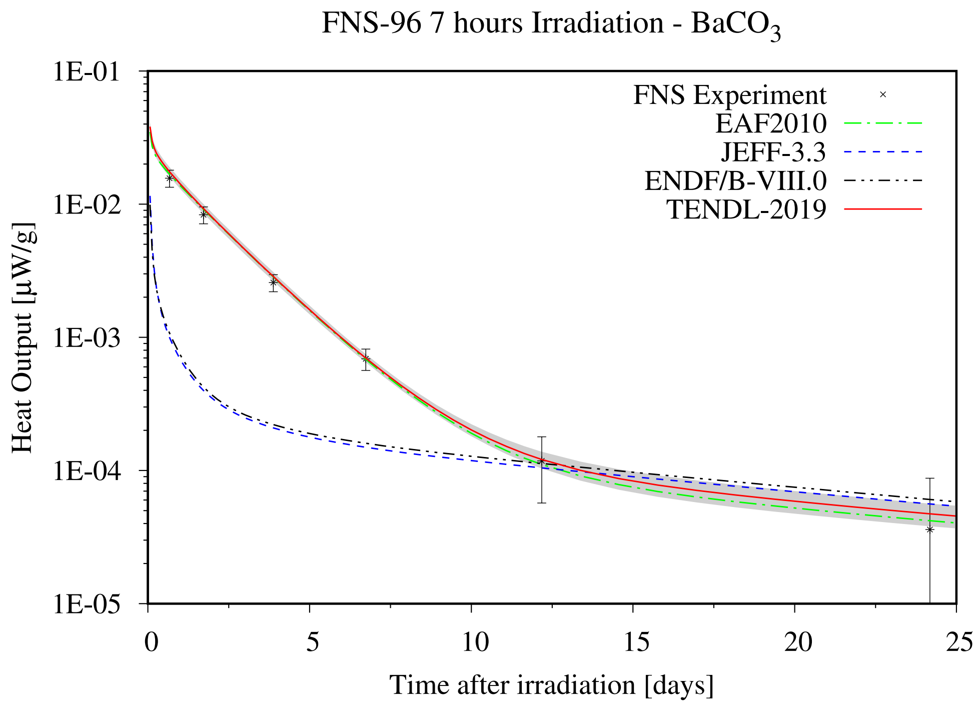
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ba137m	2.55m	Ba138(n,2n)Ba137m	96.1
		Ba137(n,n′)Ba137m	3.9
Ba131m	14.60m	Ba132(n,2n)Ba131m	99.2
Xe135m	15.29m	Ba138(n,α)Xe135m	100.0
Cs138	33.41m	Ba138(n,p)Cs138	83.1
		Ba138(n,p)Cs138m(IT)Cs138	16.9
Ba139	1.38h	Ba138(n,γ)Ba139	100.0
Ba129m	2.14h	Ba130(n,2n)Ba129m	100.0
Ba129	2.38h	Ba130(n,2n)Ba129	100.0
Xe135	9.14h	Ba138(n,α)Xe135	91.0
		Ba138(n,α)Xe135m(IT)Xe135	9.0
Ba135m	1.20d	Ba136(n,2n)Ba135m	87.6
		Ba135(n,n′)Ba135m	12.4
Ba133m	1.59d	Ba134(n,2n)Ba133m	100.0

Comments on Barium 5-minute experiments:

The 1996 sample may have contained some unidentified impurities, possibly Fluorine, which may explain the significant underestimation in the code predictions with EAF and TENDL that are not repeated in the comparison to the 2000 experiment. TENDL-2019 and EAF2010 nicely capture the profile of decay, which is a simple two nuclide picture. At short cooling times (less than around 20 minutes) and for most of the measurement points, Ba137m dominates, and an improved agreement with the experiment is observed for this experiment with TENDL-2019 in comparison to the TENDL-2017 results (by around 10%). ENDF/B-VIII.0 and JEFF-3.3 both fail to predict Ba137m production via (n,2n) reactions on Ba138 (and probably mis-attribute the Ba137m production to the stable Ba137 instead). At longer cooling times Cs138 predominates, and all library predictions converge to this contribution. However, TENDL and EAF seem to overpredict the total decay-heat for the final four measurements, but it is difficult to attribute this to a particular failing in the simulations as those two libraries predict many minor contributions from various metastable nuclides – many of which JEFF and ENDF/B miss and yet those to libraries are a better match to the experiment for those last four measurements.


FNS-00 5 Min. Irradiation - BaCO3 - TENDL-2019
FNS-00 5 Min. Irradiation - BaCO3 - EAF2010
FNS-00 5 Min. Irradiation - BaCO3 - JEFF-3.3
FNS-00 5 Min. Irradiation - BaCO3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Xe135
Ba139
N16
00 Exp
Ba133m
Ba129m
Xe135m
Ba137m
Ba131m
Ba135m
Cs138
Ba129

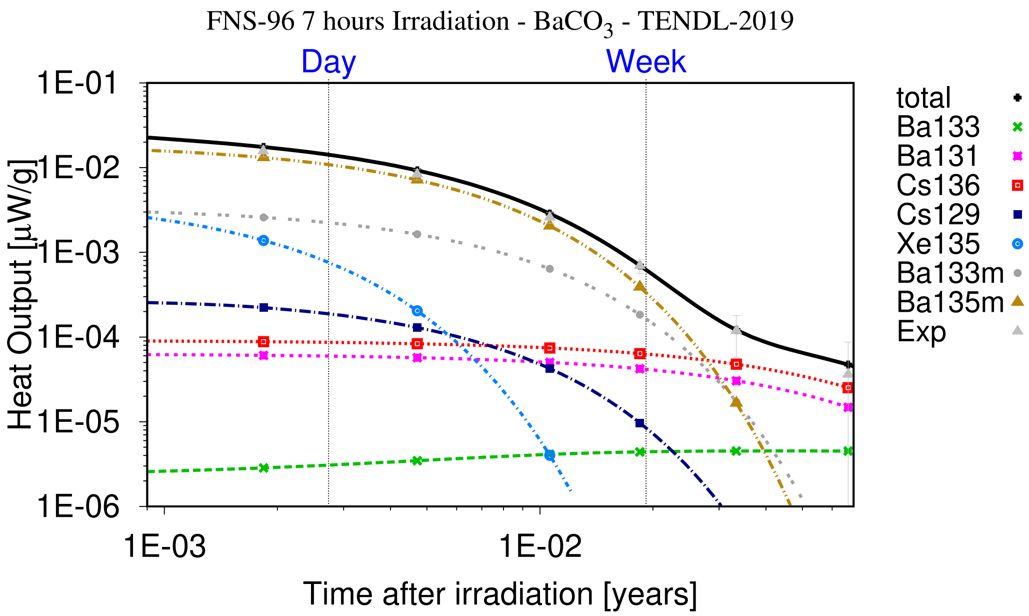

FNS-00 5 Min. Irradiation - BaCO3 - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-07
1E-06
1E-05
1E-04
1E-03
16N
137mBa
138Cs
135mXe
139Ba
129mBa
131mBa
135mBa
135Xe
133mBa
129Ba
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.67	$1.57E{-}02$ +/-15%	$1.75E{-}02$ +/-8%	0.89	14.57	0.93	15.74
1.72	$8.33E{-}03$ +/-14%	$9.26E{-}03$ +/-8%	0.90	19.70	0.91	20.90
3.88	$2.58E{-}03$ +/-15%	$2.86E{-}03$ +/-8%	0.90	11.65	0.90	12.32
6.74	$6.90E{-}04$ +/-18%	$6.98E{-}04$ +/-7%	0.99	4.31	1.01	4.62
12.18	$1.18E{-}04$ +/-52%	$1.21E{-}04$ +/-14%	0.98	1.05	1.06	1.13
24.18	$3.60E{-}05$ +/-143%	$4.73E{-}05$ +/-19%	0.76	0.59	0.86	0.64
mean % diff. from E			12	72	8	71
mean χ^2			0.32	23.41	0.21	23.71

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Ba135m	1.20d	0.90	14%	10%

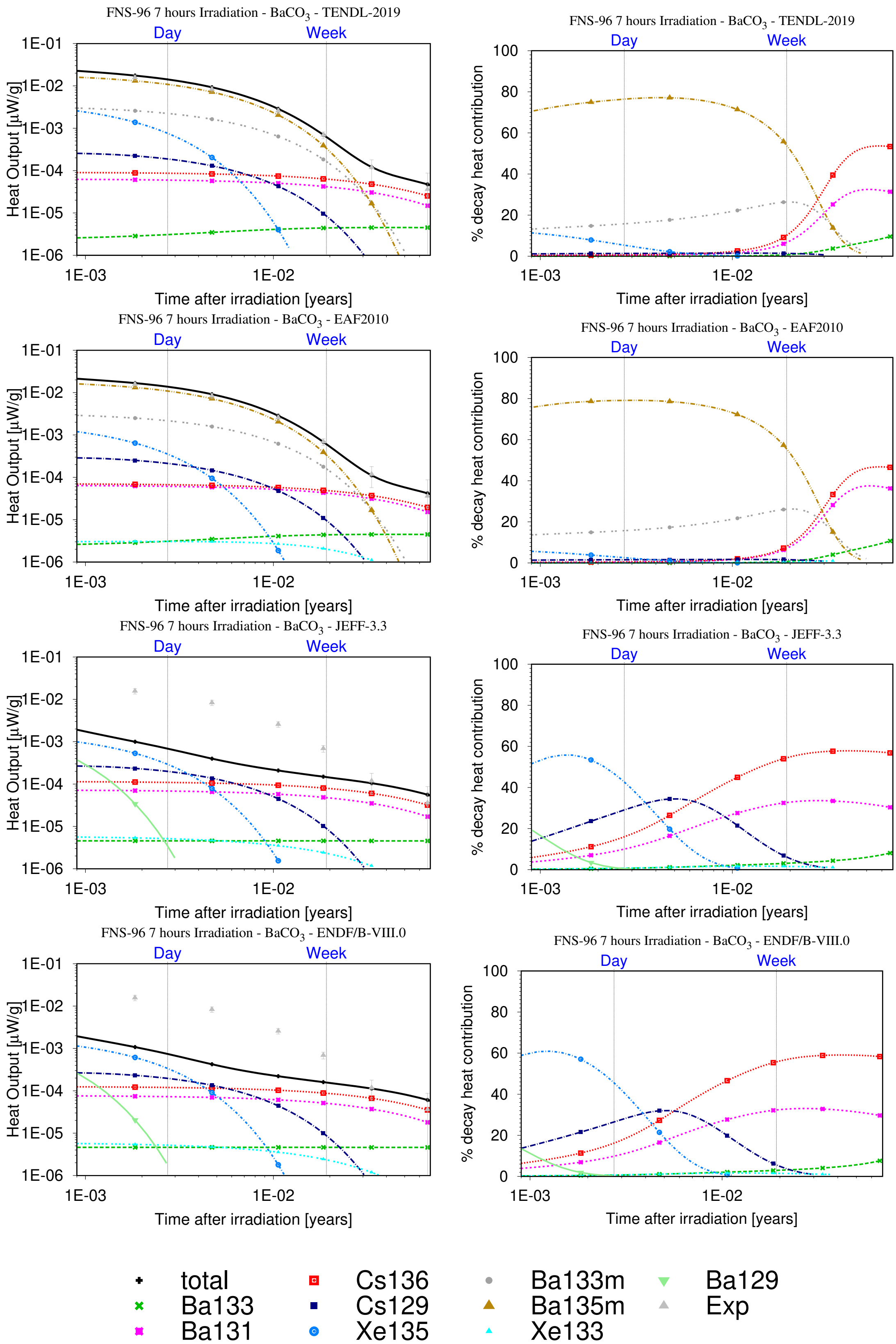


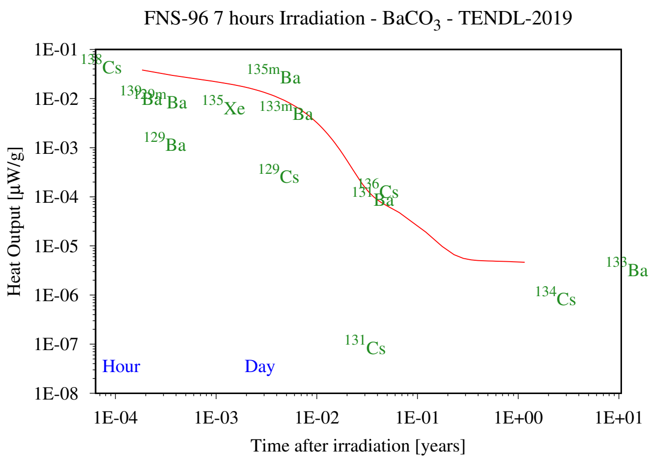
Barium,TENDL-2019 7-hours pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Ba129	2.38h	Ba130(n,2n)Ba129	100.0
Xe135	9.14h	Ba138(n,α)Xe135	53.7
		Ba138(n,α)Xe135m(IT)Xe135	46.3
Ba135m	1.20d	Ba136(n,2n)Ba135m	89.4
		Ba135(n,n$'$)Ba135m	10.6
Cs129	1.34d	Ba130(n,2n)Ba129m(β^+)Cs129	76.8
		Ba130(n,2n)Ba129(β^+)Cs129	21.7
		Ba130(n,np)Cs129	1.2
Ba133m	1.59d	Ba134(n,2n)Ba133m	100.0
Xe133	5.24d	Ba136(n,α)Xe133	91.4
		Ba136(n,α)Xe133m(IT)Xe133	4.9
		Ba137(n,nα)Xe133	3.5
Ba131	11.55d	Ba132(n,2n)Ba131m(IT)Ba131	59.4
		Ba132(n,2n)Ba131	39.6
Cs136	13.03d	Ba136(n,p)Cs136	83.5
		Ba136(n,p)Cs136m(IT)Cs136	7.1
		Ba137(n,d)Cs136	5.8
		Ba137(n,np)Cs136	2.5
		Ba137(n,d)Cs136m(IT)Cs136	1.0
Ba133	10.54y	Ba134(n,2n)Ba133	93.4
		Ba134(n,2n)Ba133m(IT)Ba133	6.6

Comments on Barium 7-hour experiments:

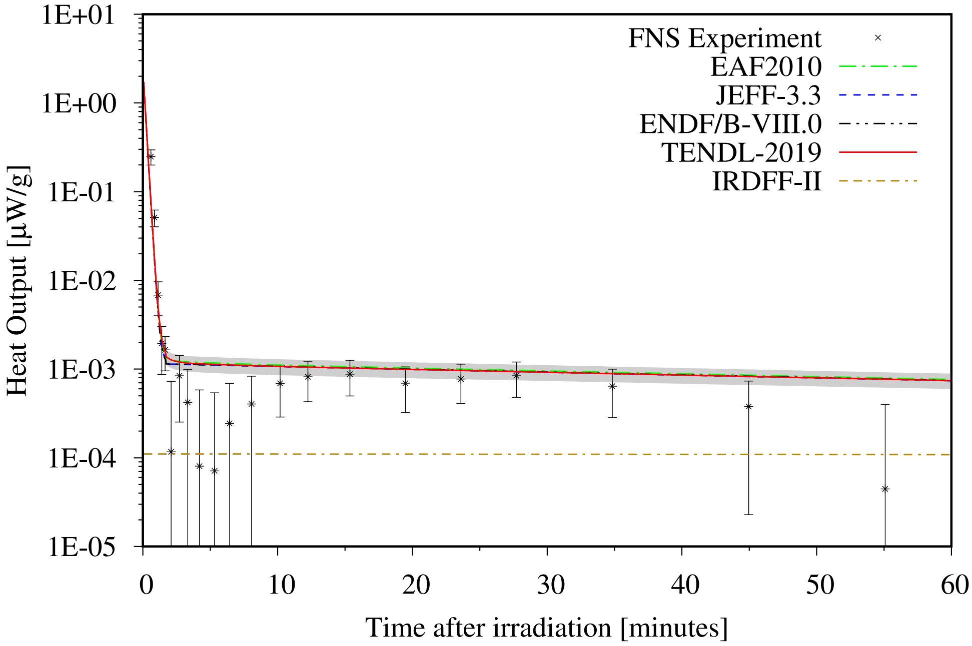
As was the case with the shorter, 5-minute experiments, ENDF/B-VIII.0 and JEFF-3.3 produce a mis-shaped decay profile, while TENDL-2019 and EAF2010 follow the experimental profile relatively well – even allowing for the large experimental uncertainty in the later cooling steps. The TENDL simulation shows that Ba135m and Ba133m are the important metastables governing the decay heat for the first few days of cooling (Bas135m from (n,2n) reactions dominates), which JEFF-3.3. and ENDF/B-VIII.0 omit. From around 2 weeks of cooling (the final two measurement times in this relatively short experiment), decay heat from Cs136 and Ba131 dominate. It is difficult to be sure which library produces the best prediction for these two nuclides because the experimental uncertainties are so large, but the decay profiles of all four seem to match the experiment in these final two data points.


FNS-96 7 hours Irradiation - BaCO3 - TENDL-2019
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
FNS-96 7 hours Irradiation - BaCO3 - EAF2010
FNS-96 7 hours Irradiation - BaCO3 - JEFF-3.3
FNS-96 7 hours Irradiation - BaCO3 - ENDF/B-VIII.0
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
total
Ba133
Ba131
Cs136
Cs129
Xe135
Ba133m
Ba135m
Xe133
Ba129
Exp


FNS-96 7 hours Irradiation - BaCO3 - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
Hour
Day
135mBa
135Xe
133mBa
129Ba
129Cs
134Cs
131Cs

Lanthanum

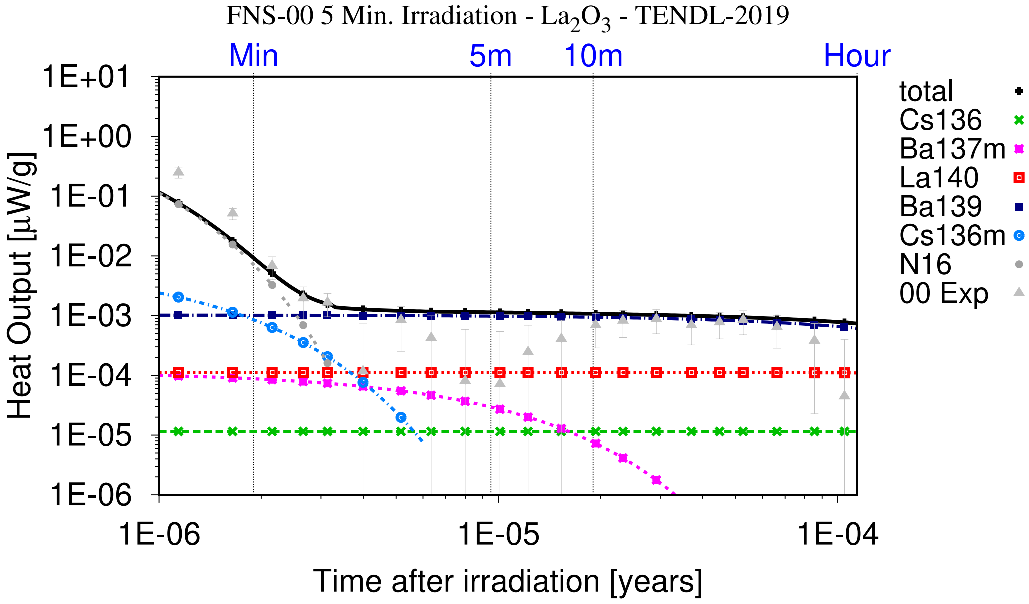
FNS-00 5 Min. Irradiation - La_2O_3



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
0.60	2.48E−01 +/-19%	7.65E−02 +/-1%	3.24	3.35	3.36	3.33	> 1000
0.87	5.11E−02 +/-22%	1.79E−02 +/-3%	2.86	3.09	3.06	3.08	462.52
1.13	6.81E−03 +/-41%	5.10E−03 +/-7%	1.34	1.56	1.47	1.56	61.65
1.40	1.94E−03 +/-55%	2.26E−03 +/-13%	0.86	1.06	0.96	1.06	17.60
1.65	1.65E−03 +/-42%	1.58E−03 +/-16%	1.04	1.27	1.15	1.27	14.91
2.10	1.17E−04 +/-524%	1.27E−03 +/-19%	0.09	0.10	0.09	0.10	1.06
2.72	8.40E−04 +/-70%	1.20E−03 +/-20%	0.70	0.74	0.69	0.74	7.61
3.33	4.22E−04 +/-135%	1.17E−03 +/-20%	0.36	0.37	0.35	0.37	3.82
4.20	8.05E−05 +/-623%	1.15E−03 +/-20%	0.07	0.07	0.07	0.07	0.73
5.32	7.13E−05 +/-659%	1.13E−03 +/-20%	0.06	0.06	0.06	0.06	0.65
6.43	2.43E−04 +/-184%	1.11E−03 +/-20%	0.22	0.22	0.21	0.22	2.21
8.07	4.05E−04 +/-106%	1.09E−03 +/-20%	0.37	0.37	0.36	0.37	3.67
10.18	6.91E−04 +/-58%	1.07E−03 +/-20%	0.65	0.64	0.62	0.65	6.27
12.25	8.20E−04 +/-48%	1.05E−03 +/-20%	0.78	0.78	0.75	0.78	7.45
15.37	8.76E−04 +/-43%	1.03E−03 +/-20%	0.85	0.85	0.82	0.86	7.96
19.48	6.92E−04 +/-53%	9.94E−04 +/-20%	0.70	0.69	0.67	0.70	6.29
23.60	7.72E−04 +/-47%	9.64E−04 +/-20%	0.80	0.79	0.77	0.80	7.03
27.72	8.40E−04 +/-43%	9.36E−04 +/-20%	0.90	0.89	0.87	0.90	7.66
34.83	6.42E−04 +/-56%	8.89E−04 +/-20%	0.72	0.72	0.70	0.72	5.86
44.95	3.78E−04 +/-94%	8.26E−04 +/-20%	0.46	0.46	0.44	0.46	3.47
55.08	4.45E−05 +/-799%	7.69E−04 +/-20%	0.06	0.06	0.06	0.06	0.41
mean % diff. from E			319	311	330	309	80
mean χ^2			2.50	2.52	2.70	2.48	4.09

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	3.24	19%	-
Ba139	1.38h	0.09	524%	23%

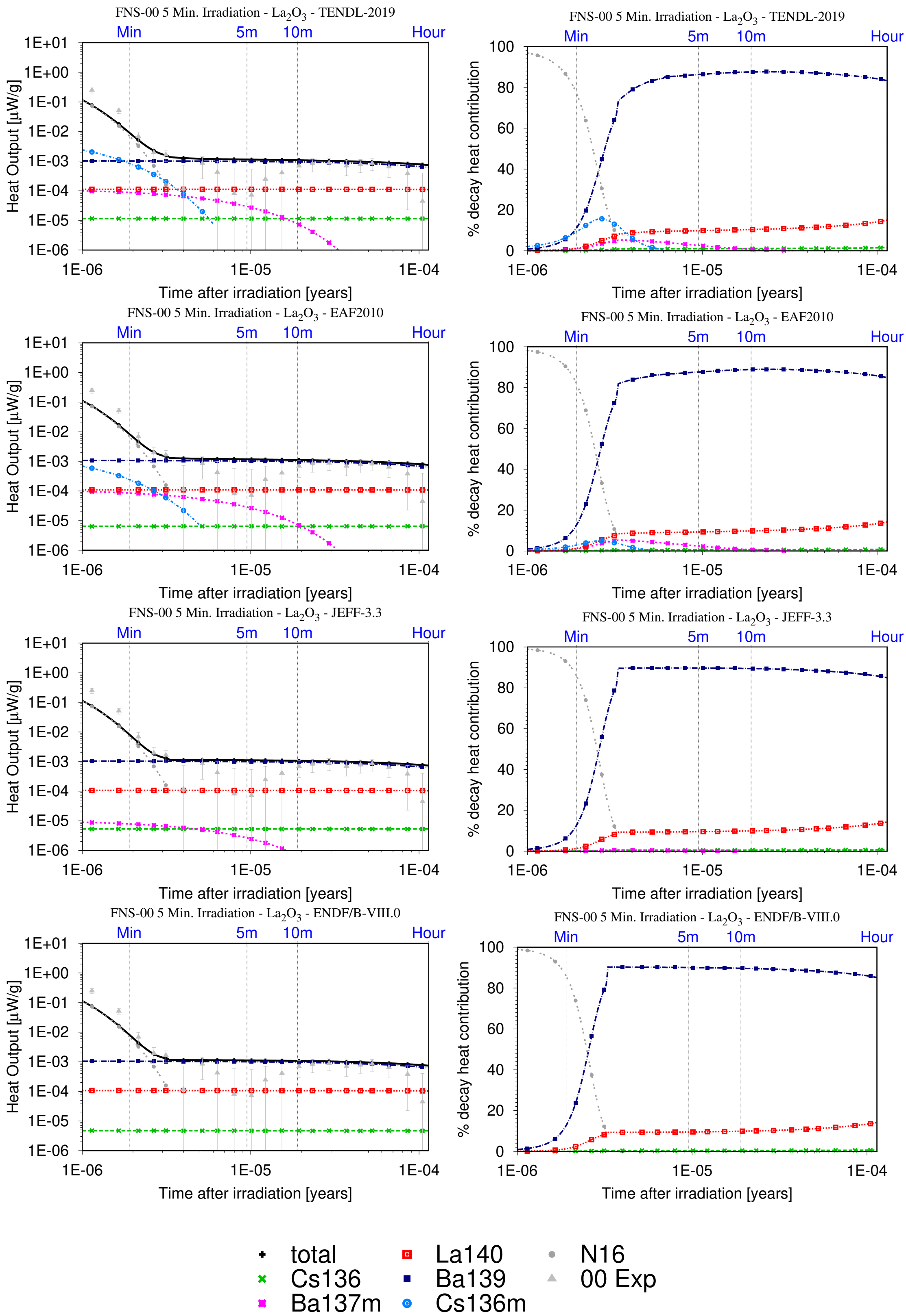


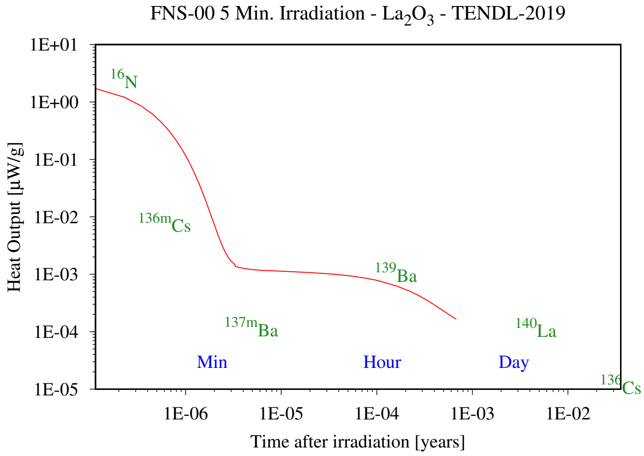
Lanthanum, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Cs136m	19.00s	La139(n,α)Cs136m	100.0
Ba137m	2.55m	La139(n,t)Ba137m	91.0
		La138(n,d)Ba137m	5.1
		La138(n,np)Ba137m	3.9
Ba139	1.38h	La139(n,p)Ba139	100.0
La140	1.68d	La139(n,γ)La140	100.0
Cs136	13.03d	La139(n,α)Cs136	89.7
		La139(n,α)Cs136m(IT)Cs136	10.3

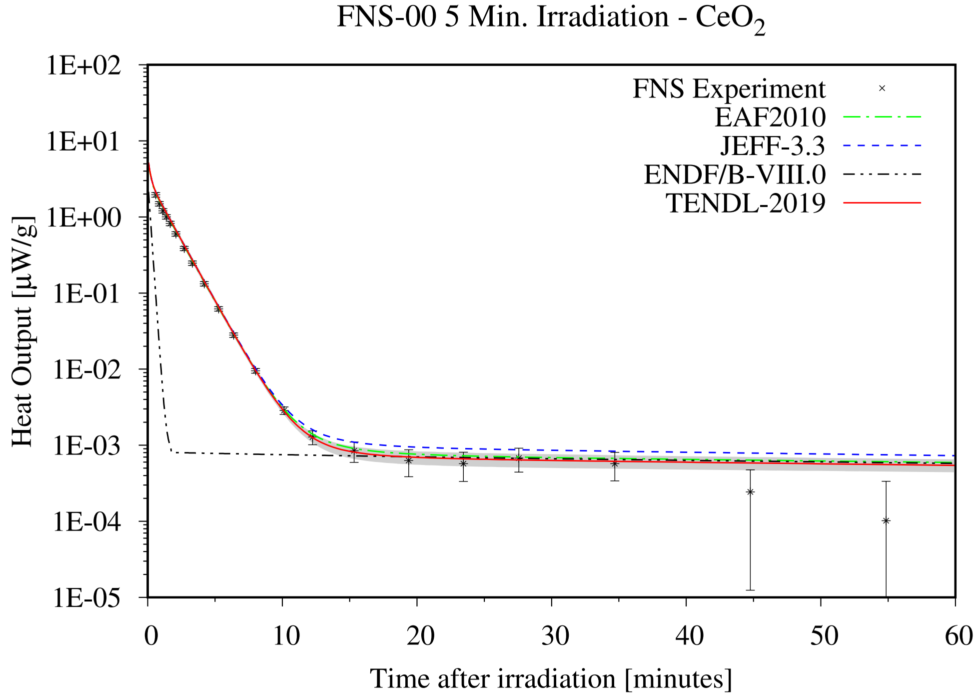
Comments on Lanthanum 5-minute experiments:

The rather large and honest experimental uncertainties do not permit an in-depth investigation for this lanthanum experiment, although the overall trend seems to be well represented by the simulations with all of the general purpose libraries. IRDFF-II is included here, but it is only able to capture the contribution from the longer-lived (relative to these experimental timescales) La140 via neutron capture on La139.


FNS-00 5 Min. Irradiation - La2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - La2O3 - EAF2010
FNS-00 5 Min. Irradiation - La2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - La2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-06
1E-05
1E-04
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
0
20
40
60
80
100
total
Cs136
Ba137m
La140
Ba139
Cs136m
N16
00 Exp


FNS-00 5 Min. Irradiation - La2O3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
136mCs
139Ba
137mBa
140La
136Cs
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

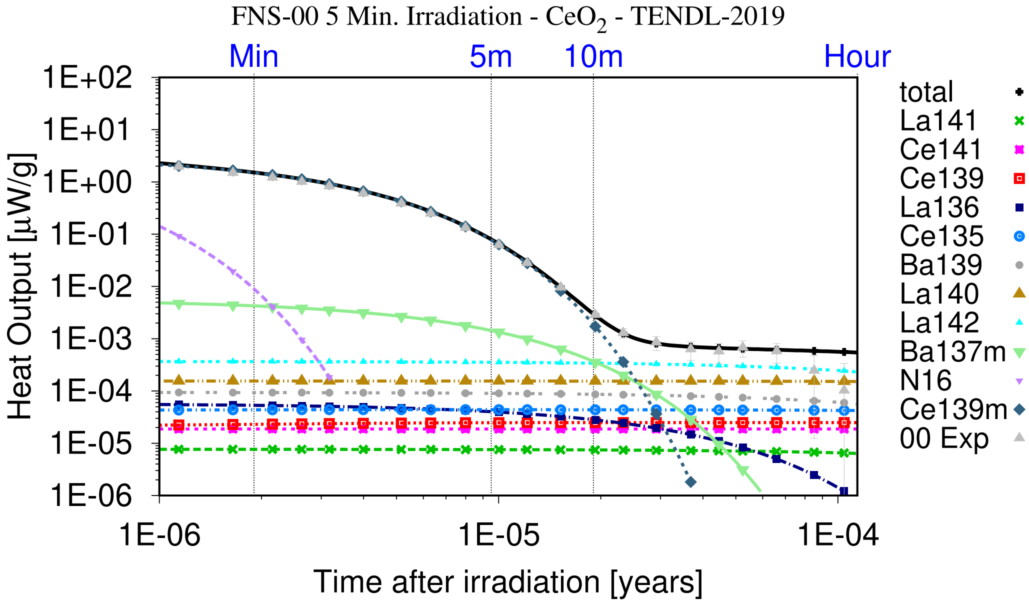
Cerium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	1.96E+00 +/-7%	2.12E+00 +/-8%	0.92	21.08	0.95	0.92
0.87	1.49E+00 +/-7%	1.68E+00 +/-8%	0.89	73.73	0.91	0.89
1.13	1.21E+00 +/-7%	1.37E+00 +/-9%	0.88	247.64	0.90	0.88
1.38	1.00E+00 +/-7%	1.14E+00 +/-9%	0.88	568.98	0.91	0.88
1.67	8.21$E-$01 +/-7%	9.20$E-$01 +/-9%	0.89	826.00	0.91	0.89
2.10	5.99$E-$01 +/-7%	6.68$E-$01 +/-9%	0.90	748.47	0.92	0.90
2.72	3.86$E-$01 +/-7%	4.24$E-$01 +/-9%	0.91	484.68	0.93	0.91
3.32	2.47$E-$01 +/-7%	2.73$E-$01 +/-9%	0.91	312.29	0.93	0.91
4.20	1.32$E-$01 +/-7%	1.43$E-$01 +/-8%	0.93	168.19	0.95	0.92
5.27	6.19$E-$02 +/-7%	6.56$E-$02 +/-8%	0.94	79.45	0.96	0.93
6.38	2.80$E-$02 +/-7%	2.95$E-$02 +/-8%	0.95	36.32	0.96	0.93
8.02	9.53$E-$03 +/-7%	9.63$E-$03 +/-8%	0.99	12.49	0.98	0.94
10.13	2.86$E-$03 +/-11%	2.79$E-$03 +/-10%	1.02	3.81	0.97	0.90
12.25	1.28$E-$03 +/-21%	1.26$E-$03 +/-15%	1.01	1.73	0.91	0.80
15.33	8.47$E-$04 +/-30%	8.11$E-$04 +/-19%	1.04	1.17	0.93	0.77
19.38	6.29$E-$04 +/-39%	7.01$E-$04 +/-20%	0.90	0.89	0.81	0.66
23.45	5.73$E-$04 +/-42%	6.63$E-$04 +/-20%	0.86	0.83	0.79	0.63
27.57	6.79$E-$04 +/-35%	6.42$E-$04 +/-20%	1.06	1.01	0.97	0.78
34.70	5.73$E-$04 +/-41%	6.15$E-$04 +/-20%	0.93	0.88	0.85	0.69
44.77	2.43$E-$04 +/-95%	5.85$E-$04 +/-20%	0.42	0.39	0.38	0.31
54.85	1.02$E-$04 +/-229%	5.58$E-$04 +/-19%	0.18	0.17	0.17	0.14
mean % diff. from E			36	95	40	59
mean χ^2			1.59	126.25	1.18	2.44

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ce139m	56.08s	0.92	7%	9%

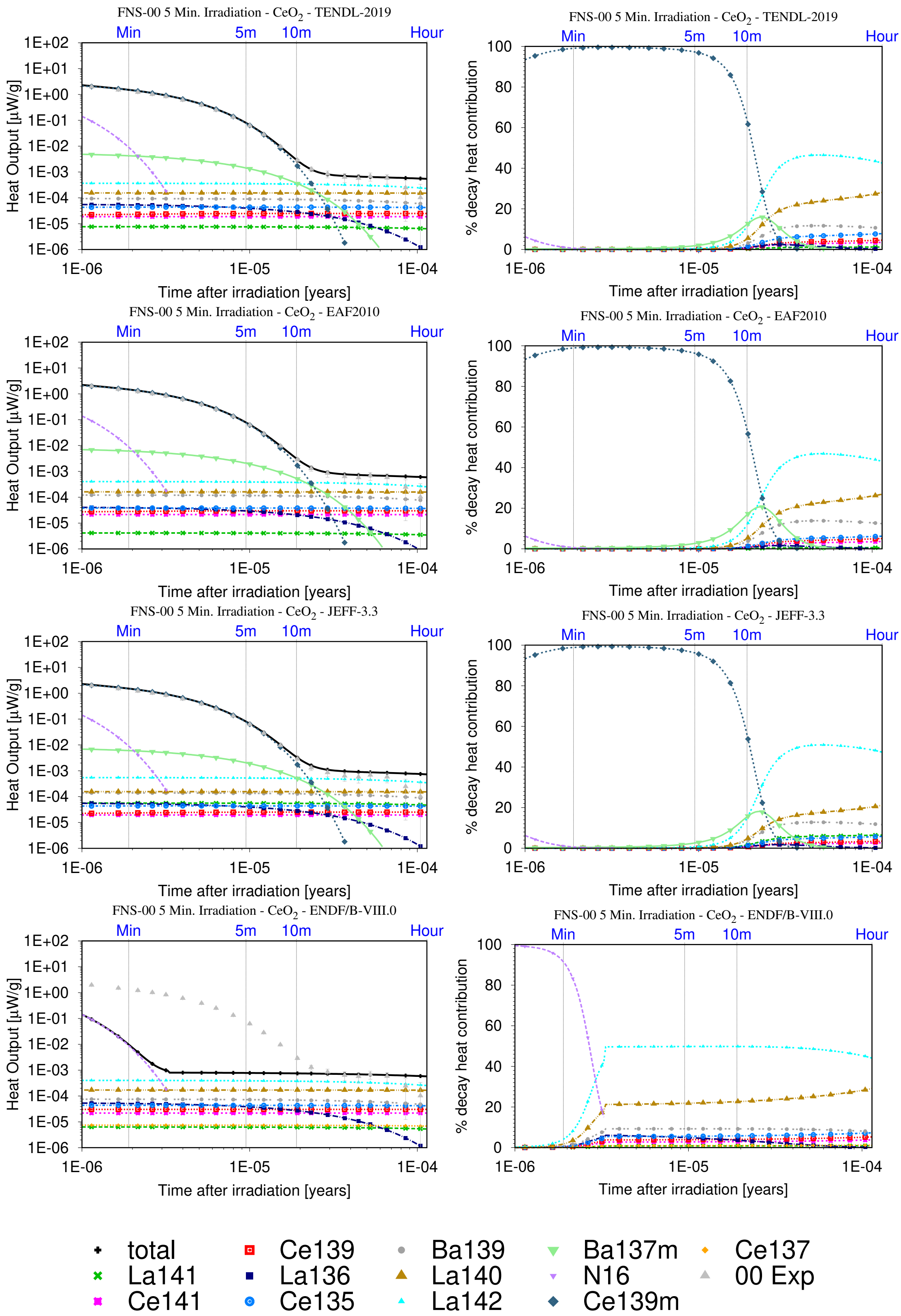


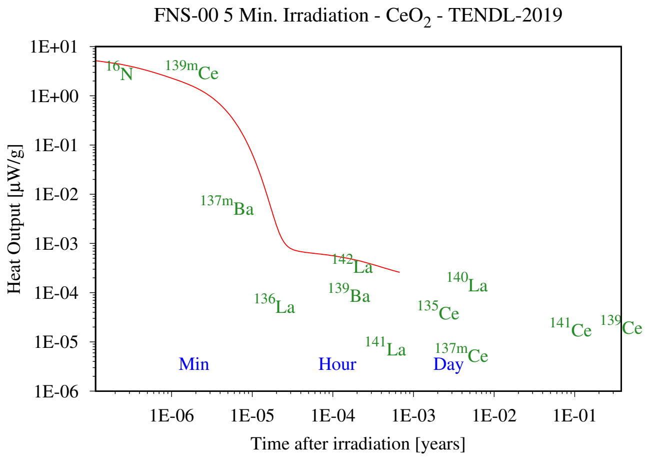
Cerium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Ce139m	56.08s	Ce140(n,2n)Ce139m	100.0
Ba137m	2.55m	Ce140(n,α)Ba137m	100.0
La136	9.87m	Ce136(n,p)La136	100.0
Ba139	1.38h	Ce142(n,α)Ba139	100.0
La142	1.52h	Ce142(n,p)La142	100.0
La141	3.92h	Ce142(n,d)La141	67.9
		Ce142(n,np)La141	32.1
Ce137	9.00h	Ce138(n,2n)Ce137	96.7
		Ce136(n,γ)Ce137	3.1
Ce135	17.70h	Ce136(n,2n)Ce135m(IT)Ce135	55.1
		Ce136(n,2n)Ce135	44.9
La140	1.68d	Ce140(n,p)La140	99.9
Ce141	32.51d	Ce142(n,2n)Ce141	98.9
		Ce140(n,γ)Ce141	1.1
Ce139	137.63d	Ce140(n,2n)Ce139m(IT)Ce139	50.6
		Ce140(n,2n)Ce139	49.4

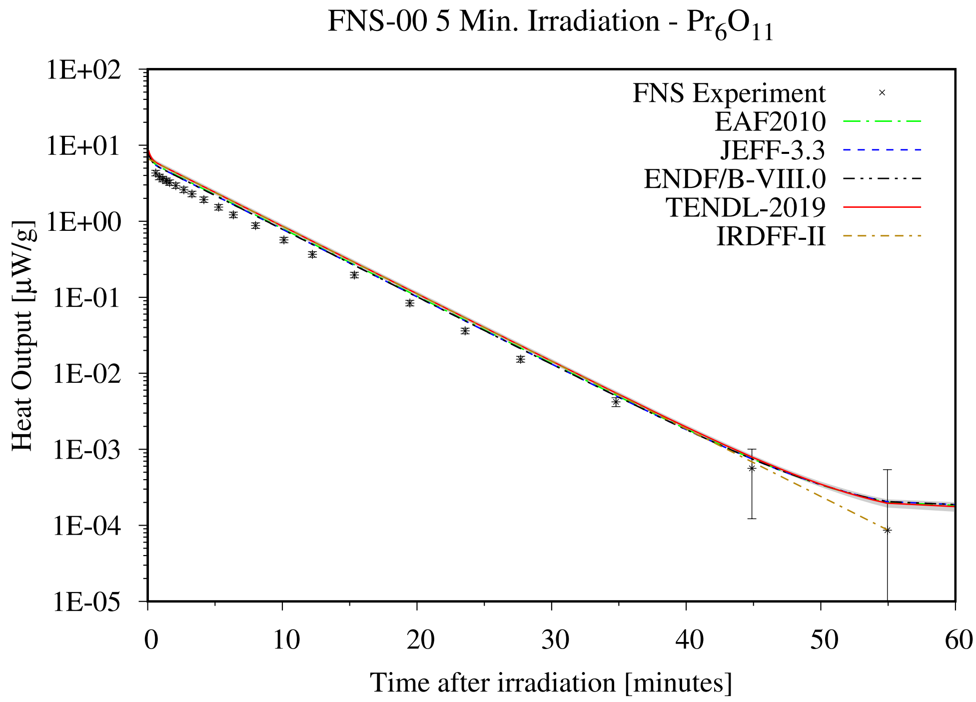
Comments on Cerium 5-minute experiments:

A good agreement to the experiment exists up to 30 minutes cooling in simulations with TENDL-2019, EAF2010, and JEFF-3.3. At later cooling times the large experimental uncertainties might explain the significant disagreement observed, especially since the simulations suggest a set of fairly constant decay-heat contributions from longer-lived (relative to the experiment timescales) nuclides (i.e. there is no reason for the significant fall in decay heat between 35 and 45 minutes, so this could be an experimental artefact). ENDF/B-VIII.0 produces a misshapen decay profile because it fails to predict the Ce139m nuclide (via (n,2n) reactions) that dominates the profile in the first 10-15 minutes of cooling.


FNS-00 5 Min. Irradiation - CeO2 - TENDL-2019
FNS-00 5 Min. Irradiation - CeO2 - EAF2010
FNS-00 5 Min. Irradiation - CeO2 - JEFF-3.3
FNS-00 5 Min. Irradiation - CeO2 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Ce139
Ba139
Ba137m
Ce137
La141
La136
La140
N16
00 Exp
Ce141
Ce135
La142
Ce139m


FNS-00 5 Min. Irradiation - CeO2 - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
16N
139mCe
137mBa
142La
140La
136La
139Ba
135Ce
141Ce
139Ce
141La
137mCe
Min
Hour
Day

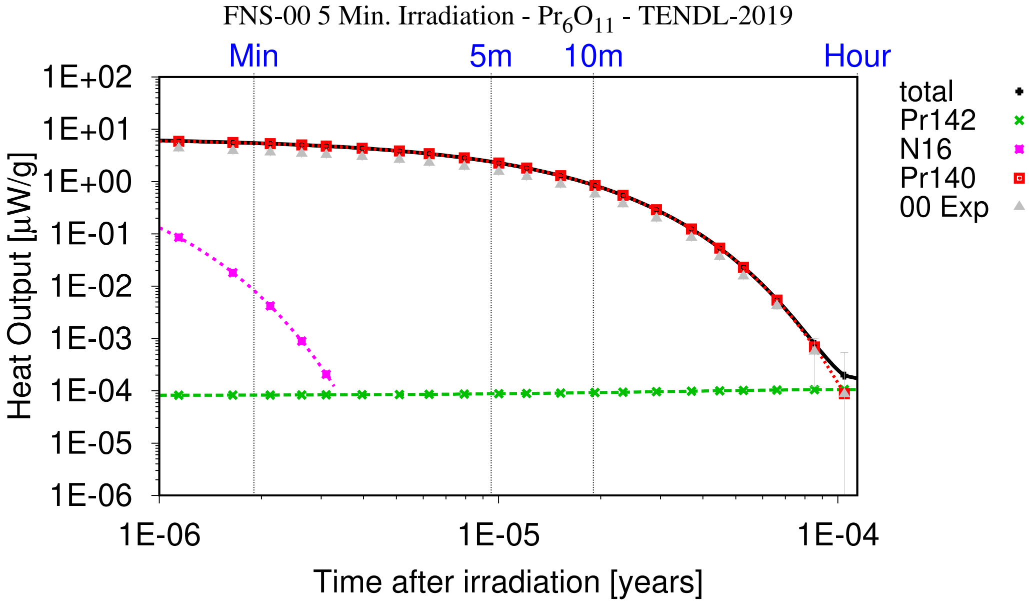
Praseodymium



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
0.60	4.31E+00 +/-9%	5.98E+00 +/-7%	0.72	0.79	0.77	0.79	0.73
0.87	3.83E+00 +/-8%	5.60E+00 +/-7%	0.68	0.75	0.73	0.75	0.69
1.12	3.60E+00 +/-8%	5.30E+00 +/-7%	0.68	0.74	0.73	0.75	0.68
1.38	3.42E+00 +/-8%	5.02E+00 +/-7%	0.68	0.75	0.73	0.75	0.68
1.63	3.22E+00 +/-8%	4.77E+00 +/-7%	0.68	0.74	0.73	0.74	0.68
2.08	2.95E+00 +/-8%	4.35E+00 +/-7%	0.68	0.74	0.73	0.74	0.68
2.68	2.60E+00 +/-8%	3.85E+00 +/-7%	0.67	0.74	0.72	0.74	0.67
3.28	2.29E+00 +/-8%	3.40E+00 +/-7%	0.67	0.74	0.72	0.74	0.67
4.17	1.92E+00 +/-8%	2.84E+00 +/-7%	0.68	0.74	0.73	0.74	0.68
5.27	1.53E+00 +/-8%	2.27E+00 +/-7%	0.68	0.74	0.73	0.74	0.68
6.37	1.22E+00 +/-8%	1.81E+00 +/-7%	0.67	0.74	0.72	0.74	0.67
8.02	8.77$E-$01 +/-8%	1.29E+00 +/-7%	0.68	0.74	0.73	0.74	0.68
10.12	5.68$E-$01 +/-8%	8.42$E-$01 +/-7%	0.67	0.74	0.72	0.74	0.67
12.23	3.67$E-$01 +/-8%	5.46$E-$01 +/-7%	0.67	0.74	0.72	0.74	0.67
15.35	1.96$E-$01 +/-8%	2.89$E-$01 +/-7%	0.68	0.75	0.73	0.75	0.68
19.47	8.40$E-$02 +/-8%	1.24$E-$01 +/-7%	0.67	0.74	0.72	0.74	0.68
23.58	3.62$E-$02 +/-8%	5.37$E-$02 +/-7%	0.67	0.74	0.72	0.74	0.67
27.70	1.53$E-$02 +/-9%	2.32$E-$02 +/-7%	0.66	0.72	0.71	0.72	0.66
34.78	4.20$E-$03 +/-13%	5.53$E-$03 +/-7%	0.76	0.83	0.81	0.83	0.77
44.88	5.63$E-$04 +/-78%	7.96$E-$04 +/-7%	0.71	0.75	0.74	0.75	0.82
54.95	8.63$E-$05 +/-526%	1.95$E-$04 +/-13%	0.44	0.42	0.43	0.42	0.98
mean % diff. from E			50	39	41	39	43
mean χ^2			27.46	14.46	16.98	14.37	27.25

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ$\mathbf{C}^{nuc}$**
Pr140	3.39m	0.72	9%	7%

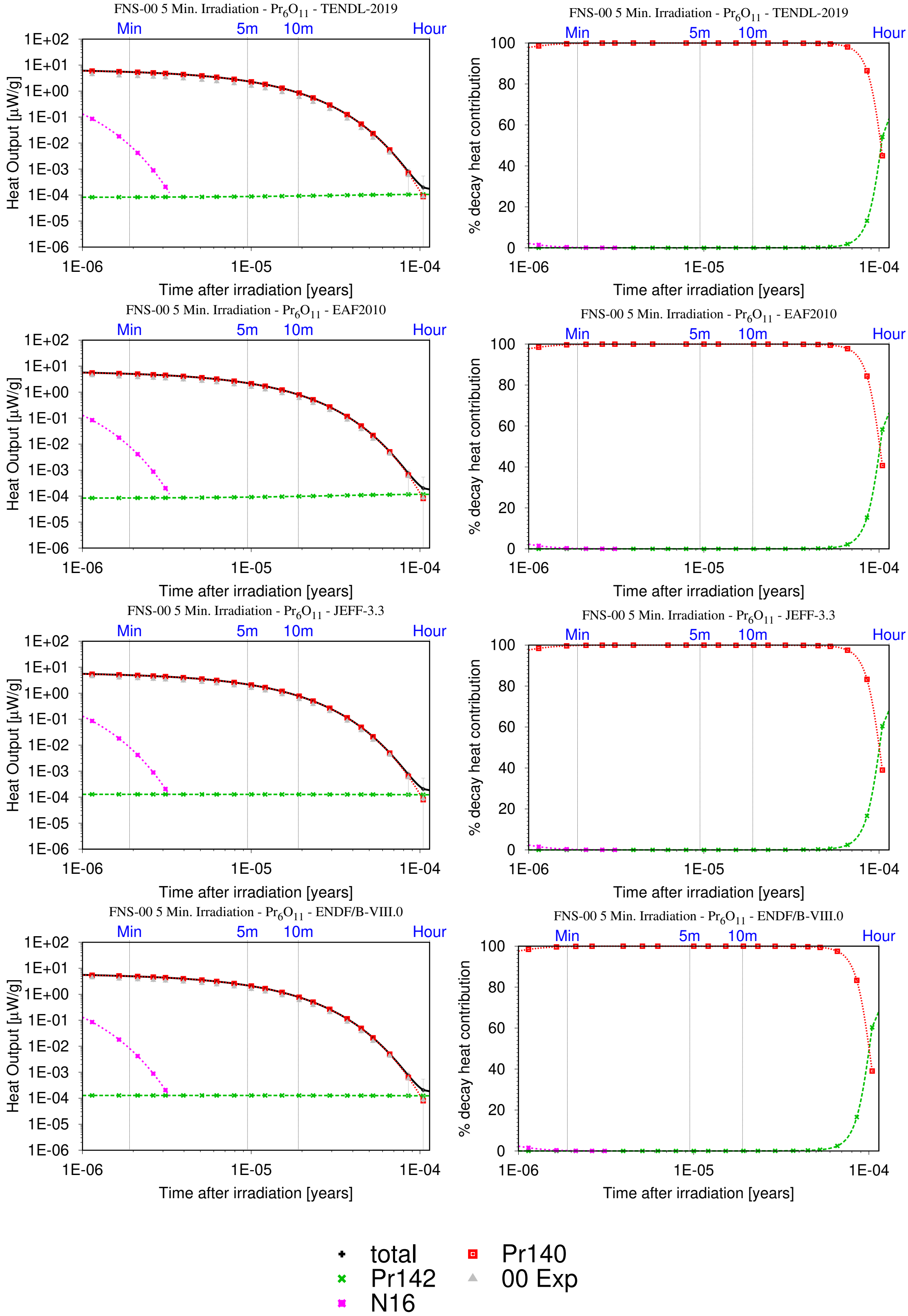


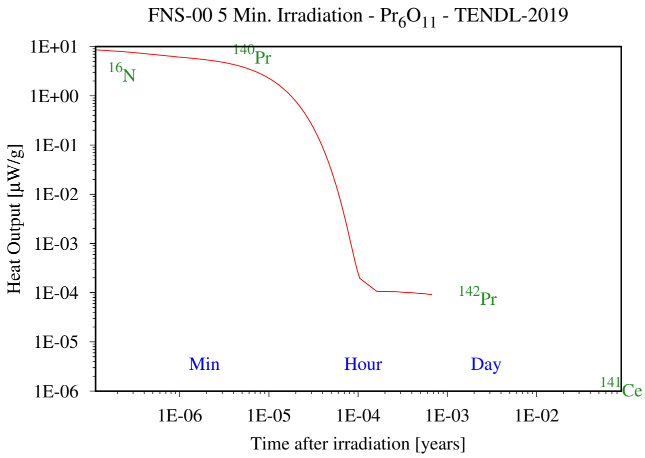
Praseodymium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Pr140	3.39m	Pr141(n,2n)Pr140	100.0
Pr142	19.12h	Pr141(n,γ)Pr142	95.5
		Pr141(n,γ)Pr142m(IT)Pr142	4.5

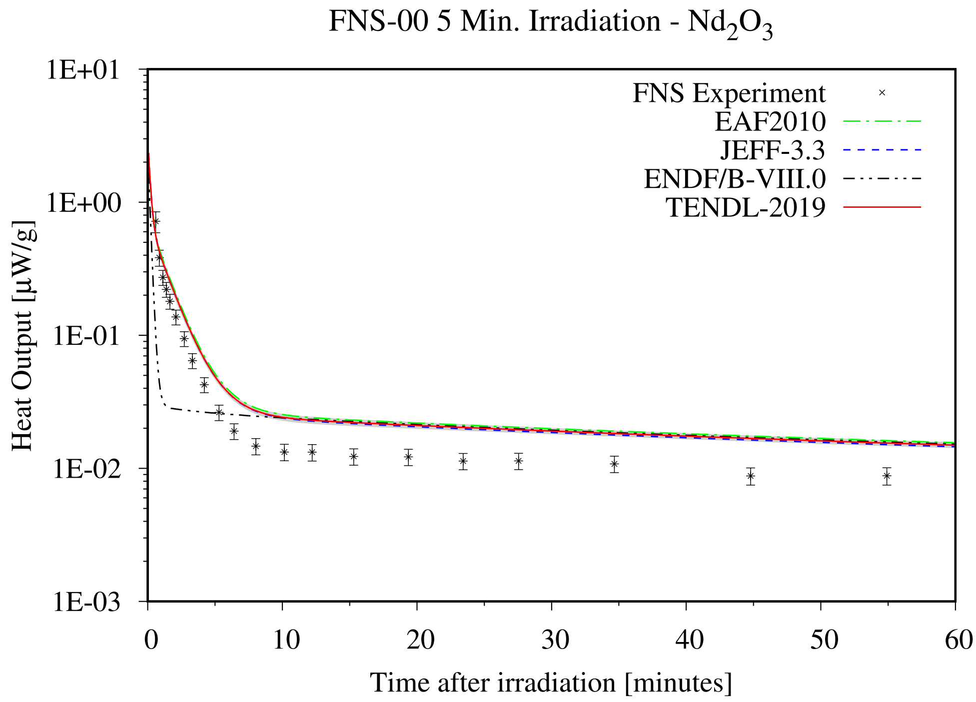
Comments on Praseodymium 5-minute experiments:

For Praseodymium, a systematic 30-50% (relative to the experiment) over-prediction exists in simulations with all libraries, indicating that the (n,2n) channel that produces the dominant Pr140 radionuclide may need to be corrected (the decay profile seems well-shaped so the decay data is reasonable). Interestingly, IRDFF-II, which includes the necessary (n,2n) reaction on Pr141 but omits the production channels for Pr142, seems to better capture the profile in the final cooling step. Even though the experimental uncertainties are too high at this time (and there could be issues with the spectrum characterisation at low energies) to make a definitive conclusion, it could be that the capture channels on Pr141 have over-estimated cross sections.


FNS-00 5 Min. Irradiation - Pr_6O_{11} - TENDL-2019
FNS-00 5 Min. Irradiation - Pr_6O_{11} - EAF2010
FNS-00 5 Min. Irradiation - Pr_6O_{11} - JEFF-3.3
FNS-00 5 Min. Irradiation - Pr_6O_{11} - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+02
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
1E-06
1E-05
1E-04
total
Pr142
N16
Pr140
00 Exp


FNS-00 5 Min. Irradiation - Pr6O11 - TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
Heat Output [µW/g]
16N
140Pr
142Pr
141Ce
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

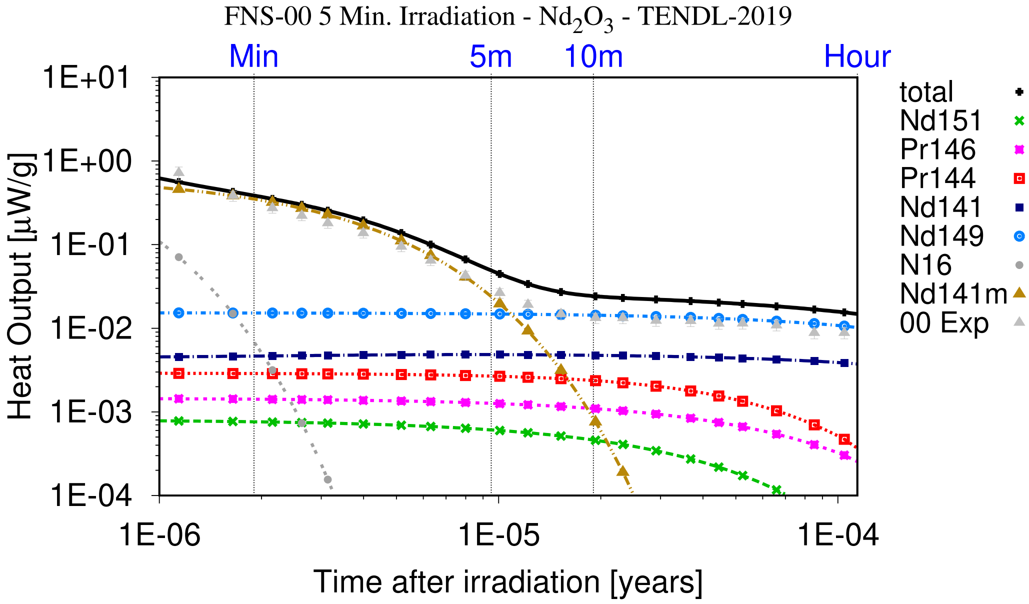
Neodymium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	7.19$E-$01 +/-18%	5.59$E-$01 +/-7%	1.29	7.18	1.24	1.29
0.87	3.83$E-$01 +/-14%	4.28$E-$01 +/-8%	0.90	8.69	0.86	0.90
1.13	2.72$E-$01 +/-13%	3.52$E-$01 +/-8%	0.77	8.50	0.74	0.77
1.38	2.21$E-$01 +/-13%	3.00$E-$01 +/-8%	0.74	7.53	0.70	0.74
1.65	1.80$E-$01 +/-13%	2.55$E-$01 +/-8%	0.71	6.32	0.67	0.71
2.10	1.37$E-$01 +/-13%	1.95$E-$01 +/-8%	0.70	4.91	0.67	0.70
2.72	9.44$E-$02 +/-13%	1.37$E-$01 +/-7%	0.69	3.44	0.65	0.69
3.32	6.44$E-$02 +/-13%	1.00$E-$01 +/-7%	0.64	2.39	0.61	0.64
4.20	4.25$E-$02 +/-13%	6.65$E-$02 +/-6%	0.64	1.61	0.61	0.64
5.30	2.63$E-$02 +/-13%	4.46$E-$02 +/-5%	0.59	1.02	0.56	0.59
6.42	1.90$E-$02 +/-14%	3.38$E-$02 +/-5%	0.56	0.75	0.54	0.57
8.03	1.47$E-$02 +/-14%	2.71$E-$02 +/-6%	0.54	0.60	0.52	0.55
10.15	1.33$E-$02 +/-14%	2.41$E-$02 +/-6%	0.55	0.55	0.53	0.56
12.22	1.32$E-$02 +/-14%	2.30$E-$02 +/-6%	0.57	0.57	0.55	0.58
15.30	1.23$E-$02 +/-14%	2.21$E-$02 +/-6%	0.56	0.55	0.53	0.57
19.37	1.22$E-$02 +/-14%	2.12$E-$02 +/-6%	0.58	0.57	0.55	0.59
23.43	1.14$E-$02 +/-14%	2.03$E-$02 +/-6%	0.56	0.55	0.54	0.57
27.55	1.14$E-$02 +/-14%	1.95$E-$02 +/-6%	0.58	0.57	0.56	0.60
34.67	1.08$E-$02 +/-14%	1.83$E-$02 +/-5%	0.59	0.58	0.57	0.61
44.78	8.78$E-$03 +/-15%	1.68$E-$02 +/-5%	0.52	0.51	0.50	0.54
54.90	8.79$E-$03 +/-15%	1.55$E-$02 +/-5%	0.57	0.56	0.54	0.58
mean % diff. from E			60	71	67	59
mean χ^2			21.32	28.96	26.41	20.02

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Nd141m	1.03m	1.29	18%	9%

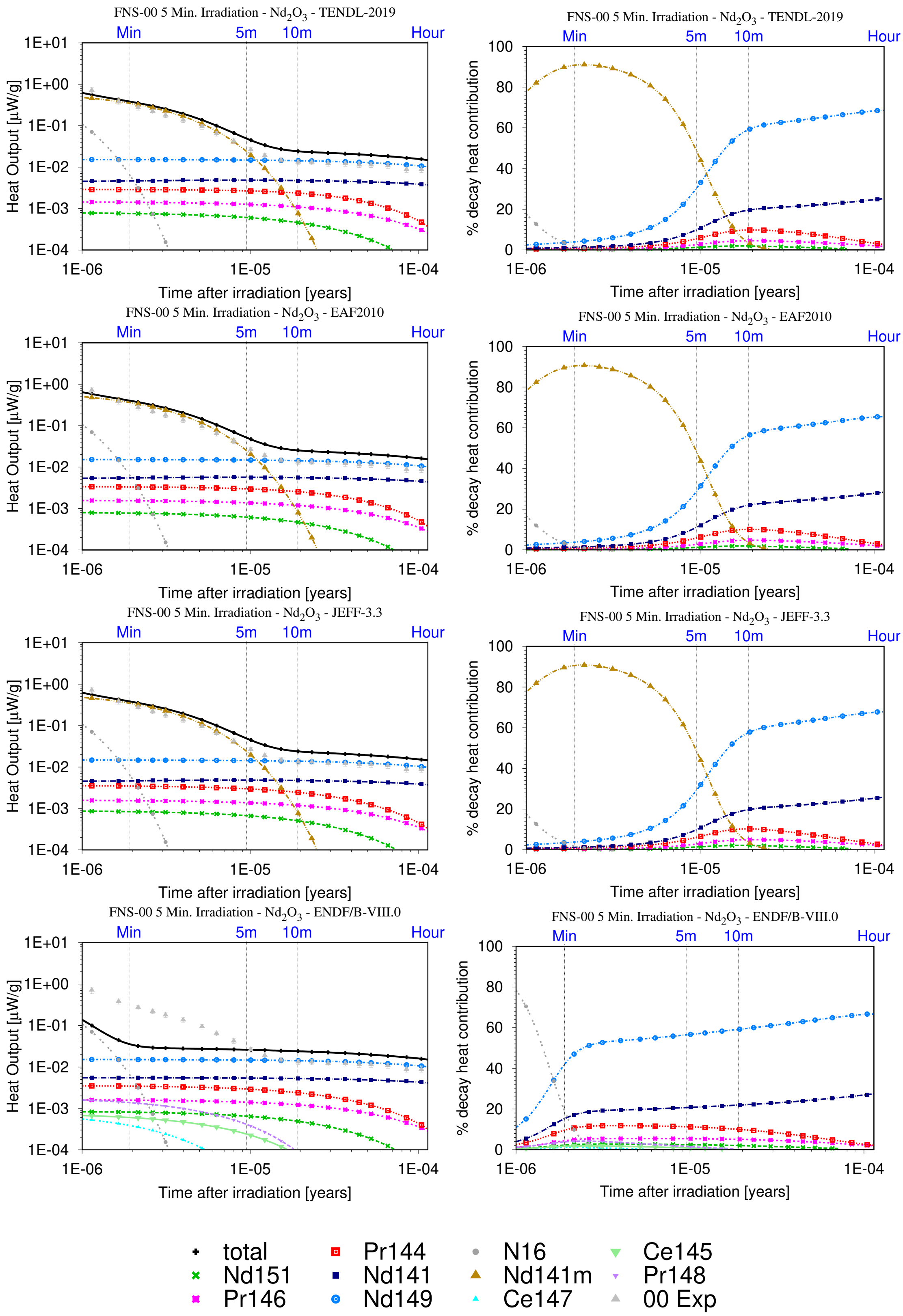


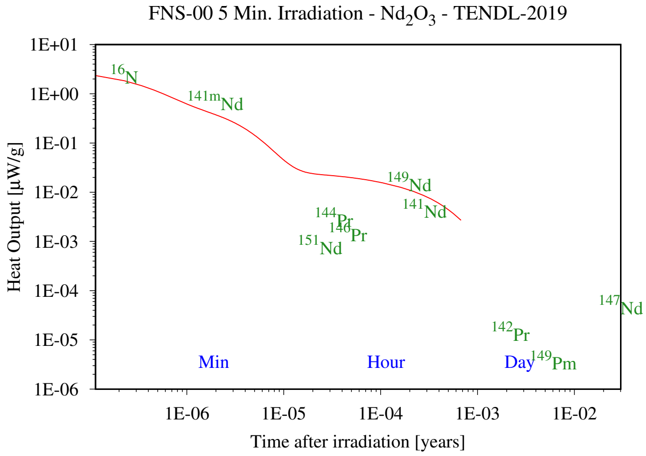
Neodymium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ce147	57.00s	Nd150(n,α)Ce147	100.0
Nd141m	1.03m	Nd142(n,2n)Nd141m	100.0
Pr148	2.29m	Nd148(n,p)Pr148	99.8
Ce145	2.95m	Nd148(n,α)Ce145	100.0
Nd151	12.44m	Nd150(n,γ)Nd151	100.0
Pr144	17.28m	Nd144(n,p)Pr144	92.0
		Nd144(n,p)Pr144m(IT)Pr144	6.6
Pr146	24.15m	Nd146(n,p)Pr146	99.9
Nd149	1.73h	Nd150(n,2n)Nd149	99.5
Nd141	2.49h	Nd142(n,2n)Nd141	66.9
		Nd142(n,2n)Nd141m(IT)Nd141	33.1

Comments on Neodymium 5-minute experiments:

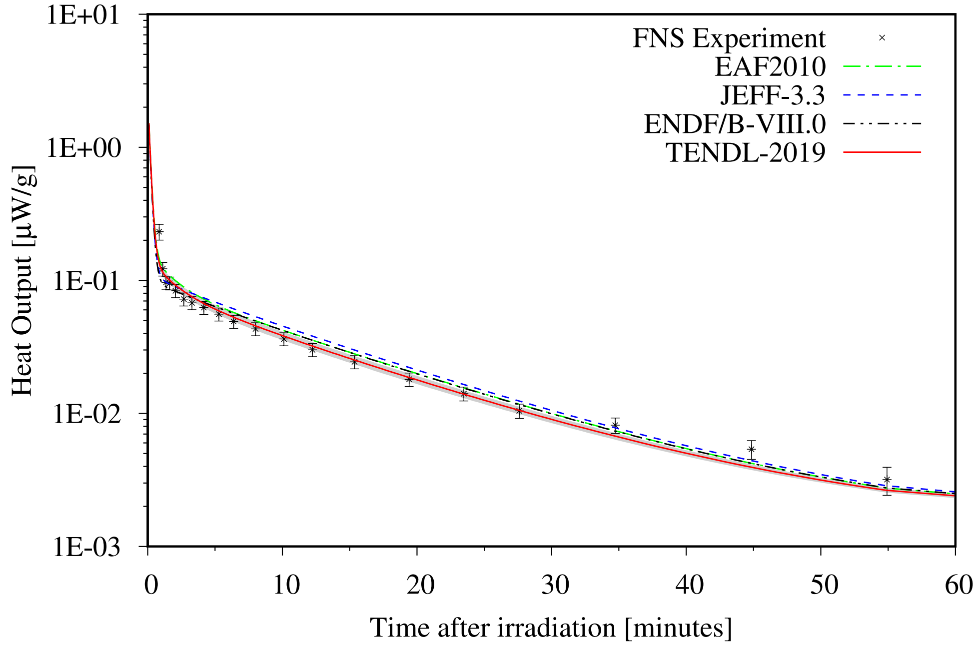
There is a rather uniform and significant 50% over-prediction with TENDL-2019 (and with the other libraries considered) from around 5 minutes of cooling onwards. This appears to be a clear case where the cross sections – particularly the Nd150(n,2n) channel for the production of the Nd149 nuclides that dominates all measurements times beyond 10 minutes – may need some adjustment. At the same time, the production of Nd141m, which dominates at sub 5-minute cooling times, is also slightly overpredicted despite the simulations following the experimental decay profile well. Since this latter nuclide is produced via a branched (n,2n) channel on Nd142 that also creates the Nd141 radionuclide, which provides around 20% of the decay heat during Nd149 dominance, that channel may also need correcting.


FNS-00 5 Min. Irradiation - Nd_2O_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Nd_2O_3 - EAF2010
FNS-00 5 Min. Irradiation - Nd_2O_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Nd_2O_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Nd151
Pr146
Pr144
Nd141
Nd149
N16
Nd141m
Ce147
Ce145
Pr148
00 Exp


FNS-00 5 Min. Irradiation - Nd2O3 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]
16N
141mNd
149Nd
141Nd
144Pr
146Pr
151Nd
147Nd
142Pr
149Pm
Min
Hour
Day

Samarium

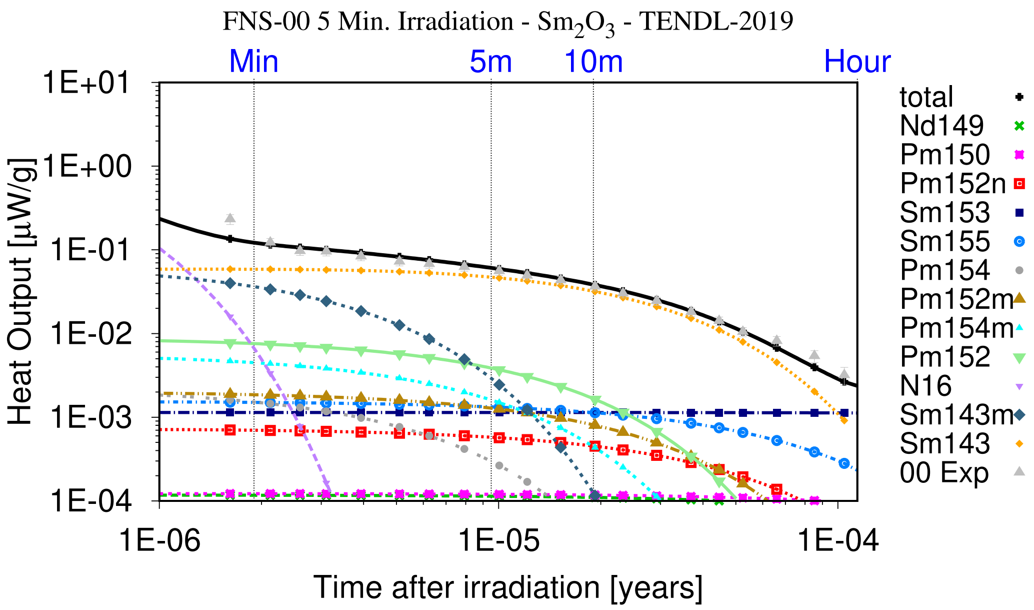
FNS-00 5 Min. Irradiation - Sm_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	2.32E−01 +/-14%	1.35E−01 +/-6%	1.71	2.13	1.59	1.98
1.12	1.22E−01 +/-12%	1.15E−01 +/-7%	1.06	1.30	0.98	1.20
1.37	9.67E−02 +/-11%	1.07E−01 +/-7%	0.91	1.08	0.84	1.00
1.63	9.53E−02 +/-11%	1.00E−01 +/-7%	0.95	1.10	0.88	1.02
2.07	8.34E−02 +/-11%	9.20E−02 +/-7%	0.91	1.01	0.84	0.93
2.68	7.23E−02 +/-11%	8.26E−02 +/-7%	0.88	0.93	0.81	0.85
3.28	6.78E−02 +/-11%	7.54E−02 +/-7%	0.90	0.92	0.83	0.85
4.17	6.24E−02 +/-11%	6.71E−02 +/-7%	0.93	0.91	0.86	0.84
5.28	5.57E−02 +/-11%	5.91E−02 +/-7%	0.94	0.90	0.87	0.83
6.38	4.91E−02 +/-11%	5.28E−02 +/-7%	0.93	0.87	0.86	0.80
8.02	4.32E−02 +/-11%	4.55E−02 +/-7%	0.95	0.87	0.87	0.81
10.12	3.63E−02 +/-11%	3.81E−02 +/-7%	0.95	0.87	0.87	0.81
12.23	3.01E−02 +/-11%	3.21E−02 +/-7%	0.94	0.85	0.85	0.79
15.37	2.44E−02 +/-11%	2.52E−02 +/-7%	0.97	0.87	0.87	0.81
19.42	1.80E−02 +/-12%	1.87E−02 +/-7%	0.97	0.87	0.87	0.81
23.48	1.41E−02 +/-12%	1.40E−02 +/-7%	1.01	0.91	0.90	0.85
27.60	1.05E−02 +/-12%	1.06E−02 +/-6%	0.99	0.90	0.89	0.84
34.73	8.15E−03 +/-13%	6.75E−03 +/-6%	1.21	1.10	1.10	1.04
44.85	5.37E−03 +/-16%	3.95E−03 +/-5%	1.36	1.27	1.27	1.22
54.92	3.18E−03 +/-24%	2.64E−03 +/-4%	1.20	1.15	1.16	1.11
mean % diff. from E			10	14	16	18
mean χ^2			1.06	1.93	2.14	2.99

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Sm143	8.75m	0.94	11%	8%

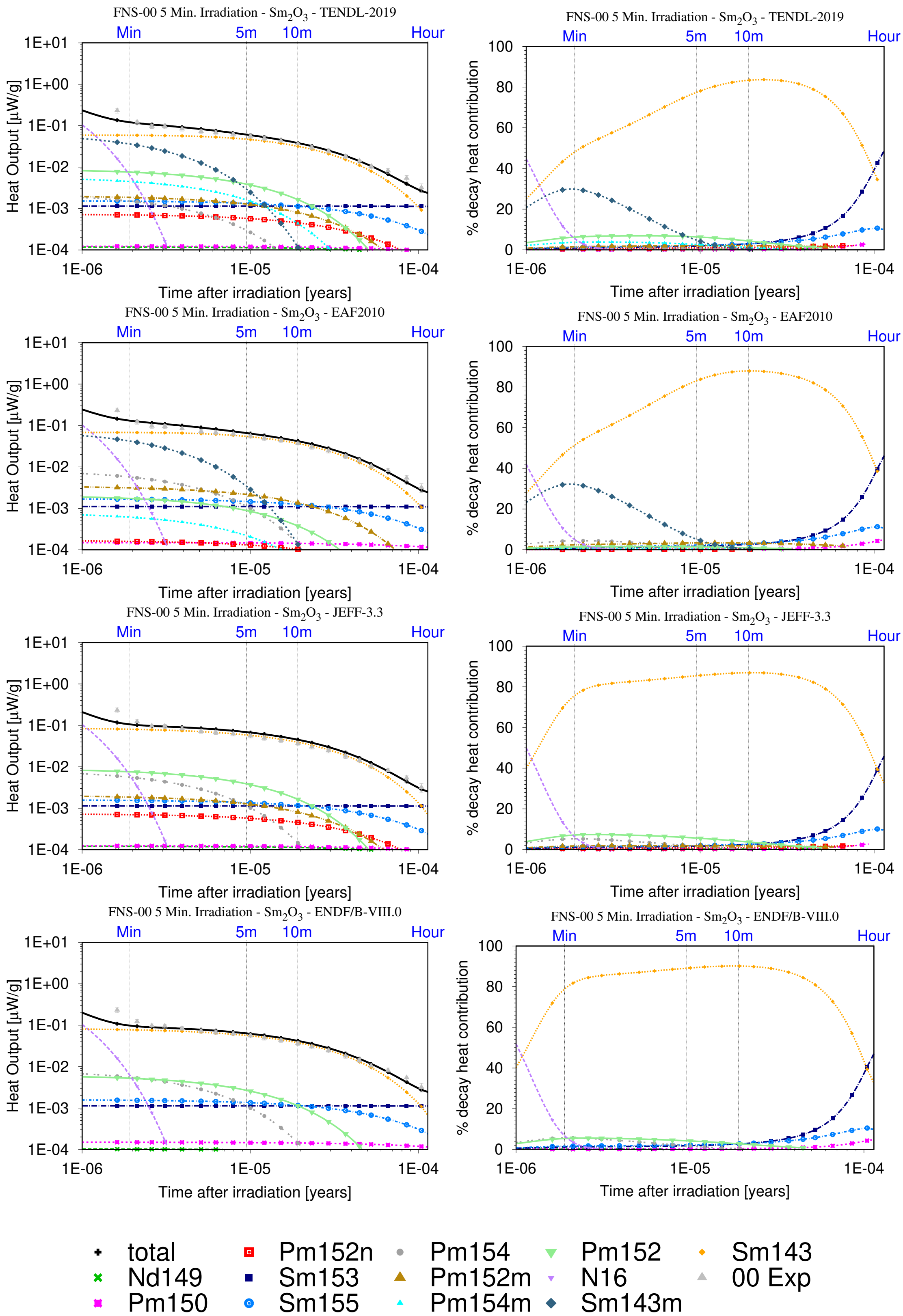


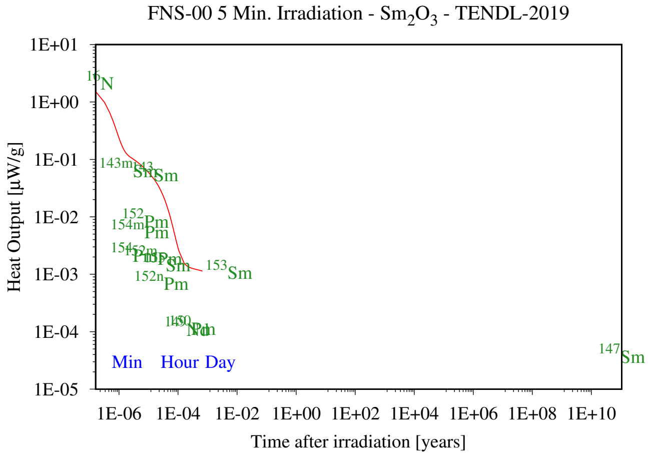
Samarium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Sm143m	1.10m	Sm144(n,2n)Sm143m	100.0
Pm154	1.70m	Sm154(n,p)Pm154	100.0
Pm154m	2.70m	Sm154(n,p)Pm154m	100.0
Pm152	4.12m	Sm152(n,p)Pm152	100.0
Pm152m	7.52m	Sm152(n,p)Pm152m	99.9
Sm143	8.75m	Sm144(n,2n)Sm143	62.0
		Sm144(n,2n)Sm143m(IT)Sm143	38.0
Pm152n	14.40m	Sm152(n,p)Pm152n	100.0
Sm155	22.30m	Sm154(n,γ)Sm155	100.0
Nd149	1.73h	Sm152(n,α)Nd149	100.0
Pm150	2.68h	Sm150(n,p)Pm150	99.8
Sm153	1.93d	Sm154(n,2n)Sm153	85.3
		Sm152(n,γ)Sm153	14.7

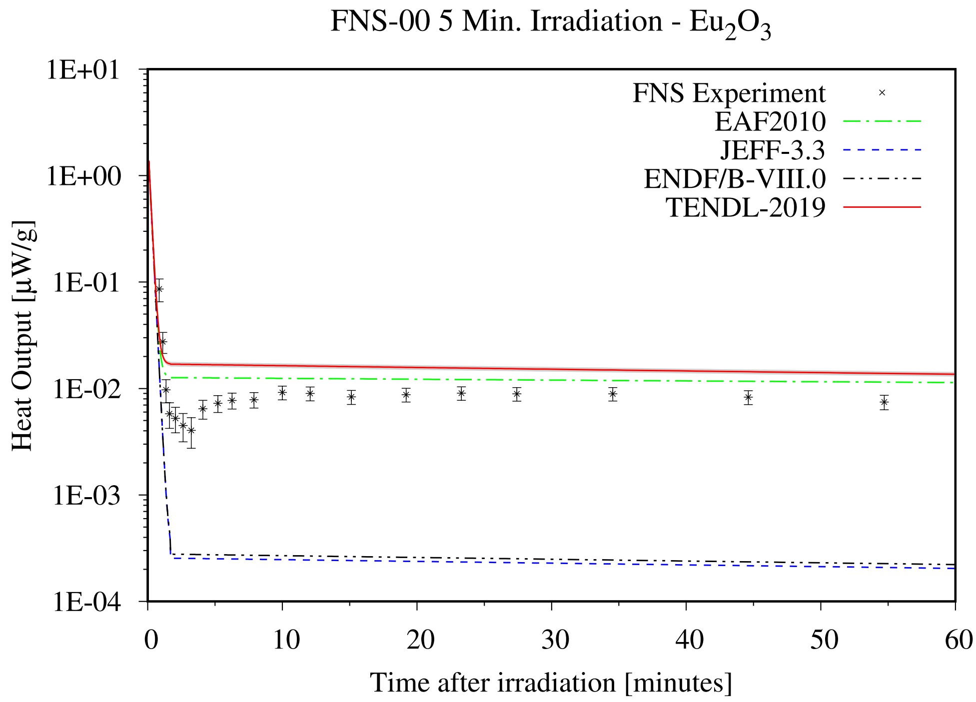
Comments on Samarium 5-minute experiments:

A good agreement exists between all the general purpose libraries and the experiment, with TENDL-2019 marginally better than the others. All libraries show the same profile of contributing nuclides, although JEFF-3.3 and ENDF/B-VIII.0 don't predict as many contributions from metastable nuclides as the other two, particularly Sm143m, which provides relatively significant contributions to the decay-heat during the first 5 minutes, and this could explain why ENDF/B and JEFF underpredict the experiment during this time.

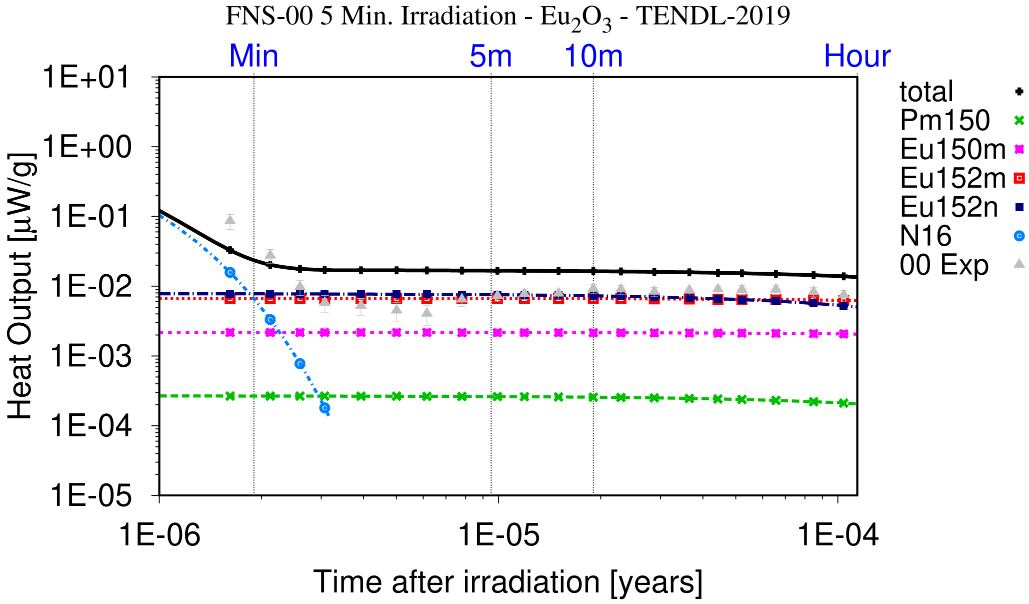

FNS-00 5 Min. Irradiation - Sm_2O_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Sm_2O_3 - EAF2010
FNS-00 5 Min. Irradiation - Sm_2O_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Sm_2O_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Nd149
Pm150
Pm152n
Sm153
Sm155
Pm154
Pm152m
Pm154m
Pm152
N16
Sm143m
Sm143
00 Exp


FNS-00 5 Min. Irradiation - Sm2O3 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
Min
Hour
Day
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-04
1E-02
1E+00
1E+02
1E+04
1E+06
1E+08
1E+10
16N
153Sm
147Sm
152nPm

Europium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	8.60E−02 +/-24%	3.28E−02 +/-3%	2.62	5.37	3.05	5.36
1.12	2.75E−02 +/-22%	2.03E−02 +/-4%	1.35	7.67	1.72	7.68
1.37	9.72E−03 +/-25%	1.77E−02 +/-5%	0.55	9.32	0.72	9.50
1.62	5.79E−03 +/-27%	1.71E−02 +/-5%	0.34	12.75	0.45	13.38
2.07	5.25E−03 +/-27%	1.69E−02 +/-5%	0.31	18.93	0.42	20.65
2.63	4.49E−03 +/-30%	1.69E−02 +/-5%	0.27	16.21	0.36	17.68
3.23	4.04E−03 +/-32%	1.68E−02 +/-5%	0.24	14.62	0.32	15.95
4.10	6.45E−03 +/-20%	1.68E−02 +/-5%	0.38	23.43	0.51	25.56
5.22	7.27E−03 +/-18%	1.67E−02 +/-5%	0.44	26.52	0.58	28.92
6.27	7.72E−03 +/-17%	1.66E−02 +/-5%	0.46	28.30	0.62	30.86
7.90	7.85E−03 +/-16%	1.65E−02 +/-5%	0.48	28.96	0.63	31.58
10.00	9.18E−03 +/-15%	1.64E−02 +/-5%	0.56	34.12	0.74	37.19
12.07	8.99E−03 +/-15%	1.63E−02 +/-5%	0.55	33.68	0.72	36.71
15.13	8.34E−03 +/-15%	1.61E−02 +/-5%	0.52	31.64	0.68	34.48
19.20	8.76E−03 +/-15%	1.58E−02 +/-5%	0.55	33.74	0.72	36.74
23.30	9.05E−03 +/-14%	1.56E−02 +/-5%	0.58	35.43	0.75	38.58
27.42	8.90E−03 +/-15%	1.53E−02 +/-5%	0.58	35.41	0.74	38.54
34.55	8.91E−03 +/-14%	1.49E−02 +/-5%	0.60	36.45	0.75	39.64
44.62	8.29E−03 +/-15%	1.44E−02 +/-5%	0.58	35.23	0.71	38.28
54.72	7.47E−03 +/-16%	1.39E−02 +/-5%	0.54	33.02	0.65	35.84
mean % diff. from E			120	95	73	95
mean χ^2			39.03	29.32	13.70	29.47

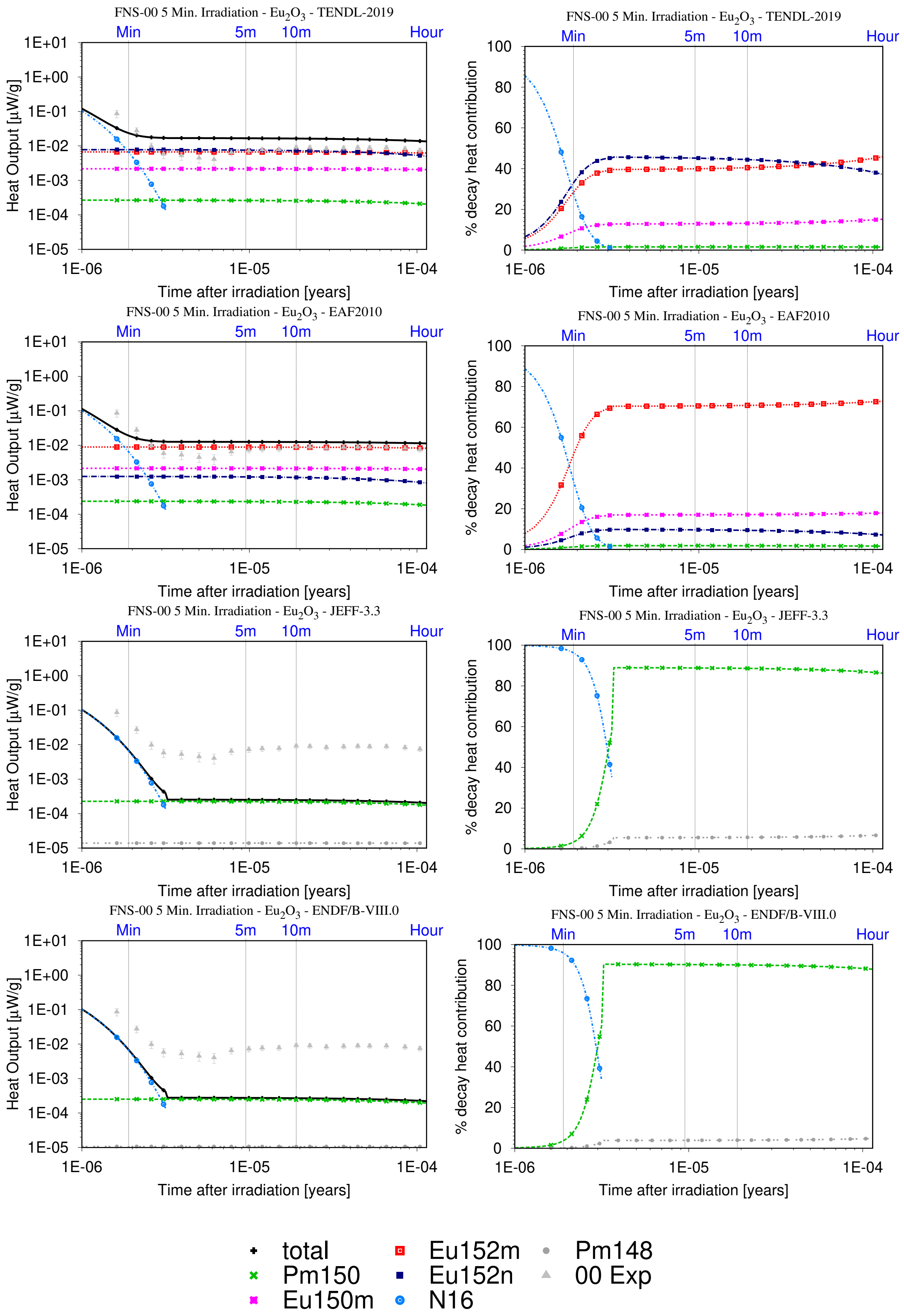


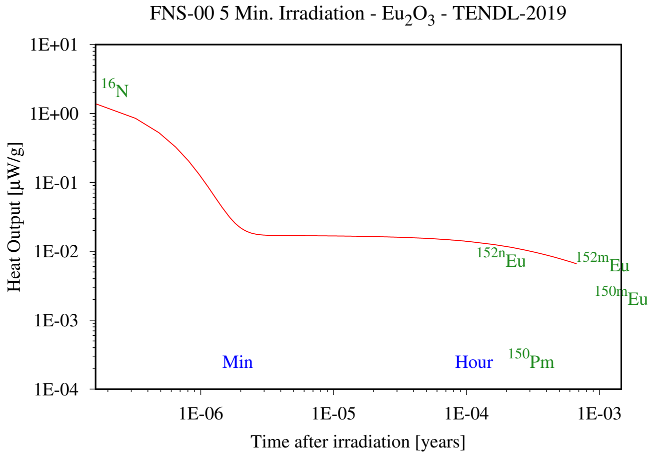
Europium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Eu152n	1.60h	Eu153(n,2n)Eu152n	99.4
Pm150	2.68h	Eu153(n,α)Pm150	100.0
Eu152m	9.27h	Eu151(n,γ)Eu152m	67.9
		Eu153(n,2n)Eu152m	32.1
Eu150m	12.80h	Eu151(n,2n)Eu150m	100.0
Pm148	5.37d	Eu151(n,α)Pm148	100.0

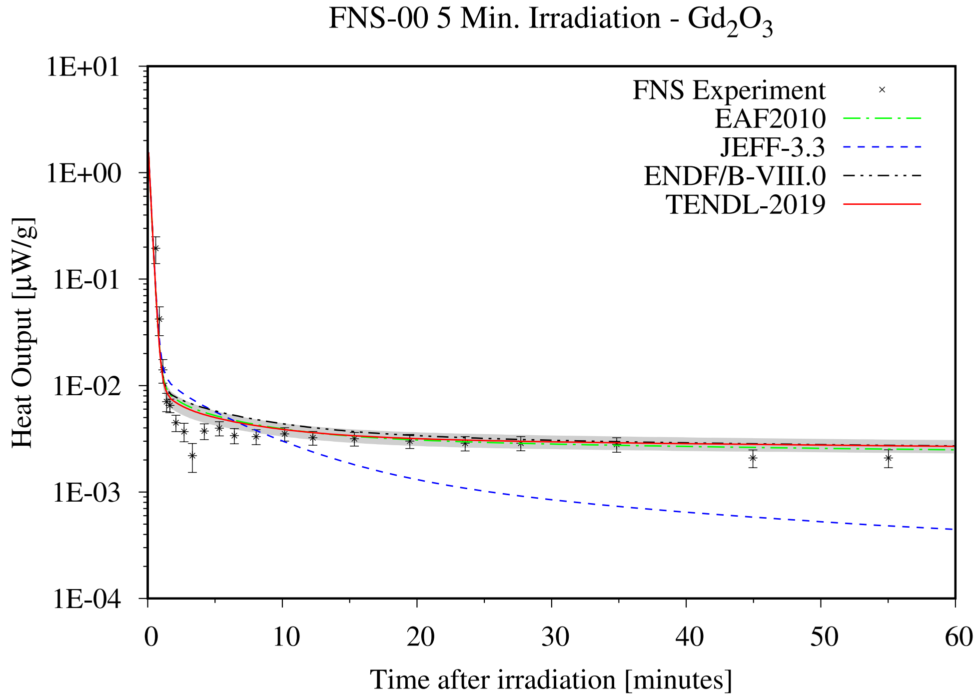
Comments on Europium 5-minute experiments:

As was observed with caesium, there is an upward trend in the decay-heat measurements at short cooling times (less than 5 minutes), which is not reproduced in the simulations with any library – either the tape contribution is overestimated or there are some missing isomeric states in the simulations. Certainly ENDF/B-VIII.0 and JEFF-3.3 have this problem as they fail to predict any of the three isomeric states that TENDL-2019 and EAF2010 find to be important (see the nuclide contribution charts), and, instead, only find the low level of decay heat attributed to the Pm150 nuclide. EAF2010 seems to be somewhat better than TENDL-2019 beyond 5 minutes of cooling and certainly those two libraries show a different distribution of the Eu152n, Eu152n, and Eu150m nuclides as a function of time – EAF2010 finds Eu152m much more predominant than TENDL-2019, which instead shows both isomeric states of Eu152 to be equally important. This demonstrates a different branching ratio within the (n,2n) cross section on Eu153, but there is too much disagreement compared to the experiment in both cases to draw any firm conclusions. Further investigation is warranted. Review of the EXFOR cross-section data shown in Figure A2 and recent findings by the authors in [19] add some further evidence for the need to re-evaluate and adjust the branching ratio (to reduce Eu152n and Eu152m production) for the ^{153}Eu(n,2n) reaction channel for future TENDL library releases.


FNS-00 5 Min. Irradiation - Eu_2O_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Eu_2O_3 - EAF2010
FNS-00 5 Min. Irradiation - Eu_2O_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Eu_2O_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Pm150
Eu150m
Eu152m
Eu152n
N16
Pm148
00 Exp


FNS-00 5 Min. Irradiation - Eu_2O_3 - TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
Heat Output [μW/g]
^{16}N
^{152n}Eu
^{152m}Eu
^{150m}Eu
Min
Hour
^{150}Pm
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

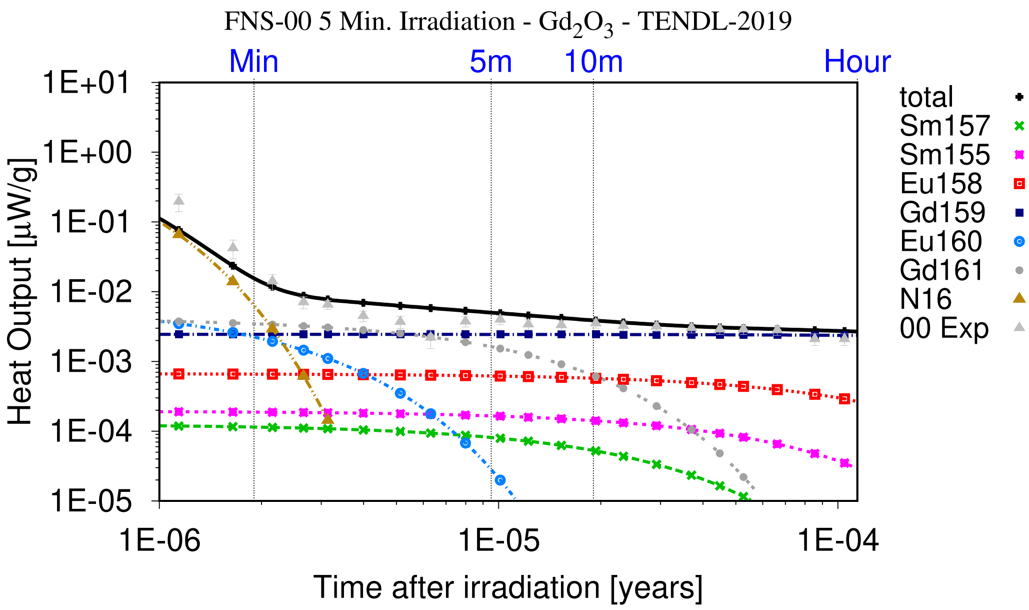
Gadolinium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	1.95$E-$01 +/-28%	7.66$E-$02 +/-3%	2.55	2.55	2.55	2.41
0.87	4.22$E-$02 +/-30%	2.36$E-$02 +/-9%	1.79	1.76	1.74	1.54
1.13	1.41$E-$02 +/-25%	1.18$E-$02 +/-15%	1.19	1.14	1.12	0.92
1.40	7.06$E-$03 +/-20%	8.77$E-$03 +/-18%	0.80	0.75	0.75	0.59
1.65	6.51$E-$03 +/-15%	7.78$E-$03 +/-18%	0.84	0.76	0.77	0.61
2.10	4.48$E-$03 +/-17%	6.92$E-$03 +/-17%	0.65	0.58	0.60	0.47
2.70	3.69$E-$03 +/-20%	6.28$E-$03 +/-17%	0.59	0.52	0.55	0.44
3.32	2.19$E-$03 +/-30%	5.82$E-$03 +/-17%	0.38	0.33	0.36	0.30
4.20	3.74$E-$03 +/-17%	5.34$E-$03 +/-16%	0.70	0.61	0.67	0.58
5.32	3.97$E-$03 +/-15%	4.90$E-$03 +/-15%	0.81	0.70	0.78	0.73
6.43	3.39$E-$03 +/-16%	4.57$E-$03 +/-15%	0.74	0.64	0.72	0.73
8.05	3.32$E-$03 +/-16%	4.20$E-$03 +/-14%	0.79	0.69	0.77	0.87
10.17	3.51$E-$03 +/-14%	3.86$E-$03 +/-14%	0.91	0.81	0.90	1.18
12.27	3.23$E-$03 +/-15%	3.62$E-$03 +/-14%	0.89	0.80	0.89	1.36
15.35	3.17$E-$03 +/-15%	3.38$E-$03 +/-14%	0.94	0.86	0.95	1.75
19.47	3.01$E-$03 +/-15%	3.19$E-$03 +/-15%	0.94	0.88	0.97	2.23
23.58	2.88$E-$03 +/-15%	3.08$E-$03 +/-15%	0.93	0.89	0.97	2.65
27.72	2.87$E-$03 +/-15%	3.00$E-$03 +/-15%	0.96	0.92	1.00	3.14
34.83	2.80$E-$03 +/-15%	2.90$E-$03 +/-15%	0.97	0.94	1.02	3.81
44.95	2.09$E-$03 +/-19%	2.80$E-$03 +/-14%	0.75	0.74	0.80	3.59
55.02	2.09$E-$03 +/-19%	2.72$E-$03 +/-14%	0.77	0.76	0.83	4.35
mean % diff. from E			33	45	35	65
mean χ^2			4.12	7.52	5.09	15.54

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	2.55	28%	-
Gd159	18.48h	0.94	15%	15%

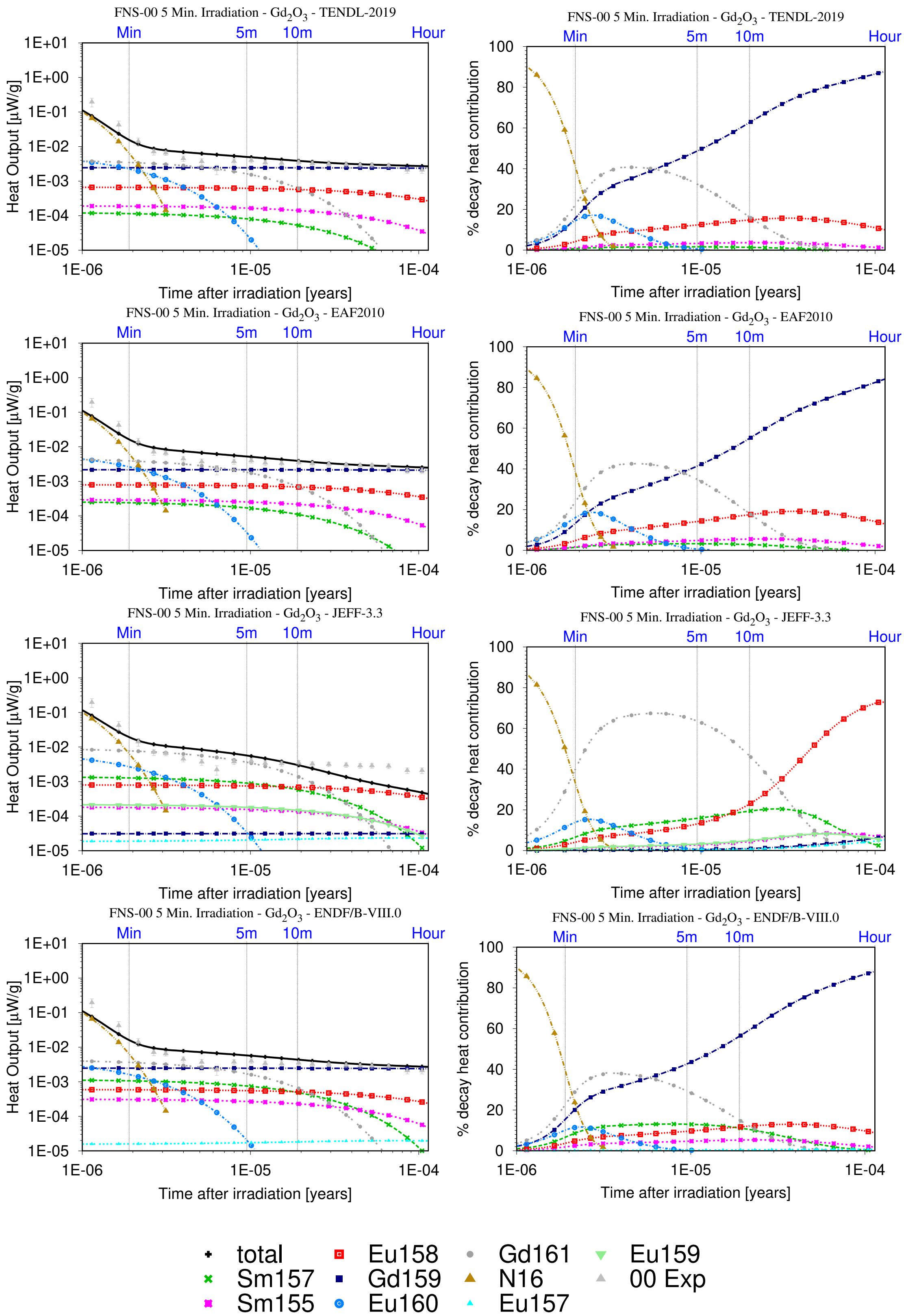


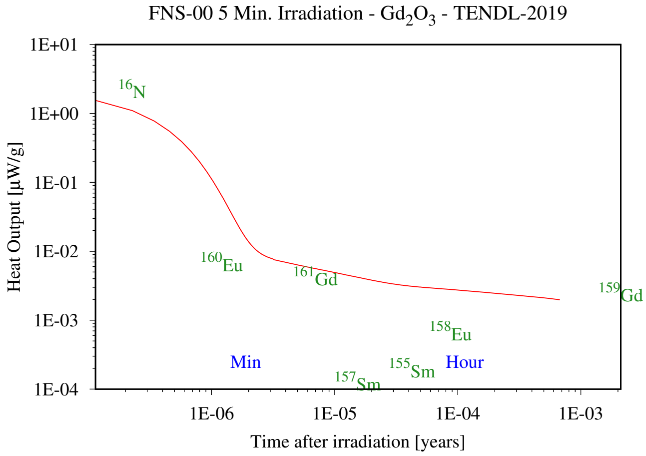
Gadolinium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Eu160	38.00s	Gd160(n,p)Eu160	100.0
Gd161	3.66m	Gd160(n,γ)Gd161	100.0
Sm157	8.07m	Gd160(n,α)Sm157	100.0
Eu159	18.10m	Gd160(n,d)Eu159	85.7
		Gd160(n,np)Eu159	14.3
Sm155	22.30m	Gd158(n,α)Sm155	100.0
Eu158	45.90m	Gd158(n,p)Eu158	99.9
Eu157	15.18h	Gd157(n,p)Eu157	90.4
		Gd158(n,d)Eu157	4.9
		Gd158(n,np)Eu157	2.7
		Gd160(n,α)Sm157(β^-)Eu157	2.0
Gd159	18.48h	Gd160(n,2n)Gd159	98.9
		Gd158(n,γ)Gd159	1.1

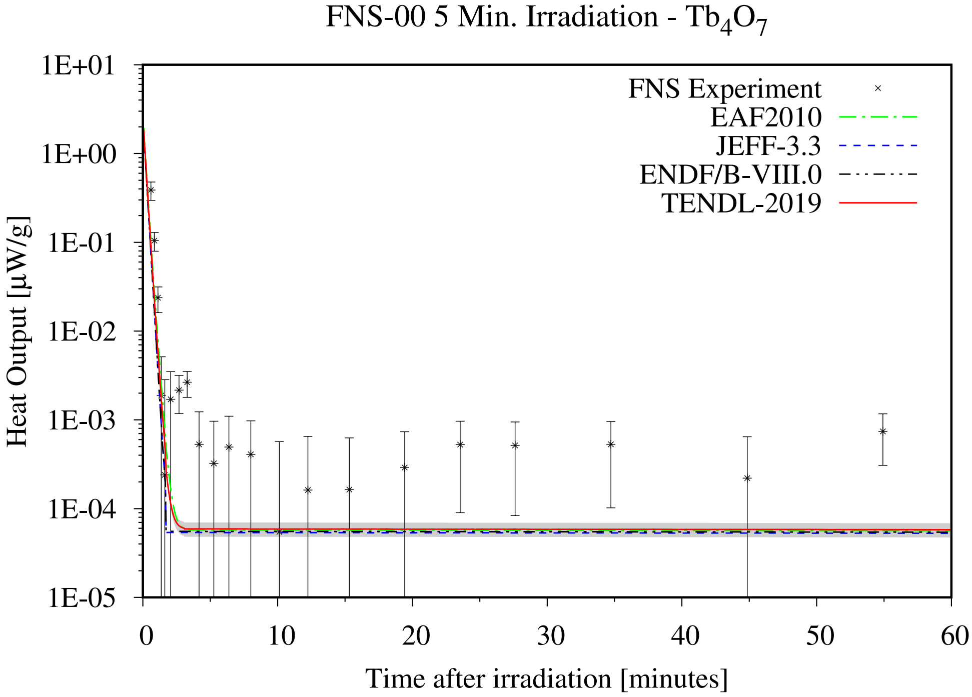
Comments on Gadolinium 5-minute experiments:

Another case with a short timescale (less than 5-minute) increase in the decay heat in the experiments. Beyond this the predictions with three of the libraries (TENDL, EAF, and ENDF/B) appear to follow the measurement profile but with a slight overprediction of one of the contributing nuclides – almost certainly the long-lived Gd159 (from (n,2n) reactions on Gd160) whose flat contribution (on this timescale) becomes more and more dominant as cooling times increase (almost 90% at 1 hour). JEFF-3.3 completely omits the reaction for this nuclide and produces a clearly very discrepant decay profile.


FNS-00 5 Min. Irradiation - Gd2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Gd2O3 - EAF2010
FNS-00 5 Min. Irradiation - Gd2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Gd2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Sm157
Sm155
Eu158
Gd159
Eu160
Gd161
N16
Eu157
Eu159
00 Exp


FNS-00 5 Min. Irradiation - Gd2O3 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
16N
160Eu
161Gd
159Gd
158Eu
155Sm
157Sm
Min
Hour
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

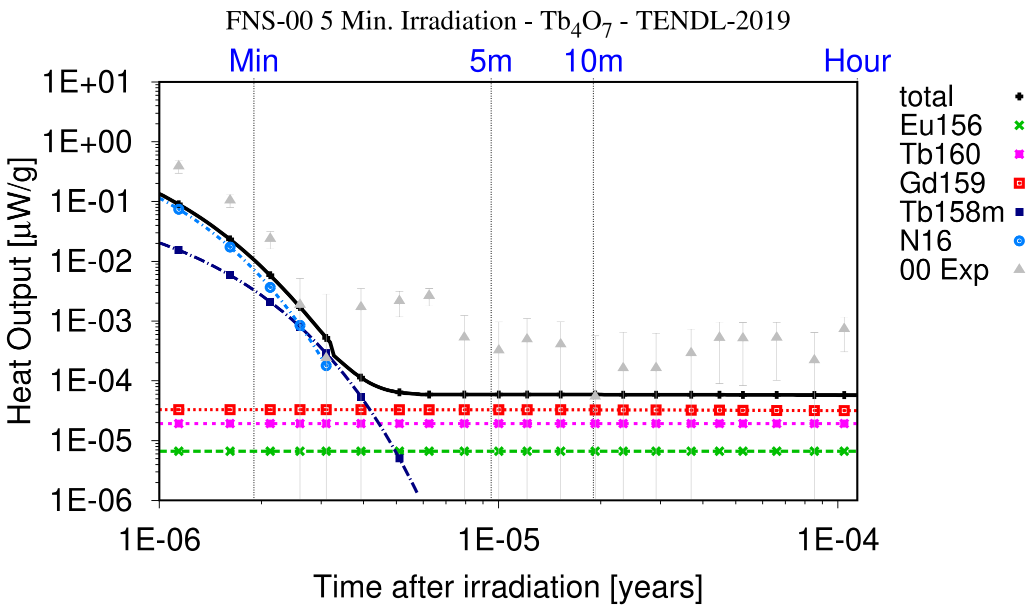
Terbium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	$3.88E{-}01$ +/-23%	$9.00E{-}02$ +/-1%	4.31	5.23	3.71	5.20
0.85	$1.04E{-}01$ +/-24%	$2.33E{-}02$ +/-2%	4.48	6.03	3.59	6.00
1.12	$2.38E{-}02$ +/-32%	$5.82E{-}03$ +/-2%	4.09	6.43	3.00	6.40
1.37	$1.88E{-}03$ +/-174%	$1.71E{-}03$ +/-3%	1.10	2.08	0.74	2.06
1.63	$2.41E{-}04$ +/-1077%	$5.27E{-}04$ +/-4%	0.46	1.00	0.29	0.98
2.07	$1.70E{-}03$ +/-105%	$1.14E{-}04$ +/-10%	14.96	30.76	10.14	31.66
2.68	$2.16E{-}03$ +/-46%	$6.49E{-}05$ +/-17%	33.36	39.05	31.90	40.19
3.28	$2.65E{-}03$ +/-32%	$5.91E{-}05$ +/-18%	44.81	47.81	46.09	49.21
4.17	$5.31E{-}04$ +/-132%	$5.91E{-}05$ +/-18%	8.98	9.58	9.23	9.86
5.27	$3.23E{-}04$ +/-199%	$5.91E{-}05$ +/-18%	5.47	5.83	5.62	6.00
6.38	$4.94E{-}04$ +/-122%	$5.90E{-}05$ +/-18%	8.37	8.93	8.61	9.19
8.02	$4.08E{-}04$ +/-139%	$5.90E{-}05$ +/-18%	6.92	7.38	7.12	7.60
10.13	$5.46E{-}05$ +/-942%	$5.90E{-}05$ +/-18%	0.93	0.99	0.95	1.02
12.25	$1.62E{-}04$ +/-302%	$5.89E{-}05$ +/-18%	2.75	2.93	2.83	3.02
15.32	$1.64E{-}04$ +/-283%	$5.89E{-}05$ +/-18%	2.78	2.97	2.86	3.06
19.43	$2.90E{-}04$ +/-154%	$5.88E{-}05$ +/-18%	4.93	5.26	5.07	5.41
23.55	$5.27E{-}04$ +/-83%	$5.87E{-}05$ +/-18%	8.98	9.58	9.23	9.86
27.62	$5.14E{-}04$ +/-84%	$5.86E{-}05$ +/-18%	8.78	9.36	9.03	9.64
34.73	$5.29E{-}04$ +/-81%	$5.85E{-}05$ +/-18%	9.05	9.66	9.31	9.94
44.85	$2.20E{-}04$ +/-193%	$5.83E{-}05$ +/-18%	3.78	4.03	3.89	4.15
54.92	$7.40E{-}04$ +/-59%	$5.81E{-}05$ +/-18%	12.74	13.58	13.10	13.99
mean % diff. from E			78	76	84	76
mean χ^2			2.34	2.56	2.17	2.56

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
N16	7.13s	4.31	23%	-

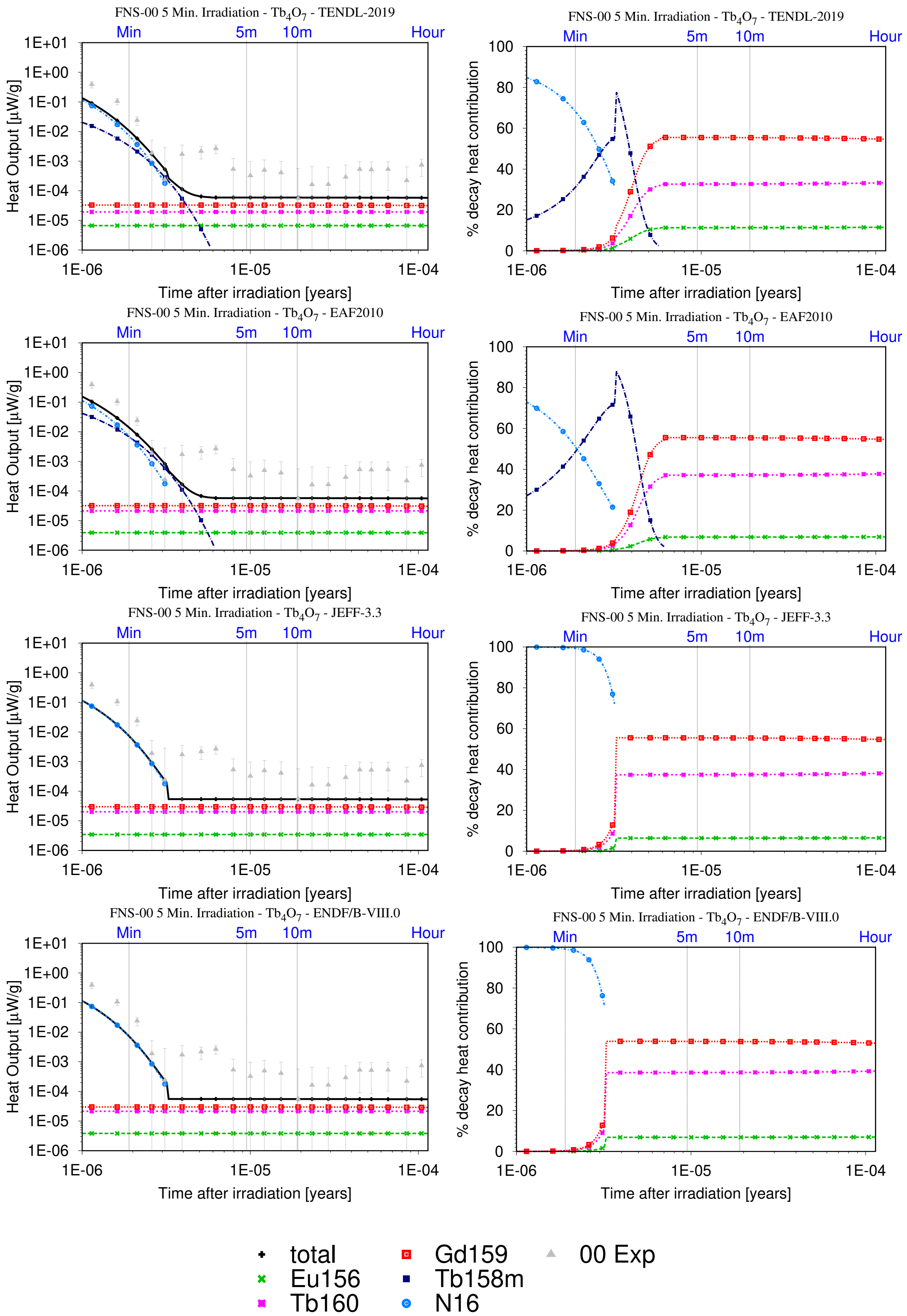


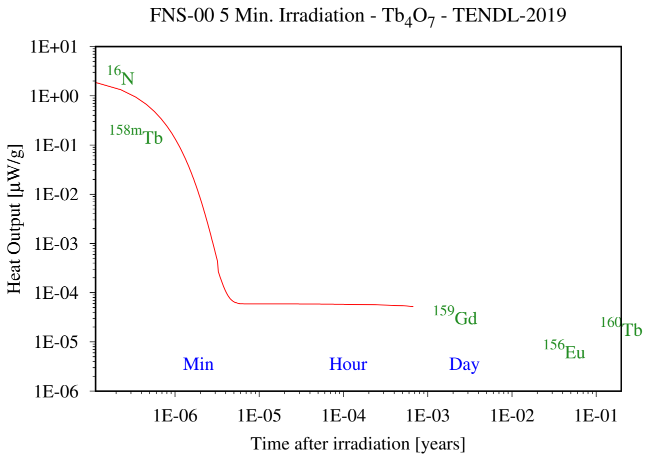
Terbium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Tb158m	10.80s	Tb159(n,2n)Tb158m	100.0
Gd159	18.48h	Tb159(n,p)Gd159	100.0
Eu156	15.19d	Tb159(n,α)Eu156	100.0
Tb160	72.28d	Tb159(n,γ)Tb160	100.0

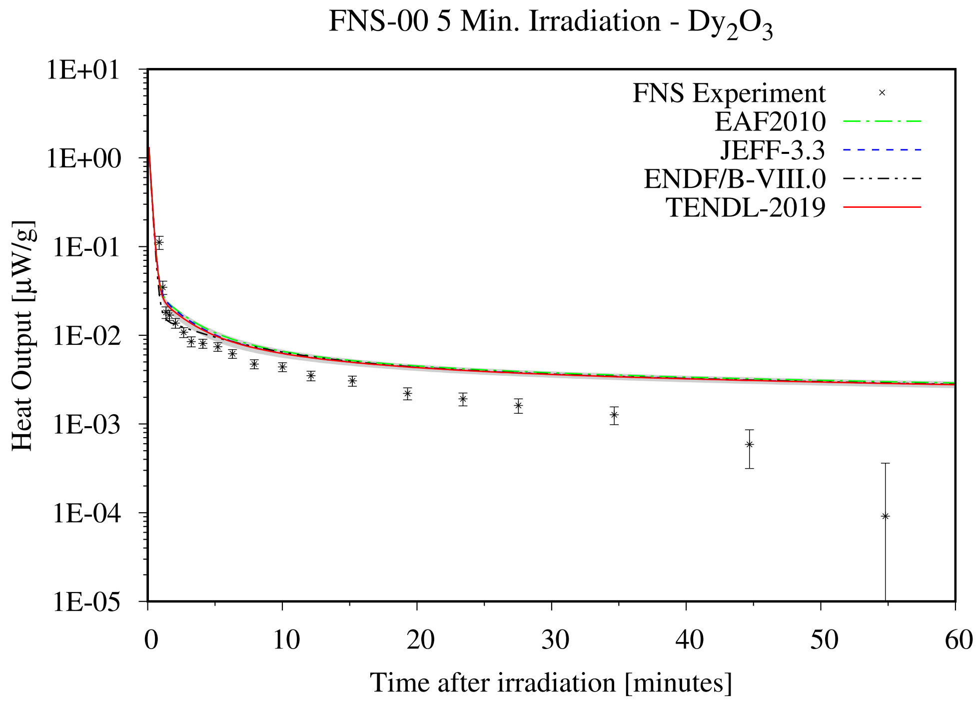
Comments on Terbium 5-minute experiments:

None of the included libraries perform particularly well (IRDFF-II is omitted because it contains no terbium reactions), although the overall profile of each, nearly identical, curve seems to match the experimental profile (but not the heat level). The contribution from the short-lived Tb158m, which only TENDL and EAF predict, is completely swamped by N16 from oxygen (and so it is difficult to assess the prediction quality), and the plateau beyond around three minutes of cooling, which comes from Gd159 and Tb160 decay heat, seems to be a severe underprediction of the experiment. However, the associated measurements should be viewed with caution due to the large, uneven uncertainties.


FNS-00 5 Min. Irradiation - Tb4O7 - TENDL-2019
FNS-00 5 Min. Irradiation - Tb4O7 - EAF2010
FNS-00 5 Min. Irradiation - Tb4O7 - JEFF-3.3
FNS-00 5 Min. Irradiation - Tb4O7 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Eu156
Tb160
Gd159
Tb158m
N16
00 Exp


FNS-00 5 Min. Irradiation - Tb4O7 - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
16N
158mTb
159Gd
156Eu
160Tb
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]

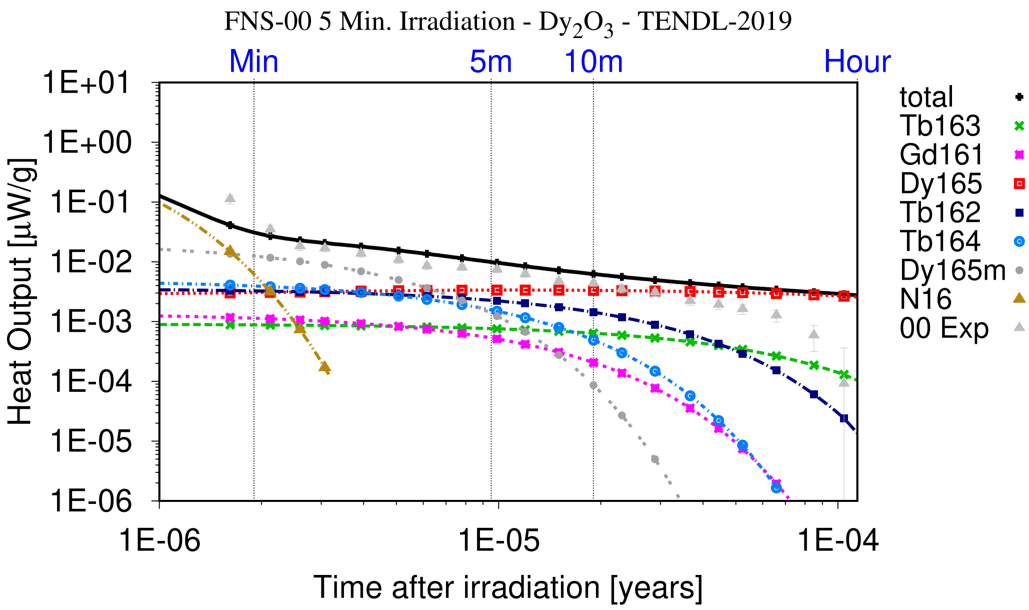
Dysprosium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	$1.12E{-}01$ +/-17%	$4.10E{-}02$ +/-8%	2.73	3.69	2.59	2.59
1.12	$3.48E{-}02$ +/-17%	$2.70E{-}02$ +/-11%	1.29	1.93	1.19	1.20
1.37	$1.81E{-}02$ +/-15%	$2.28E{-}02$ +/-12%	0.80	1.20	0.73	0.74
1.62	$1.69E{-}02$ +/-13%	$2.06E{-}02$ +/-13%	0.82	1.19	0.75	0.76
2.07	$1.37E{-}02$ +/-13%	$1.80E{-}02$ +/-13%	0.76	1.04	0.70	0.72
2.67	$1.08E{-}02$ +/-13%	$1.55E{-}02$ +/-14%	0.70	0.88	0.64	0.66
3.23	$8.50E{-}03$ +/-13%	$1.36E{-}02$ +/-14%	0.63	0.74	0.57	0.60
4.10	$8.08E{-}03$ +/-12%	$1.15E{-}02$ +/-14%	0.70	0.77	0.65	0.68
5.20	$7.42E{-}03$ +/-11%	$9.64E{-}03$ +/-13%	0.77	0.79	0.71	0.75
6.30	$6.20E{-}03$ +/-11%	$8.41E{-}03$ +/-13%	0.74	0.73	0.69	0.73
7.92	$4.74E{-}03$ +/-12%	$7.21E{-}03$ +/-12%	0.66	0.64	0.62	0.65
10.02	$4.39E{-}03$ +/-11%	$6.23E{-}03$ +/-10%	0.71	0.68	0.67	0.70
12.13	$3.50E{-}03$ +/-12%	$5.58E{-}03$ +/-10%	0.63	0.61	0.60	0.63
15.20	$3.07E{-}03$ +/-13%	$4.95E{-}03$ +/-9%	0.62	0.61	0.59	0.62
19.30	$2.21E{-}03$ +/-15%	$4.40E{-}03$ +/-8%	0.50	0.50	0.48	0.50
23.42	$1.92E{-}03$ +/-17%	$4.02E{-}03$ +/-8%	0.48	0.47	0.46	0.47
27.53	$1.62E{-}03$ +/-19%	$3.75E{-}03$ +/-8%	0.43	0.43	0.41	0.43
34.65	$1.27E{-}03$ +/-23%	$3.42E{-}03$ +/-8%	0.37	0.37	0.36	0.37
44.70	$5.88E{-}04$ +/-46%	$3.10E{-}03$ +/-8%	0.19	0.19	0.18	0.19
54.80	$9.15E{-}05$ +/-296%	$2.87E{-}03$ +/-9%	0.03	0.03	0.03	0.03
mean % diff. from E			228	228	244	231
mean χ^2			27.53	27.40	33.99	29.03

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Dy165	2.33h	0.48	17%	9%

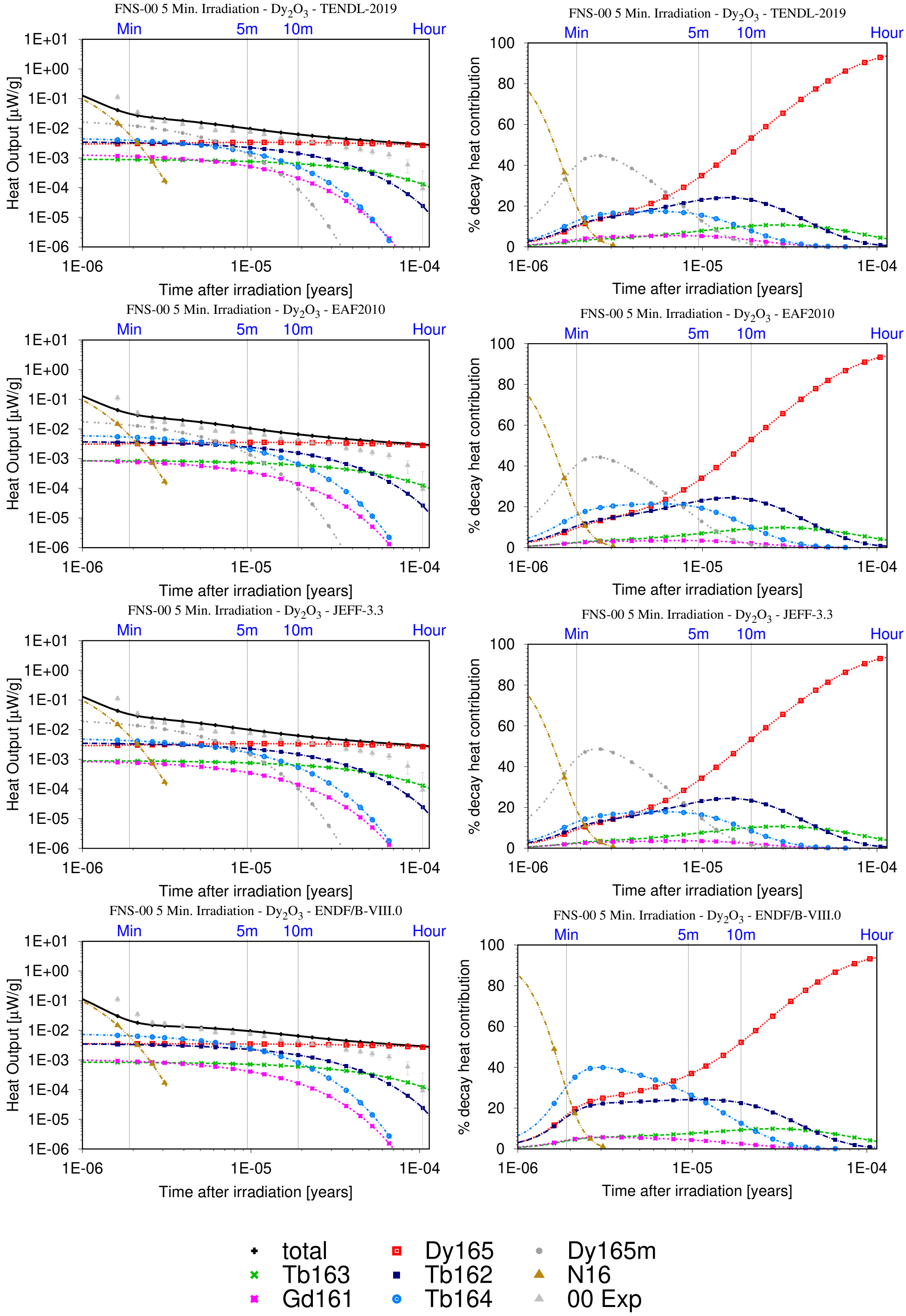


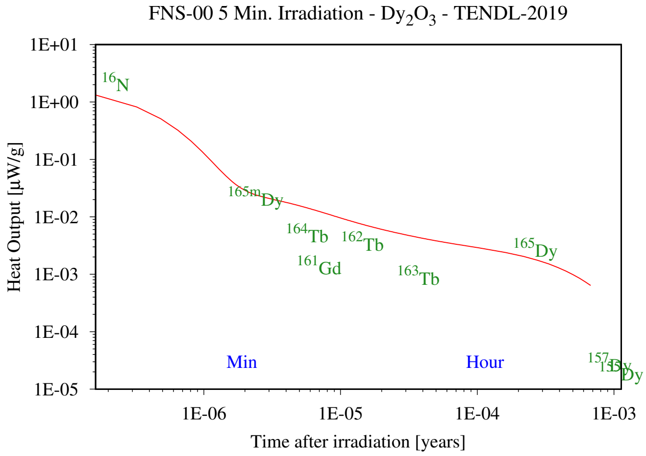
Dysprosium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Dy165m	1.26m	Dy164(n,γ)Dy165m	100.0
Tb164	3.00m	Dy164(n,p)Tb164	100.0
Gd161	3.66m	Dy164(n,α)Gd161	100.0
Tb162	7.60m	Dy162(n,p)Tb162	93.2
		Dy163(n,d)Tb162	4.7
		Dy163(n,np)Tb162	1.9
Tb163	19.50m	Dy163(n,p)Tb163	93.8
		Dy164(n,d)Tb163	4.8
		Dy164(n,np)Tb163	1.4
Dy165	2.33h	Dy164(n,γ)Dy165m(IT)Dy165	50.1
		Dy164(n,γ)Dy165	49.9

Comments on Dysprosium 5-minute experiments:

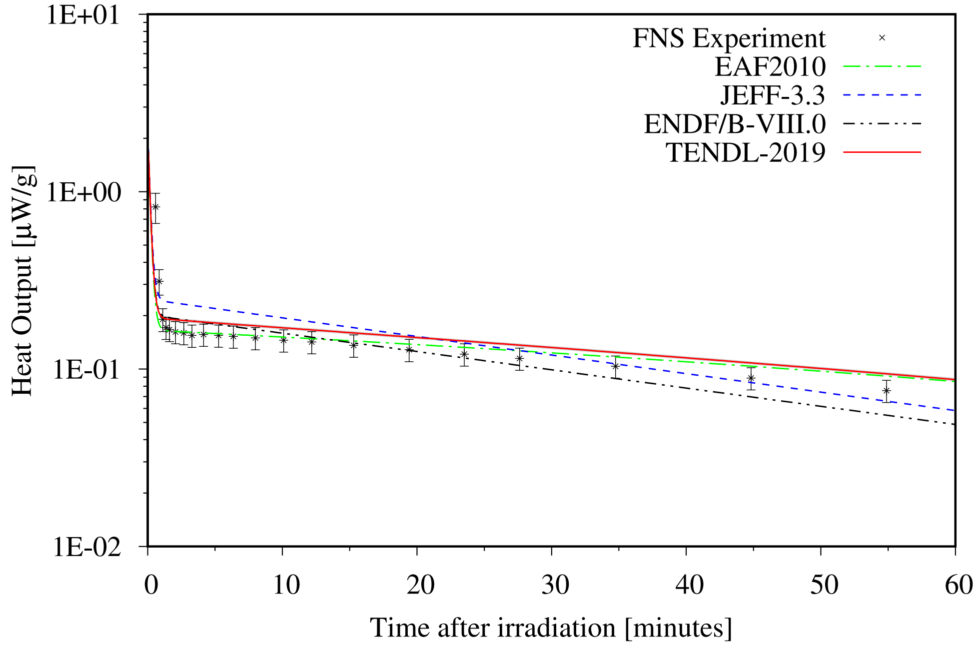
All libraries massively overpredict the experimental decay heat at cooling times beyond around 1 minute (at shorter times the contribution from N16 seems to be underpredicted). The culprit is the constant, swamping contribution from Dy165 (its half-life is beyond the timescale of the experiment), whose decay profile does not match the experimental profile, which falls away throughout the measurement. In fact, the measurement profile would be better matched by the other decaying contributions from Tb162 and Tb163 (from (n,p) reactions), suggesting that the Dy165 should not be there at all and giving cause to question the neutron capture cross sections that produce it in the simulations (EAF, TENDL, and JEFF also predict significant Dy165m production via the same channel, and this too seems an overprediction).


FNS-00 5 Min. Irradiation - Dy2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Dy2O3 - EAF2010
FNS-00 5 Min. Irradiation - Dy2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Dy2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Tb163
Gd161
Dy165
Tb162
Tb164
Dy165m
N16
00 Exp


FNS-00 5 Min. Irradiation - Dy2O3 - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
16N
165mDy
164Tb
162Tb
161Gd
163Tb
165Dy
Min
Hour

Holmium

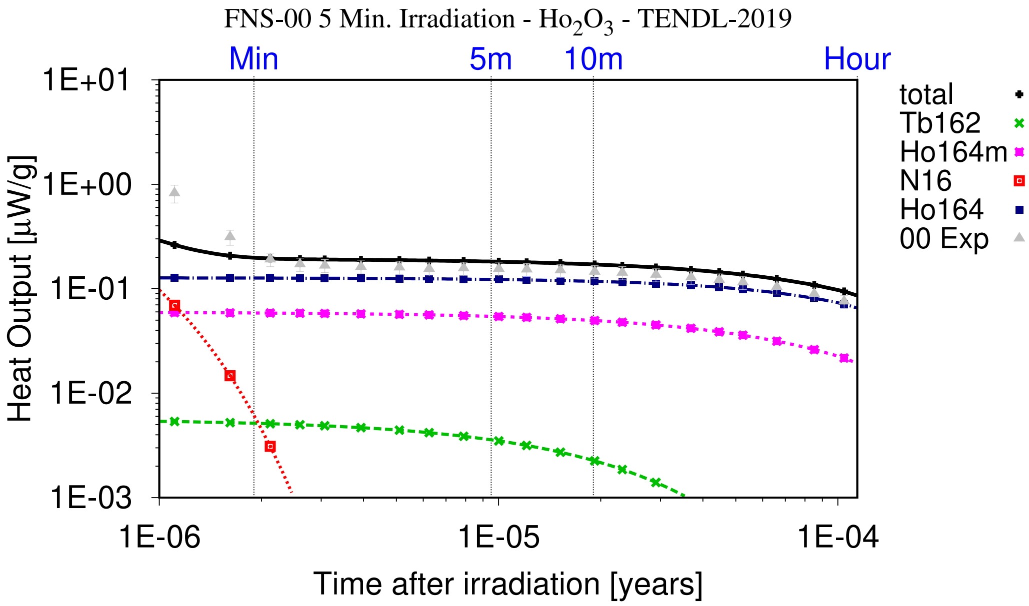
FNS-00 5 Min. Irradiation - Ho_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	8.20E−01 +/-19%	2.63E−01 +/-2%	3.12	3.06	3.51	2.62
0.85	3.12E−01 +/-16%	2.07E−01 +/-2%	1.51	1.47	1.74	1.21
1.12	1.91E−01 +/-15%	1.95E−01 +/-2%	0.98	0.95	1.14	0.78
1.37	1.71E−01 +/-14%	1.92E−01 +/-2%	0.89	0.87	1.04	0.71
1.62	1.67E−01 +/-14%	1.91E−01 +/-2%	0.87	0.86	1.02	0.70
2.07	1.62E−01 +/-14%	1.89E−01 +/-2%	0.86	0.84	0.99	0.69
2.68	1.60E−01 +/-14%	1.88E−01 +/-2%	0.85	0.84	0.99	0.69
3.28	1.55E−01 +/-14%	1.86E−01 +/-2%	0.83	0.83	0.96	0.68
4.15	1.57E−01 +/-14%	1.84E−01 +/-2%	0.85	0.86	0.98	0.70
5.27	1.55E−01 +/-14%	1.81E−01 +/-2%	0.85	0.87	0.98	0.71
6.37	1.53E−01 +/-14%	1.79E−01 +/-2%	0.85	0.88	0.98	0.72
8.00	1.50E−01 +/-14%	1.75E−01 +/-2%	0.86	0.90	0.97	0.73
10.10	1.45E−01 +/-14%	1.71E−01 +/-2%	0.85	0.92	0.96	0.75
12.18	1.42E−01 +/-14%	1.66E−01 +/-2%	0.86	0.94	0.96	0.77
15.30	1.36E−01 +/-14%	1.60E−01 +/-2%	0.85	0.97	0.94	0.80
19.42	1.29E−01 +/-14%	1.52E−01 +/-2%	0.85	1.01	0.93	0.83
23.52	1.21E−01 +/-14%	1.44E−01 +/-2%	0.84	1.05	0.92	0.86
27.62	1.15E−01 +/-14%	1.36E−01 +/-2%	0.84	1.10	0.91	0.90
34.75	1.04E−01 +/-14%	1.24E−01 +/-2%	0.83	1.17	0.89	0.97
44.82	8.90E−02 +/-14%	1.08E−01 +/-2%	0.82	1.28	0.86	1.06
54.88	7.56E−02 +/-14%	9.41E−02 +/-2%	0.80	1.37	0.83	1.14
mean % diff. from E			20	17	11	31
mean χ^2			2.15	1.71	1.29	5.29

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$T_{1/2}$	E/C	%ΔE	%ΔC^{nuc}
Ho164	28.60m	0.80	14%	3%

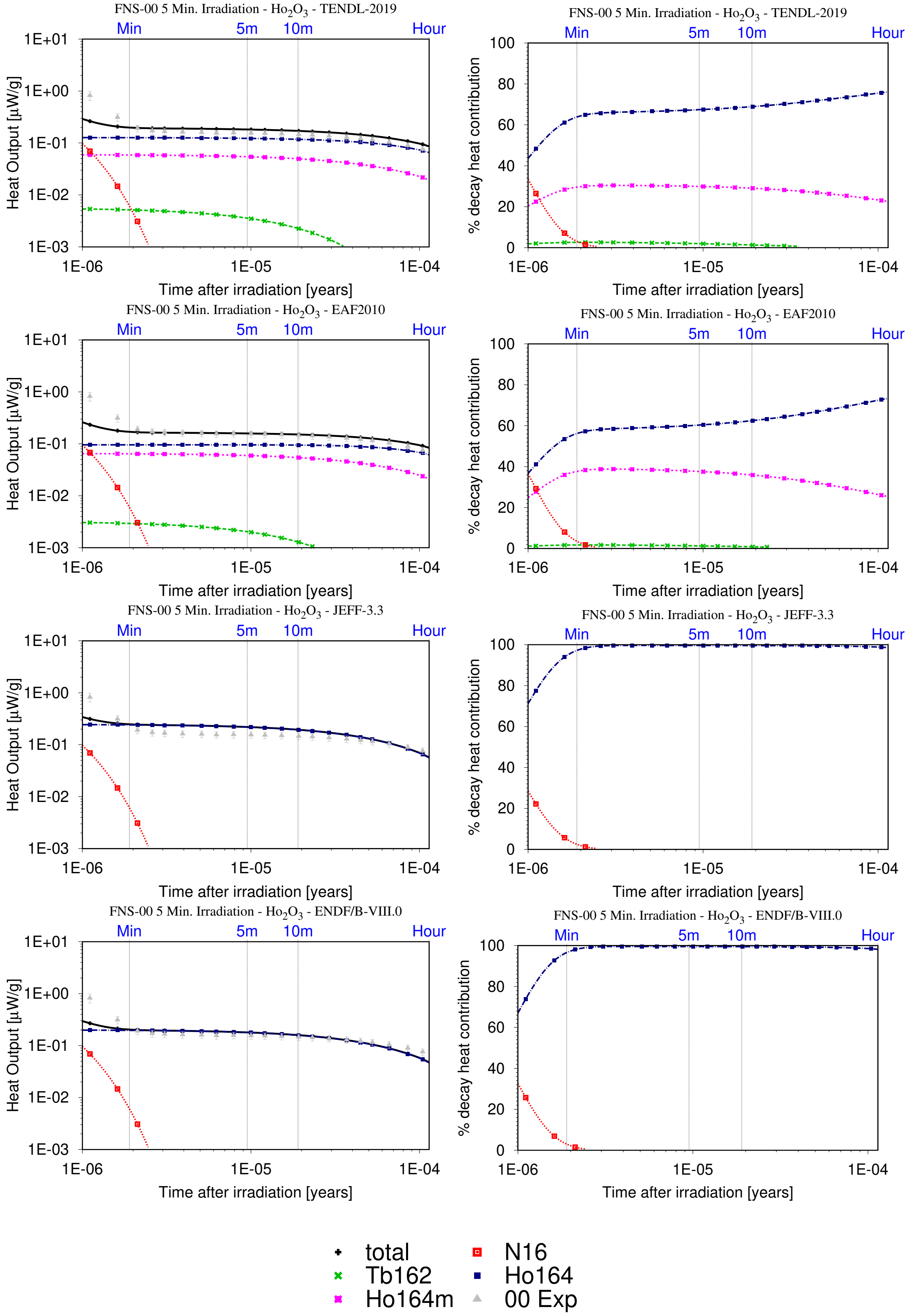


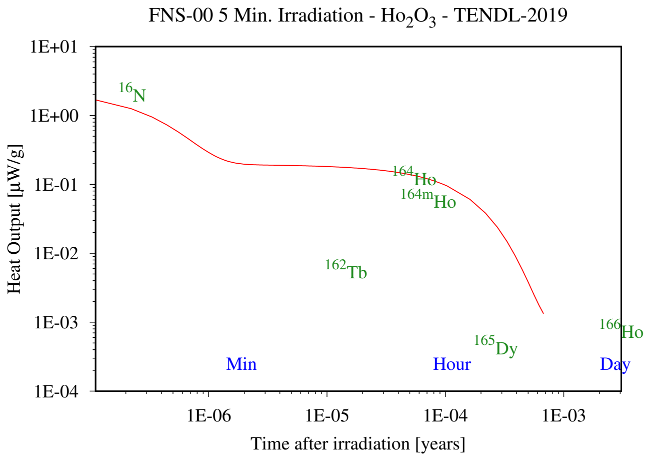
Holmium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Tb162	7.60m	Ho165(n,α)Tb162	100.0
Ho164	28.60m	Ho165(n,2n)Ho164	95.8
		Ho165(n,2n)Ho164m(IT)Ho164	4.2
Ho164m	37.61m	Ho165(n,2n)Ho164m	100.0

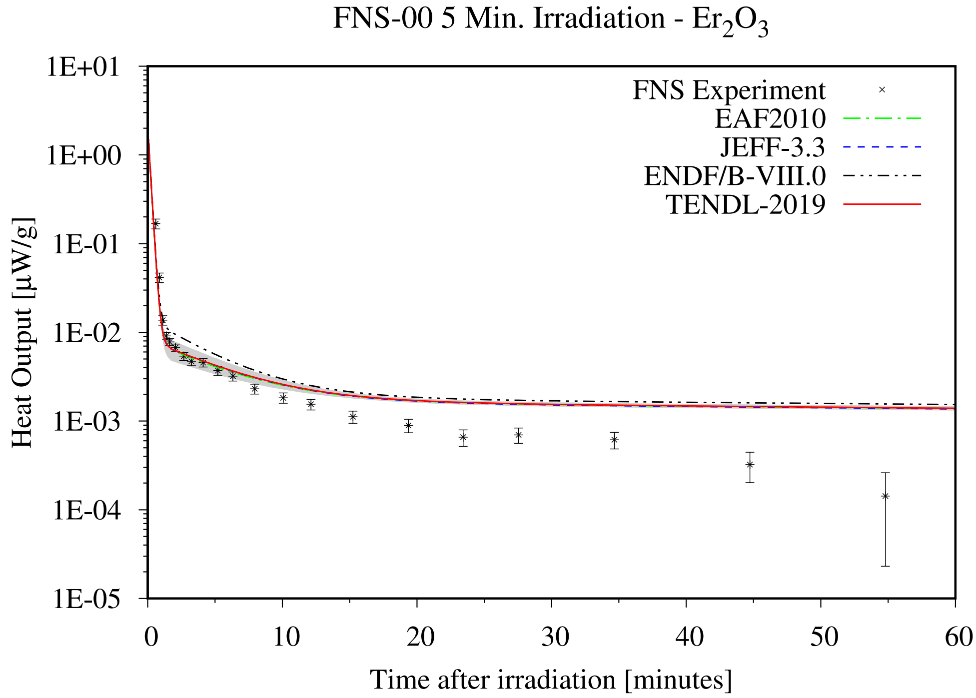
Comments on Holmium 5-minute experiments:

TENDL-2019 and EAF2010 give a better match to the experimental profile than either JEFF-3.3 or ENDF/B-VIII.0, although ENDF/B, by chance, manages to have a slightly lower average deviation than TENDL-2019 with a clearly incorrect decay profile. EAF2010 is very good overall (ignoring the usual underprediction of N16 contributions at short timescales). For this lanthanide, the experiment gives a nice example of the importance of the correct branching ratios in an (n,2n) reaction that produces a ground-state and metastable with similar (but not identical) half-lives. The subtle ratio between the slightly longer-lived Ho164m and the ground-state it decays to is crucial in correctly predicting the profile. The fact that TENDL-2019 overpredicts slightly more than EAF2010 suggests that the (n,2n) channel on Ho165 and its branching ratio should be checked. Importantly, the time-evolution is a good match and it is worth remembering that a correction in the decay data has improved matters compared to earlier libraries [20].


FNS-00 5 Min. Irradiation - Ho2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Ho2O3 - EAF2010
FNS-00 5 Min. Irradiation - Ho2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Ho2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Tb162
Ho164m
N16
Ho164
00 Exp


FNS-00 5 Min. Irradiation - Ho2O3 - TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
Heat Output [µW/g]
16N
164Ho
164mHo
162Tb
165Dy
166Ho
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
Time after irradiation [years]

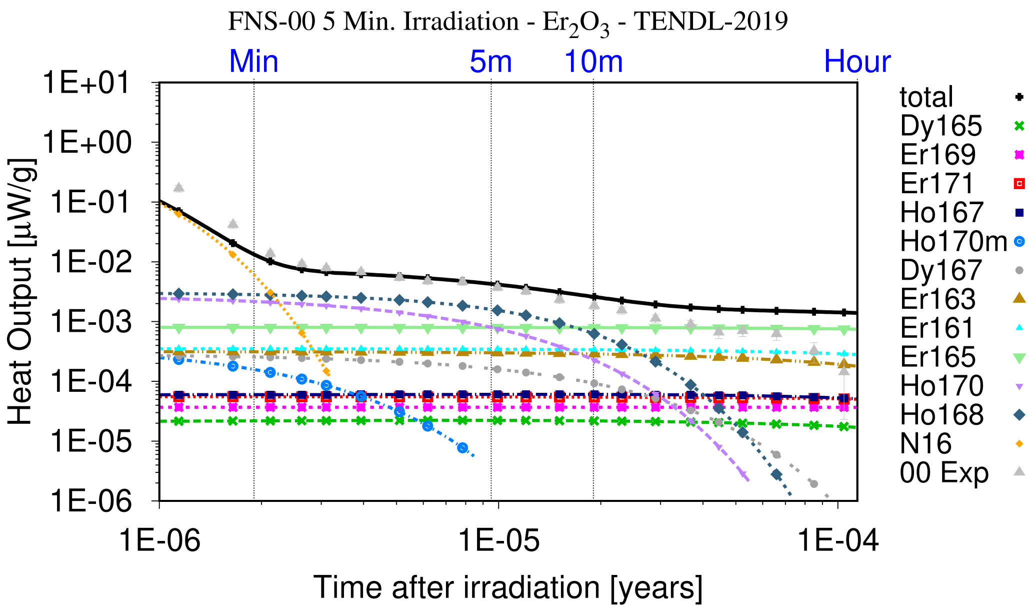
Erbium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	$1.68E{-}01$ +/-13%	$7.01E{-}02$ +/-3%	2.40	2.25	2.42	2.40
0.87	$4.15E{-}02$ +/-12%	$2.06E{-}02$ +/-10%	2.02	1.65	2.02	2.03
1.12	$1.37E{-}02$ +/-12%	$1.02E{-}02$ +/-19%	1.35	0.95	1.34	1.35
1.38	$9.10E{-}03$ +/-10%	$7.51E{-}03$ +/-25%	1.21	0.79	1.21	1.22
1.63	$7.79E{-}03$ +/-9%	$6.76E{-}03$ +/-26%	1.15	0.75	1.16	1.16
2.07	$6.71E{-}03$ +/-10%	$6.22E{-}03$ +/-26%	1.08	0.71	1.10	1.09
2.68	$5.39E{-}03$ +/-10%	$5.73E{-}03$ +/-25%	0.94	0.64	0.97	0.95
3.25	$4.73E{-}03$ +/-11%	$5.32E{-}03$ +/-24%	0.89	0.62	0.92	0.89
4.12	$4.57E{-}03$ +/-11%	$4.76E{-}03$ +/-22%	0.96	0.70	1.00	0.97
5.22	$3.70E{-}03$ +/-11%	$4.16E{-}03$ +/-21%	0.89	0.68	0.92	0.89
6.33	$3.20E{-}03$ +/-12%	$3.67E{-}03$ +/-19%	0.87	0.69	0.90	0.88
7.95	$2.31E{-}03$ +/-13%	$3.11E{-}03$ +/-16%	0.74	0.62	0.77	0.75
10.07	$1.83E{-}03$ +/-13%	$2.59E{-}03$ +/-12%	0.71	0.61	0.72	0.71
12.13	$1.54E{-}03$ +/-14%	$2.25E{-}03$ +/-10%	0.69	0.61	0.70	0.69
15.25	$1.12E{-}03$ +/-16%	$1.93E{-}03$ +/-7%	0.58	0.53	0.59	0.59
19.37	$8.93E{-}04$ +/-17%	$1.72E{-}03$ +/-6%	0.52	0.48	0.52	0.52
23.43	$6.57E{-}04$ +/-21%	$1.62E{-}03$ +/-6%	0.40	0.37	0.41	0.41
27.55	$6.98E{-}04$ +/-20%	$1.57E{-}03$ +/-6%	0.45	0.41	0.45	0.45
34.67	$6.16E{-}04$ +/-21%	$1.51E{-}03$ +/-6%	0.41	0.37	0.41	0.41
44.73	$3.24E{-}04$ +/-37%	$1.46E{-}03$ +/-6%	0.22	0.20	0.22	0.22
54.80	$1.42E{-}04$ +/-84%	$1.42E{-}03$ +/-6%	0.10	0.09	0.10	0.10
mean % diff. from E			103	129	101	101
mean χ^2			22.28	35.83	21.63	21.46

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
N16	7.13s	2.40	13%	-

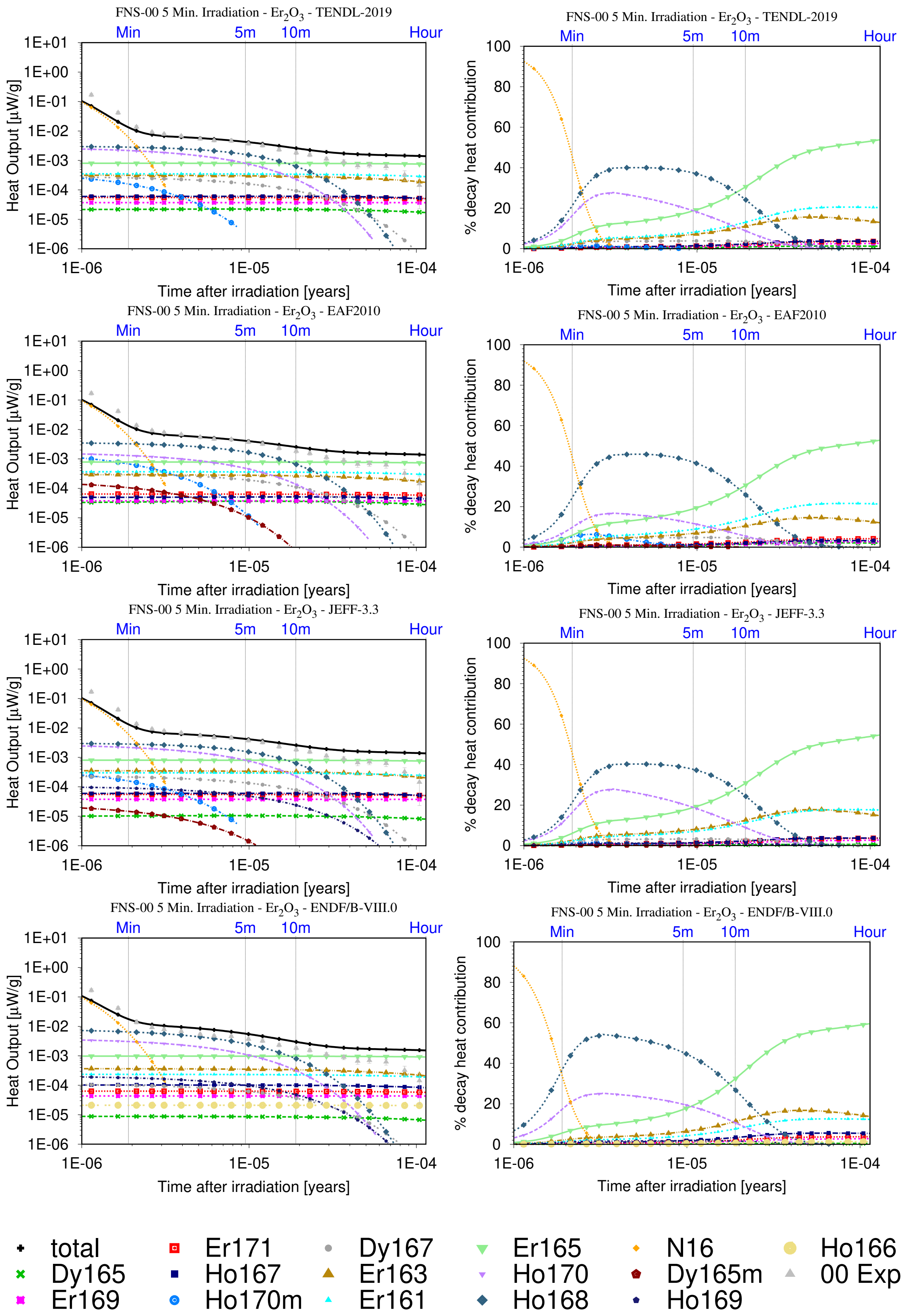


Erbium, TENDL-2019 5-minute pathway analysis

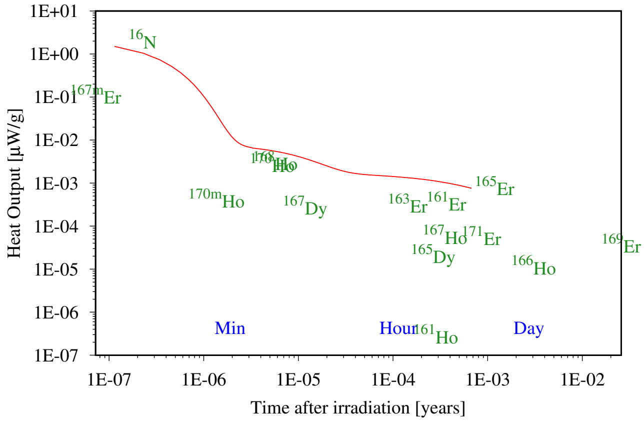
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Ho170m	43.00s	Er170(n,p)Ho170m	100.0
Dy165m	1.26m	Er168(n,α)Dy165m	100.0
Ho170	2.78m	Er170(n,p)Ho170	100.0
Ho168	2.99m	Er168(n,p)Ho168	66.1
		Er168(n,p)Ho168m(IT)Ho168	33.6
Ho169	4.40m	Er170(n,d)Ho169	82.5
		Er170(n,np)Ho169	17.5
Dy167	6.20m	Er170(n,α)Dy167	100.0
Er163	1.25h	Er164(n,2n)Er163	99.4
Dy165	2.33h	Er168(n,α)Dy165	84.1
		Er168(n,α)Dy165m(IT)Dy165	15.9
Ho167	3.10h	Er167(n,p)Ho167	91.6
		Er168(n,d)Ho167	4.5
		Er170(n,α)Dy167(β^-)Ho167	2.3
		Er168(n,np)Ho167	1.6
Er161	3.21h	Er162(n,2n)Er161	100.0
Er171	7.52h	Er170(n,γ)Er171	100.0
Er165	10.36h	Er166(n,2n)Er165	99.6
Ho166	1.12d	Er166(n,p)Ho166	97.5
		Er167(n,d)Ho166	1.5
Er169	9.40d	Er170(n,2n)Er169	98.5
		Er168(n,γ)Er169	1.5

Comments on Erbium 5-minute experiments:

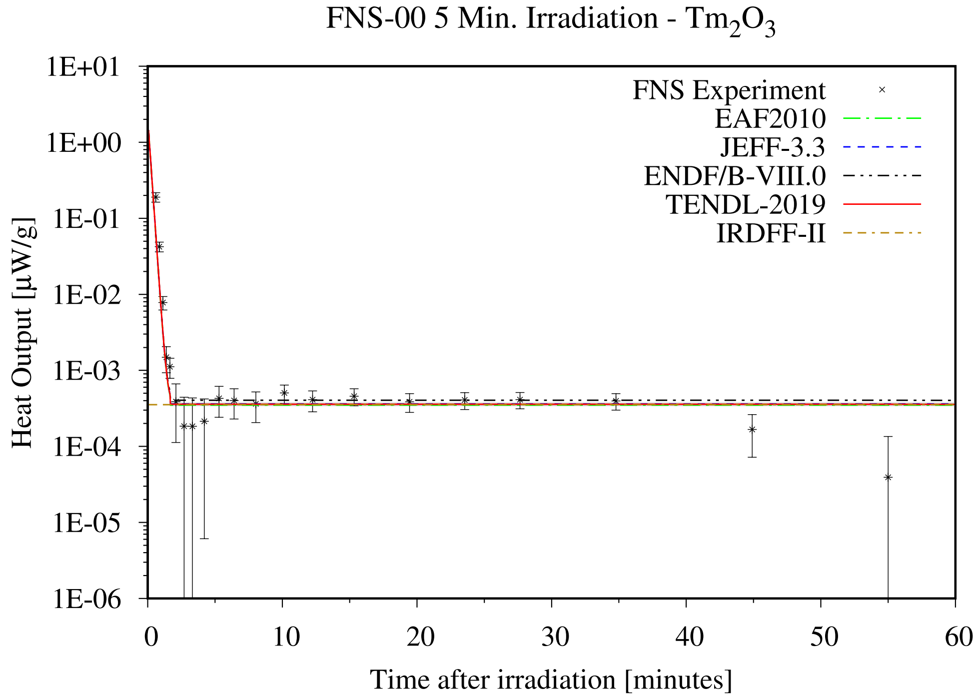
At first glance the obvious disagreement in the shape profile of the measured decay-heat and the simulations is suggestive of a problem with the underlying half-life data for some nuclide, which would be a rare and interesting example if confirmed. However, closer inspection of the nuclide contributions from the simulations suggest, instead, that there could be an over-estimation of Er165 production via (n,2n) reactions, which dominates the simulated decay-heat beyond 10 minutes of cooling – precisely the region where the simulations are clearly discrepant from the experimental measurements. If this channel was adjusted downwards, then the simulations would be a much better match to the experiment.


FNS-00 5 Min. Irradiation - Er2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Er2O3 - EAF2010
FNS-00 5 Min. Irradiation - Er2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Er2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-06
1E-05
1E-04
total
Dy165
Er169
Er171
Ho167
Ho170m
Dy167
Er163
Er161
Er165
Ho170
Ho168
N16
Dy165m
Ho169
Ho166
00 Exp

FNS-00 5 Min. Irradiation - Er_2O_3 - TENDL-2019



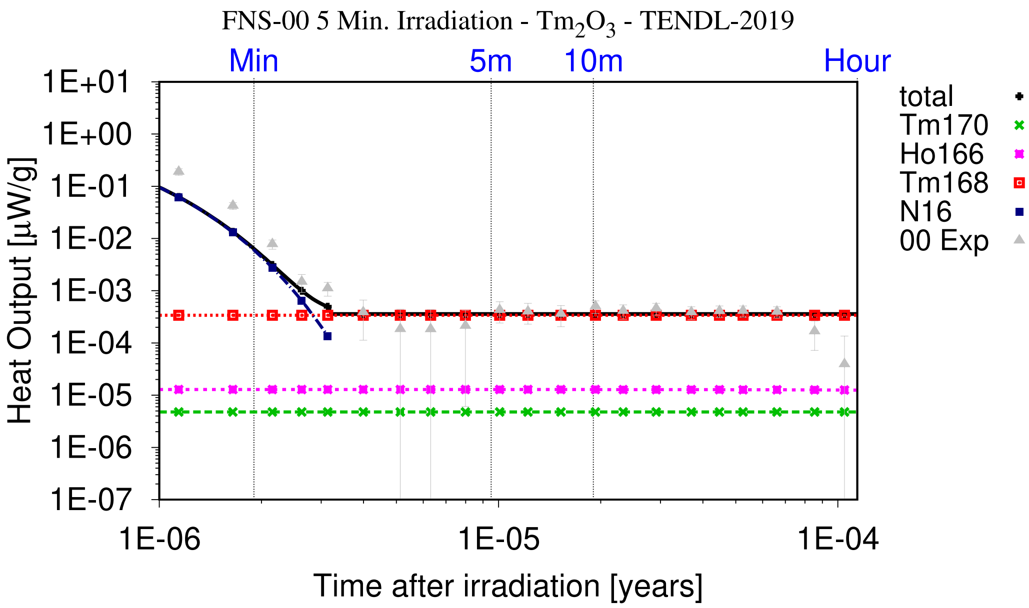
Thulium



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
0.60	1.90$E-$01 +/-14%	6.22$E-$02 +/-0%	3.05	3.07	3.11	3.05	536.93
0.87	4.24$E-$02 +/-15%	1.34$E-$02 +/-0%	3.15	3.16	3.22	3.16	119.92
1.13	7.78$E-$03 +/-20%	3.17$E-$03 +/-1%	2.45	2.47	2.56	2.49	22.02
1.38	1.49$E-$03 +/-38%	1.02$E-$03 +/-2%	1.45	1.42	1.52	1.48	4.21
1.65	1.12$E-$03 +/-30%	4.98$E-$04 +/-4%	2.24	2.07	2.33	2.25	3.15
2.10	3.88$E-$04 +/-71%	3.58$E-$04 +/-5%	1.08	0.96	1.11	1.07	1.10
2.70	1.85$E-$04 +/-140%	3.58$E-$04 +/-5%	0.52	0.46	0.53	0.51	0.52
3.32	1.84$E-$04 +/-136%	3.58$E-$04 +/-5%	0.51	0.45	0.53	0.51	0.52
4.20	2.14$E-$04 +/-97%	3.58$E-$04 +/-5%	0.60	0.53	0.61	0.59	0.60
5.30	4.29$E-$04 +/-44%	3.58$E-$04 +/-5%	1.20	1.06	1.23	1.18	1.21
6.42	4.01$E-$04 +/-43%	3.58$E-$04 +/-5%	1.12	0.99	1.15	1.11	1.13
8.03	3.62$E-$04 +/-43%	3.58$E-$04 +/-5%	1.01	0.89	1.04	1.00	1.03
10.15	5.04$E-$04 +/-27%	3.58$E-$04 +/-5%	1.41	1.24	1.44	1.39	1.43
12.25	4.11$E-$04 +/-31%	3.58$E-$04 +/-5%	1.15	1.01	1.18	1.14	1.16
15.33	4.57$E-$04 +/-25%	3.58$E-$04 +/-5%	1.28	1.13	1.31	1.26	1.29
19.45	3.87$E-$04 +/-28%	3.58$E-$04 +/-5%	1.08	0.95	1.11	1.07	1.09
23.55	4.07$E-$04 +/-25%	3.58$E-$04 +/-5%	1.14	1.01	1.17	1.13	1.15
27.65	4.12$E-$04 +/-24%	3.58$E-$04 +/-5%	1.15	1.02	1.18	1.14	1.17
34.78	3.97$E-$04 +/-25%	3.58$E-$04 +/-5%	1.11	0.98	1.14	1.10	1.12
44.90	1.67$E-$04 +/-57%	3.58$E-$04 +/-5%	0.47	0.41	0.48	0.46	0.47
55.00	3.92$E-$05 +/-245%	3.58$E-$04 +/-5%	0.11	0.10	0.11	0.11	0.11
mean % diff. from E			76	83	76	77	84
mean χ^2			3.63	3.83	3.70	3.66	6.96

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	3.05	14%	-
Tm168	93.10d	1.08	71%	5%

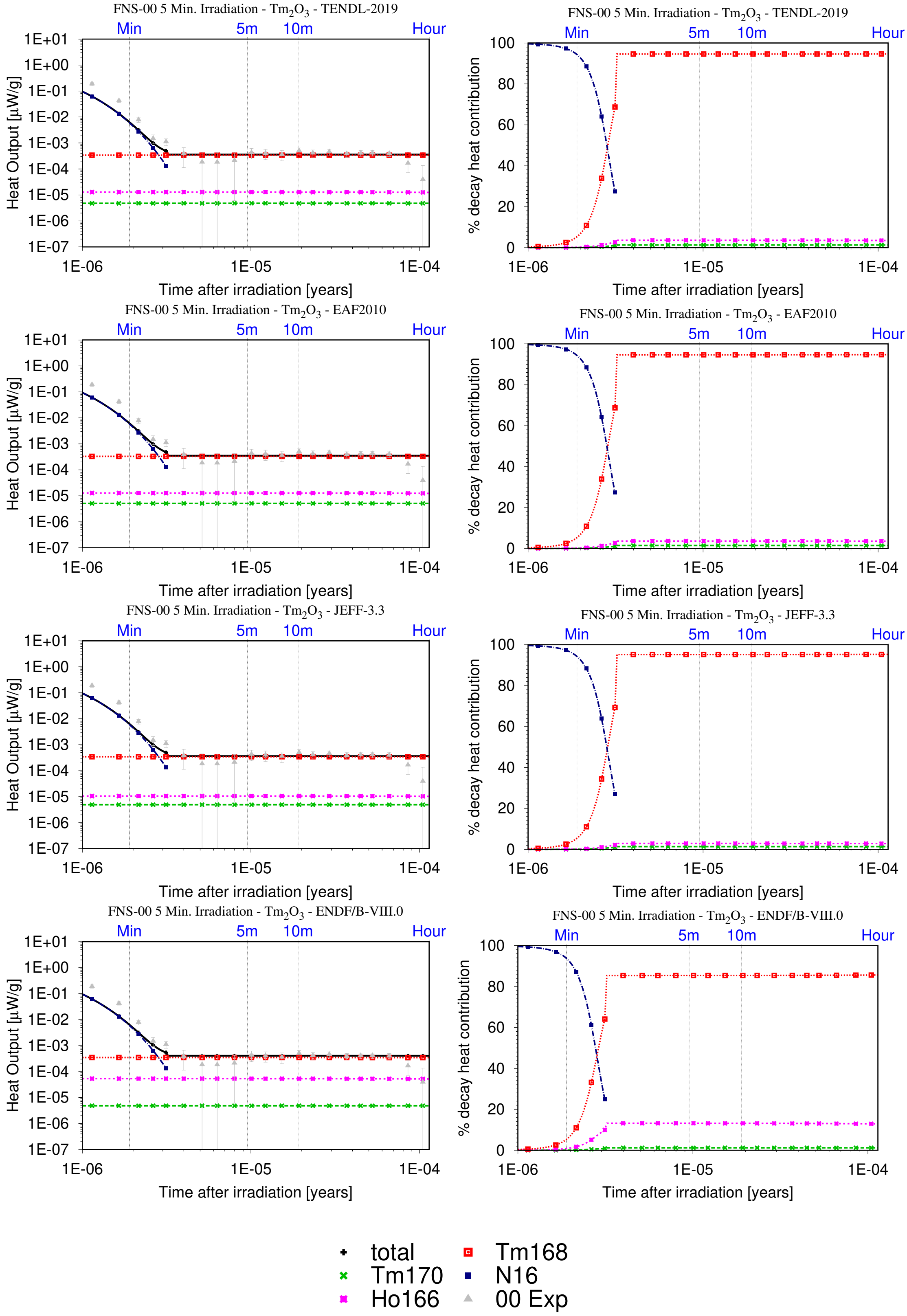


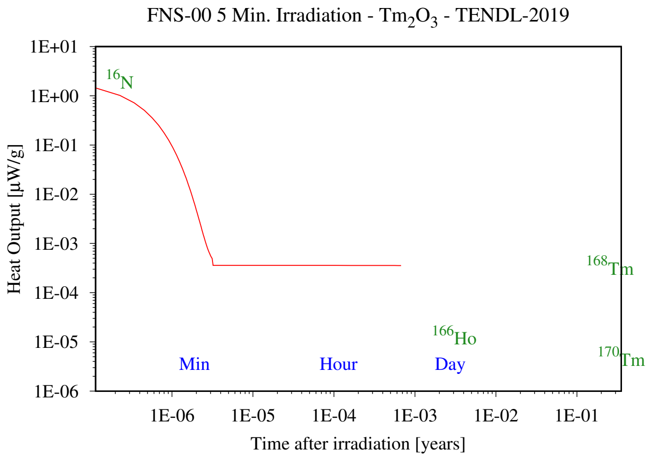
Thulium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
N16	7.13s	O16(n,p)N16	100.0
Ho166	1.12d	Tm169(n,α)Ho166	100.0
Tm168	93.10d	Tm169(n,2n)Tm168	100.0
Tm170	128.61d	Tm169(n,γ)Tm170	100.0

Comments on Thulium 5-minute experiments:

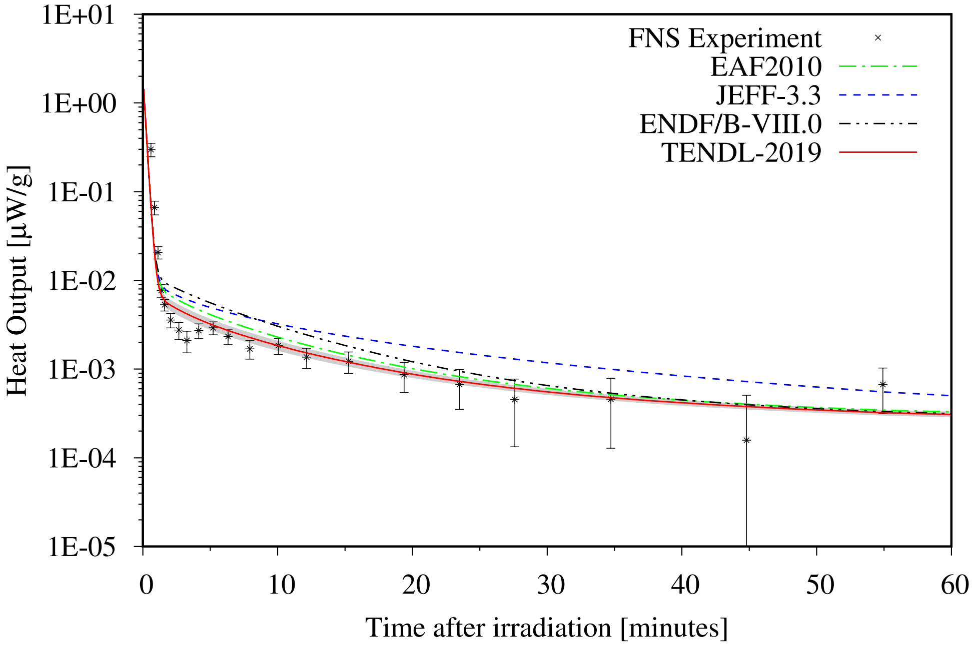
A rare example in the lanthanides where IRDFF-II is able to simulate the experiment reasonably. As usual, no library is able to capture the measured response from N16 decay-heat at very short timescales (could there be some missing contributions from isomeric states?), but they all agree on the dominant, constant contribution from Tm168 at all cooling times beyond around 1.5 minutes (nearly 100% at all times where N16 does not contribute). The overall agreement, as measured by the mean % difference, does not look good, but this can be attributed to experimental problems, which see very high uncertainties below 10 minutes of cooling, some random fluctuations, and then a significant drop in decay-heat (again with high uncertainties) beyond 40 minutes of cooling – the simulations particularly disagree with this and there is no obvious reason to expect it.


FNS-00 5 Min. Irradiation - Tm2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Tm2O3 - EAF2010
FNS-00 5 Min. Irradiation - Tm2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Tm2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Tm170
Ho166
Tm168
N16
00 Exp


FNS-00 5 Min. Irradiation - Tm2O3 - TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
Heat Output [µW/g]
16N
168Tm
166Ho
170Tm
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]

Ytterbium

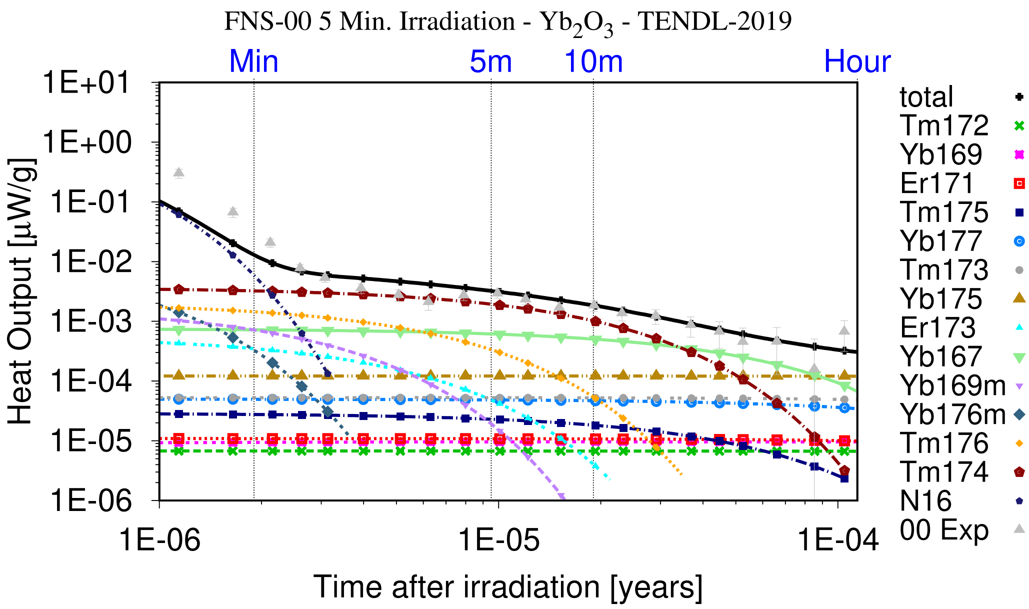
FNS-00 5 Min. Irradiation - Yb_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	$2.99E{-}01$ +/-17%	$6.95E{-}02$ +/-2%	4.30	4.18	4.26	4.16
0.87	$6.64E{-}02$ +/-18%	$2.03E{-}02$ +/-5%	3.27	2.84	3.04	2.94
1.12	$2.07E{-}02$ +/-16%	$9.38E{-}03$ +/-10%	2.20	1.61	1.86	1.79
1.37	$7.71E{-}03$ +/-16%	$6.83E{-}03$ +/-13%	1.13	0.74	0.91	0.86
1.62	$5.31E{-}03$ +/-15%	$5.90E{-}03$ +/-14%	0.90	0.56	0.71	0.66
2.07	$3.57E{-}03$ +/-18%	$5.21E{-}03$ +/-14%	0.68	0.41	0.54	0.49
2.67	$2.75E{-}03$ +/-22%	$4.63E{-}03$ +/-14%	0.59	0.35	0.46	0.42
3.27	$2.10E{-}03$ +/-27%	$4.16E{-}03$ +/-14%	0.50	0.29	0.39	0.35
4.15	$2.72E{-}03$ +/-19%	$3.62E{-}03$ +/-14%	0.75	0.43	0.59	0.50
5.22	$2.92E{-}03$ +/-17%	$3.10E{-}03$ +/-14%	0.94	0.54	0.74	0.61
6.32	$2.33E{-}03$ +/-19%	$2.70E{-}03$ +/-14%	0.86	0.50	0.68	0.54
7.93	$1.69E{-}03$ +/-24%	$2.25E{-}03$ +/-14%	0.75	0.44	0.60	0.45
10.05	$1.84E{-}03$ +/-21%	$1.82E{-}03$ +/-13%	1.01	0.61	0.81	0.57
12.15	$1.36E{-}03$ +/-26%	$1.51E{-}03$ +/-12%	0.90	0.57	0.74	0.49
15.27	$1.23E{-}03$ +/-27%	$1.19E{-}03$ +/-11%	1.03	0.68	0.86	0.53
19.38	$8.66E{-}04$ +/-37%	$9.06E{-}04$ +/-10%	0.96	0.68	0.82	0.47
23.50	$6.69E{-}04$ +/-48%	$7.27E{-}04$ +/-9%	0.92	0.71	0.81	0.44
27.60	$4.53E{-}04$ +/-71%	$6.06E{-}04$ +/-8%	0.75	0.61	0.67	0.35
34.73	$4.57E{-}04$ +/-72%	$4.76E{-}04$ +/-8%	0.96	0.86	0.89	0.46
44.80	$1.58E{-}04$ +/-221%	$3.78E{-}04$ +/-7%	0.42	0.40	0.39	0.22
54.92	$6.70E{-}04$ +/-53%	$3.23E{-}04$ +/-7%	2.08	2.03	1.95	1.21
mean % diff. from E			37	88	57	107
mean χ^2			4.01	20.60	8.09	15.75

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	4.30	17%	-



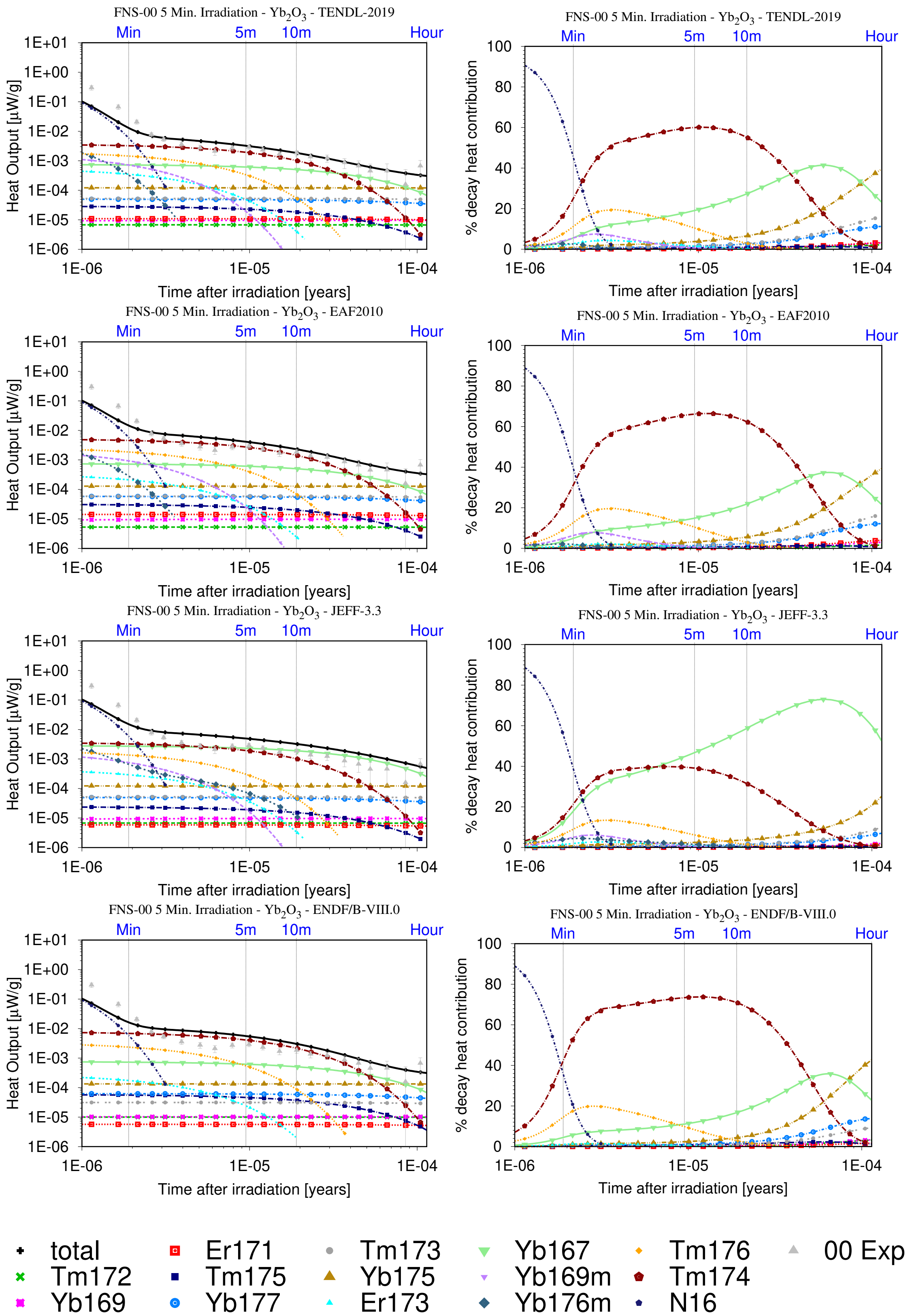
Ytterbium, TENDL-2019 5-minute pathway analysis

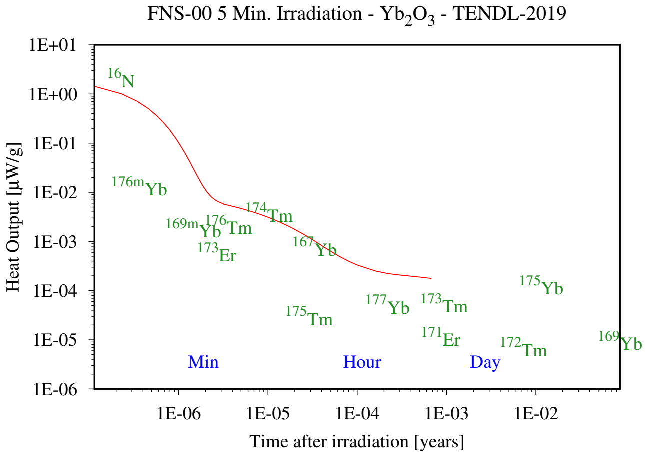
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Yb176m	11.40s	Yb176(n,n′)Yb176m	100.0
Yb169m	46.00s	Yb170(n,2n)Yb169m	98.8
Er173	1.40m	Yb176(n,α)Er173	100.0
Tm176	1.90m	Yb176(n,p)Tm176	100.0
Tm174	5.40m	Yb174(n,p)Tm174	99.7
Tm175	15.17m	Yb176(n,d)Tm175	80.6
		Yb176(n,np)Tm175	19.4
Yb167	17.50m	Yb168(n,2n)Yb167	100.0
Yb177	1.91h	Yb176(n,γ)Yb177	72.0
		Yb176(n,γ)Yb177m(IT)Yb177	28.0
Er171	7.52h	Yb174(n,α)Er171	100.0
Tm173	8.24h	Yb173(n,p)Tm173	94.6
		Yb176(n,α)Er173(β^-)Tm173	2.4
		Yb174(n,d)Tm173	2.1
Tm172	2.65d	Yb172(n,p)Tm172	90.7
		Yb173(n,d)Tm172	5.4
		Yb173(n,np)Tm172	3.7
Yb175	4.18d	Yb176(n,2n)Yb175	98.4
		Yb174(n,γ)Yb175	1.6
Yb169	32.01d	Yb170(n,2n)Yb169	77.2
		Yb170(n,2n)Yb169m(IT)Yb169	20.1
		Yb168(n,γ)Yb169	2.0

Comments on Ytterbium 5-minute experiments:

The best agreement here is seen with TENDL-2019 simulations, followed by EAF2010 – both give nice agreement to the experimental profile, even allowing for the large experimental uncertainties beyond 20 minutes of cooling (the low χ^2 deviations demonstrate this). ENDF/B-VIII.0 and JEFF-3.3 overpredict, but for different reasons; ENDF/B-VIII.0 over-produces the short-lived Tm174 nuclide (via (n,p) reactions) and so is wrong in the 1-10 minute cooling phase. Meanwhile, results of Tm174 production with JEFF-

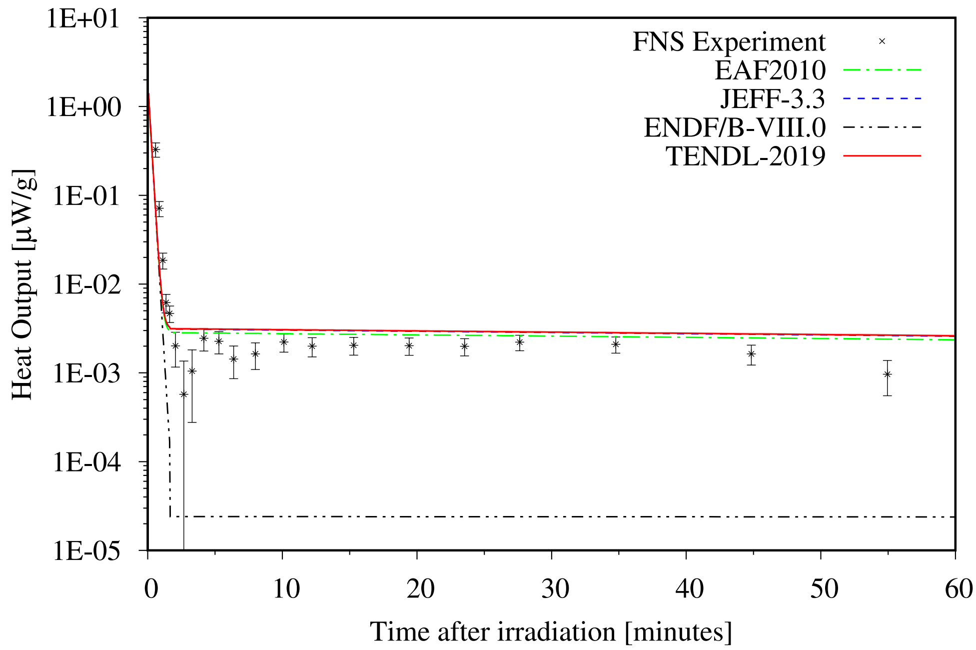
3.3 look reasonable, whereas over-production of the Yb167 nuclide (via (n,2n) on Yb168) is apparent, causing an overprediction beyond 10 minutes of cooling.


FNS-00 5 Min. Irradiation - Yb_2O_3 - TENDL-2019
FNS-00 5 Min. Irradiation - Yb_2O_3 - EAF2010
FNS-00 5 Min. Irradiation - Yb_2O_3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Yb_2O_3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Tm172
Yb169
Er171
Tm175
Yb177
Tm173
Yb175
Er173
Yb167
Yb169m
Yb176m
Tm176
Tm174
N16
00 Exp


FNS-00 5 Min. Irradiation - Yb2O3 - TENDL-2019
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
Heat Output [μW/g]
16N
176mYb
169mYb
176Tm
173Er
174Tm
167Yb
175Tm
177Yb
173Tm
171Er
175Yb
172Tm
169Yb
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

Lutetium

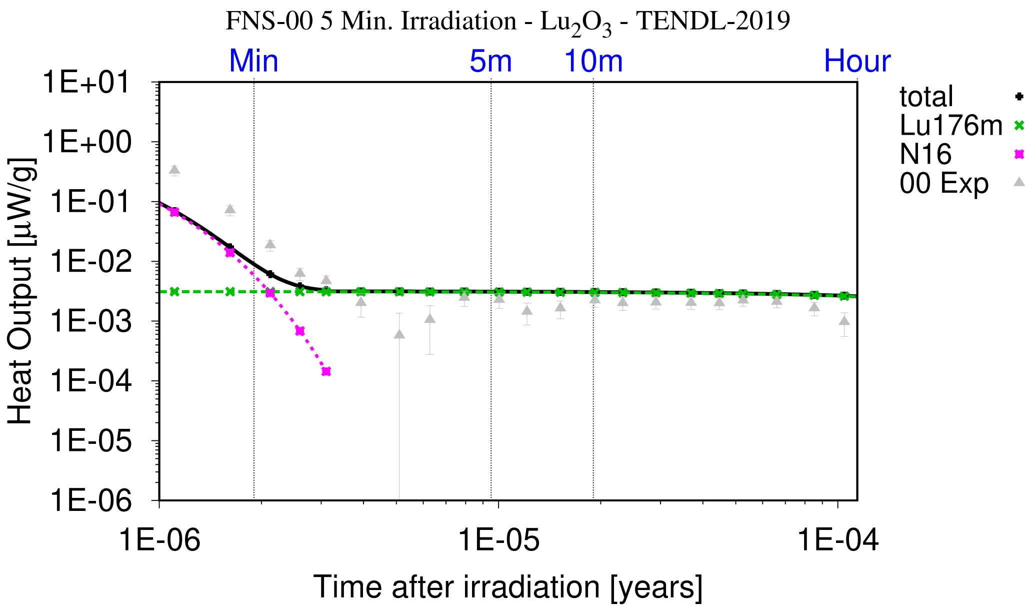
FNS-00 5 Min. Irradiation - Lu_2O_3



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	3.29$E-$01 +/-18%	6.93$E-$02 +/-0%	4.75	5.00	4.86	4.75
0.85	7.14$E-$02 +/-19%	1.71$E-$02 +/-1%	4.17	5.13	4.32	4.18
1.12	1.86$E-$02 +/-20%	6.08$E-$03 +/-2%	3.05	6.28	3.26	3.06
1.37	6.19$E-$03 +/-24%	3.82$E-$03 +/-2%	1.62	8.65	1.77	1.63
1.63	4.67$E-$03 +/-21%	3.29$E-$03 +/-3%	1.42	26.80	1.57	1.43
2.07	2.01$E-$03 +/-42%	3.14$E-$03 +/-3%	0.64	83.70	0.71	0.65
2.68	5.73$E-$04 +/-137%	3.13$E-$03 +/-3%	0.18	23.84	0.20	0.18
3.30	1.05$E-$03 +/-74%	3.13$E-$03 +/-3%	0.33	43.50	0.37	0.34
4.17	2.45$E-$03 +/-28%	3.12$E-$03 +/-3%	0.79	101.95	0.87	0.79
5.28	2.27$E-$03 +/-28%	3.11$E-$03 +/-3%	0.73	94.52	0.81	0.74
6.38	1.43$E-$03 +/-40%	3.10$E-$03 +/-3%	0.46	59.58	0.51	0.47
8.00	1.63$E-$03 +/-33%	3.08$E-$03 +/-3%	0.53	68.00	0.59	0.54
10.12	2.23$E-$03 +/-23%	3.06$E-$03 +/-3%	0.73	92.75	0.81	0.73
12.22	2.00$E-$03 +/-24%	3.04$E-$03 +/-3%	0.66	83.33	0.73	0.66
15.30	2.05$E-$03 +/-23%	3.01$E-$03 +/-3%	0.68	85.32	0.75	0.69
19.42	2.02$E-$03 +/-22%	2.97$E-$03 +/-3%	0.68	84.29	0.75	0.69
23.53	1.99$E-$03 +/-22%	2.94$E-$03 +/-3%	0.68	82.96	0.75	0.68
27.63	2.21$E-$03 +/-20%	2.90$E-$03 +/-3%	0.76	92.44	0.85	0.77
34.77	2.10$E-$03 +/-21%	2.83$E-$03 +/-3%	0.74	87.73	0.82	0.75
44.83	1.64$E-$03 +/-25%	2.75$E-$03 +/-3%	0.60	68.53	0.66	0.60
54.95	9.65$E-$04 +/-43%	2.66$E-$03 +/-3%	0.36	40.43	0.40	0.37
mean % diff. from E			86	95	72	84
mean χ^2			6.54	14.16	5.04	6.37

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
N16	7.13s	4.75	18%	-
Lu176m	3.63h	1.62	24%	3%

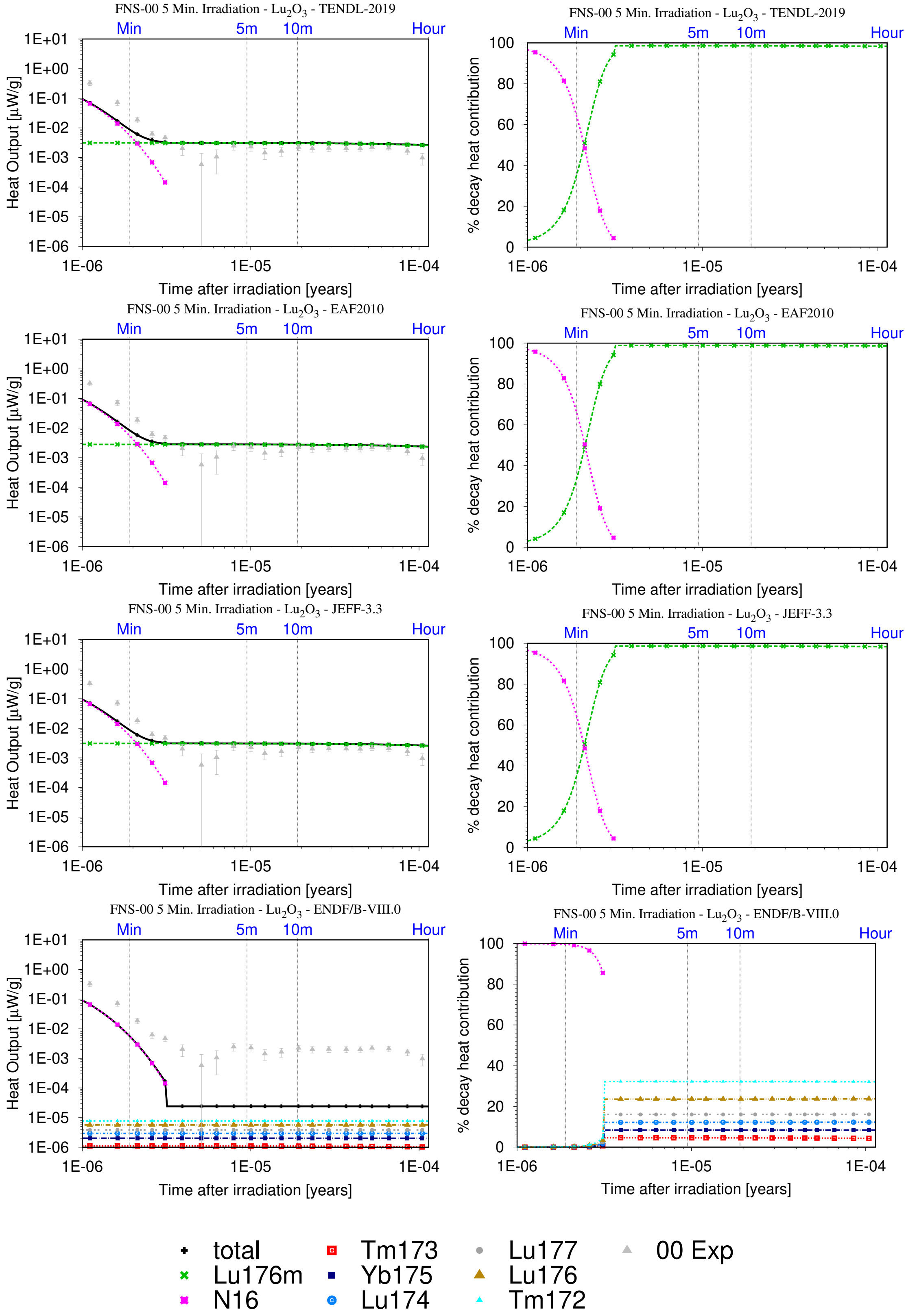


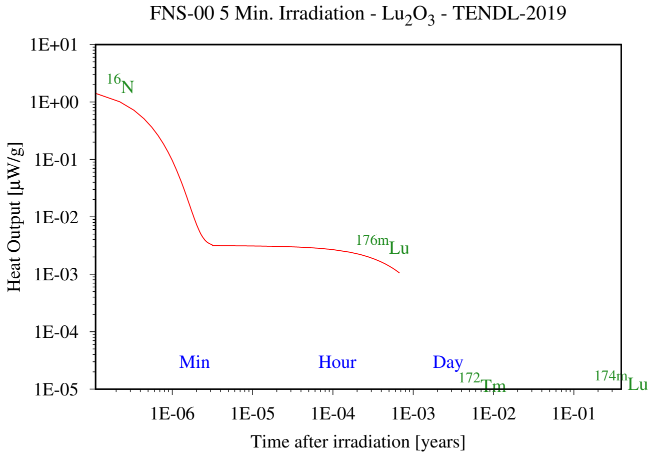
Lutetium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Lu176m	3.63h	Lu175(n,γ)Lu176m	90.2
		Lu176(n,n$'$)Lu176m	9.8
Tm173	8.24h	Lu176(n,α)Tm173	100.0
Tm172	2.65d	Lu175(n,α)Tm172	99.9
Yb175	4.18d	Lu175(n,p)Yb175	99.4
Lu177	6.65d	Lu176(n,γ)Lu177	100.0
Lu174	3.56y	Lu175(n,2n)Lu174	99.9
Lu176	4.0 10^{10}y	no pathways found	

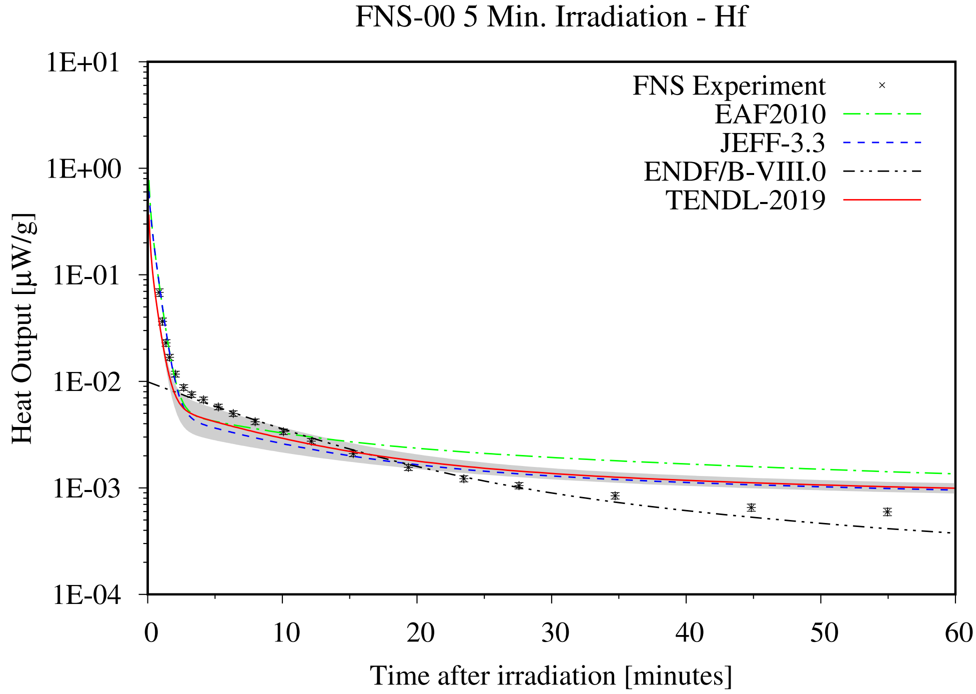
Comments on Lutetium 5-minute experiments:

There is some structure in the experimental results that are not captured by the simulations, particularly below 5 minutes of cooling – the high quoted uncertainties suggest that there may have been problems in the experiment (such as an incorrect level of tape subtraction). ENDF/B-VIII.0 does not include the reaction channels to produce the Lu176m metastable that the other libraries predict to provide almost the entirety of the decay heat from Lutetium itself. This is clearly discrepant as the profile with the other libraries is a reasonable match to the experiment, although they mostly overpredict. There could be a justifiable need to correct one of the identified channels for Lu176m production. Notice that the absence of Lu176m production with ENDF/B, causes the identification of many minor nuclides (that are thus included in the pathway analysis), which otherwise are not important for the simulations with other libraries.


FNS-00 5 Min. Irradiation - Lu2O3 - TENDL-2019
FNS-00 5 Min. Irradiation - Lu2O3 - EAF2010
FNS-00 5 Min. Irradiation - Lu2O3 - JEFF-3.3
FNS-00 5 Min. Irradiation - Lu2O3 - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Lu176m
N16
Tm173
Yb175
Lu174
Lu177
Lu176
Tm172
00 Exp


FNS-00 5 Min. Irradiation - Lu2O3 - TENDL-2019
Heat Output [μW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
176mLu
Min
Hour
Day
172Tm
174mLu
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]

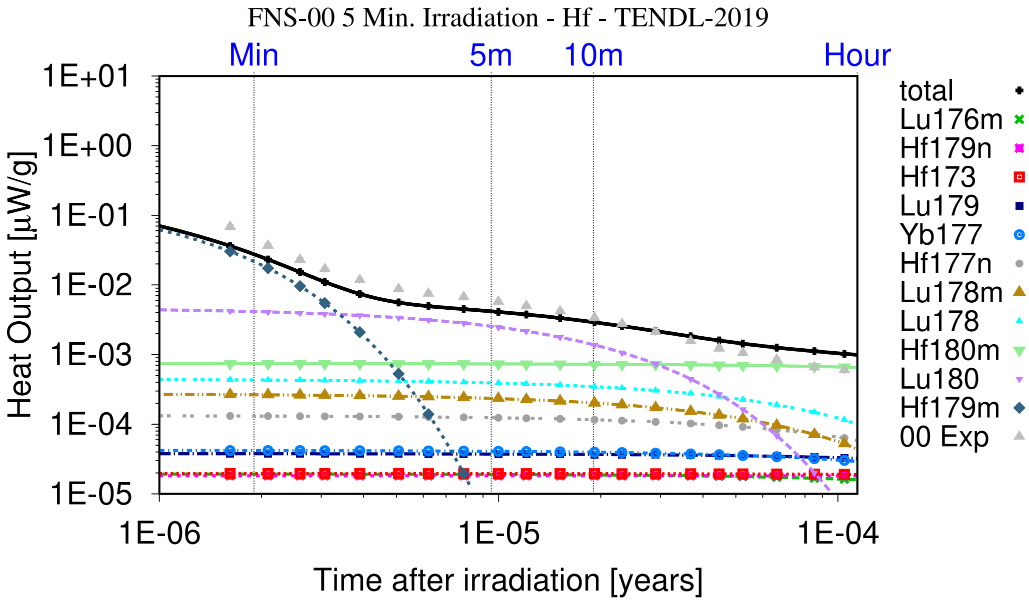
Hafnium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	6.84E−02 +/-8%	3.64E−02 +/-9%	1.88	7.58	0.83	0.83
1.10	3.65E−02 +/-8%	2.32E−02 +/-11%	1.57	4.16	0.74	0.74
1.37	2.30E−02 +/-7%	1.53E−02 +/-15%	1.50	2.70	0.78	0.78
1.62	1.68E−02 +/-7%	1.11E−02 +/-19%	1.52	2.03	0.88	0.90
2.05	1.17E−02 +/-6%	7.44E−03 +/-27%	1.57	1.48	1.13	1.18
2.67	8.75E−03 +/-6%	5.60E−03 +/-33%	1.56	1.18	1.42	1.53
3.27	7.51E−03 +/-6%	4.96E−03 +/-34%	1.51	1.08	1.50	1.66
4.15	6.71E−03 +/-6%	4.50E−03 +/-34%	1.49	1.05	1.50	1.71
5.25	5.76E−03 +/-6%	4.10E−03 +/-33%	1.40	1.01	1.39	1.61
6.35	4.99E−03 +/-6%	3.77E−03 +/-31%	1.32	0.98	1.28	1.51
7.98	4.18E−03 +/-6%	3.35E−03 +/-29%	1.25	0.96	1.16	1.41
10.08	3.37E−03 +/-6%	2.91E−03 +/-26%	1.16	0.95	1.03	1.30
12.15	2.75E−03 +/-6%	2.57E−03 +/-24%	1.07	0.93	0.91	1.19
15.27	2.10E−03 +/-6%	2.18E−03 +/-20%	0.96	0.92	0.78	1.06
19.37	1.55E−03 +/-6%	1.83E−03 +/-16%	0.85	0.94	0.65	0.92
23.48	1.22E−03 +/-7%	1.60E−03 +/-14%	0.76	0.96	0.56	0.82
27.58	1.05E−03 +/-7%	1.44E−03 +/-12%	0.73	1.04	0.52	0.77
34.72	8.44E−04 +/-7%	1.26E−03 +/-11%	0.67	1.15	0.47	0.70
44.83	6.53E−04 +/-8%	1.12E−03 +/-11%	0.58	1.23	0.41	0.61
54.95	5.96E−04 +/-8%	1.03E−03 +/-11%	0.58	1.44	0.42	0.60
mean % diff. from E			33	22	46	30
mean χ^2			28.06	20.60	74.47	24.47

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Hf179m	18.67s	1.88	8%	7%

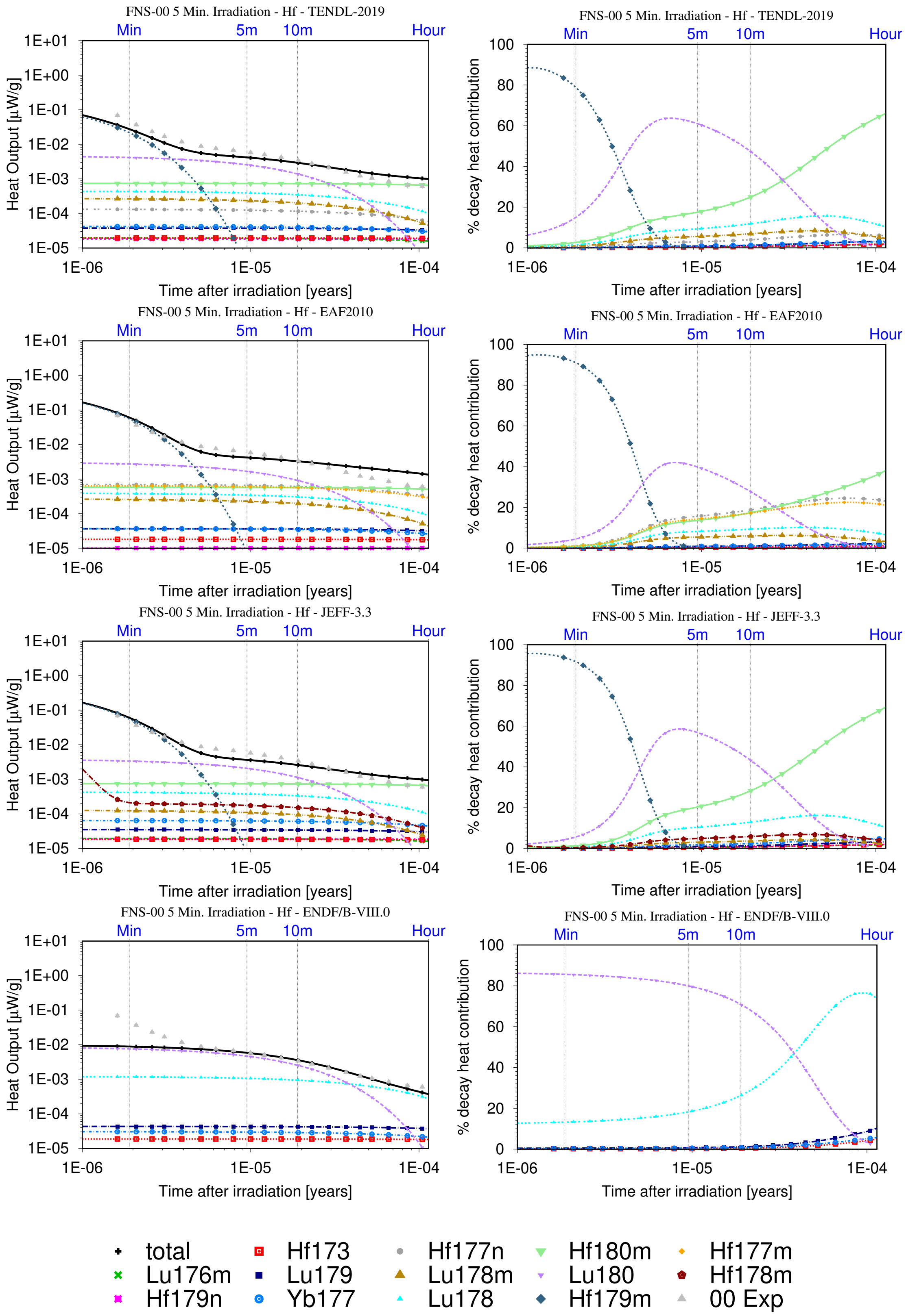

FNS-00 5 Min. Irradiation - Hf - TENDL-2019
Min
5m
10m
Hour
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
Heat Output [µW/g]
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Lu176m
Hf179n
Hf173
Lu179
Yb177
Hf177n
Lu178m
Lu178
Hf180m
Lu180
Hf179m
00 Exp

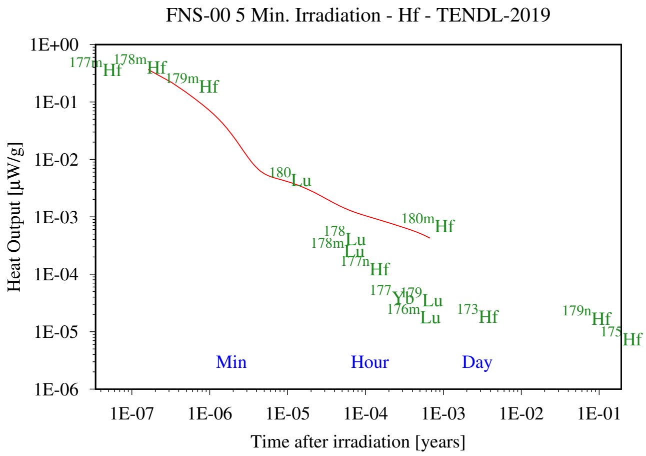
Hafnium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Hf177m	1.08s	Hf178(n,2n)Hf177m	89.8
		Hf177(n,n′)Hf177m	10.0
Hf178m	4.00s	Hf179(n,2n)Hf178m	77.1
		Hf178(n,n′)Hf178m	20.2
		Hf180(n,3n)Hf178m	1.6
		Hf177(n,γ)Hf178m	1.2
Hf179m	18.67s	Hf180(n,2n)Hf179m	83.8
		Hf179(n,n′)Hf179m	9.3
		Hf178(n,γ)Hf179m	6.9
Lu180	5.70m	Hf180(n,p)Lu180	100.0
Lu178m	23.10m	Hf178(n,p)Lu178m	77.1
		Hf179(n,d)Lu178m	13.7
		Hf179(n,np)Lu178m	8.1
		Hf180(n,t)Lu178m	1.2
Lu178	28.40m	Hf178(n,p)Lu178	94.7
		Hf179(n,d)Lu178	3.4
		Hf179(n,np)Lu178	1.5
Hf177n	51.39m	Hf177(n,n′)Hf177n	90.9
		Hf178(n,2n)Hf177n	6.6
		Hf176(n,γ)Hf177n	2.5
Yb177	1.91h	Hf180(n,α)Yb177	92.8
		Hf180(n,α)Yb177m(IT)Yb177	7.2
Lu176m	3.63h	Hf176(n,p)Lu176m	73.5
		Hf177(n,d)Lu176m	16.2
		Hf177(n,np)Lu176m	9.1
		Hf178(n,t)Lu176m	1.2
Lu179	4.59h	Hf179(n,p)Lu179	89.5
		Hf180(n,d)Lu179	6.5
		Hf180(n,np)Lu179	4.0
Hf180m	5.50h	Hf180(n,n′)Hf180m	98.1
		Hf179(n,γ)Hf180m	1.9
Hf173	23.90h	Hf174(n,2n)Hf173	100.0
Hf179n	25.10d	Hf180(n,2n)Hf179n	90.1
		Hf179(n,n′)Hf179n	9.8

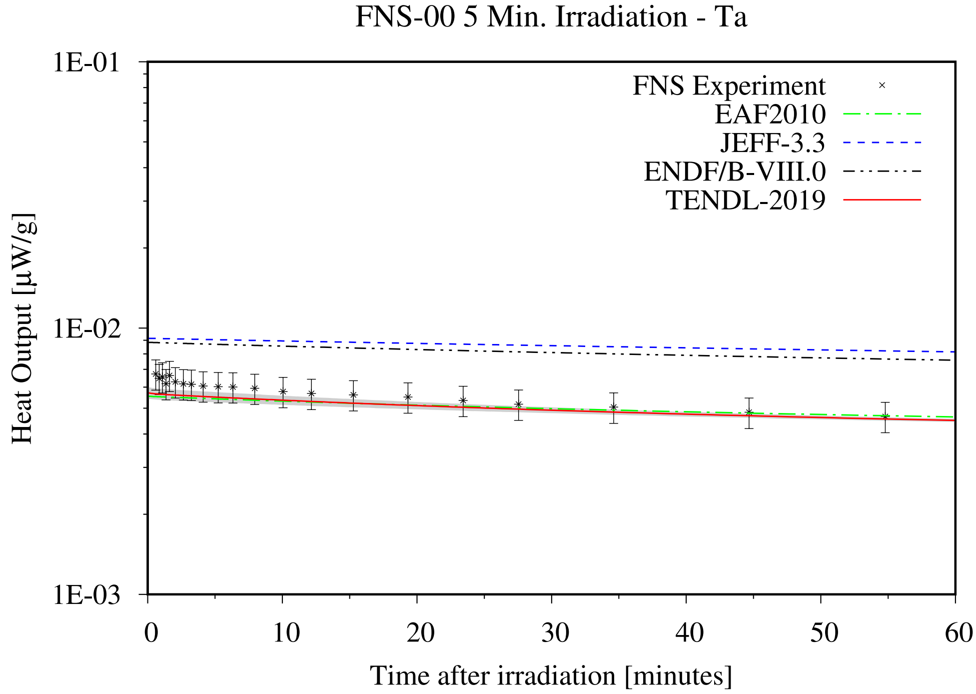
Comments on Hafnium 5-minute experiments:

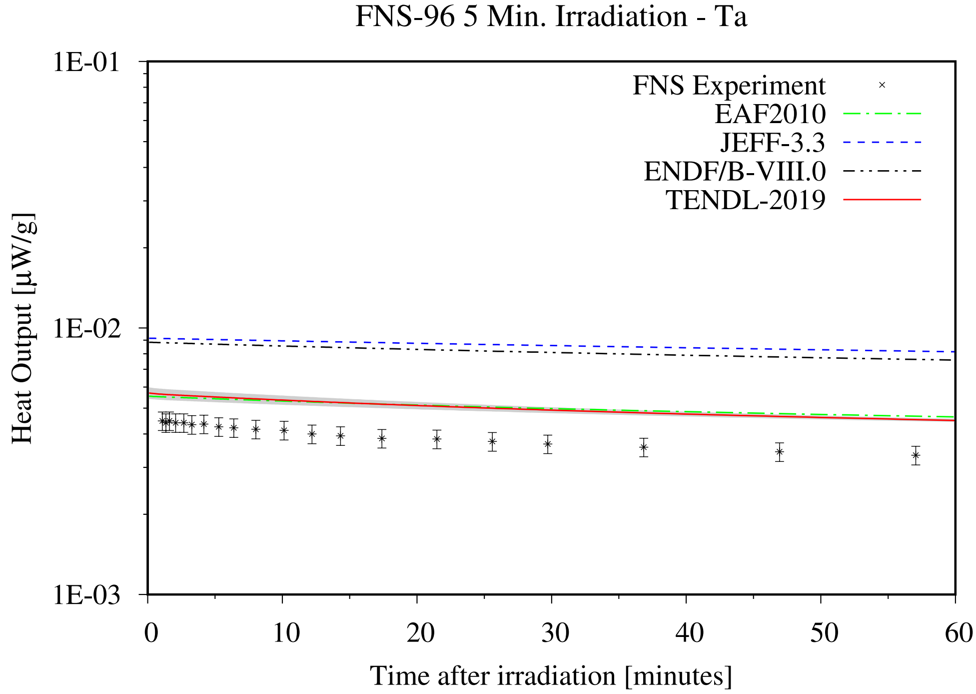
The predicted contribution from Hf179m in the first ~2 minutes of cooling is a good fit to the experiment in simulations with EAF2010 and JEFF-3.3 – ENDF/B-VIII.0 fails to capture the production of this nuclide from a combination of Hf180(n,2n) and Hf178(n,γ), while TENDL-2019 seems to underpredict compared to the better result seen with TENDL-2017. At longer cooling times none of the simulated profiles is a good match for the shape of the decay evolution. One possibility, in examining the nuclide contribution charts of TENDL and EAF, is that a greater production of Lu180 could provide a closer match to the experiment between 2 and around 15 minutes of cooling, while a reduction in Hf180m would solve the overprediction at later cooling times and leave the Lu178 to dominate, whose profile seems to better fit the decay profile in the experiment for the last few cooling steps. A careful reassessment of the Hf180(n,p), Hf180(n,n′) reaction channels for the production of Lu180 and Hf180m, respectively, is advised.


FNS-00 5 Min. Irradiation - Hf - TENDL-2019
FNS-00 5 Min. Irradiation - Hf - EAF2010
FNS-00 5 Min. Irradiation - Hf - JEFF-3.3
FNS-00 5 Min. Irradiation - Hf - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Hf173
Hf177n
Hf180m
Hf177m
Lu176m
Lu179
Lu178m
Lu180
Hf178m
Hf179n
Yb177
Lu178
Hf179m
00 Exp


FNS-00 5 Min. Irradiation - Hf - TENDL-2019
Heat Output [µW/g]
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
177mHf
178mHf
179mHf
180Lu
180mHf
178Lu
178mLu
177nHf
177Yb
179Lu
176mLu
173Hf
179nHf
175Hf
Min
Hour
Day

Tantalum

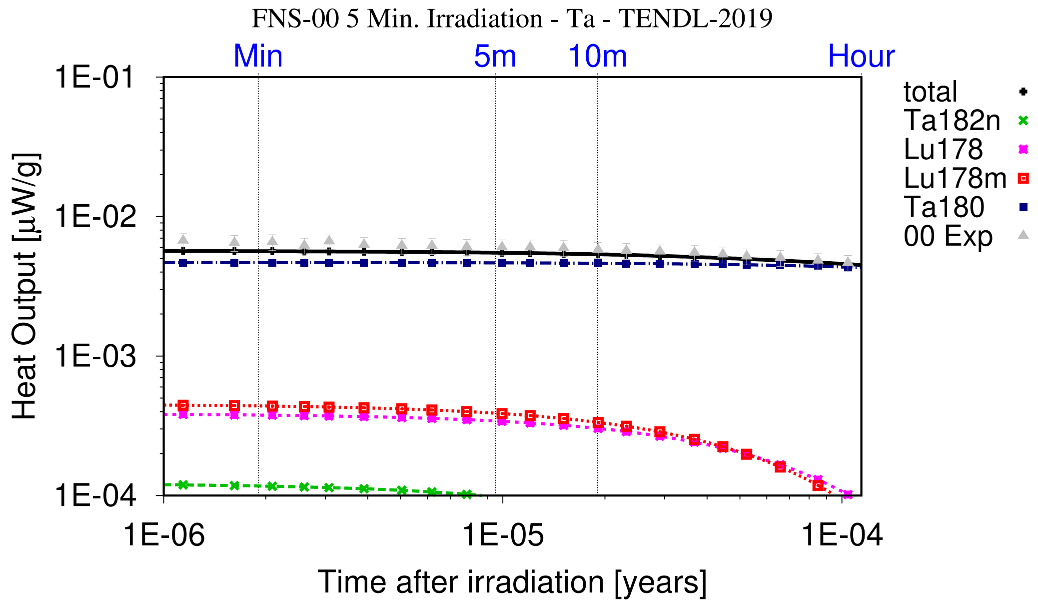

FNS-00 5 Min. Irradiation - Ta
1E-01
1E-02
1E-03
Heat Output [µW/g]
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019


FNS-96 5 Min. Irradiation - Ta
1E-01
1E-02
1E-03
Heat Output [µW/g]
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.60	6.72E−03 +/-13%	5.66E−03 +/-5%	1.19	0.76	1.22	0.74
0.85	6.47E−03 +/-13%	5.65E−03 +/-5%	1.14	0.73	1.17	0.71
1.10	6.56E−03 +/-13%	5.64E−03 +/-5%	1.16	0.74	1.19	0.72
1.37	6.18E−03 +/-13%	5.63E−03 +/-5%	1.10	0.70	1.12	0.68
1.62	6.64E−03 +/-13%	5.62E−03 +/-5%	1.18	0.76	1.21	0.73
2.05	6.28E−03 +/-13%	5.60E−03 +/-5%	1.12	0.72	1.14	0.69
2.65	6.17E−03 +/-13%	5.58E−03 +/-5%	1.11	0.70	1.13	0.68
3.25	6.15E−03 +/-13%	5.56E−03 +/-5%	1.11	0.70	1.13	0.68
4.12	6.06E−03 +/-13%	5.54E−03 +/-4%	1.09	0.70	1.11	0.67
5.23	6.02E−03 +/-13%	5.50E−03 +/-4%	1.09	0.69	1.11	0.67
6.33	6.01E−03 +/-13%	5.47E−03 +/-4%	1.10	0.69	1.11	0.67
7.95	5.94E−03 +/-13%	5.42E−03 +/-4%	1.10	0.69	1.11	0.66
10.05	5.77E−03 +/-13%	5.36E−03 +/-4%	1.08	0.67	1.09	0.65
12.17	5.68E−03 +/-13%	5.30E−03 +/-4%	1.07	0.67	1.08	0.64
15.28	5.62E−03 +/-13%	5.23E−03 +/-4%	1.07	0.67	1.08	0.63
19.33	5.51E−03 +/-13%	5.13E−03 +/-3%	1.07	0.66	1.07	0.63
23.43	5.35E−03 +/-13%	5.04E−03 +/-3%	1.06	0.65	1.05	0.61
27.55	5.18E−03 +/-13%	4.96E−03 +/-3%	1.04	0.64	1.03	0.60
34.62	5.05E−03 +/-13%	4.84E−03 +/-2%	1.04	0.63	1.03	0.59
44.67	4.83E−03 +/-13%	4.69E−03 +/-2%	1.03	0.62	1.01	0.58
54.78	4.66E−03 +/-13%	4.56E−03 +/-1%	1.02	0.61	0.99	0.57
mean % diff. from E			8	46	9	53
mean χ^2			0.50	13.05	0.63	17.36

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ta180	8.08h	1.19	13%	1%

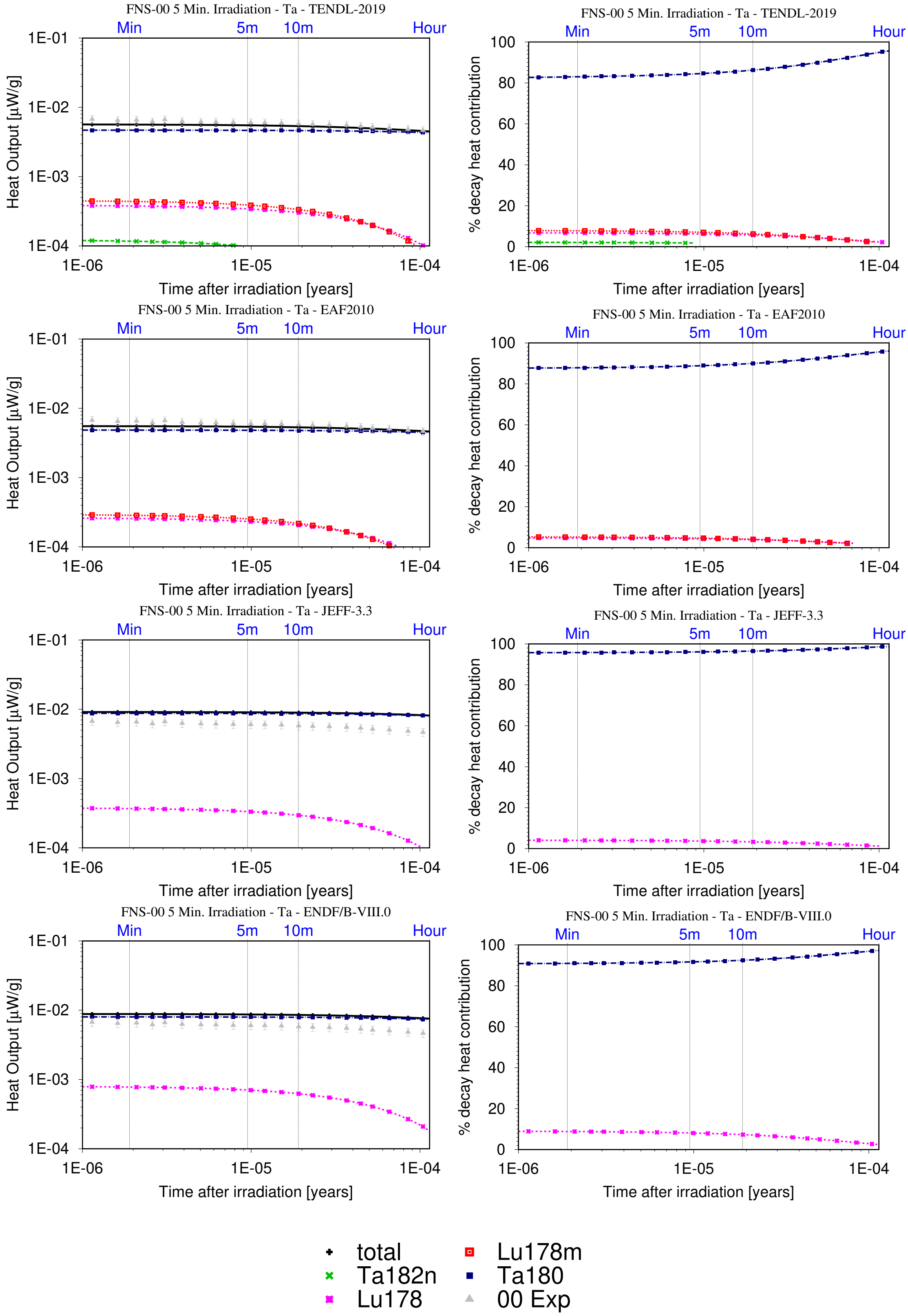


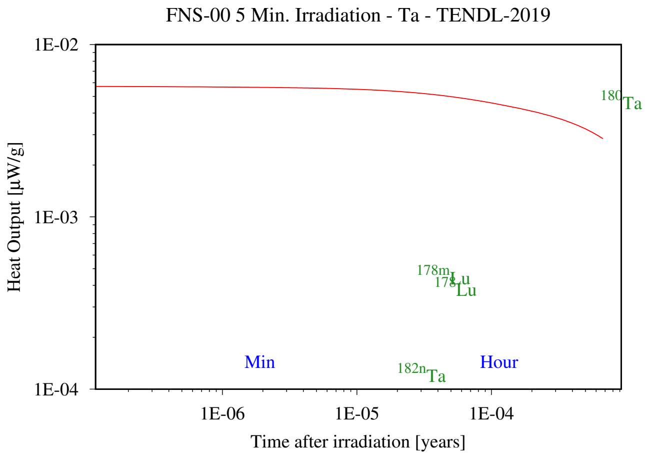
Tantalum, TENDL-2019 5-minute pathway analysis

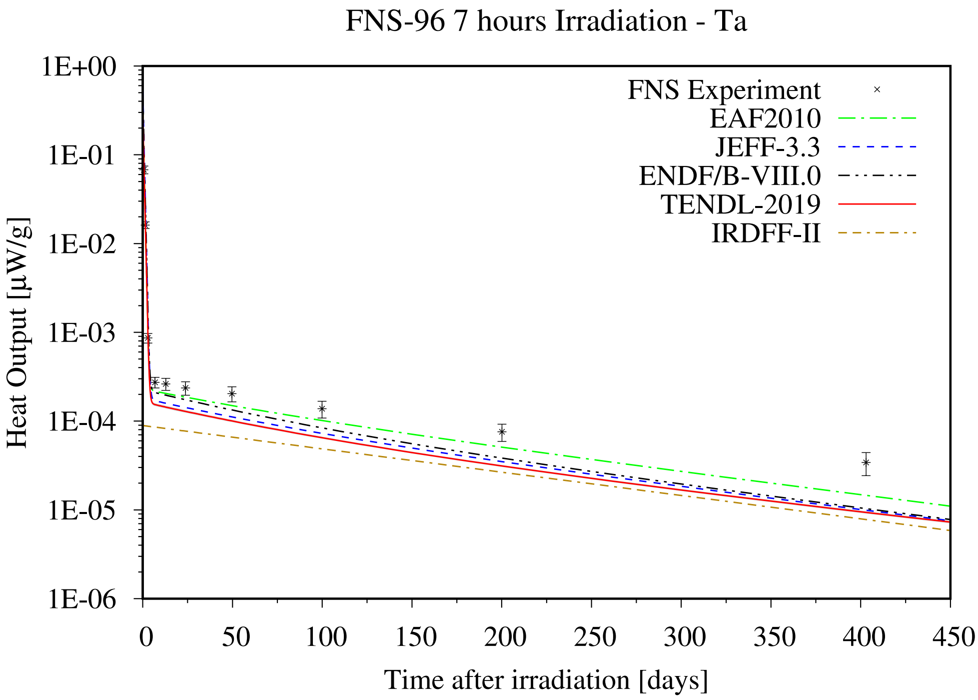
Product	$T_{1/2}$	Pathways	Path %
Ta182n	15.84m	Ta181(n,γ)Ta182n	100.0
Lu178m	23.10m	Ta181(n,α)Lu178m	100.0
Lu178	28.40m	Ta181(n,α)Lu178	100.0
Ta180	8.08h	Ta181(n,2n)Ta180	100.0

Comments on Tantalum 5-minute experiments:

There are some noticeable and unexplained differences between the decay heat levels of the two 5-minute experiments for tantalum. The fact that the code predictions with TENDL-2019 (and EAF2010) agree very well with the more recent 2000 experiment suggests that the experimental techniques may have been improved between 1996 and 2000 leading to the latter being more representative of reality. TENDL-2019 and EAF2010 are both within the (rather large) experimental uncertainty for the 2000 experiment, while ENDF/B-VIII.0 and JEFF-3.3 both overpredict the result by more than 40% on average. This is again a situation where these two libraries sum the contributions of (n,2n) channels. In this case ENDF/B-VIII.0 and JEFF-3.3 assume that all of the (n,2n) reactions on Ta182 produce the unstable, short-lived ground-state Ta180, while in fact around half should have produced the stable Ta180m "metastable", which does not contribute to decay heat. This is a glaring error because the stability of Ta180m is such an unusual and well-known anomaly that it should have been easy to get this correct.


FNS-00 5 Min. Irradiation - Ta - TENDL-2019
FNS-00 5 Min. Irradiation - Ta - EAF2010
FNS-00 5 Min. Irradiation - Ta - JEFF-3.3
FNS-00 5 Min. Irradiation - Ta - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
1E-01
1E-02
1E-03
1E-04
0
20
40
60
80
100
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Ta182n
Lu178
Lu178m
Ta180
00 Exp

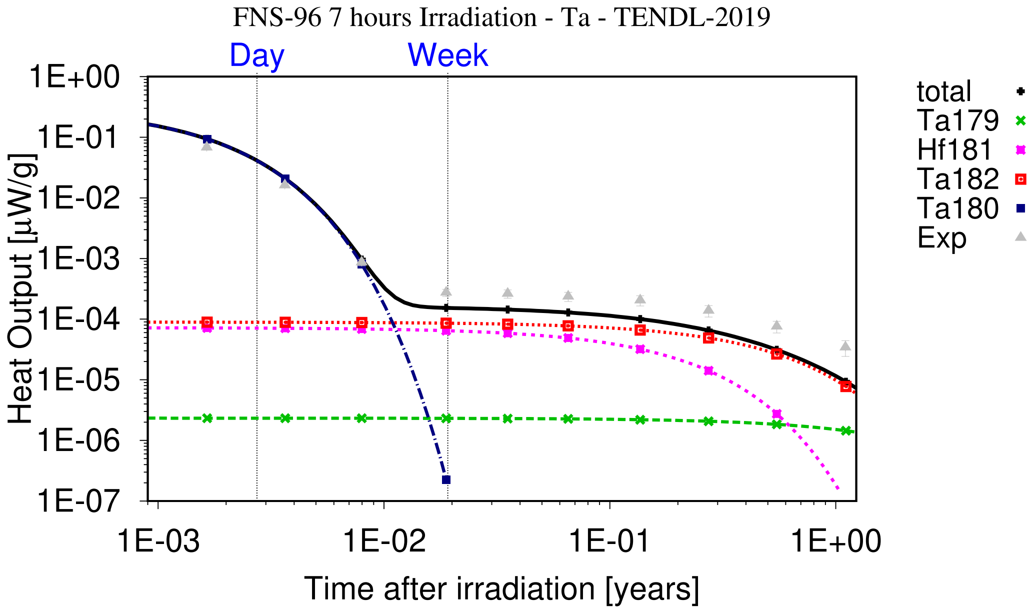

FNS-00 5 Min. Irradiation - Ta - TENDL-2019
Heat Output [µW/g]
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
Time after irradiation [years]
180Ta
178mLu
178Lu
182nTa
Min
Hour



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Days	μW/g	μW/g	E/C	E/C	E/C	E/C	E/C
0.60	$6.79E{-}02$ +/-10%	$9.37E{-}02$ +/-1%	0.72	0.43	0.71	0.40	764.45
1.33	$1.62E{-}02$ +/-9%	$2.09E{-}02$ +/-1%	0.77	0.45	0.76	0.42	182.77
2.91	$8.64E{-}04$ +/-12%	$9.61E{-}04$ +/-1%	0.90	0.53	0.83	0.53	9.87
6.88	$2.73E{-}04$ +/-14%	$1.53E{-}04$ +/-3%	1.78	1.30	1.26	1.61	3.20
12.88	$2.63E{-}04$ +/-15%	$1.44E{-}04$ +/-3%	1.83	1.34	1.28	1.65	3.18
23.88	$2.36E{-}04$ +/-17%	$1.29E{-}04$ +/-3%	1.84	1.36	1.27	1.66	3.06
49.72	$2.04E{-}04$ +/-19%	$1.00E{-}04$ +/-3%	2.03	1.53	1.36	1.83	3.09
99.91	$1.38E{-}04$ +/-21%	$6.50E{-}05$ +/-3%	2.12	1.64	1.36	1.89	2.83
200.13	$7.57E{-}05$ +/-22%	$3.12E{-}05$ +/-2%	2.42	1.98	1.49	2.16	2.85
402.97	$3.42E{-}05$ +/-29%	$9.28E{-}06$ +/-3%	3.69	3.35	2.38	3.49	4.44
mean % diff. from E			45	61	30	71	77
mean χ^2			7.92	45.35	4.91	57.49	38.31

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Ta180	8.08h	0.72	10%	1%
Ta182	114.71d	2.12	21%	3%

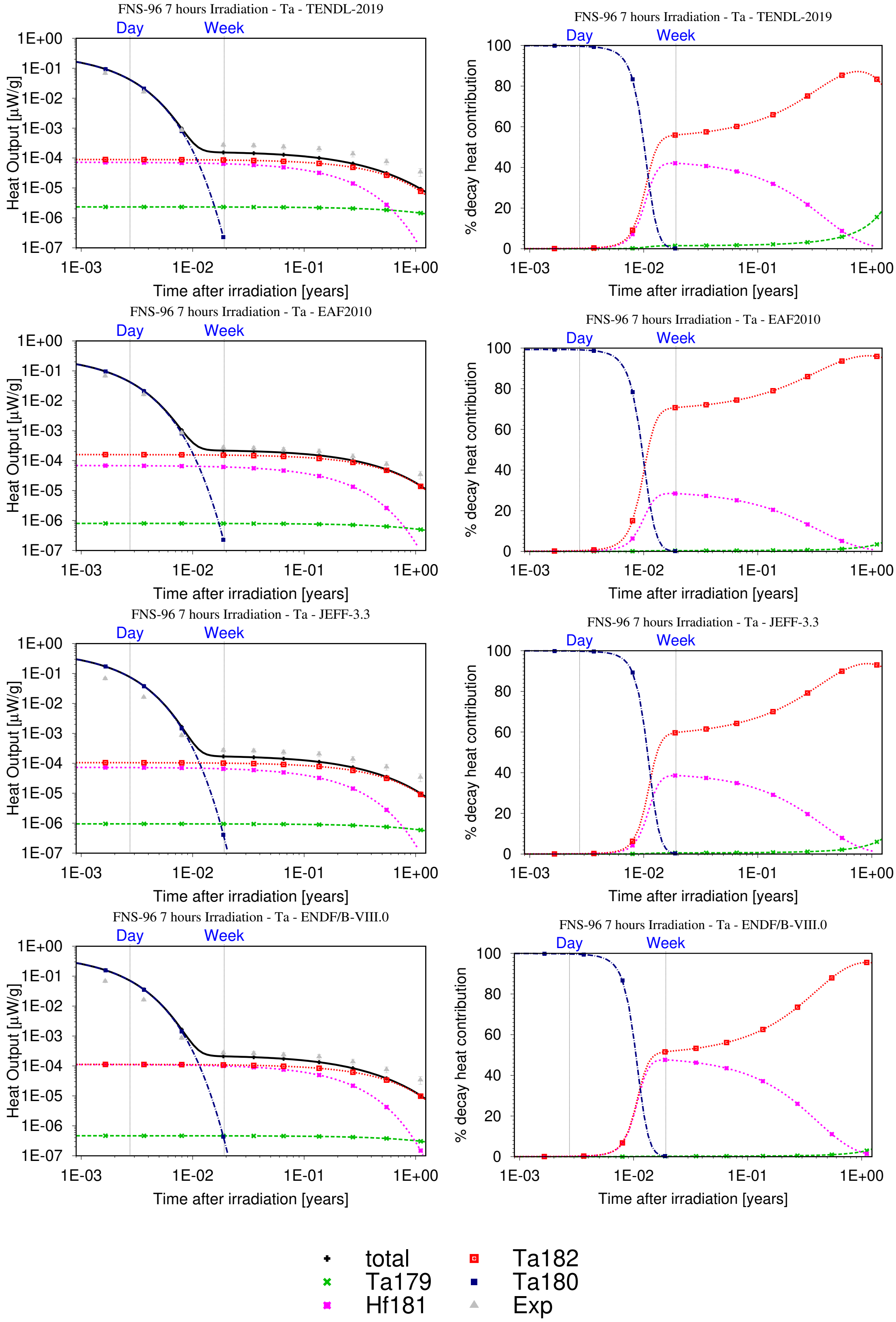


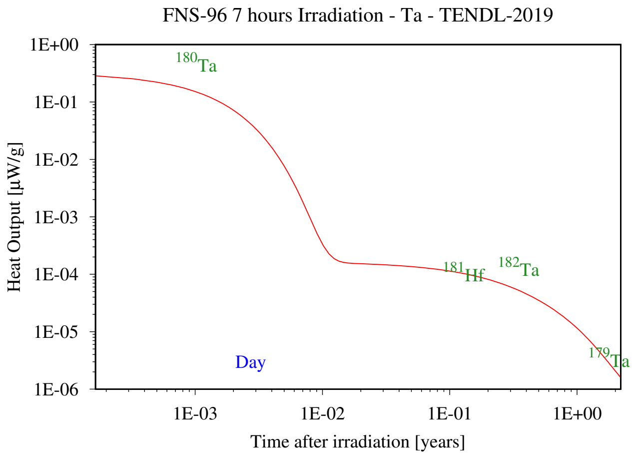
Tantalum,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Ta180	8.08h	Ta181(n,2n)Ta180	100.0
Hf181	42.38d	Ta181(n,p)Hf181	100.0
Ta182	114.71d	Ta181(n,γ)Ta182	55.9
		Ta181(n,γ)Ta182m(IT)Ta182	41.4
		Ta181(n,γ)Ta182n(IT)Ta182m(IT)Ta182	2.7
Ta179	1.61y	Ta181(n,3n)Ta179	99.2

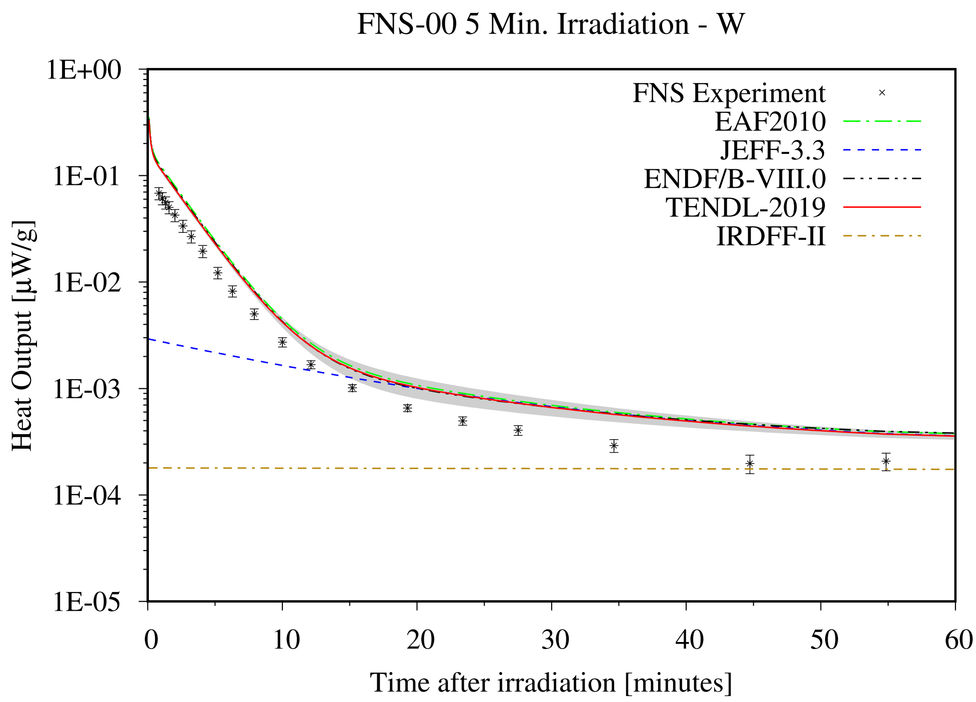
Comments on Tantalum 7-hour experiments:

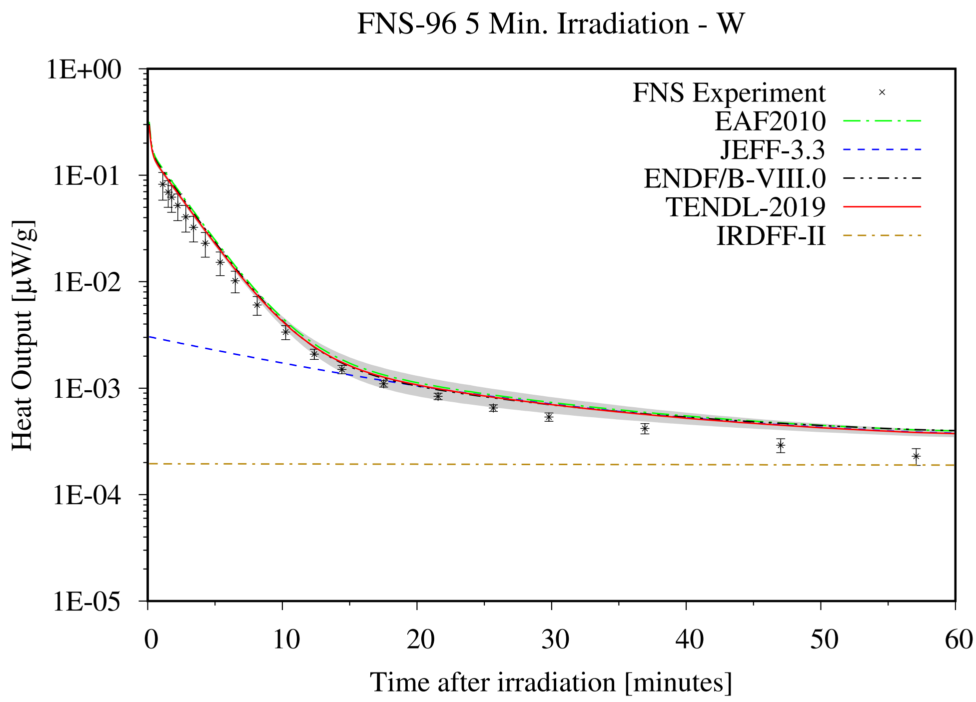
The decay profile seems properly shaped by first the heat from Ta180 at cooling times less than 3 days, and then contributions from Hf181 and predominantly Ta182 at later times. However, the Ta180 production seems to overestimate the experiment, while a 50% or more underprediction is evident at later cooling times. Potentially, both the (n,2n) and neutron capture channels on Ta181 should be reassessed. IRDFF-II only includes the ground-state branch of the neutron capture reaction (whose evaluation is closer to TENDL in the MeV region) to Ta182, and so underpredicts to a greater extent than the other libraries.


FNS-96 7 hours Irradiation - Ta - TENDL-2019
FNS-96 7 hours Irradiation - Ta - EAF2010
FNS-96 7 hours Irradiation - Ta - JEFF-3.3
FNS-96 7 hours Irradiation - Ta - ENDF/B-VIII.0
Day
Week
Heat Output [μW/g]
% decay heat contribution
Time after irradiation [years]
1E-07
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
1E+00
0
20
40
60
80
100
total
Ta179
Hf181
Ta182
Ta180
Exp


FNS-96 7 hours Irradiation - Ta - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
180Ta
181Hf
182Ta
179Ta
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Tungsten

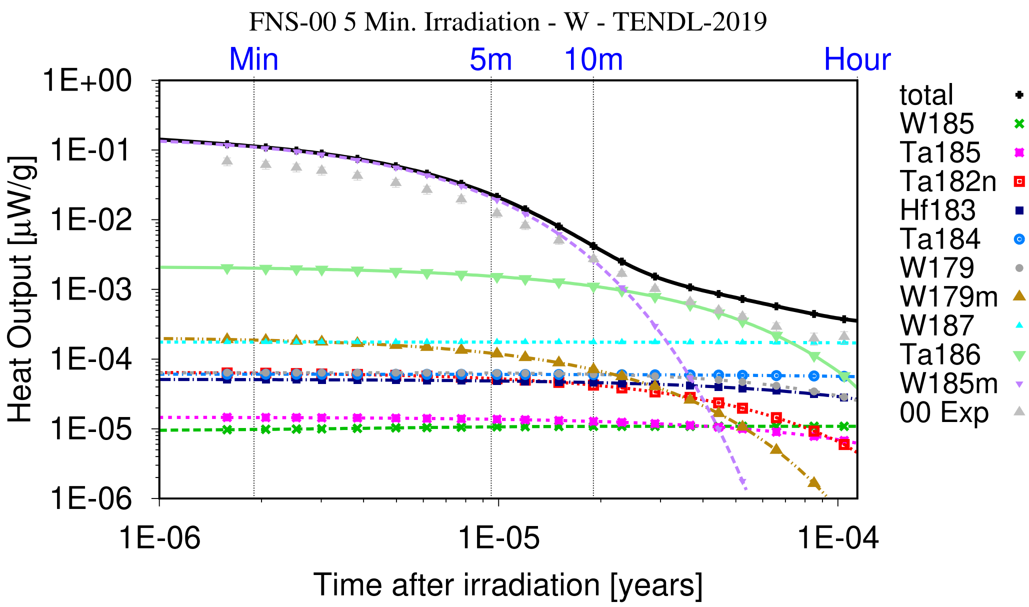

FNS-00 5 Min. Irradiation - W
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - W
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
Time after irradiation [minutes]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
0
10
20
30
40
50
60

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
0.83	6.83E−02 +/-13%	1.21E−01 +/-5%	0.56	0.55	0.52	24.52	380.56
1.08	6.11E−02 +/-13%	1.09E−01 +/-5%	0.56	0.54	0.52	22.29	340.80
1.33	5.57E−02 +/-13%	9.85E−02 +/-5%	0.57	0.55	0.53	20.63	310.79
1.58	5.03E−02 +/-13%	8.90E−02 +/-5%	0.56	0.55	0.53	18.90	280.44
2.02	4.25E−02 +/-13%	7.47E−02 +/-5%	0.57	0.55	0.53	16.39	237.05
2.62	3.36E−02 +/-13%	5.87E−02 +/-5%	0.57	0.56	0.53	13.44	187.63
3.23	2.67E−02 +/-13%	4.59E−02 +/-5%	0.58	0.57	0.54	11.09	149.29
4.08	1.95E−02 +/-13%	3.28E−02 +/-5%	0.59	0.58	0.55	8.49	108.82
5.20	1.22E−02 +/-12%	2.13E−02 +/-5%	0.57	0.56	0.53	5.68	68.26
6.30	8.22E−03 +/-12%	1.41E−02 +/-6%	0.58	0.57	0.54	4.07	45.94
7.92	5.02E−03 +/-11%	8.00E−03 +/-7%	0.63	0.61	0.59	2.72	28.05
10.02	2.73E−03 +/-10%	4.19E−03 +/-11%	0.65	0.64	0.61	1.66	15.26
12.13	1.68E−03 +/-9%	2.51E−03 +/-15%	0.67	0.67	0.63	1.14	9.39
15.20	1.01E−03 +/-8%	1.53E−03 +/-20%	0.66	0.67	0.63	0.80	5.69
19.30	6.55E−04 +/-8%	1.07E−03 +/-22%	0.61	0.62	0.58	0.63	3.68
23.40	4.96E−04 +/-9%	8.61E−04 +/-21%	0.58	0.58	0.55	0.57	2.80
27.52	4.05E−04 +/-11%	7.27E−04 +/-19%	0.56	0.56	0.53	0.55	2.29
34.63	2.91E−04 +/-14%	5.72E−04 +/-15%	0.51	0.50	0.49	0.50	1.65
44.73	1.97E−04 +/-20%	4.44E−04 +/-11%	0.44	0.43	0.42	0.44	1.12
54.85	2.08E−04 +/-19%	3.73E−04 +/-8%	0.56	0.52	0.53	0.55	1.19
mean % diff. from E			74	77	85	78	81
mean χ^2			38.49	41.19	50.93	42.69	58.00

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	**$T_{1/2}$**	**E/C**	**%ΔE**	**%ΔC^{nuc}**
W185m	1.67m	0.56	13%	5%

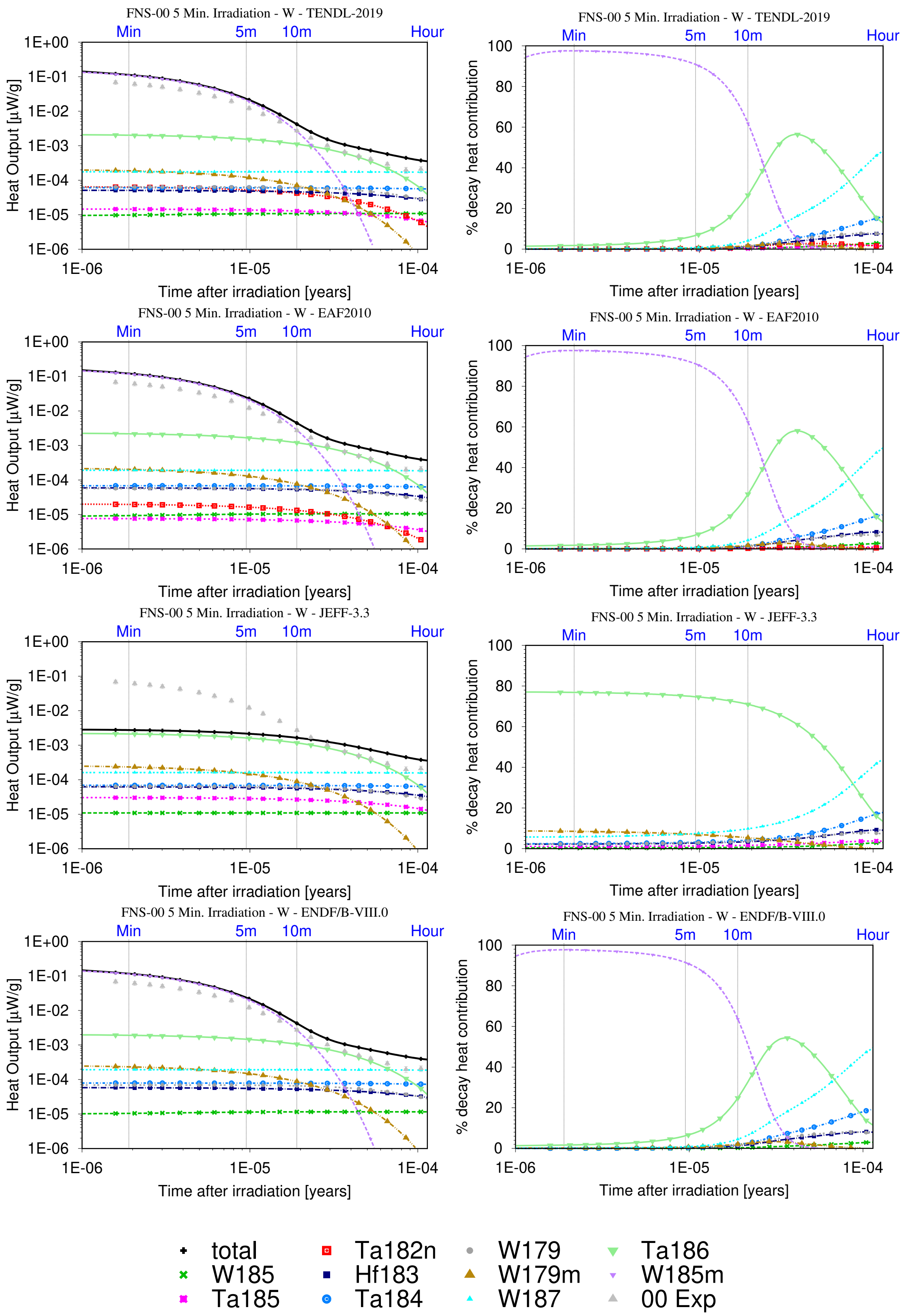


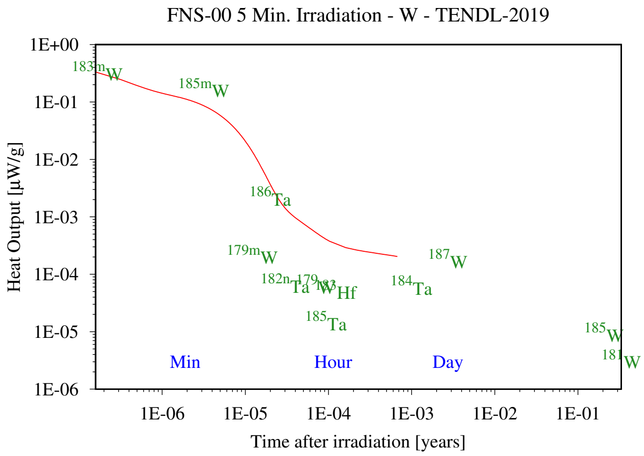
Tungsten, TENDL-2019 5-minute pathway analysis

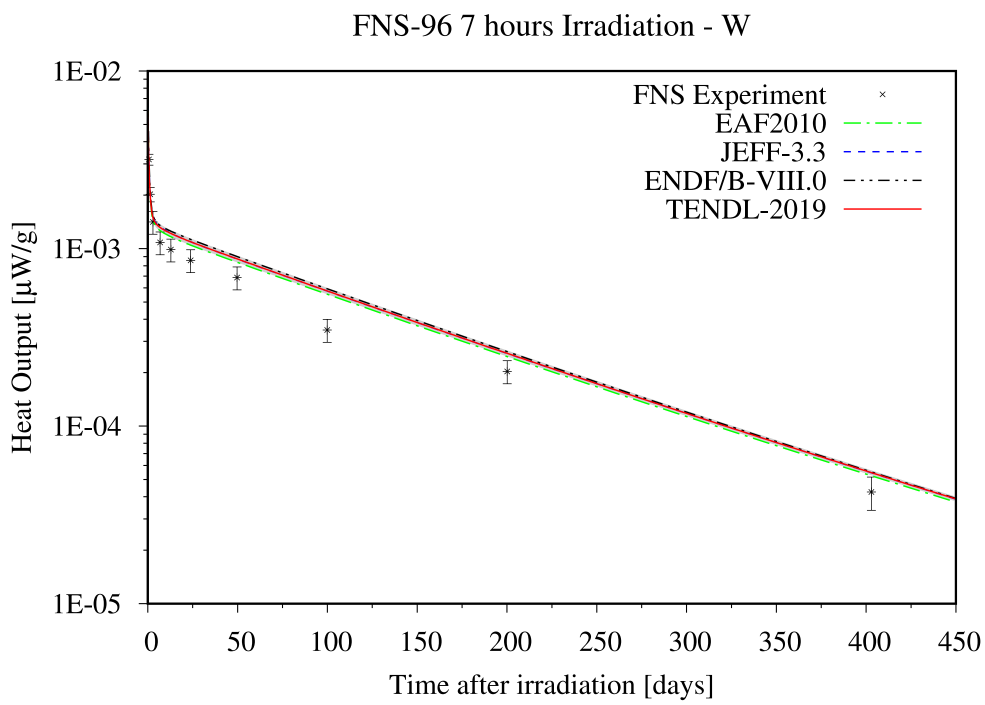
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
W185m	1.67m	W186(n,2n)W185m	99.9
W179m	6.40m	W180(n,2n)W179m	100.0
Ta186	10.50m	W186(n,p)Ta186	100.0
Ta182n	15.84m	W182(n,p)Ta182n	91.2
		W183(n,d)Ta182n	6.6
		W183(n,np)Ta182n	1.5
W179	37.05m	W180(n,2n)W179	93.9
		W180(n,2n)W179m(IT)W179	6.1
Ta185	48.99m	W186(n,d)Ta185	78.8
		W186(n,np)Ta185	21.2
Hf183	1.07h	W186(n,α)Hf183	100.0
Ta184	8.70h	W184(n,p)Ta184	99.7
W187	23.85h	W186(n,γ)W187	100.0
W185	75.12d	W186(n,2n)W185	74.6
		W186(n,2n)W185m(IT)W185	24.6

Comments on Tungsten 5-minute experiments:

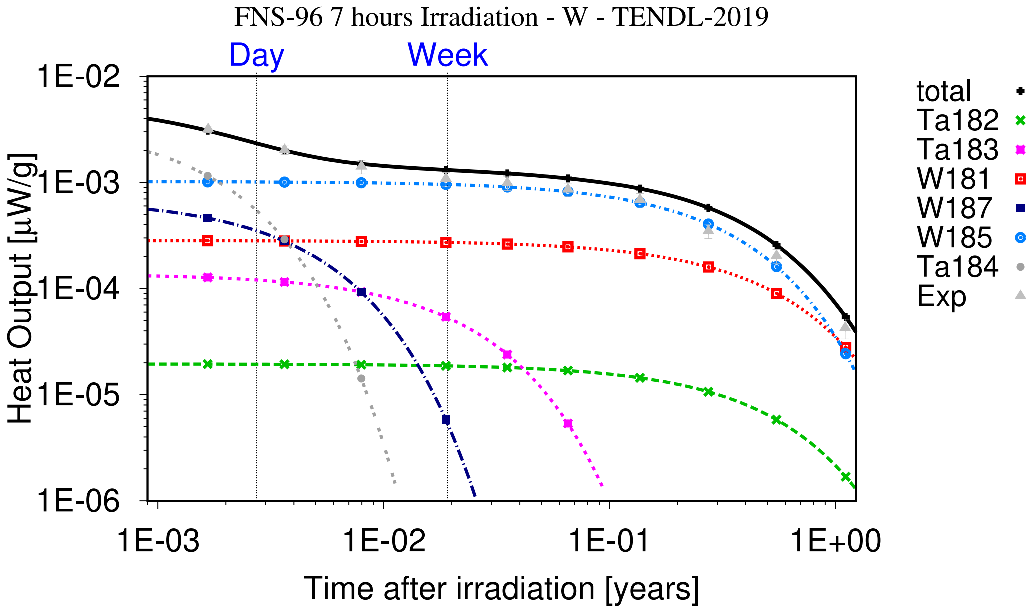
A better than expected level of agreement is observed for this particularly troublesome, in nuclear data terms, element even at short cooling time for ENDF/B-VIII.0, TENDL-2019, and EAF2010. The decay profile predicted with those libraries nicely follows the experimental shape, although the systematic over-prediction on both experimental batches (more in the 2000 case) suggests that there needs to be some re-evaluation and in-depth analysis of the major production routes involved, in particular the (n,2n) channel to produce W185m, which dominates (generally more than 90%) all cooling times less than 10 minutes with those libraries. JEFF-3.3 clearly misrepresents the decay-shape by missing the production of W185m. Analysis of the available differential data for the entire W186(n,2n) channel in EXFOR reveals that the currently evaluated cross section for W185m in TENDL-2019 (and ENDF/B-VIII.0, EAF2010) is higher than the majority of data around 14 MeV, with EXFOR data falling largely outside of the TENDL-2019 uncertainty band (the data at 14 MeV could be biased by the one anomalously high data point at 15 MeV). If the experimental measurements are to be believed then they would indicate that the W186(n,2n)W185m production channel needs to be re-evaluated slightly ($\sim$0.85 factor), particularly at 14 MeV.
All general purpose libraries are in reasonable agreement with one another for the longer-term profile, predicting first Ta186 and then W187 dominance, but again, overprediction is evident. IRDFF-II is only able to capture the contribution of the longer lived W187 radionuclide, whose production via neutron capture on W186 has important dosimetry applications.


FNS-00 5 Min. Irradiation - W - TENDL-2019
FNS-00 5 Min. Irradiation - W - EAF2010
FNS-00 5 Min. Irradiation - W - JEFF-3.3
FNS-00 5 Min. Irradiation - W - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
W185
Ta185
Ta182n
Hf183
Ta184
W179
W179m
W187
Ta186
W185m
00 Exp


FNS-00 5 Min. Irradiation - W - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.61	3.17$E-03$ +/-7%	3.08$E-03$ +/-11%	1.03	0.90	1.00	0.99
1.33	2.02$E-03$ +/-9%	2.00$E-03$ +/-7%	1.01	0.94	1.02	0.99
2.91	1.41$E-03$ +/-15%	1.50$E-03$ +/-5%	0.94	0.91	0.98	0.93
6.88	1.08$E-03$ +/-15%	1.31$E-03$ +/-4%	0.82	0.80	0.86	0.82
12.87	9.86$E-04$ +/-15%	1.22$E-03$ +/-4%	0.81	0.79	0.85	0.81
23.87	8.58$E-04$ +/-15%	1.09$E-03$ +/-4%	0.79	0.76	0.82	0.79
49.71	6.87$E-04$ +/-15%	8.75$E-04$ +/-4%	0.78	0.76	0.82	0.79
99.90	3.48$E-04$ +/-15%	5.78$E-04$ +/-4%	0.60	0.59	0.63	0.60
200.12	2.03$E-04$ +/-15%	2.57$E-04$ +/-4%	0.79	0.77	0.82	0.79
402.95	4.26$E-05$ +/-21%	5.39$E-05$ +/-3%	0.79	0.78	0.82	0.79
mean % diff. from E			23	27	19	23
mean χ^2			3.68	4.72	2.65	3.68

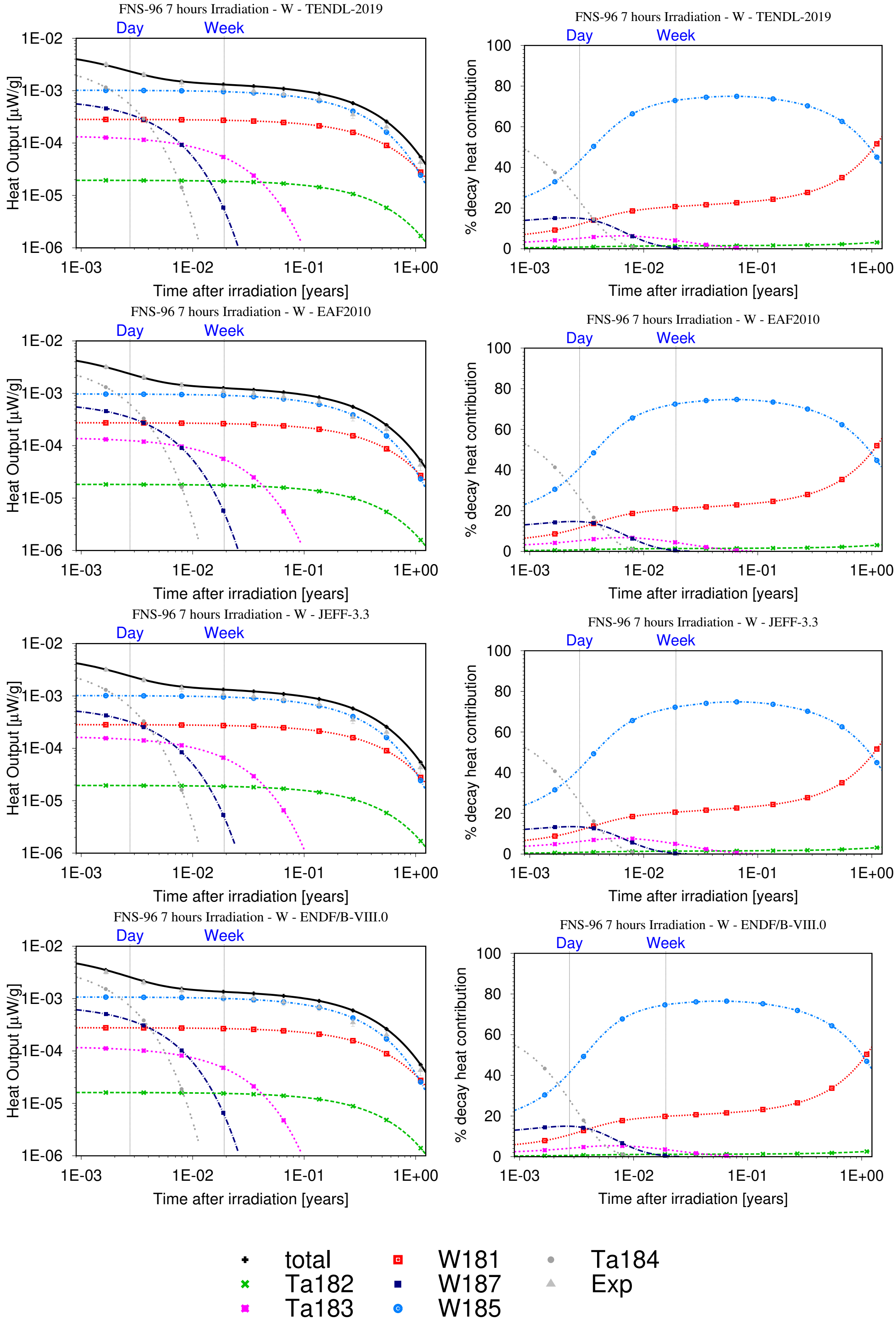


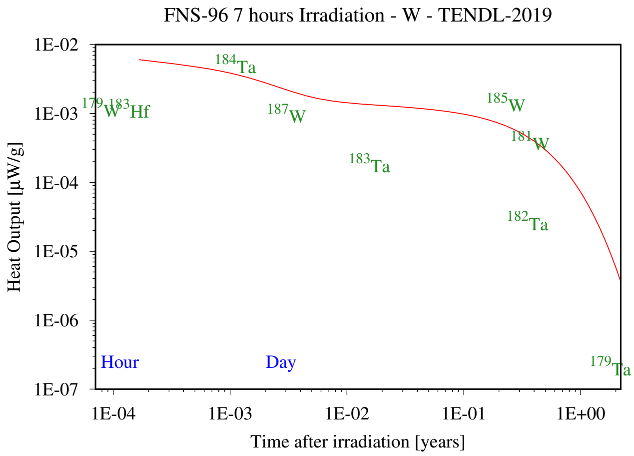
Tungsten,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Ta184	8.70h	W184(n,p)Ta184	99.8
W187	23.85h	W186(n,γ)W187	100.0
Ta183	5.09d	W183(n,p)Ta183	81.4
		W186(n,α)Hf183(β^-)Ta183	11.4
		W184(n,d)Ta183	5.3
		W184(n,np)Ta183	2.0
W185	75.12d	W186(n,2n)W185	63.8
		W186(n,2n)W185m(IT)W185	36.0
Ta182	114.71d	W182(n,p)Ta182m(IT)Ta182	45.6
		W182(n,p)Ta182	42.9
		W182(n,p)Ta182n(IT)Ta182m(IT)Ta182	7.4
		W183(n,d)Ta182m(IT)Ta182	1.3
W181	120.99d	W182(n,2n)W181	99.4

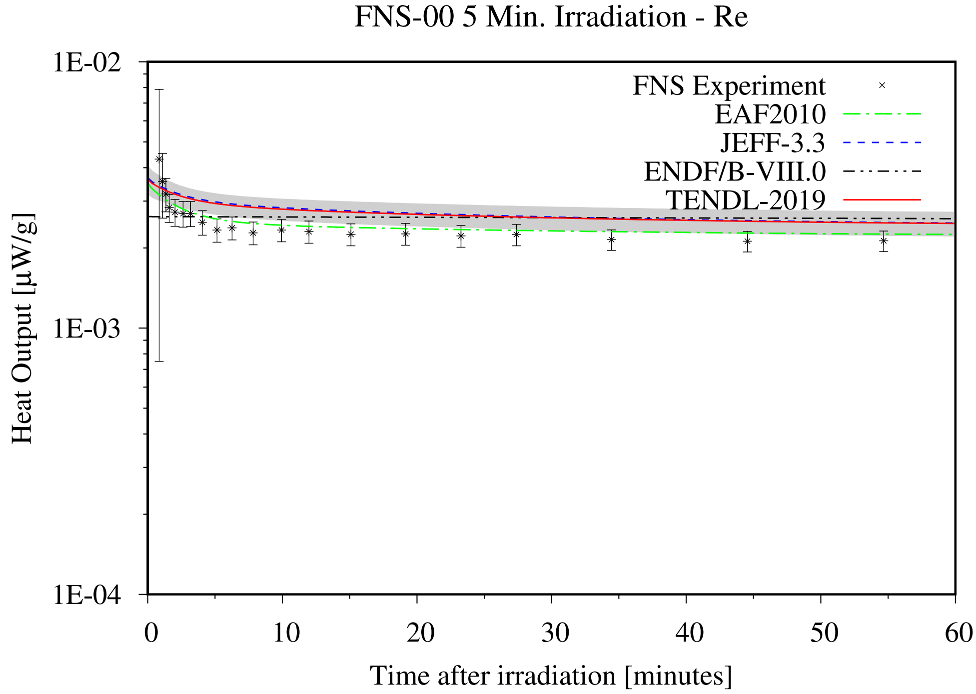
Comments on Tungsten 7-hour experiments:

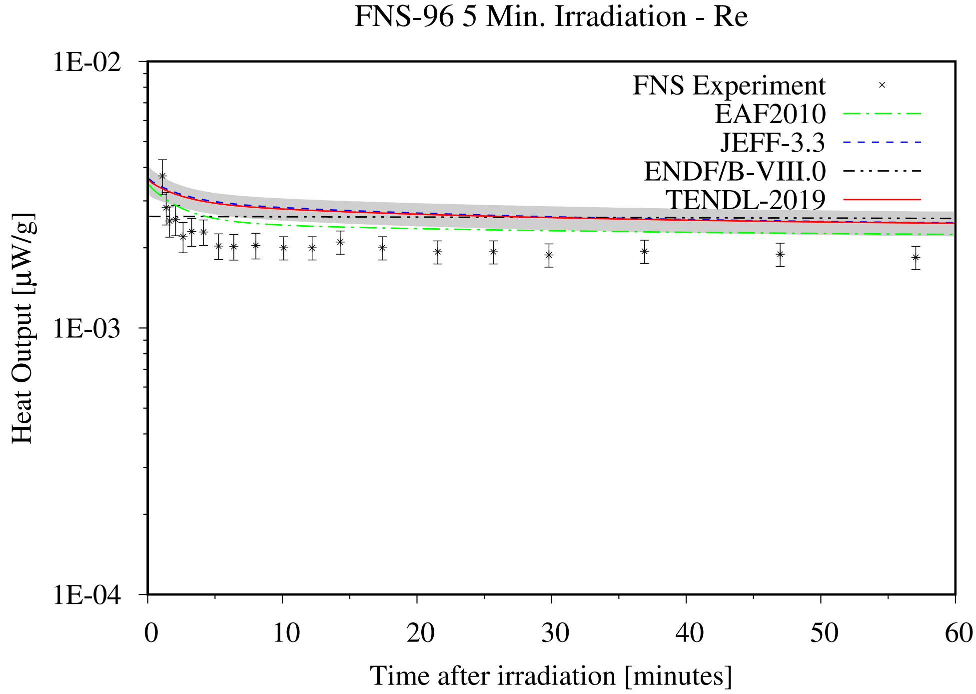
There seems to be a systematic 20-30% overestimation with all libraries in the production of W185, which is significant at all cooling times, but particularly dominant beyond 1 day of cooling. Production of this nuclide is via the same (n,2n) channel that caused overprediction of W185m in the 5-minute experiment, adding further evidence of the need to re-evaluate that channel. However, simulations with all libraries are in good agreement with the experiment during the first few days of cooling, where Ta184 (via (n,p) reactions on W184) is dominant. Note that it could, in fact, be W181, rather than W185, that is overpredicted here, since that nuclide contributes around 20% to the decay heat for much of the profile (and increases near the end), but again it would be an (n,2n) channel (this time on W182) that needs adjustment (TENDL-2019 appears to overestimate the EXFOR experimental cross section data for this channel).


FNS-96 7 hours Irradiation - W - TENDL-2019
FNS-96 7 hours Irradiation - W - EAF2010
FNS-96 7 hours Irradiation - W - JEFF-3.3
FNS-96 7 hours Irradiation - W - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-02
1E-03
1E-04
1E-05
1E-06
1E-01
1E+00
100
80
60
40
20
0
total
Ta182
Ta183
W181
W187
W185
Ta184
Exp

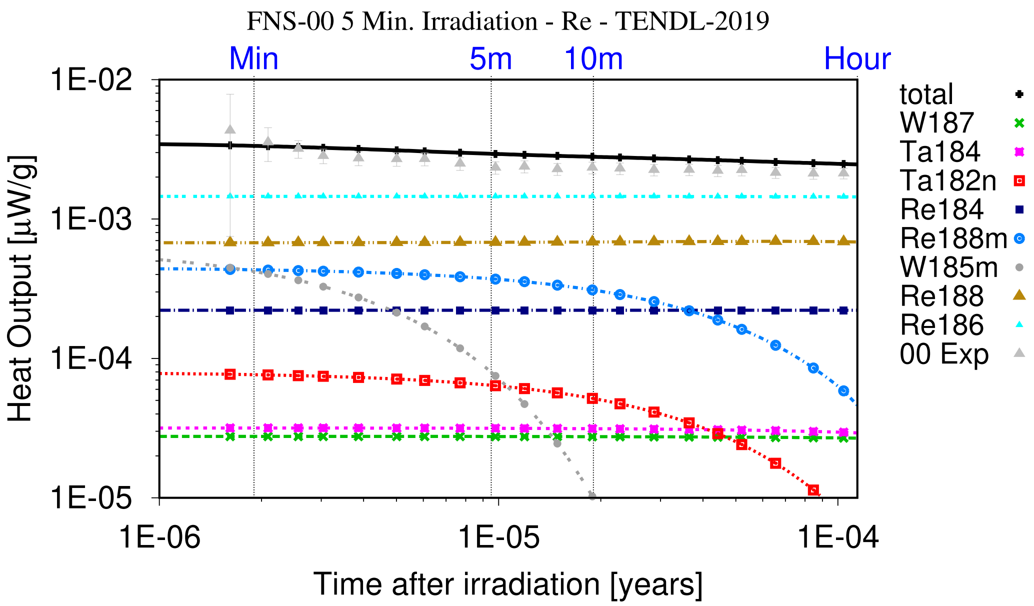

FNS-96 7 hours Irradiation - W - TENDL-2019
Heat Output [μW/g]
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
Time after irradiation [years]
1E-04
1E-03
1E-02
1E-01
1E+00
184Ta
179W
183Hf
187W
185W
181W
183Ta
182Ta
179Ta
Hour
Day

Rhenium


FNS-00 5 Min. Irradiation - Re
Heat Output [µW/g]
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019


FNS-96 5 Min. Irradiation - Re
Heat Output [µW/g]
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	4.31E−03 +/-83%	3.38E−03 +/-11%	1.28	1.64	1.36	1.26
1.10	3.55E−03 +/-27%	3.33E−03 +/-11%	1.07	1.36	1.15	1.05
1.35	3.19E−03 +/-14%	3.28E−03 +/-10%	0.97	1.22	1.05	0.96
1.60	2.84E−03 +/-12%	3.24E−03 +/-10%	0.87	1.08	0.95	0.86
2.03	2.72E−03 +/-12%	3.18E−03 +/-10%	0.86	1.04	0.94	0.84
2.63	2.69E−03 +/-11%	3.11E−03 +/-9%	0.86	1.03	0.96	0.85
3.18	2.69E−03 +/-11%	3.06E−03 +/-9%	0.88	1.03	0.99	0.87
4.05	2.50E−03 +/-11%	2.99E−03 +/-9%	0.83	0.95	0.94	0.82
5.15	2.33E−03 +/-10%	2.93E−03 +/-9%	0.80	0.89	0.91	0.79
6.27	2.38E−03 +/-10%	2.89E−03 +/-9%	0.82	0.91	0.95	0.81
7.83	2.28E−03 +/-10%	2.84E−03 +/-9%	0.80	0.87	0.92	0.79
9.93	2.33E−03 +/-10%	2.80E−03 +/-10%	0.83	0.89	0.96	0.82
11.98	2.30E−03 +/-10%	2.76E−03 +/-10%	0.83	0.88	0.96	0.82
15.10	2.25E−03 +/-9%	2.72E−03 +/-10%	0.83	0.86	0.94	0.82
19.17	2.26E−03 +/-9%	2.68E−03 +/-10%	0.84	0.87	0.96	0.83
23.27	2.22E−03 +/-9%	2.64E−03 +/-10%	0.84	0.85	0.95	0.83
27.38	2.25E−03 +/-9%	2.61E−03 +/-10%	0.86	0.86	0.96	0.85
34.45	2.15E−03 +/-9%	2.57E−03 +/-10%	0.84	0.83	0.93	0.83
44.55	2.12E−03 +/-9%	2.52E−03 +/-10%	0.84	0.82	0.93	0.84
54.67	2.13E−03 +/-9%	2.48E−03 +/-11%	0.86	0.82	0.94	0.85
mean % diff. from E			18	15	7	19
mean χ^2			3.31	2.07	0.34	3.75

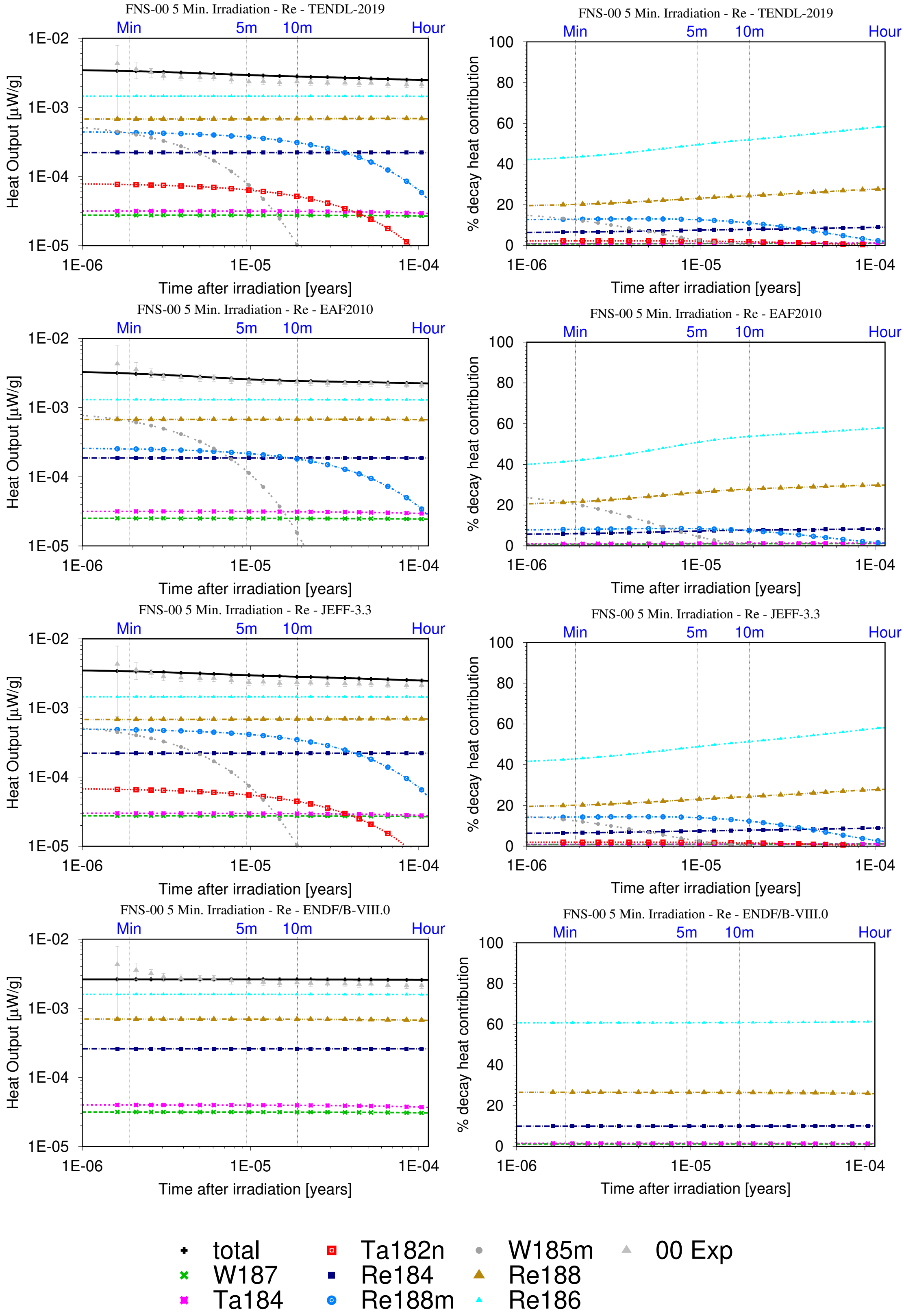


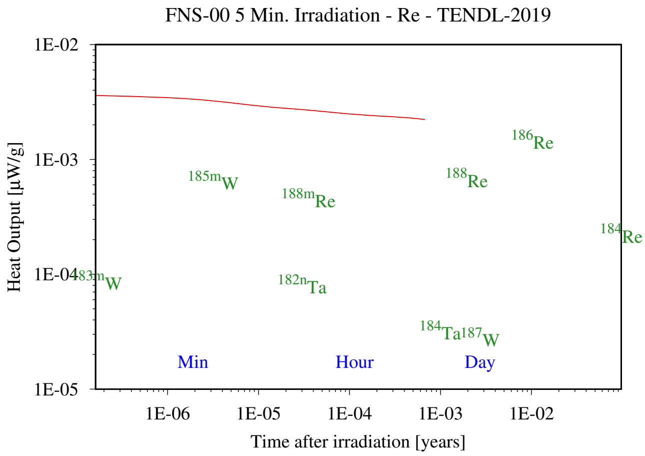
Rhenium, TENDL-2019 5-minute pathway analysis

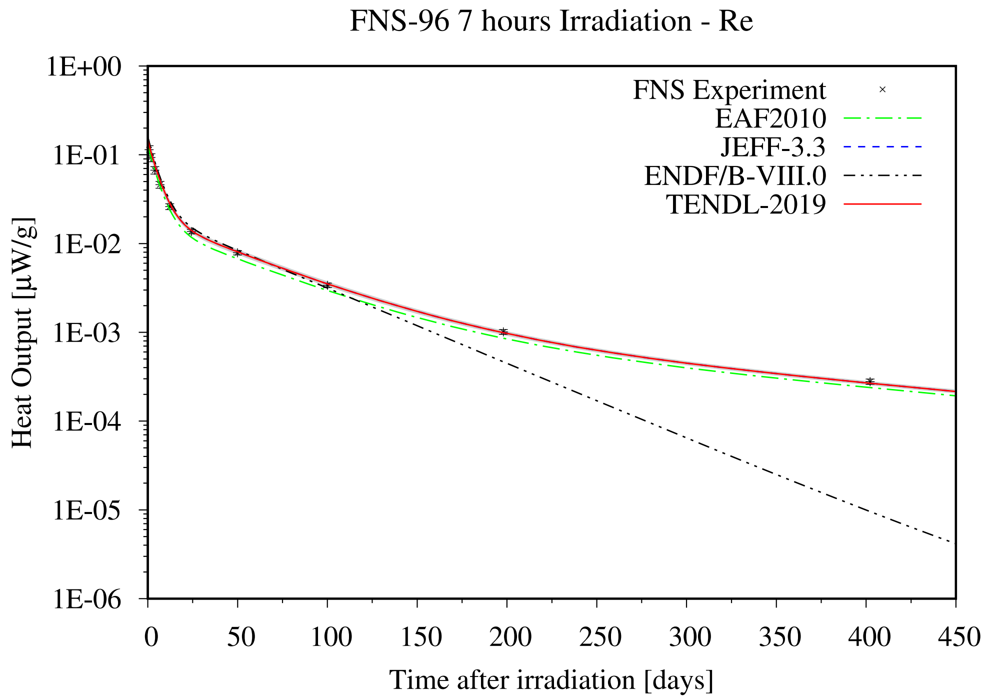
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
W185m	1.67m	Re185(n,p)W185m	90.9
		Re187(n,t)W185m	9.1
Ta182n	15.84m	Re185(n,α)Ta182n	100.0
Re188m	18.60m	Re187(n,γ)Re188m	100.0
Ta184	8.70h	Re187(n,α)Ta184	100.0
Re188	16.98h	Re187(n,γ)Re188	99.4
W187	23.85h	Re187(n,p)W187	100.0
Re186	3.75d	Re187(n,2n)Re186	95.2
		Re185(n,γ)Re186	4.8
Re184	35.40d	Re185(n,2n)Re184	100.0

Comments on Rhenium 5-minute experiments:

EAF2010 shows very good agreement to the 2000 batch of the 5 minute experiments on rhenium, nearly within the experimental uncertainties. The experimental result from the 1996 batch is significantly different, which is unexplained, but EAF2010 is still the best performer. The other three libraries considered are all in reasonable agreement with one-another, but overpredict the production of Re186, in particular, relative to EAF2010 and thus show a greater overprediction of both experimental batches compared to that legacy library. A re-evaluation of the predominant (n,2n) channel on Re187 may be required. There may also be a slight overprediction of the capture channel on the same target with all libraries, leading to an over-production of Re188, which contributes at least 20% of the decay-heat at all times and in all simulations (even EAF2010 is not in exact agreement with the 2000 experimental batch and so Re188 is an obvious culprit).


FNS-00 5 Min. Irradiation - Re - TENDL-2019
FNS-00 5 Min. Irradiation - Re - EAF2010
FNS-00 5 Min. Irradiation - Re - JEFF-3.3
FNS-00 5 Min. Irradiation - Re - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
total
Ta182n
W185m
00 Exp
W187
Re184
Re188
Ta184
Re188m
Re186

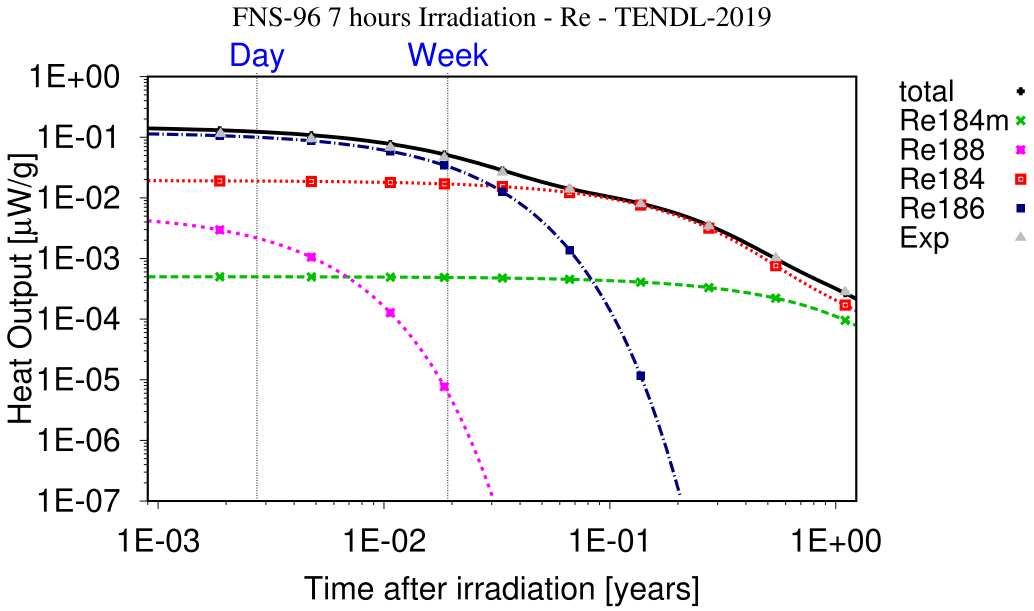

FNS-00 5 Min. Irradiation - Re - TENDL-2019
1E-02
1E-03
1E-04
1E-05
Heat Output [μW/g]
183mW
185mW
188mRe
182nTa
186Re
188Re
184Re
184Ta
187W
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.69	1.14$E-$01 +/-11%	1.30$E-$01 +/-16%	0.88	0.81	1.00	0.87
1.74	9.32$E-$02 +/-10%	1.08$E-$01 +/-15%	0.86	0.80	0.99	0.86
3.90	6.71$E-$02 +/-10%	7.74$E-$02 +/-15%	0.87	0.80	1.00	0.87
6.76	4.61$E-$02 +/-9%	5.21$E-$02 +/-13%	0.88	0.82	1.03	0.88
12.21	2.61$E-$02 +/-8%	2.85$E-$02 +/-9%	0.92	0.84	1.08	0.92
24.22	1.37$E-$02 +/-6%	1.41$E-$02 +/-7%	0.97	0.89	1.16	0.97
49.97	7.88$E-$03 +/-6%	8.08$E-$03 +/-7%	0.98	0.94	1.17	0.98
100.10	3.39$E-$03 +/-6%	3.52$E-$03 +/-7%	0.96	1.07	1.14	0.96
197.96	1.01$E-$03 +/-6%	9.92$E-$04 +/-6%	1.02	2.17	1.18	1.02
402.17	2.78$E-$04 +/-7%	2.67$E-$04 +/-5%	1.04	28.92	1.17	1.04
mean % diff. from E			8	29	8	8
mean χ^2			1.18	31.23	2.75	1.18

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Re186	3.75d	0.88	11%	19%
Re184	35.40d	0.97	6%	7%

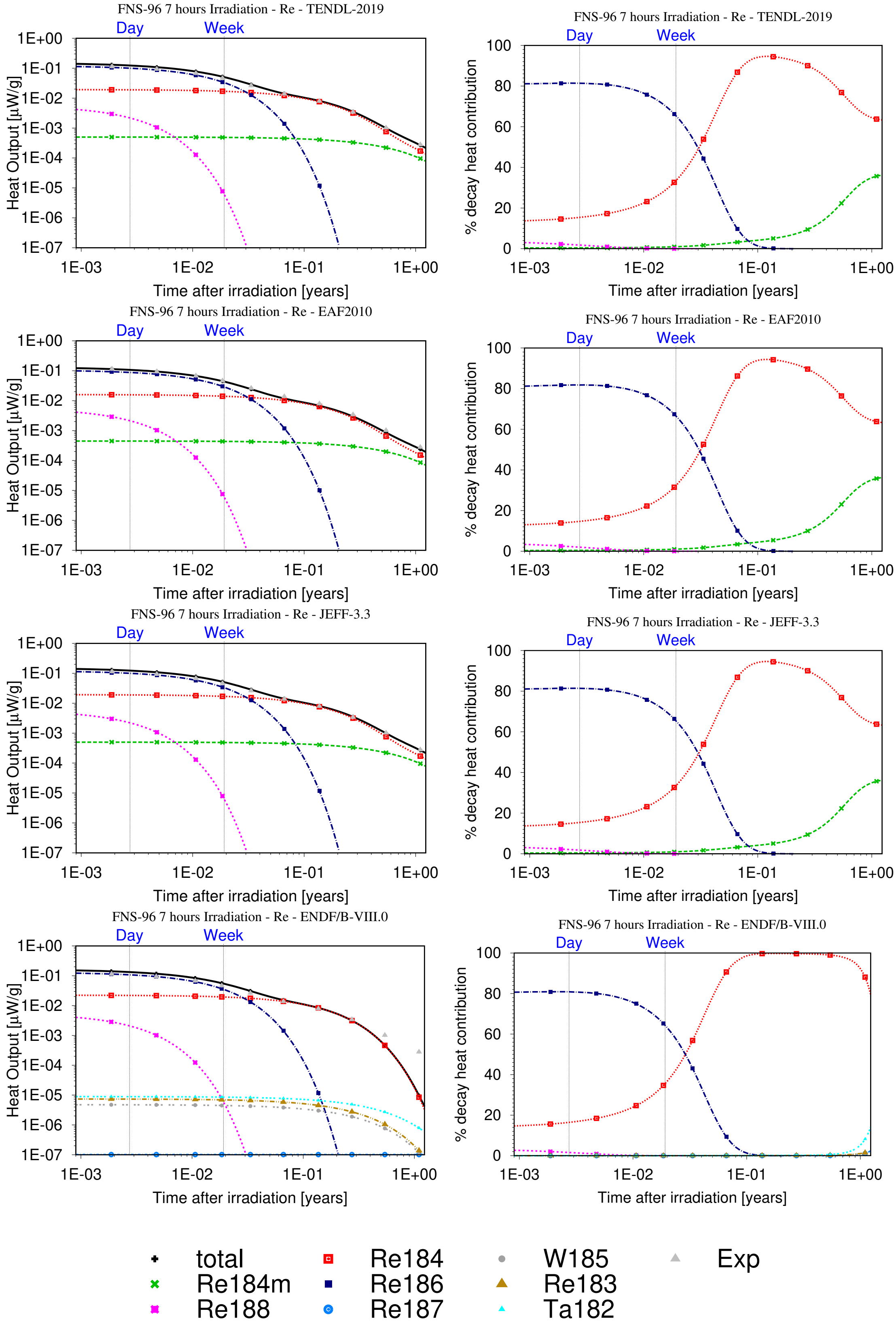


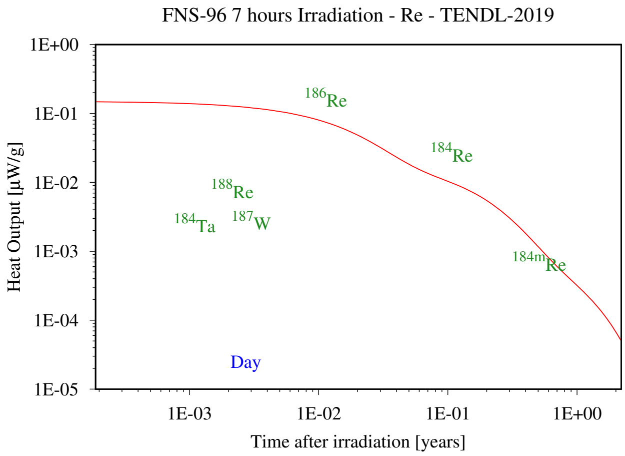
Rhenium,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Re188	16.98h	Re187(n,γ)Re188	71.1
		Re187(n,γ)Re188m(IT)Re188	28.9
Re186	3.75d	Re187(n,2n)Re186	99.6
Re184	35.40d	Re185(n,2n)Re184	100.0
Re183	70.00d	Re185(n,3n)Re183	100.0
W185	75.12d	Re185(n,p)W185	67.0
		Re185(n,p)W185m(IT)W185	29.6
		Re187(n,t)W185m(IT)W185	2.2
		Re187(n,t)W185	1.2
Ta182	114.71d	Re185(n,α)Ta182m(IT)Ta182	45.7
		Re185(n,α)Ta182n(IT)Ta182m(IT)Ta182	27.3
		Re185(n,α)Ta182	27.0
Re184m	168.01d	Re185(n,2n)Re184m	100.0
Re187	$4.4\ 10^{10}$y	no pathways found	

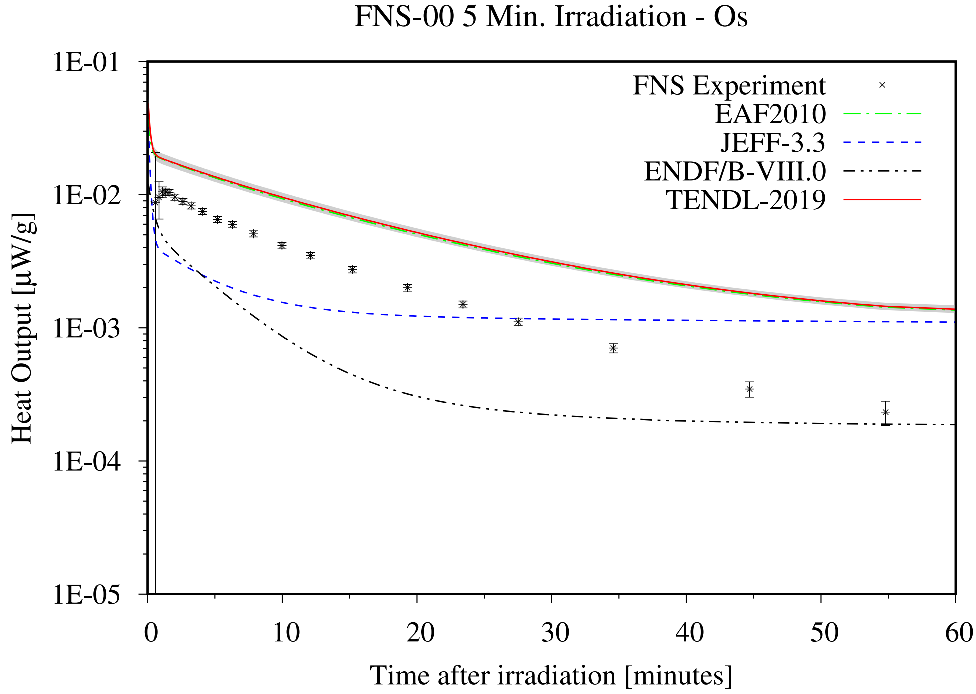
Comments on Rhenium 7-hour experiments:

A much better agreement, compared to the 5-minutes analysis, with TENDL-2019, JEFF-3.3 (which can be barely distinguished from the TENDL results), and EAF2010 for measured cooling times starting from 0.69 days. Note in this case the unusual occurrence of metastable isomer having a half-life greater than the ground (Re184m vs. Re184). The decay heat from this Re184m metastable becomes a significant factor in the final two experimental cooling times and ENDF/B-VIII.0's failure to produce it in simulations explains why that library is so discrepant beyond 100 days of cooling. Re186 dominates at cooling times less than 1 week, and all four libraries do a reasonable job of capturing the experiment in this region (EAF2010 is best here, while TENDL-2019 and JEFF-3.3 are better in the Re184 region). Overall, the relevant (n,2n) channels probably need further work to improve the agreement.


FNS-96 7 hours Irradiation - Re - TENDL-2019
FNS-96 7 hours Irradiation - Re - EAF2010
FNS-96 7 hours Irradiation - Re - JEFF-3.3
FNS-96 7 hours Irradiation - Re - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
100
80
60
40
20
0
total
Re184
W185
Exp
Re184m
Re186
Re183
Re188
Re187
Ta182


FNS-96 7 hours Irradiation - Re - TENDL-2019
Heat Output [μW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
186Re
184Re
188Re
184Ta
187W
184mRe
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

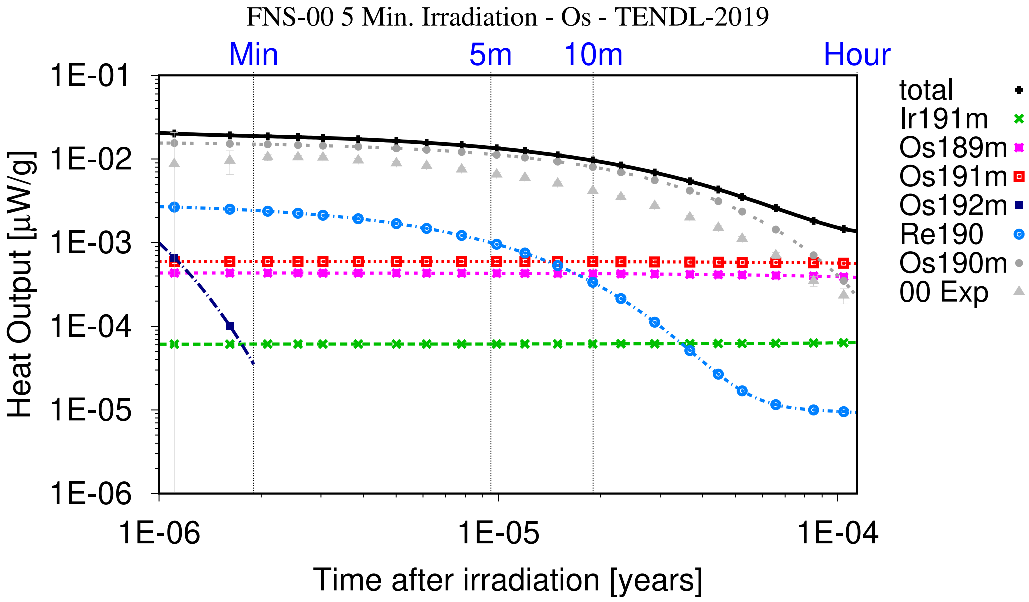
Osmium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.58	8.70E−03 +/-138%	2.02E−02 +/-9%	0.43	1.31	0.44	1.87
0.85	9.54E−03 +/-31%	1.92E−02 +/-9%	0.50	1.71	0.50	2.43
1.10	1.05E−02 +/-9%	1.86E−02 +/-9%	0.56	2.13	0.57	2.86
1.35	1.04E−02 +/-6%	1.83E−02 +/-9%	0.57	2.33	0.58	2.95
1.60	1.04E−02 +/-5%	1.79E−02 +/-9%	0.58	2.49	0.59	3.04
2.03	9.59E−03 +/-5%	1.72E−02 +/-9%	0.56	2.56	0.56	2.98
2.63	8.88E−03 +/-5%	1.64E−02 +/-9%	0.54	2.70	0.55	2.99
3.23	8.24E−03 +/-5%	1.56E−02 +/-9%	0.53	2.83	0.53	3.00
4.10	7.48E−03 +/-5%	1.46E−02 +/-9%	0.51	3.05	0.52	3.02
5.20	6.51E−03 +/-5%	1.34E−02 +/-8%	0.48	3.28	0.49	2.95
6.30	5.96E−03 +/-5%	1.24E−02 +/-8%	0.48	3.68	0.49	2.99
7.87	5.08E−03 +/-5%	1.11E−02 +/-8%	0.46	4.15	0.47	2.88
9.98	4.15E−03 +/-5%	9.59E−03 +/-8%	0.43	4.78	0.44	2.66
12.08	3.49E−03 +/-5%	8.36E−03 +/-8%	0.42	5.44	0.43	2.45
15.20	2.74E−03 +/-6%	6.88E−03 +/-8%	0.40	6.14	0.41	2.09
19.30	2.00E−03 +/-6%	5.41E−03 +/-8%	0.37	6.27	0.38	1.62
23.42	1.50E−03 +/-6%	4.33E−03 +/-7%	0.35	5.73	0.36	1.25
27.52	1.11E−03 +/-7%	3.52E−03 +/-7%	0.32	4.77	0.32	0.95
34.58	7.04E−04 +/-8%	2.58E−03 +/-6%	0.27	3.36	0.28	0.61
44.70	3.47E−04 +/-13%	1.83E−03 +/-6%	0.19	1.78	0.19	0.31
54.80	2.33E−04 +/-21%	1.45E−03 +/-6%	0.16	1.23	0.16	0.21
mean % diff. from E			160	63	155	80
mean χ^2			501.94	127.59	467.62	118.99

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Os190m	9.90m	0.43	138%	9%

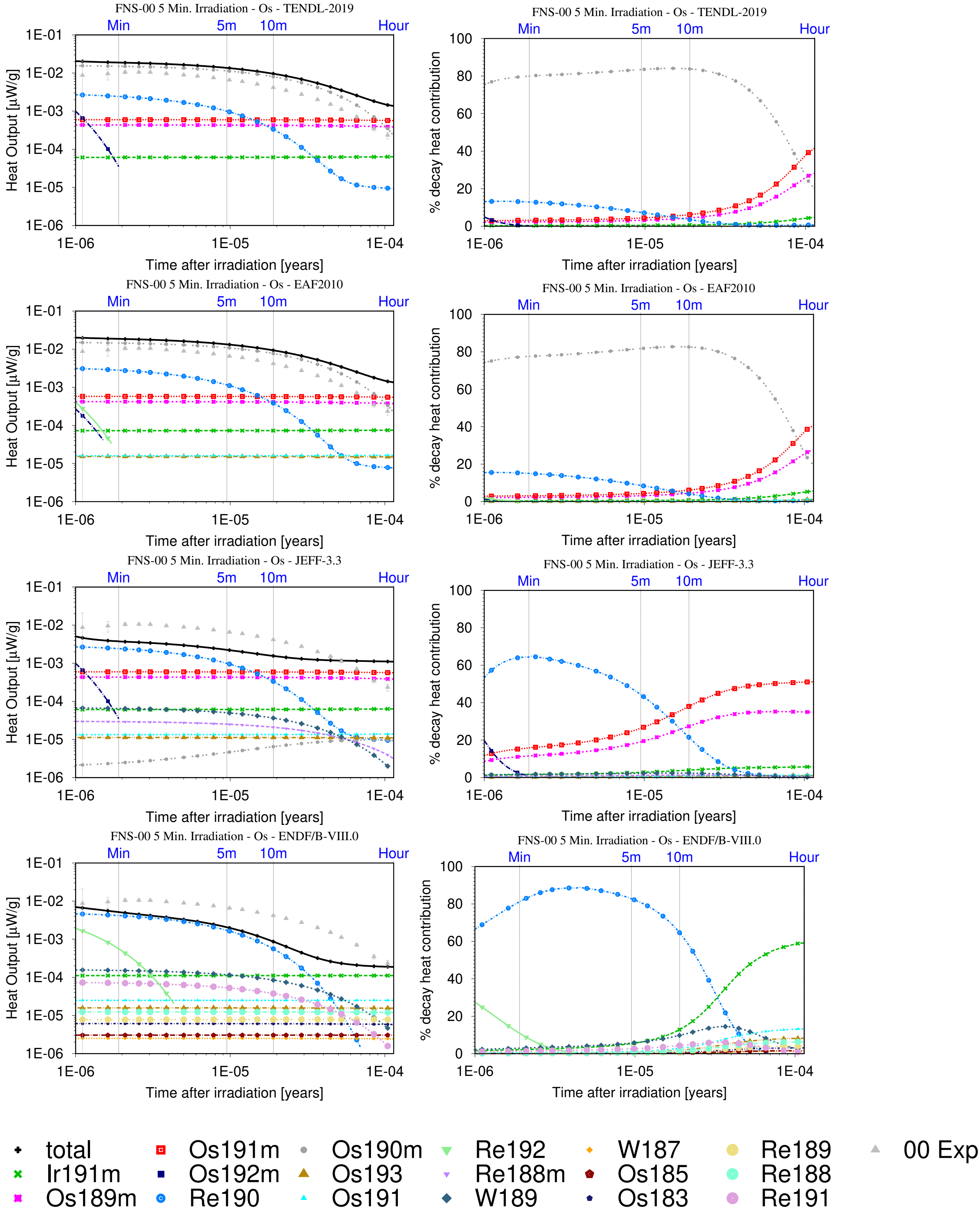


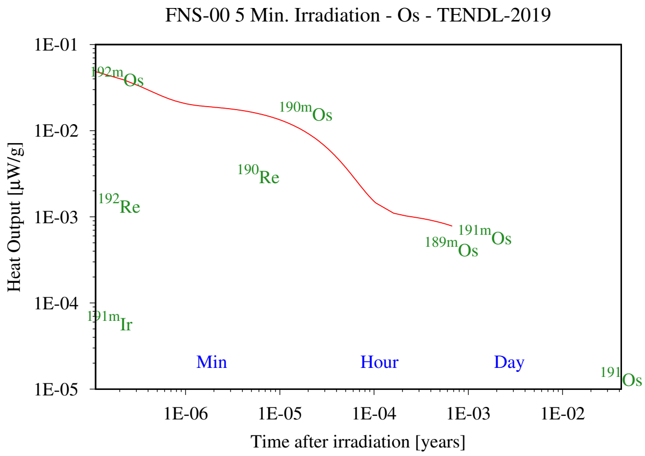
Osmium, TENDL-2019 5-minute pathway analysis

Product	$T_{1/2}$	Pathways	Path %
Ir191m	4.90s	Os192(n,2n)Os191(β^-)Ir191m	99.6
Os192m	5.90s	Os192(n,n′)Os192m	100.0
Re192	6.20s	Os192(n,p)Re192	100.0
Re190	3.10m	Os190(n,p)Re190	99.8
Re191	9.70m	Os192(n,d)Re191	86.5
		Os192(n,np)Re191	13.5
Os190m	9.90m	Os190(n,n′)Os190m	96.4
		Os192(n,3n)Os190m	3.2
W189	11.49m	Os192(n,α)W189	100.0
Re188m	18.60m	Os188(n,p)Re188m	86.7
		Os189(n,d)Re188m	8.8
		Os189(n,np)Re188m	4.4
Os189m	5.81h	Os190(n,2n)Os189m	92.7
		Os189(n,n′)Os189m	7.2
Os183	13.00h	Os184(n,2n)Os183	100.0
Os191m	13.10h	Os192(n,2n)Os191m	98.9
		Os190(n,γ)Os191m	1.1
Re188	16.98h	Os188(n,p)Re188	78.1
		Os189(n,d)Re188	12.7
		Os189(n,np)Re188	5.2
		Os188(n,p)Re188m(IT)Re188	3.3
W187	23.85h	Os190(n,α)W187	100.0
Re189	1.01d	Os189(n,p)Re189	97.6
		Os190(n,d)Re189	1.6
Os193	1.25d	Os192(n,γ)Os193	100.0
Os191	15.30d	Os192(n,2n)Os191	99.6
Os185	93.80d	Os186(n,2n)Os185	98.6
		Os187(n,3n)Os185	1.2

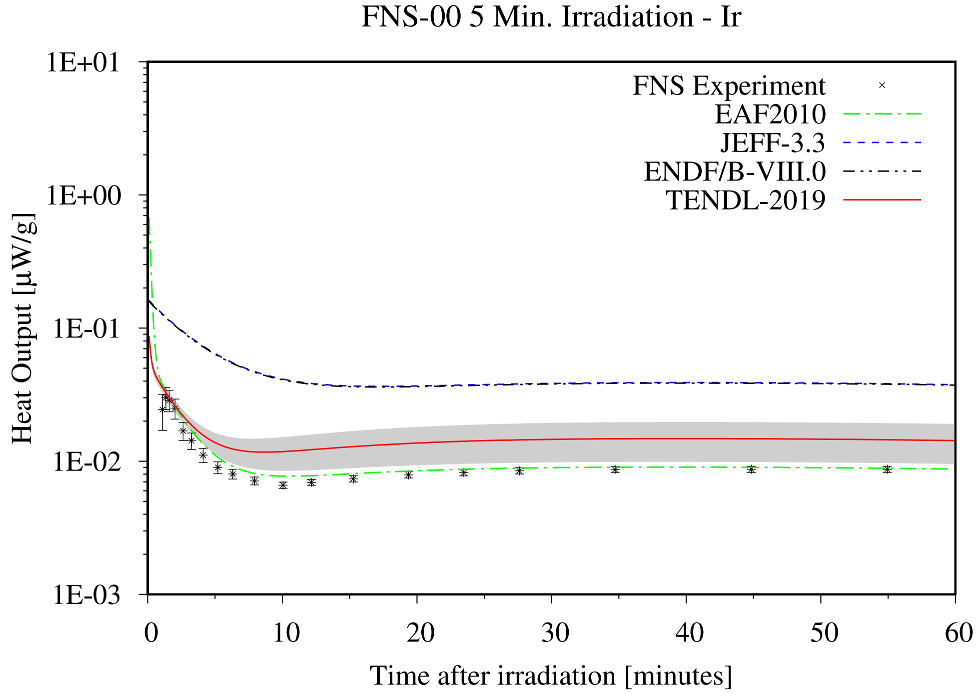
Comments on Osmium 5-minute experiments:

While JEFF-3.3 provides a significantly better comparison to the experimental decay heat magnitude in comparison to EAF2010, in reality it completely mis-represents the shape profile of the time evolution. EAF2010 is much better in this respect and it predicts that Os190m is the main contributor to the decay heat during all but the final experimental cooling time measured. Clearly, the production of this radionuclide via (n,n′) reactions on Os190 is massively overpredicted by the EAF2010 library, but it nonetheless gives the proper shape to the evolution. This channel has been embedded in TENDL-2019 (and that library closely follows EAF), however it still needs further analysis and scale-correction to be able to properly match the experiment. ENDF/B-VIII.0 has even greater trouble predicting this experiment, as it does not even generate the contributions from the Os191m and Os189m metastables that JEFF and TENDL find as the underlying base of decay heat. On the other hand, the high discrepancy between the experiment and simulations in the final few cooling times, where those metastables become important, show that the production channels of these are also in need of re-analysis.


FNS-00 5 Min. Irradiation - Os - TENDL-2019
FNS-00 5 Min. Irradiation - Os - EAF2010
FNS-00 5 Min. Irradiation - Os - JEFF-3.3
FNS-00 5 Min. Irradiation - Os - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Ir191m
Os189m
Os191m
Os192m
Re190
Os190m
Os193
Os191
Re192
Re188m
W189
W187
Os185
Os183
Re189
Re188
Re191
00 Exp


FNS-00 5 Min. Irradiation - Os - TENDL-2019
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
192mOs
190mOs
190Re
192Re
191mOs
189mOs
191mIr
Min
Hour
Day
191Os
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

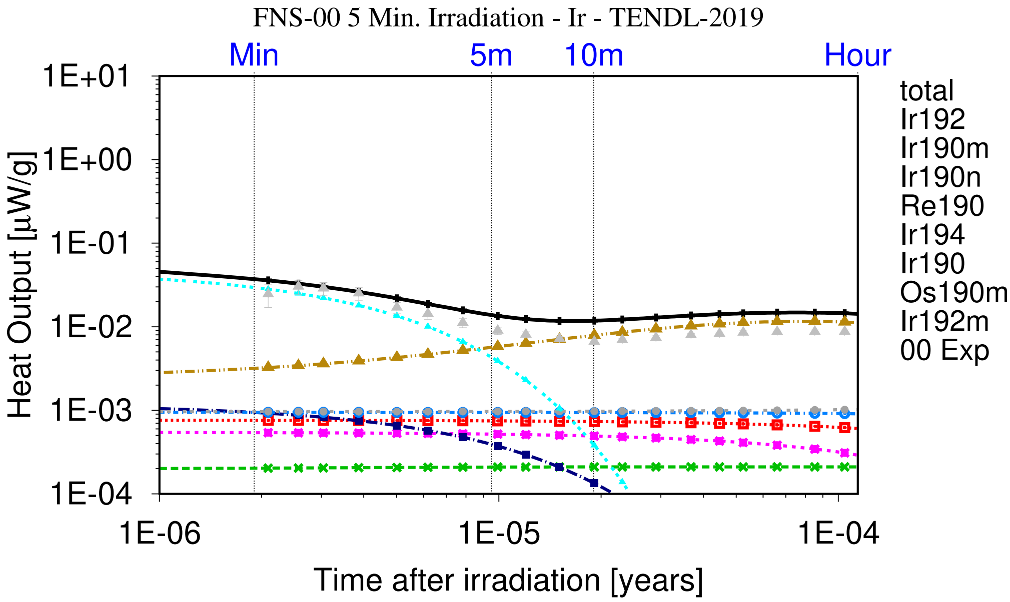
Iridium



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
1.10	2.44E−02 +/-30%	3.58E−02 +/-9%	0.68	0.19	0.65	0.19
1.35	3.01E−02 +/-19%	3.28E−02 +/-9%	0.92	0.25	0.90	0.25
1.60	2.87E−02 +/-18%	3.01E−02 +/-9%	0.95	0.25	0.95	0.25
2.03	2.50E−02 +/-17%	2.61E−02 +/-10%	0.96	0.24	0.97	0.24
2.63	1.69E−02 +/-15%	2.19E−02 +/-11%	0.77	0.18	0.81	0.18
3.25	1.43E−02 +/-14%	1.87E−02 +/-12%	0.76	0.17	0.83	0.17
4.12	1.11E−02 +/-12%	1.57E−02 +/-15%	0.71	0.15	0.83	0.15
5.22	8.98E−03 +/-10%	1.35E−02 +/-19%	0.67	0.15	0.84	0.14
6.32	8.02E−03 +/-8%	1.24E−02 +/-22%	0.65	0.15	0.88	0.15
7.93	7.13E−03 +/-7%	1.18E−02 +/-26%	0.61	0.15	0.88	0.15
10.05	6.61E−03 +/-5%	1.18E−02 +/-28%	0.56	0.16	0.86	0.16
12.15	6.92E−03 +/-5%	1.22E−02 +/-30%	0.57	0.18	0.89	0.18
15.27	7.38E−03 +/-5%	1.29E−02 +/-31%	0.57	0.20	0.91	0.20
19.37	7.91E−03 +/-5%	1.36E−02 +/-32%	0.58	0.22	0.94	0.22
23.48	8.22E−03 +/-5%	1.41E−02 +/-32%	0.58	0.22	0.94	0.22
27.60	8.48E−03 +/-5%	1.45E−02 +/-33%	0.59	0.22	0.95	0.22
34.72	8.66E−03 +/-5%	1.48E−02 +/-33%	0.59	0.23	0.96	0.22
44.83	8.70E−03 +/-5%	1.48E−02 +/-33%	0.59	0.23	0.97	0.22
54.93	8.70E−03 +/-5%	1.45E−02 +/-33%	0.60	0.23	0.98	0.23
mean % diff. from E			52	419	13	425
mean χ^2			94.41	3453.56	2.29	3550.01

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC^{nuc}**
Ir192m	1.44m	0.68	30%	8%
Os190m	9.90m	0.58	5%	42%

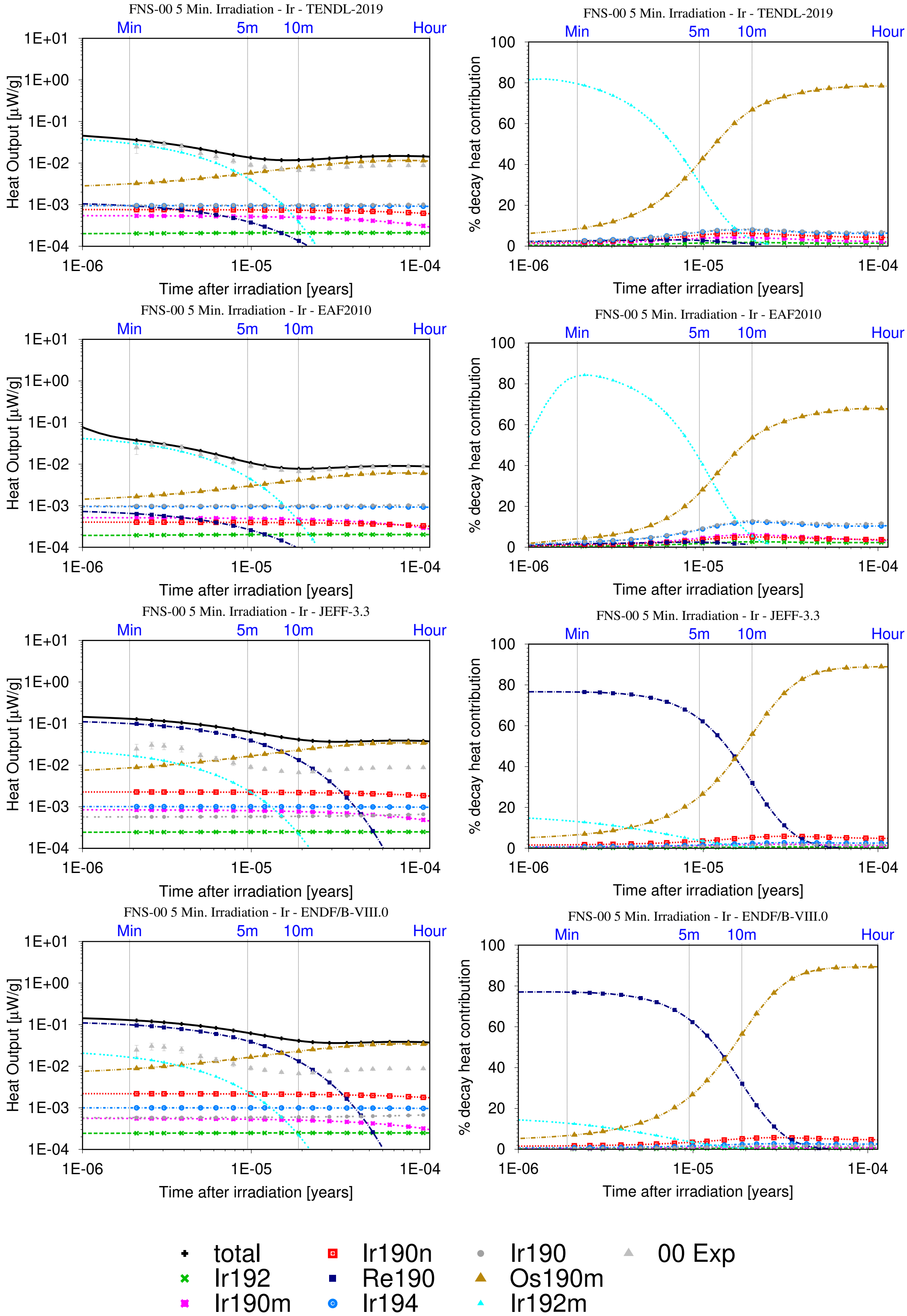


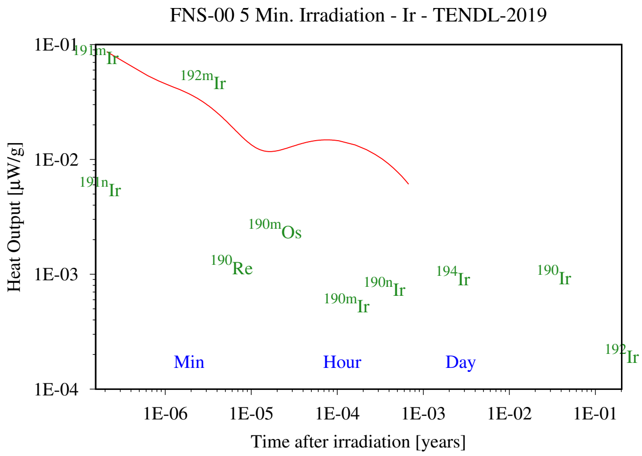
Iridium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Ir192m	1.44m	Ir193(n,2n)Ir192m	66.2
		Ir191(n,γ)Ir192m	33.8
Re190	3.10m	Ir193(n,α)Re190	99.6
Os190m	9.90m	Ir191(n,2n)Ir190n(β^+)Os190m	87.4
		Ir191(n,d)Os190m	11.5
		Ir191(n,np)Os190m	1.1
Ir190m	1.12h	Ir191(n,2n)Ir190m	100.0
Ir190n	3.09h	Ir191(n,2n)Ir190n	100.0
Ir194	19.30h	Ir193(n,γ)Ir194	99.9
Ir190	12.00d	Ir191(n,2n)Ir190	99.6
Ir192	73.80d	Ir193(n,2n)Ir192	86.5
		Ir193(n,2n)Ir192m(IT)Ir192	6.5
		Ir191(n,γ)Ir192	3.7
		Ir191(n,γ)Ir192m(IT)Ir192	3.3

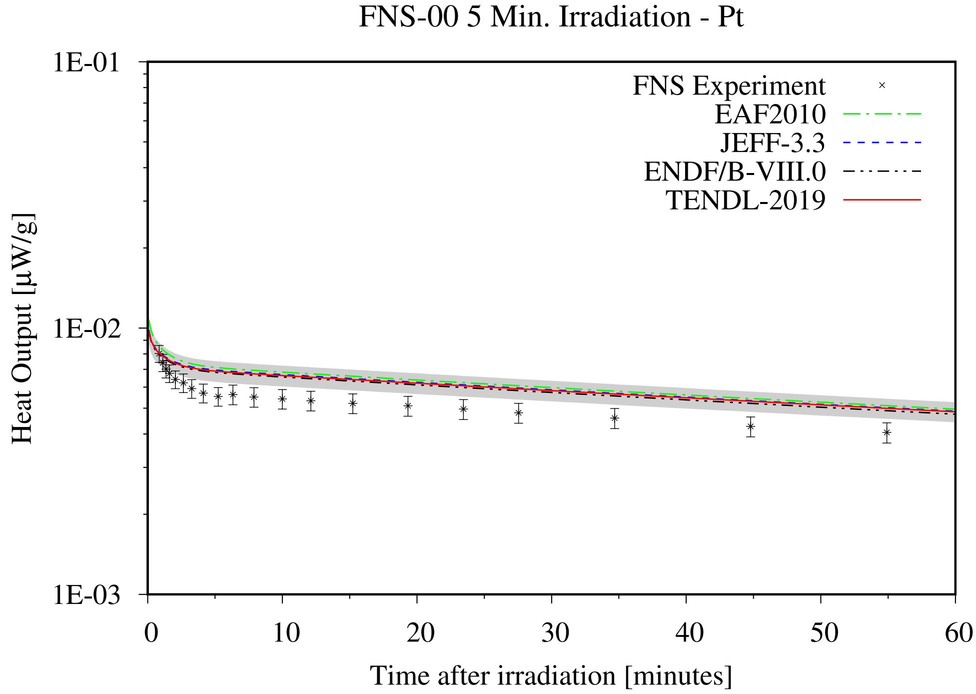
Comments on Iridium 5-minute experiments:

EAF2010 and now TENDL-2019 are the only libraries that matches the experiment in this case, demonstrating that the observed decay-heat comes from Ir192m at short cooling times (less than 5 minutes) and then from Os190m at longer times; growth of the latter as Ir190n decays explains why the decay-heat increases in the experiments and simulations between 5 and 15 minutes of cooling. All other nuclides are shown to only provide minor contributions to the decay heat. TENDL-2019 has been dramatically improved in comparison to TENDL-2017, which didn't capture the Os190m production correctly, but EAF2010 is still much better. Adjustment of the (n,2n) channel on Ir191 is probably warranted in TENDL to reduce Ir90n production (perhaps a branching issue?). Meanwhile JEFF-3.3 and ENDF/B-VIII.0 both predict the importance of Os190m, although they overpredict its production via (n,2n) reactions on Ir191 (primarily via the Ir190n metastable). More dramatically, they predict the dominance of a completely different nuclide, Re190, at short decay times of less than 5 minutes.


FNS-00 5 Min. Irradiation - Ir - TENDL-2019
FNS-00 5 Min. Irradiation - Ir - EAF2010
FNS-00 5 Min. Irradiation - Ir - JEFF-3.3
FNS-00 5 Min. Irradiation - Ir - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Ir192
Ir190m
Ir190n
Re190
Ir194
Ir190
Os190m
Ir192m
00 Exp


FNS-00 5 Min. Irradiation - Ir - TENDL-2019
Heat Output [μW/g]
1E-01
1E-02
1E-03
1E-04
191mIr
192mIr
191nIr
190mOs
190Re
190nIr
190mIr
194Ir
190Ir
192Ir
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]

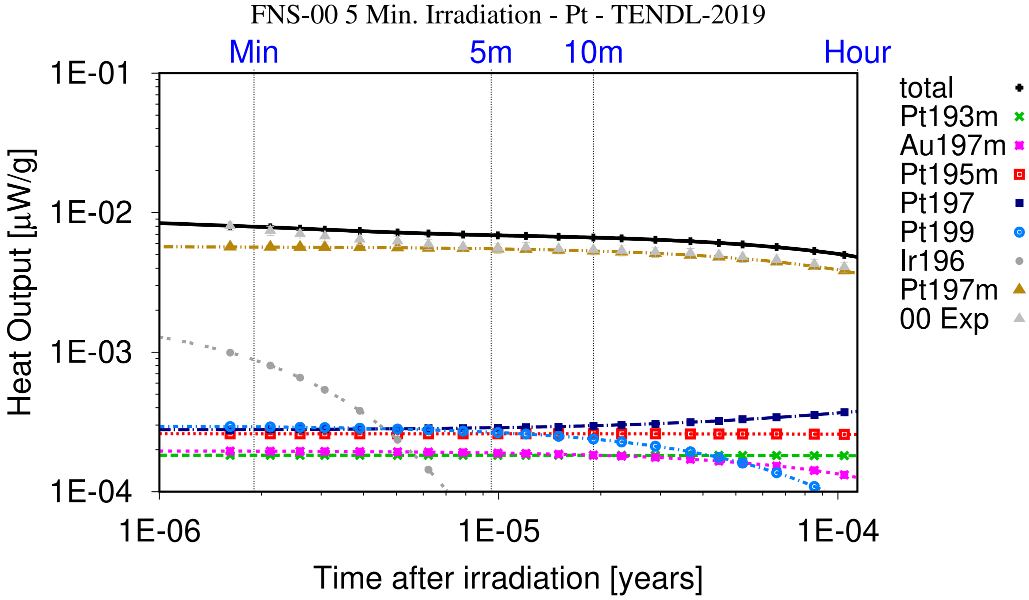
Platinum



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	$8.02E{-}03$ +/-7%	$8.06E{-}03$ +/-9%	0.99	1.01	0.94	0.99
1.12	$7.41E{-}03$ +/-7%	$7.85E{-}03$ +/-9%	0.94	0.95	0.89	0.94
1.37	$7.02E{-}03$ +/-8%	$7.69E{-}03$ +/-9%	0.91	0.92	0.87	0.91
1.62	$6.76E{-}03$ +/-8%	$7.56E{-}03$ +/-9%	0.89	0.90	0.85	0.89
2.05	$6.41E{-}03$ +/-8%	$7.38E{-}03$ +/-9%	0.87	0.88	0.83	0.86
2.65	$6.23E{-}03$ +/-8%	$7.21E{-}03$ +/-9%	0.86	0.87	0.83	0.86
3.27	$5.93E{-}03$ +/-8%	$7.09E{-}03$ +/-9%	0.84	0.85	0.81	0.83
4.13	$5.70E{-}03$ +/-8%	$6.97E{-}03$ +/-9%	0.82	0.83	0.79	0.81
5.23	$5.53E{-}03$ +/-8%	$6.88E{-}03$ +/-9%	0.80	0.81	0.78	0.80
6.33	$5.63E{-}03$ +/-8%	$6.81E{-}03$ +/-9%	0.83	0.84	0.80	0.82
7.90	$5.51E{-}03$ +/-8%	$6.73E{-}03$ +/-9%	0.82	0.83	0.79	0.81
10.00	$5.42E{-}03$ +/-8%	$6.63E{-}03$ +/-9%	0.82	0.83	0.79	0.81
12.12	$5.34E{-}03$ +/-9%	$6.54E{-}03$ +/-9%	0.82	0.83	0.79	0.81
15.23	$5.22E{-}03$ +/-9%	$6.41E{-}03$ +/-9%	0.81	0.83	0.79	0.81
19.33	$5.11E{-}03$ +/-9%	$6.24E{-}03$ +/-9%	0.82	0.83	0.80	0.81
23.45	$4.96E{-}03$ +/-9%	$6.07E{-}03$ +/-9%	0.82	0.83	0.80	0.81
27.55	$4.81E{-}03$ +/-9%	$5.92E{-}03$ +/-9%	0.81	0.82	0.79	0.81
34.68	$4.59E{-}03$ +/-9%	$5.65E{-}03$ +/-9%	0.81	0.83	0.79	0.81
44.78	$4.27E{-}03$ +/-9%	$5.31E{-}03$ +/-9%	0.80	0.82	0.78	0.80
54.90	$4.06E{-}03$ +/-9%	$5.00E{-}03$ +/-9%	0.81	0.83	0.79	0.81
mean % diff. from E			19	17	23	20
mean χ^2			5.62	4.79	8.02	6.16

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Pt197m	1.59h	0.87	8%	11%

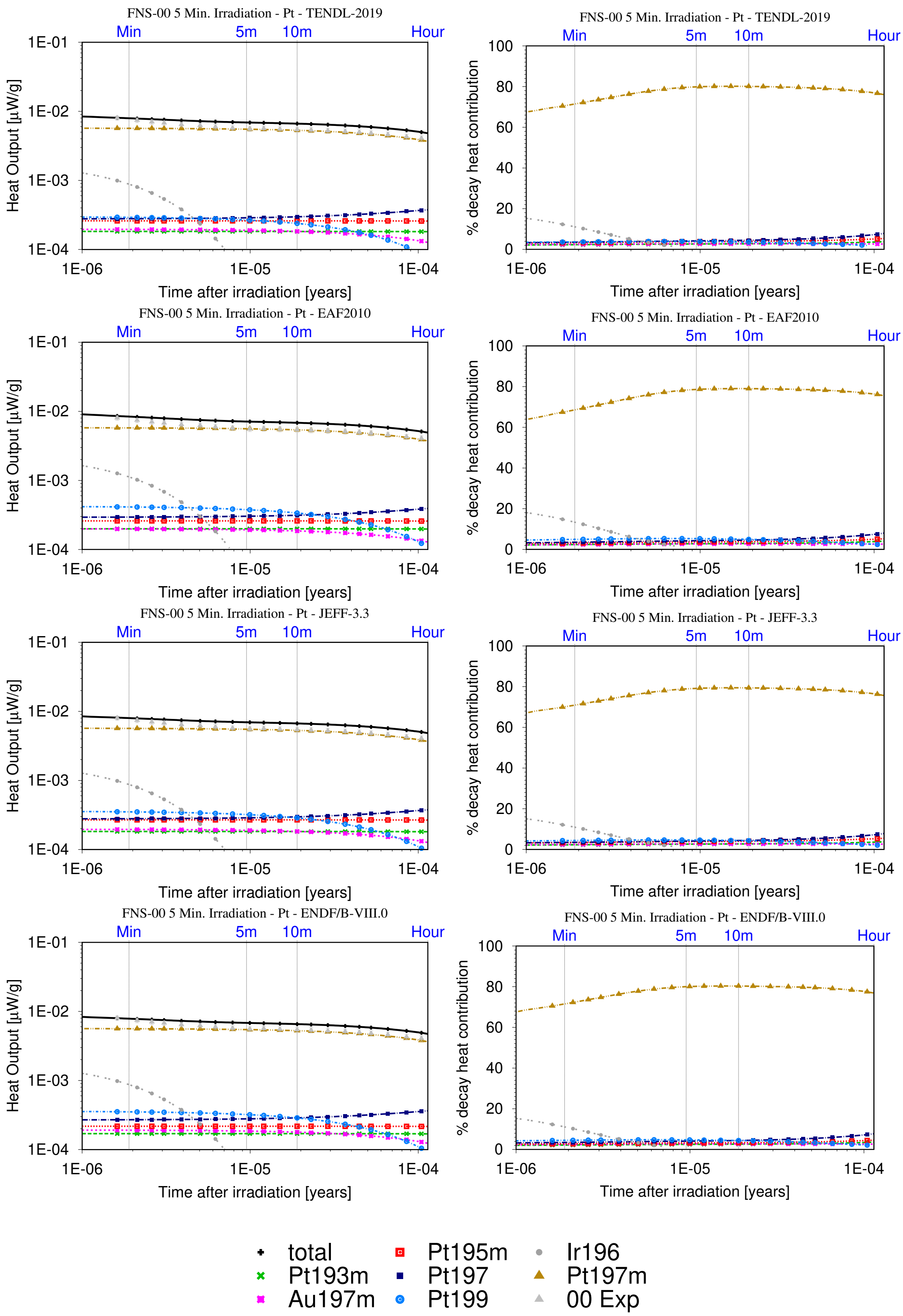


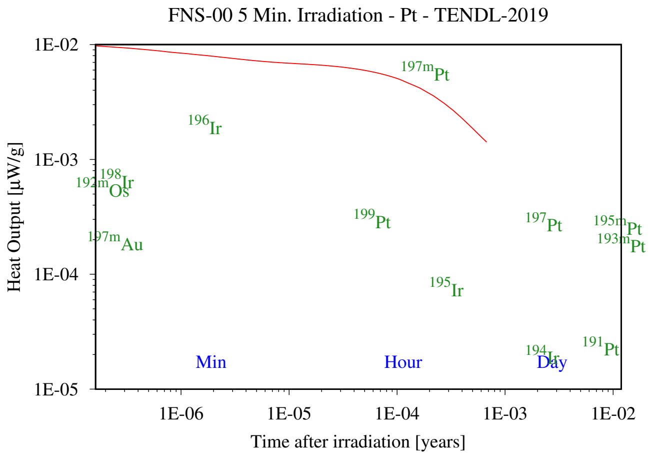
Platinum, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Au197m	7.74s	Pt198(n,2n)Pt197m(β^-)Au197m	99.7
Ir196	52.00s	Pt196(n,p)Ir196	100.0
Pt199	30.80m	Pt198(n,γ)Pt199	94.1
		Pt198(n,γ)Pt199m(IT)Pt199	5.9
Pt197m	1.59h	Pt198(n,2n)Pt197m	99.7
Pt197	19.89h	Pt198(n,2n)Pt197	95.5
		Pt196(n,γ)Pt197	2.4
		Pt198(n,2n)Pt197m(IT)Pt197	2.1
Pt195m	4.02d	Pt196(n,2n)Pt195m	84.7
		Pt195(n,n$'$)Pt195m	15.2
Pt193m	4.34d	Pt194(n,2n)Pt193m	99.6

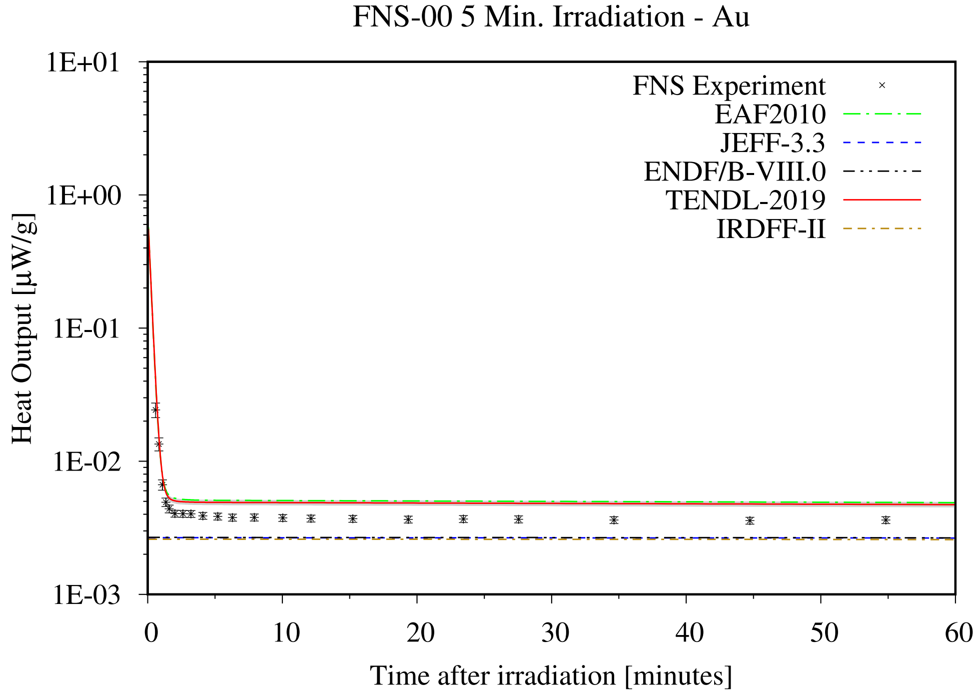
Comments on Platinum 5-minute experiments:

Since the only nuclide predicted to contribute significantly to the decay-heat by all libraries is Pt197m at all cooling times, the discrepancy between the simulations and experiment must be attributed to incorrect production rates of that nuclide. With TENDL-2019 (and the other libraries) there appears to be around a 20% overprediction in the decay-heat from Pt197m, although the experimental uncertainty and TENDL-2019 error bands do at least overlap. A case for correction of the (n,2n) reaction channel on Pt198 (maybe the branching ratio of that channel is wrong).

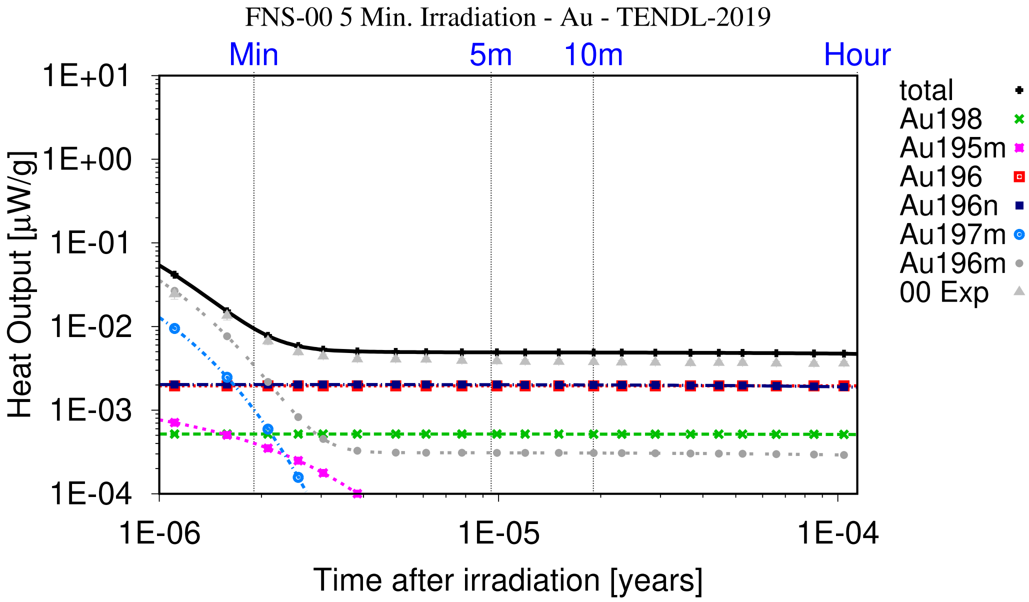

FNS-00 5 Min. Irradiation - Pt - TENDL-2019
FNS-00 5 Min. Irradiation - Pt - TENDL-2019
FNS-00 5 Min. Irradiation - Pt - EAF2010
FNS-00 5 Min. Irradiation - Pt - EAF2010
FNS-00 5 Min. Irradiation - Pt - JEFF-3.3
FNS-00 5 Min. Irradiation - Pt - JEFF-3.3
FNS-00 5 Min. Irradiation - Pt - ENDF/B-VIII.0
FNS-00 5 Min. Irradiation - Pt - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-01
1E-02
1E-03
1E-04
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Pt193m
Au197m
Pt195m
Pt197
Pt199
Ir196
Pt197m
00 Exp


FNS-00 5 Min. Irradiation - Pt - TENDL-2019
Heat Output [μW/g]
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]
197mPt
196Ir
198Ir
192mOs
197mAu
199Pt
197Pt
195mPt
193mPt
195Ir
194Ir
191Pt
Min
Hour
Day

Gold



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	2.43E−02 +/-13%	4.16E−02 +/-6%	0.58	9.06	0.60	9.10	9.34
0.83	1.35E−02 +/-11%	1.52E−02 +/-5%	0.88	5.02	0.91	5.05	5.18
1.10	6.66E−03 +/-9%	7.73E−03 +/-4%	0.86	2.48	0.85	2.50	2.56
1.35	4.93E−03 +/-7%	5.84E−03 +/-4%	0.84	1.84	0.81	1.85	1.90
1.60	4.39E−03 +/-7%	5.28E−03 +/-4%	0.83	1.64	0.79	1.65	1.69
2.02	4.05E−03 +/-6%	5.04E−03 +/-5%	0.80	1.51	0.77	1.52	1.56
2.62	4.03E−03 +/-6%	4.96E−03 +/-5%	0.81	1.51	0.78	1.51	1.55
3.22	4.02E−03 +/-6%	4.93E−03 +/-5%	0.82	1.50	0.79	1.51	1.55
4.10	3.89E−03 +/-6%	4.92E−03 +/-5%	0.79	1.45	0.76	1.46	1.50
5.20	3.85E−03 +/-6%	4.91E−03 +/-5%	0.78	1.44	0.76	1.44	1.48
6.30	3.78E−03 +/-6%	4.90E−03 +/-5%	0.77	1.41	0.74	1.42	1.45
7.92	3.79E−03 +/-6%	4.90E−03 +/-5%	0.77	1.41	0.75	1.42	1.46
10.03	3.75E−03 +/-6%	4.89E−03 +/-5%	0.77	1.40	0.74	1.41	1.45
12.13	3.72E−03 +/-6%	4.88E−03 +/-5%	0.76	1.39	0.74	1.40	1.43
15.23	3.70E−03 +/-6%	4.87E−03 +/-5%	0.76	1.38	0.73	1.39	1.43
19.35	3.66E−03 +/-6%	4.86E−03 +/-5%	0.75	1.37	0.73	1.37	1.41
23.45	3.68E−03 +/-6%	4.84E−03 +/-5%	0.76	1.38	0.73	1.38	1.42
27.55	3.67E−03 +/-6%	4.83E−03 +/-5%	0.76	1.37	0.73	1.38	1.41
34.63	3.62E−03 +/-6%	4.81E−03 +/-5%	0.75	1.35	0.73	1.36	1.40
44.73	3.58E−03 +/-6%	4.77E−03 +/-5%	0.75	1.34	0.72	1.35	1.38
54.83	3.62E−03 +/-6%	4.74E−03 +/-5%	0.76	1.36	0.74	1.36	1.40
mean % diff. from E			29	37	33	37	39
mean χ^2			21.21	28.67	27.97	29.13	31.83

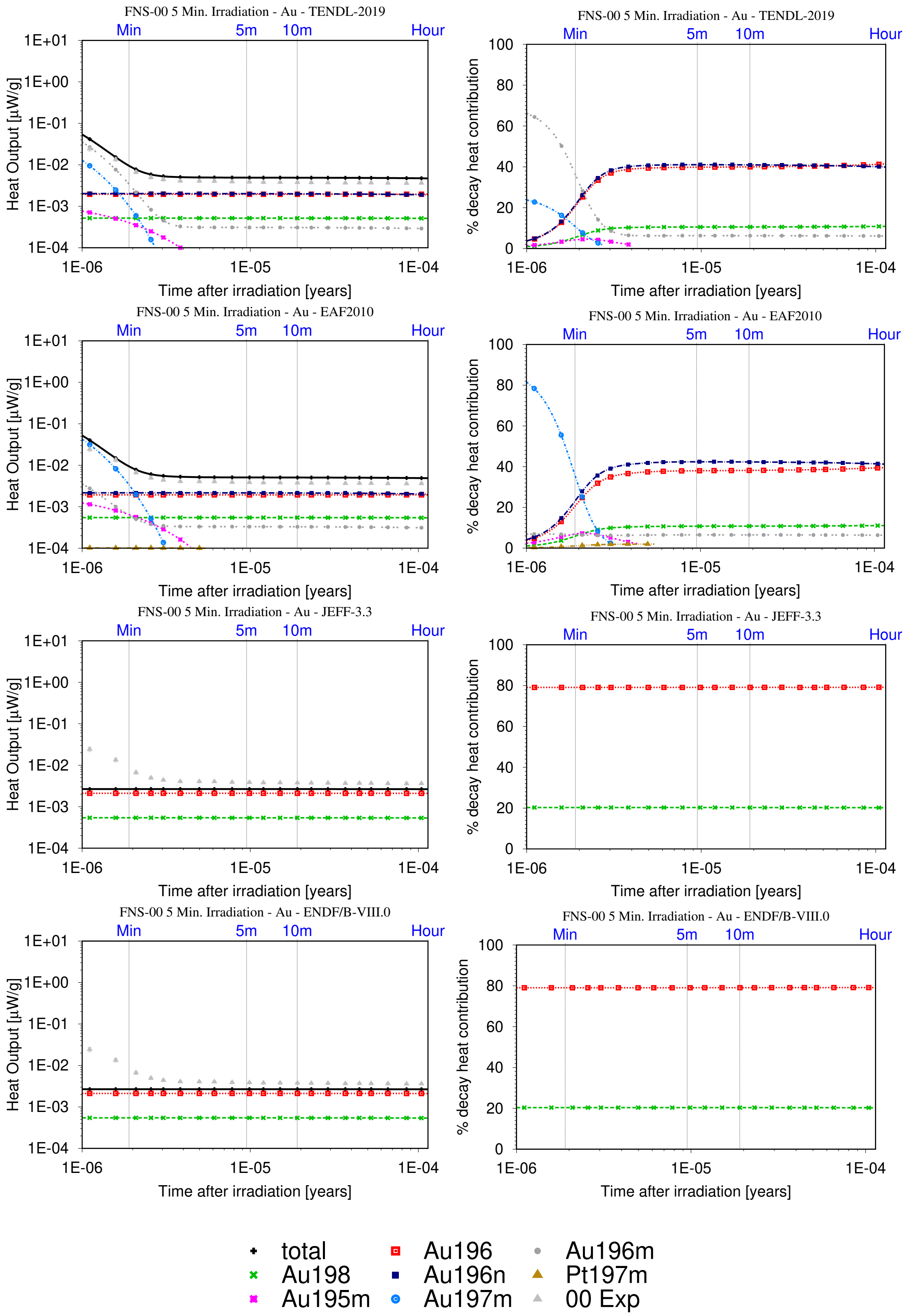


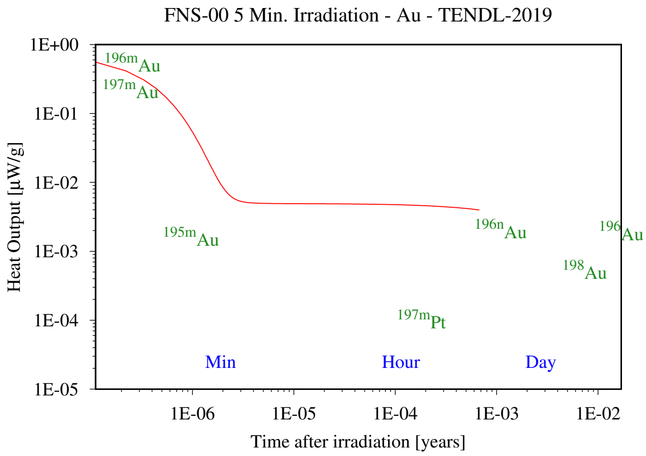
Gold, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Au197m	7.74s	Au197(n,n′)Au197m	100.0
Au196m	8.10s	Au197(n,2n)Au196m	99.9
Au195m	30.49s	Au197(n,3n)Au195m	100.0
Pt197m	1.59h	Au197(n,p)Pt197m	100.0
Au196n	9.60h	Au197(n,2n)Au196n	100.0
Au198	2.69d	Au197(n,γ)Au198	100.0
Au196	6.18d	Au197(n,2n)Au196m(IT)Au196	65.0
		Au197(n,2n)Au196	35.0

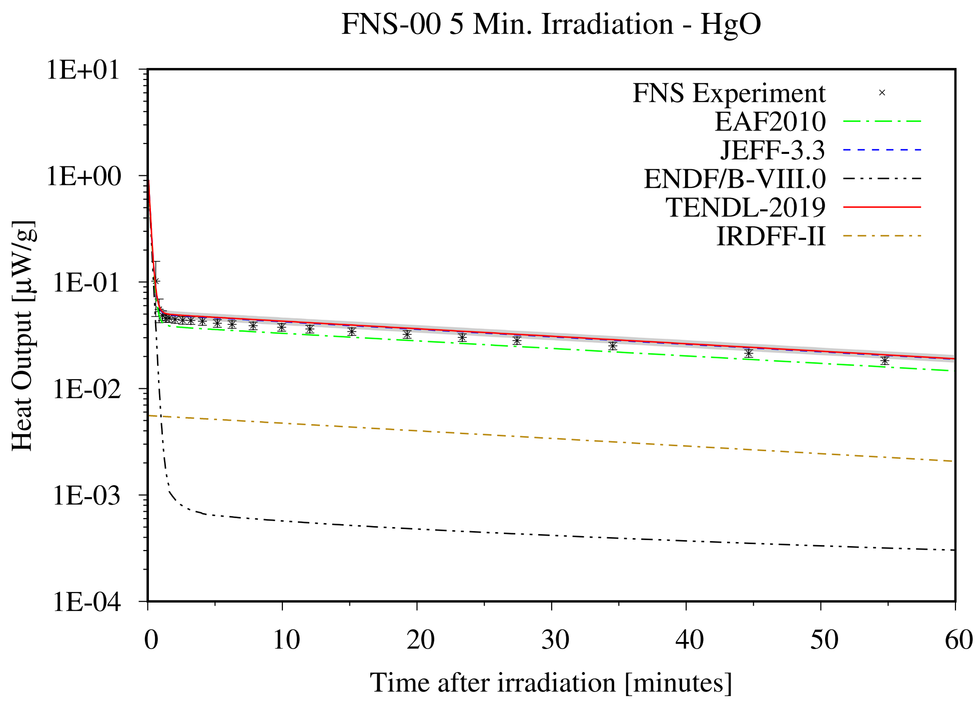
Comments on Gold 5-minute experiments:

No library prediction is particularly good, but at least TENDL-2019 and EAF2010 produce the correct two-step decay profile, with dominance in the first 1 minute of cooling by a short-lived nuclide, followed by nearly equal contributions from Au196 and Au196n at all remaining cooling times. Interestingly, while the two libraries agree on the contributing nuclides for the second stage, they predict different nuclides for the first 1 minute: TENDL-2019 predicts that Au196m should be dominant, while EAF2010 predicts in is Au197m. These nuclides have nearly identical half-lives and so the profile of each seems to capture the measurement profile well – it is difficult to judge which is correct, although TENDL-2019 also shows a minor Au197m contribution; further analysis is warranted.
Overall, both TENDL-2019 and EAF2010 overpredict by about 30% the experimental values. Meanwhile JEFF-3.3, ENDF/B-VIII.0, and IRDFF-II only capture Au196 production (i.e. the usual absence of metastable production channels) and thus underpredict (coincidently by about 30%) at all cooling times. all underpredict by a similar percentage.
Incorrect branching ratios for (n,2n) to Au196, Au196m, and Au196n in TENDL-2019 could still be the source of overprediction with that library.


FNS-00 5 Min. Irradiation - Au - TENDL-2019
FNS-00 5 Min. Irradiation - Au - EAF2010
FNS-00 5 Min. Irradiation - Au - JEFF-3.3
FNS-00 5 Min. Irradiation - Au - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
% decay heat contribution
100
80
60
40
20
0
1E-06
1E-05
1E-04
Time after irradiation [years]
total
Au198
Au195m
Au196
Au196n
Au197m
Au196m
Pt197m
00 Exp


FNS-00 5 Min. Irradiation - Au - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
196mAu
197mAu
195mAu
196nAu
196Au
198Au
197mPt
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]

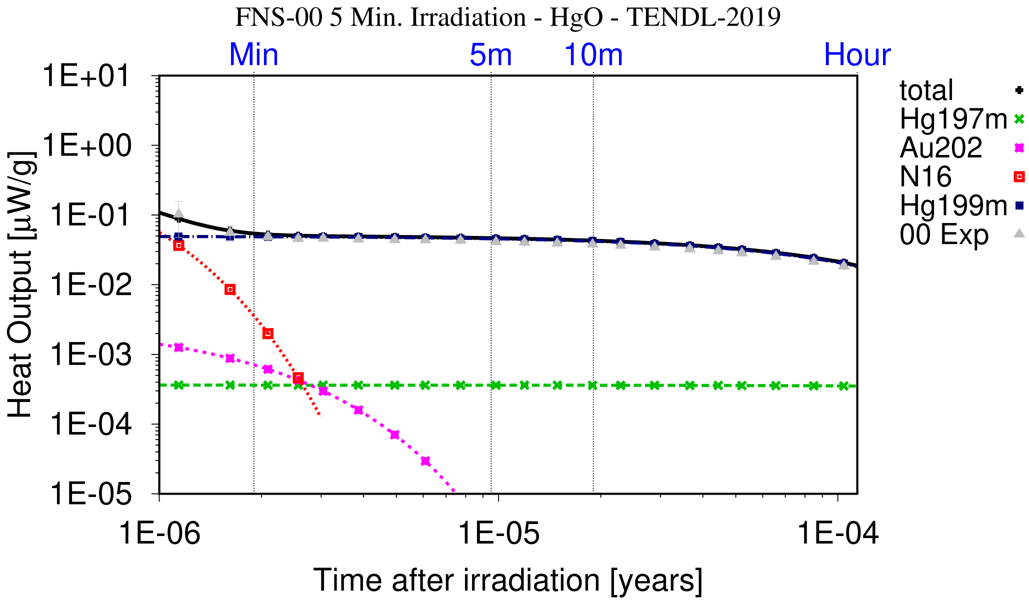
Mercury



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
0.60	1.02$E-$01 +/-53%	8.85$E-$02 +/-5%	1.15	2.63	1.32	1.16	18.48
0.85	5.54$E-$02 +/-25%	5.96$E-$02 +/-7%	0.93	5.41	1.14	0.94	10.08
1.10	4.85$E-$02 +/-11%	5.25$E-$02 +/-8%	0.92	14.30	1.17	0.94	8.86
1.35	4.56$E-$02 +/-8%	5.06$E-$02 +/-8%	0.90	27.12	1.15	0.91	8.37
1.60	4.58$E-$02 +/-8%	4.98$E-$02 +/-8%	0.92	42.47	1.18	0.93	8.44
2.03	4.46$E-$02 +/-8%	4.92$E-$02 +/-8%	0.91	49.13	1.17	0.92	8.28
2.60	4.38$E-$02 +/-8%	4.87$E-$02 +/-8%	0.90	55.59	1.17	0.91	8.21
3.20	4.35$E-$02 +/-8%	4.81$E-$02 +/-8%	0.90	60.19	1.18	0.92	8.24
4.07	4.28$E-$02 +/-8%	4.74$E-$02 +/-8%	0.90	64.03	1.17	0.91	8.22
5.17	4.10$E-$02 +/-8%	4.65$E-$02 +/-8%	0.88	64.02	1.15	0.89	8.01
6.27	4.00$E-$02 +/-8%	4.57$E-$02 +/-8%	0.88	64.40	1.14	0.89	7.97
7.83	3.89$E-$02 +/-8%	4.45$E-$02 +/-8%	0.87	65.03	1.14	0.88	7.94
9.95	3.76$E-$02 +/-8%	4.30$E-$02 +/-8%	0.88	65.94	1.14	0.89	7.96
12.05	3.62$E-$02 +/-8%	4.15$E-$02 +/-8%	0.87	66.15	1.13	0.88	7.93
15.17	3.43$E-$02 +/-8%	3.95$E-$02 +/-8%	0.87	66.25	1.13	0.88	7.90
19.27	3.23$E-$02 +/-8%	3.69$E-$02 +/-8%	0.87	66.68	1.14	0.88	7.95
23.37	3.01$E-$02 +/-8%	3.45$E-$02 +/-8%	0.87	66.18	1.14	0.88	7.95
27.43	2.82$E-$02 +/-8%	3.23$E-$02 +/-8%	0.87	65.46	1.14	0.88	7.96
34.55	2.51$E-$02 +/-8%	2.88$E-$02 +/-8%	0.87	63.73	1.14	0.88	7.97
44.65	2.14$E-$02 +/-8%	2.44$E-$02 +/-8%	0.87	60.69	1.14	0.88	8.00
54.75	1.83$E-$02 +/-8%	2.08$E-$02 +/-8%	0.88	57.58	1.15	0.89	8.09
mean % diff. from E			13	95	13	11	88
mean χ^2			2.30	129.54	2.30	1.85	103.75

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Hg199m	42.10m	0.93	25%	8%

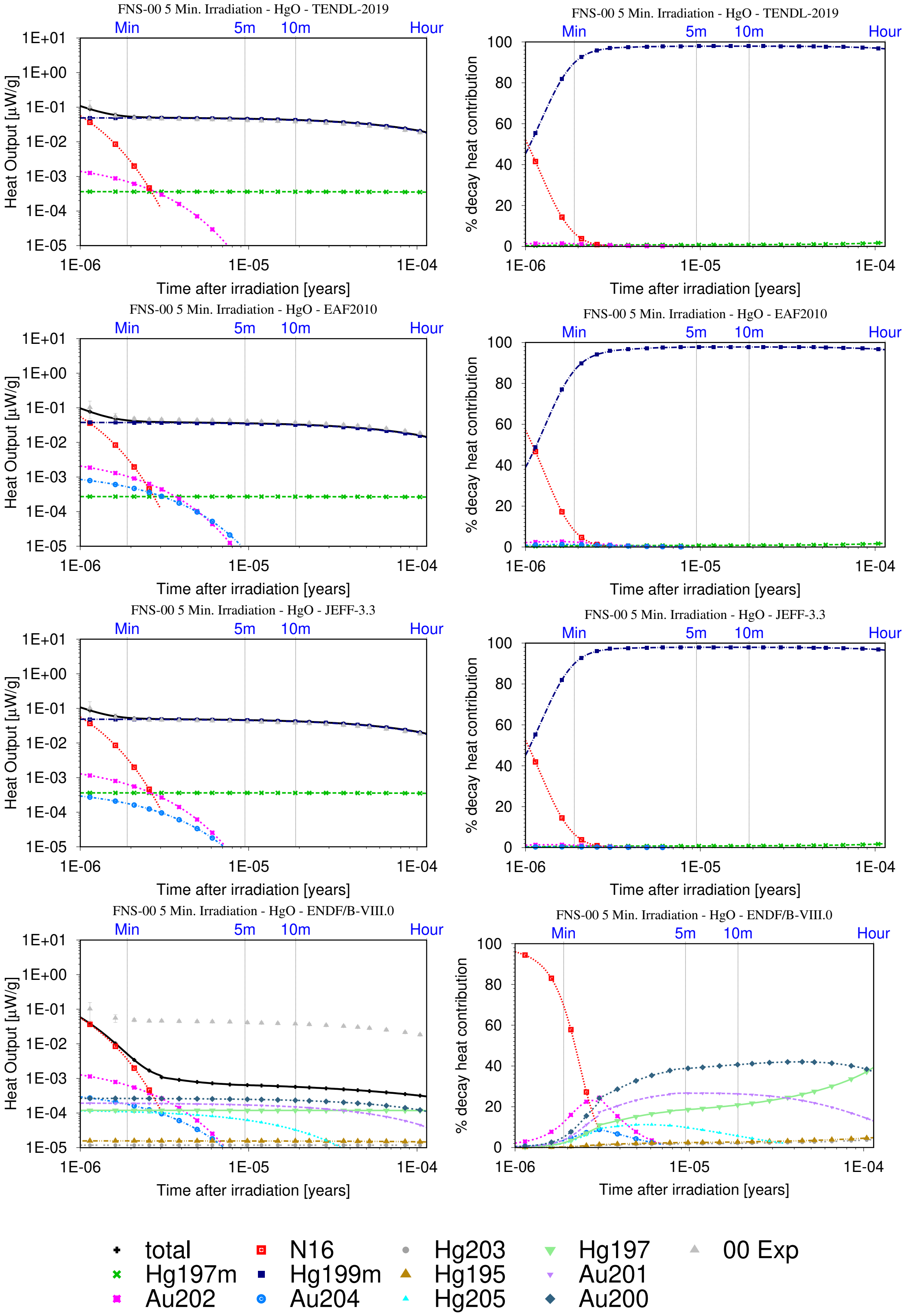


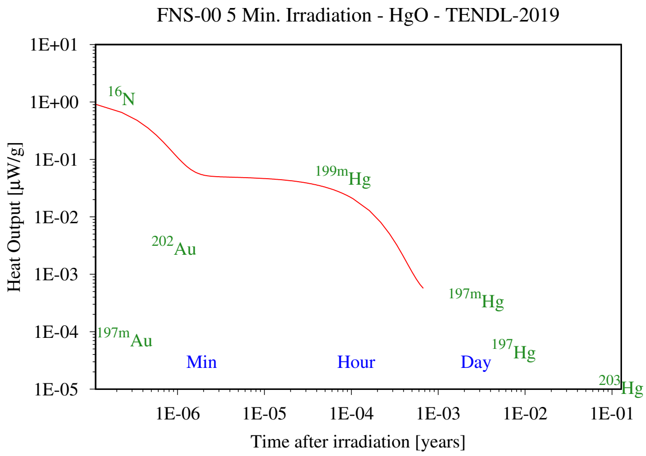
Mercury, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Au202	28.80s	Hg202(n,p)Au202	100.0
Au204	39.79s	Hg204(n,p)Au204	100.0
Hg205	5.20m	Hg204(n,γ)Hg205	100.0
Au201	26.00m	Hg201(n,p)Au201	97.0
		Hg202(n,d)Au201	2.3
Hg199m	42.10m	Hg200(n,2n)Hg199m	87.3
		Hg199(n,n′)Hg199m	12.5
Au200	48.40m	Hg200(n,p)Au200	98.9
Hg195	9.90h	Hg196(n,2n)Hg195	99.9
Hg197m	23.90h	Hg198(n,2n)Hg197m	100.0
Hg197	2.69d	Hg198(n,2n)Hg197	99.3
Hg203	46.62d	Hg204(n,2n)Hg203	99.4

Comments on Mercury 5-minute experiments:

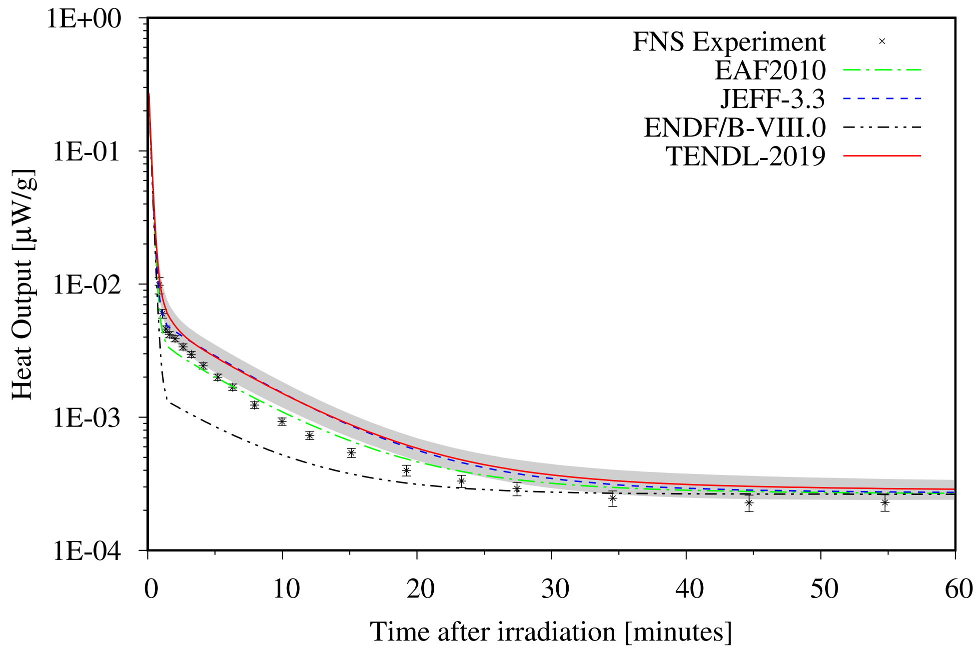
A textbook case exemplifying the problem (for ENDF/B-VIII.0) when missing the production of isomeric states. TENDL-2019, JEFF-3.3, and EAF2010 all agree regarding the complete dominance of the Hg199m nuclide (at all but the first cooling step where the usual N16 signal is seen), produced by a combination of (n,2n) reactions on Hg200 and (n,n′) reactions on Hg199, but ENDF/B-VIII.0 does not include either of these channels and so massively underpredicts relative to the experiment. The other libraries are not perfect and there could be justification for modifying some of the production cross sections for this uniquely predominant metastable. IRDFF-II includes only the (n,n′) reaction channel on Hg199 for this simulation which explains underprediction of the experiment with that library.


FNS-00 5 Min. Irradiation - HgO - TENDL-2019
FNS-00 5 Min. Irradiation - HgO - EAF2010
FNS-00 5 Min. Irradiation - HgO - JEFF-3.3
FNS-00 5 Min. Irradiation - HgO - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
100
80
60
40
20
0
total
N16
Hg203
Hg197
00 Exp
Hg197m
Hg199m
Hg195
Au201
Au202
Au204
Hg205
Au200


FNS-00 5 Min. Irradiation - HgO - TENDL-2019
Heat Output [µW/g]
1E+01
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
16N
199mHg
202Au
197mHg
197mAu
197Hg
203Hg
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
Time after irradiation [years]

Thallium

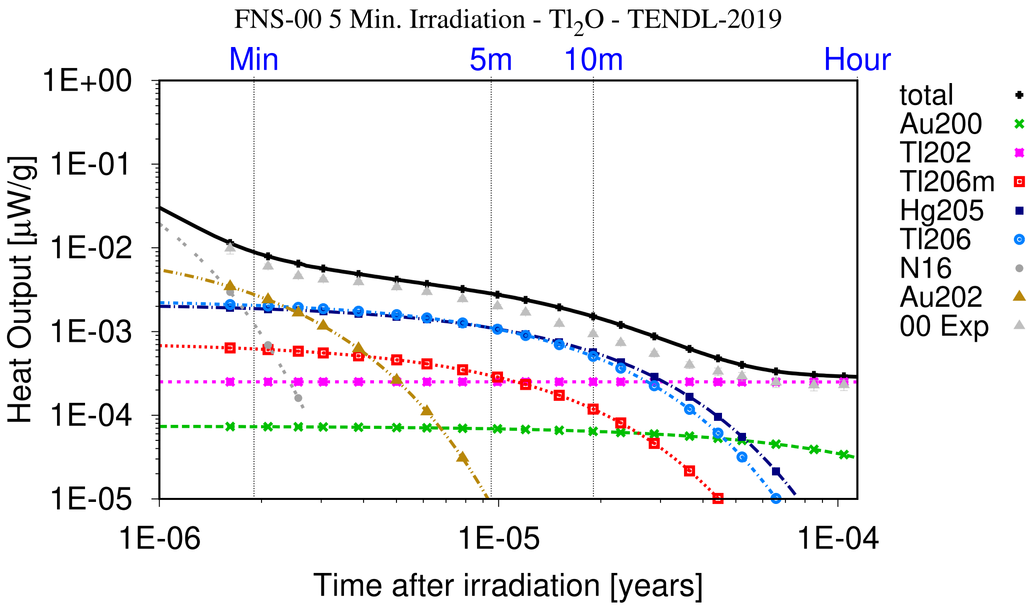
FNS-00 5 Min. Irradiation - Tl_2O



Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	9.81$E-$03 +/-14%	1.14$E-$02 +/-25%	0.86	2.26	1.43	1.17
1.10	5.99$E-$03 +/-7%	7.90$E-$03 +/-27%	0.76	2.91	1.37	1.02
1.35	4.59$E-$03 +/-6%	6.49$E-$03 +/-26%	0.71	3.07	1.26	0.90
1.60	4.17$E-$03 +/-5%	5.66$E-$03 +/-24%	0.74	3.23	1.26	0.88
2.03	3.89$E-$03 +/-5%	4.86$E-$03 +/-23%	0.80	3.18	1.27	0.88
2.63	3.38$E-$03 +/-5%	4.16$E-$03 +/-23%	0.81	2.98	1.21	0.84
3.23	2.97$E-$03 +/-5%	3.70$E-$03 +/-23%	0.80	2.82	1.16	0.80
4.12	2.43$E-$03 +/-5%	3.22$E-$03 +/-23%	0.76	2.58	1.08	0.74
5.22	2.00$E-$03 +/-6%	2.76$E-$03 +/-23%	0.72	2.40	1.02	0.71
6.32	1.68$E-$03 +/-6%	2.39$E-$03 +/-23%	0.70	2.28	0.99	0.69
7.93	1.23$E-$03 +/-6%	1.94$E-$03 +/-23%	0.64	1.97	0.89	0.63
9.98	9.29$E-$04 +/-6%	1.52$E-$03 +/-22%	0.61	1.78	0.84	0.61
12.05	7.29$E-$04 +/-7%	1.20$E-$03 +/-21%	0.61	1.63	0.83	0.61
15.12	5.41$E-$04 +/-8%	8.77$E-$04 +/-20%	0.62	1.44	0.82	0.63
19.22	3.99$E-$04 +/-9%	6.20$E-$04 +/-19%	0.64	1.24	0.82	0.66
23.32	3.31$E-$04 +/-11%	4.79$E-$04 +/-19%	0.69	1.13	0.85	0.73
27.43	2.91$E-$04 +/-12%	4.00$E-$04 +/-20%	0.73	1.04	0.86	0.77
34.55	2.47$E-$04 +/-13%	3.34$E-$04 +/-21%	0.74	0.92	0.83	0.79
44.67	2.28$E-$04 +/-14%	3.03$E-$04 +/-20%	0.75	0.86	0.82	0.80
54.77	2.29$E-$04 +/-14%	2.91$E-$04 +/-18%	0.79	0.87	0.85	0.83
mean % diff. from E			40	44	18	33
mean χ^2			37.27	69.42	6.42	30.90

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Tl202	12.24d	0.75	14%	5%

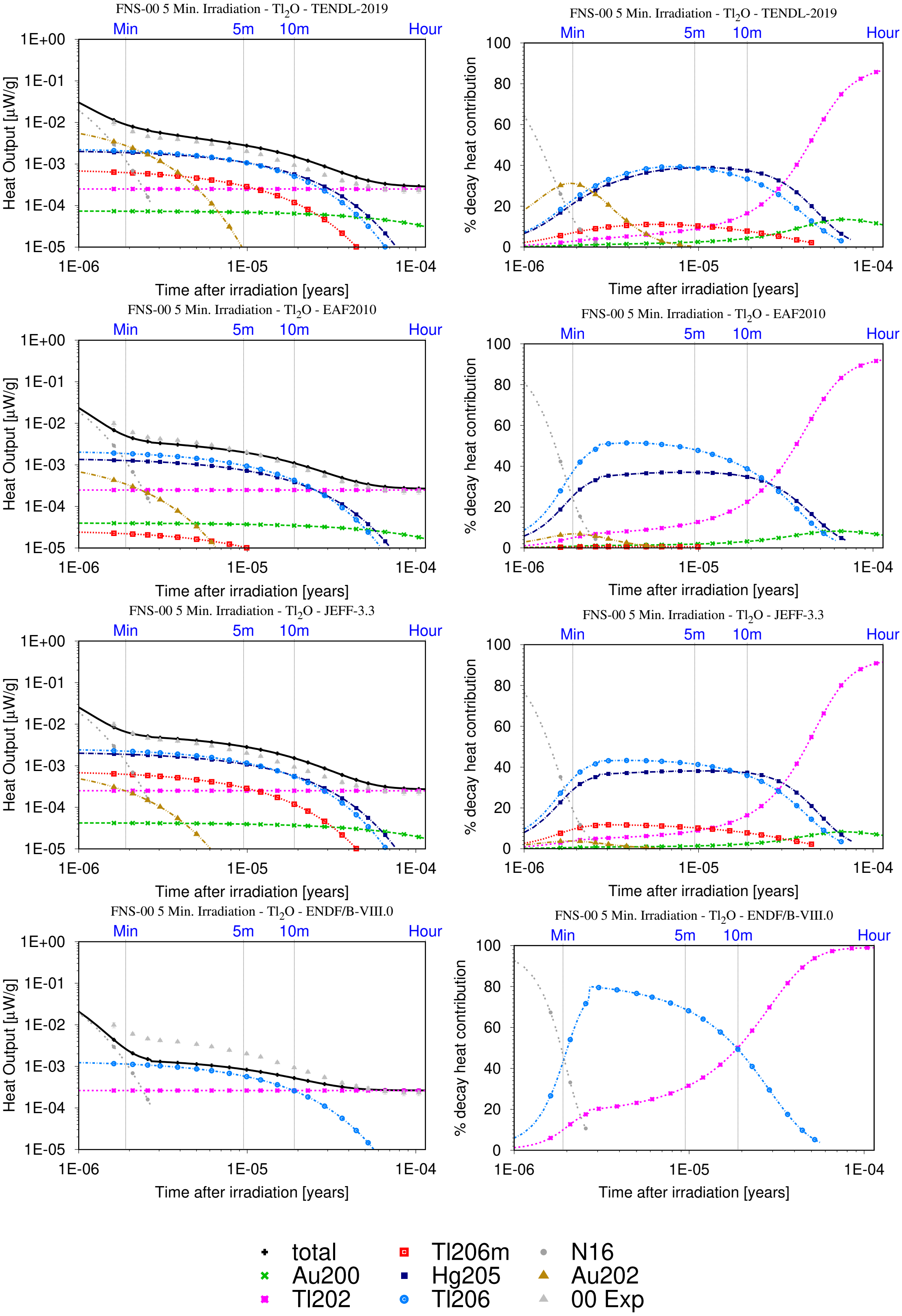


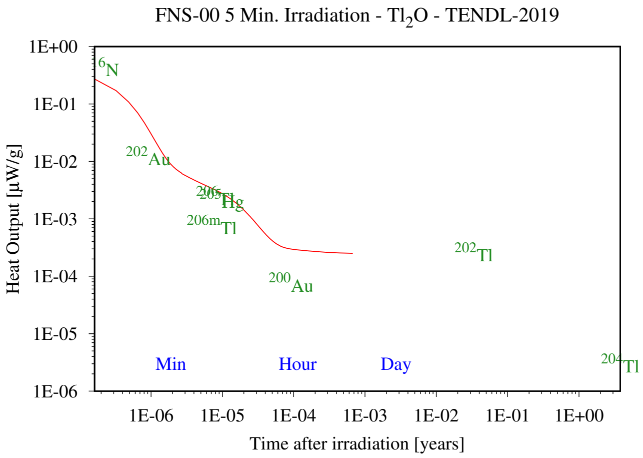
Thallium, TENDL-2019 5-minute pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
N16	7.13s	O16(n,p)N16	100.0
Au202	28.80s	Tl205(n,α)Au202	100.0
Tl206m	3.76m	Tl205(n,γ)Tl206m	100.0
Tl206	4.20m	Tl205(n,γ)Tl206	97.7
		Tl205(n,γ)Tl206m(IT)Tl206	2.3
Hg205	5.20m	Tl205(n,p)Hg205	100.0
Au200	48.40m	Tl203(n,α)Au200	100.0
Tl202	12.24d	Tl203(n,2n)Tl202	100.0

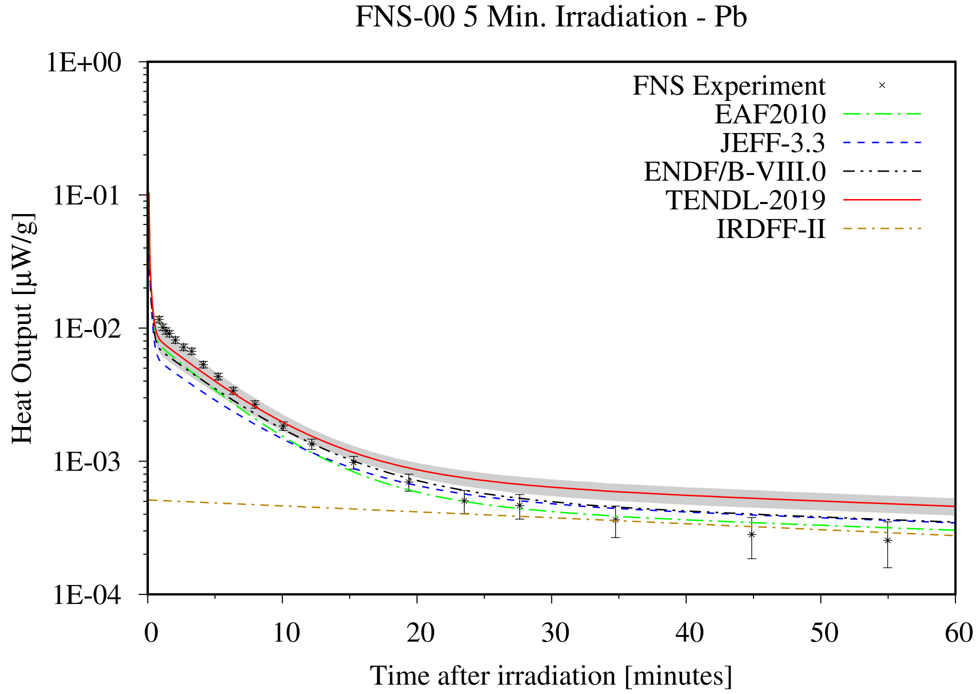
Comments on Thallium 5-minute experiments:

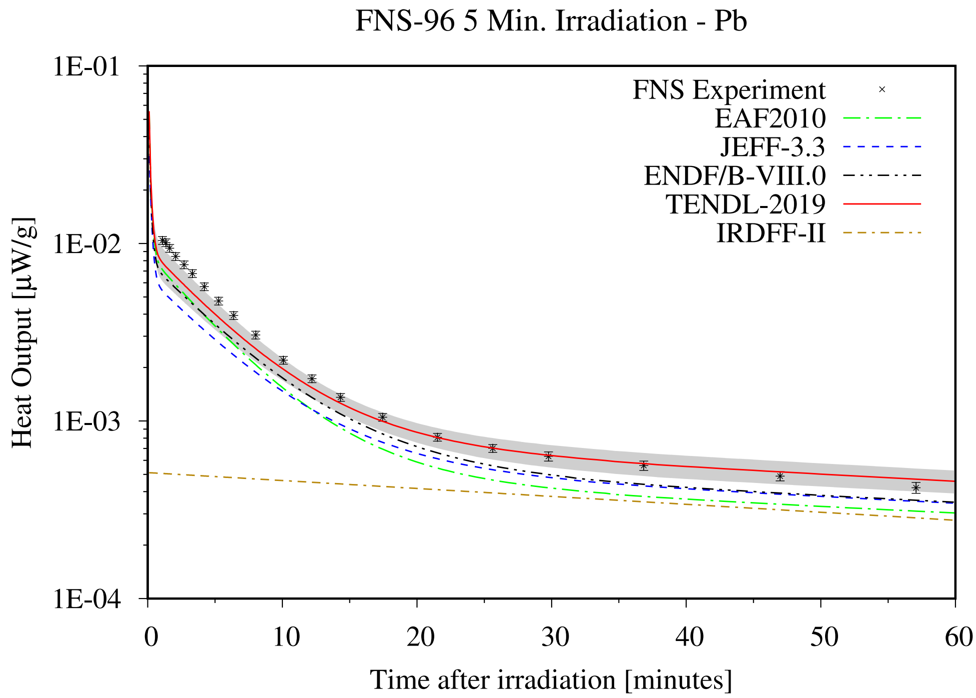
Reasonable shape agreement for TENDL-2019 and JEFF-3.3, but only EAF2010 can be considered to produce a good overall agreement to the experiment. For TENDL-2019, in particular, the large discrepancies for cooling times between 1 and 30 minutes suggest that the production routes for the Hg205 and Tl206 nuclides that contribute and dominate almost equally in this time range may need re-evaluation. ENDF/B-VIII.0 clearly mis-represents the profile at cooling times below 30 minutes because, surprisingly, it does not contain the (n,p) channel to produce Hg205 from Tl205.


FNS-00 5 Min. Irradiation - Tl2O - TENDL-2019
FNS-00 5 Min. Irradiation - Tl2O - EAF2010
FNS-00 5 Min. Irradiation - Tl2O - JEFF-3.3
FNS-00 5 Min. Irradiation - Tl2O - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
0
20
40
60
80
100
total
Au200
Tl202
Tl206m
Hg205
Tl206
N16
Au202
00 Exp


FNS-00 5 Min. Irradiation - Tl2O - TENDL-2019
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
6N
202Au
206Hg
205Hg
206mTl
202Tl
200Au
204Tl
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Lead


FNS-00 5 Min. Irradiation - Pb
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E+00
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]

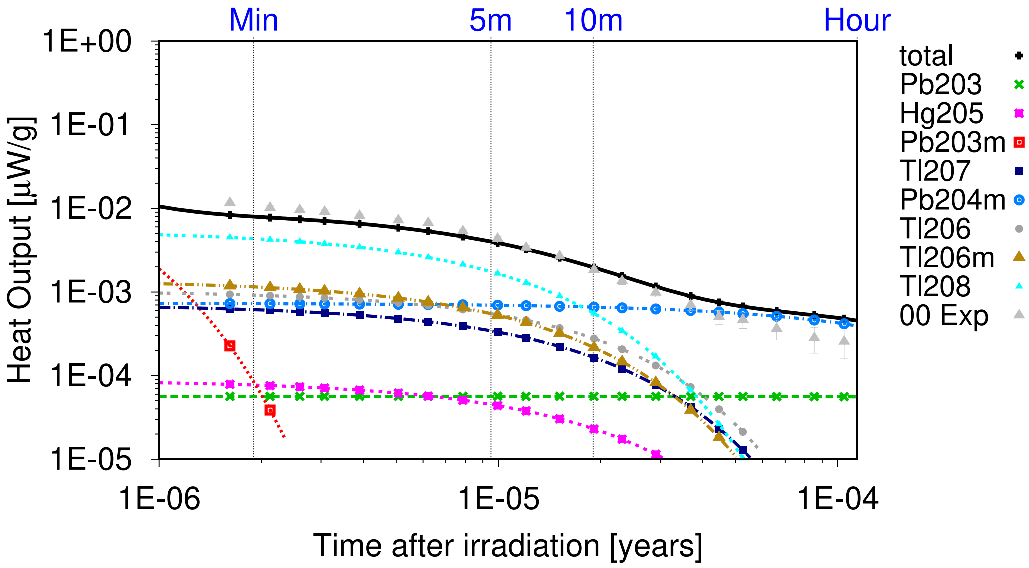

FNS-96 5 Min. Irradiation - Pb
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
IRDFF-II
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
0
10
20
30
40
50
60
Time after irradiation [minutes]

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
0.85	1.16$E-$02 +/-6%	8.33$E-$03 +/-21%	1.39	1.64	1.52	2.00	22.87
1.12	1.01$E-$02 +/-6%	7.76$E-$03 +/-21%	1.31	1.53	1.43	1.88	20.05
1.37	9.53$E-$03 +/-6%	7.38$E-$03 +/-21%	1.29	1.51	1.42	1.85	18.87
1.62	9.09$E-$03 +/-6%	7.06$E-$03 +/-21%	1.29	1.50	1.42	1.84	18.05
2.05	8.14$E-$03 +/-6%	6.55$E-$03 +/-21%	1.24	1.45	1.38	1.78	16.24
2.67	7.19$E-$03 +/-6%	5.88$E-$03 +/-20%	1.22	1.41	1.37	1.73	14.42
3.27	6.69$E-$03 +/-6%	5.31$E-$03 +/-20%	1.26	1.45	1.43	1.78	13.51
4.13	5.32$E-$03 +/-6%	4.60$E-$03 +/-19%	1.16	1.33	1.33	1.62	10.85
5.23	4.33$E-$03 +/-6%	3.85$E-$03 +/-18%	1.12	1.28	1.32	1.56	8.92
6.35	3.39$E-$03 +/-6%	3.25$E-$03 +/-17%	1.04	1.18	1.25	1.43	7.06
7.97	2.67$E-$03 +/-6%	2.57$E-$03 +/-16%	1.04	1.17	1.28	1.41	5.67
10.07	1.84$E-$03 +/-7%	1.96$E-$03 +/-14%	0.94	1.06	1.20	1.26	3.99
12.18	1.35$E-$03 +/-9%	1.54$E-$03 +/-13%	0.87	0.99	1.16	1.16	2.98
15.30	9.80$E-$04 +/-11%	1.16$E-$03 +/-12%	0.84	0.98	1.18	1.11	2.24
19.40	6.98$E-$04 +/-15%	8.91$E-$04 +/-12%	0.78	0.94	1.15	1.03	1.66
23.52	5.04$E-$04 +/-19%	7.50$E-$04 +/-13%	0.67	0.83	1.01	0.89	1.25
27.63	4.65$E-$04 +/-21%	6.70$E-$04 +/-14%	0.69	0.88	1.05	0.92	1.21
34.75	3.63$E-$04 +/-27%	5.91$E-$04 +/-15%	0.61	0.80	0.94	0.82	1.01
44.87	2.82$E-$04 +/-34%	5.28$E-$04 +/-15%	0.53	0.70	0.81	0.71	0.87
54.97	2.55$E-$04 +/-38%	4.80$E-$04 +/-15%	0.53	0.70	0.81	0.71	0.88
mean % diff. from E			29	23	21	31	66
mean χ^2			8.07	15.04	13.50	30.60	152.21

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%Δ**$\mathbf{C}^{nuc}$
Pb204m	1.13h	0.67	20%	17%

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

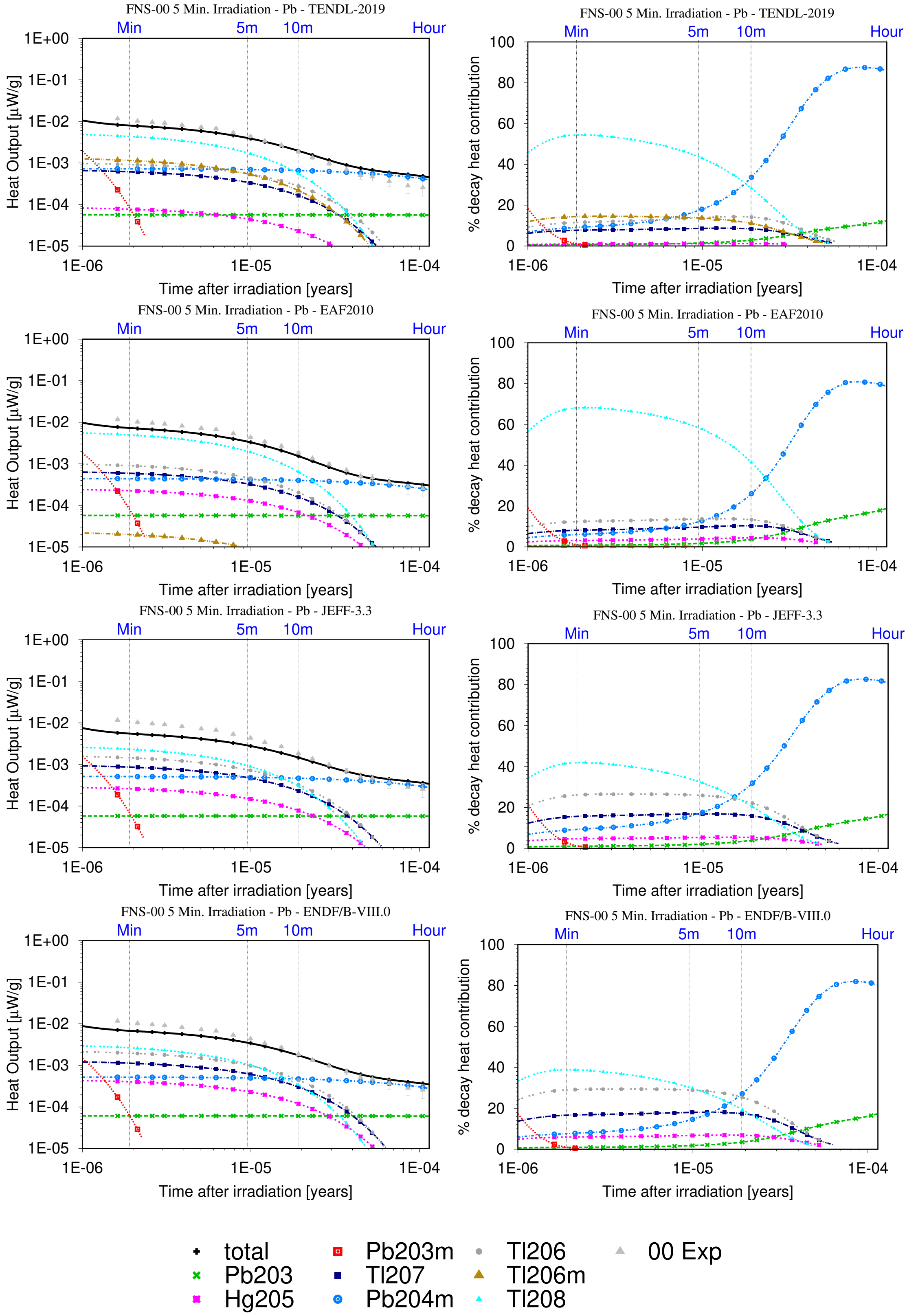


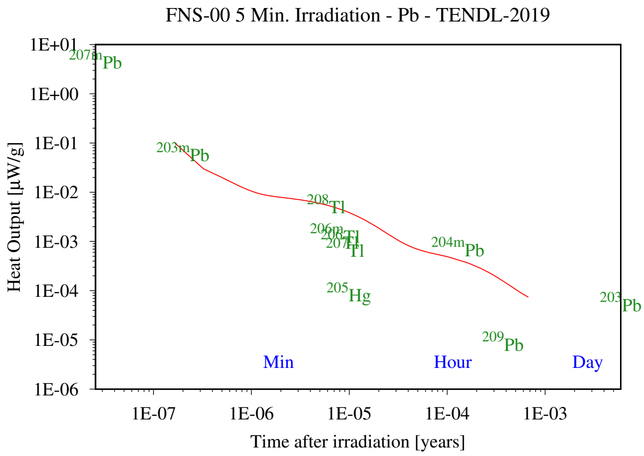
Lead, TENDL-2019 5-minute pathway analysis

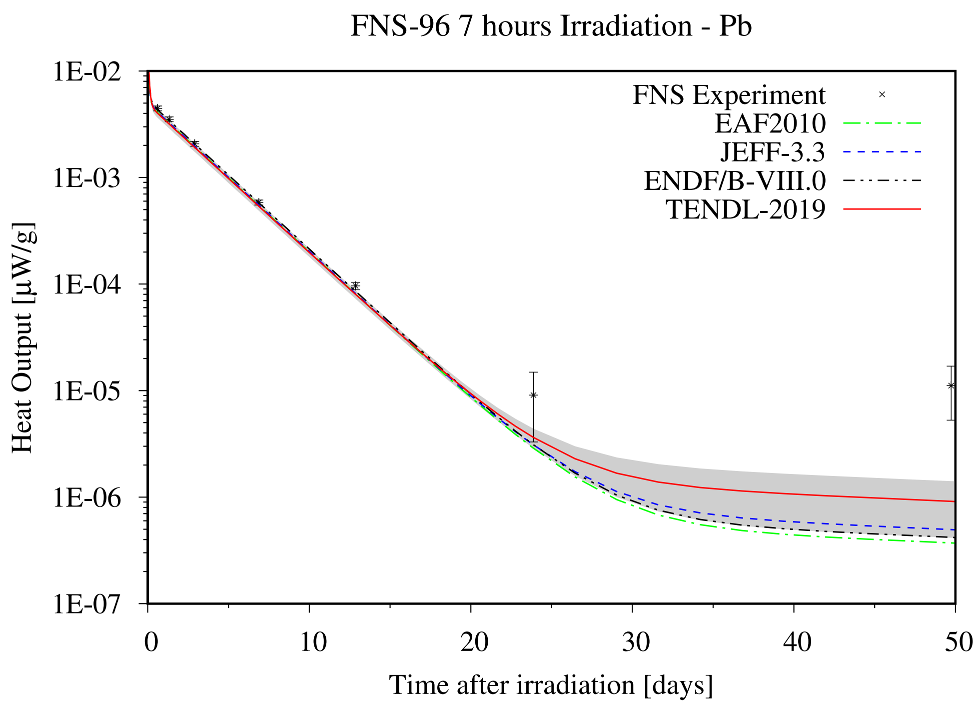
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Pb203m	6.29s	Pb204(n,2n)Pb203m	97.4
		Pb204(n,2n)Pb203n(IT)Pb203m	2.6
Tl208	3.05m	Pb208(n,p)Tl208	100.0
Tl206m	3.76m	Pb206(n,p)Tl206m	99.1
Tl206	4.20m	Pb206(n,p)Tl206	87.6
		Pb206(n,p)Tl206m(IT)Tl206	9.7
		Pb207(n,d)Tl206	1.9
Tl207	4.77m	Pb207(n,p)Tl207	47.0
		Pb207(n,p)Tl207m(IT)Tl207	41.9
		Pb208(n,d)Tl207	6.2
		Pb208(n,np)Tl207	2.6
		Pb208(n,d)Tl207m(IT)Tl207	2.0
Hg205	5.20m	Pb208(n,α)Hg205	100.0
Pb204m	1.13h	Pb204(n,n$'$)Pb204m	100.0
Pb203	2.16d	Pb204(n,2n)Pb203m(IT)Pb203	51.3
		Pb204(n,2n)Pb203	47.3
		Pb204(n,2n)Pb203n(IT)Pb203m(IT)Pb203	1.4

Comments on Lead 5-minute experiments:

The experimental data sets are somewhat different from one-another, resulting in a very different comparison to the simulations. The 1996 experiment seems to be better captured by the simulations (particularly from TENDL-2019) at cooling times beyond 10 minutes. The more recent, 2000 experiment is overpredicted by the simulations (with all libraries) at these cooling times. This is an interesting deviation from the previous comparison [7] with earlier version of the libraries, where, instead, the 2000 experiment was better captured by the simulations. For TENDL, this appears to originate from a 30% increase in the total cross section associated with the (n,n$'$) reaction on Pb204 between TENDL-2014 and TENDL-2017, that remained in TENDL-2019, which leads to an increase in Pb204m production and its contribution to the decay heat (at long cooling times, when this nuclide dominates, the total decay heat has increased by this same $\sim$30% factor). However, in both batches the short term heat predictions, dominated by decay heat of Tl208 from (n,p) reactions on Pb208 in the simulations, seem to be low compared with the measured ones (as was the case in [7]). After 30 minutes of cooling EAF2010 and IRDFF-II yield the closest match to the experiment – Pb204(n,$'$)Pb204m is an important dosimetry reaction and is included in the official IRDFF-II release.


FNS-00 5 Min. Irradiation - Pb - TENDL-2019
FNS-00 5 Min. Irradiation - Pb - EAF2010
FNS-00 5 Min. Irradiation - Pb - JEFF-3.3
FNS-00 5 Min. Irradiation - Pb - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E+00
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-05
1E-04
100
80
60
40
20
0
total
Pb203
Hg205
Pb203m
Tl207
Pb204m
Tl206
Tl206m
Tl208
00 Exp

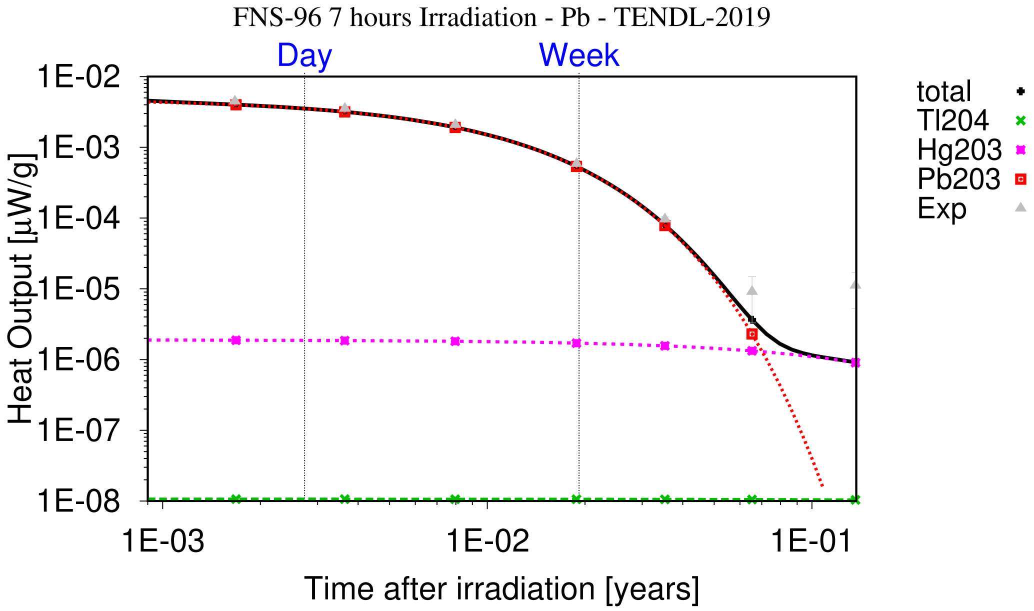

FNS-00 5 Min. Irradiation - Pb - TENDL-2019
Heat Output [μW/g]
Time after irradiation [years]
207mPb
203mPb
208Tl
206mTl
207Tl
205Hg
204mPb
209Pb
203Pb
Min
Hour
Day



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.61	$4.46E{-}03$ +/-5%	$4.01E{-}03$ +/-9%	1.11	1.03	1.09	1.08
1.33	$3.52E{-}03$ +/-5%	$3.18E{-}03$ +/-9%	1.11	1.03	1.09	1.08
2.91	$2.08E{-}03$ +/-5%	$1.92E{-}03$ +/-9%	1.08	1.00	1.06	1.06
6.88	$5.83E{-}04$ +/-5%	$5.38E{-}04$ +/-9%	1.08	1.01	1.07	1.06
12.87	$9.62E{-}05$ +/-8%	$8.01E{-}05$ +/-9%	1.20	1.12	1.19	1.18
23.88	$9.09E{-}06$ +/-64%	$3.64E{-}06$ +/-21%	2.50	2.92	3.15	2.93
49.73	$1.11E{-}05$ +/-53%	$9.14E{-}07$ +/-54%	12.17	26.52	29.93	22.40
mean % diff. from E			29	26	30	29
mean χ^2			2.84	0.98	2.33	2.07

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Pb203	2.16d	1.11	5%	9%
Hg203	46.62d	12.17	53%	55%

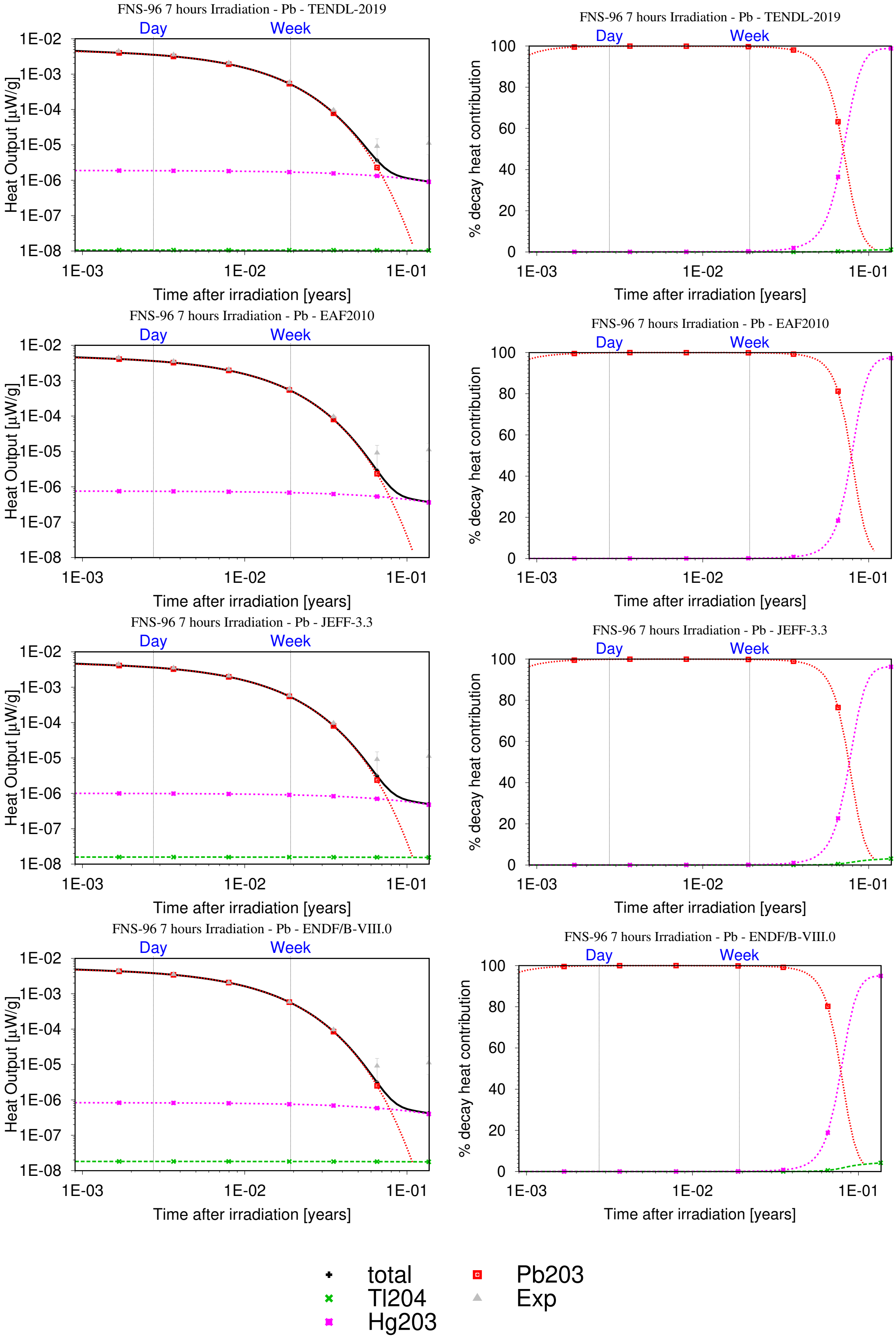


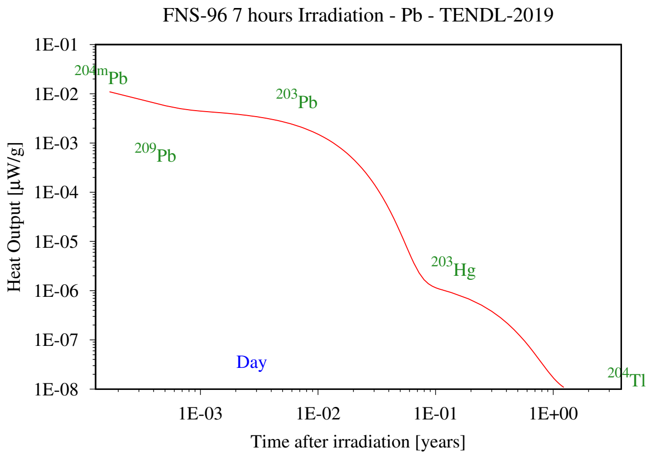
Lead,TENDL-2019 7-hours pathway analysis

Product	**$T_{1/2}$**	**Pathways**	**Path %**
Pb203	2.16d	Pb204(n,2n)Pb203m(IT)Pb203	51.7
		Pb204(n,2n)Pb203	47.1
		Pb204(n,2n)Pb203n(IT)Pb203m(IT)Pb203	1.2
Hg203	46.62d	Pb206(n,α)Hg203	99.9
Tl204	3.79y	Pb204(n,p)Tl204	99.5

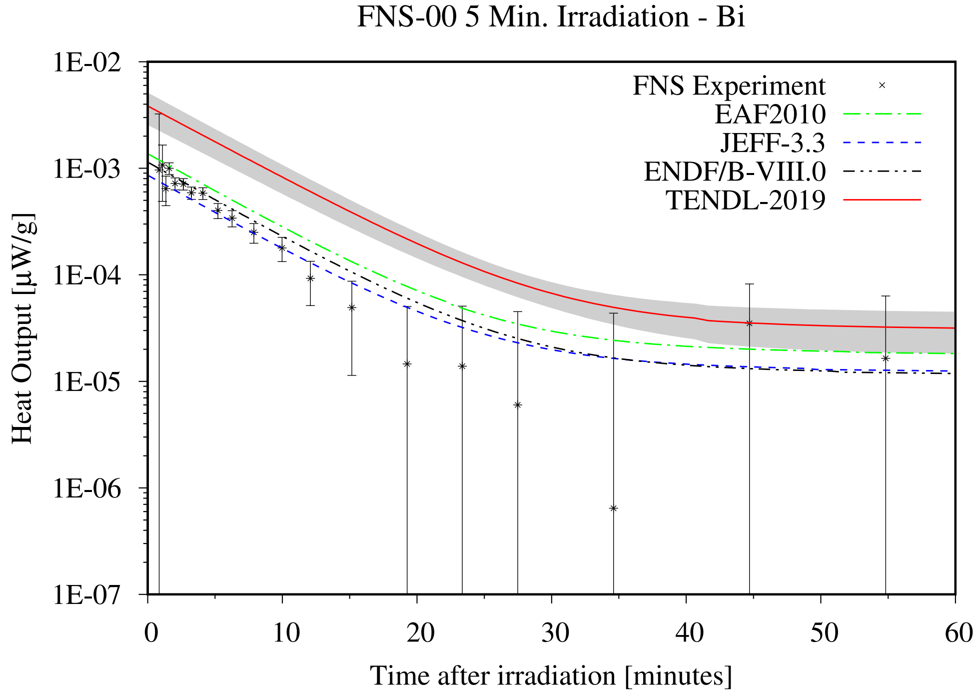
Comments on Lead 7-hour experiments:

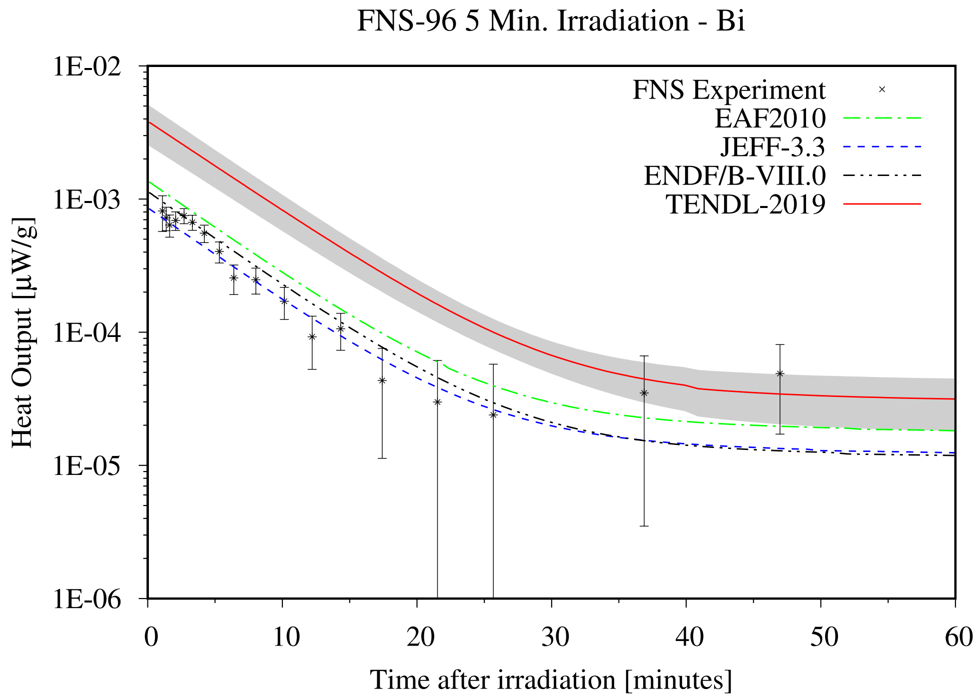
At shorter cooling times (below around 15 days) there is good agreement between the simulations and experiment (this is particularly clear in the nuclide contribution plots). However, at longer times (beyond around 20 days) – associated with the final two experimental data points – the simulations diverge (consistently with each other) from the experiment. This could be due to an unreported impurity in the sample, although an underestimation of Hg203 production from (n,α) reactions on Pb206 is not completely eliminated as a potential issue. In general, the experimental data is scarce and discrepant, and the experimental uncertainties are very large for these last points so more definitive analysis is not possible.


FNS-96 7 hours Irradiation - Pb - TENDL-2019
Day
Week
Heat Output [µW/g]
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
1E-03
1E-02
1E-01
Time after irradiation [years]
FNS-96 7 hours Irradiation - Pb - TENDL-2019
% decay heat contribution
100
80
60
40
20
0
FNS-96 7 hours Irradiation - Pb - EAF2010
FNS-96 7 hours Irradiation - Pb - JEFF-3.3
FNS-96 7 hours Irradiation - Pb - ENDF/B-VIII.0
total
Tl204
Hg203
Pb203
Exp


FNS-96 7 hours Irradiation - Pb - TENDL-2019
Heat Output [µW/g]
1E-01
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
204mPb
203Pb
209Pb
203Hg
204Tl
Day
1E-03
1E-02
1E-01
1E+00
Time after irradiation [years]

Bismuth

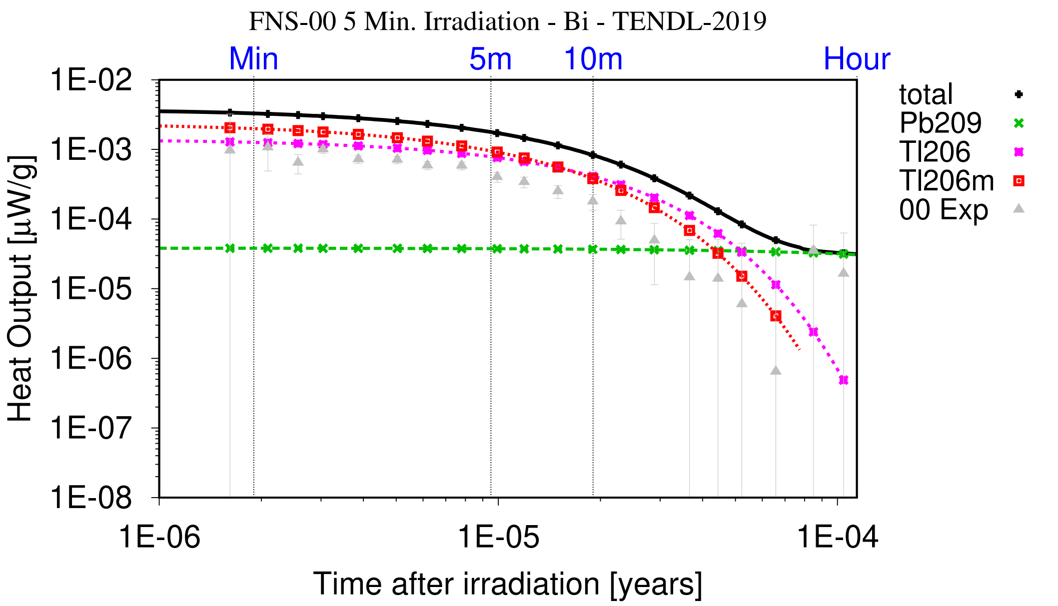

FNS-00 5 Min. Irradiation - Bi
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
0
10
20
30
40
50
60


FNS-96 5 Min. Irradiation - Bi
Heat Output [µW/g]
Time after irradiation [minutes]
FNS Experiment
EAF2010
JEFF-3.3
ENDF/B-VIII.0
TENDL-2019
1E-02
1E-03
1E-04
1E-05
1E-06
0
10
20
30
40
50
60

Times	FNS EXP. 5 mins	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Min.	μW/g	μW/g	E/C	E/C	E/C	E/C
0.85	9.65E−04 +/-235%	3.37E−03 +/-33%	0.29	0.97	0.81	1.29
1.10	1.07E−03 +/-54%	3.24E−03 +/-33%	0.33	1.12	0.93	1.49
1.35	6.44E−04 +/-31%	3.12E−03 +/-33%	0.21	0.70	0.58	0.93
1.60	1.00E−03 +/-12%	3.00E−03 +/-33%	0.33	1.14	0.95	1.51
2.03	7.20E−04 +/-13%	2.81E−03 +/-33%	0.26	0.88	0.73	1.16
2.65	7.12E−04 +/-12%	2.55E−03 +/-33%	0.28	0.96	0.80	1.27
3.25	5.89E−04 +/-13%	2.33E−03 +/-32%	0.25	0.87	0.73	1.16
4.10	5.83E−04 +/-13%	2.04E−03 +/-32%	0.29	0.99	0.82	1.31
5.22	4.02E−04 +/-16%	1.72E−03 +/-32%	0.23	0.82	0.68	1.08
6.27	3.41E−04 +/-17%	1.46E−03 +/-31%	0.23	0.82	0.68	1.08
7.88	2.51E−04 +/-21%	1.14E−03 +/-31%	0.22	0.78	0.64	1.02
9.98	1.79E−04 +/-26%	8.30E−04 +/-30%	0.22	0.77	0.63	1.01
12.08	9.27E−05 +/-45%	6.05E−04 +/-30%	0.15	0.55	0.45	0.71
15.17	4.92E−05 +/-77%	3.85E−04 +/-29%	0.13	0.46	0.37	0.59
19.27	1.46E−05 +/-247%	2.17E−04 +/-28%	0.07	0.24	0.19	0.29
23.37	1.39E−05 +/-266%	1.30E−04 +/-26%	0.11	0.37	0.29	0.43
27.48	6.00E−06 +/-653%	8.37E−05 +/-26%	0.07	0.24	0.17	0.26
34.60	6.43E−07 +/-6683%	4.96E−05 +/-31%	0.01	0.04	0.03	0.04
44.70	3.50E−05 +/-134%	3.54E−05 +/-40%	0.99	2.66	1.75	2.55
54.82	1.64E−05 +/-285%	3.23E−05 +/-42%	0.51	1.36	0.88	1.29
mean % diff. from E			799	189	282	175
mean χ^2			189.54	1.00	3.76	1.01

TENDL-2019 FNS-00 5 Min. nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	**%ΔC**^{nuc}
Pb209	3.25h	0.99	134%	43%

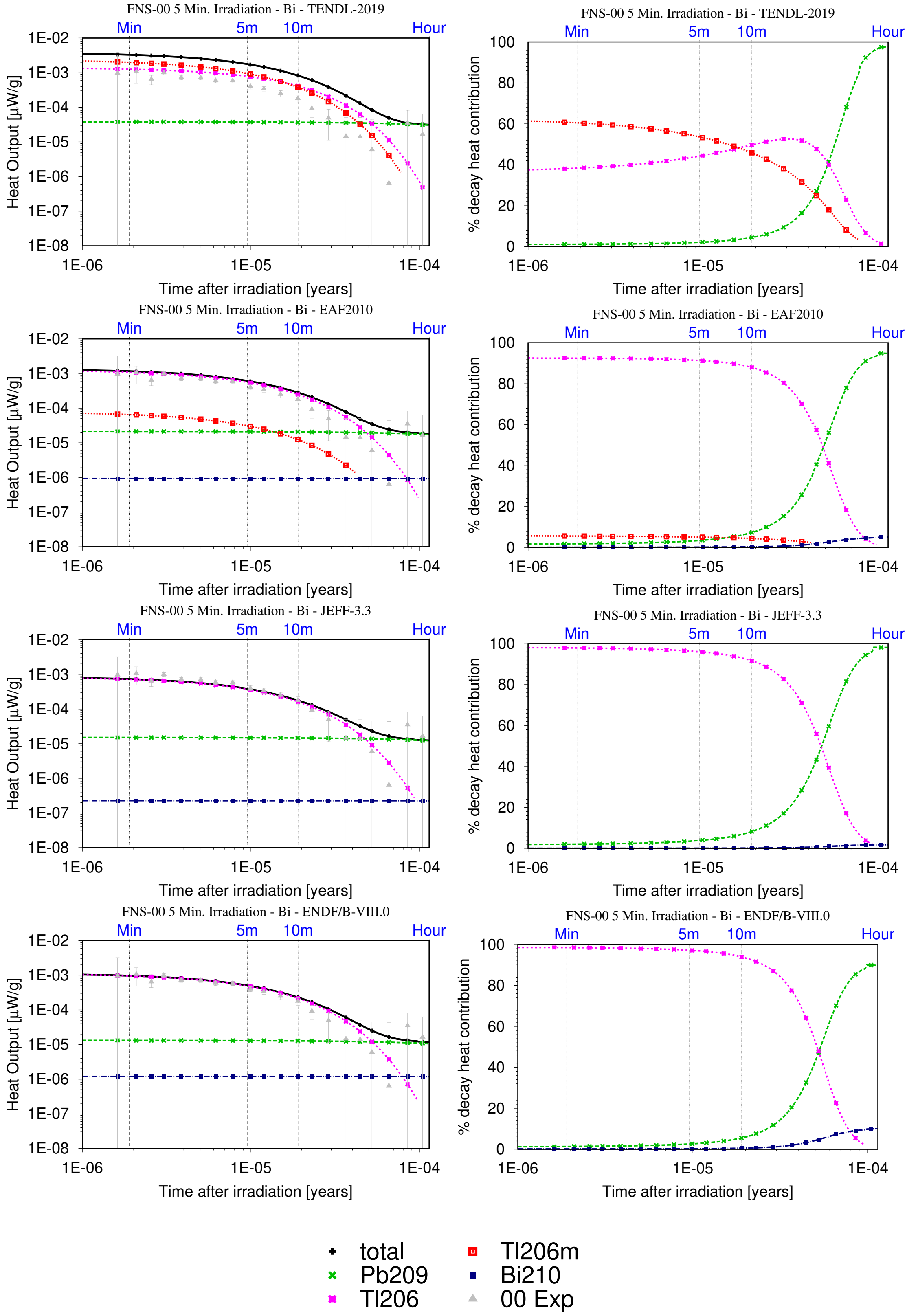


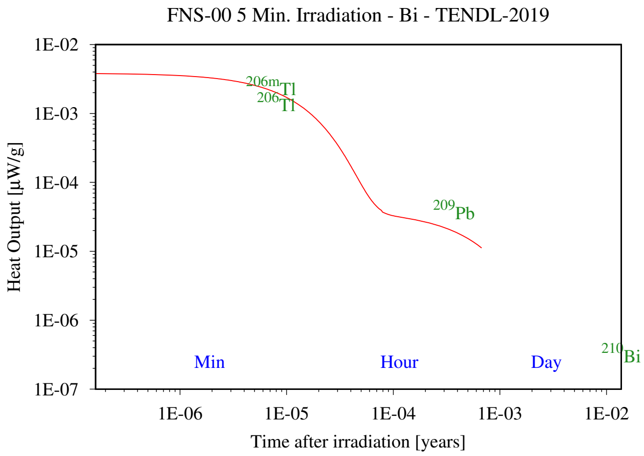
Bismuth, TENDL-2019 5-minute pathway analysis

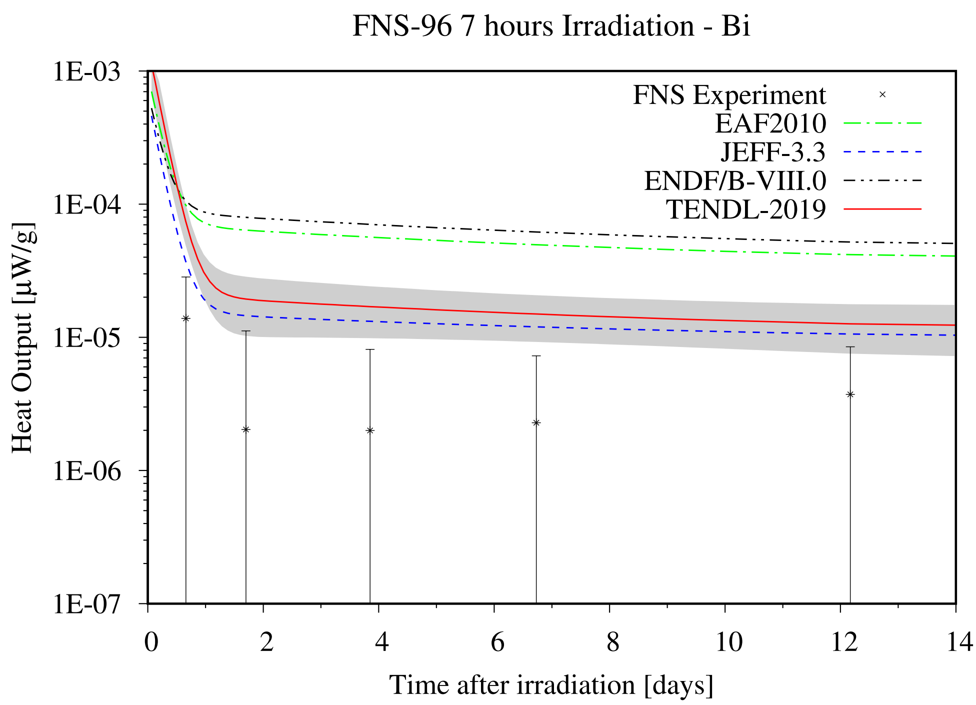
Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Tl206m	3.76m	Bi209(n,α)Tl206m	100.0
Tl206	4.20m	Bi209(n,α)Tl206	87.5
		Bi209(n,α)Tl206m(IT)Tl206	12.5
Pb209	3.25h	Bi209(n,p)Pb209	100.0
Bi210	5.01d	Bi209(n,γ)Bi210	100.0

Comments on Bismuth 5-minute experiments:

Some large differences and uncertainties can be seen between the two experimental datasets. This is particularly true at cooling times beyond around 20 minutes. At shorter decay times (where the experimental uncertainties are lower), simulations with JEFF-3.3, EAF2010, and ENDF/B-VIII.0 are in reasonably good agreement with the experimental profile and measurements, while TENDL-2019 sits apart. While the former three predict near-complete dominance of Tl206 during the first 20-30-minutes of cooling, TENDL-2019 instead predicts a combined contribution from Tl206 and its first-level metastable – all via (n,α) reactions on Bi209. The overprediction by TENDL-2019 suggests that the branching ratio for this channel with that library is wrong (EAF2010 also predicts Tl206m, but at a much lower level).
Nothing can be gleaned from the later cooling steps, particular with respect to the production of Pb209 – there is too much uncertainty.


FNS-00 5 Min. Irradiation - Bi - TENDL-2019
FNS-00 5 Min. Irradiation - Bi - EAF2010
FNS-00 5 Min. Irradiation - Bi - JEFF-3.3
FNS-00 5 Min. Irradiation - Bi - ENDF/B-VIII.0
Min
5m
10m
Hour
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
total
Pb209
Tl206
Tl206m
Bi210
00 Exp

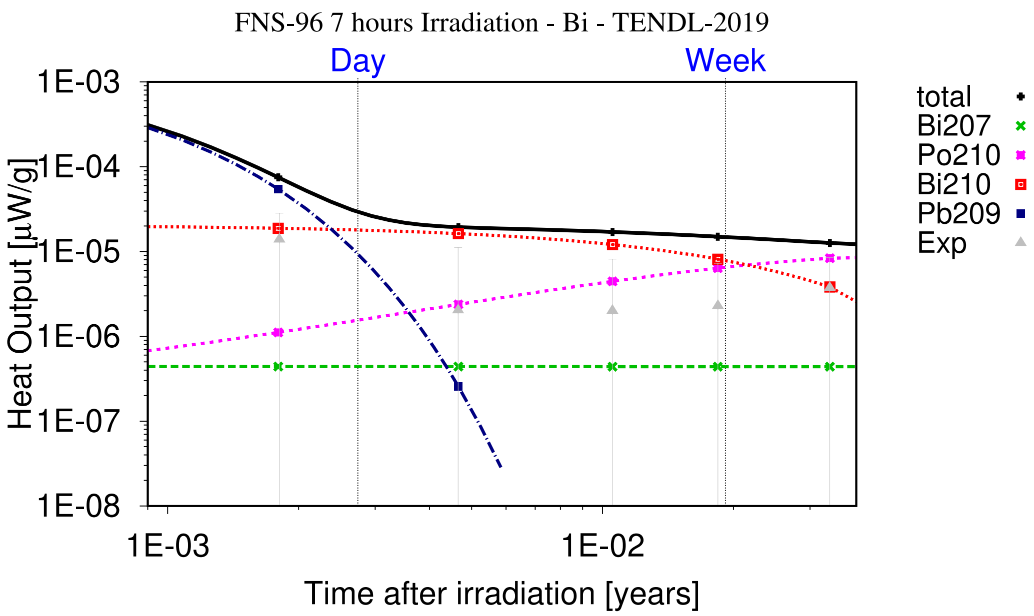

FNS-00 5 Min. Irradiation - Bi - TENDL-2019
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
Heat Output [µW/g]
206mTl
206Tl
209Pb
210Bi
Min
Hour
Day
1E-06
1E-05
1E-04
1E-03
1E-02
Time after irradiation [years]



Times	FNS EXP. 7 hrs	TENDL-2019		ENDF/B-VIII.0	EAF2010	JEFF-3.3
Days	μW/g	μW/g	E/C	E/C	E/C	E/C
0.66	$1.39E{-}05$ +/-105%	$7.48E{-}05$ +/-34%	0.19	0.13	0.14	0.37
1.70	$2.03E{-}06$ +/-451%	$1.94E{-}05$ +/-47%	0.10	0.03	0.03	0.14
3.85	$2.00E{-}06$ +/-307%	$1.70E{-}05$ +/-42%	0.12	0.03	0.04	0.15
6.73	$2.28E{-}06$ +/-218%	$1.50E{-}05$ +/-38%	0.15	0.04	0.05	0.19
12.17	$3.73E{-}06$ +/-128%	$1.26E{-}05$ +/-40%	0.30	0.07	0.09	0.35
mean % diff. from E			568	2363	1896	391
mean χ^2			7.44	96.52	62.63	2.73

TENDL-2019 FNS-96 7-hours nuclide E/C analysis

Product	$\mathbf{T_{1/2}}$	**E/C**	**%ΔE**	$\%\Delta C^{nuc}$
Bi210	5.01d	0.10	451%	56%

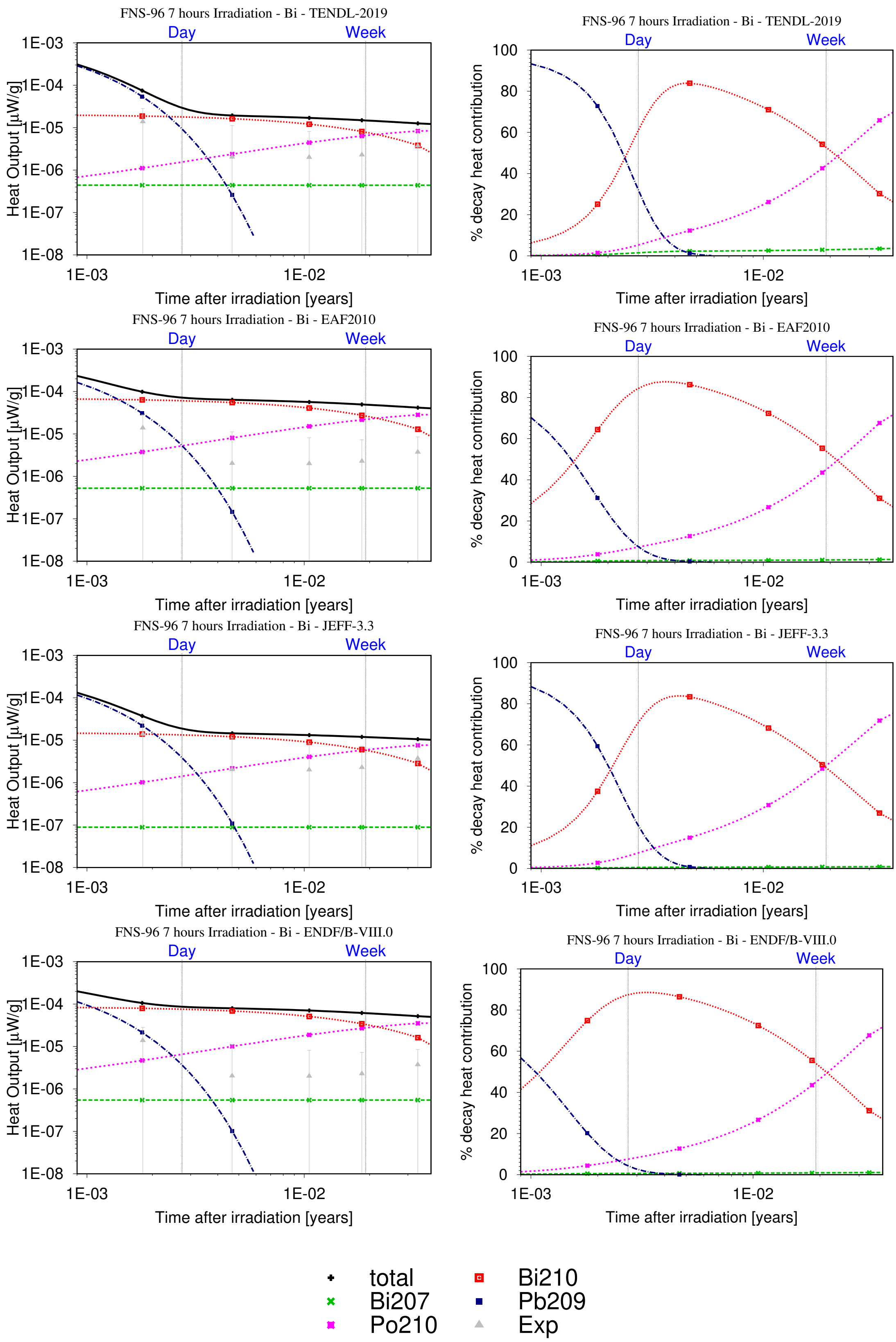


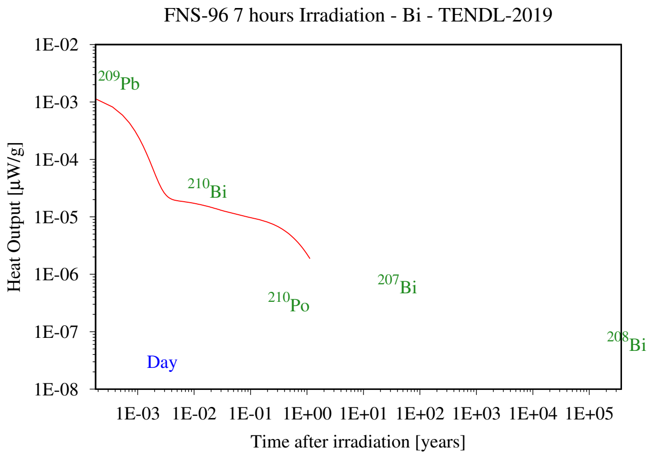
Bismuth,TENDL-2019 7-hours pathway analysis

Product	$\mathbf{T_{1/2}}$	**Pathways**	**Path %**
Pb209	3.25h	Bi209(n,p)Pb209	100.0
Bi210	5.01d	Bi209(n,γ)Bi210	100.0
Po210	138.39d	Bi209(n,γ)Bi210(β^-)Po210	100.0
Bi207	31.76y	Bi209(n,3n)Bi207	100.0

Comments on Bismuth 7-hour experiments:

A poor C/E agreement on this important element, but the experimental uncertainties are very large. As with the 5 minute experiments on bismuth, the simulations overpredict (to a varying degree depending on the library), although it is difficult to draw any conclusions about library deficiencies with such large experimental uncertainties.


FNS-96 7 hours Irradiation - Bi - TENDL-2019
FNS-96 7 hours Irradiation - Bi - EAF2010
FNS-96 7 hours Irradiation - Bi - JEFF-3.3
FNS-96 7 hours Irradiation - Bi - ENDF/B-VIII.0
Day
Week
Heat Output [µW/g]
% decay heat contribution
Time after irradiation [years]
1E-03
1E-02
1E-04
1E-05
1E-06
1E-07
1E-08
0
20
40
60
80
100
total
Bi207
Po210
Bi210
Pb209
Exp


FNS-96 7 hours Irradiation - Bi - TENDL-2019
Heat Output [μW/g]
1E-02
1E-03
1E-04
1E-05
1E-06
1E-07
1E-08
209Pb
210Bi
210Po
207Bi
208Bi
Day
1E-03 1E-02 1E-01 1E+00 1E+01 1E+02 1E+03 1E+04 1E+05
Time after irradiation [years]

5 Summary Tables

Here we present two summary tables, based on the 2000 5-minute and 1996 7-hour results, respectively. For each material we calculate a rough indicative measure of the quality of agreement between each nuclear library considered and the experimental results. This measure is the time-averaged absolute % difference between each calculated decay heat and its corresponding experimental value. In other words, each value in the following tables is calculated via:

$$\langle \%\Delta^x \rangle = \frac{1}{n_t} \sum_{t=1}^{n_t} \frac{100|C_t^x - E_t|}{E_t}, \quad (1)$$

where $\%\Delta^x$ is the % difference for library x, n_t is the total number of experimental points (times), C_t^x is the calculated decay heat at time t for library x, and E_t is the experimental measurement at t. Where there are no calculated values – due to deficiencies in a particular library – then the assumed difference contribution is 100%, which is mathematically correct but is perhaps a conservative estimate since in situations where a library severely overestimates the % difference may be much more than 100%. Note that the values in the summary tables below, and in the final row of the comparison tables for each material where they are also given, have been rounded to the nearest %. In the summary tables a colour coding is applied to the values, with green indicating a better than 10% agreement on average, orange better than 50%, and red worse than this.

Table of mean % differences from FNS-00 5 minute experiments, indicating the quality of agreement for different libraries for cooling times ranging from a few minutes up to 1 hour. Note that a blank entry under the IRDFF-II heading indicates cases where that library is not able to provide a meaningful result.

material	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Fluorine	2	2	8	2	34
Sodium	27	45	25	21	72
Magnesium	6	6	5	6	27
Aluminium	13	8	8	14	25
Silicon	10	13	6	7	30
Phosphorus	5	12	11	7	78
Sulphur	29	54	63	24	
Chlorine	13	44	32	44	
Potassium	4	15	25	6	
Calcium	19	14	13	18	
Scandium	7	63	9	7	
Titanium	3	7	3	3	52
Vanadium	14	14	13	14	87
Chromium	17	14	10	13	
Manganese	4	17	13	24	83
Iron	7	5	9	10	7
SS304	3	1	4	2	44

material	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
SS316	6	4	1	5	42
Cobalt	6	4	10	6	99
Inconel-600	5	15	14	10	78
Nickel	14	39	7	7	83
Nickel-chrome	5	13	8	4	93
Copper	5	2	7	5	3
Zinc	11	6	3	13	
Gallium	2	3	9	2	
Germanium	9	12	27	8	
Arsenic	14	19	16	8	
Selenium	8	32	17	9	
Bromine	2	27	4	2	
Rubidium	2	94	7	2	
Strontium	10	35	9	8	
Yttrium	22	55	19	60	58
Zirconium	10	5	16	74	87
Niobium	10	97	7	10	39
Molybdenum	2	6	32	13	
Ruthenium	4	29	3	27	
Rhodium	245	110	240	302	97
Palladium	12	66	23	32	
Silver	6	88	10	51	
Cadmium	17	63	5	60	
Indium	123	213	104	226	90
Tin	12	52	11	28	
Antimony	24	66	22	78	
Tellurium	3	170	6	2	
Iodine	85	79	86	96	90
Caesium	67	59	63	58	
Barium	16	79	17	77	
Lanthanum	319	311	330	309	80
Cerium	36	95	40	59	
Praseodymium	50	39	41	39	43
Neodymium	60	71	67	59	
Samarium	10	14	16	18	
Europium	120	95	73	95	
Gadolinium	33	45	35	65	
Terbium	78	76	84	76	
Dysprosium	228	228	244	231	
Holmium	20	17	11	31	
Erbium	103	129	101	101	
Thulium	76	83	76	77	84
Ytterbium	37	88	57	107	
Lutetium	86	95	72	84	

material	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Hafnium	33	22	46	30	
Tantalum	8	46	9	53	
Tungsten	74	77	85	78	81
Rhenium	18	15	7	19	
Osmium	160	63	155	80	
Iridium	52	419	13	425	
Platinum	19	17	23	20	
Gold	29	37	33	37	39
Mercury	13	95	13	11	88
Thallium	40	44	18	33	
Lead	29	23	21	31	66
Bismuth	799	189	282	175	

Table of mean % differences from FNS-96 7 hour experiments, indicating the quality of agreement for different libraries for cooling times ranging from a few days up to approximately 1 year. Note that a blank entry under the IRDFF-II heading indicates cases where that library is not able to provide a meaningful result.

material	TENDL-2019	ENDF/B-VIII.0	EAF2010	JEFF-3.3	IRDFF-II
Sodium	14	17	24	5	21
Aluminium	47	47	47	100	98
Sulphur	5	5	4	5	7
Potassium	152	191	232	160	120
Calcium	6	7	15	6	
Titanium	7	7	8	7	19
Vanadium	25	24	23	25	78
Chromium	24	24	24	27	
Manganese	4	6	6	4	1
Iron	9	9	3	9	13
SS304	7	9	3	6	20
SS316	7	10	4	6	23
Cobalt	10	6	12	5	9
Inconel-600	3	4	3	3	14
Nickel	2	5	4	4	13
Nickel-chrome	2	4	4	3	14
Copper	8	8	4	8	8
Strontium	10	13	11	10	
Yttrium	16	15	14	30	18
Zirconium	5	10	7	7	
Niobium	7	98	4	8	10
Molybdenum	14	27	8	30	
Tin	22	51	23	61	
Barium	12	72	8	71	
Tantalum	45	61	30	71	77
Tungsten	23	27	19	23	
Rhenium	8	29	8	8	
Lead	29	26	30	29	
Bismuth	568	2363	1896	391	

6 Discussion

From such a validation exercise a lot of information can be extracted from the results. However, its uniqueness and specificities require caution to be applied when drawing or projecting conclusions from the results.

The time dependence of the comparison has been clearly established and it is not surprising to see some fluctuations in the degree of agreement with cooling time. This is due to the fact that the set of predominant radionuclides evolves with time in direct relation with their appropriate half-lives. A clear picture emerges in that the comparative results for short cooling times, less than one hour, tend to be worse than the results for cooling times greater than a day but shorter than a year. This was expected, since the nuclear database (production cross sections and decay data) tends to be less qualified for these short-lived nuclides. This is due to difficulties encountered when assessing short half-life isotopes and isomers. Having said that, the agreement reached on the prediction of some short lived isomers is rather good for, in particular, TENDL – a specificity that is unique to a properly assembled nuclear data file that contains all necessary branching ratios. Other libraries often miss such information. The overall results are surprisingly good on exotic material samples, even more so when allowing for certain experimental difficulties.

What has been clearly demonstrated by this validation exercise is that the calculational method used by the FISPACT-II to predict the decay power and associated uncertainty of structural materials under a hard fusion neutron field is adequate. When the nuclear data are known with sufficient accuracy the code predictions are within the boundaries defined by the experimental uncertainty. However, nuclear databases, TENDL-2019, EAF2010, JEFF-3.3, ENDF/B-VIII.0, and IRDFF-II tend to give different results because of variation in the data they contain for the cross sections and decay of the radionuclides involved. The majority of the results are satisfactory and give credit to the work performed in assembling such large libraries. However, the level of accuracy of the cross sections tested by this validation exercise span from a few percent, which is acceptable, to orders of magnitude, which is not. When the latter case occurs then very specific and time consuming studies need to be performed before any action is taken to correct the nuclear databases. Such remarks are in line with the results of earlier international code comparisons on decay heat, including [10, 11] and some performed on fission fuel materials [21].

All the cross section paths linked with an E/C values greater than 10% have been analysed in line with other validation studies, (FNG Frascati, SNEG-13 Sergiev Posad, D-Be Cyclotron Karlsruhe, etc.) and compared with the experimental database EXFOR [22]. If the results corroborate one another there will be more incentive and firm grounds to apply an appropriate correction in the next generation of general-purpose nuclear data-files.

In contrast, some of the other libraries, such as JEFF-3.3 and ENDF/B-VIII.0, generally contain data for less of the isomeric states, which seriously impairs their ability to properly simulate any responses when these are predominant. This is particularly obvious at short cooling times. The legacy EAF2010 library still performs surprisingly well in most cases – there are very few examples where it is outperformed by TENDL-2019. However, the lack of an ongoing development plan for this library means that it is not viable in the long-term (there is no plan to improve its content or completeness) and the new technology-based approaches for TENDL-2019 and others have longevity. Furthermore, the EAF libraries are unable to provide resonance parameters that are useful for self-shielding (and probability tables) in the unresolved resonance range (URR). Nor can it provide kerma, dpa cross sections, or recoil and emitted particle spectra, and it is not fully compatible with the industry standard ENDF-6 or newly developed GNDS file formats. On the other hand, the fact that it has taken almost 10-years to reach a stage where TENDL is able to reproduce the sturdiness of EAF libraries is testament to the latter's quality and the dedication of the evaluators involved.

IRDFF-II is able to produce reasonable predictions for some FNS experiments despite its limited, but targeted, 54-isotopes, 119-reaction cross section database. While this validation exercise can be considered a fair test of that library, there a many instances and time frames where such a special library cannot, nor is it supposed to, deliver outside its field of reference although the overall quality of its content is undeniable for its purpose (with the caveats identified concerning the overprediction of Co59, Al27, V51, etc.).

6.1 Uncertainties in the calculations

The TENDL-2019 library contains 2813 target nuclides ranging from ^{1}H to ^{291}Mc with all reactions kinematically allowed up to 200 MeV. Meanwhile the associated decay library contains data for 3875 nuclides, that may be produced by any combination of reactions and decays. Crucially covariance information for each reaction type is uniquely stored (in mf-33,40) for incident particles with energies from 10^{-5}eV up to 200 MeV. Above the upper energy of the resolved resonance range, for each of the 2813 isotopes, a Monte Carlo method, in which the covariance data come from uncertainties of the nuclear model calculations, is used. Short-range, self-scaling variance components are also specified for each (mt) reaction type. The data format used to store the variance-covariance information has been made fully compliant with the ENDF-6 format [17] description and the files are read directly by FISPACT-II without any further intermediate processing. Variance and covariance data are re-used by FISPACT-II to create uncertainty predictions and sensitivity analyses [23].

In this report, systematic experimental uncertainty, calculational uncertainty and E over C values have been quoted and calculated in a way that allows a direct comparison to be made. The method used for the generation of qualitative variance information in TENDL-2019, compared to what was done in EAF2010 uncertainty file is a significant achievement, when the calculational uncertainties quoted in the tables are of the same order of the E/C values. This demonstrates that the method chosen to calculate these uncertainties in the TALYS code system is not only valid but adequate. Of course, the same remarks as for the cross section and decay data file apply; even if the bulk of the data seems to be satisfactory, certain specific data entries need to be revisited in line with the findings of this validation exercise and other studies.

7 Conclusions

The experimental time-dependent decay-power measurement program at JAEA FNS combined with the code simulations performed in this study provide a unique check of the calculational method and nuclear databases associated with the prediction of decay power for the set of material samples analysed. The results of the comparison give confidence in most of the decay heat values calculated, although the predominantly 14 MeV neutron spectrum in FNS means that the low neutron energy reactions of importance in other devices have not yet been fully considered [24]. This statement limits the scope of validation and possible conclusions reached in this study to the decay power predicted through the identified pathways. However, it covers the decay data of all the isotopes involved irrespective of their production routes.

The experimental uncertainty, calculational uncertainty and E/C values have been systematically evaluated, presented, and analyzed. Their direct comparison demonstrates that the method chosen to calculate and propagate uncertainties in the FISPACT-II code system is verified and validated (V&V), and that the uncertainties file could be further improved in some cases.

A set of deficiencies and discrepancies have been identified in various cross sections, and these may require some corrective actions to be taken. These corrections and/or amendments will benefit the next generation of the library cross sections, associated variance and covariances. A large proportion of the decay powers calculated in this validation exercise with TENDL-2019 are in good agreement (within a few %) with the experimental values for cooling times spanning from tens of seconds up to, uniquely, cooling times of more than a year.

Maintenance and testing of inventory code systems for activation, transmutation and source term calculations, and the associated general purpose cross section libraries, is essential for many projects in order to present a sound and well validated safety assessment. Licensing authorities will require evidence of experimental validation. However, the relevance of the experimental irradiation conditions and set-up to those that are likely to exist in a device needs to be carefully considered in order for such an assessment and validation to be applicable to the data predicted for the next generation of nuclear devices.

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Appendix A

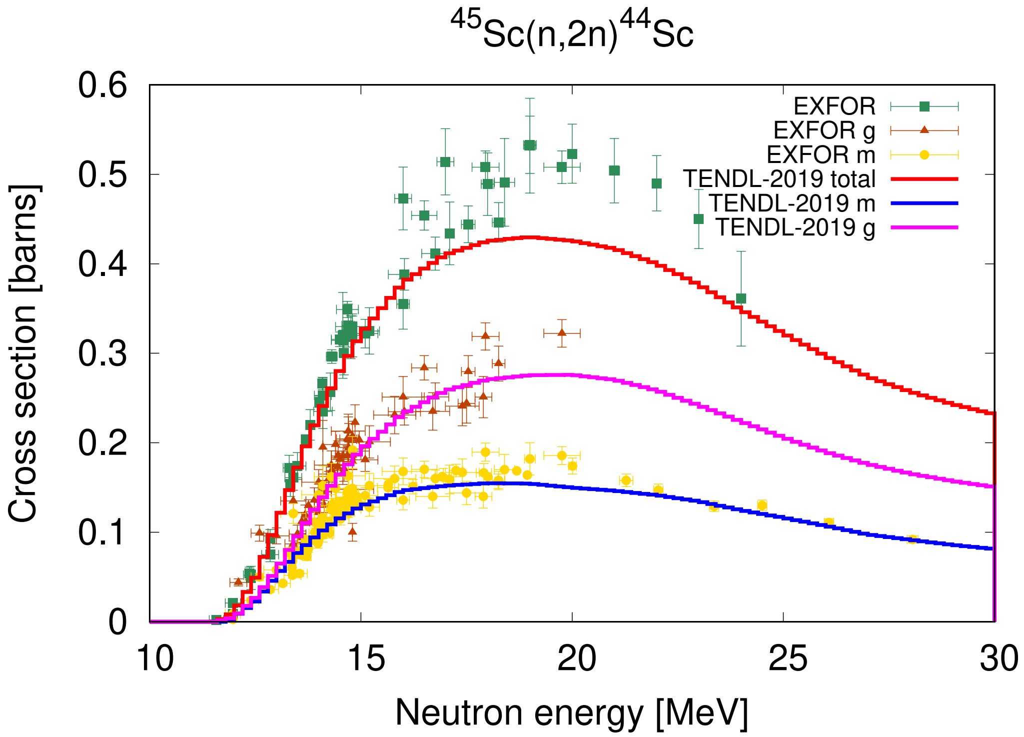

Figure A1: Sc45(n,2n) reaction cross section plot.

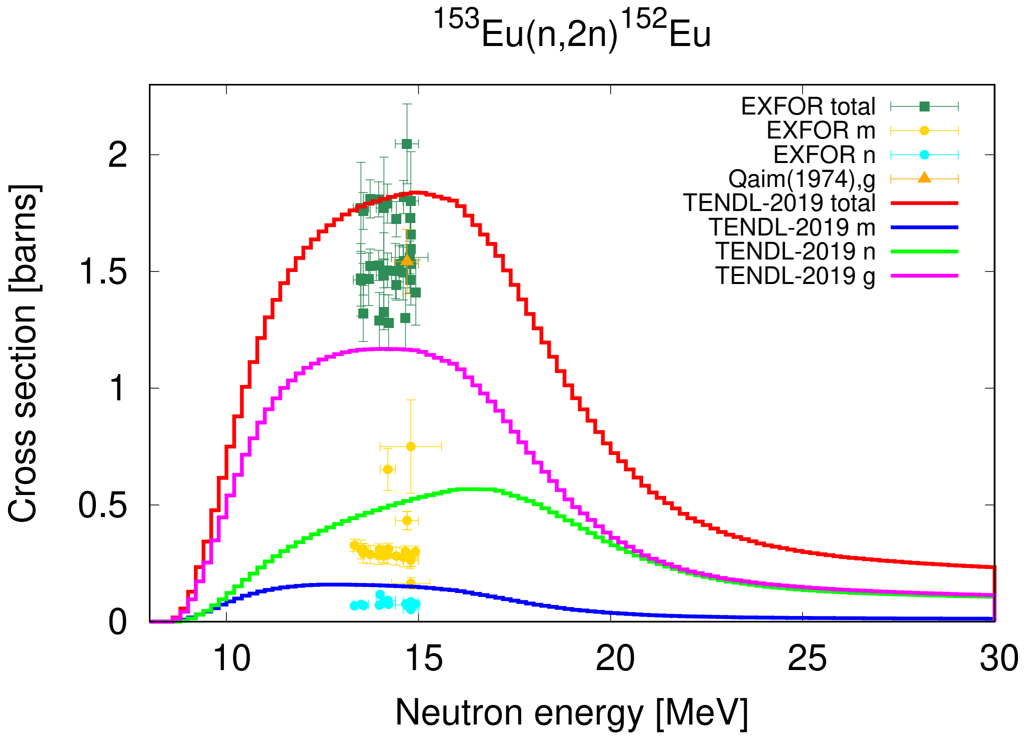

Figure A2: Eu153(n,2n) reaction cross section plot.