Scoping of material damage with FISPACT-II and different nuclear data libraries: transmutation, activation, and PKAs

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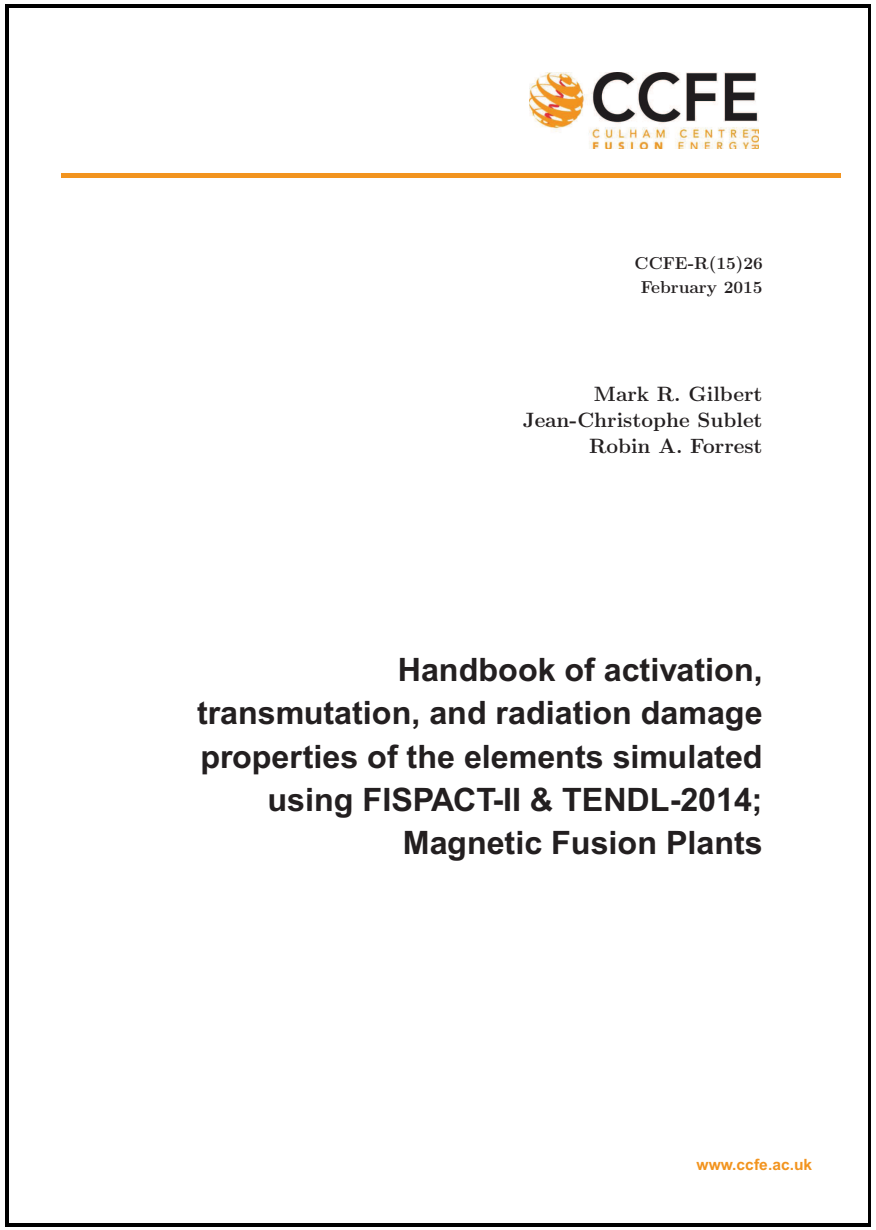
Outline

- Automated infrastructure for scoping inventory simulations
  - Multiple materials handbooks
- Activity – library comparisons, fusion vs. fission
- Transmutation – library comparisons, fusion vs. fission
- PKA distributions from SPECTRA-PKA
  - library comparisons, fusion vs. fission
  - cumulative distributions & cascade splitting
  - per-channel damage calculations

Background

- A reference document of typical responses of the elements to fusion neutron irradiation is a useful tool during material selection exercises for conceptual DEMO (and beyond) designs
- This has resulted in the repeated production of handbooks presenting inventory simulation results – showing activation and transmutation response
- However, the creation of previous versions of the handbook (1992-3, 2004, 2009) was time-consuming, used document software that was cumbersome for a graph/table-dominated report, and required significant error-prone user-manipulation of data
- A new automated infrastructure – to run simulations, process the results, create figures and tables, and compile into a report – has been developed to overcome these short-comings and also provide a platform for extensions and improvements



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CCFE-R(15)26
February 2015

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Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Magnetic Fusion Plants

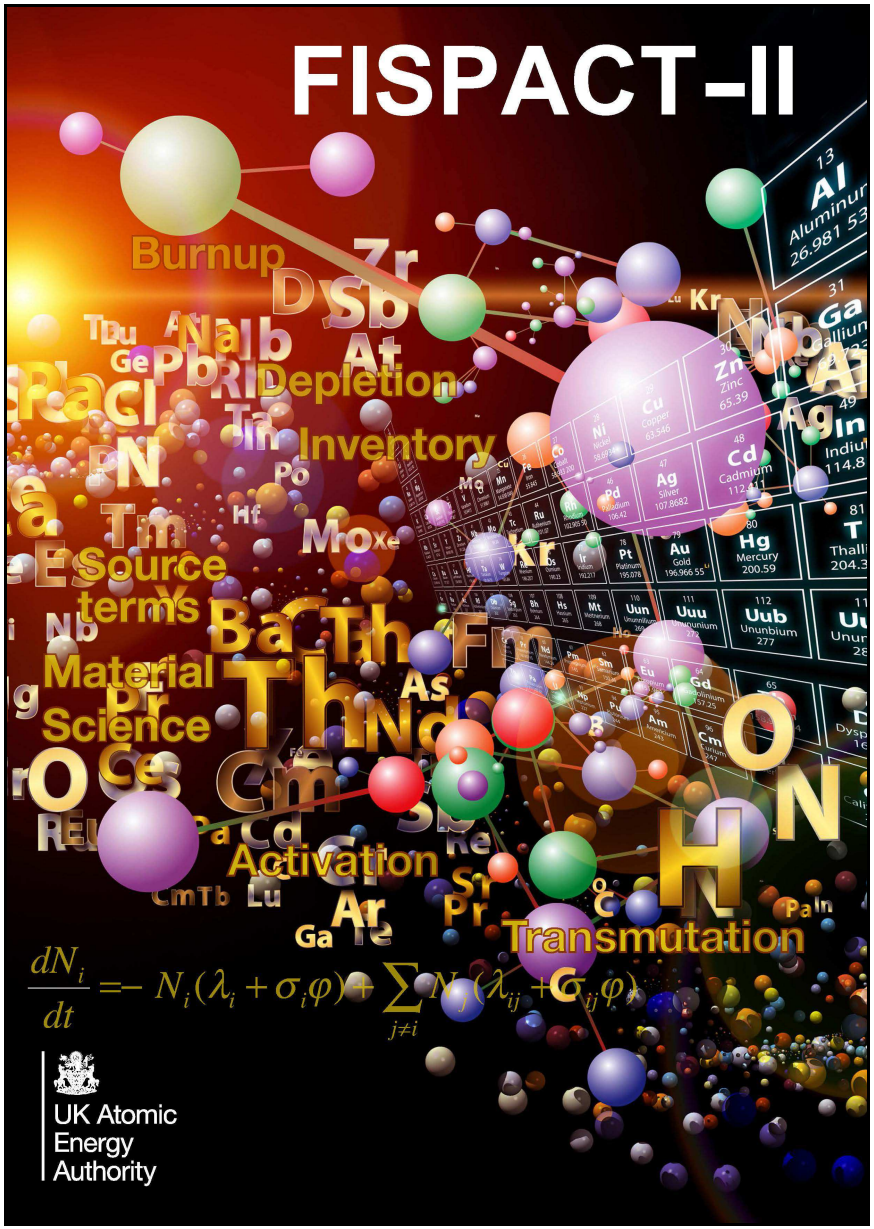
www.ccfe.ac.uk

- First version of new materials handbook created using TENDL-2014[§] nuclear data library and the FISPACT-II inventory simulator
- Data for all naturally occurring elements from hydrogen to bismuth under typical predicted DEMO conditions
- 695 pages in main report + a 521 page PKA supplement
- Available to download from

  http://www.ccfe.ac.uk/fispact.aspx

CCFE-R(15)26.pdf

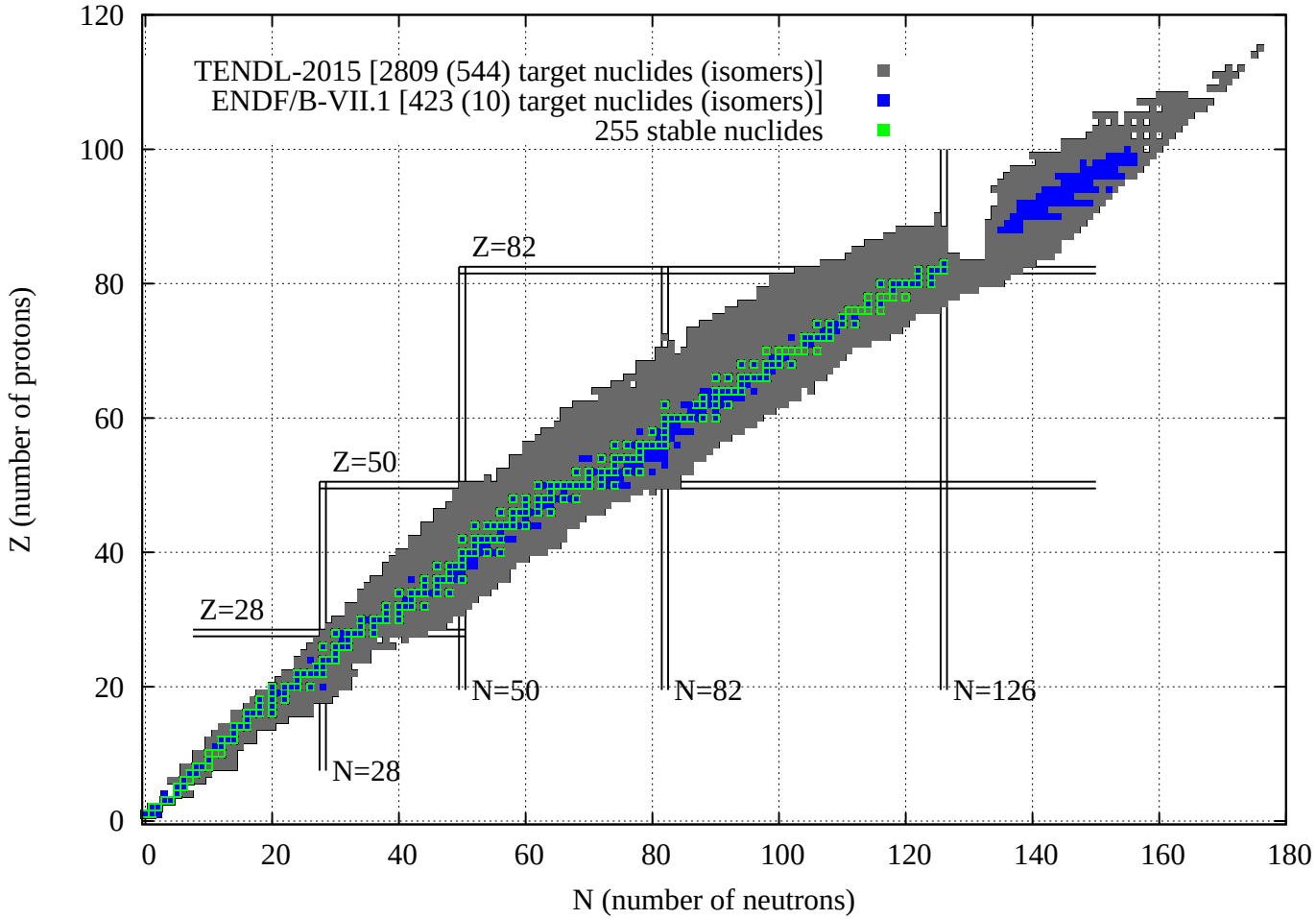
[§] update with TENDL-2015 available soon
PKA – primary knock-on atom



- enhanced multiphysics platform for predicting the inventory changes in materials under both neutron and charged-particle interactions
  - calculates activation, transmutation, burn-up, dpa, PKAs, gas production, and more
- employs the most up-to-date nuclear data libraries in ENDF format:
  - including TENDL-2015 & 2014, JEFF-3.2, JENDL-4.0, ENDF/B-VII.1, and CENDL-3.1
  - includes decay and fission-yield data (GEFY-5.2)

TENDL-2015[§]

- Target nuclide coverage in TENDL libraries is more complete than elsewhere:



- Many more isomeric states are included as both targets (parents) and daughters of reactions – vital for correct prediction of activity

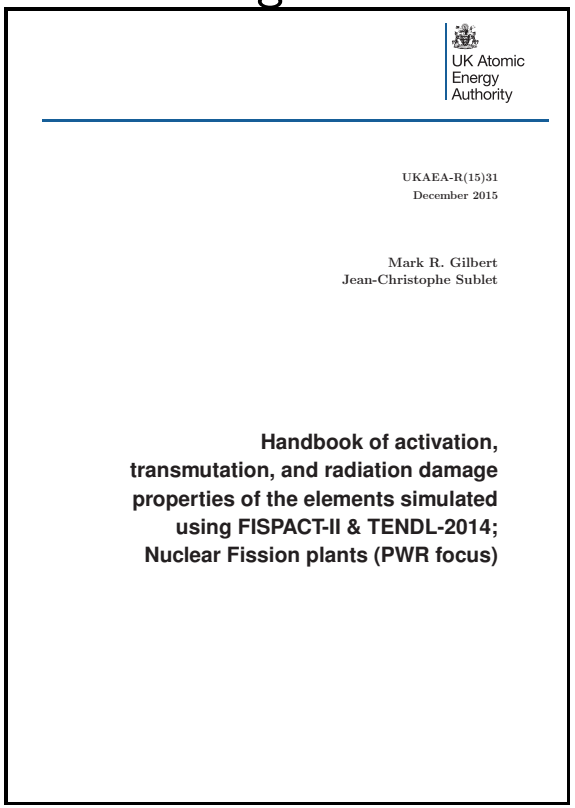
[§] A. J. Koning, D. Rochman, *et al.*
Available from ftp://ftp.nrg.eu/pub/www/talys/t15/

Handbook layout for each element:

1. Tabulated DEMO first wall activation response
   - % contributions of important radionuclides to various radiological quantities as a function of cooling time
2. Graphs of DEMO activation response
   - decay evolution of total activity, heat, and γ-dose under three different spectra & compared to Fe + indicative dominant nuclide contributions
   - new for 2016 – nuclide contributions as a function of time
3. Importance diagrams
   - spectrum independent mapping of important radionuclides in the neutron-energy vs. decay time phase-space
4. DEMO first wall transmutation response
   - time evolution under irradiation of initially-pure elemental composition
   - nuclide concentration map at 2 full power years
5. DEMO first wall PKA distributions
   - time=0 spectra plotted as both elemental and isotopic sums
6. Reaction pathways
   - major production pathways for important radionuclides at four characteristic neutron-energy ranges

Other handbooks

- The automated system makes the production of additional handbooks straightforward:


UK Atomic Energy Authority

UKAEA-R(15)31
December 2015

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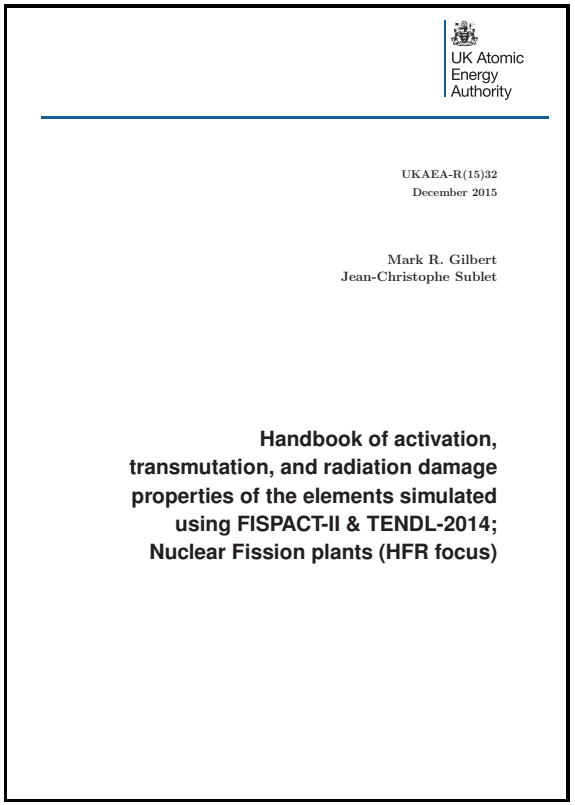
Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission plants (PWR focus)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UKAEA-R(15)32
December 2015

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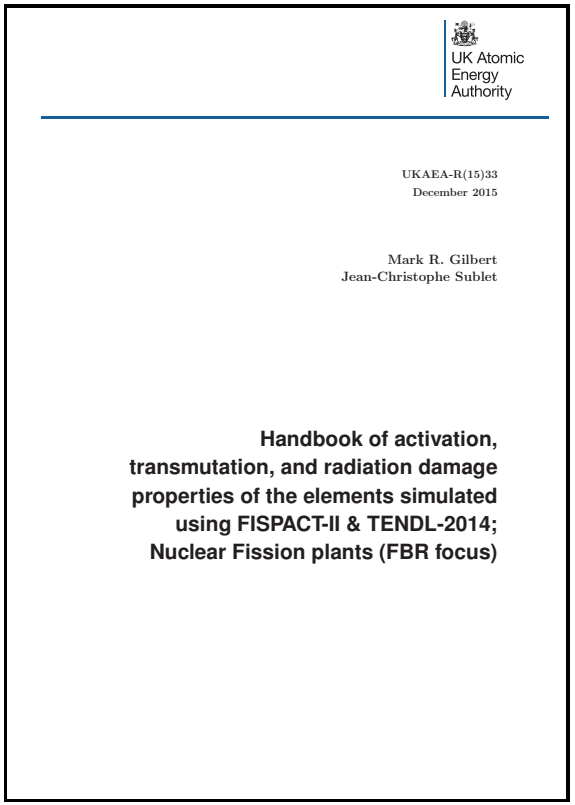
Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission plants (HFR focus)


UK Atomic Energy Authority

UKAEA-R(15)33
December 2015

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Jean-Christophe Sublet

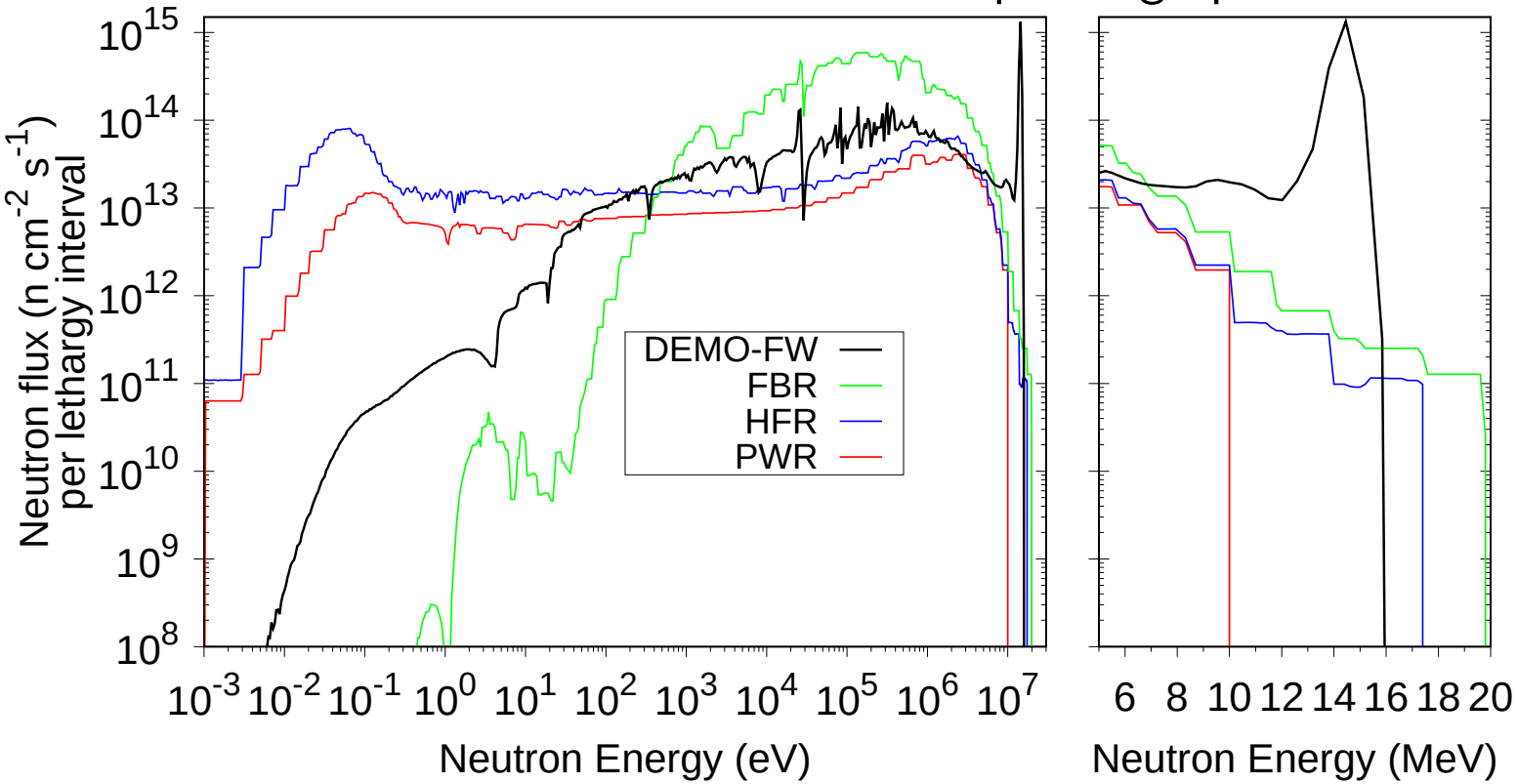
Handbook of activation, transmutation, and radiation damage properties of the elements simulated using FISPACT-II & TENDL-2014; Nuclear Fission plants (FBR focus)

- three other "nuclear physics materials handbooks" for fission environments (UKAEA-R(15)31-33[§]):
  - PWR (Paluel), FBR (superphenix), and HFR (Petten) reactors

[§] Also downloadable from `http://www.ccfe.ac.uk/fispact.aspx`

Other handbooks

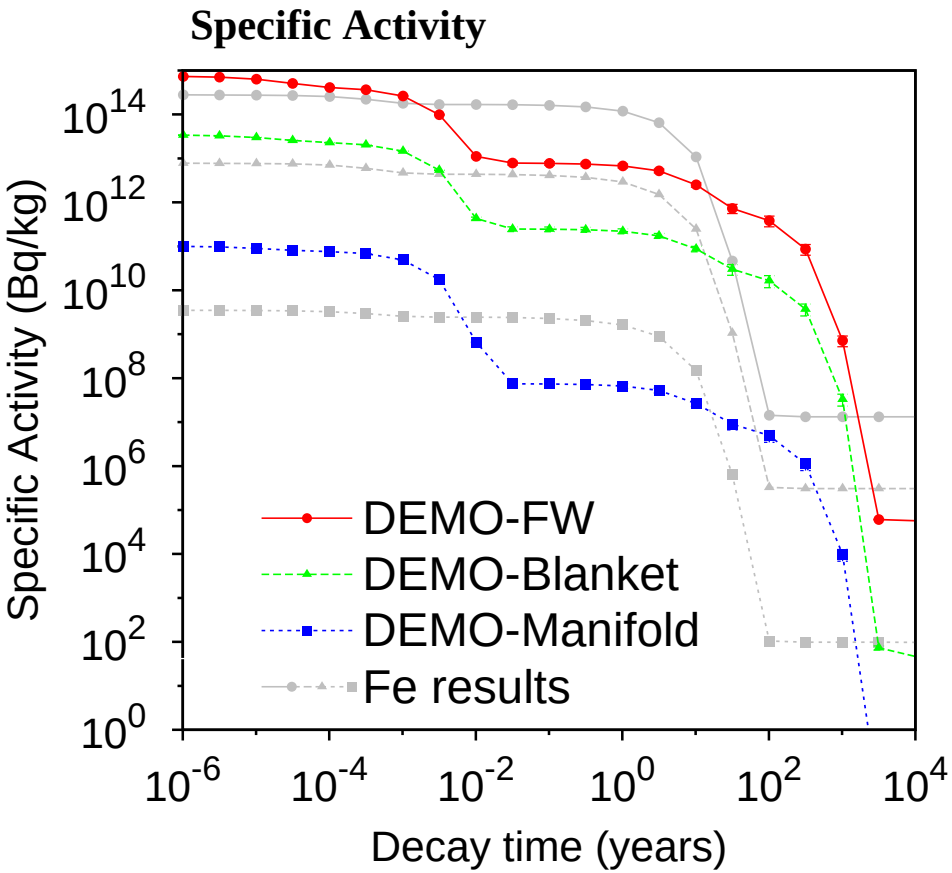
- In each fission handbook the main spectrum is used for the activation tables and transmutation results...
- with results from all three in the activation response graphs

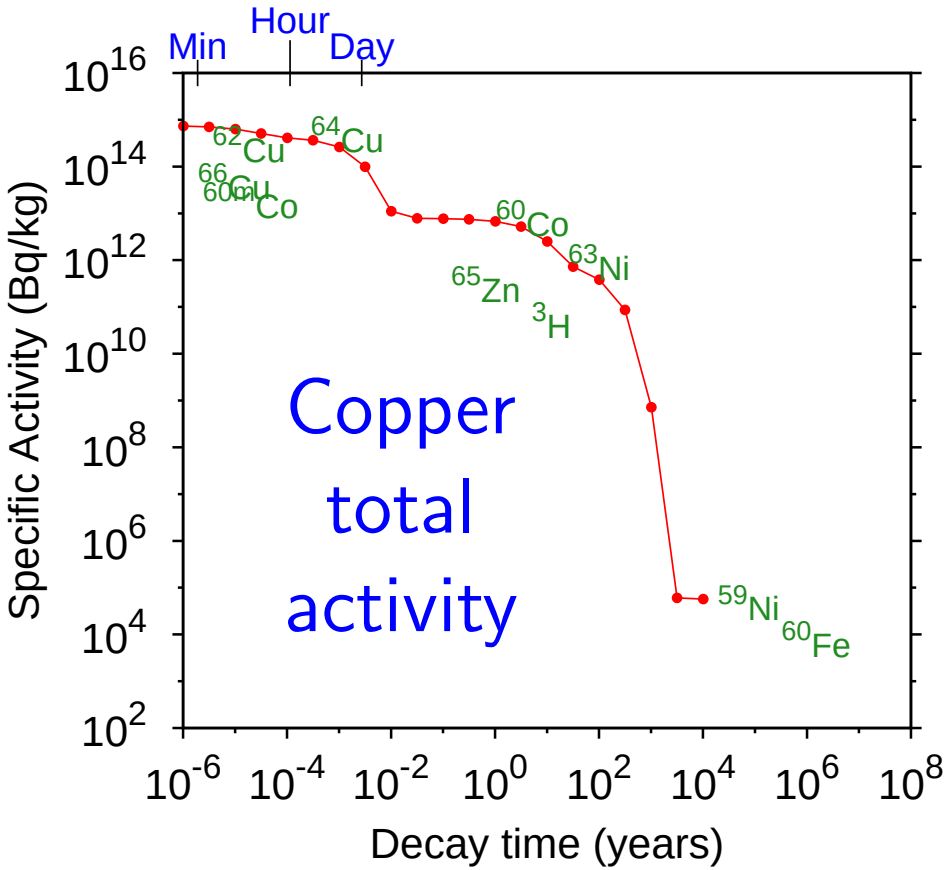


- all four TENDL-2014 reports have also been reproduced using JEFF-3.2, JENDL-4.0, & ENDF/B-VII.1
- almost 250,000 separate FISPACT-II calculations in total for 16 reports

Activation response – example output

- Decay curves following 2 fpy irradiations under 3 different DEMO conditions
- Plots for specific (total) activity, γ dose rate and heat output
- Second plot shows shows contributing radionuclides and where they are important

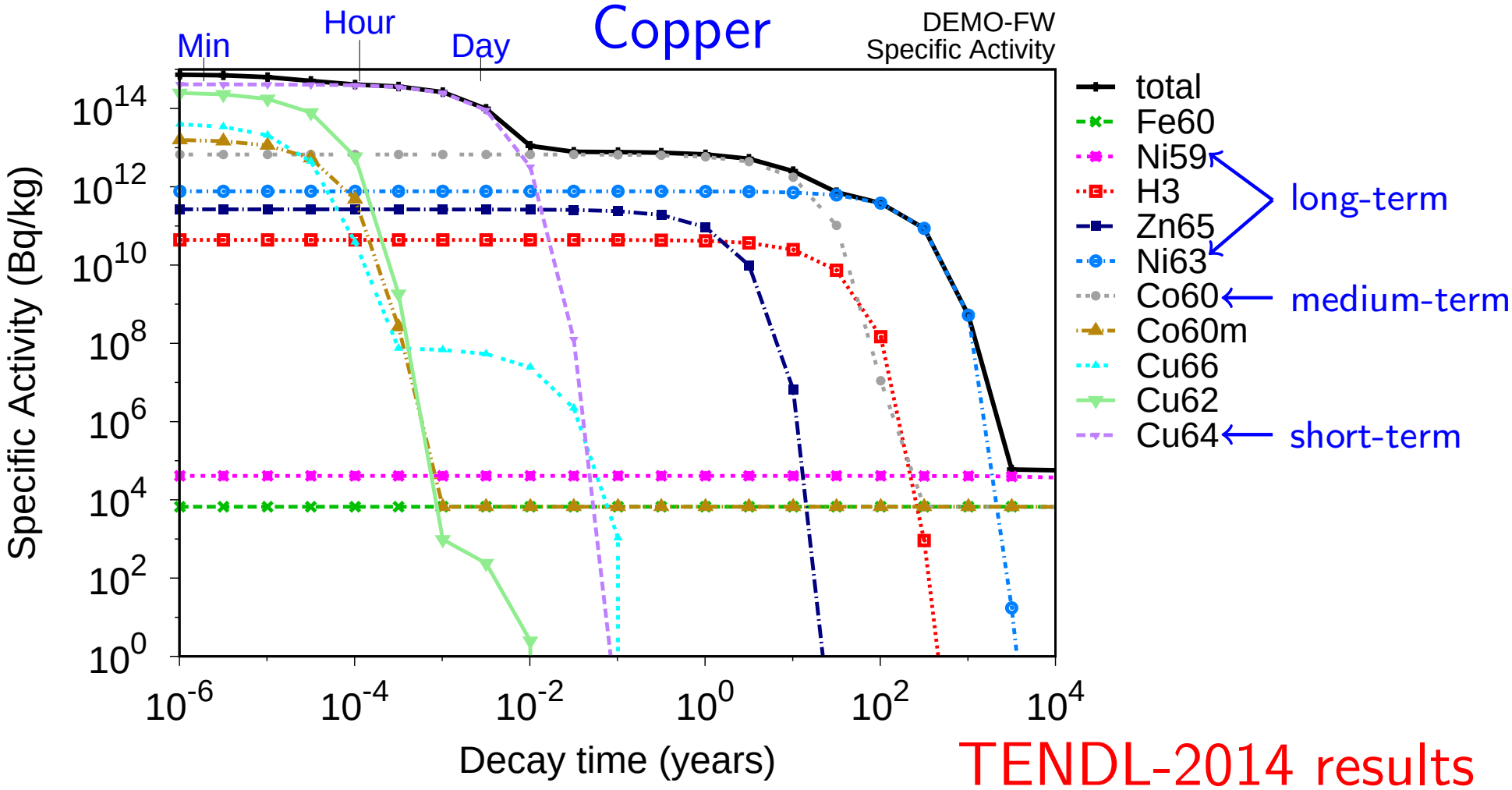




TENDL-2014 results

Activation response – full nuclide contributions

- Newly developed automation to plot (dominant) nuclide contributions as a function of time



TENDL-2014 results

- shows which nuclides are important and when

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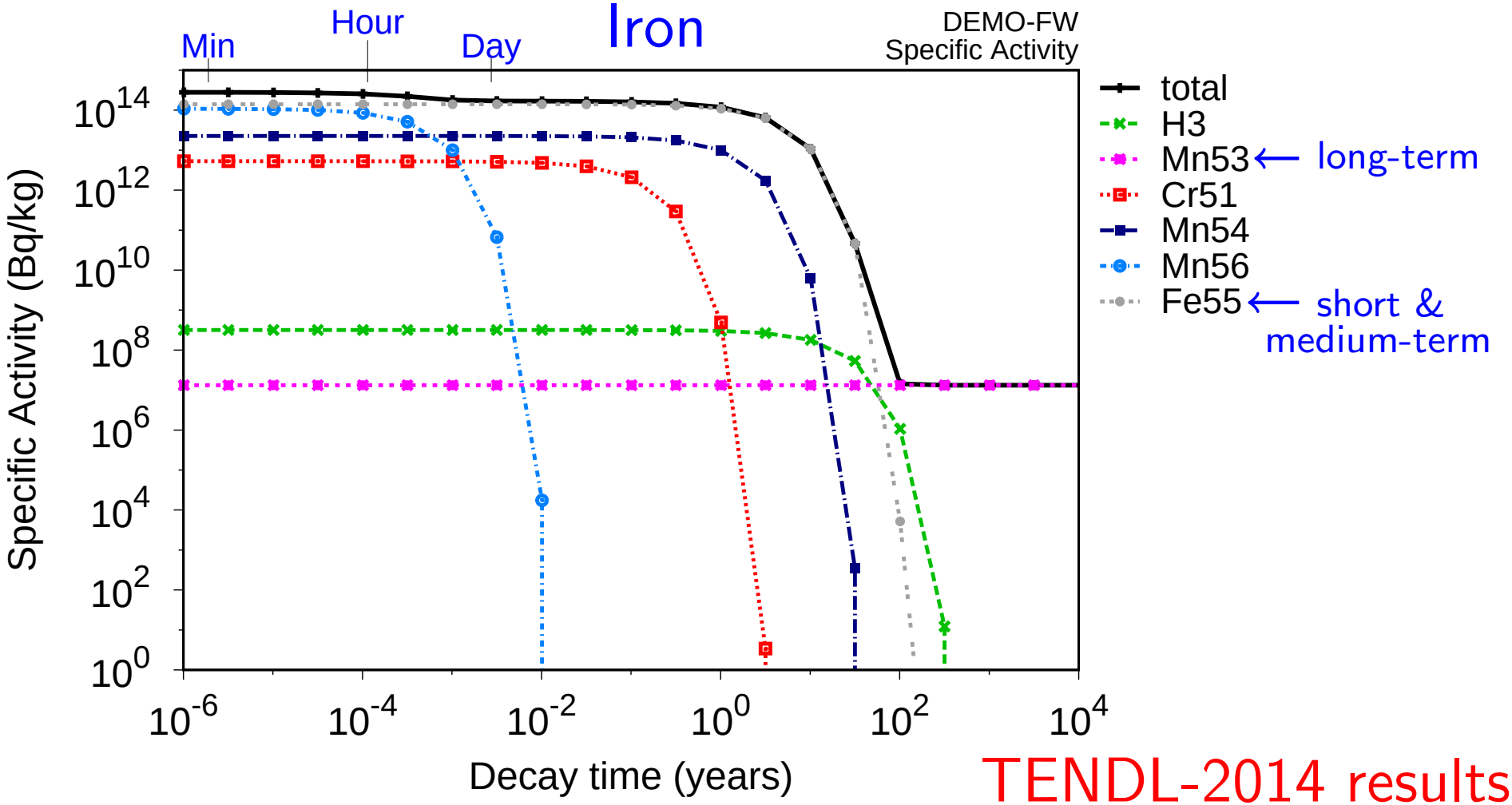

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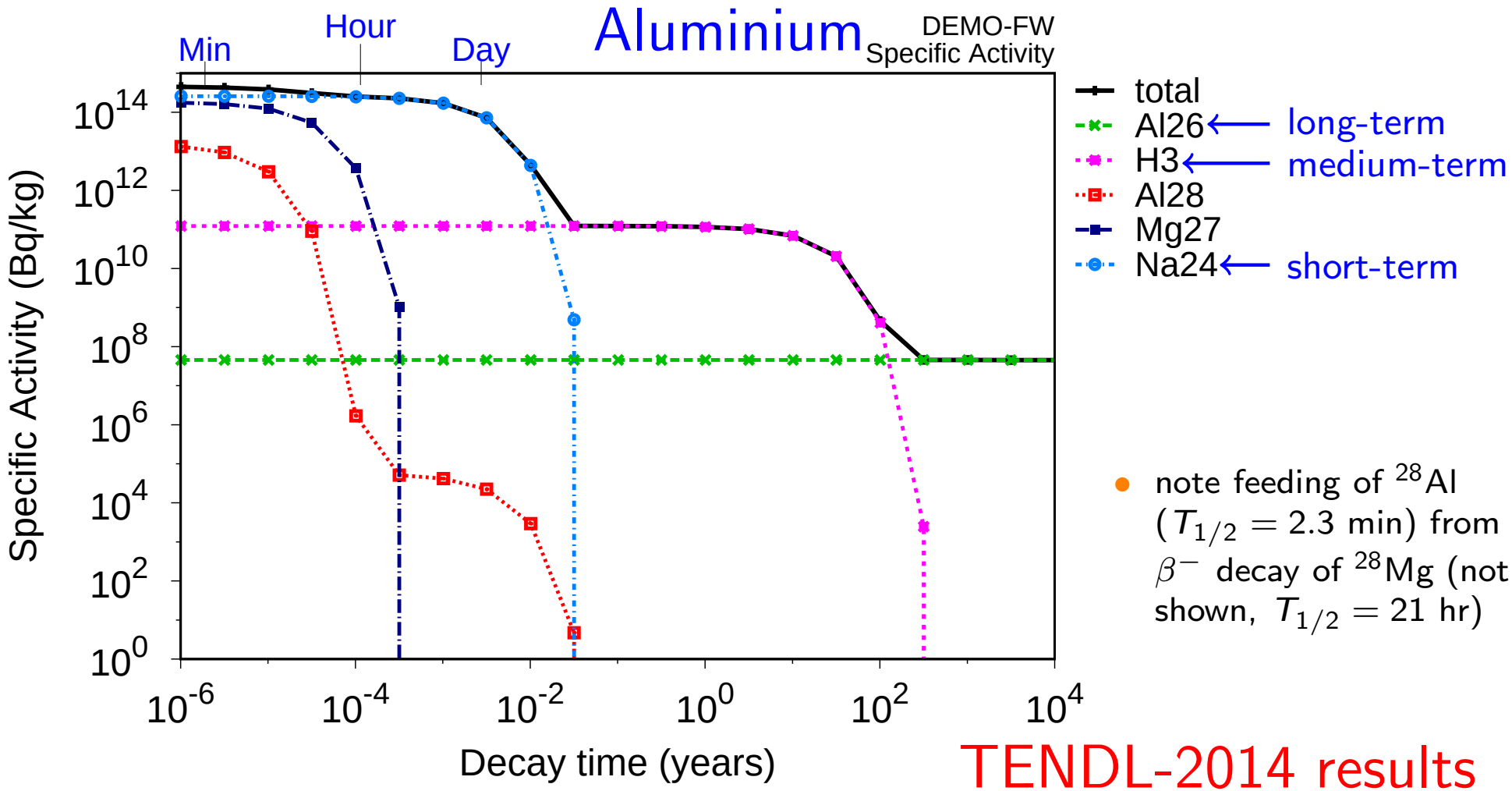

- note feeding of ^{28}Al ($T_{1/2} = 2.3$ min) from β^- decay of ^{28}Mg (not shown, $T_{1/2} = 21$ hr)

TENDL-2014 results

- shows which nuclides are important and when

Activation response – full nuclide contributions

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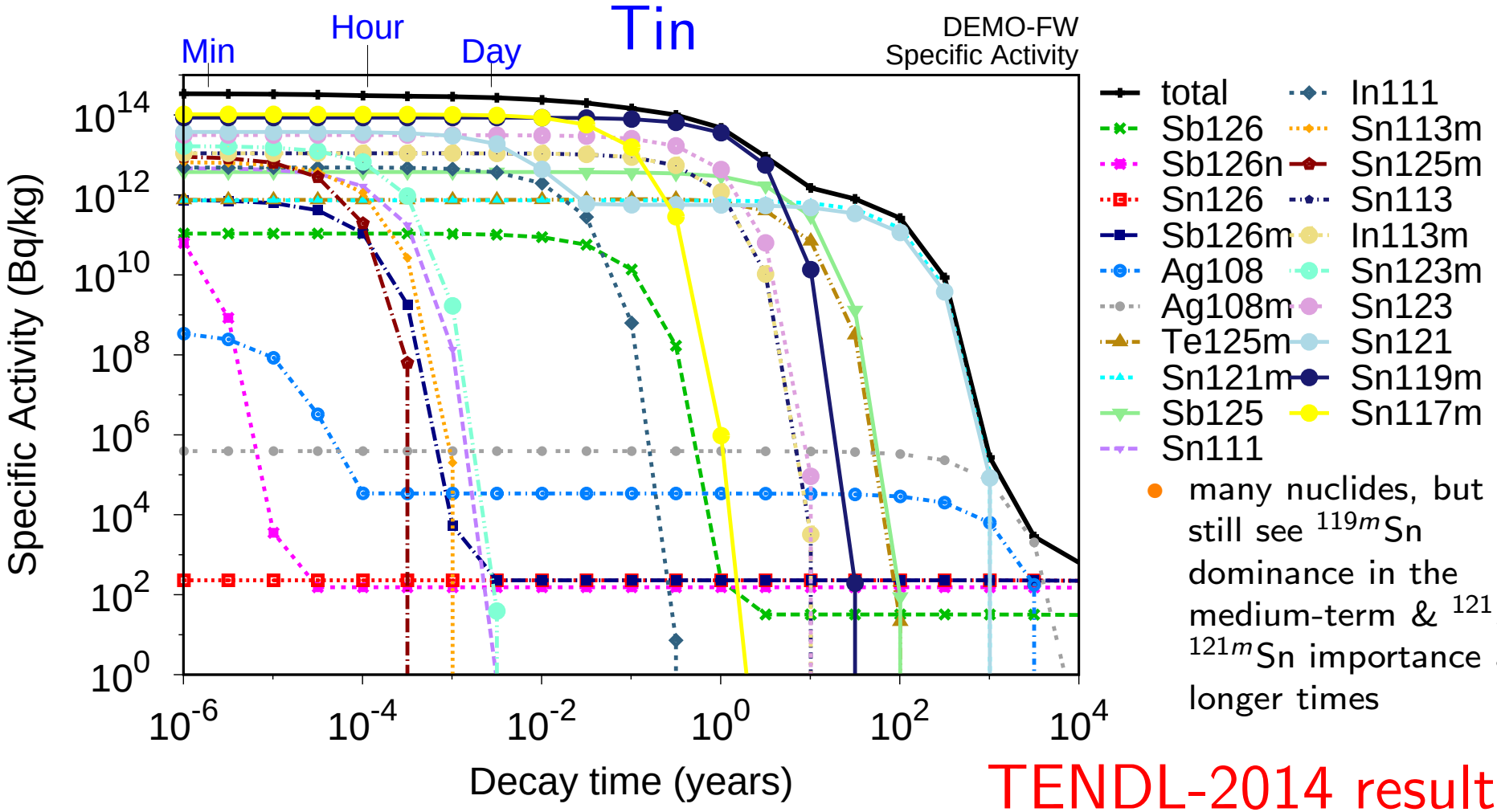


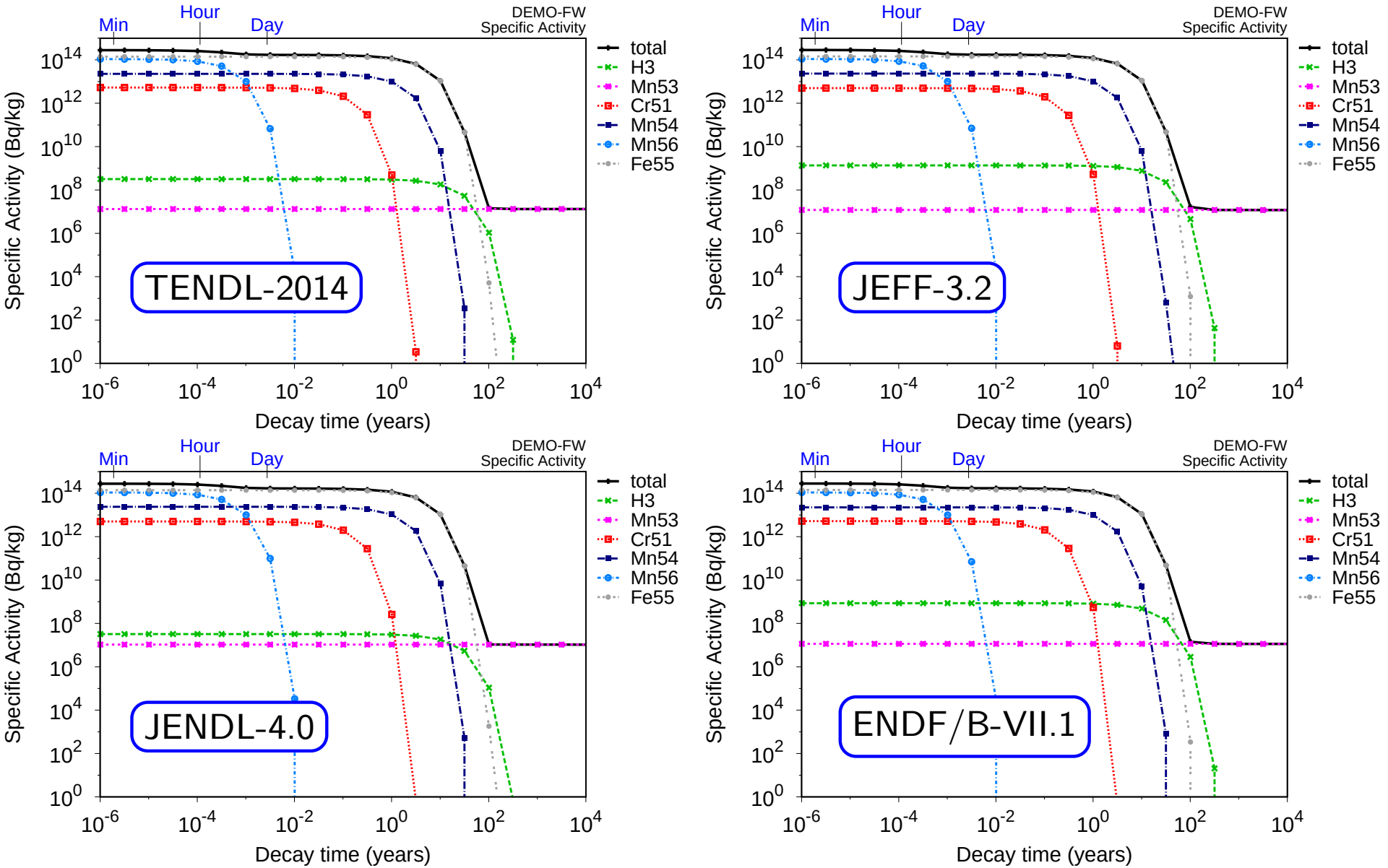
- many nuclides, but can still see ^{119m}Sn dominance in the medium-term & ^{121}Sn, ^{121m}Sn importance at longer times

TENDL-2014 results

- but picture can be very complex!!

Iron

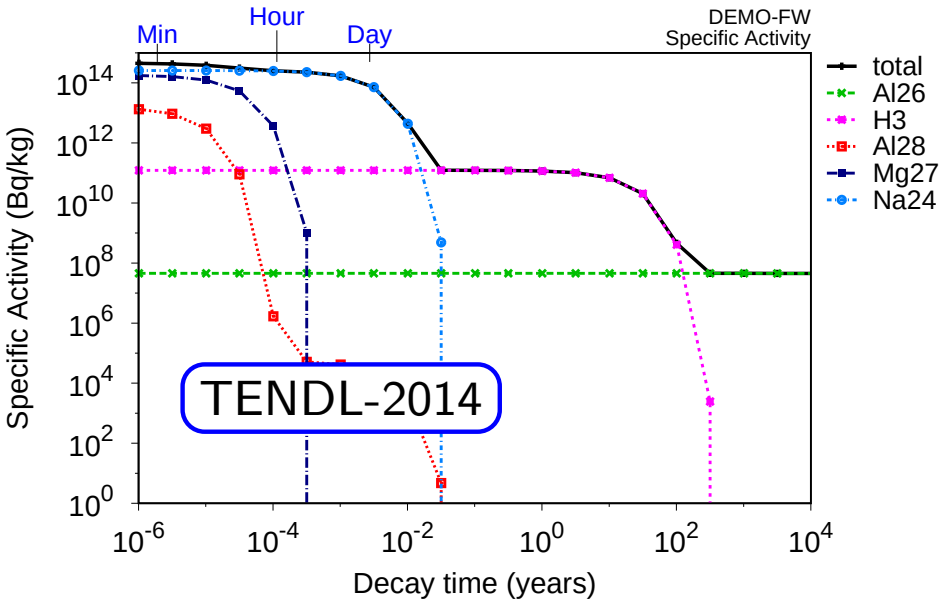
Variation with library

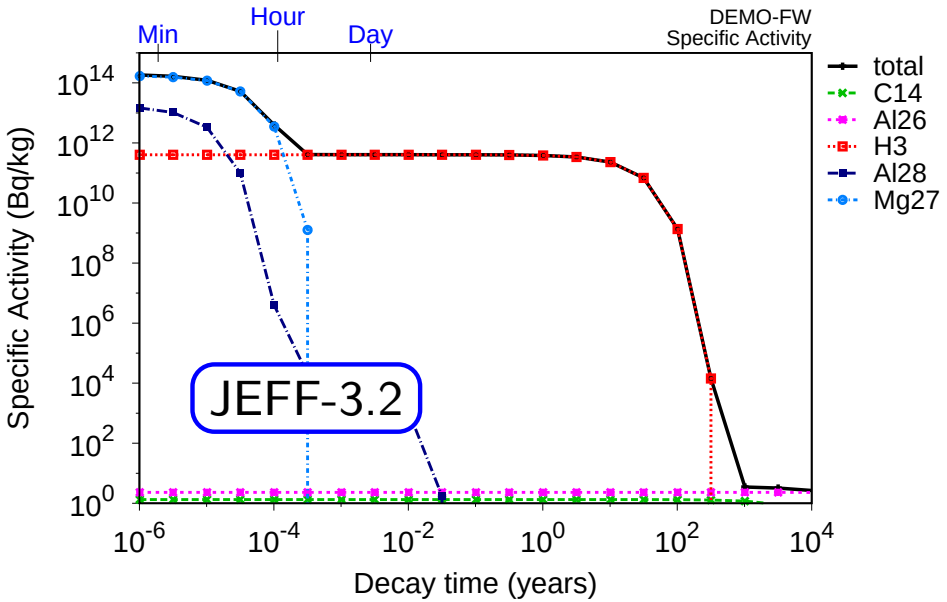


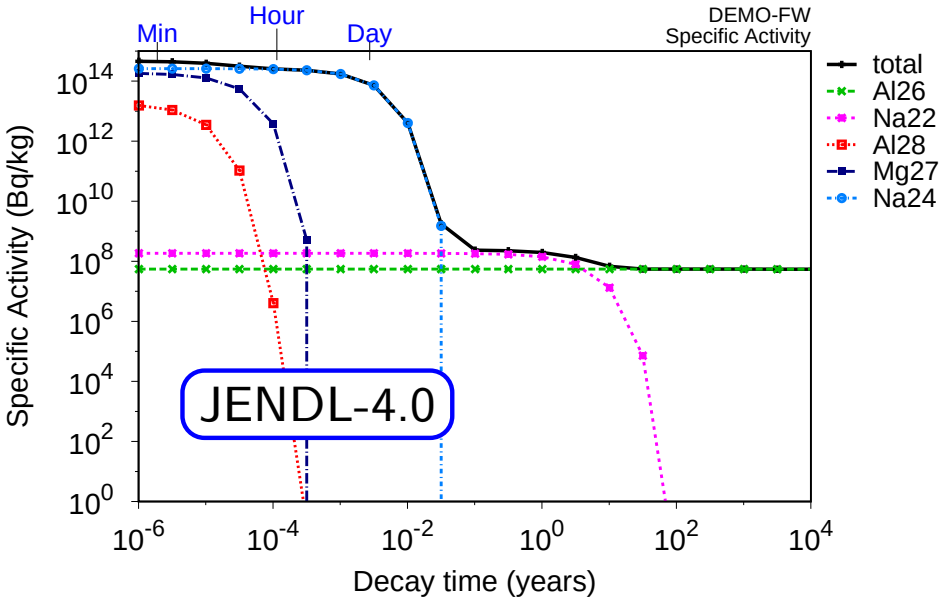
- Fe shows nearly identical response with all libraries

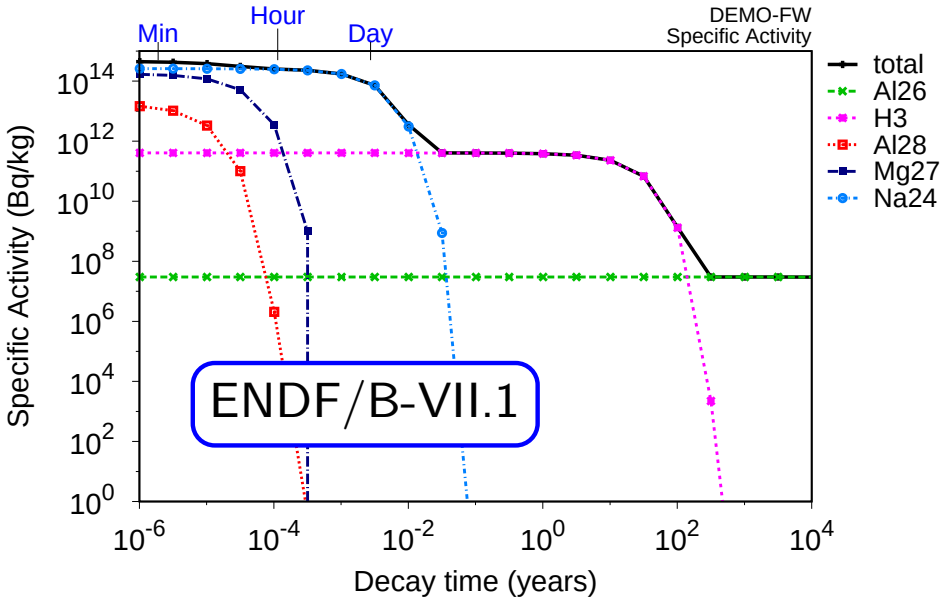
Aluminium

Variation with library





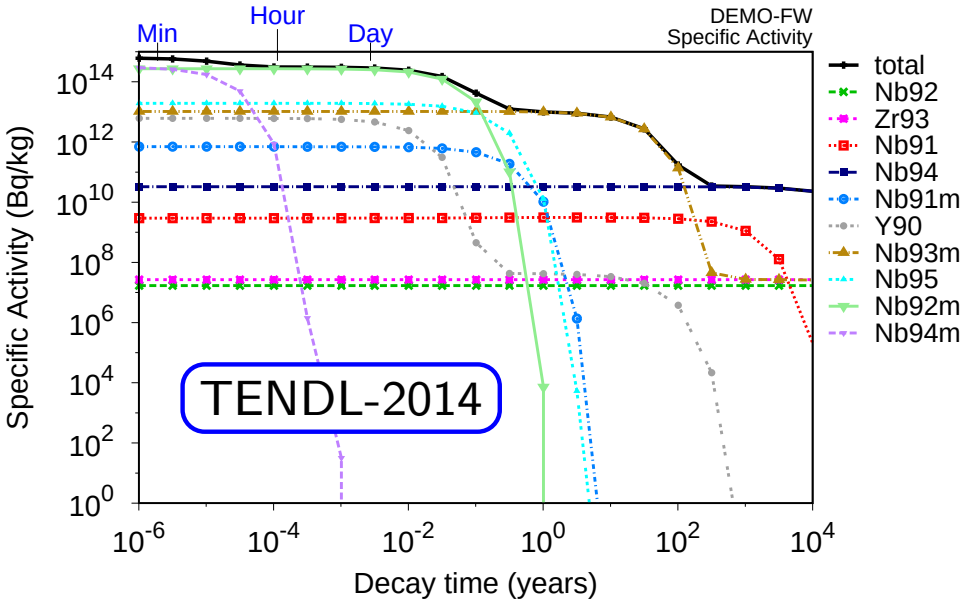


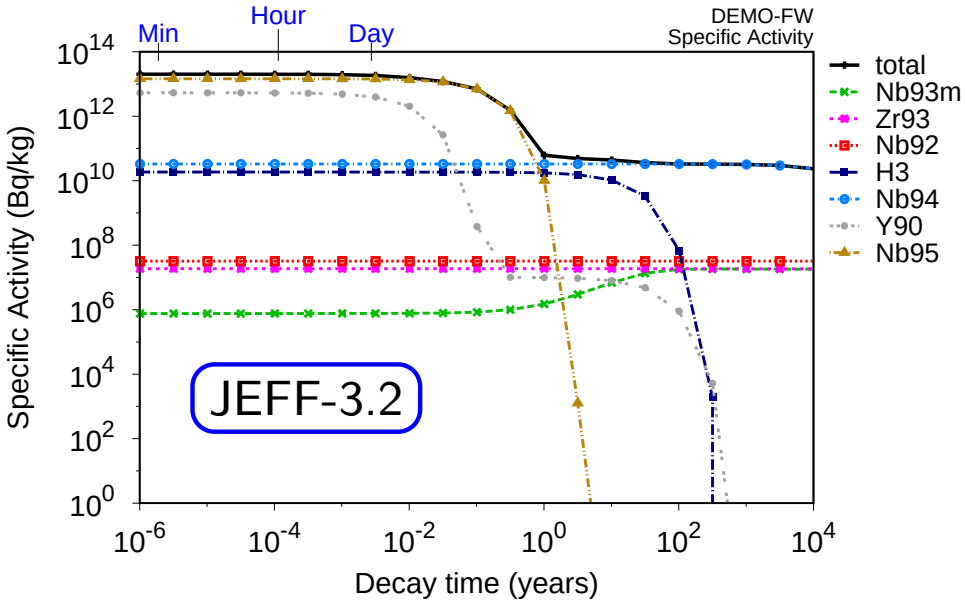


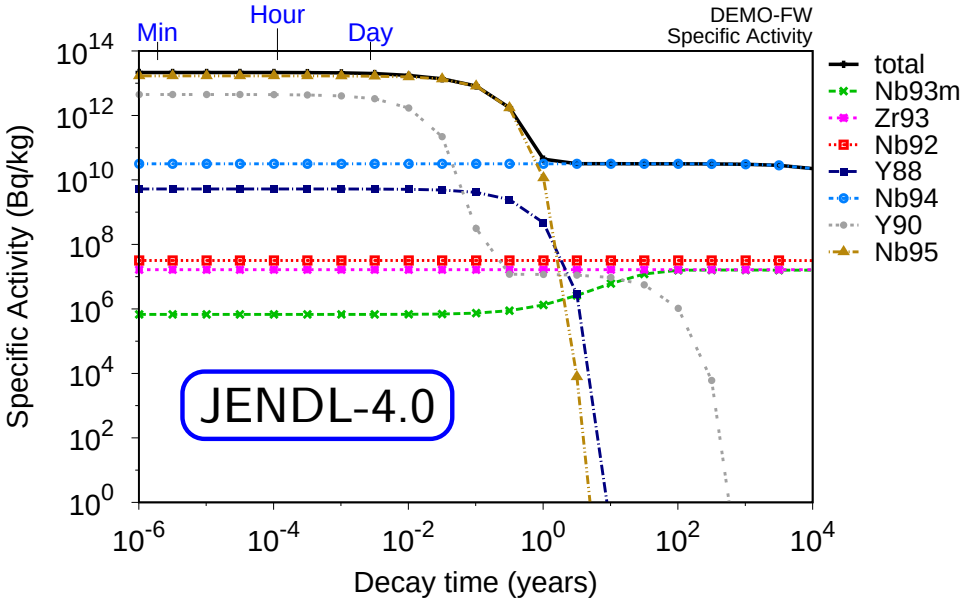
- JEFF-3.2 appears to under-produce ^{26}Al (n,2n)
- JENDL-4.0 is missing tritium production channel

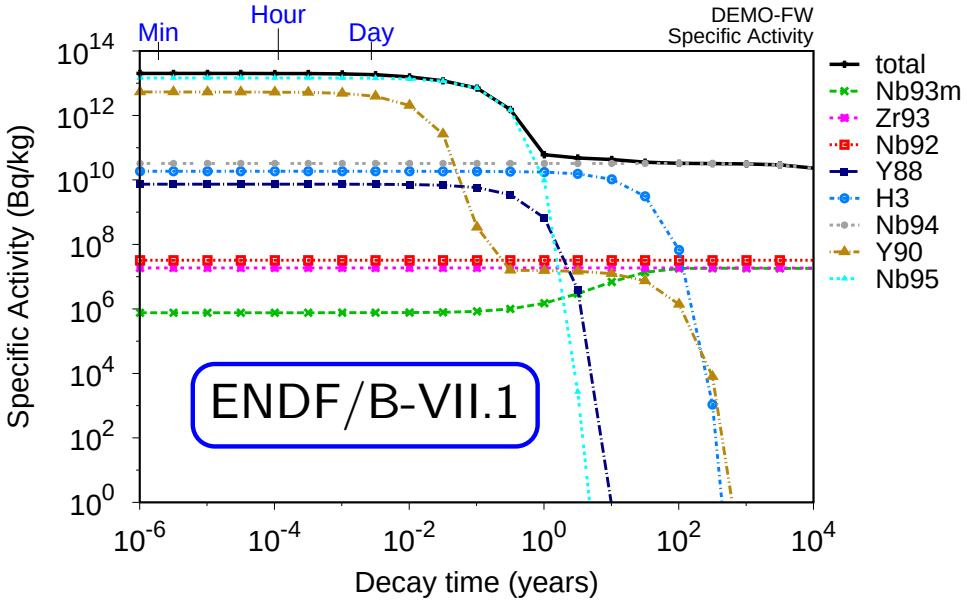
Niobium

Variation with library





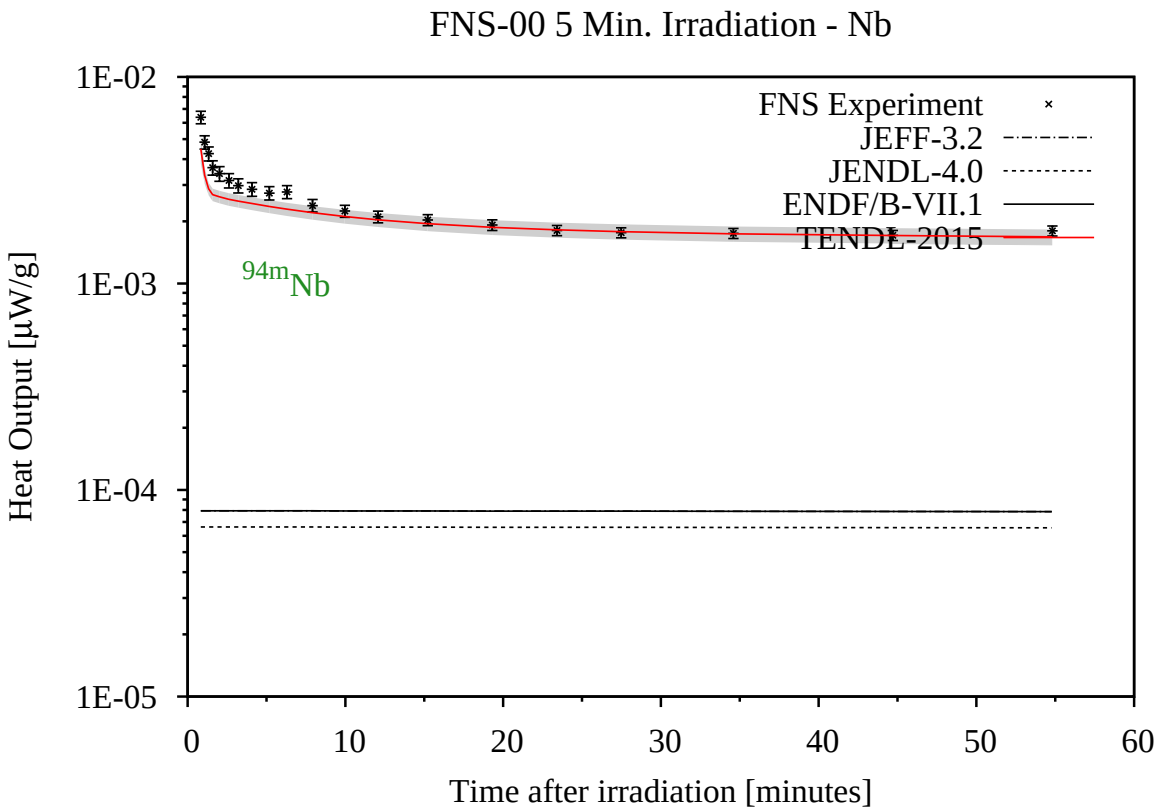




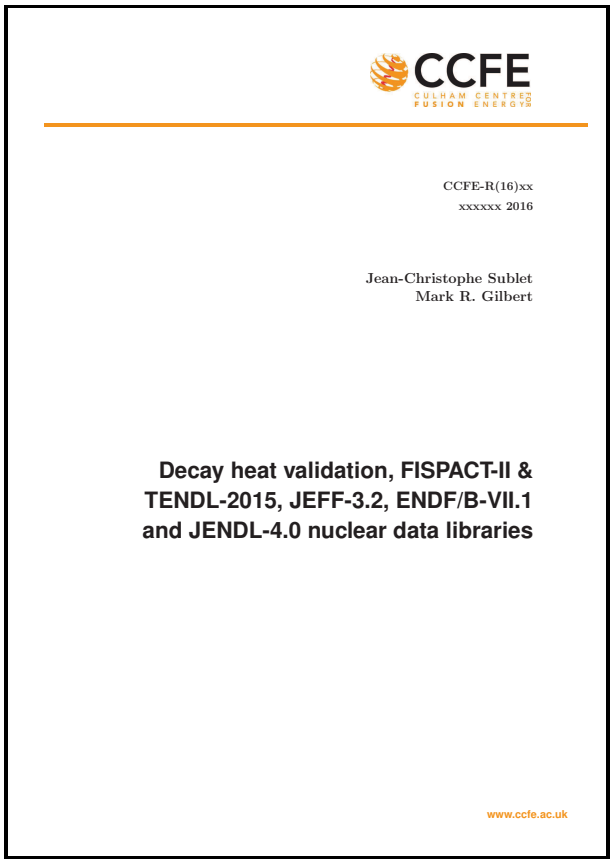
- missing isomeric states for Nb in all but TENDL

FISPACT-II & TENDL validation

- Comparison of experimentally-measured decay heat (FNS JAERI) to FISPACT-II predictions with TENDL-2015 and other (legacy) libraries[§]:



Niobium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Decay heat validation, FISPACT-II & TENDL-2015, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries

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- Only TENDL has open reaction channels to the necessary isomeric states
- ^{94m}Nb at short decay times

[§]report in preparation

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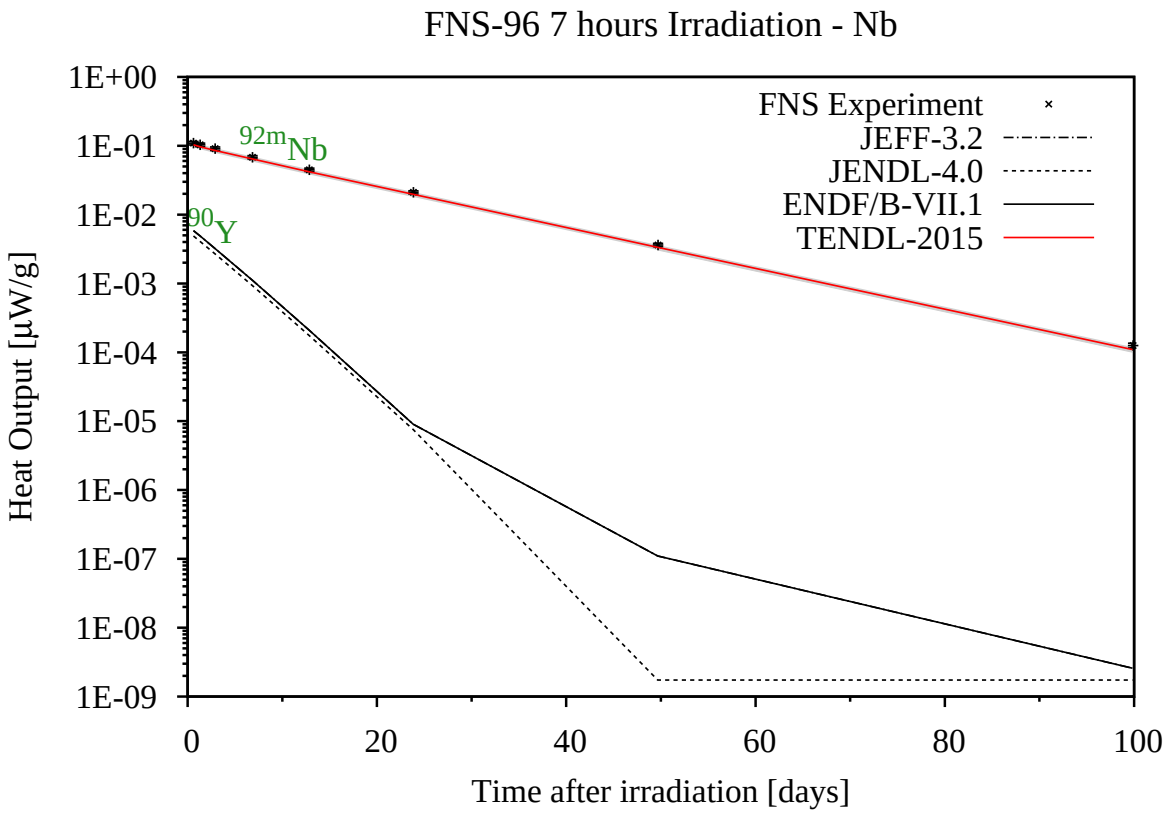
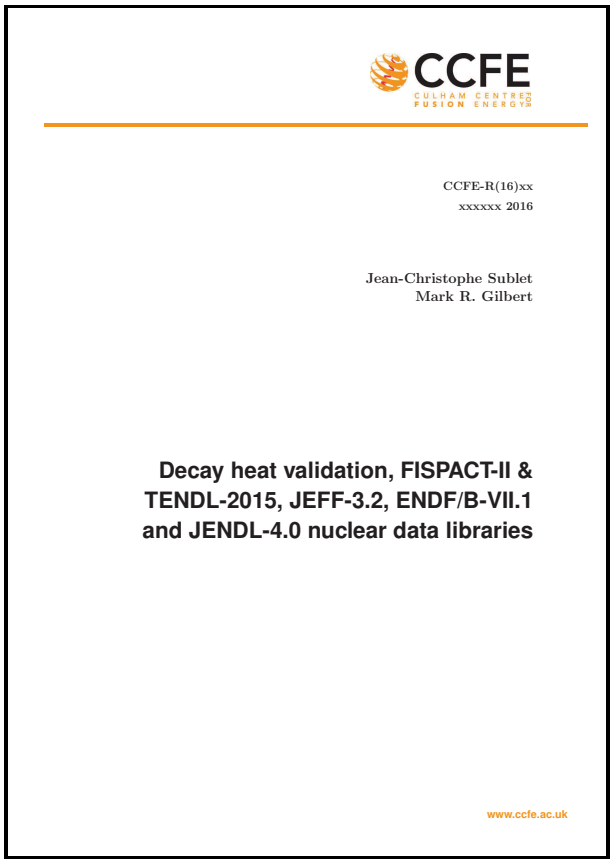


Niobium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- Only TENDL has open reaction channels to the necessary isomeric states
- ^{92m}Nb at longer times

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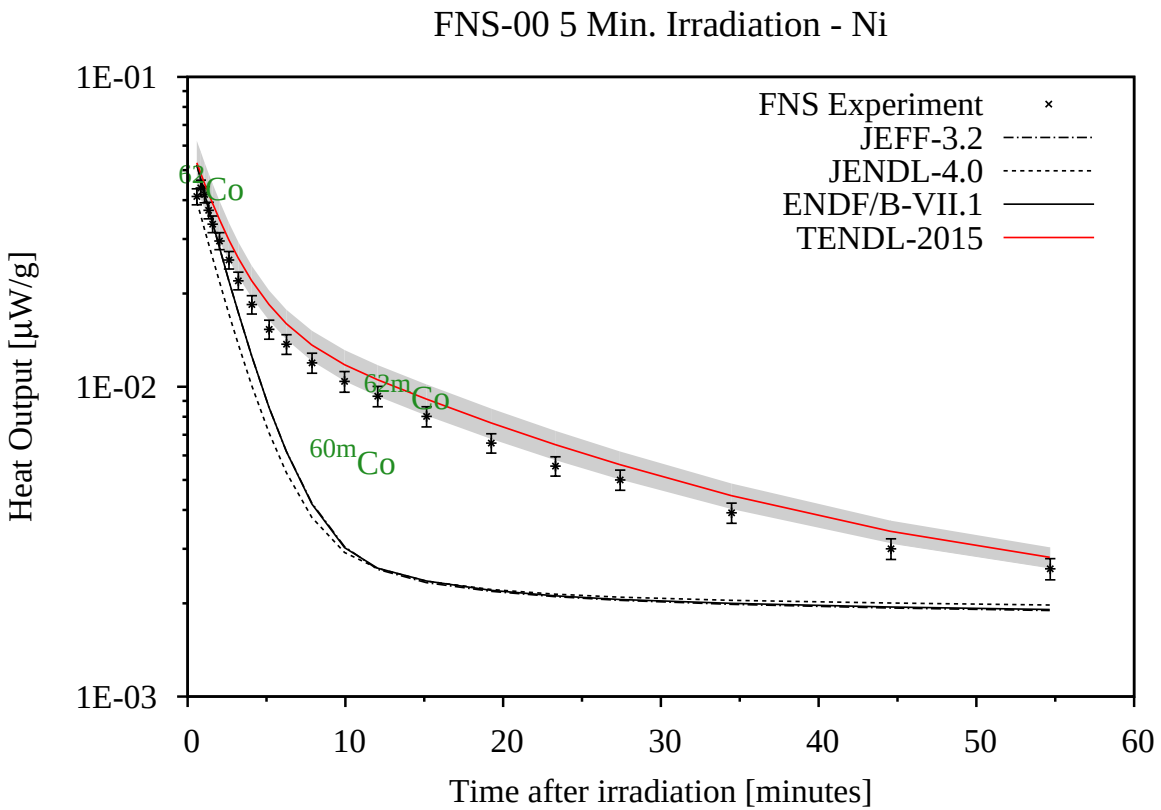
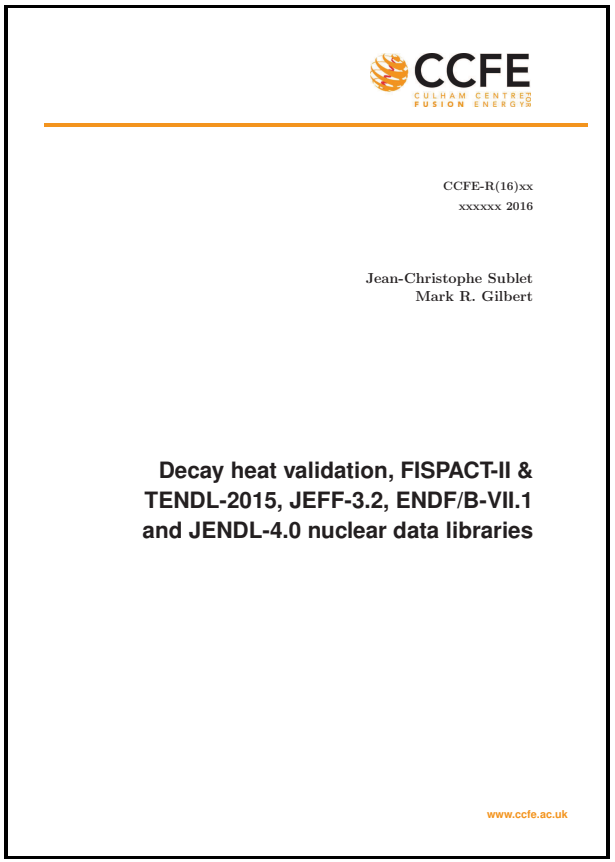


Nickel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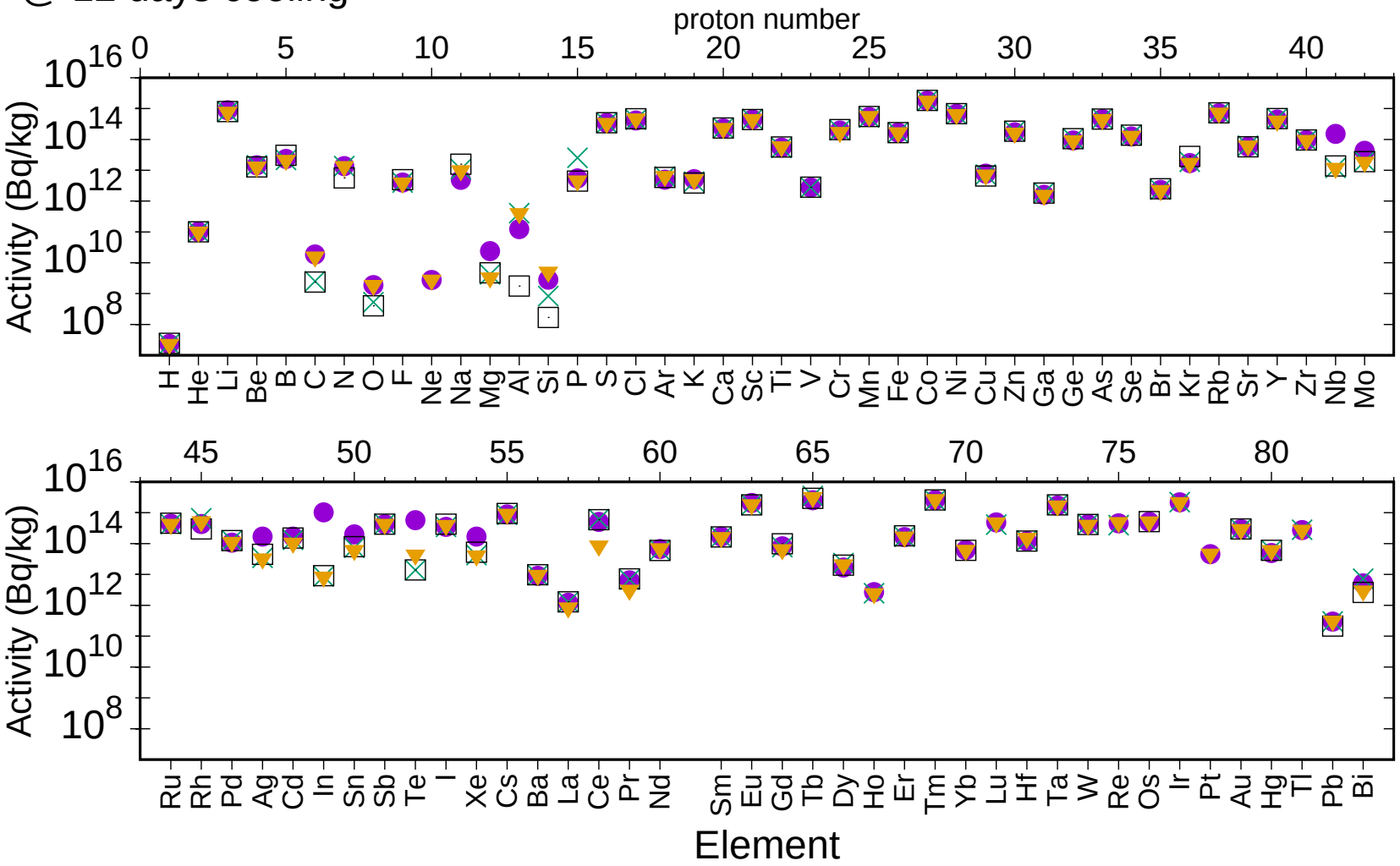
- Other examples include the absence of cobalt isomers produced by irradiating Ni

[§]report in preparation

Activation global results

- time snapshot of activity during cooling[§] for all materials:

@ 12 days cooling

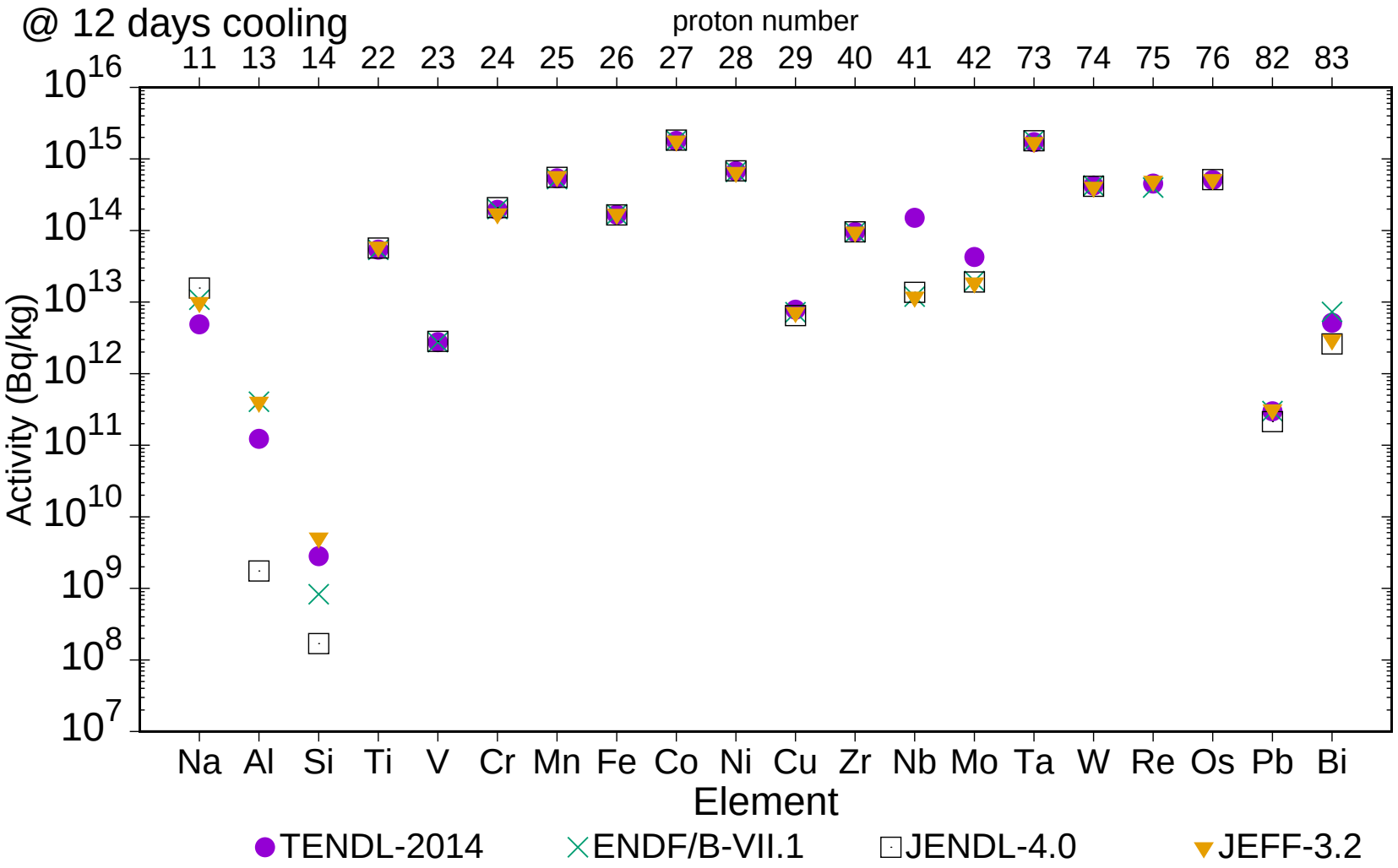


too much data! ●TENDL-2014 ×ENDF/B-VII.1 □JENDL-4.0 ▼JEFF-3.2

[§]after 2 fpy in FW DEMO conditions

Activation global results

- time snapshot of activity during cooling[§] for selected materials:



- Some important material show significant variation with library

[§]after 2 fpy in FW DEMO conditions

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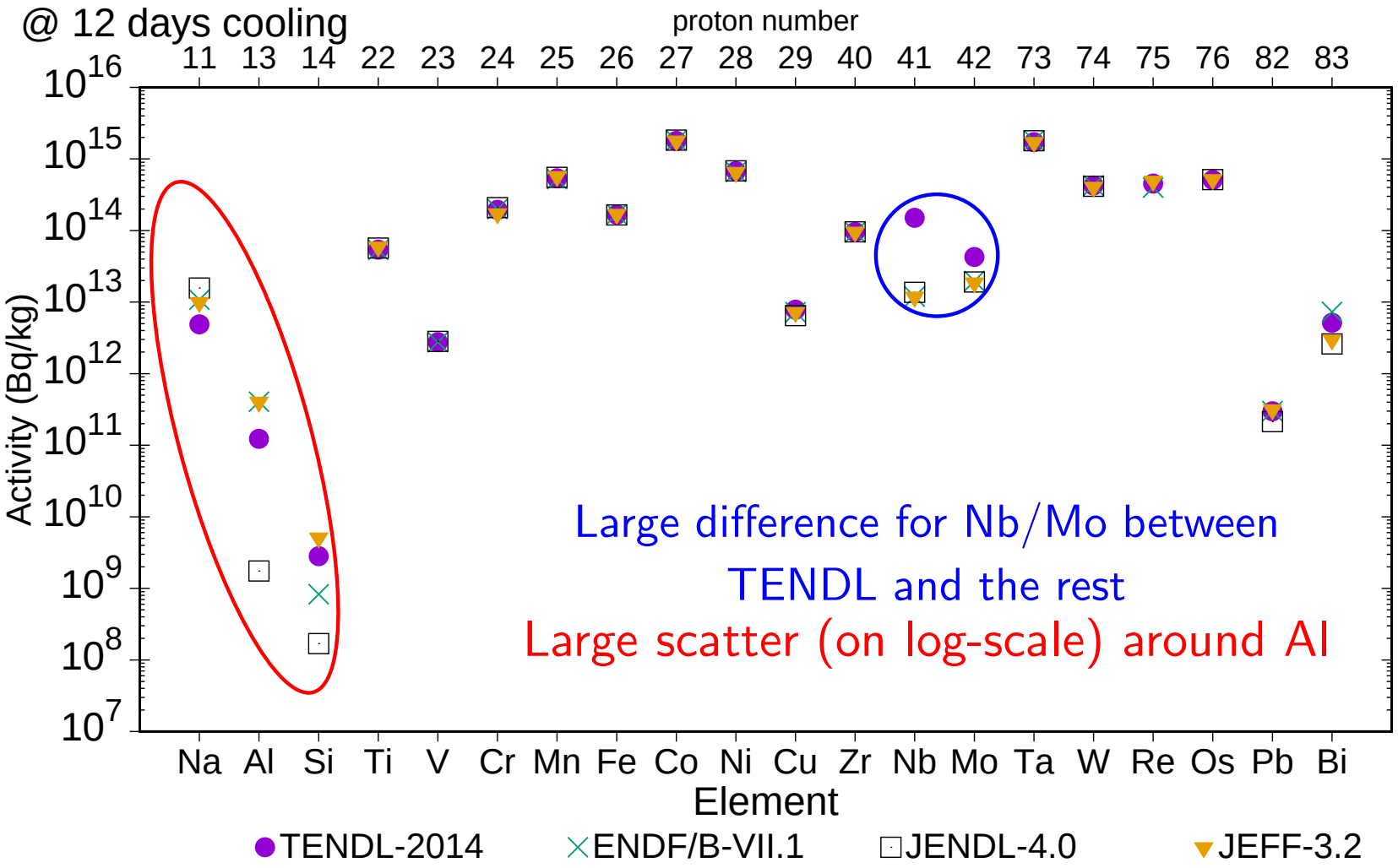

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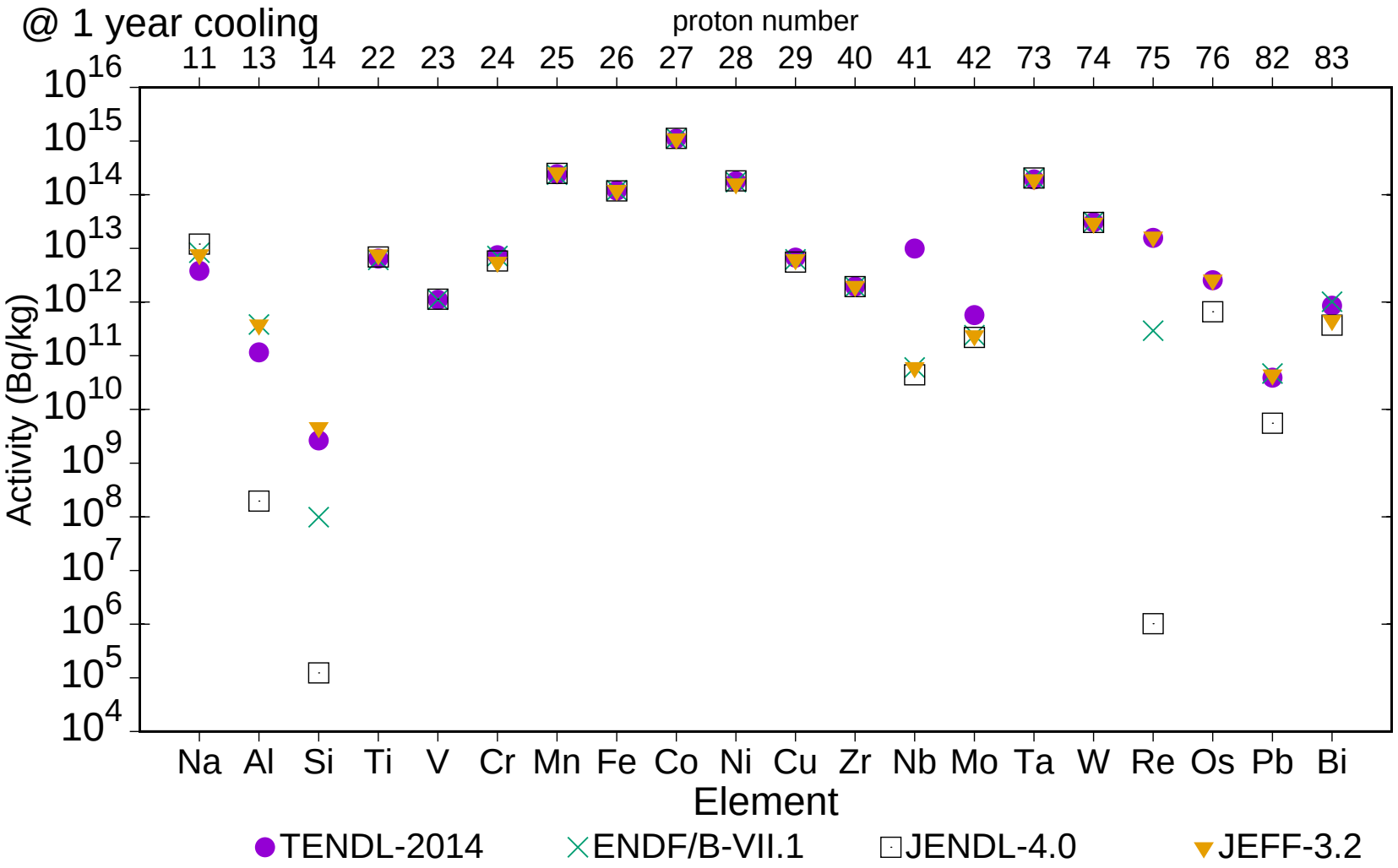

- can even get worse at longer cooling times

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Activation global results

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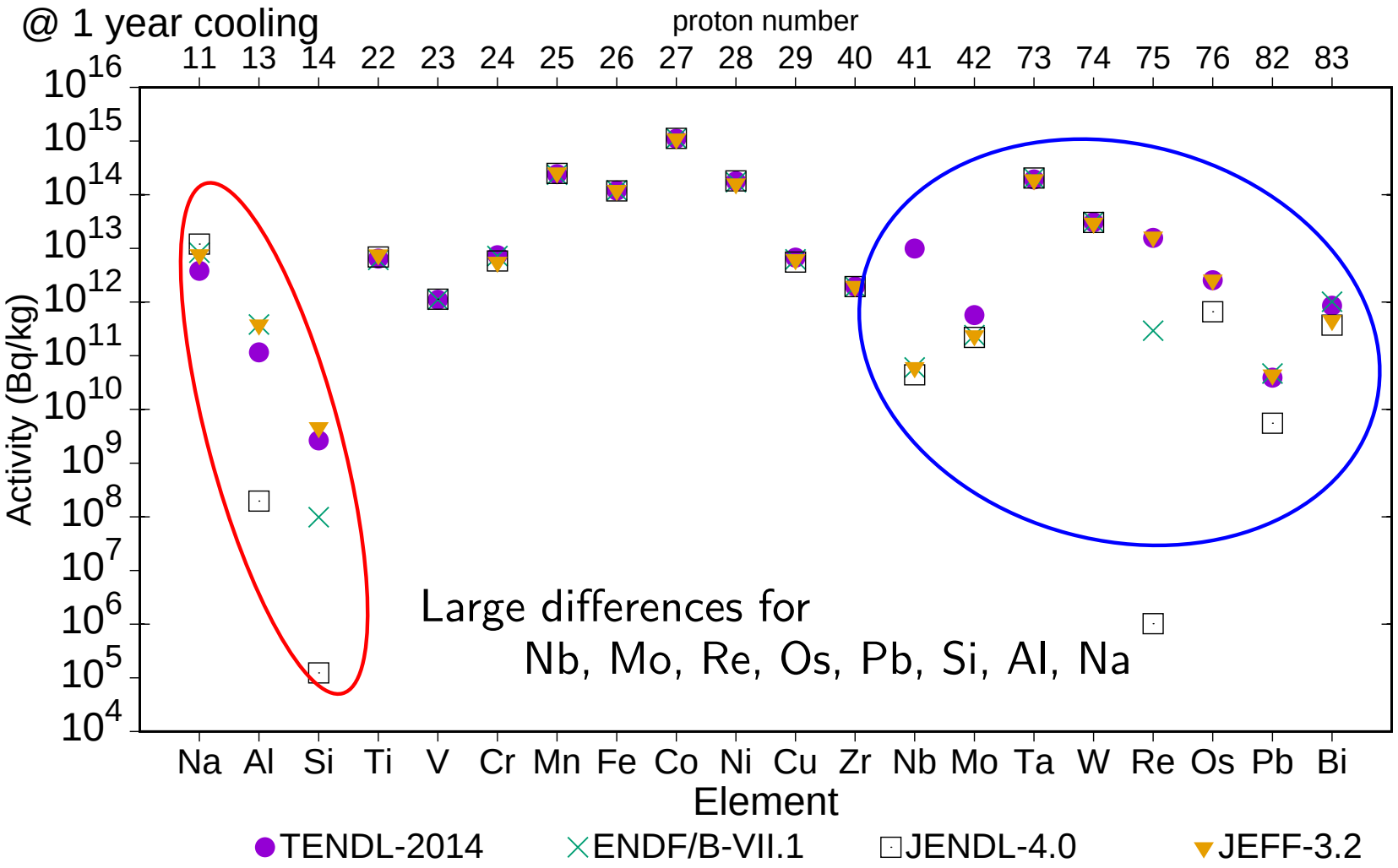
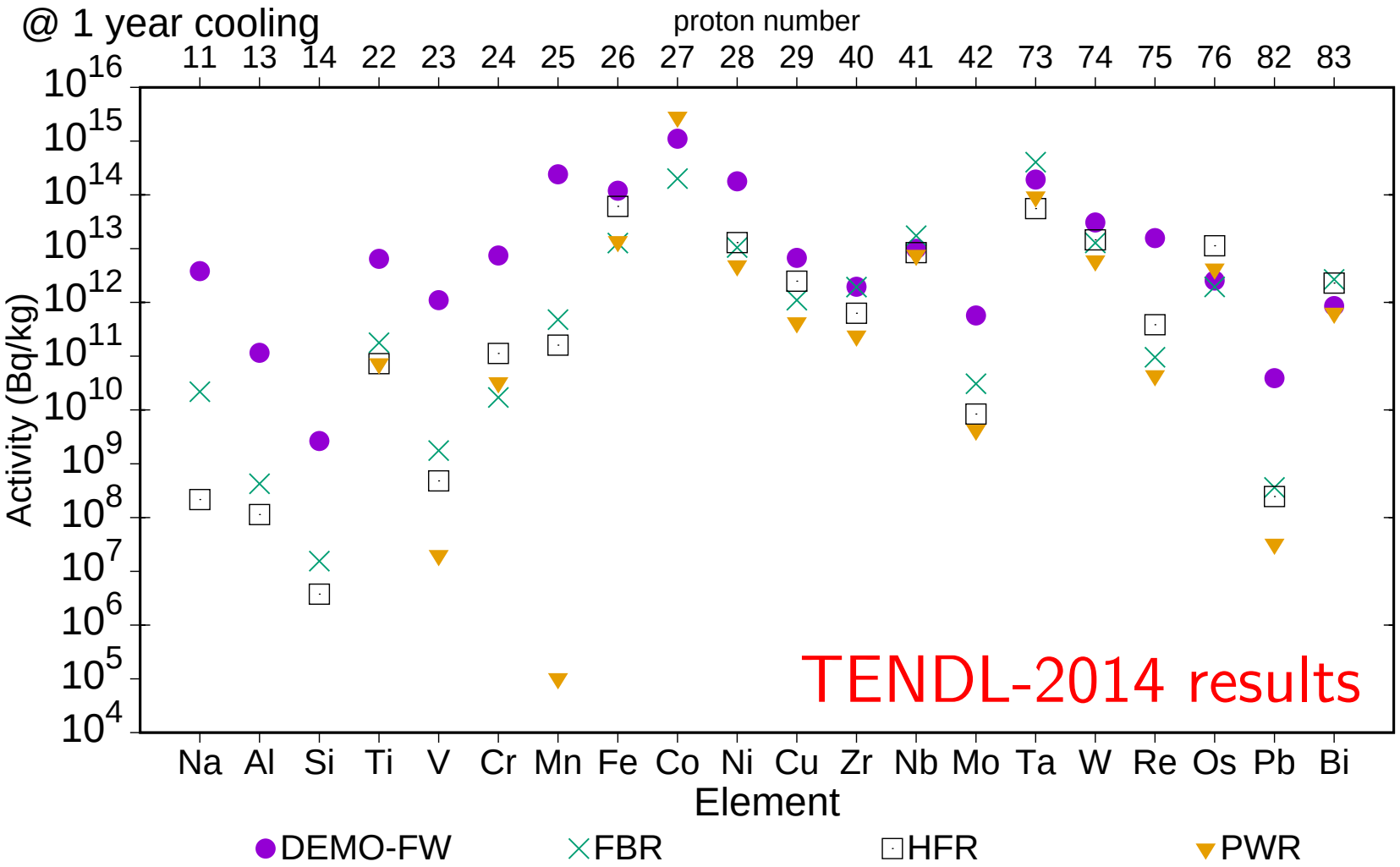


- can even get worse at longer cooling times

[§]after 2 fpy in FW DEMO conditions

Activation global results – fusion vs. fission

- time snapshot of activity during cooling[§] for selected materials:

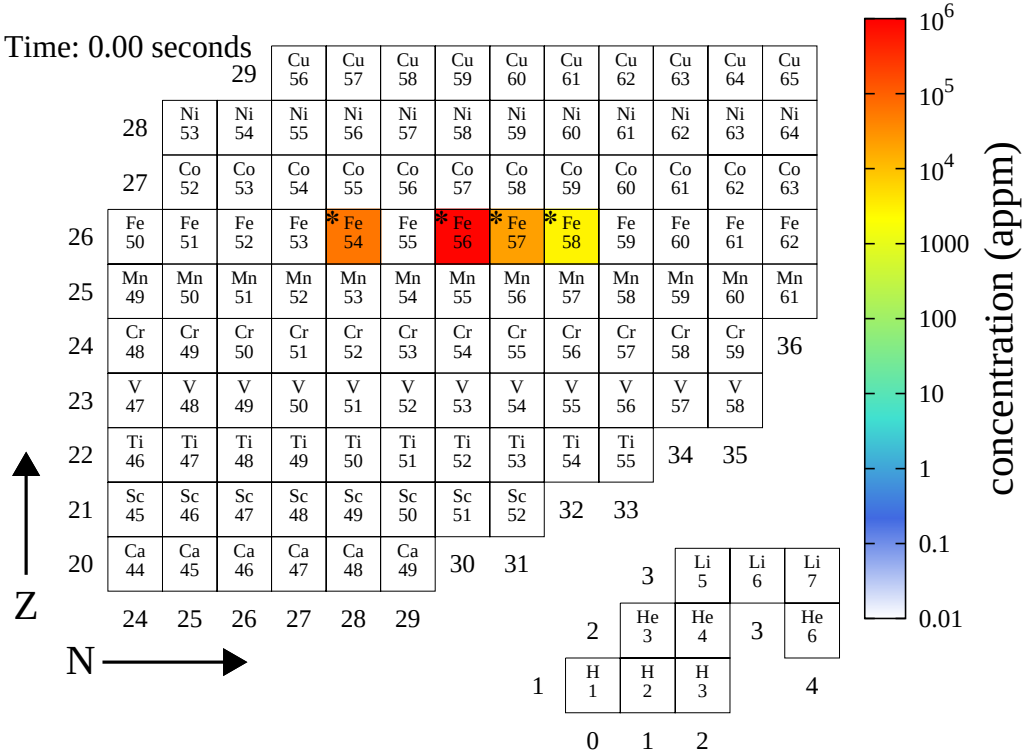


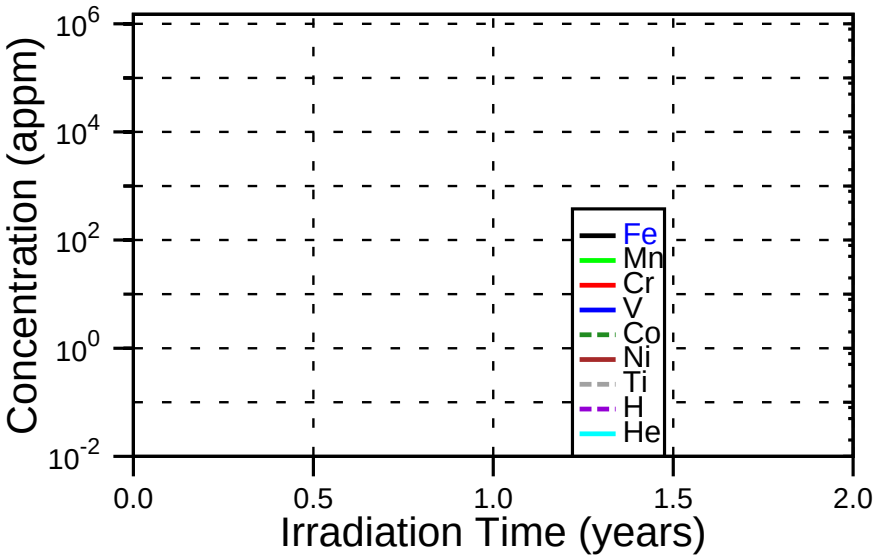
- Fusion mostly more active, but with exceptions

[§]after 2 fpy in each scenario

Transmutation

- The output of FISPACT-II gives a detailed, isotopically-separated break-down of the composition as a function of time under irradiation





- plotted in the handbooks at both the elemental (line chart) and isotopic (nuclide chart[§]) level
- production of impurities, particularly gases, under irradiation is a significant "damage" mechanism

DEMO-FW, TENDL-2014 results

appm - atomic parts per million
* nuclide present in input composition
[§] Gilbert, Packer, Sublet, Forrest, *Nucl. Sci. Eng.* **177** (2014) 291–306

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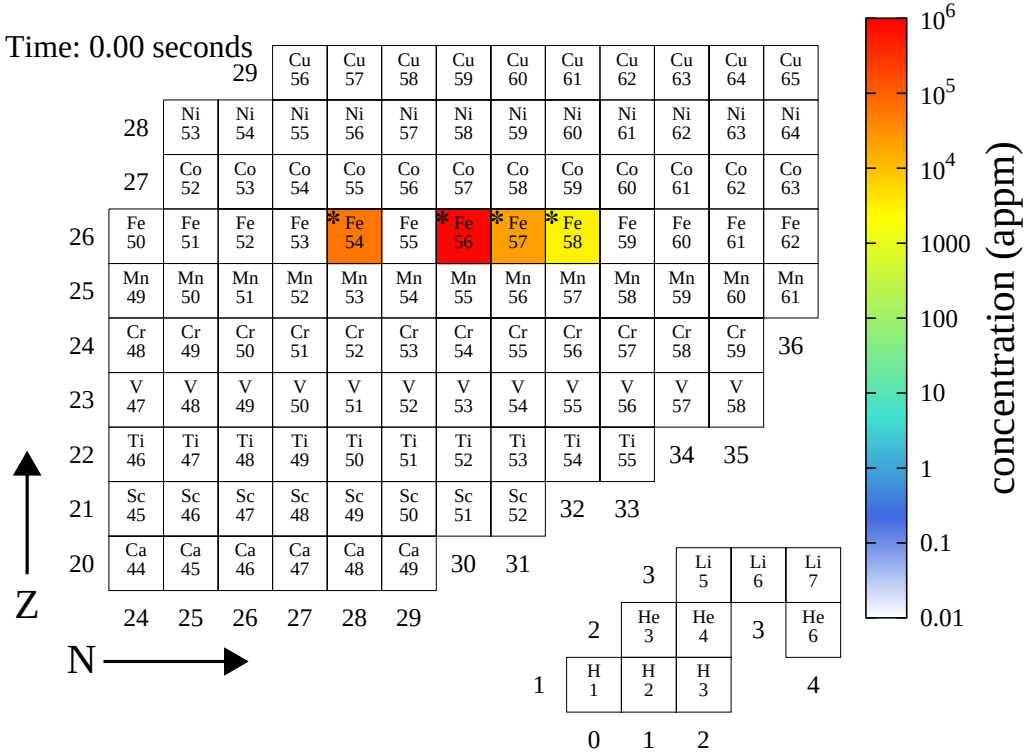

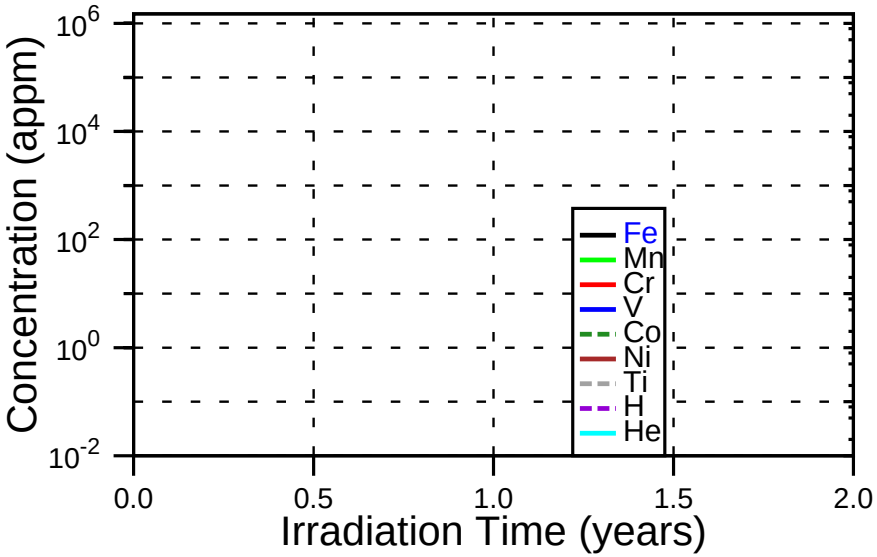

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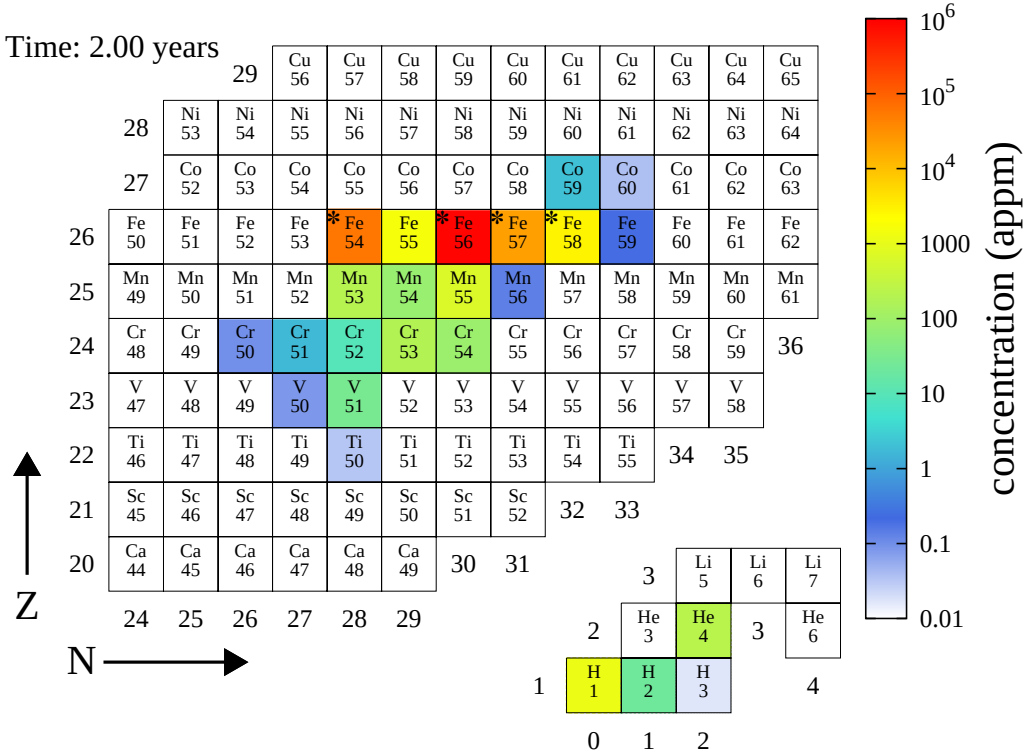
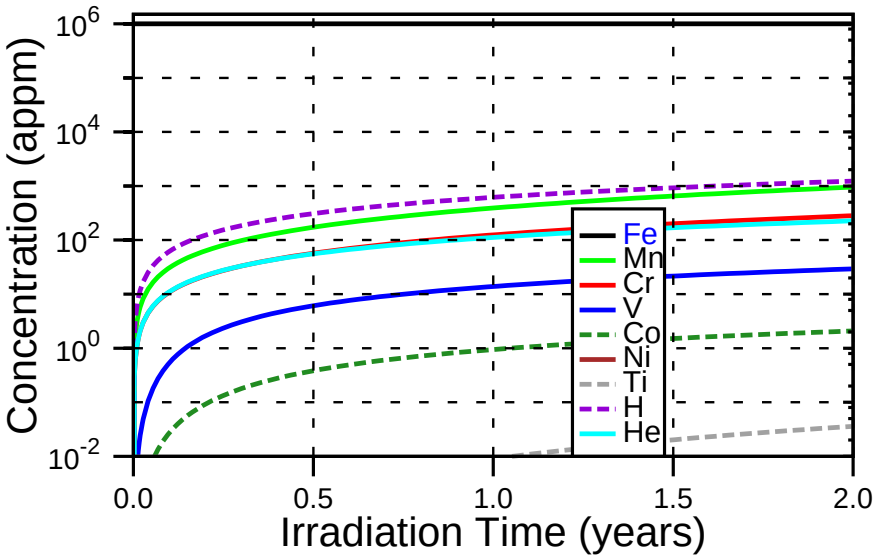
- The output of FISPACT-II gives a detailed, isotopically-separated break-down of the composition as a function of time under irradiation





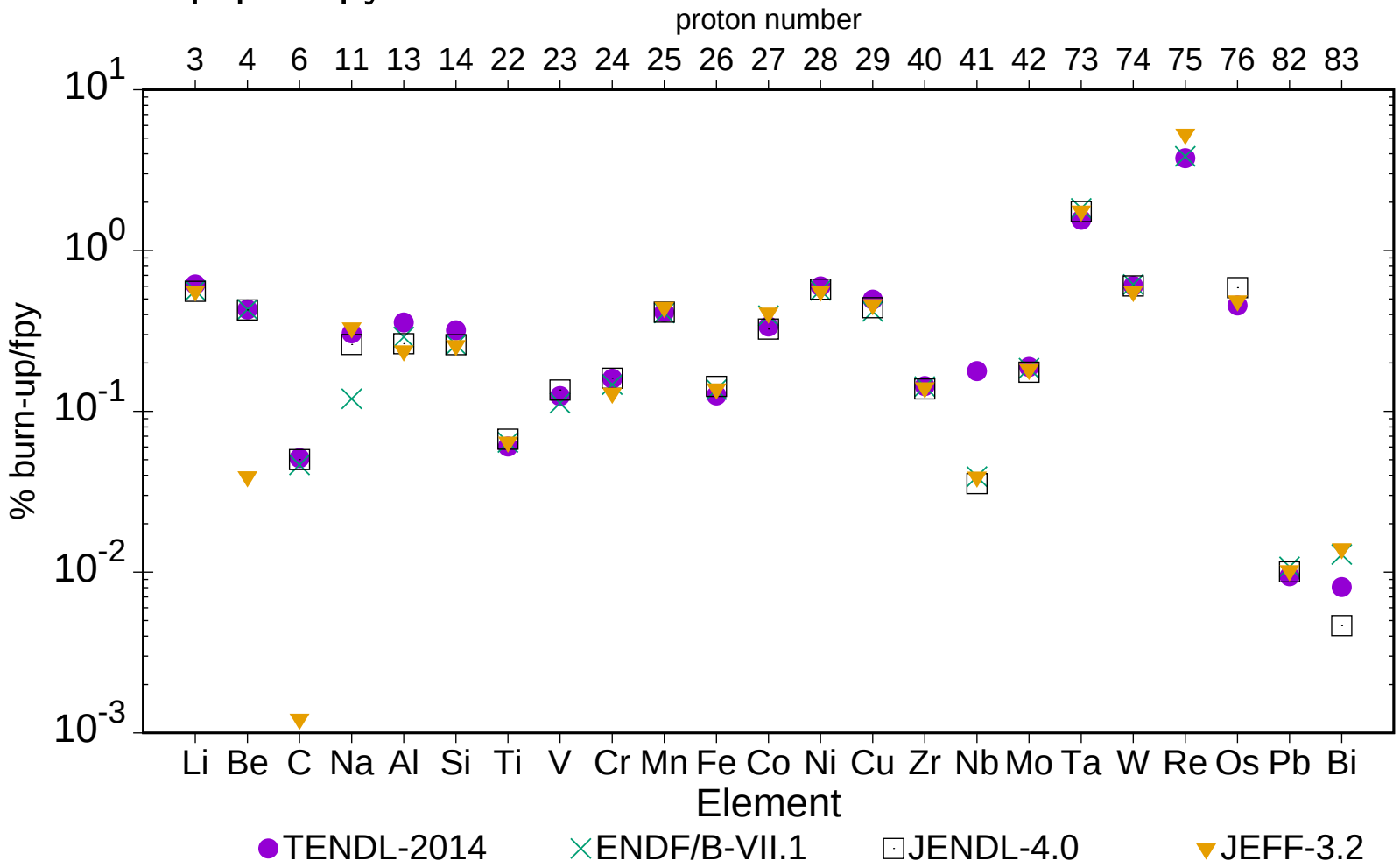
- plotted in the handbooks at both the elemental (line chart) and isotopic (nuclide chart[§]) level – after 2 fpy
- production of impurities, particularly gases, under irradiation is a significant "damage" mechanism

DEMO-FW, TENDL-2014 results

appm - atomic parts per million
* nuclide present in input composition
[§] Gilbert, Packer, Sublet, Forrest, *Nucl. Sci. Eng.* **177** (2014) 291–306

Transmutation – library variation

- % burn-up per fpy for selected elements[§]:

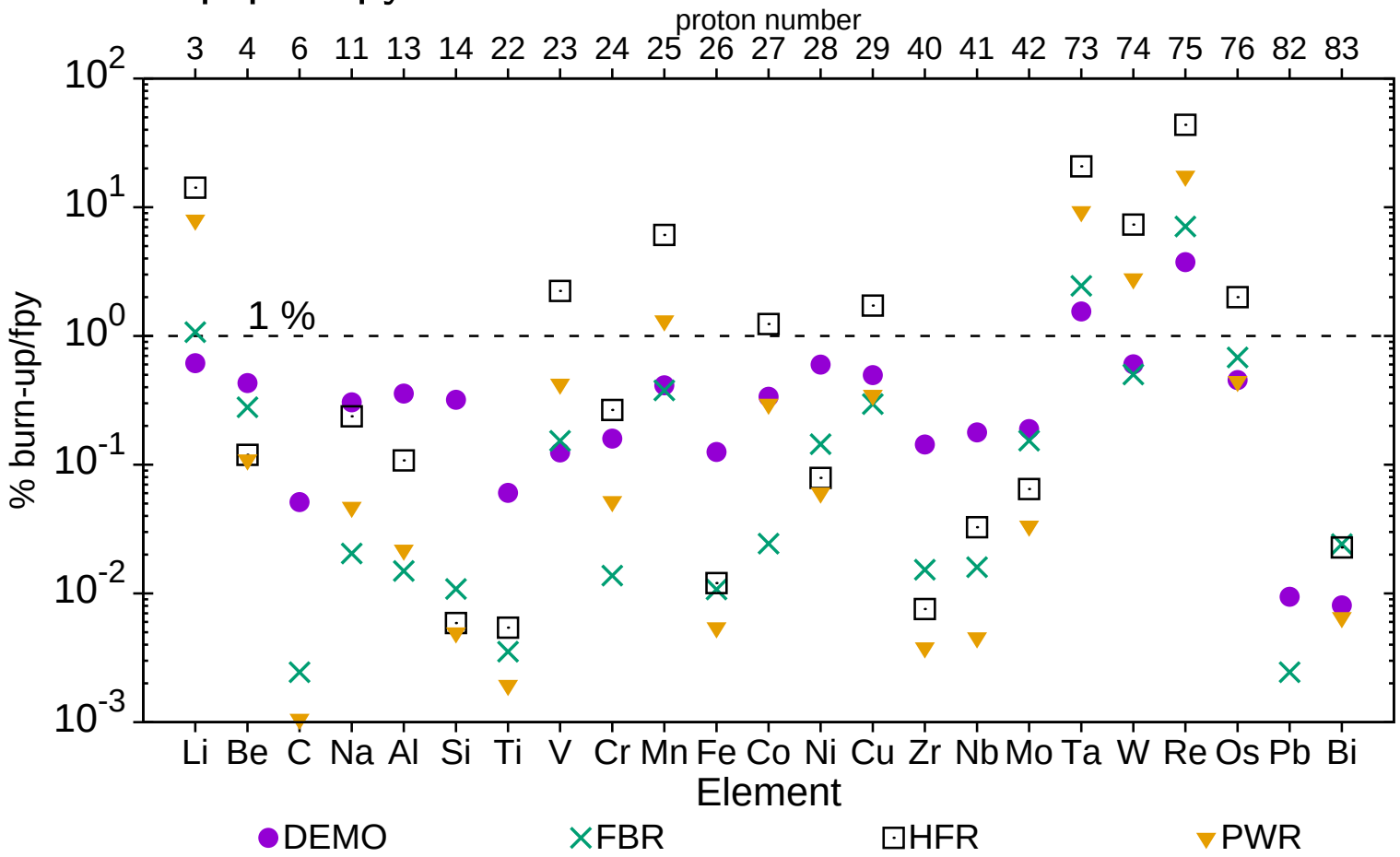


- Good, order-of-magnitude agreement between libraries for most materials, but some important materials (e.g. C, Nb) show large variation

[§]in FW DEMO conditions
fpy - full power years

Transmutation – environment variation

- % burn-up per fpy for selected elements[§]:

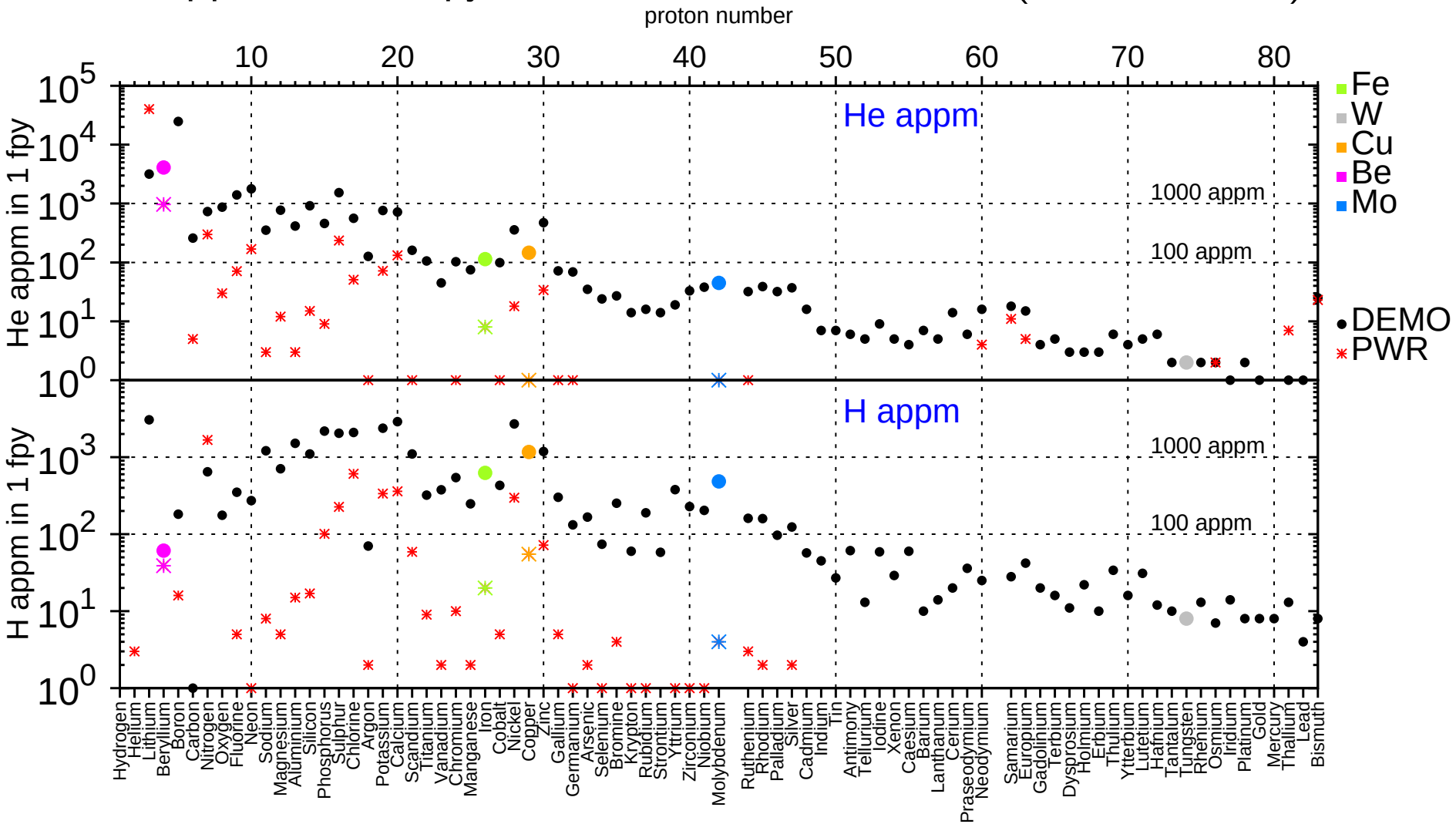


- Fission spectra are moderated ("softer") than fusion & combined with high-flux in HFR produces greater burn-up rates in many elements ⇒ spectrum modification (via shielding) required to match fusion in experimental campaigns

[§]TENDL-2014 results
fpy - full power years

Gas production – fusion vs. fission

- Gas appm after 1 fpy in DEMO FW and PWR§ (TENDL-2014):



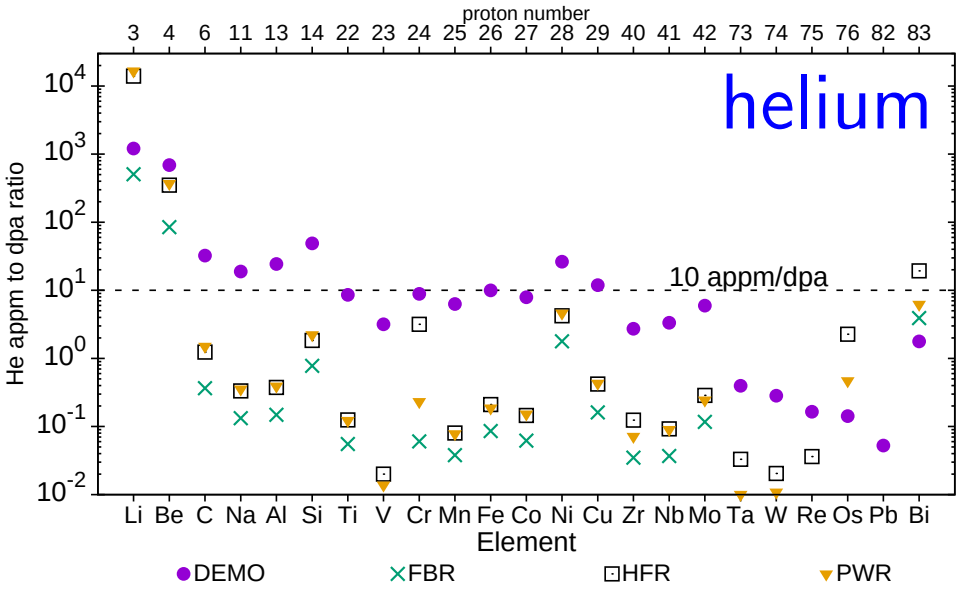
- gas production is significantly higher under fusion neutrons

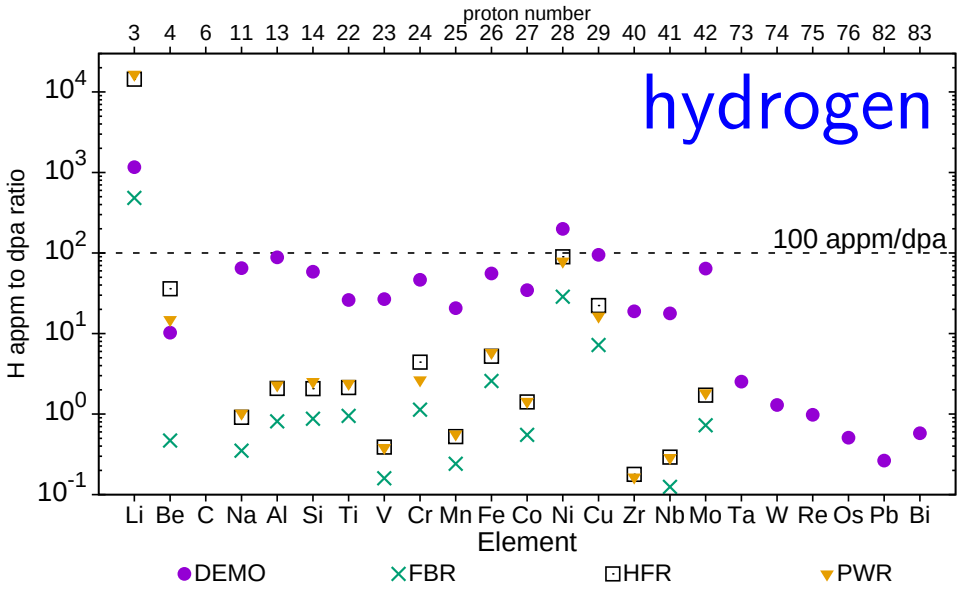
- with very few exceptions

§fuel assembly average

Gas production (selected) – fusion vs. fission

- Gas-to-dpa ratios (TENDL-2014):

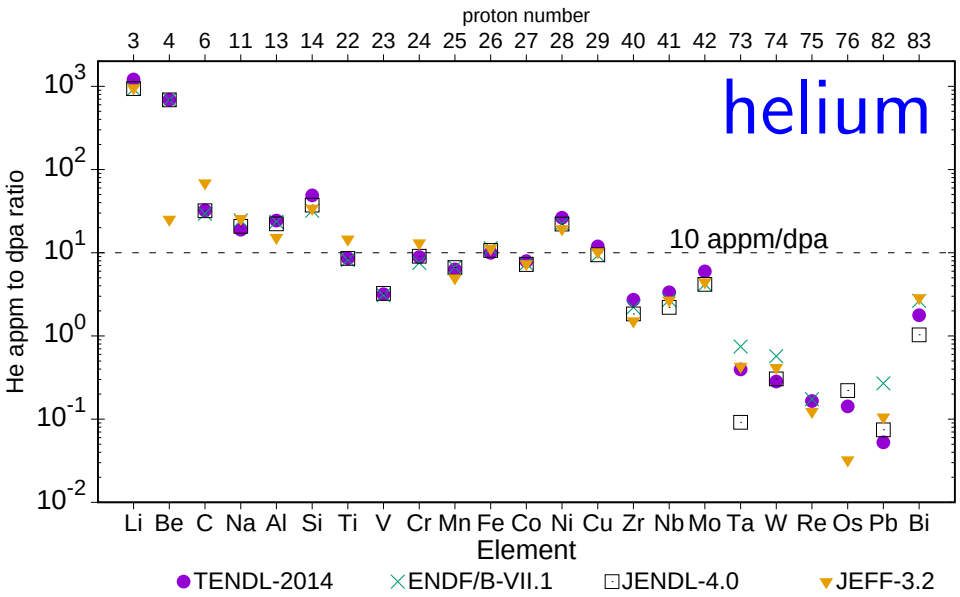


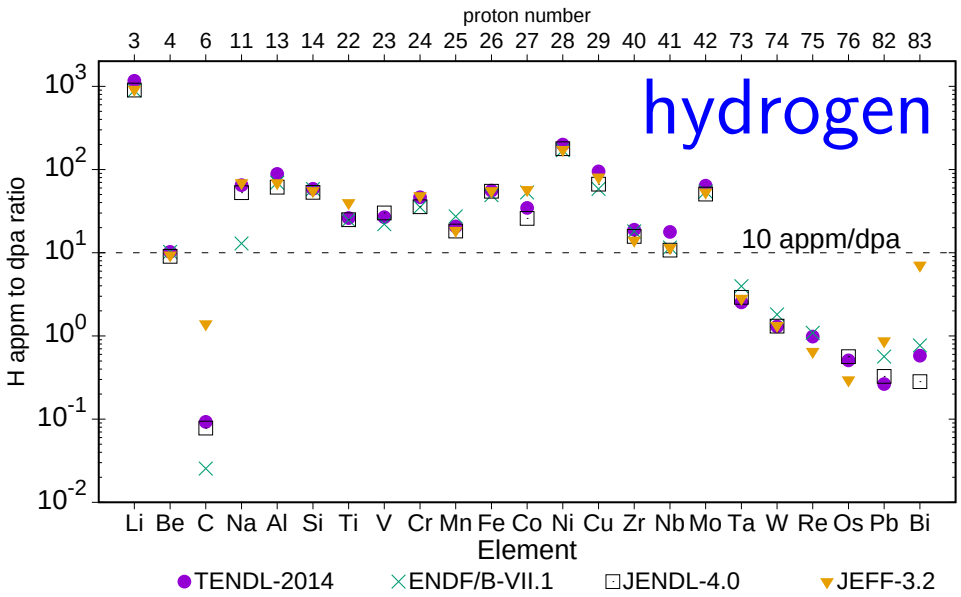


- even when scaled by (NRT) dpa rates, the difference between fusion and fission is high
- makes it difficult to realise correct (for fusion) gas production rates in actual (thermal) fission environments

Gas production (selected) – library comparison

- Gas-to-dpa ratios under DEMO FW conditions:

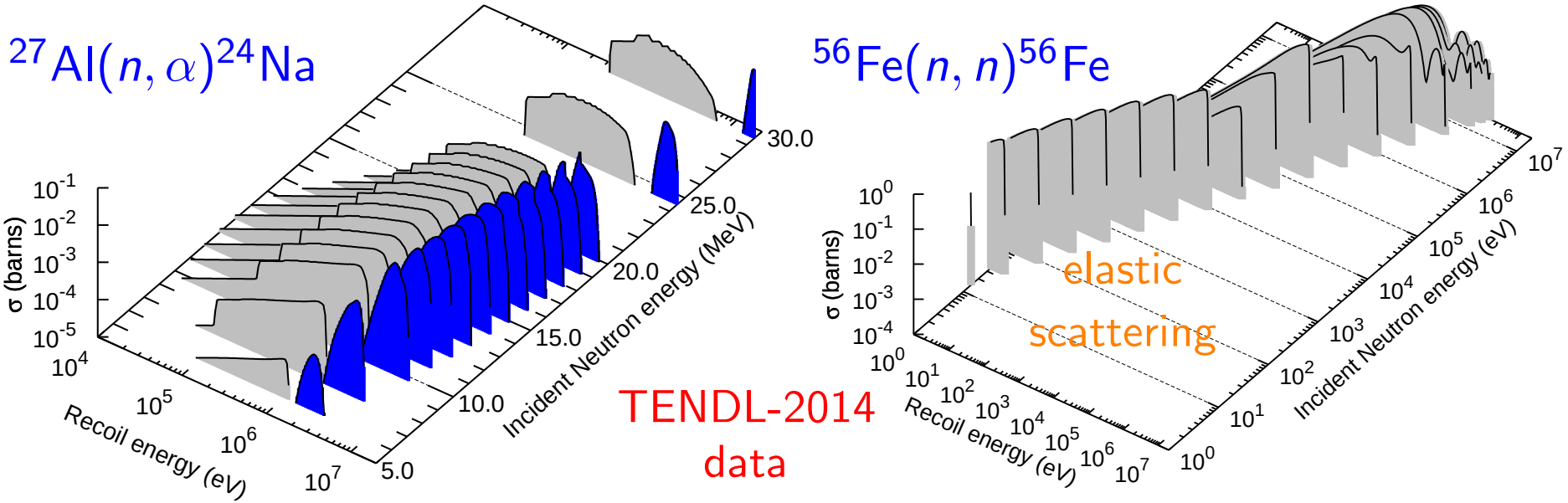




- Generally good agreement between libraries for the important materials (same order-of-magnitude)
- but more variation when gas production and/or dpa rates are low
  - note hydrogen production from carbon, in particular

PKAs: Computational approach

- Motivation: energy distributions of primary knock-on atom (PKA) fluxes provides more information to materials modelling than dpa
- Neutron interaction recoil matrices $M^{x\to y} \equiv \{m_{ij}^{x\to y}\}$ calculated using NJOY[§] (via GROUPR) $\longrightarrow$ using pointwise nuclear data
  - $m_{ij}^{x\to y}$ is the recoil cross section (in barns) for a recoil energy E_i of daughter y resulting from an incident neutron energy E_j on parent x
  - for each target (parent) isotope there will be a set of $M^{x\to y}$



[§]2012.50 (+ local update) version of the nuclear data processing system developed at LANL

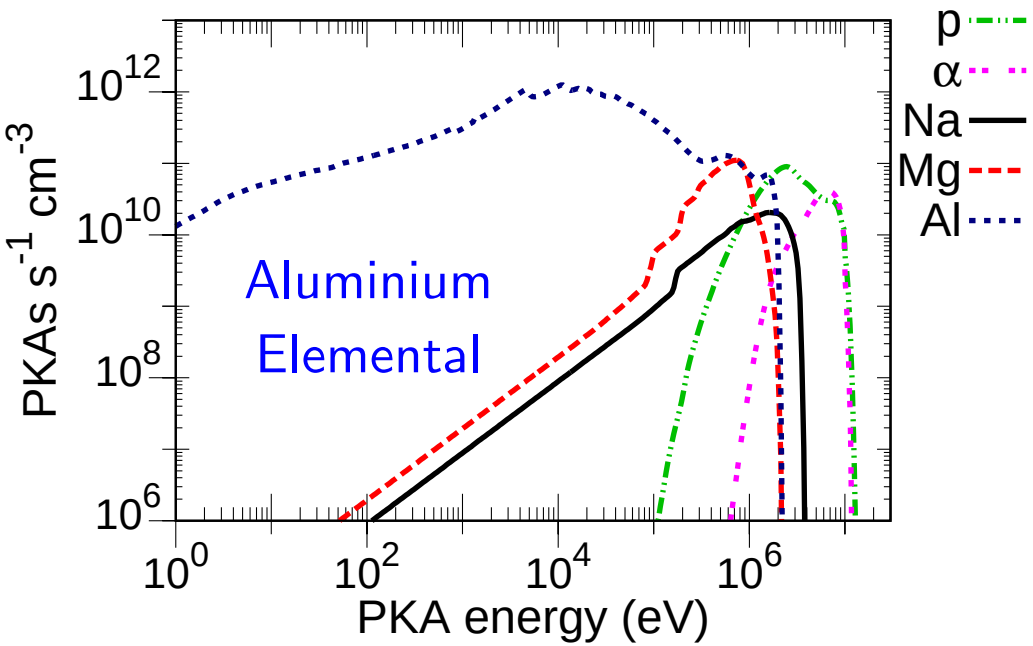
PKAs: Computational approach

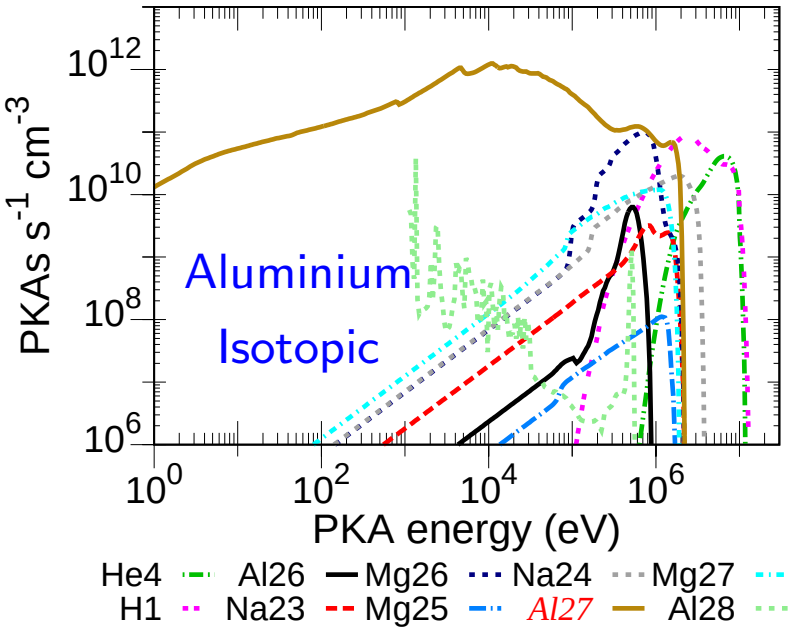
- Collapsing with a neutron irradiation spectrum $\{\phi_j\}$ gives the recoil-energy spectrum $R^{x\to y}(E)$:

"PKA-spectrum" under neutron irradiation

$$\equiv R^{x\to y}(E) \equiv \{r_i^{x\to y}\} = \left\{ \sum_j m_{ij}^{x\to y} \phi_j \right\}$$

- processing done with newly written SPECTRA-PKA[§] code





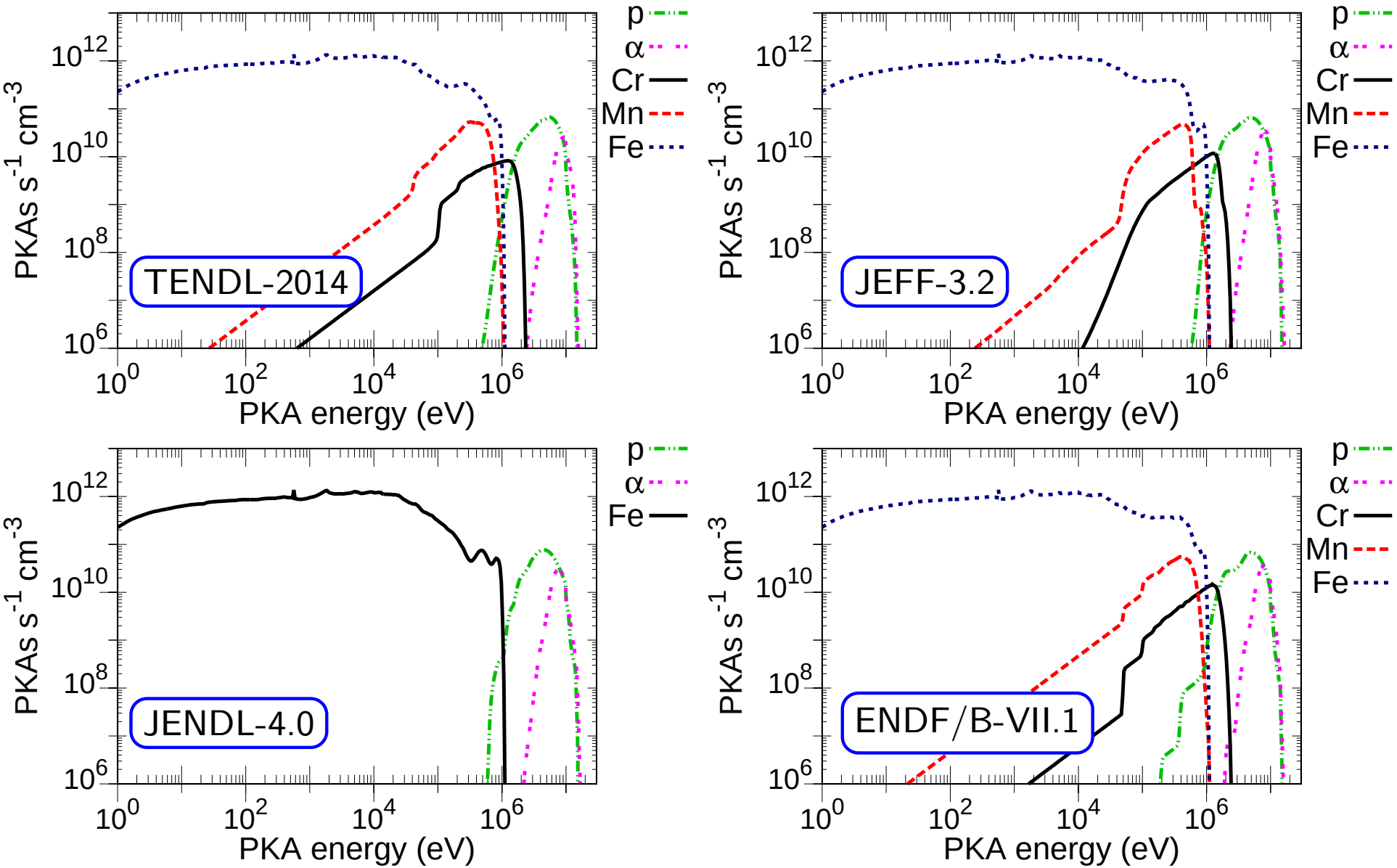
[§] Gilbert *et al.*, *JNM* **467** (2015) 121-134

- PKA spectra of Al under DEMO first wall conditions with TENDL-2014
- many different recoil species (even with just Al27 target)

Iron

PKA distributions – elemental

DEMO-FW

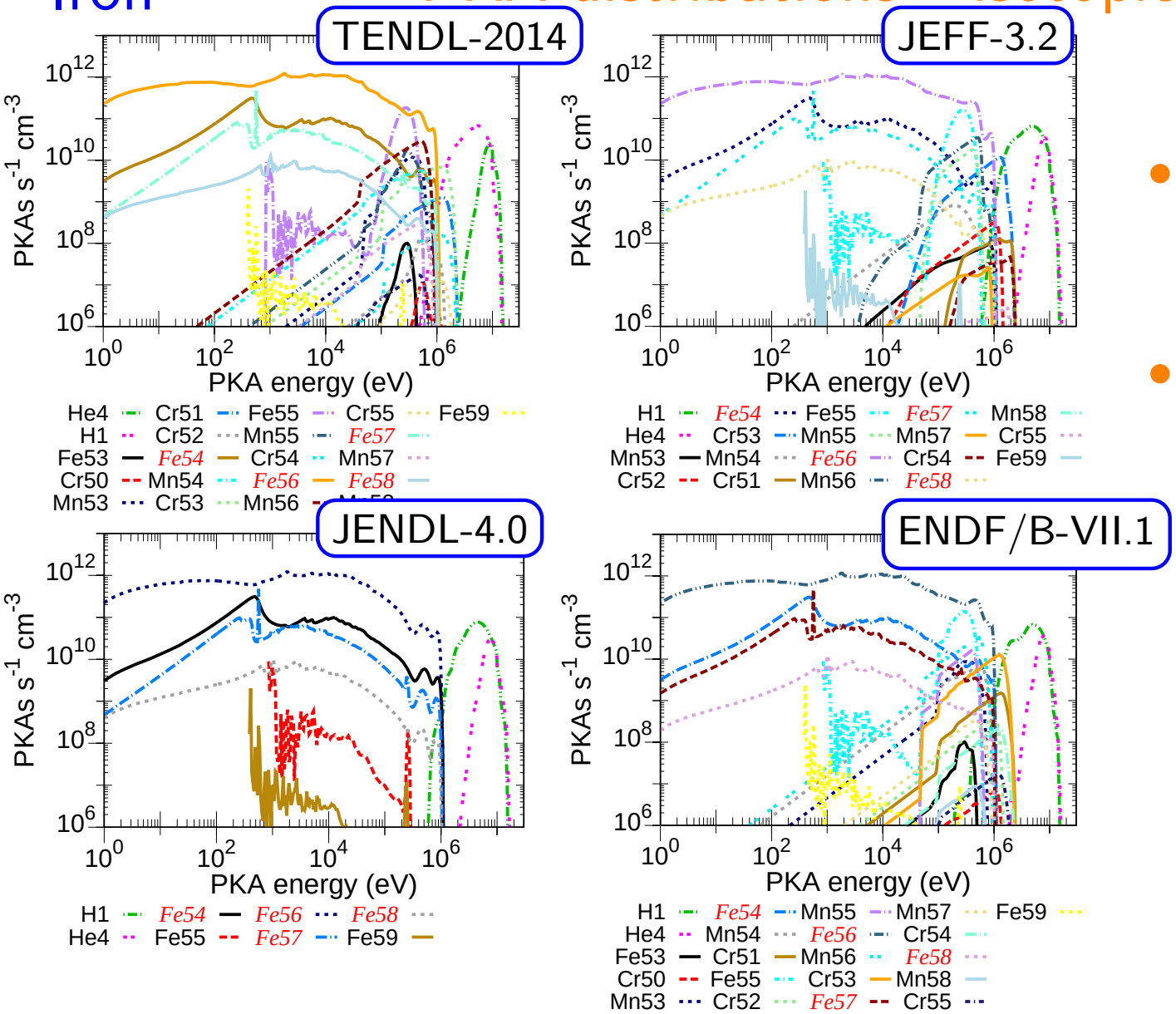


- Missing channels in JENDL-4.0?

Iron

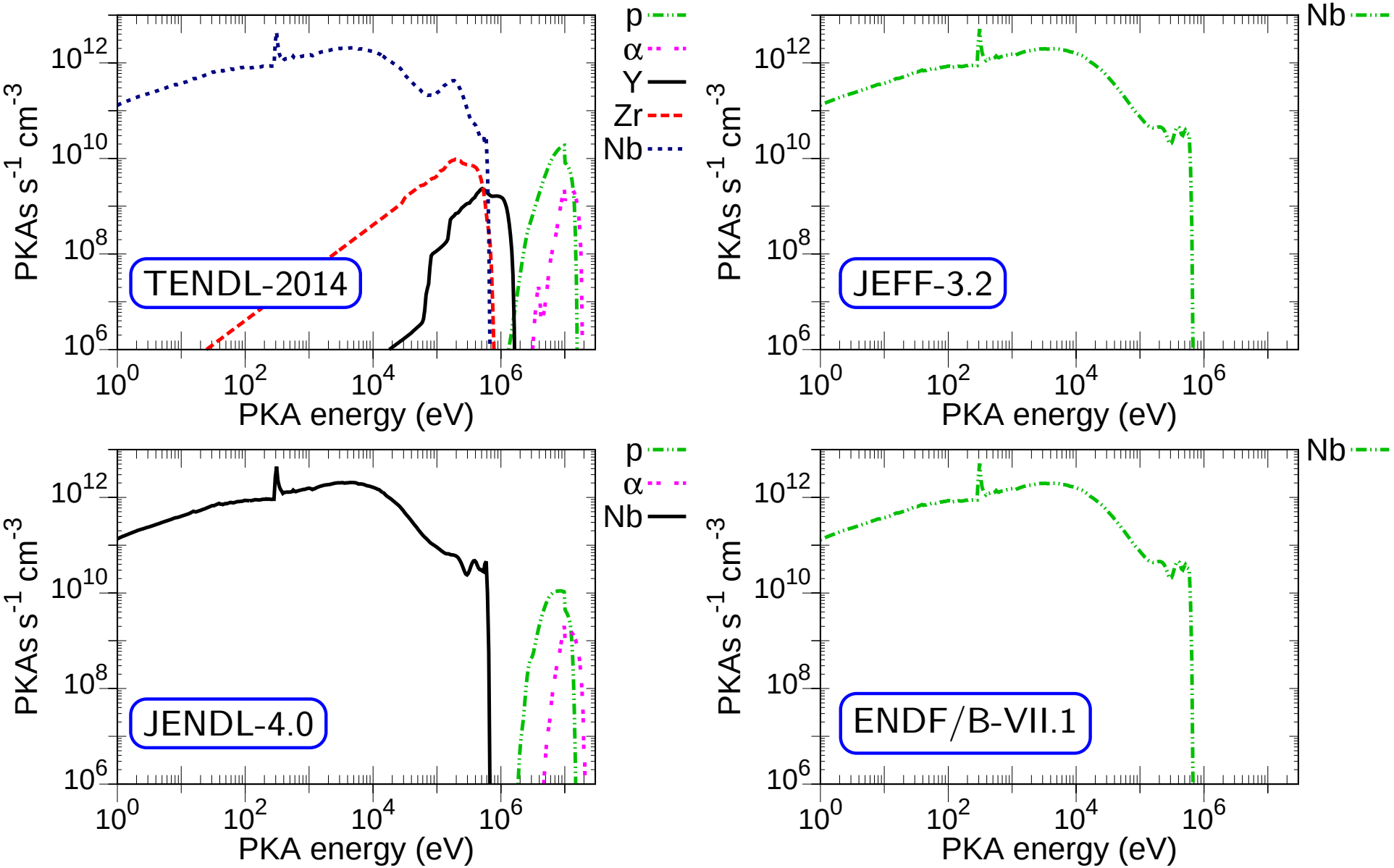
PKA distributions – isotopic

DEMO-FW



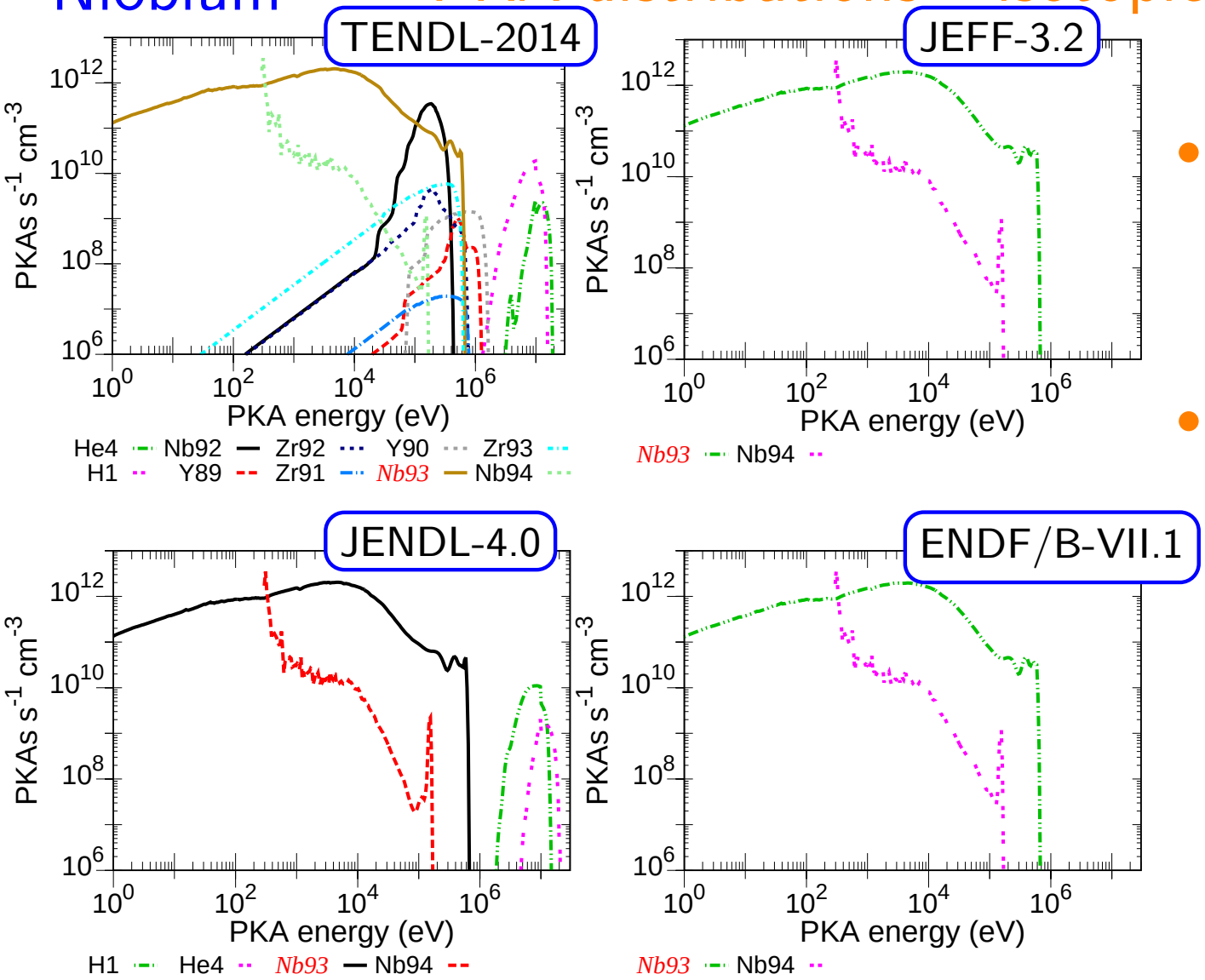
- fewer isotopes with PKA distributions from JENDL-4.0
- but the dominance of scattering channels might hide this discrepancy from total damage functions (e.g. kerma)

Niobium PKA distributions – elemental DEMO-FW



- Missing attributions in all but TENDL?

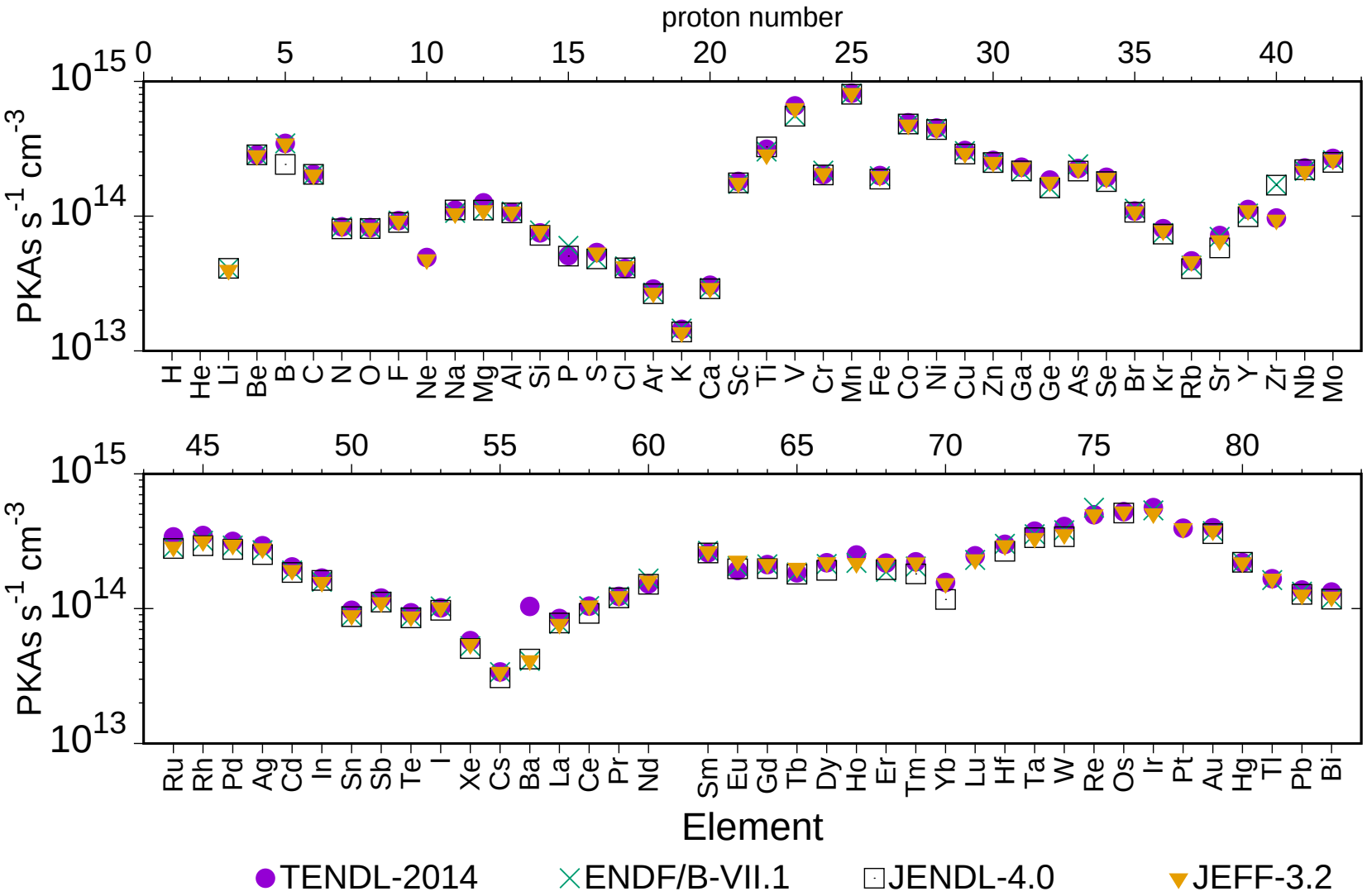
Niobium PKA distributions – isotopic DEMO-FW



- Only TENDL-2014 and JENDL-4.0 have high energy gas recoils
- JEFF-3.2 and ENDF/B-VII.1 seem to have incomplete, for material science, files (^{94}Nb generated via (n,γ) xs approximation)

Total PKA rates – library comparison

- total heavy PKAs* for all materials§



*above 10 eV & excluding proton and alpha recoils
§FW DEMO conditions

Total PKA rates – library comparison

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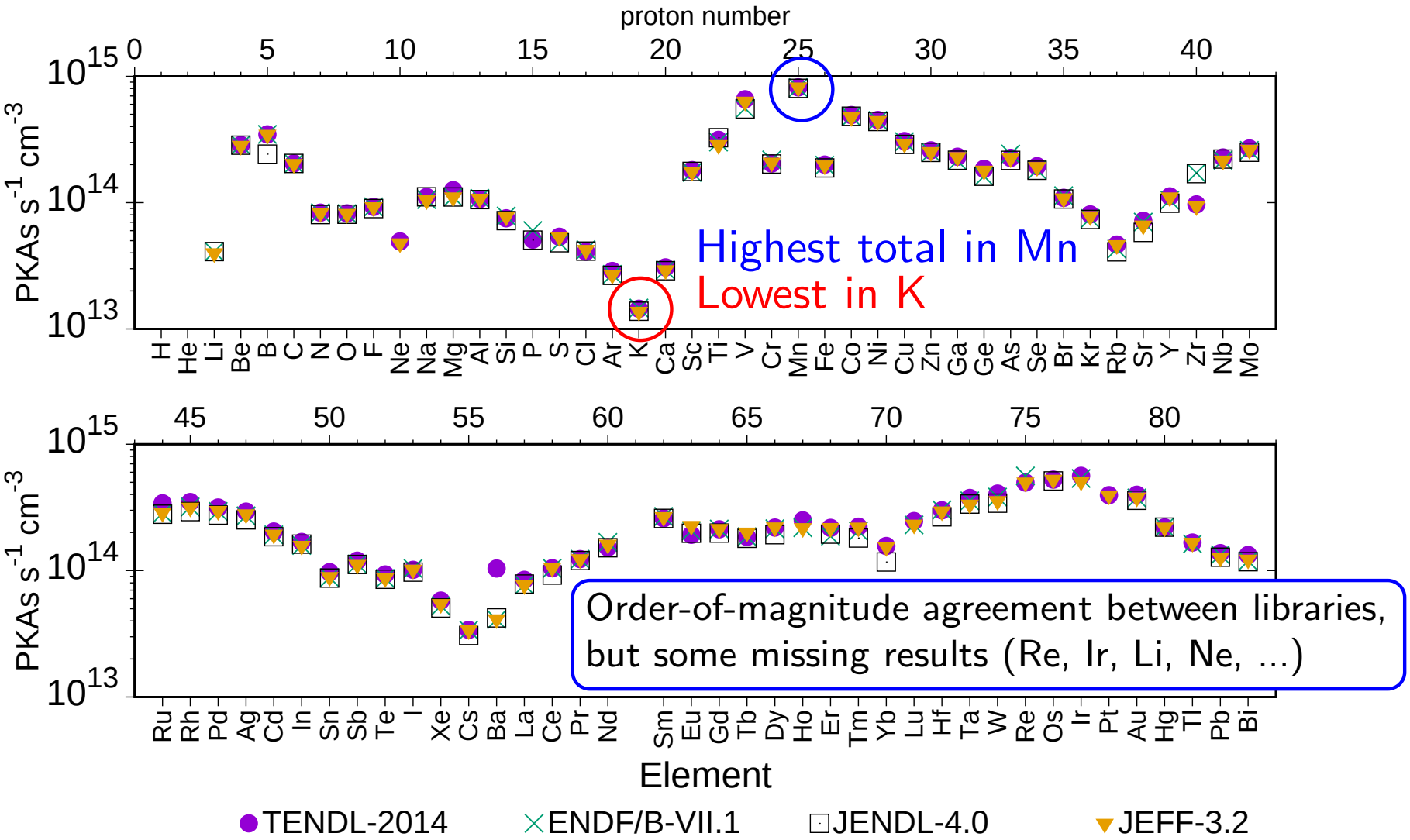
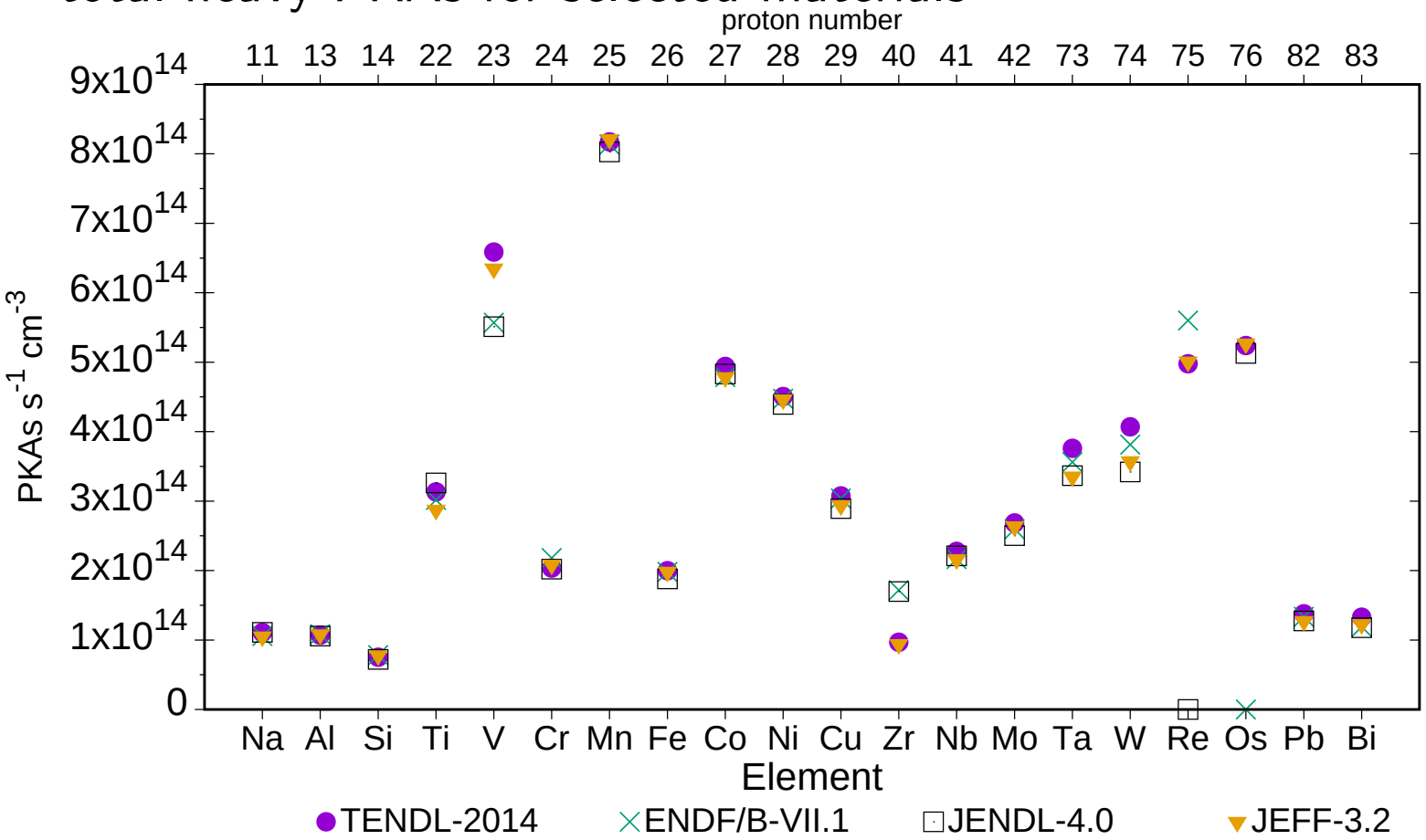


Order-of-magnitude agreement between libraries, but some missing results (Re, Ir, Li, Ne, ...)

*above 10 eV & excluding proton and alpha recoils
§FW DEMO conditions

Total PKA rates – library comparison

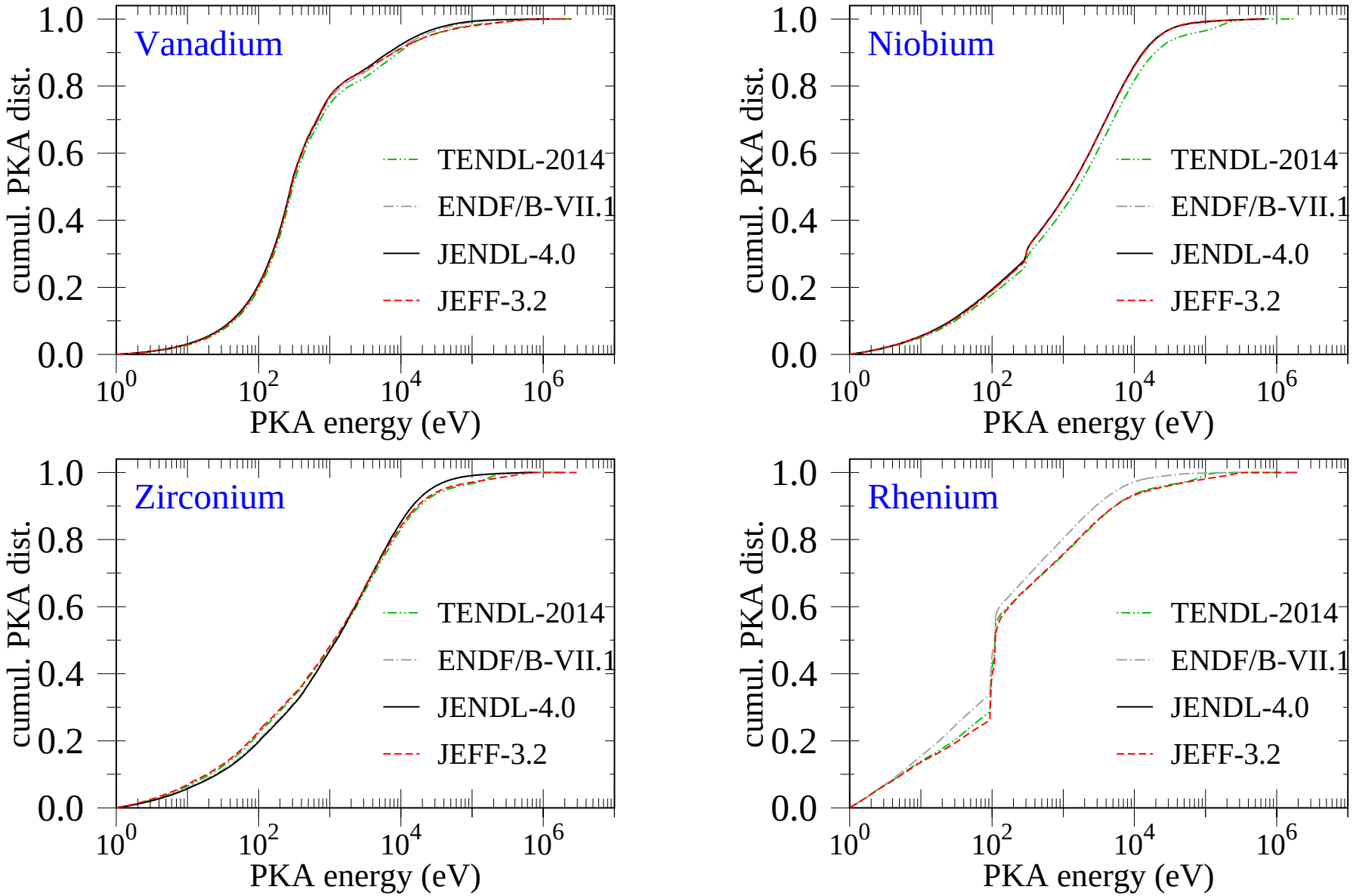
- total heavy PKAs for selected materials



- Too many isomeric states (> 3)in ^{90}Zr file caused processing failure in NJOY (already patched)
- Agreement in Nb despite missing channels in non-TENDL libraries

Excluding proton and alpha recoils
FW DEMO conditions

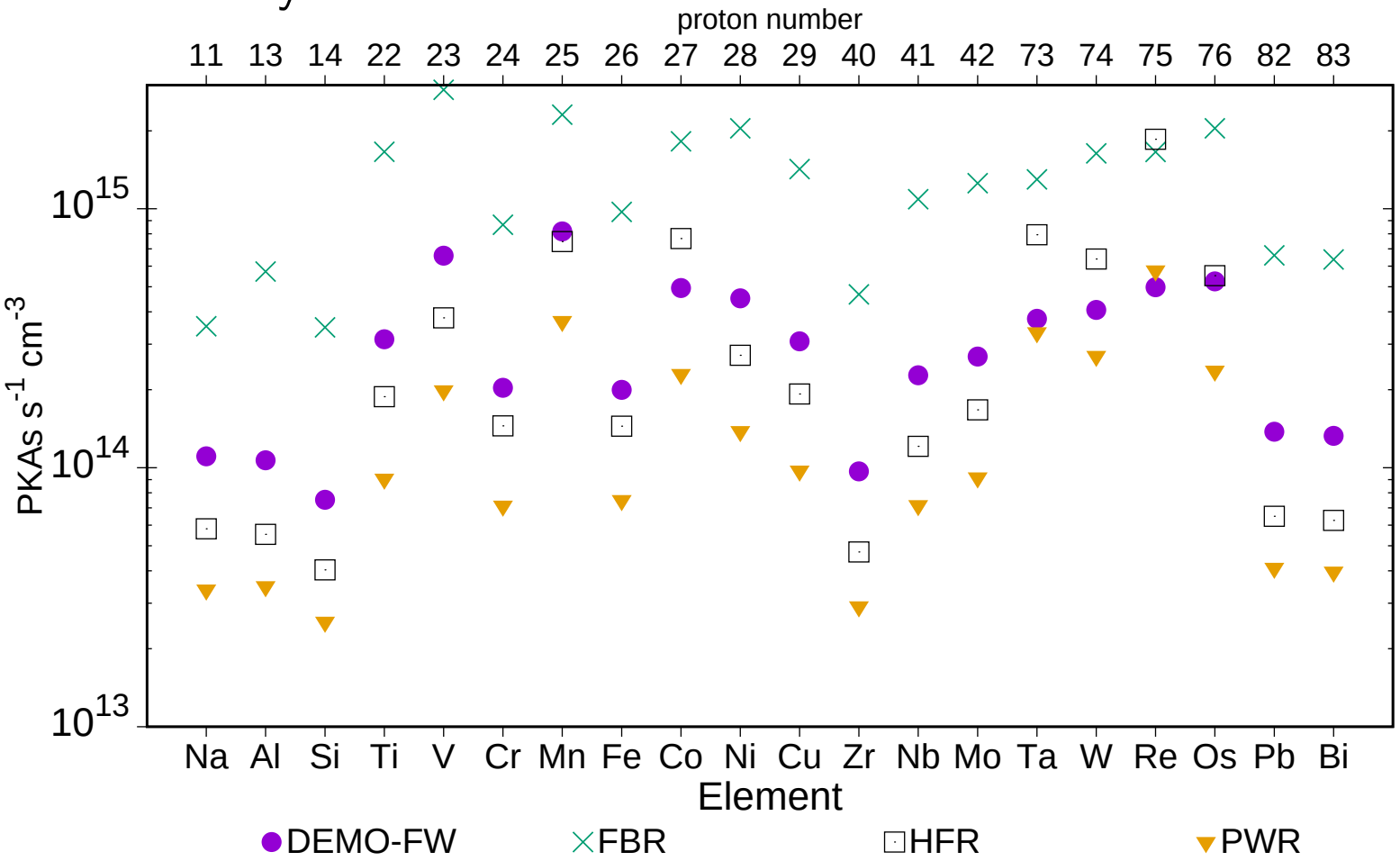
DEMO-FW Cumulative PKA distributions (CPDs)



- CPDs show the relative energy distribution of PKAs
- despite differences in total rates, CPDs are similar

Total PKA rates – fusion vs. fission

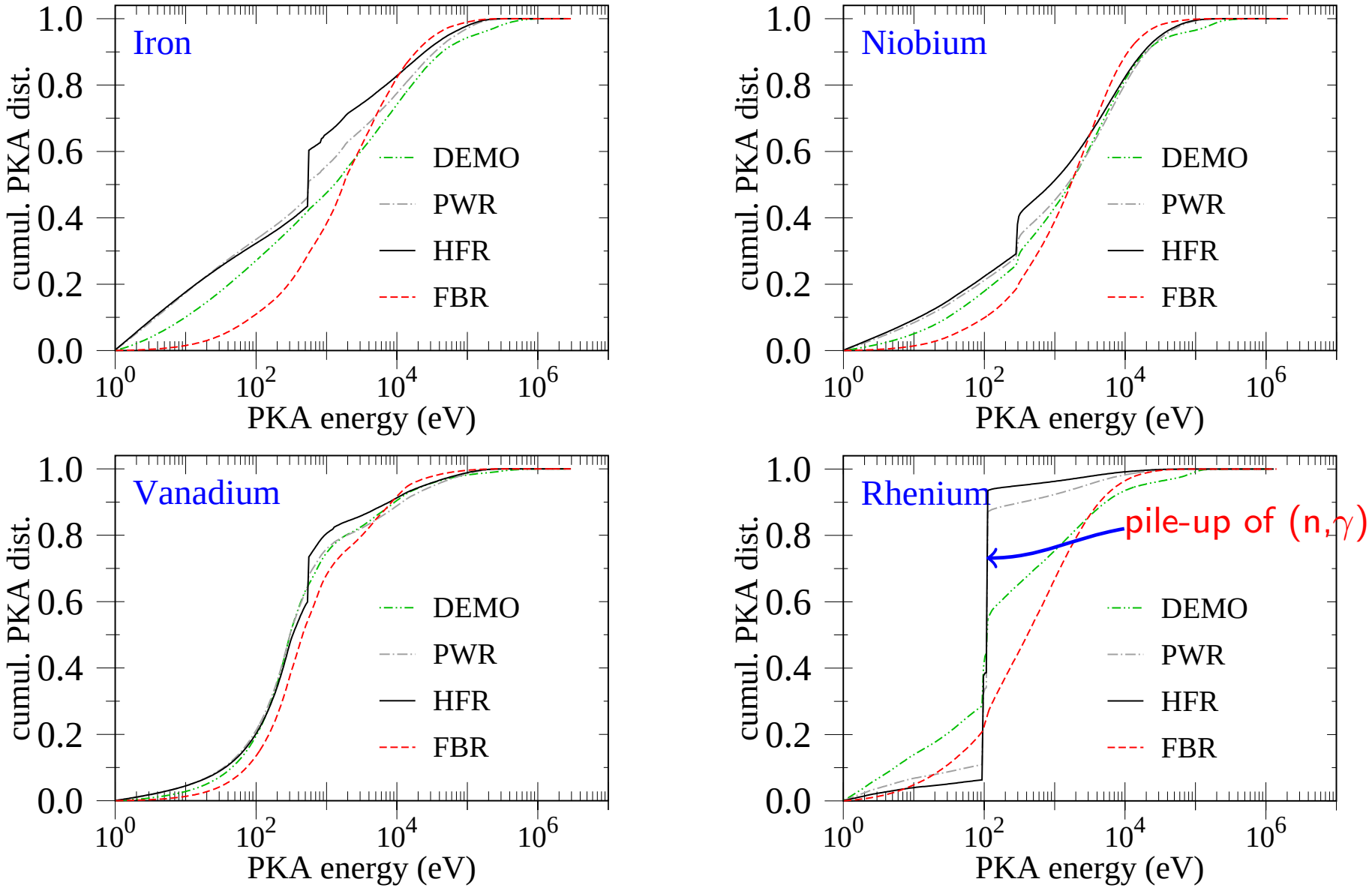
- total heavy PKAs for selected materials



- FBR spectrum produces highest rates due to high, fast flux (compare with HFR where high, soft flux instead produced high transmutation)
- "existing" fission (PWR) the lowest

CPDs: fusion vs. fission

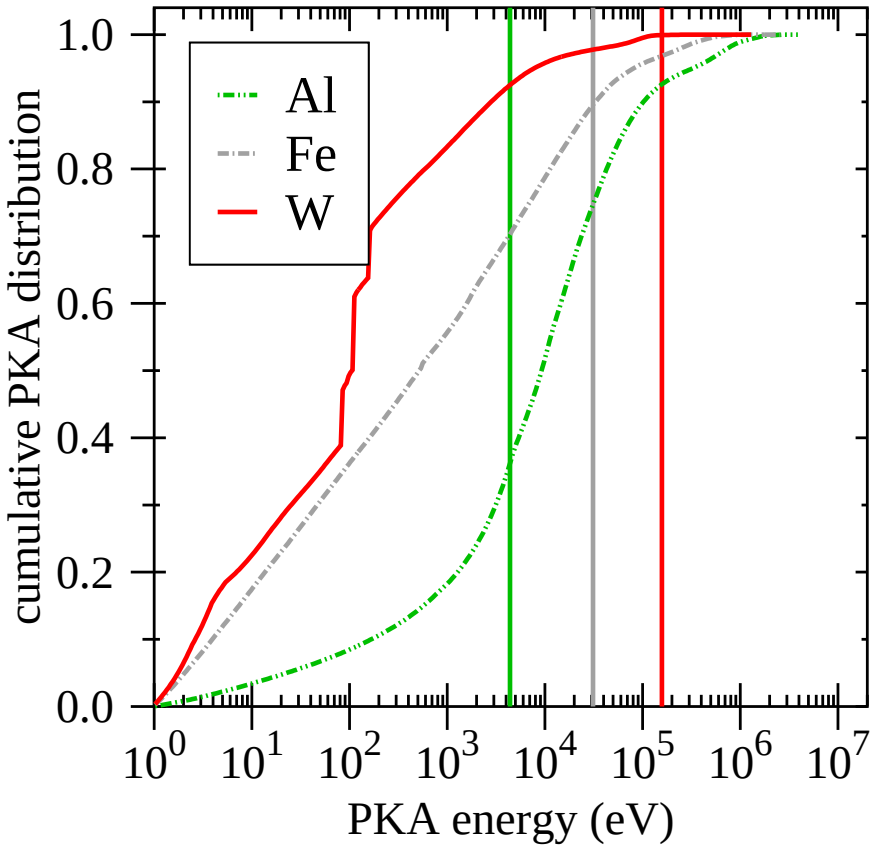
TENDL-2014



- FPR missing low and high energy parts due to peaked spectrum

CPDs – application to damage modelling

- Recent work[§] has defined the threshold energy for sub-cascade formation (cascade fragmentation) to occur
- we can compare this to CPDs to see what fraction (if any) of PKAs will result in sub-cascade formation



- Vertical lines are the fragmentation thresholds (same colours as curves)
- Fraction of PKAs above threshold (roughly) follows mass trend
- e.g. in Al 63% of PKAs are above threshold, in Fe only 10%, and in W less that 0.1%

DEMO FW, TENDL-2014 results

[§] De Backer, Sand, Nordlund, Luneville, Simeone, Dudarev, *EPL* (2016) submitted

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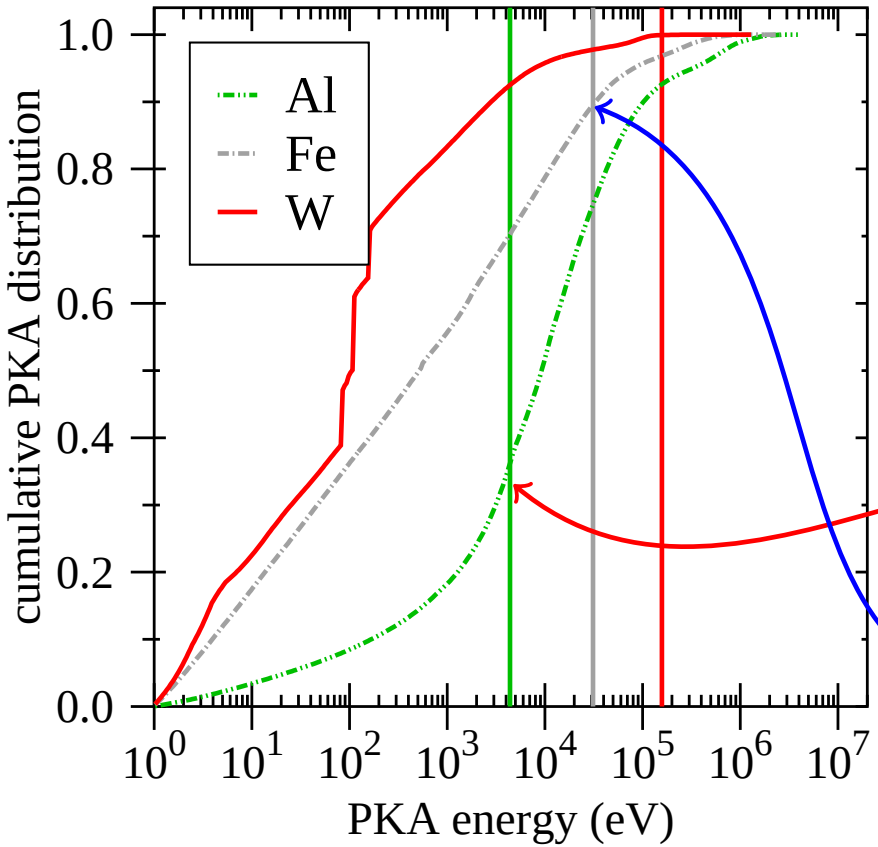

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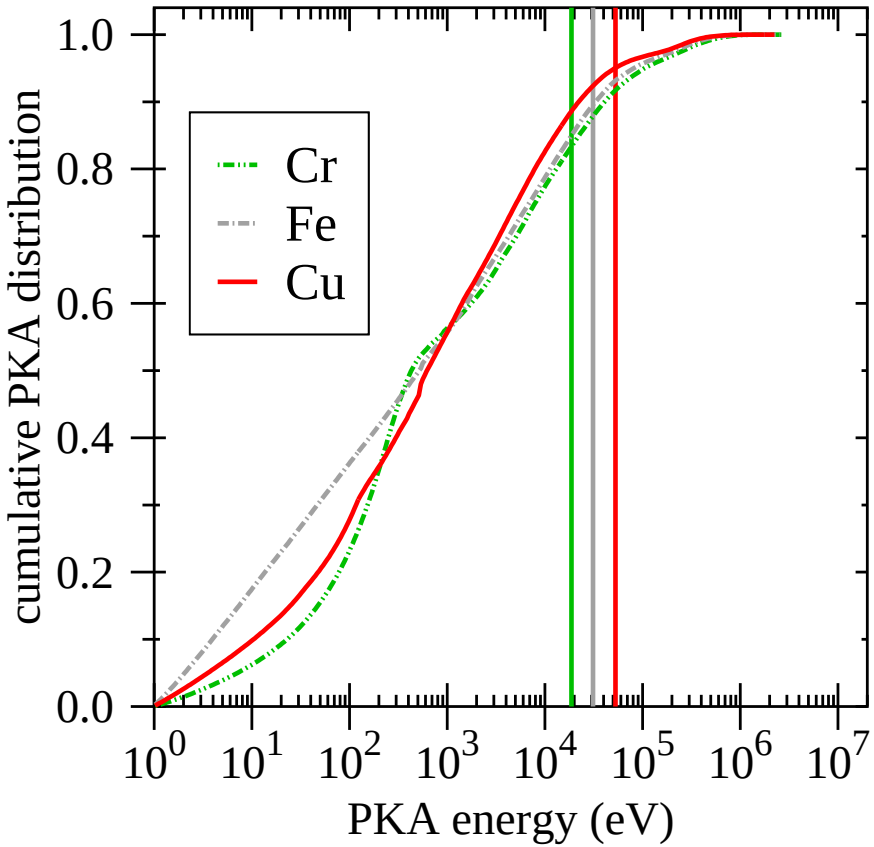

- In near-mass elements the picture is fairly similar.
- Fractions above threshold:
  17% Cr
  10% Fe
  5% Cu

DEMO FW, TENDL-2014 results

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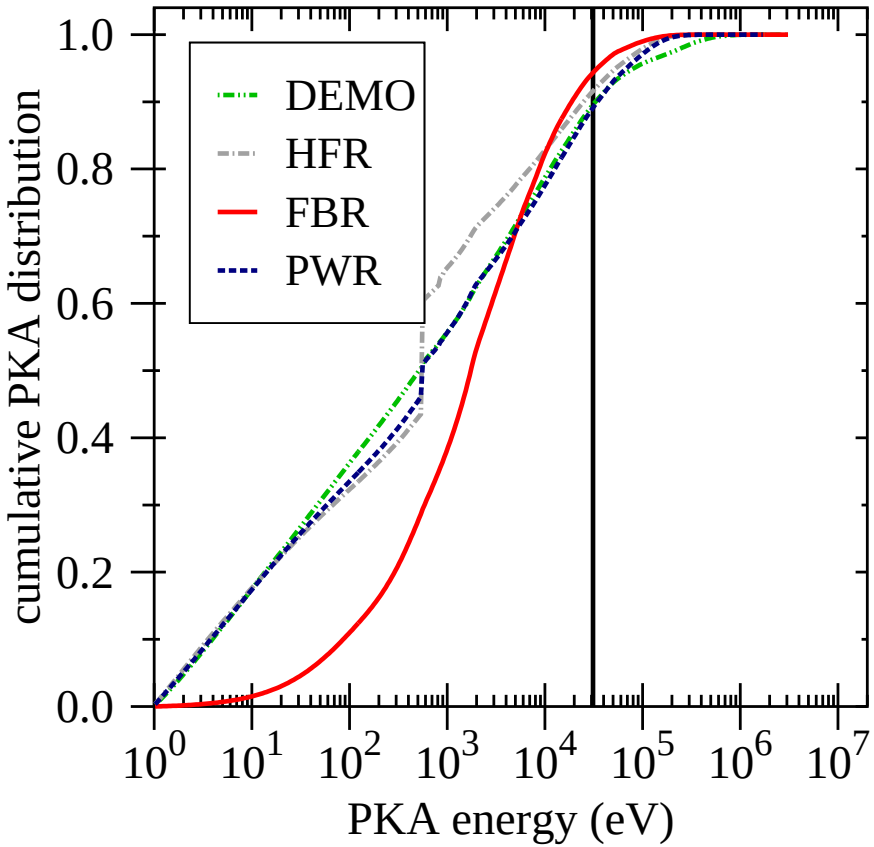


- In Fe there is not much difference between fusion and fission.
- Fractions above threshold:
  10% DEMO
  8% HFR
  6% FBR
  11% PWR

TENDL-2014 results

[§] De Backer, Sand, Nordlund, Luneville, Simeone, Dudarev, *EPL* (2016) submitted

Damage energy & dpa from SPECTRA-PKA

- The displacement energy in the NRT-dpa formula is normally calculated using the total damage kerma cross section (from NJOY)
- However, with SPECTRA-PKA, it is possible to calculate the damage contribution as a function of reaction channel
  - a new & novel capability
- Standard LSS[§] formula to account for electronic loss and convert PKA energy into damage energy – including correct treatment of parent and daughter mass
- displacement-energy rate accumulated and summed using PKA rate at each damage energy. NRT formula can be applied to the total
- For a given reaction channel, the total displacement energy is:

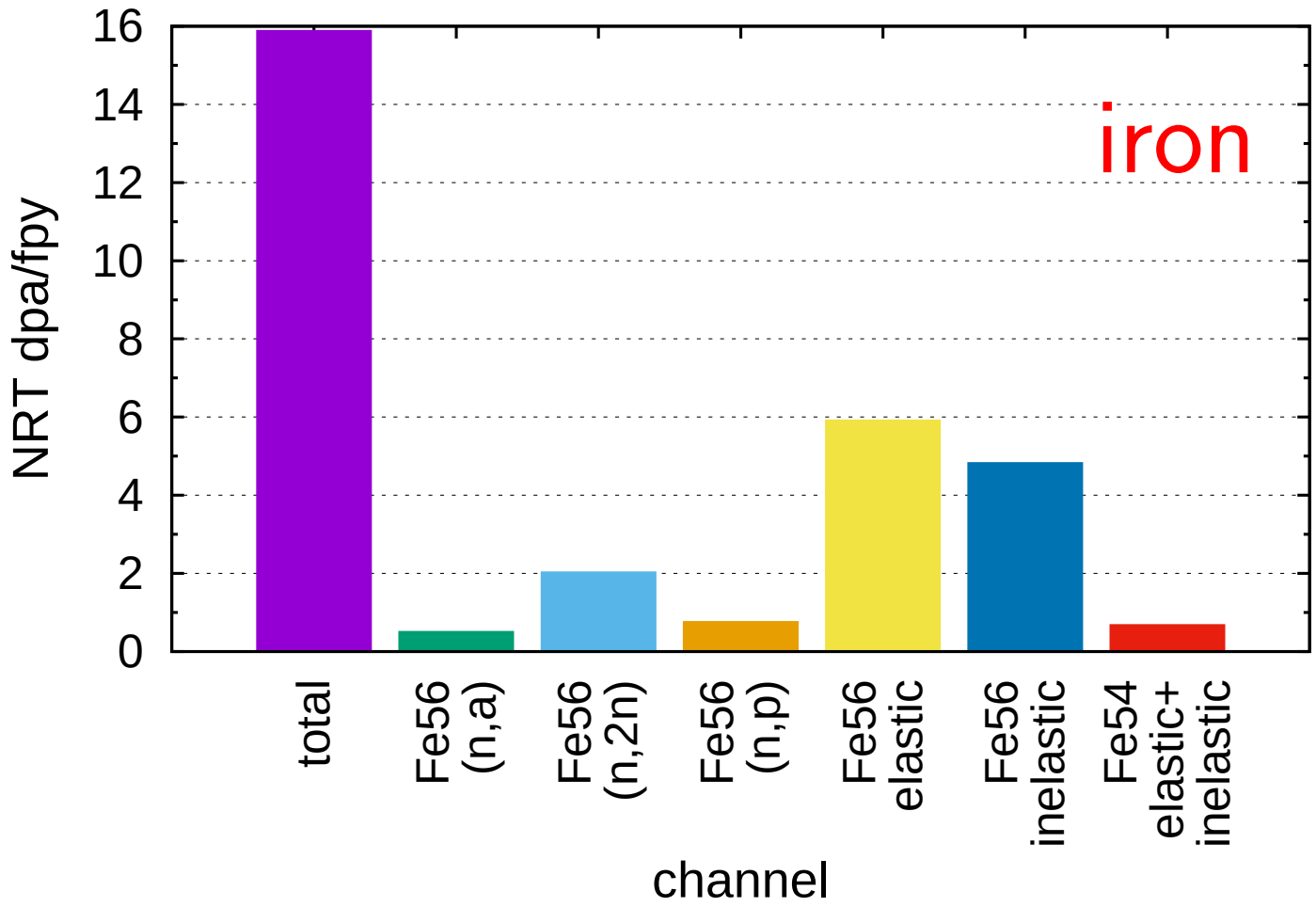
$$\sum_i T^{LSS}(E_i^{pka}) R_i^{pka},$$

where $T^{LSS}(E^{pka})$ is the LSS equivalent energy for PKA energy E^{pka}, and R_i^{pka} is number of PKAs at energy E_i^{pka}

[§] Lindhard, Scharff, Schiøtt, *Mat. Fys. Medd. Dan. Vid. Selsk.* **33** (1963) 1–42

Damage energy from SPECTRA-PKA

- Channel contributions to NRT dpa/fpy* for Fe§ under DEMO FW conditions:



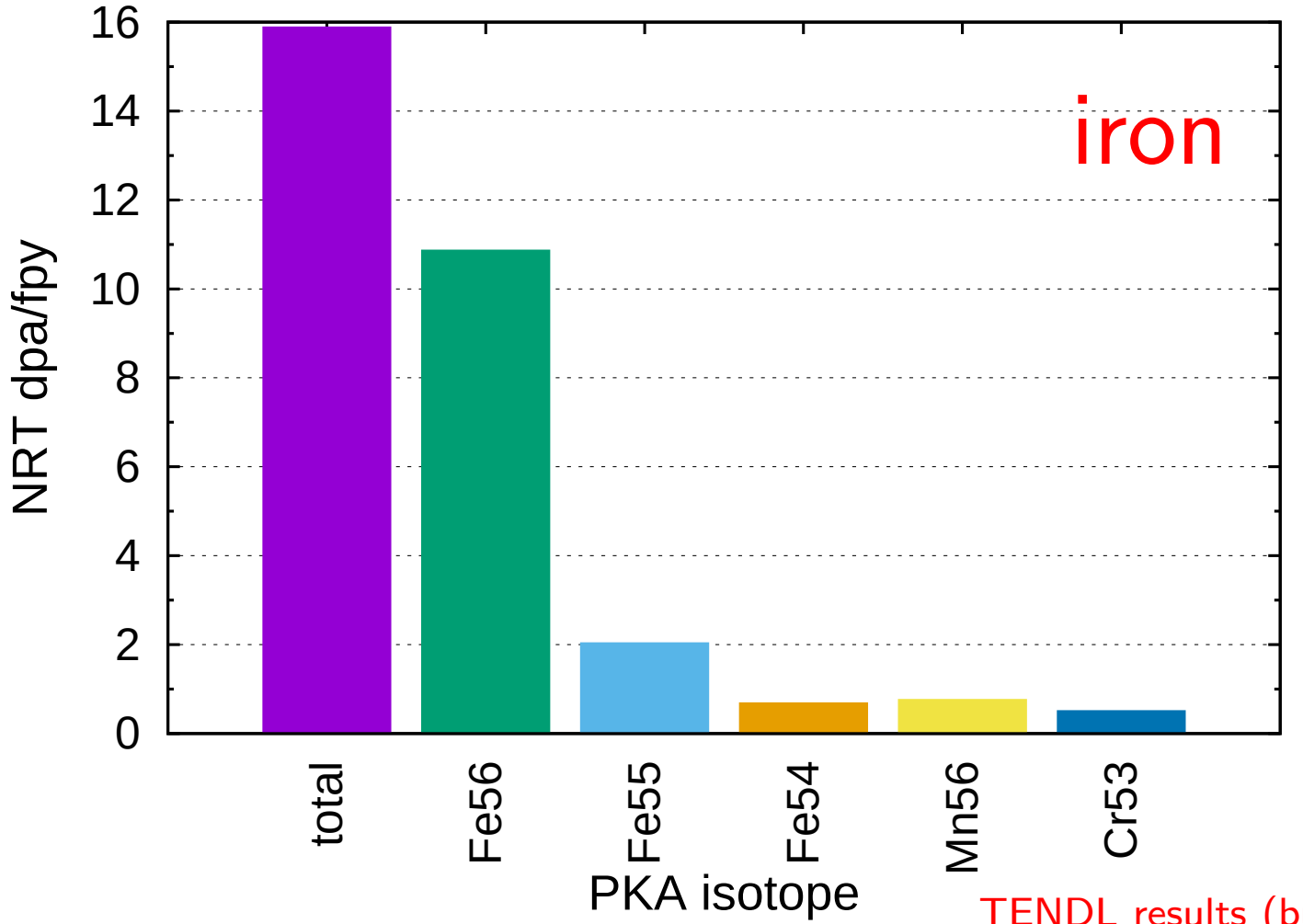
- Largest contributions are from scattering of ^{56}Fe (91.2 atm.%)
- ^{56}Fe(n,2n) also important (13%)
- total agrees with value obtained from standard approach – FISPACT-II & total damage kerma

TENDL results (but ENDF/B-VII.1 similar)

*fpy – full power years
§ $E_d = 40$ eV

Damage energy from SPECTRA-PKA

- Nuclide contributions to NRT dpa/fpy* for Fe§ under DEMO FW conditions:



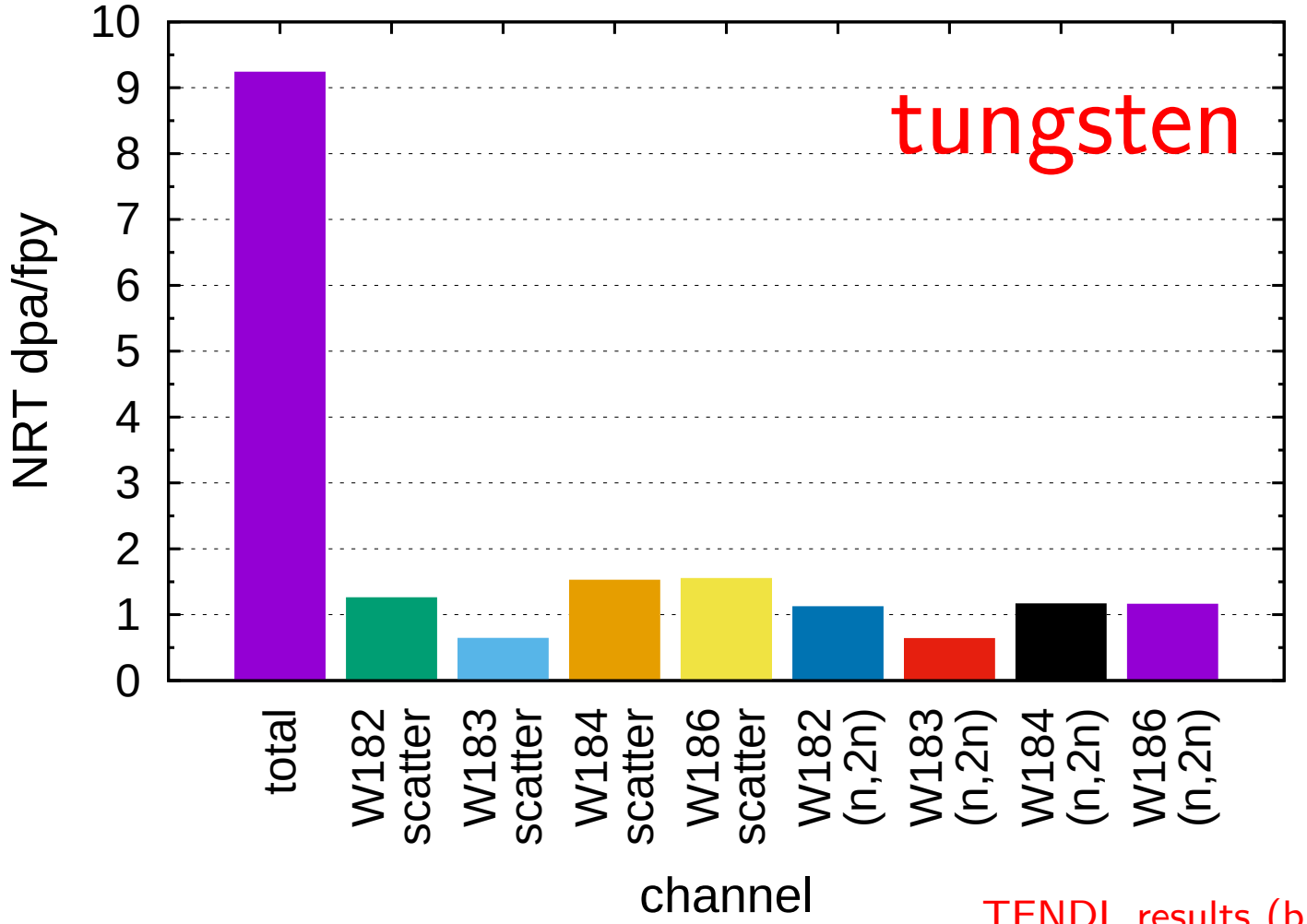
- the per-channel dpas summed by daughter indicate the proportion of damage from different recoiling species
- dominated by Fe nuclides, but with a contribution from ^{56}Mn & ^{53}Cr

TENDL results (but ENDF/B-VII.1 similar)

*fpy – full power years
§ $E_d = 40$ eV

Damage energy from SPECTRA-PKA

- Channel contributions to NRT dpa/fpy for W[§] under DEMO FW conditions:



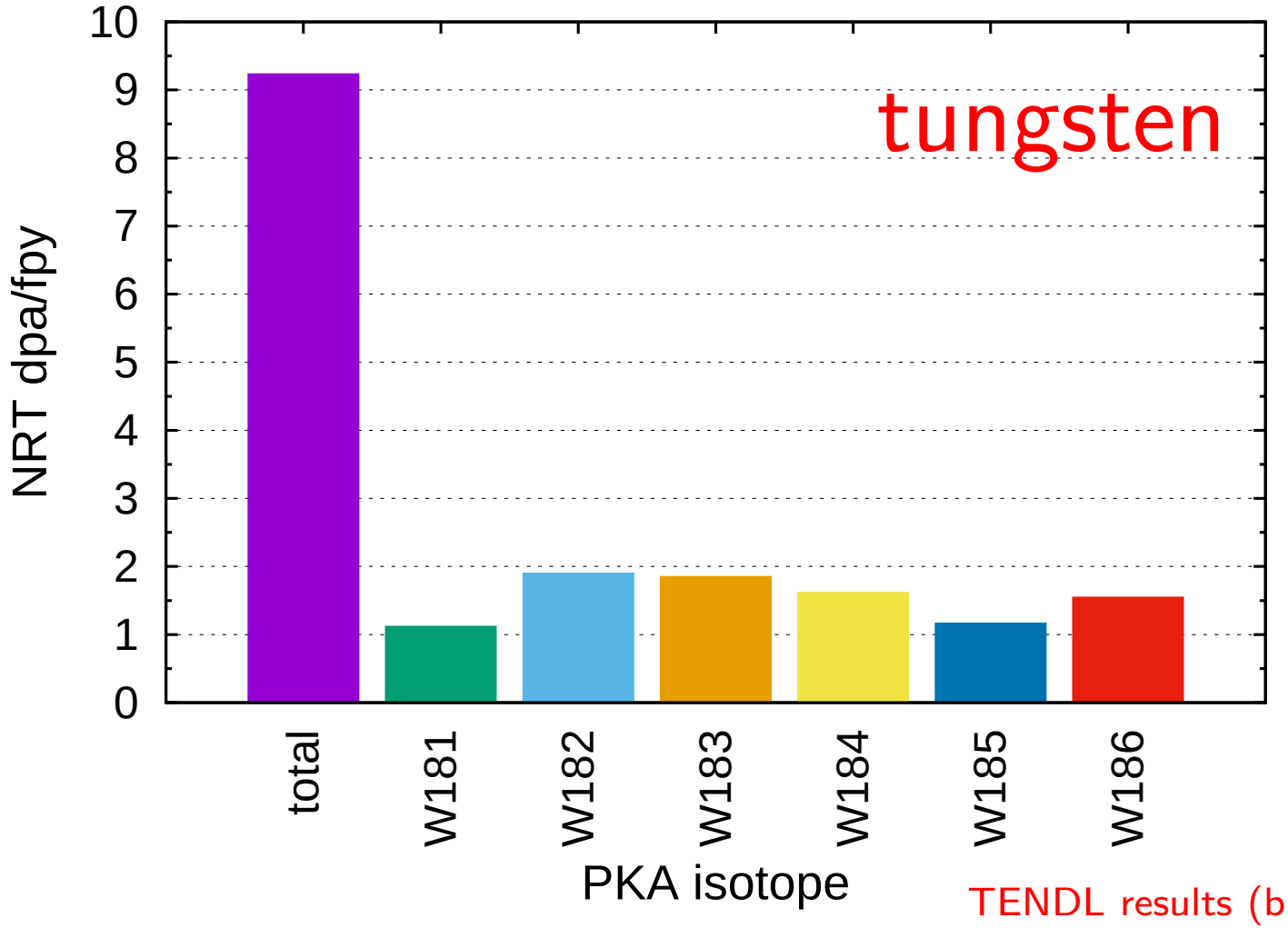
- In W, (n,2n) contributes as much as elastic/inelastic scattering

TENDL results (but ENDF/B-VII.1 similar)

[§] $E_d = 55$ eV

Damage energy from SPECTRA-PKA

- Nuclide contributions to NRT dpa/fpy for W[§] under DEMO FW conditions:



- no significant contributions from reactions that produce isotopes of other elements

TENDL results (but ENDF/B-VII.1 similar)

[§] $E_d = 55$ eV

Summary (1)

- Automated simulation, processing, and reporting structure provides the flexibility to perform scoping studies
  - for different libraries
  - for different irradiation conditions/environments
- The data from different versions can be collated and compared
- For key elements, the major international libraries generally produce similar results for activation, transmutation (including gas production), and PKA distributions
  - but there are some missing reaction channels in the other (legacy) libraries in comparison to TENDL
- The predicted fusion conditions will produce more activation than fission, but not necessarily the highest burn-up (HFR) or PKA rates (FBR)

Summary (2)

- Comparison of cumulative PKA distributions to sub-cascade formation thresholds demonstrates that lighter elements will have much greater cascade splitting
- SPECTRA-PKA and processed libraries can be used to calculate per-channel contributions to displacement energy (& dpa)
  - a new & novel capability
  - providing new insight into the distribution of damage production